Propositions belonging to the thesis of Hilda van der Veen

Stellingen behorende bij het proefschrift van Hilda van der Veen

1. The creativity that originates from interdisciplinary cooperation is not sufficiently cultivated in the Netherlands.

Interdisciplinaire samenwerking is in Nederland een te weinig benutte bron van creativiteit.

2. The unpredictability of Bi-Lanczos makes the method invaluable.

Het gedrag van Bi-Lanczos is onvoorspelbaar en dat maakt de methode onmisbaar.

3. The idea that mathematics is horrible, difficult or unfeminine is a result of an indoctrination not based on reality.

De gedachte dat wiskunde griezelig, moeilijk of onvrouwelijk is, is het gevolg van een niet op de werkelijkheid gebaseerde indoctrinatie.

4. Disconnecting the mathematical problem from the application facilitates the solution thereof.

Het wiskundige probleem loskoppelen van de toepassing vergemakkelijkt de oplossing ervan.

5. Scientific research should not be valued on its applicability.

Wetenschappelijk onderzoek zou niet beoordeeld moeten worden op de toepasbaarheid.[4][6]

6. Lack of empathy hinders the integration of women in male dominated areas.

De integratie van vrouwen in door mannen gedomineerde omgevingen wordt bemoeilijkt door een gebrek aan inlevingsvermogen bij mannen.

7. A 'pas de deux' has more quality than the sum of each separate part. Likewise, in technical areas, men and women should integrate.

Een 'pas de deux' is meer dan de som der delen. Evenzo zouden mannen en vrouwen in de techniek moeten integreren.
8. As long as macho (aggressively masculine) behavior is accepted women are not yet treated equally.

Zolang macho (aggressief mannelijk) gedrag wordt geaccepteerd is er van gelijke sexe behandeling nog geen sprake.[1]

9. Sexual harassment is differently interpreted by women and men. An official accusation by a woman is therefore often ridiculed.

Ongewenste intimiteit wordt door vrouwen en mannen verschillend geïnterpreteerd. Een officiële aanklacht door een vrouw wordt daarom vaak belachelijk gemaakt.[5]

10. Sorrow leads to enlightenment, but the gain is based on loss.

Verdriet geeft inzicht maar niet zonder verlies. [3][2]

References

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The significance and use of eigenvalues and eigenvectors in the numerical analysis of elasto-plastic soils
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Hilda van der Veen
To my brother Harro

Sorrow leads to enlightenment
but the gain is based on loss
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Chapter 1

Introduction

The world’s population continues to grow and the space available for building and infrastructure is therefore getting sparser. To increase the available space, possibilities are to make artificial islands or to build underground structures. The soil behavior is of major importance for these structures. Another engineering field which requires a good knowledge of soil behavior is the oil industry. For instance, borehole stability analysis is an important subject in this field of research.

Soil behavior can be studied in a laboratory. However, this can become time consuming when newly prepared specimens are necessary for each test. Another way to look at the deformation of soil and predict its behavior in practical situations is by constructing a numerical model based on laboratory findings. With a single numerical model several tests can be performed. A numerical model for soil is constructed from a material model and a spatial discretization. The material model consists of relations between strains and stresses or displacements and forces. With the finite element method the continuous problem is discretized and solved on a computer.

Soil is a complex material. Stress-strain relations are nonlinear due, amongst others, to plastic behavior. The numerical modeling of soil deformation may encounter difficulties like divergence of the iterative procedure and unstable solutions. In this research the possible causes of these difficulties are investigated and solutions are sought to avoid them.

1.1 Scope

The features of soil which are important in this study are its plastic behavior and its friction. To describe plasticity an elasto-plastic model is adopted that separates elastic behavior from plastic behavior with a yield function. The
typical frictional behavior of sand necessitates the use of a constitutive model which gives rise to nonsymmetric material and structural matrices. In particular, a so-called nonassociated flow rule causes the nonsymmetry needed to capture inelastic volume effects like dilatancy and contraction.

Eigenvalues and eigenvectors describe important properties of a matrix and therefore of the characteristics of the underlying problem. On a material level the matrix that relates strains to stresses is of interest. After discretization large matrices evolve that describe the load-displacement behavior. The size of the matrices in the finite element computations is such that an iterative eigenvalue and eigenvector procedure is needed.

1.2 Aims

Material models in which frictional effects become important normally result in a constitutive relation where the tangent stiffness tensor that sets the relation between the stress rate tensor and the strain rate tensor becomes nonsymmetric. As a result, the structural tangent stiffness matrix that is obtained after discretization of the boundary value problem, becomes nonsymmetric. In principle, nonsymmetric matrices allow for complex eigenvalues. However, on physical grounds it is hard to imagine that complex eigenvalues would arise. Since the structural stiffness matrix is filled by real numbers, the complex eigenvalues, if they exist, must be complex conjugate. This would require the eigenvectors to be complex conjugates and it is hard to attach any physical significance to a complex displacement vector under static loading conditions [3]. The following questions regarding the material model thus arise:

- Do complex eigenvalues exist in the elasto-plastic material matrix?
- If they exist, how do they relate to eigenvalues of the structural tangent stiffness matrix?

Other problems in the numerical modeling are caused by possible instabilities of the solution and loss of uniqueness, i.e. the presence of bifurcation points. A bifurcation point in the solution path is usually a consequence of the symmetry of the boundary value problem and a homogeneous distribution of material parameters. At a certain load level, there may be more than one possible solution, what implies that the structural matrix is singular. In practice, a bifurcation point is never exactly encountered, but negative pivots in the iterative solution procedure indicate loss of uniqueness of the homogeneous solution. Eigenvectors associated to negative eigenvalues can then be used to perturb the solution vector and to excite a solution related to a proper inhomogeneous deformation [4, 19]. This procedure is called branch switching. In more recent

Eigenvector perturbation is different from material perturbation that is often used in engineering practice [17]. The material parameters of one of the elements of the mesh are then perturbed. This, however, influences the peak load before bifurcation, and moreover, deformation may turn out to be different from what was expected or observed in practice. In other words, the deformation may be different from the original intrinsic bifurcation mode of the material. The focus in this thesis is therefore on eigenvector perturbation. In particular, the following questions are addressed:

- What is the significance of eigenvalues and eigenvectors in the numerical modeling of soil?
- Which eigenvalue and eigenvector methods are available and can they be improved?
- How can the branch switch procedure be improved?

Summarizing, the study aims at the validation of material models for soil using eigenvalues and eigenvectors. Also, the eigenvector-based branch switch procedure is further improved in order to go beyond bifurcation points. Moreover, the concept of bifurcation and stability is investigated with help of eigenvalues and eigenvectors.

1.3 Outline

In the second chapter a short introduction is given of the concept of plasticity for soils and of the Drucker-Prager yield surface. Nonassociated plasticity is discussed and the elasto-plastic material matrix is set up. It is investigated whether the eigenvalues of this matrix are real or complex. Chapter 3 briefly discusses the main ingredients of the finite element method. Some examples are introduced that are frequently referred to in the remainder of this thesis. In Chapter 4 a connection is made between the eigenvalue analysis of the elasto-plastic material matrix and some numerical examples. The stress history of finite element tests are compared to the eigenvalue distribution computed in Chapter 2.

The iterative eigenvalue methods for nonsymmetric matrices are described in Chapter 5. First the Lanczos [21] method is introduced after which Arnoldi’s method and the Bi-Lanczos method are discussed. The Bi-Lanczos method is then refined resulting in the BILAP0 method. In Chapter 6 the perturbation techniques are described, that is, an already established method [4] and its generalization as well as newly developed techniques. The perturbation methods are thoroughly tested and compared to each other. Some computational
difficulties are further analyzed in Chapter 7. In this chapter the question of
stability, bifurcation and negative pivots or eigenvalues is also addressed.

Chapter 8 is an evaluation of this research with the conclusions and some
reflections.

Due to the combination of linear algebra and soil mechanics the notation used
in this thesis is a mixture of both linear algebra and soil mechanics style con-
ventions. In general bold lower case letters, greek or roman, denote vectors and
bold upper case letters denote matrices. Other letters are scalars or functions.
The letters i, j, k, l and m are reserved for iteration indices, except for the letter
i that is also used to denote complex variables. In the following alphabetical
list most vectors, matrices, functions and scalars used in this thesis are briefly
described.

\textbf{b} \quad \text{Body force.}
\textbf{B} \quad \text{Differential operator} \ L \ \text{times the interpolation matrix} \ N.
\textbf{c} \quad \text{Cohesion or characteristic polynomial.}
\textbf{D, D}_{e}, \textbf{D}_{e,p} \quad \text{Discriminant, elasticity matrix and elasto-plastic material matrix.}
\textbf{e} \quad \text{Identity vector.}
\textbf{E} \quad \text{Stiffness parameters or Young’s modulus.}
\textbf{f, f} \quad \text{Yield function and force vector.}
\textbf{g, g} \quad \text{Plastic potential function and body force per unit of mass.}
\textbf{G} \quad \text{Shear modulus.}
\textbf{H, H} \quad \text{Hardening parameter and Hessenberg matrix.}
\textbf{i, j} \quad \text{Newton-Raphson iteration counters.}
\textbf{I, I} \quad \text{Invariants of the stress matrix and identity matrix.}
\textbf{k} \quad \text{Eigenvalue method counter or constant in yield function.}
\textbf{K, K} \quad \text{Krylov subspace and tangent stiffness matrix.}
\textbf{L} \quad \text{Differential operator.}
\textbf{l, m, m} \quad \text{Eigenvalue method counters and direction of plastic flow.}
\textbf{n, n} \quad \text{Total number of degrees of freedom and normal vector (of yield
surface).}
\textbf{N} \quad \text{Matrix of interpolation functions.}
\textbf{p} \quad \text{Hydrostatic axis.}
\textbf{P} \quad \text{Potential energy function.}
\textbf{q} \quad \text{Fixed force vector or Lanczos and Arnoldi iteration vector.}
\textbf{Q} \quad \text{Matrix orthogonal Lanczos or Arnoldi iteration vectors.}
\textbf{r} \quad \text{Rayleigh quotient.}
\textbf{R} \quad \text{Upper triangular Schur matrix.}
\textbf{s, S, S} \quad \text{Schur vector, matrix of orthogonal Schur vectors and surface.}
\textbf{t} \quad \text{Traction.}
\textbf{T} \quad \text{Three-diagonal matrix.}
1.3. OUTLINE

$\mathbf{u}$ Displacement or deformation vector.
$\mathbf{v}, \mathbf{w}$ Right and left Bi-Lanczos iteration vectors.
$V, \mathbf{V}, W$ Volume, matrix of right and left Bi-Lanczos iteration vectors.
$\mathbf{x}, \mathbf{y}$ Right and left eigenvectors.
$\mathbf{Z}$ Matrix of orthogonal Schur vectors.

$\alpha, \beta$ Constant in yield function and plastic potential function.
$\epsilon, \epsilon$ Machine precision and strain vector.
$\delta$ Kronecker delta.
$\lambda, \Lambda$ Eigenvalues and diagonal matrix of eigenvalues.
$\mu$ Length of the force vector increment.
$\nu$ Poisson's ratio.
$\omega$ Inner products of right and left Bi-Lanczos iteration vectors.
$\Omega, \Omega$ Matrix of inner products of right and left Bi-Lanczos iteration vectors and notation for area.
$\phi, \psi$ Angle of internal friction and dilatancy angle.
$\phi, \psi$ Right and left eigenvectors of Ritz matrix.
$\rho$ Density.
$\theta$ Eigenvalues of Ritz matrix.
$\sigma, \Sigma$ Stress vector and stress matrix.
Chapter 2

Elasto-Plasticity

A numerical simulation involves many different aspects like discretization, interpolation, integration, etc., that may cause instabilities or inaccuracies. In this chapter the beginning of any numerical modeling process is analyzed, namely the material model. For soils this basically consists of an elasto-plastic constitutive relation including a yield surface. Stresses and strains in a body due to loading or prescribed displacements are related via the elasto-plastic constitutive law, whereas the yield surface distinguishes stresses that cause elastic deformation from those that cause plastic deformation. In particular a Drucker-Prager yield surface is used to set up the elasto-plastic material matrix relating strain rates and stress rates.

This chapter includes an introduction to stresses, principal values and the Drucker-Prager yield function for plastic behavior (Sections 2.1.1, 2.1.2). A more thorough and complete analysis of these subjects can be found in e.g. [23]. The elasto-plastic matrix is set up in Section 2.1.3 followed by an analysis of its eigenvalues in Section 2.2. In particular conditions are set up for isotropic and orthotropic plane-stress and plane-strain configurations that guarantee real eigenvalues of the elasto-plastic material matrix.

2.1 Material model

For the construction of an elasto-plastic model describing the partially elastic, partially plastic deformation behavior of soil a yield surface is needed. It is often set up in terms of invariants or principal values of the stress matrix.

This section introduces the stress matrix and explains the computation of its principal values, used for the construction of a yield surface according to the Drucker-Prager concept [12]. This is followed by the derivation of the elasto-
plastic material matrix. In the last part of this Section (2.1.4) the two material configurations are described that are used throughout this research.

2.1.1 Stress

The stresses due to a force in a three-dimensional body can be characterized by the nine stress components on a unit cube, see Figure 2.1, where the three orthogonal directions are denoted by $x, y, z$ as is common practice in engineering. Due to symmetry it holds that $\sigma_{ij} = \sigma_{ji}$ and thus only six stress components are different. They are arranged in the stress matrix $\Sigma$ as follows:

$$\Sigma = \begin{bmatrix}
\sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\
\sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\
\sigma_{zx} & \sigma_{zy} & \sigma_{zz}
\end{bmatrix}.$$  \hspace{1cm} (2.1)

The eigenvalues of the stress matrix $\Sigma$ are called principal values, denoted by $\sigma_1, \sigma_2$ and $\sigma_3$. For a symmetric matrix the principal values are equivalent to the normal stresses in a coordinate system for which shear stresses vanish. The cubic polynomial that defines the principal values or eigenvalues $\lambda$ of the stress matrix $\Sigma$ reads:

$$c(\lambda) = \lambda^3 - \lambda^2(\sigma_{yy} + \sigma_{zz} + \sigma_{xx})$$
$$+ \lambda(\sigma_{yy}\sigma_{zz} + \sigma_{yy}\sigma_{xx} + \sigma_{xx}\sigma_{zz} - \sigma_{xy} - \sigma_{yz} - \sigma_{xz})$$
$$- 2\sigma_{xy}\sigma_{xz}\sigma_{yz} - \sigma_{xx}\sigma_{yy}\sigma_{zz} + \sigma_{xx}\sigma_{yz}^2 + \sigma_{zz}\sigma_{xy}^2 + \sigma_{yy}\sigma_{xz}^2.$$  \hspace{1cm} (2.2)

The characteristic polynomial of the diagonal principal value matrix is:

$$c(\lambda) = \lambda^3 - \lambda^2(\sigma_1 + \sigma_2 + \sigma_3) + \lambda(\sigma_1\sigma_2 + \sigma_1\sigma_3 + \sigma_2\sigma_3) - \sigma_1\sigma_2\sigma_3.$$  \hspace{1cm} (2.3)
Comparing the factors of (2.2) and (2.3), it follows readily that:

\[ I_1 = \sigma_{yy} + \sigma_{zz} + \sigma_{xx} = \sigma_1 + \sigma_2 + \sigma_3, \]  
\[ I_2 = \sigma_{yy}\sigma_{zz} + \sigma_{yy}\sigma_{xx} + \sigma_{xx}\sigma_{zz} - \sigma_{xy}^2 - \sigma_{yz}^2 - \sigma_{xz}^2 = \sigma_1\sigma_2 + \sigma_1\sigma_3 + \sigma_2\sigma_3, \]  
\[ I_3 = \sigma_{xx}\sigma_{yy}\sigma_{zz} + 2\sigma_{xy}\sigma_{xz}\sigma_{yz} - \sigma_{xx}\sigma_{yx}^2 - \sigma_{zz}\sigma_{zy}^2 - \sigma_{xy}\sigma_{xz}^2 = \sigma_1\sigma_2\sigma_3. \]  

Values \( I_1, I_2, I_3 \) are called the invariants of the stress matrix because these values are unchanged under rotation of the coordinate axes, just like the principal values are. The invariants are used for the construction of a yield surface (Section 2.1.2) and for the computation of eigenvalues of the elasto-plastic matrix that is introduced in Section 2.1.3.

### 2.1.2 Yield surface

Stresses in a body induce elastic and possibly plastic deformations. The stresses that are located on a yield surface cause plastic deformations, and stresses within the surface elastic deformations. Stresses outside the yield surface are not allowed. For different materials there are differently shaped yield surfaces. For soils the Mohr-Coulomb and the Drucker-Prager yield surface are commonly used. A more sophisticated surface is for example embodied in the Cam-Clay model [27] for the description of plastic deformation of clay.

This study is limited to the use of the Drucker-Prager yield surface, which has the shape of a cone in principal stress space (Fig. 2.2) and is defined by a yield function \( f_{DP} \). It is a smooth interpretation of Mohr’s theory of rupture [23], according to which failure or rupture occurs on a plane in a body if the shear stress and normal stress on that plane reach a critical combination. The Drucker-Prager yield function depends on the hydrostatic pressure \( p = I_1/3 \), the central axis of the Drucker-Prager cone.

The shape of the yield surface is influenced by the cohesion and friction angle of the material. A hardening or softening rule on the friction angle leads to a larger or smaller opening of the cone and a hardening or softening rule on the cohesion translates the cone along its hydrostatic axis.

The Drucker-Prager yield surface can be set up with the invariants of the stress matrix (eq. (2.4)). The surface defines those stresses that yield plastic deformation:

\[ f_{DP} = \sqrt{I_1^2 - 3I_2 + \alpha I_1 / 3 - k} = 0, \]  
\[ (2.5) \]
Figure 2.2: Drucker-Prager yield function.

with

$$\alpha = \frac{6 \sin \phi}{3 - \sin \phi}, \quad k = \frac{6c \cos \phi}{3 - \sin \phi},$$  \hspace{1cm} (2.6)$$

where $\phi$ is the angle of friction and $c$ the cohesion. For stresses that obey $f_{DP} = 0$ the deformation is elastoplastic. If $f_{DP} < 0$ then the deformation is elastic. Stresses outside the yield surface ($f_{DP} > 0$) are not allowed. It is possible that an intermediate stress state outside the yield surface is found during the convergence process of a numerical approximation. These stresses must be projected back onto the surface, see for example [30].

In an elastoplastic formulation as adopted here, the total strain is a combination of elastic and plastic strains. The rate of the (rate-independent) plastic strain is described by a flow rule that is obtained from a plastic potential function $g$:

$$m_{ij} = \frac{\partial g}{\partial \sigma_{ij}}.$$  \hspace{1cm} (2.7)$$

If $m_{ij}$ is associated with the yield criterion, i.e. $f = g$, then the flow rule is said to be associated. A flow rule derived from a plastic potential $g$ that is distinct from $f$ is accordingly called a nonassociated flow rule.
2.1.3 Elasto-plasticity

A constitutive law describes the relation between stresses $\sigma$ and strains $\varepsilon$ where $\sigma$ is a vector of stresses:

$$
\sigma^T = [\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{xz}, \sigma_{yz}].
$$

(2.8)

The elastic response is described by Hooke's law: $\sigma = D_\varepsilon \varepsilon$. The plastic response is more complex and results in nonlinear relations. The total elasto-plastic response is given by:

$$
\dot{\sigma} = D_{ep} \dot{\varepsilon}, \quad D_{ep} = D_\varepsilon - \frac{D_\varepsilon m n^T D_\varepsilon}{H + n^T D_\varepsilon m},
$$

(2.9)

in which $H$ is a hardening parameter. The two vectors $m$ and $n$ are respectively the direction of plastic flow derived from the plastic potential, and the normal to the yield surface. The plastic potential is chosen as:

$$
g_{Dp} = \sqrt{I_1^2 - 3I_2} + \beta I_1/3 - k,
$$

(2.10)

with

$$
\beta = \frac{6 \sin \psi}{3 - \sin \psi},
$$

(2.11)

so that if $\beta = \alpha$ the material obeys an associated flow rule, cf. equation (2.5).

The angle $\psi$ is called the dilatancy angle. The normal to the yield surface $n$ is constructed by taking the derivative of equation (2.5):

$$
n = \left\{ \frac{\partial f_{Dp}}{\partial \sigma_{ij}} \right\} = \frac{1}{2 \sqrt{I_1^2 - 3I_2}} \left\{ \frac{\partial (I_1^2 - 3I_2)}{\partial \sigma_{ij}} \right\} + \frac{\alpha}{3} \left\{ \frac{\partial I_1}{\partial \sigma_{ij}} \right\}.
$$

(2.12)

The direction of the plastic flow $m$ differs from $n$ only by the used angle and can therefore be expressed as:

$$
m = n + \frac{(\beta - \alpha)}{3} \left\{ \frac{\partial I_1}{\partial \sigma_{ij}} \right\}.
$$

(2.13)

Note that matrix $D_{ep}$ is singular by definition if hardening parameter $H$ is zero as can be verified by post-multiplication with $m$:

$$
D_{ep} m = D_\varepsilon m - \frac{D_\varepsilon m n^T D_\varepsilon m}{n^T D_\varepsilon m} = D_\varepsilon m - D_\varepsilon m = 0.
$$

(2.14)

In Section 2.2 eigenvalues of this matrix are computed and stress regions are defined in which complex eigenvalues may appear.
2.1.4 Plane-stress and plane-strain configurations

In this work two stress configurations are considered. Both configurations are a simplification of a three-dimensional state to two dimensions. Plane-strain is a typical assumption that is often utilized in soils: only a normal stress and no shear stresses are taken into account for the third dimension ($\sigma_{xz} = \sigma_{yz} = 0$). The other configuration is called plane-stress and applies more to thin-walled structures. A plane-stress configuration excludes all stress in third dimension, i.e. $\sigma_{xz} = \sigma_{yz} = \sigma_{zz} = 0$. The relations in equation (2.4) can be simplified according to each of the stress states.

The plane-stress case is included in the eigenvalue analyses of Section 2.2 but is not used in the finite element applications.

In a plane-strain situation, the invariants of the stress matrix (eq. (2.4)) can be simplified to:

$$
I_1 = \sigma_{yy} + \sigma_{zz} + \sigma_{xx} = \sigma_1 + \sigma_2 + \sigma_3, \\
I_2 = \sigma_{yy} \sigma_{zz} + \sigma_{yy} \sigma_{xx} + \sigma_{xx} \sigma_{zz} - \sigma_{xy}^2 = \sigma_1 \sigma_2 + \sigma_1 \sigma_3 + \sigma_2 \sigma_3, \\
I_3 = \sigma_{xx} \sigma_{yy} \sigma_{zz} - \sigma_{zz} \sigma_{xy}^2 = \sigma_1 \sigma_2 \sigma_3.
$$

In case of a plane-stress distribution, the invariants of the stress matrix become:

$$
I_1 = \sigma_{yy} + \sigma_{xx} = \sigma_1 + \sigma_2, \\
I_2 = \sigma_{yy} \sigma_{xx} - \sigma_{xy}^2 = \sigma_1 \sigma_2.
$$

Invariant $I_3$ is no longer relevant because any stress component with a subscript $z$ vanishes and consequently the stress matrix (eq. (2.1)) is only of the size $2 \times 2$. With only two non-zero principal stresses $\sigma_1$ and $\sigma_2$, the yield surface in principal stress space is reduced to an oval line, Figure 2.3(a). All possible stress combinations that yield plastic deformation can now be visualized. The surface covering all these stress combinations is an ellipsoid, Figure 2.3(b).

2.2 Eigenvalue Analysis

In this chapter the plane-stress and plane-strain distributions will be investigated in more detail, by computing and evaluating the eigenvalues of the associated elasto-plastic matrix $D_{ep}$, eq. (2.9). Hardening is not taken into account because, as will be shown in Section 4.1, it does not give qualitatively different results.

For each stress distribution two cases are analyzed, namely isotropy and orthotropy. In contrast to an isotropic material, an orthotropic material has different material stiffness parameters in orthogonal directions.
Figure 2.3: Plane-stress yield surface for principal stresses (to the left) and all stresses (to the right).
2.2.1 Plane-stress configuration

A plane-stress configuration is defined by two principal values \( \sigma_1, \sigma_2 \) and three stresses \( \sigma_{xx}, \sigma_{yy}, \sigma_{xy} \). The third principal value \( \sigma_3 \) and stresses with a subscript \( z \) are zero. Considering equation (2.16), vectors \( \mathbf{n} \) and \( \mathbf{m} \), defined by equations (2.12), (2.13), can be simplified to:

\[
\mathbf{n} = \begin{bmatrix}
\frac{\partial f_{DP}}{\partial \sigma_{xx}} \\
\frac{\partial f_{DP}}{\partial \sigma_{yy}} \\
\frac{\partial f_{DP}}{\partial \sigma_{xy}}
\end{bmatrix} = \frac{1}{2\sqrt{I_1^3 - 3I_2}} \begin{bmatrix}
2I_1 - 3\sigma_{yy} \\
2I_1 - 3\sigma_{xx} \\
6\sigma_{xy}
\end{bmatrix} + \frac{\alpha}{3} \begin{bmatrix}
1 \\
1 \\
0
\end{bmatrix},
\]

with \( I_1, I_2 \) as in equation (2.16), and:

\[
\mathbf{m} = \mathbf{n} + (\beta - \alpha)[1, 1, 0]^T / 3. \tag{2.18}
\]

The elasto-plastic stiffness matrix \( \mathbf{D}_{ep} \), equation (2.9), is of size \( 3 \times 3 \) and, because of the singularity of the matrix (eq. (2.14)), at least one zero eigenvalue \( \lambda \) must exist and the characteristic polynomial can be written as the product of \( \lambda \) times a second degree polynomial.

The rest of this section is split into two parts. The first part deals with isotropic plane-stress conditions and the second part with orthotropic plane-stress conditions.

Isotropic plane-stress

The entries of the elasticity matrix \( \mathbf{D}_e \) are defined by two parameters: Young’s modulus \( E \) and Poisson’s ratio \( \nu \), and \( \mathbf{D}_e \) reads:

\[
\mathbf{D}_e = \frac{E}{(1 + \nu)(1 - 2\nu)} \begin{bmatrix}
(1 - \nu) & \nu & 0 \\
\nu & (1 - \nu) & 0 \\
0 & 0 & (1 - 2\nu)/2
\end{bmatrix}. \tag{2.19}
\]

As a consequence, the characteristic polynomial of \( \mathbf{D}_{ep} \) is a multiple of \( E/(1 + \nu)(1 - 2\nu) \) (eq. (2.9)) and this factor can be left out of the computations. The discriminant of the characteristic polynomial of the elasto-plastic matrix \( \mathbf{D}_{ep} \) is further simplified by multiplication with \( \mathbf{n}^T \mathbf{D}_e \mathbf{m} \). It then becomes:

\[
D = \frac{1}{4}(1 - 2\nu)^2 \{2\nu(u - \nu)(u + 2w) \\
+ 4\nu^2w(u - \nu) + \nu^2(u - \nu)^2 + (u - 2\nu w)^2\}, \tag{2.20}
\]

were the following abbreviations have been used:

\[
u = m_1 n_1 + m_2 n_2, \quad \nu = m_1 n_2 + m_2 n_1, \quad \nu = m_3 n_3. \tag{2.21}
\]
By definition $u + w$ and $w$ are positive. The term $(u - v)$ is also positive, which becomes clear if the identity is used that $m_1 = n_1 + (\beta - \alpha)/3$ and $m_2 = n_2 + (\beta - \alpha)/3$:

$$u - v = n_1^2 + (n_1 + n_2)(\beta - \alpha)/3$$
$$+ n_2^2 - 2n_1n_2 - (n_1 + n_2)(\beta - \alpha)/3 = (n_1 - n_2)^2.$$ (2.22)

Therefore all terms in expression (2.20) for the discriminant of the characteristic polynomial of the isotropic elasto-plastic material matrix are positive. Consequently, all its eigenvalues are real.

### Orthotropic plane-stress

The elasticity matrix that describes the relation between strains and stresses is diagonal for an elastic response if no contraction exists. Because of the different stiffness parameters in orthogonal directions, the elasticity matrix can be written as:

$$D_e = \begin{bmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & G \end{bmatrix},$$ (2.23)

where coupling effects have been ignored. Parameters $E_1$ and $E_2$ are stiffness values, and $G$ is the shear modulus. The rank-1 update of this diagonal matrix defined by equation (2.9) may have a specific property, captured in the following lemma.

**Lemma 1** Let $A$ be an $n \times n$ diagonal matrix. The nonsymmetric rank-1 update $A + uv^T$ is similar to a symmetric matrix if the products $u_i v_i$ are all positive.

The lemma is proved in Appendix A.1, page 23.

Matrix $D_{ep}$ can be related to Lemma 1 by setting $u = D_e m/n^T D_e m$ and $v = n^T D_e$. Because the entries of $D_e$ are positive, Lemma 1 implies that only if the signs of one of the elements of $m$ and $n$ differ complex eigenvalues may appear. In many applications $m_i n_i > 0$ but if $m$ and $n$ are different vectors (nonassociated plasticity) the product can be negative.

The characteristic polynomial of $D_{ep}$ is of the third degree with one zero eigenvalue: $c(\lambda) = \lambda^3 + B\lambda^2 + C\lambda$. Complexity of the eigenvalues $\lambda$ now depends on the sign of the discriminant $B^2 - 4C$ which, after some elaboration and
multiplication with \( \{n^T D_e m\}^2 \), can be written as:

\[
D = 2E_1 E_2 (G - E_1)(G - E_3)m_1 n_1 m_2 n_2 \\
+ 2E_1 G (E_2 - E_1)(E_2 - G)m_1 n_1 m_3 n_3 \\
+ 2E_2 G (E_1 - E_2)(E_1 - G)m_2 n_2 m_3 n_3 + E_1^2 (E_2 - G)^2 (m_1 n_1)^2 \\
+ E_2^2 (E_1 - G)^2 (m_2 n_2)^2 + G^2 (E_1 - E_2)^2 (m_3 n_3)^2.
\]

(2.24)

If an isotropic material without contraction is considered, so that \( E_2 = E_1 = E \), equation (2.24) simplifies to:

\[
D = E^2 (E - G)^2 (m_1 n_1 + m_2 n_2)^2.
\]

(2.25)

This discriminant is always positive and so the eigenvalues of \( D_e \) are real.

However, for orthotropic materials \( E_1 \neq E_2 \) and the analysis is more difficult. Now, three reformulations of expression (2.24) are distinguished, all of which consist of a square and an additional term. One of these is:

\[
D = \{ E_1 (E_2 - G)m_1 n_1 + E_2 (E_1 - G)m_2 n_2 + G (E_1 - E_2)m_3 n_3 \}^2 \\
+ 4E_1 G (E_2 - E_1)(E_2 - G)m_1 n_1 m_3 n_3.
\]

(2.26)

This formulation provides the following sufficient conditions that assure a positive discriminant:

\[
\begin{align*}
\{ \ E_2 < E_1 < G \ & \lor \ G < E_1 < E_2 \ & \} \ & \land \ & m_1 n_1 m_3 n_3 > 0, \ (2.27) \\
\{ \ E_2 < G < E_1 \ & \lor \ E_1 < G < E_2 \ & \} \ & \land \ & m_1 n_1 m_3 n_3 > 0, \\
\{ \ E_1 < E_2 < G \ & \lor \ G < E_2 < E_1 \ & \} \ & \land \ & m_1 n_1 m_3 n_3 < 0.
\end{align*}
\]

If one of these conditions holds real eigenvalues are guaranteed. If a similar analysis is performed for the other formulations of (2.24) and if the fact that by definition \( m_3 n_3 > 0 \) is used, the combined sufficient conditions that assure a positive discriminant become:

\[
\begin{align*}
\{ \ G < E_1 < E_2 \ & \lor \ E_2 < E_1 < G \ & \} \ & \land \ & m_1 n_1 > 0, \ (2.28) \\
\{ \ G < E_2 < E_1 \ & \lor \ E_1 < E_2 < G \ & \} \ & \land \ & m_1 n_1 < 0, \\
\{ \ G < E_2 < E_1 \ & \lor \ E_1 < E_2 < G \ & \} \ & \land \ & m_2 n_2 > 0, \\
\{ \ G < E_1 < E_2 \ & \lor \ E_2 < E_1 < G \ & \} \ & \land \ & m_2 n_2 < 0.
\end{align*}
\]

The combination for which \( G \) has a value between \( E_1 \) and \( E_2 \) cancels because in that case any value of \( m_1 n_1 \) or \( m_2 n_2 \) results in a positive value of \( D \) (eq. (2.24)).
2.2. EIGENVALUE ANALYSIS

From a physical point of view $G < E_i$, and therefore only four situations need to be considered. If the conditions are not fulfilled, complex eigenvalues may appear.

From Lemma 1 it is known that complex eigenvalues can only appear if one of the elements of $m$ and $n$ have a different sign. Conditions (2.28) lead to a similar conclusion with some extra restrictions. Therefore, only some negative products $m_i n_i$ could possibly lead to complex eigenvalues.

Vector $m$ is closely related to $n$ and is different in sign only for a finite set of stresses. A lower bound for $m_i n_i$, $i = 1, 2$ can be defined. The product $m_i n_i$ equals $n_i^2 + n_i(\beta - \alpha)/3$ and attains its minimum where $2n_i + (\beta - \alpha)/3 = 0$, that is when $n_i = (\alpha - \beta)/6$. The product $m_i n_i$ then becomes:

$$m_i n_i = \frac{(\alpha - \beta)^2}{36} + \frac{(\alpha - \beta)(\beta - \alpha)}{18} = -\frac{(\alpha - \beta)^2}{36}. \quad (2.29)$$

The difference between $\alpha$ and $\beta$ is therefore the main factor of influence for the possible existence of complex eigenvalues.

For plane-stress conditions, the yield surface in the non-principal stress space has the form of an ellipsoid (see Figure 2.3(b)). Since $m_3$ and $n_3$ are equal and always appear together, and since they are the only $m_i, n_i$ depending on $\sigma_{xy}$ (see equation (2.17)), the shear stress $\sigma_{xy}$ is present only in squared form in the characteristic polynomial of the elasto-plastic matrix $D_{ep}$. Therefore, the eigenvalues of the upper and lower part of the ellipsoid are the same. Figure 2.4 is a view from above of these eigenvalues. There are two non-zero eigenvalues. For the choice of $E_1$, $E_2$ and $G$ denoted in Figure 2.4 and according to conditions (2.28), complex eigenvalues may arise only in the areas where $m_1 n_1 < 0$ and $m_2 n_2 > 0$. Some complex eigenvalues indeed appear. They are denoted by holes and come in complex conjugate pairs.

2.2.2 Plane-strain configuration

In case of a plane-strain configuration one more stress direction is accounted for: $\sigma_{zz}$. Vectors $m$ and $n$ now have four elements (eq. (2.12)):

$$n = \frac{1}{2\sqrt{I_1^2 - 3I_2}} \begin{bmatrix} 2I_1 - 3\sigma_{yy} - 3\sigma_{zz} \\ 2I_1 - 3\sigma_{xx} - 3\sigma_{zz} \\ 2I_1 - 3\sigma_{xx} - 3\sigma_{yy} \\ 6\sigma_{xy} \end{bmatrix} + \frac{\alpha}{3} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 0 \end{bmatrix}, \quad (2.30)$$

with $I_1, I_2, I_3$ as in equation (2.15), and

$$m = n + (\beta - \alpha)[1, 1, 1, 0]^T / 3. \quad (2.31)$$
Figure 2.4: Eigenvalue distribution $\lambda_1$ and $\lambda_2$ for orthotropic plane-stress conditions. Material parameters: $E_1 = 50, E_2 = 60, G = 30, \phi = \pi/9, \psi = 0$, cohesion=0.01. Between the two inclined lines it holds that $m_1 n_1 < 0$. 
2.2. EIGENVALUE ANALYSIS

Again the following text is split into a part about isotropic plane-strain conditions and a part about orthotropc plane-strain conditions.

**Isotropic plane-strain**

For isotropic plane-strain conditions, certain combinations of the elements of \( \mathbf{n} \) and \( \mathbf{m} \) (eq. (2.30)) simplify the eigenvalue computations considerably. Introducing the parameters:

\[
\begin{align*}
    u &= m_1 n_1 + m_2 n_2 + m_3 n_3, \\
    v &= m_1 n_2 + m_1 n_3 + m_2 n_1 + m_2 n_3 + m_3 n_1 + m_3 n_2, \\
    w &= m_4 n_4,
\end{align*}
\]

(2.32)

it can be shown that (see Appendix A.2, page 25):

\[
\begin{align*}
    u &= \frac{3}{2} + \frac{\alpha \beta}{3} - \frac{w}{2}, \\
    v &= -\frac{3}{2} + \frac{2 \alpha \beta}{3} + \frac{w}{2}.
\end{align*}
\]

(2.33)

The discriminant of the elasto-plastic material matrix can therefore be expressed in terms of \( w \) only.

Taking into account \( \sigma_{zz} \), the elasticity matrix for plane-strain conditions has one column and row more than the one resulting from plane-stress conditions. It is of the form:

\[
\mathbf{D}_e = \frac{E}{(1 + \nu)(1 - 2\nu)} \begin{bmatrix}
1 - \nu & \nu & \nu & 0 \\
\nu & 1 - \nu & \nu & 0 \\
\nu & \nu & 1 - \nu & 0 \\
0 & 0 & 0 & (1 - 2\nu)/2
\end{bmatrix}.
\]

(2.34)

The constant \( E/(1 + \nu)(1 - 2\nu) \) can again be left out of the analysis. After multiplication with \((1 + \nu)(1 - 2\nu)\mathbf{n}^T \mathbf{D}_e \mathbf{m} / E \), the characteristic polynomial of \( \mathbf{D}_{ep} \) can be written as:

\[
c(\lambda) = \lambda(\lambda - 1 + 2\nu) \{A\lambda^2 + B\lambda + C\}.
\]

(2.35)

Apart from the zero eigenvalue there is a constant eigenvalue that is equal to \( 1 - 2\nu \). After multiplication with \( 2\mathbf{n}^T \mathbf{D}_e \mathbf{m} / (\lambda(\lambda - 1 + 2\nu)) \) the discriminant \( B^2 - 4AC \) becomes:

\[
D = \frac{(1 - 2\nu)^2}{144} \left[\left\{9(4\nu + 1) - 3w(1 - 2\nu) - 2\alpha \beta (\nu + 1)\right\}^2 - 24\alpha \beta (\nu + 1)(1 + 4\nu)(w - 3)\right].
\]

(2.36)

Because \( w \leq 3 \) (Appendix A.2, page 25) and because \( \nu \) is usually between zero and a half, the analysis is completed and it can be concluded that for isotropic materials all eigenvalues of the elasto-plastic matrix are real, irrespective of the value of the dilatancy angle.
Orthotropic plane-strain

For orthotropic materials the discussion is limited to the case with no Poisson effect \((\nu = 0)\), as was done for the plane-stress configuration. In a plane-strain configuration, the elasticity matrix has then four different diagonal entries. The first three entries, \(E_1, E_2, E_3\), signify the stiffness parameters in orthogonal directions and the fourth entry, \(G\), signifies a shear modulus. All four stiffness moduli are positive.

The appropriate characteristic polynomial of the elasto-plastic matrix \(D_{ep}\) is of degree four, with one zero root. The higher order of the characteristic polynomial makes the analysis more difficult, and unfortunately to such an extent, that only a numerical analysis could be carried out. This means that for certain material parameters the eigenvalues of \(D_{ep}\) were computed, thereby studying the possible occurrence of complex eigenvalues.

As a consequence of Lemma 1 (page 15), the only region where complex eigenvalues can be found is where the product \(m_i n_i, i = 1, 3\) is negative. For the numerical analysis of the eigenvalues of \(D_{ep}\) one ring of the Drucker-Prager cone has been chosen, Figure 2.2. On such a ring the invariants \(I_1\) and \(I_2\) are constant:

**Lemma 2** On the circular rings of the Drucker-Prager cone (Fig. 2.2) that have the hydrostatic axis as normal it holds that \(I_1\) and \(I_2\) are constant.

**Proof:**
The normal of such a ring and the plane in which the ring lies is expressed by \((1,1,1)\), i.e. the direction of the hydrostatic axis \(p\). The inner product of \((1,1,1)\) with any point on the plane gives the same value by definition. The point \((p,p,p)\) is on this plane and the inner product therefore equals \(3p\). Because \(I_1 = 3p\) and \(I_2\) is uniquely defined by \(I_1\) via the Drucker-Prager yield function (eq. (2.5)), the lemma is true.

The eigenvalues of \(D_{ep}\) are computed by varying \(\sigma_{xx}\) and \(\sigma_{yy}\) within the limit given by a fixed \(I_1\). The stress component \(\sigma_{zz}\) then follows from this value of \(I_1\) and with the Drucker-Prager yield function \(f_{DP}\) (eq. (2.5)) the second variant \(I_2\) can be obtained as well as \(\sigma_{xy}\) (eq. (2.15)).

Between the black lines in Figure 2.5 the product \(n_i m_i\) is negative and complex eigenvalues may appear in this area. Note that the eigenvalues are representative for the eigenvalues of any circular mesh line of the cone for a fixed internal friction angle (see Section 4.1). As with the plane-stress case complex eigenvalues emerge in conjugate pairs.
Figure 2.5: Complex eigenvalues for orthotropic plane-strain conditions. Between the black lines the product $m_i n_i$ is negative. Material parameters: $E_1 = 55, E_2 = 60, E_3 = 50, G = 30; \sin \psi = 0.1; \sin \phi = 0.3; \text{cohesion} = 0.0001.$
Appendix A.1

Proof of Lemma 1

In this appendix Lemma 1, page 15 is proved.

Suppose that the characteristic polynomial of $A + uv^T$ contains only terms in which $u_i$ and $v_i$ are combined, i.e. cross products like $u_i v_j$, $i \neq j$ or terms with only $u_i$ or $v_i$ do not appear. Analogously, the characteristic polynomial of the symmetric matrix $A + zz^T$ then contains only combinations of the products $z_i z_i$. Setting $z_i = \sqrt{|u_i v_i|}$ it then follows that $A + uv^T$ is similar to the symmetric matrix $A + zz^T$ if $u_i v_i > 0$. It is now shown that indeed the characteristic polynomial of $A + uv^T$ consists uniquely of terms in which $u_i$ and $v_i$ are combined.

The characteristic polynomial of $A + uv^T$ is equal to the determinant of $B = A + uv^T - \lambda I$ with $I$ the identity matrix. For the computation of a determinant the following formula can be used[35]:

$$\det(B) = \sum_{\pi:\pi!} \prod_{i=1}^n b_{i\pi(i)} \det(P_\pi). \quad (2.37)$$

The columns of $P_\pi$ are a permutation of the columns of the identity matrix with the ordering according to the permutation $\pi = (\pi(1), \ldots, \pi(n))$ of the numbers $(1, \ldots, n)$. Thus $\det(P_\pi)$ is either 1 or -1. The sum is taken over all $n!$ permutations $\pi$.

A diagonal element $b_{i\pi(i)}, i = \pi(i)$ of the matrix $B$ equals $a_{ii} + u_i v_i - \lambda_i$ and thus contains only combined $u_i v_i$. An off-diagonal element $b_{i\pi(i)}, i \neq \pi(i)$ equals $u_i v_{\pi(i)}$. Equation 2.37 can be reordered so that the diagonal terms are separated from the off-diagonal terms:

$$\det(B) = \sum_{\pi:\pi!} \left\{ \prod_{i \in \omega_1(\pi)} (a_{ii} - \lambda + u_i v_i) \prod_{j \in \omega_2(\pi)} u_j v_{\pi(j)} \right\} \det(P_\pi). \quad (2.38)$$
The set $\omega_1$ consists of the elements of $\pi$ for which it holds that $i = \pi(i)$. The set $\omega_2$ is the rest so that $\omega_1 \cup \omega_2 = \pi$ and $\omega_1 \cap \omega_2 = \emptyset$. It now remains to show that the second product in equation (2.38) contains both $u_j$ and $v_j$ for all $j \in \omega_2$.

Suppose that $j = 1 \in \omega_2$ then 1 cannot be an element of $\omega_1$ because $\omega_1 \cap \omega_2 = \emptyset$. This means that $v_1$ is not contained in the first product. However, the right hand side of equation (2.38) includes $v_1$ and it must therefore be contained in the second product. This line of reasoning holds for any $j \in \omega_2$. Thus equation (2.38) can be written as:

$$
\det(B) = \sum_{\pi=\pi_1} \left\{ \prod_{i \in \omega_1(\pi)} (a_{ii} - \lambda + u_i v_i) \prod_{j \in \omega_2(\pi)} u_j v_j \right\} \det(P_\pi), \quad (2.39)
$$

and the lemma is proved.
Appendix A.2

Parameter elaborations

In this appendix the expressions for $u, v$ and $w$ of Section 2.32 (page 19) are further developed to show how $u, v$ can be expressed as functions of $w$ and to show that $w \leq 3$. The following notations were introduced:

\[ u = m_1n_1 + m_2n_2 + m_3n_3, \]  
\[ v = m_1n_2 + m_1n_3 + m_2n_1 + m_2n_3 + m_3n_1 + m_3n_2, \]  
\[ w = m_4n_4. \]  

Writing $\mathbf{m} = \mathbf{n} + (\beta - \alpha)[1, 1, 1, 0]^T/3$ and using equation (2.30) and $n_1 + n_2 + n_3 = \alpha$, the following simplifications are obtained:

\[ u = n_1^2 + n_2^2 + n_3^2 + (n_1 + n_2 + n_3)(\beta - \alpha)/3 \]
\[ = n_1^2 + n_2^2 + n_3^2 + \alpha(\beta - \alpha)/3, \]  
\[ v = 2n_1n_2 + 2n_1n_3 + 2n_2n_3 + 2\alpha(\beta - \alpha)/3, \]  

such that:

\[ u + v = (n_1 + n_2 + n_3)^2 + \alpha(\beta - \alpha) = \alpha \beta. \]

Moreover, the last component of $\mathbf{m}$ and $\mathbf{n}$ is the same and therefore:

\[ w = \frac{36\sigma_{xy}^2}{4(I_1^2 - 3I_2)}. \]
Because:

\[
\begin{align*}
    n_1^2 + n_2^2 + n_3^2 &= \frac{1}{4(I_1^2 - 3I_2)} \left\{ 12I_1^2 + 18(\sigma_{xx}^2 + \sigma_{yy}^2 + \sigma_{zz}^2) \\
    &\quad - 24I_1(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}) \\
    &\quad + 18(\sigma_{xx}\sigma_{yy} + \sigma_{xx}\sigma_{zz} + \sigma_{yy}\sigma_{zz}) \right\} + \frac{\alpha^2}{3} \\
    &= \frac{1}{4(I_1^2 - 3I_2)} \left\{ -12I_1^2 + 18(I_1^2 - I_2 - \sigma_{xy}^2) \right\} + \frac{\alpha^2}{3} \\
    &= \frac{3}{2} + \frac{\alpha^2}{3} - \frac{18\sigma_{xy}^2}{4(I_1^2 - 3I_2)},
\end{align*}
\]

it follows that:

\[
2u + w = 3 + \frac{2\alpha^2}{3} + \frac{2\alpha(\beta - \alpha)}{3} = 3 + \frac{2\alpha\beta}{3}.
\]  \hspace{1cm} (2.46)

With equations (2.43), (2.46) \( u \) and \( v \) can be expressed in terms of \( w \):

\[
u = \frac{3}{2} + \frac{\alpha\beta}{3} - \frac{w}{2}, \quad v = -\frac{3}{2} + \frac{2\alpha\beta}{3} + \frac{w}{2}.
\]  \hspace{1cm} (2.47)

Finally, note that \( w \leq 3 \). This can be verified by substituting:

\[
6\sigma_{xy}^2 = 2(I_1^2 - 3I_2) - \left\{ (\sigma_{xx} - \sigma_{yy})^2 + (\sigma_{xx} - \sigma_{zz})^2 + (\sigma_{yy} - \sigma_{zz})^2 \right\},
\]  \hspace{1cm} (2.48)

into equation (2.44).
Chapter 3

Finite element model

The continuum problem associated to soil deformation is in general too complex to solve analytically. If the finite element method is chosen as the numerical tool, the computation can be characterized by the following steps. First, the area is subdivided into disjunct elements. The elements are connected via the edges such that all elements together exactly constitute the whole area. Relations are set up for each element and are then assembled into a global discrete system. The deformation of soil has a nonlinear character and the discrete system is solved with an iterative method.

In this chapter the above mentioned steps are investigated in more detail. However, no attempt is made to describe and explain the finite element method in all its facets or to give a general introduction. Only the aspects of interest for this study are described briefly. More complete information can be found for example in the books by Zienkiewicz and Taylor [42] or Crisfield [7, 8] for an engineering point of view or Strang and Fix [36] for a mathematical point of view.

In the last section of this chapter some examples of finite element problems are presented. These are used extensively in the remainder of this work.

3.1 Material laws

A body in space may experience two kinds of forces: a force on the surface, for example due to contact, and a force in the interior of the body, e.g. gravity. A body force \( \mathbf{b} \) is expressed per unit of mass, so that if \( \mathbf{b} \) acts on a volume element \( dV \) with density \( \rho \) the total force becomes \( \mathbf{b} \rho dV \). A surface element has a normal \( \mathbf{n} \) indicating its orientation and a force on the surface is therefore described by \( t(\mathbf{n})dS \) where \( S \) is the surface of the element on which \( t \), called the surface traction, acts.
Body forces and surface tractions induce accelerations on the body and the forces and accelerations are related by the global equation of motion (balance of linear momentum). Denoting the space occupied by an arbitrary part of the body by \( \Omega \) and its surface by \( \partial \Omega \), the global force equation reads\([23]\):

\[
\int_\Omega \rho b \, dV + \int_{\partial \Omega} t(n) \, dS = \int_\Omega \rho a \, dV,
\]

(3.1)

where \( a = \ddot{u} \) and \( u \) the displacement vector.

The surface traction \( t \) can be expressed as the product of the Cauchy stress matrix \( \Sigma \) \([23]\), introduced in Section 2.1.1, with the outward normal vector \( n \) of the surface:

\[
t(n) = \Sigma n.
\]

(3.2)

Due to the balance of angular momentum \([42]\) \( \Sigma \) is symmetric. For further elaboration of the equation of motion (3.1) it is more convenient to change to indicial notation. The Cauchy stress matrix is then denoted by \( \sigma_{ij} \) and if ever an index is repeated, summation is implied. This means that equation (3.2) in indicial notation reads: \( t_{ij}(n_j) = \sigma_{ij} n_j \). Using this type of notation and also equation (3.2), the equation of motion (3.1) becomes:

\[
\int_\Omega \rho b_i \, dV + \int_{\partial \Omega} \sigma_{ij} n_j \, dS = \int_\Omega \rho a_i \, dV.
\]

(3.3)

Gauss’ theorem implies that:

\[
\int_{\partial \Omega} \sigma_{ij} n_j \, dS = \int_\Omega \sigma_{ij,j} \, dV.
\]

(3.4)

where \( \sigma_{ij,j} \) is the notation for the derivative of \( \sigma_{ij} \) in the direction of the \( j^{th} \) variable. With Gauss’ theorem as stated above, equation (3.3) can be simplified to:

\[
\int_\Omega (\rho b_i + \sigma_{ij,j} - \rho a_i) \, dV = 0.
\]

(3.5)

This equation embodies a fundamental law that should be independent of how a given body is defined. Thus, for this integral to be zero for any region \( \Omega \), the integrand must zero and this leads to the local equations of motion (local balance of linear momentum, due to Cauchy):

\[
\rho b_i + \sigma_{ij,j} - \rho a_i = 0.
\]

(3.6)

If the accelerations in the material are omitted and writing \( g_i = \rho b_i \) this equation becomes:

\[
\sigma_{ij,j} + g_i = 0.
\]

(3.7)
3.2. DISCRETIZATION

Figure 3.1: Triangular element (a) without and (b) with curved edges. Rectangular element (c) without and (d) with curved edges. The 'x's denote (a) 1, (b) 3, (c) 2x2 and (d) 3x3 integration points for Gauss integration.

The kinematic equations describe the relation between displacements \( u \) and strains. This relation reads, for small deformations:

\[
\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}),
\]  

(3.8)

where \( \epsilon_{ij} \) are engineering strains. Like the stress matrix \( \sigma_{ij} \), the strain matrix \( \epsilon_{ij} \) is symmetric: \( \epsilon_{ij} = \epsilon_{ji} \).

Summarizing, modeling of soil deformation involves constitutive equations (Section 2.1.3), kinematic equations, the equilibrium of force (balance of linear and angular momentum) and boundary conditions. A practical and efficient approach to solve all equations and constraints at the same time, is offered by the finite element method. The next section discusses this approach.

3.2 Discretization

The elements form the building blocks of the finite element method. In two dimensions, their basic form is usually either triangular or quadrilateral. The edges are straight for the simpler elements and curved for more complex elements. Figure 3.1 shows a triangular and a quadrilateral element with and without curved edges.

The nodal degrees of freedom (translations and rotations) of element \( l \) are denoted by \( u^{l_0} \). The global displacement within element \( l \) is denoted by \( u^l \) and is computed with the interpolation matrix \( N_l \):

\[
u^l = N_l u^{l_0}.
\]  

(3.9)

The elements of matrix \( N_l \) are functions of nodal coordinates.

A numerical solution is sought to the equilibrium equation, eq. (3.7). The finite element method provides a framework for this problem. It consists of
reformulation of the equilibrium equation as a variational problem by setting the integral of the equilibrium equations multiplied with a test function equal to zero (Galerkin’s approach). In solid mechanics the test functions are called variations and are preceded by $\delta$. Note that formulation of the minimum potential energy function or the principal of virtual work may lead to the same variational problem.

3.2.1 Weak formulation

Inside the element $\sigma_{ij,j} + g_i = 0$ must be satisfied whereas on the surface it must hold that $\sigma_{ij}n_j - t_i = 0$ with $t_i$ the surface tractions and $n_j$ the normal of the surface. Instead of solving these equations exactly, a weak formulation is set up. This means that the equilibrium equation inside an element and that $\sigma_{ij}n_j - t_i = 0$ on its surface are multiplied with virtual displacements $\delta u_i$ and then integrated over the whole area or its boundary, whichever is appropriate.

Let $V$ denote volume and $S$ surface, $\Omega_e$ the volume taken up by an element and $\partial \Omega_e$ its surface. The weak formulation of the equilibrium equations according to Galerkin then becomes:

$$ \int_{\Omega_e} \delta u_i (\sigma_{ij,j} + g_i) dV - \int_{\partial \Omega_e} \delta u_i (\sigma_{ij} n_j - t_i) dS = 0. \quad (3.10) $$

Gauss’ theorem implies that:

$$ \int_{\partial \Omega_e} \delta u_i \sigma_{ij} n_j dS = \int_{\Omega_e} (\delta u_i \sigma_{ij})_j dV. \quad (3.11) $$

Equation (3.11) can be further simplified using the notation for strains from equation (3.8):

$$ \int_{\Omega_e} (\delta u_i \sigma_{ij})_j dV = \int_{\Omega_e} \delta \varepsilon_{ij} \sigma_{ij} dV + \int_{\Omega_e} \sigma_{ij,j} \delta u_i dV. \quad (3.12) $$

Equations (3.11) and (3.12) can be used to reformulate (3.10):

$$ - \int_{\Omega_e} \delta \varepsilon_{ij} \sigma_{ij} dV + \int_{\Omega_e} \delta u_i g_i dV + \int_{\partial \Omega_e} \delta u_i t_i dS = 0. \quad (3.13) $$

It is now more convenient to switch back from indicial to vector notation. This means that $u_i$ is written as $u$, $\varepsilon_{ij}$ as $\varepsilon$ and so on. In particular, $\sigma_{ij}$ becomes $\sigma$, a vector whose elements are the entries of the stress matrix introduced in Section 2.1.1: $\sigma^T = [\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{xz}, \sigma_{yz}]$. Equation (3.13) then reads:

$$ - \int_{\Omega_e} \delta \varepsilon^T \sigma dV + \int_{\Omega_e} \delta u^T g dV + \int_{\partial \Omega_e} \delta u^T t dS = 0. \quad (3.14) $$
3.2. DISCRETIZATION

The left-most integral can be interpreted as the variation of internal energy (strain energy) whereas the two other integrals express the virtual work done by the external forces. In the examples considered in this research the body forces are not taken into account. Therefore, the second term of equation (3.14) vanishes. The integral is evaluated numerically in integration points and the number and location of these points define the order and type of integration. In this research Gauss integration is used [42], see also Figure 3.1.

The aim of the finite element formulation is to obtain an expression relating forces to displacements. The constitutive law was formulated in rate equations in Section 2.1.3 but is linearized in practice as follows:

$$\dot{\sigma} = D_{ep} \epsilon \Rightarrow \sigma = \dot{\sigma} + D_{ep} \Delta \epsilon,$$  \hspace{1cm} (3.15)

where $\dot{\sigma}$ is fixed and $\Delta \epsilon$ a small strain increment. Matrix $D_{ep}$ is nonsymmetric in case of nonassociated plasticity. In the previous section (eq. (3.9)) it was stated that $u' = N_l u'^n$. The kinematic equation (3.8) in more compact form reads: $\epsilon = L^T u$. The differential operator $L$ is made up of derivatives in space coordinates. The size and form depend on the configuration. For two-dimensional plane-stress conditions $L$ reads:

$$L = \begin{bmatrix} \partial/\partial x & 0 & \partial/\partial y \\ 0 & \partial/\partial y & \partial/\partial x \end{bmatrix},$$  \hspace{1cm} (3.16)

whereas for plane-strain it holds that:

$$L = \begin{bmatrix} \partial/\partial x & 0 & 0 \\ 0 & \partial/\partial y & 0 \\ 0 & 0 & \partial/\partial x \end{bmatrix}. \hspace{1cm} (3.17)$$

Using $\epsilon = L^T u$ it follows that:

$$\epsilon'^n = L^T N_l u'^n = B u'^n \text{ with } B = L^T N_l. \hspace{1cm} (3.18)$$

With equation (3.18) and the linearized constitutive equation (3.15), equation (3.14) becomes for element $l$:

$$\int_{\Omega_e} \delta \epsilon'^n T \sigma dV = \int_{\Omega_e} \delta \epsilon'^n T (\dot{\sigma} + D_{ep} \Delta \epsilon'^n) dV$$

$$= \int_{\Omega_e} \delta u'^n T B^T D_{ep} B \Delta u'^n dV + \int_{\Omega_e} \delta u'^n T B^T \dot{\sigma} dV \hspace{1cm} (3.19)$$

$$= \int_{\partial \Omega_e} (N_l \delta u'^n)^T t dS.$$

The integral with the fixed stress vector $\dot{\sigma}$ can be interpreted as a body force and assembled with the integral of surface tractions. The nodal displacements
do not depend on the space variables and can be taken out of the integral. Defining:

\[ K' = \int_{\Omega_e} B^T D_{cp} B dV, \]

\[ \Delta f' = \int_{\partial \Omega_e} N_i^T t dS - \int_{\Omega_e} B^T \dot{\sigma} dV, \]

equation (3.19) becomes:

\[ \delta u^{ln} \cdot T K' \Delta u^{ln} = \delta u^{ln} \cdot T \Delta f'. \]

(3.22)

This relation holds for a specific element. The relation of all elements together is now expressed as:

\[ \delta u^T \{ K \Delta u - \Delta f \} = 0. \]

(3.23)

In \( K \) and \( f \) all element contributions are assembled and \( u \) is the vector of all nodal displacements. The equation must hold for every virtually admissible nodal displacement vector \( \delta u \) and thus \( K \Delta u = \Delta f \) must hold.

### 3.2.2 Newton-Raphson iteration

Starting with a force on the surface, the finite element equations allow for the computation of a displacement vector that results in equilibrium. However, the constitutive relation is nonlinear. Therefore, a discrepancy arises between the external force vector and the internal forces that result from the computed displacement. This discrepancy can be eliminated or at least diminished by the application of an iterative procedure. The Newton-Raphson method is a common choice for this purpose.

In the Newton-Raphson iterative procedure the total force is applied in small increments. Equation (3.23) can therefore also be written as:

\[ K_i \Delta_i u = \mu_i q, \]

(3.24)

where \( \Delta_i \) now denotes the \( i \)th increment of the Newton-Raphson iteration. Vector \( q \) is fixed during the whole process, whereas parameter \( \mu_i \) can be different for every increment. The Newton-Raphson method starts with the tangent stiffness matrix of the previous converged iteration. The stresses and strains resulting from an applied force via this old tangent stiffness matrix are used to set up a new tangent stiffness matrix. The difference between the internal and external force vector is then used to find an adjustment of the displacement vector after which the iteration is performed once more. This is repeated until the difference between the internal and external forces is negligible.
3.3 Bifurcation of the displacement field

Bifurcation of the load-displacement path is defined as loss of uniqueness of the incremental equilibrium, which means that a certain force increment is in equilibrium with more than one displacement increment. Bifurcation points can be classified in two ways: discontinuous and continuous. For a discontinuous bifurcation the force increment is related to the displacement increments via different tangent stiffness matrices. For a continuous bifurcation the same tangent stiffness matrix relates the displacement increments to the force increment. The focus of this research is on continuous bifurcation.

If there are at least two solutions, subtracting the appropriate finite element relations as presented in equation (3.24) for two force/displacement equilibrium paths and leaving out the subscripts gives the bifurcation condition:

\[
\begin{align*}
\mathbf{K}\Delta^1 \mathbf{u} = & \quad \mu \mathbf{q} \\
\mathbf{K}\Delta^2 \mathbf{u} = & \quad \mu \mathbf{q}
\end{align*}
\]  \quad \Rightarrow \quad \mathbf{K}(\Delta^1 \mathbf{u} - \Delta^2 \mathbf{u}) = \mathbf{K}\Delta \mathbf{u}_\Delta = 0. \tag{3.25}

The subscript \( \Delta \) indicates the difference between the two displacement increments. Equation (3.25) implies that \( \mathbf{K} \) is singular, i.e. at least one eigenvalue must equal zero. Let \( \lambda_k, k = 1, \ldots, k \) be the zero eigenvalues and \( \mathbf{x}_k, \mathbf{y}_k \) the associated right and left eigenvectors. Because \( \mathbf{K} \) is singular, a nontrivial solution of equation (3.25) exists if either \( \mu = 0 \) or \( \mathbf{q} \) lies in the column space of \( \mathbf{K} \) so that \( \mathbf{y}_k^T \mathbf{q} = 0 \) for all \( j \). The latter can be understood as follows. If \( \mathbf{K}\Delta \mathbf{u} = \mu \mathbf{q} \in \text{span}\{\mathbf{x}_{k+1}, \ldots, \mathbf{x}_n\} \) and because \( \mathbf{y}_m^T \mathbf{x}_k = \delta_{mk} \) it follows that \( \mathbf{y}_k^T \mathbf{K}\Delta \mathbf{u} = \mu \mathbf{y}_k^T \mathbf{q} = 0 \). It can be concluded that equation (3.25) is satisfied if either one of the following is true:

1. \( \mu = 0 \),
2. \( \mathbf{y}_k^T \mathbf{q} = 0 \),
3. \( \mathbf{y}_k^T \mathbf{q} = 0 \) and \( \mu = 0 \). \tag{3.26}

The first possibility is called a limit point, whereas the second possibility determines a bifurcation point. The third possibility is that a limit point is a bifurcation point as well. In this thesis attention is paid to the second possibility.

Note that for the examples of this work, zero eigenvalues or an exact bifurcation point are never found. This is due to the fact that neither the material
model nor the load incrementation are continuous. Therefore, a change from loading to unloading results in a change of tangent stiffness matrix and a discontinuity in the slope of the load-displacement curve.

**Potential energy and stability**

For elastic materials there is a clear relation between the potential energy and instability which is provided by the potential energy function $P$. Expanded in a Taylor series around a stable solution $\mathbf{u}$ this function reads [7]:

$$
P(\mathbf{u} + \Delta \mathbf{u}) = P(\mathbf{u}) + \left( \frac{\partial P}{\partial \mathbf{u}_i} \right)^T \Delta \mathbf{u} + \frac{1}{2} \Delta \mathbf{u}^T \left( \frac{\partial^2 P}{\partial \mathbf{u}_i \partial \mathbf{u}_j} \right) \Delta \mathbf{u} + \ldots$$

$$
\approx P(\mathbf{u}) + \mathbf{p}_1^T \Delta \mathbf{u} + \frac{1}{2} \Delta \mathbf{u}^T \mathbf{p}_2 \Delta \mathbf{u}.
$$

(3.27)

The vector $\mathbf{p}_1$ is the out-of-balance force and $\mathbf{p}_1^T \Delta \mathbf{u}$ should be zero in an equilibrium state. The term $\mathbf{p}_2$ is equal to the structural stiffness matrix $\mathbf{K}$. In order to have a stable equilibrium, a small energy change $P(\mathbf{u} + \Delta \mathbf{u}) - P(\mathbf{u})$ should be positive for any small $\Delta \mathbf{u}$. This means that $\Delta \mathbf{u}^T \mathbf{K} \Delta \mathbf{u}$ must be positive, and thus $\mathbf{K}$ must be positive definite. Although relation (3.27) only holds for elastic materials the information provided by the pivots of $\mathbf{K}$ may still be useful.

The condition for stability proposed by Hill [18] is of a more general nature. Hill postulates that for any infinitesimal displacement the increase in internal energy should exceed the work of the external forces. This can be translated into [9]:

$$
\Delta \sigma^T \Delta \varepsilon > 0,
$$

(3.28)

for a small increment of stresses $\Delta \sigma$ and a small increment of strains $\Delta \varepsilon$. Loss of stability is not necessarily equal to loss of uniqueness [9]. In other words, if the material becomes unstable, there is not necessarily another solution related to a positive definite tangent stiffness matrix. In general bifurcation or loss of uniqueness is preceded by loss of stability. Another matter of consideration is that positive definiteness is needed to guarantee stability for any small displacement. But in practice only one particular loading case is considered. Thus, if $\mathbf{K}$ becomes indefinite this may not be noticed in the material behavior for the load or displacement increment considered.

If $\mathbf{K}$ is normal ($\mathbf{KK}^T = \mathbf{K}^T \mathbf{K}$), positive definiteness implies positive pivots (from the Gaussian elimination process used for solving the finite element equations) as well as positive eigenvalues (see Golub and van Loan [15], pp. 141, 314). If $\mathbf{K}$ is not normal, positive definiteness no longer implies positive eigenvalues.
However, uniqueness of the incremental solution can be related to positive eigenvalues of $\mathbf{K}$, even if $\mathbf{K}$ is not normal. It has been assumed in the examples of Chapter 6 that a bifurcation point is passed if at least one eigenvalue of $\mathbf{K}$ turns negative. In almost all tests a bifurcation was indeed present and another path was found. A few problems where negative eigenvalues, negative pivots and bifurcation did not coincide, are further analyzed in Chapter 7.

### 3.4 Examples

In this section three different types of problems are discussed briefly. The first problem is that of pure shear, the second concerns biaxial compression and the third is the borehole stability problem. Certain discretizations or material parameters are proposed that are often used in the following chapters. It holds for all problems that the deformation is elastic, becomes plastic and stays homogeneous until a bifurcation point has been reached. Only plane-strain problems were considered so that all problems are two-dimensional with only a normal stress in the third direction.

The first example is primarily chosen as test case for the proposed branch switch methods. In Figure 3.2(a) the loading case is shown, a typical discretization is shown in Figure 3.2(b) and the element that has been used is displayed in Figure 3.2(c). Note that the right and left sides of this element are linked by dependence relations in order to behave identically with respect to the horizontal and vertical displacement so as to simulate the one-dimensional underlying configuration. With six linear elements the total number of nodal degrees of
freedom is 28, but only eleven are free. During homogeneous deformations the rod may shorten, but is not allowed to bend. The element is a simple rectangular element with straight edges, nodes only on the corners of the element and a $2 \times 2$ Gauss integration is used.

Softening is applied to the cohesion. During loading it holds that if the softening parameter goes from zero to ten, the cohesion diminishes from 0.01 to 0.001. Young’s modulus equals 1.8625N/mm$^2$ and Poisson’s ratio $\nu = 0.49$.

In the second example the specimen is free to move in the horizontal direction and is compressed in the vertical direction. Due to the fact that there is only normal stress and no strains in the direction normal to the free surface this problem is referred to as the biaxial compression test. The particular configurations for this problem are shown in Figure 3.3.

Table 3.1 shows the type and number of elements (#el), the dimensions, the degrees of freedom (DOF) and the Poisson ratio $\nu$ for a specific discretization. In Table 3.1 QQ is an abbreviation of quadrilateral quadratic and TQ triangular quadratic. In the latter case the area is subdivided into $6 \times 12$ rectangles that

<table>
<thead>
<tr>
<th>type</th>
<th>#el</th>
<th>Dim.</th>
<th>DOF</th>
<th>free</th>
<th>$\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>QQ</td>
<td>6 \times 12</td>
<td>60 \times 120 mm</td>
<td>506</td>
<td>479</td>
<td>0.49</td>
</tr>
<tr>
<td>QQ</td>
<td>12 \times 24</td>
<td>120 \times 240 mm</td>
<td>1874</td>
<td>1873</td>
<td>0.3</td>
</tr>
<tr>
<td>TQ</td>
<td>4 \times 6 \times 12</td>
<td>60 \times 120 mm</td>
<td>1226</td>
<td>1199</td>
<td>0.49</td>
</tr>
</tbody>
</table>
Figure 3.4: Borehole stability problem with (a) a quarter of a horizontal cross section, (b) a three-dimensional representation and (c) typical discretizations.

are each subdivided into four triangles.

Softening is again applied to the cohesion. During loading it holds that if the softening parameter goes from zero to one hundred, the cohesion decreases from 0.01 to 0.001. Young’s modulus equals 1.8625N/mm² and sin φ = 0.3.

The third and last example is the borehole stability problem. In search for oil, holes are drilled after which the bore is removed. Upon removal of the bore deformation occurs in the horizontal plane that may destroy the hole. Of interest is the strength of the hole and possible deformation modes in the cross section. These depend on the depth of the hole. Figure 3.4 shows a quarter of a horizontal cross section and a three-dimensional representation of the problem.

If the area is divided into 25 elements along the hole boundary, and 80 along the straight sides and if each element is subdivided into four quadratic triangles, then the total number of degrees of freedom is 8182 of which 8100 are non-prescribed.

Some remarks

In the graphs that give the relation between loading and displacement the slopes decrease as loading or prescribed displacement increase. The graphs become flatter until the bifurcation point is reached. The load-displacement graph of the borehole stability problem has an almost flat top.

If nothing is done at bifurcation the solution continues on the homogeneous
branch which is unstable. This branch has a slightly negative slope. In Chapter 6 it is explained how a proper post-bifurcation behavior can be computed and how this relates to load-displacement graphs and deformations.

For some of the tests a Cosserat[6] continuum will be used. This means that besides the two translational degrees of freedom there is an extra rotational degree of freedom in a node. This type of continuum may help to overcome mesh dependency of the solution in case of problems with material softening [16].
Chapter 4

A material-type eigenvalue analysis of numerical solutions

In this chapter some stress paths of finite element computations are analyzed and linked to the eigenvalue analysis of Section 2.2. This eigenvalue analysis consisted of computing the eigenvalues of the elastoplastic material matrix $D_{ep}$ for a certain ring of the Drucker-Prager cone (Figure 2.2). On this ring the first invariant $I_1$ is constant as well as the second invariant $I_2$ (Lemma 2, page 20). Also, this ring is related to a specific cohesion.

In a numerical computation with softening on the cohesion, $I_1$ and $I_2$ constantly change. In this chapter it is explained how these different states can all be related to one particular $I_1, I_2$ with fixed cohesion. It is then possible to see how and where a finite element calculation develops in the eigenvalue plots of Section 2.2. Particular attention is paid to the regions where complex eigenvalues were found in the analysis of Section 2.2. If an example would enter into one of these regions this could cause numerical difficulties.

The mapping of a $I_1, I_2$ combination with a particular cohesion onto a reference configuration can be done without influencing the eigenvalue analysis. This is explained in Section 4.1. The evolution of some examples in the reference configuration is discussed in Section 4.2. Because complex eigenvalues of the elastoplastic matrix were found only for orthotropy, the material model chosen for the examples is that of plane-strain orthotropy.
4.1 Computational setup

For fixed dilatancy and friction angles and for fixed Young’s moduli, a finite element computation produces stress states after every Newton-Raphson iteration that relate to a particular \( I_1, I_2 \)-combination and a cohesion. In this section it is explained how such a stress state can be mapped onto a reference state, so that the results of all Newton-Raphson iterations can be compared in one single image.

The whole set of possible stress distributions defined by a specific value of \( I_1, I_2, \phi \) and \( \psi \), presents a filled oval in the \( \sigma_{xx}, \sigma_{yy} \) space. The oval’s center is the hydrostatic pressure \( p \) and its radius follows from the constraint that \( \sigma_{xy}^2 \) must be positive. During a nonlinear calculation with softening on the cohesion, every Newton-Raphson iteration results in a different stress distribution associated to a particular value for \( I_1 \) and a specific cohesion. To show the whole process in one image, every converged stress distribution is transformed to the reference distribution defined by \( I_1^* = 0 \) and \( c^* = 0.01 \), where the superscript \( * \) is used to indicate the reference values. As a consequence \( I_2^* = -k^2/3 \) (see eq. (2.5)), where \( k \) depends on \( c^* \) according to equation (2.6).

Given \( \{\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}\} \) from a converged state of the Newton Raphson process (see Section 3.2.2), the values of \( I_1 \) and \( I_2 \) can be obtained with equations (2.15) as well as the hydrostatic pressure \( p \). All possible stress combinations in \( \sigma_{xx}, \sigma_{yy} \) space are described by an oval. Another way to describe an oval is with center point, radius and angle. With the hydrostatic pressure \( p \) as center point the description of the oval becomes:

\[
\sigma_{xx} = p + r \cos \theta, \quad (4.1)
\]
\[
\sigma_{yy} = p + r \sin \theta, \quad (4.2)
\]
\[
\sigma_{zz} = p - r \sin \theta - r \cos \theta, \quad (4.3)
\]
\[
\sigma_{xy}^2 = \sigma_{xx} \sigma_{yy} + \sigma_{xx} \sigma_{zz} + \sigma_{yy} \sigma_{zz} - I_2
\]
\[
= 3p^2 - r^2 \cos \theta \sin \theta - r^2 \sin^2 \theta - r^2 \cos^2 \theta - I_2 \quad (4.4)
\]
\[
= I_1^2/3 - I_2 - r^2(1 + \cos \theta \sin \theta),
\]
for a given cohesion and hydrostatic pressure \( p \). Therefore, \( \sigma_{xy}^2 \) attains its maximum at \( r = 0 \) and vanishes when:

\[
r = \sqrt{(I_1^2 - 3I_2)/3(1 + \cos \theta \sin \theta)} \equiv R. \quad (4.5)
\]

For the reference state oval, \((I_1^* = 0)\), the radius associated with \( \sigma_{xy}^2 = 0 \) is given by:

\[
R^* = \sqrt{-I_2/(1 + \cos \theta \sin \theta)}. \quad (4.6)
\]
The stresses found in a numerical computation are now expressed by \( p, r \) and \( \theta \). During the transformation to the reference state \( p \) and \( r \) change, but \( \theta \) is fixed. The stress values in the reference state are denoted by a superscript \( r \) and can be computed from the original stress values via:

\[
\sigma^{*}_{xx} = \frac{(\sigma_{xx} - p)R^*}{R}, \\
\sigma^{*}_{yy} = \frac{(\sigma_{yy} - p)R^*}{R}, \\
\sigma^{*}_{zz} = \frac{(\sigma_{zz} - p)R^*}{R},
\]

(4.7) \hspace{1cm} (4.8) \hspace{1cm} (4.9)

after which \( \sigma^{*}_{xy} \) can be computed from \( I_2^* \). The eigenvalues of the elastic-plastic matrix \( D_{ep} \) are the same in the original state and in the reference state. That is, the normals \( m, n \) that make up \( D_{ep} \) (eq. (2.9)) are unchanged by the transformation. Filling in equation (2.30) (page 17) for both stress distributions gives for example for \( n_1 \):

\[
n_1 = \frac{2I_1^* - 3\sigma^{*}_{yy} - 3\sigma^{*}_{zz}}{2\sqrt{(I_1^*)^2 - 3I_2^*}} + \frac{\alpha}{3} = \frac{-3(\sigma_{yy} + \sigma_{zz} - 2p)\sqrt{-I_2^*}}{2\sqrt{-3I_2^*} \sqrt{I_1^*/3 - I_2}} + \frac{\alpha}{3} \\
= \frac{2I_1 - 3\sigma_{yy} - 3\sigma_{zz}}{2\sqrt{I_1^2 - 3I_2}} + \frac{\alpha}{3}.
\]

(4.10)

Elaborations for \( n_2, n_3 \) and \( n_4 \) lead to similar relations.

The next section describes some examples of plane-strain orthotropy. The stress values after a Newton-Raphson iterations are transformed according to the method given above and then compared with the eigenvalue analysis of Section 2.2.

### 4.2 Examples

In Section 2.2.2 eigenvalues were computed of the plane-strain orthotropic material matrix with material properties that lead to complex eigenvalues. This configuration is chosen as reference state onto which the stress states of the examples discussed in this section are mapped.

In the eigenvalue analysis of Section 2.2.2 the Young’s moduli were set to 50 and 60 N/mm² and the shear modulus to 30 N/mm². The cohesion is 0.0001 N/mm² and \( \sin \phi = 0.3, \sin \psi = 0.1 \). The examples discussed here refer to the examples introduced in Section 3.4.

In the first example the pure shear problem is considered. The numerical computation is performed until negative pivots are found. A small amount of strain
Figure 4.1: Stress paths and complex eigenvalues in the reference stress configuration. Material parameters: \(E_1 = 55, E_2 = 60, E_3 = 50, G = 30; \sin \psi = 0.1; \sin \phi = 0.3; \) cohesion = .0001.

hardening is included. The total loading is subdivided into nine steps and in each step all four stress components in one of the integration points are computed. These stresses are then mapped onto the reference state. Even though these stresses lie close to the combinations associated to complex eigenvalues, none of the stresses are actually in this area. This is visualized in Figure 4.1('o'), where the shear stress \(\sigma_{xy}\) is plotted against the normal stresses \(\sigma_{xx}, \sigma_{yy}\). The holes in the figure denote the areas where at least one of the three eigenvalues of the material matrix was complex (see also Fig. 2.5).

The second example is the biaxial compression test with a fine mesh of twelve by twenty-four quadrilaterals. The finite element computation is continued until the Newton-Raphson iteration fails to converge for the given step size.

The sides of the specimen are free to move. As a result the shear stress is zero during homogeneous deformation. In the visualization of the eigenvalues the stress path is therefore situated on the outer border of the image in \(\sigma_{xx}, \sigma_{yy}\) space. As Figure 4.1('+') shows, the stresses in this example remain far away from the critical zone.

For the example of the borehole stability problem a mesh is chosen that is composed of 2000 triangles with nodes in the corners and on the middle
of the edges. The plasticity spreads quickly throughout all the elements and the computation is continued until the Newton-Raphson iteration no longer converges. The stresses found are situated close to the outer border, see Figure 4.1('\circ'). There is a large drop in value of the shear stress $\sigma_{xy}$ near to the side, and the shear stress in this example is of the same order as the other (normal) stresses $\sigma_{xx}, \sigma_{yy}$.

It was shown that the examples discussed do not enter the range where the eigenvalues of the elasto-plastic material matrix $D_{xp}$ are complex in case of plane-strain orthotropy without contraction. However, the eigenvalues of this matrix are not related directly to the eigenvalues of the tangent stiffness matrix $K$ constructed after discretization (3.2). In Chapter 6 some examples are presented for which complex eigenvalues of $K$ were found when the bifurcation point was approached.
Chapter 5

Eigenvalue and eigenvector methods

In the previous chapter an eigenvalue analysis at material level was related to numerical examples in order to see how possible complex eigenvalues of the elasto-plastic material matrix relate to stress situations found in a finite element computation.

The second part of the research, which starts here, consists of an eigenvalue analysis at structural level. Eigenvalues and eigenvectors found in this process are used for computing post-bifurcation equilibrium paths. In this chapter eigenvalue methods are introduced that can be used for large and sparse matrices that evolve from a finite element discretization.

There are various methods for computing the eigenvalues and eigenvectors of large matrices. Some methods aim at computing all eigenvalues and eigenvectors, e.g. Householder and QR ([15], Sec. 5.1, 5.2), while other methods have a more iterative quality like the Jacobi ([15], Sec. 8.4) and the power or subspace method [13, 29]. The finite element description of the deformation of soil gives rise to large and sparse matrices of which only some eigenvalues and eigenvectors are of interest, often less than ten percent. For this kind of matrices the Lanczos type methods have turned out to be the most attractive because of their convergence properties and reasonable cost.

In this section the symmetric Lanczos method [21] is first described. Then two generalizations are discussed that can handle nonsymmetric matrices, namely the Arnoldi and the Bi-Lanczos method. The Bi-Lanczos method suffers from spurious eigenvalues and for this reason an adaptation of the Bi-Lanczos method is proposed, namely the BILAPO method.
5.1 Lanczos method for symmetric matrices

The Lanczos method [21] reduces a symmetric matrix $\mathbf{K}$ to a symmetric tridiagonal form $\mathbf{T}$ of which the eigenvalues $\theta$ are successively better estimates of the eigenvalues $\lambda$ of the original matrix. The reduction is performed with an orthogonal matrix $\mathbf{Q}$ and the question is: how can such a matrix $\mathbf{Q}$ be constructed so that it generates a reduced matrix $\mathbf{T}$ whose eigenvalues are successively better estimates of those of $\mathbf{K}$?

The smallest and largest eigenvalues, $\lambda_1$ and $\lambda_n$ respectively, of any symmetric matrix $\mathbf{K} \in \mathbb{R}^{n \times n}$ are the minimum and maximum of the Rayleigh quotient $r$:

$$
\lambda_1 = \min_{z \neq 0} r(z, \mathbf{K}) = \min_{z \neq 0} \frac{z^T \mathbf{K} z}{z^T z}, \quad \lambda_n = \max_{z \neq 0} r(z, \mathbf{K}) = \max_{z \neq 0} \frac{z^T \mathbf{K} z}{z^T z}.
$$

(5.1)

A method that is set up to approximate the eigenvalues of $\mathbf{K}$ by construction of a reduced matrix whose eigenvalues are successively better estimates should improve the estimates of the two Rayleigh quotients in every iteration. After $k$ iterations, the reduction can be written as $\mathbf{Q}_k^T \mathbf{K} \mathbf{Q}_k$, with $\mathbf{Q}_k \in \mathbb{R}^{n \times k}$ and $\mathbf{Q}_k^T \mathbf{Q}_k = \mathbf{I}_k$ where $\mathbf{I}_k$ is the identity matrix of size $k \times k$. The approximated Rayleigh quotients are then:

$$
m_k = \min_{z \neq 0} \frac{z^T \mathbf{Q}_k^T \mathbf{K} \mathbf{Q}_k z}{z^T z} = \min_{z \neq 0} r(\mathbf{Q}_k z, \mathbf{K}) \geq \lambda_1,
$$

(5.2)

$$
M_k = \max_{z \neq 0} \frac{z^T \mathbf{Q}_k^T \mathbf{K} \mathbf{Q}_k z}{z^T z} = \max_{z \neq 0} r(\mathbf{Q}_k z, \mathbf{K}) \leq \lambda_n.
$$

(5.3)

The inequalities on the right hold because $m_k$ and $M_k$ are obtained by searching a vector space of dimension $k$ whereas $\lambda_1$ and $\lambda_n$ are found by searching an $n$-dimensional vector space. A next iteration vector results in the best improvement if it is set up in the direction of the derivative $\nabla r$ of the Rayleigh quotient $r$ because $m_k$ diminishes most rapidly in the direction of $-\nabla r$ and $M_k$ increases most rapidly in the direction of $\nabla r$. The derivative of a Rayleigh quotient $r$ equals:

$$
\nabla r(z, \mathbf{K}) = \nabla \left\{ \frac{z^T \mathbf{K} z}{z^T z} \right\} = \frac{2}{z^T z} \mathbf{K} z - \frac{2(z^T \mathbf{K} z)}{(z^T z)^2} z.
$$

(5.4)

Consequently, the derivative $\nabla r$ lies in the space spanned by the vectors $\mathbf{K} z$ and $z$. Thus, if matrix $\mathbf{Q}_k$ is expanded with a new column $\mathbf{q}_{k+1}$ such that the expansion reflects the direction of $\nabla r$, the minimum and maximum Rayleigh quotients will both have improved.

Finding a new vector in the direction of $\mathbf{K} z$ and $z$ can be translated to expanding a Krylov space with one more vector. A Krylov matrix (named
after A.N. Krylov [20]) is constructed from a matrix $K \in \mathbb{R}^{n \times n}$ and vector $q_1$ as follows:

$$
\mathcal{K}(K, q_1, n) = [q_1, Kq_1, K^2q_1, \ldots, K^{n-1}q_1].
$$

(5.5)

A Krylov subspace for $k \leq n$ then reads:

$$
\mathcal{K}_k(K, q_1, k) = \text{span}\{q_1, Kq_1, K^2q_1, \ldots, K^{k-1}q_1\}.
$$

(5.6)

The equivalence of expanding the set of orthogonal vectors $q_m, m = 1, \ldots, k$ with $q_{k+1}$ and the expansion of the Krylov subspace $\mathcal{K}_k(K, q_1, k)$ can be expressed by:

$$
\text{span}\{q_1, q_2, \ldots, q_k, q_{k+1}\} = \text{span}\{q_1, Kq_1, \ldots, K^{k-1}q_1, K^kq_1\}.
$$

(5.7)

Put differently: the most efficient way of generating an orthogonal set of vectors that reduce $K$ to a matrix whose eigenvalues are successively better approximates of the eigenvalues of $K$ is equivalent to finding an orthogonal basis for the Krylov subspace of $K$ and $q_1$.

To find an orthogonal basis of the Krylov subspace $\mathcal{K}_k$ in an efficient way, the tri-diagonalization of $K$ is examined and related to the $QR$ decomposition of $\mathcal{K}_k$. The tri-diagonalization of a matrix $K$ with an orthogonal matrix can be expressed by:

$$
Q^TKQ = T, \quad \text{and} \quad K = QTQ^T,
$$

(5.8)

with $T \in \mathbb{R}^{n \times n}$ the tri-diagonal matrix and $Q \in \mathbb{R}^{n \times n}$; whereas a $QR$ factorization reads:

$$
K = QR,
$$

(5.9)

with $R \in \mathbb{R}^{n \times n}$ an upper triangular matrix. From the $QR$ decomposition it is known that it provides a unique orthogonal basis ([15], Sec. 5.2.6). Consider now the tri-diagonalization of $K$ in the Krylov matrix $\mathcal{K}(K, q_1, n)$:

$$
\mathcal{K}(K, q_1, n) = [q_1, Kq_1, K^2q_1, \ldots, K^{n-1}q_1]
$$

$$
= [q_1, QTQ^Tq_1, QT^2Q^Tq_1, \ldots, QT^{n-1}Q^Tq_1],
$$

(5.10)

because $Q^TQ = I$. Since $q_1$ is the first column of matrix $Q$: $q_1 = Qe_1$ with $e_1$ a vector of length $n$ with all zeros except for a one in the first entry and $Q^Tq_1 = e_1$, the tri-diagonalization can be simplified to:

$$
\mathcal{K}(K, q_1, n) = Q[e_1, Te_1, T^2e_1, \ldots, T^{n-1}e_1].
$$

(5.11)
In the right hand side of this equation the orthogonal matrix $Q$ multiplies an upper triangular matrix and the relation to the $QR$ decomposition of $K$ is found. Thus, an orthogonal basis for $K$ can be computed efficiently by tri-diagonalizing $K$. The Lanczos method is now derived according to these concepts and principles.

The symmetric Lanczos method

The aim is to reduce matrix $K$ to a tri-diagonal form $T$ with an orthogonal matrix $Q$. If the reduction is completed ($k = n$) it can be written as $KQ = QT$ where:

$$
Q = \begin{bmatrix}
\vdots & \vdots & \cdots & \vdots \\
q_1 & q_2 & \cdots & q_n \\
\vdots & \vdots & \cdots & \vdots
\end{bmatrix}, \quad T = \begin{bmatrix}
\alpha_1 & \beta_1 & & 0 \\
\beta_1 & \alpha_2 & \ddots & \\
& \ddots & \ddots & \beta_{n-1} \\
0 & & \beta_{n-1} & \alpha_n
\end{bmatrix}.
$$

(5.12)

The Lanczos iteration can be obtained by equating the $k^{th}$ column on both sides of $KQ = QT$ and then elaborating the orthogonality condition. Equating the $k^{th}$ column on both sides gives for $2 \leq k \leq n - 1$:

$$
Kq_k = Q \begin{bmatrix}
0 & \cdots & 0 & \beta_{k-1} & \alpha_k & \beta_k & 0 & \cdots & 0
\end{bmatrix}^T
= \beta_{k-1}q_{k-1} + \alpha_k q_k + \beta_k q_{k+1},
$$

(5.13)

and thus:

$$
\beta_k q_{k+1} = Kq_k - \alpha_k q_k - \beta_{k-1} q_{k-1}.
$$

(5.14)

Pre-multiplication of equation (5.13) with the $k^{th}$ vector $q_k$ and elaborating the orthogonality condition $q_m^T q_l = \delta_{ml}$ where $\delta_{ml}$ is the Kronecker delta, then leads to:

$$
q_k^T Kq_k = \beta_{k-1} q_{k-1}^T q_k + \alpha_k q_k^T q_k + \beta_k q_{k+1}^T q_k = \alpha_k.
$$

(5.15)

Thus, at any stage of the iteration the next orthogonal vector $q_{k+1}$ of the tri-diagonalization can be obtained by first computing $\alpha_k$ using equation (5.15) and then elaborating equation (5.14). One matrix-vector product $Kq_k$ needs to be computed and the result can be used in both expressions.

Computations of eigenvalues and eigenvectors

The eigenvalues of $T$ are indeed successively better estimates of the eigenvalues of matrix $K$. The eigenvalues are also called Ritz values and $T$ the Ritz matrix.
The approximation can be verified by substituting the eigenvalue problem for \( T \) into the Lanczos relation at iteration \( k \). At iteration \( k \) it holds that:

\[
KQ_k = Q_k T_k + \beta_k q_{k+1} e_k^T,
\]  
(5.16)

where \( Q_k \in \mathbb{R}^{n \times k} \), \( T_k \in \mathbb{R}^{k \times k} \) and \( e_k \) is an identity vector of length \( k \) with all zeros except for a one in the \( k^{th} \) entry. The eigenvalue problem for \( T_k \) is denoted by \( T_k \phi_l = \theta_l \phi_l \) for eigenvalue \( \theta_l \) with associated eigenvector \( \phi_l \). Post-multiplication of equation (5.16) with \( \phi_l \) gives:

\[
KQ_k \phi_l = Q_k T_k \phi_l + \beta_k q_{k+1} e_k^T \phi_l = Q_k \theta_l \phi_l + \beta_k \phi_{kl} q_{k+1},
\]  
(5.17)

where \( \phi_{kl} \) is the last entry (entry \( k \)) of the \( l^{th} \) eigenvector. Setting \( x_l = Q_k \phi_l \) the approximate eigenvalue problem for \( K \) is obtained:

\[
Kx_l = \theta_l x_l + \beta_k \phi_{kl} q_{k+1},
\]  
(5.18)

and the eigenvalues of \( T \) are shown to be approximate eigenvalues of \( K \) if \( \beta_k \phi_{kl} q_{k+1} \) is small. The eigenvectors \( x \) are called Ritz vectors. How good the approximation is depends on the size of \( \beta_k \phi_{kl} \):

\[
\| Kx_l - \theta_l x_l \|_2 = \beta_k \phi_{kl} .
\]  
(5.19)

Either this (absolute residual) norm or the norm scaled by \( \| \theta_l x_l \|_2 \) (relative residual norm) can be used as termination criterion in the eigenvalue computation. The norm \( \| x_l \|_2 \) in that scaling can be simplified to:

\[
\| x_l \|_2 = \| Q_k \phi_l \|_2 = \| \phi_l \|_2 .
\]  
(5.20)

Thus, the eigenvectors \( x \) of \( K \) need not be constructed, in order to obtain the relative residual norm of an eigenpair of \( K \).

## 5.2 Eigenvalue methods for nonsymmetric matrices

The deformation of soil is described more accurately with a nonassociated flow rule than with an associated flow rule, see Section 2.1.2. Therefore, the system matrix \( K \) is usually nonsymmetric. There are two natural ways of extending the Lanczos method so that it can handle nonsymmetric eigenvalue problems.

The matrices that define the Lanczos method are the orthogonal reduction matrix \( Q \) and the tri-diagonal matrix \( T \). The method of Arnoldi [2] conserves the orthogonality of the reduction and therefore loses the tri-diagonality of the reduced matrix, whereas the Bi-Lanczos [40] method conserves the tri-diagonality and therefore loses the orthogonality of the reduction. Both methods are discussed in more detail in the following subsections.

An attractive alternative to the Lanczos based eigenvalue methods can be the more recently developed Jacobi-Davidson method [33].
5.2.1 Arnoldi’s method

In Arnoldi’s method [2] the orthogonality of the reduction is conserved. Therefore, matrix $K$ is no longer reduced to tri-diagonal form but instead to upper Hessenberg form. An upper Hessenberg matrix $H$ is upper triangular with one more non-zero sub-diagonal:

$$H = \begin{bmatrix}
h_{11} & h_{12} & \cdots & h_{1n} \\
\beta_1 & h_{22} & \ddots & \vdots \\
& \ddots & \ddots & h_{(n-1)n} \\
0 & \beta_{n-1} & h_{nn}
\end{bmatrix}.$$  \hspace{1cm} (5.21)

The matrix of iteration vectors still obeys $Q^TQ = I$ and the total transformation after $k = n$ iterations is denoted by $KQ = QH$. Equating the $k^{th}$ column in $KQ = QH$ for $2 \leq k \leq n - 1$ gives:

$$Kq_k = Q\begin{bmatrix} h_{1k} \cdots h_{kk} & \beta_k & 0 & \cdots & 0 \end{bmatrix}^T$$
$$= \sum_{l=1}^{k} h_{lk}q_l + \beta_kq_{k+1},$$  \hspace{1cm} (5.22)

so that:

$$\beta_k q_{k+1} = Kq_k - \sum_{l=1}^{k} h_{lk}q_l.$$  \hspace{1cm} (5.23)

Each of the entries $h_{mk}$ can be computed at iteration $k$ by pre-multiplication of equation (5.22) with the appropriate $q_m$ and using the orthogonality condition $q_m^Tq_l = \delta_{ml}$:

$$q_m^T Kq_k = \sum_{l=1}^{k} h_{lk}q_m^Tq_l + \beta_kq_m^Tq_{k+1} = h_{mk}. $$  \hspace{1cm} (5.24)

Naturally, the matrix-vector product $Kq_k$ needs only be computed once at iteration $k$.

Per iteration the method of Arnoldi consists of $k$ vector dot products and one matrix-vector multiplication. The cost per iteration therefore increases with every step. If many iterations are necessary, a restart procedure may be a good alternative in order to limit the cost of the vector dot products, see for example Sorensen [34] and Lehoucq [22].
Computations of eigenvalues and eigenvectors

Eigenvalues and eigenvectors can be computed from the Hessenberg matrix \( H \) by substituting the eigenvalue problem of \( H \) into the relation summarizing all Arnoldi iterations. Replacing \( T \) by \( H \) in equations (5.16) and (5.17) results in the appropriate equations. An estimate of the accuracy of an eigenpair can then be obtained using equations (5.18)-(5.20) that were set up for the symmetric Lanczos method.

Since \( K \) is nonsymmetric there is also a left eigenproblem with left eigenvectors that are orthogonal to the right eigenvectors. This problem cannot be solved directly with Arnoldi's method. Of course, executing Arnoldi's method twice, once with \( K \) and once with \( K^T \) provides both right and left eigenvectors.

In this work, eigenvalues and eigenvectors of \( H \) were computed with LAPACK [1] routine HQR2.

5.2.2 Bi-Lanczos method

In the Bi-Lanczos method [21] or two-sided Lanczos method a reduction to tri-diagonal form is obtained by weakening the orthogonality condition of the iteration vectors to a bi-orthogonality condition. In other words: two sets of iteration vectors evolve that are mutually orthogonal. The right iteration vectors are denoted by \( V = \{ v_m \} \) and the left iteration vectors by \( W = \{ w_m \} \). The normalized bi-orthogonality or duality condition then implies that \( W^T V = I \). The right and left eigenvectors of \( K \) also obey the bi-orthogonality relation: \( y_i^T x_j = \delta_{ij} \).

If matrix \( K \) is nonsymmetric, the resulting tri-diagonal matrix is also nonsymmetric. The entries on the diagonal are again denoted by \( \alpha_k \), the entries on the lower diagonal by \( \beta_k \) and the entries on the upper diagonal by \( \gamma_k \). In order to obtain the entries on both the upper and lower diagonals two relations are set up, one with an ordinary matrix-vector product and one with the transposed matrix-vector product. After \( k = n \) iterations the reduction can be summarized as:

\[
KV = VT, \quad K^T W = WT^T. \tag{5.25}
\]

Equating the \( k^{th} \) column on both sides of both equations gives the \( k^{th} \) right and left iteration of the Bi-Lanczos method:

\[
\begin{align*}
Kv_k &= V \begin{bmatrix} 0 & \cdots & 0 & \gamma_{k-1} & \alpha_k & \beta_k & 0 & \cdots & 0 \end{bmatrix}^T \\
&= \gamma_{k-1} v_{k-1} + \alpha_k v_k + \beta_k v_{k+1},
\end{align*}
\]

so that:

\[
\beta_k v_{k+1} = Kv_k - \gamma_{k-1} v_{k-1}, \tag{5.27}
\]
and:
\[
K^T w_k = W \begin{bmatrix} 0 & \cdots & 0 & \beta_{k-1} & \alpha_k & \gamma_k & 0 & \cdots & 0 \end{bmatrix}^T
\]
\[= \beta_{k-1} w_{k-1} + \alpha_k w_k + \gamma_k w_{k+1}, \tag{5.28}
\]
so that:
\[
\gamma_k w_{k+1} = K^T w_k - \alpha_k w_k - \beta_{k-1} w_{k-1}.	ag{5.29}
\]
Parameters $\beta_k$ and $\gamma_k$ can be chosen freely as long as $w_k^T v_k = 1$, but not all choices are advisable because of stability and accuracy reasons. In this research $\beta$ and $\gamma$ are chosen such that $\|v_k\|_2 = 1$.

Elaborating the duality condition gives the relation for $\alpha_k$. Either equation (5.26) can be pre-multiplied by $w_k^T$ or equation (5.28) by $v_k^T$ to give:
\[
\alpha_k = w_k^T K v_k. \tag{5.30}
\]
For a practical implementation of the Bi-Lanczos method the reader is referred to Golub and van Loan [15] (Sec. 9.4.3) or Saad [29].

Note that The Bi-Lanczos method is set up around two matrix-vector products per iteration and four vector updates. The cost per iteration is thus constant, in contrast to the cost per iteration for Arnoldi’s method.

**Computations of eigenvalues and eigenvectors**

At the end of Section 5.1 it was explained how the eigenvalues and eigenvectors of $K$ can be computed from the eigenvalues and eigenvectors of $T$ if $K$ is symmetric. For the Bi-Lanczos method this is done in a similar fashion. The two relations that summarize the right and left Bi-Lanczos iterations read (eqs. (5.26),(5.28)):
\[
K V_k = V_k T_k + \beta_k v_{k+1} e_k^T, \quad K^T W_k = W_k T_k^T + \gamma_k w_{k+1} e_k^T, \tag{5.31}
\]
where $V_k, W_k \in \mathbb{R}^{n \times k}$, $T_k \in \mathbb{R}^{k \times k}$ and $e_k$ an identity vector of length $k$ with all zeros except for a one in the $k^{th}$, i.e. last, entry. Substituting the right and left eigenvalue problems $T \phi_i = \theta_i \phi_i, T^T \psi_i = \theta_i \psi_i$ for eigenvalue $\theta_i$ and right and left eigenvectors $\phi_i, \psi_i$ of the tri-diagonal matrix $T$ in equation (5.31) gives:
\[
K V_k \phi_i = V_k T_k \phi_i + \beta_k v_{k+1} e_k^T \phi_i = \theta_i V_k \phi_i + \beta_k \phi_{kl} v_{k+1}, \tag{5.32}
\]
\[
K^T W_k \psi_i = W_k T_k^T \psi_i + \gamma_k w_{k+1} e_k^T \psi_i = \theta_i W_k \psi_i + \gamma_k \psi_{kl} w_{k+1},
\]
where $\phi_{kl}$ and $\psi_{kl}$ are the last entries (entry $k$) of the $l^{th}$ right and left eigenvector. Setting $x_l = V_k \phi_l$ and $y_l = W_k \psi_l$ the approximate right and left eigenvalue problem for $K$ follow:
\[
K x_l = \theta_l x_l + \beta_k \phi_{kl} v_{k+1}, \quad K^T y_l = \theta_l y_l + \gamma_k \psi_{kl} w_{k+1}, \tag{5.33}
\]
with the norms:

\[ \| \mathbf{Kx}_t - \theta_t \mathbf{x}_t \|_2 = \| \beta_k \mathbf{phi}_t \|_2 \| \mathbf{v}_{k+1} \|_2, \]  
(5.34)

\[ \| \mathbf{K}^T \mathbf{y}_t - \theta_t \mathbf{y}_t \|_2 = \| \gamma_k \mathbf{psi}_t \|_2 \| \mathbf{w}_{k+1} \|_2. \]  
(5.35)

The values \( \| \mathbf{v}_{k+1} \|_2 \) and \( \| \mathbf{w}_{k+1} \|_2 \) depend on the scaling of the iterations vectors (in this research:
\( \| \mathbf{v}_{k+1} \|_2 = 1, \| \mathbf{w}_{k+1} \|_2 \neq 1 \)).

A relative residual norm can be obtained by dividing by \( \| \theta_t \mathbf{x}_t \|_2 \) and \( \| \theta_t \mathbf{y}_t \|_2 \) respectively. Because the eigenvectors are not orthogonal this expression cannot be further simplified as was done for the Arnoldi method. This means that to compute a relative residual norm the eigenvectors of \( \mathbf{K} \) need to be constructed from the eigenvectors of \( \mathbf{T} \).

The eigenproblem of \( \mathbf{T} \) was solved by constructing a \( QR \)-decomposition and then extracting the eigenvalues from the upper triangular matrix. This may seem inefficient for a tri-diagonal matrix, but a stable method that exploits the nonsymmetric tri-diagonality is not known. The appropriate LAPACK [1] routines used were DHSEQR and DHSEIN.

The Bi-Lanczos iteration vectors suffer from loss of bi-orthogonality which translates into spurious eigenvalues, i.e. eigenvalues that are multiple in the tri-diagonal matrix but not in \( \mathbf{K} \). An efficient way to eliminate this inaccuracy is provided by the BILAP0 method discussed in the next subsection.

Another problem with the Bi-Lanczos method arises whenever \( \mathbf{w}_t^T \mathbf{v}_k \) is zero or almost zero. This is called serious or near serious breakdown and can be circumvented by using the Look-Ahead concept in the Bi-Lanczos method [26].

### 5.2.3 Bi-Lanczos with partial orthogonalization

When Lanczos first introduced his method in 1950 [21] it was quickly discovered that the orthogonality of the iteration vectors is usually soon lost [40] for the symmetric as well as the nonsymmetric Lanczos iteration. At that time the only alternative known to solve this problem was re-orthogonalization of the iteration vectors at every step. This works well and the symmetric Lanczos with full re-orthogonalization is still a popular method. However, for nonsymmetric matrices full re-orthogonalization means that the number of operations is twice as much as that of Arnoldi’s method, due to the double matrix-vector product and the double set of iteration vectors. The Bi-Lanczos method therefore soon lost popularity.

In 1979 an adaptation of the re-orthogonalization of the Lanczos method was introduced called selective re-orthogonalization [25]. In this method the iteration vectors were set explicitly orthogonal against (almost) converged eigenvectors. Another efficiency improvement is provided by the method of partial orthogonalization, introduced in 1984 by Simon [31],[32]. In order to follow the
loss of orthogonality a cheap recurrence relation is updated in every iteration. Only when the loss of bi-orthogonality becomes too severe, the new iteration vectors are set explicitly orthogonal against all the old iteration vectors.

This method of partial orthogonalization was recently applied to the non-symmetric Lanczos method [10], [38] and is discussed hereafter.

The BILAP0 method

The iteration vectors of the basic Bi-Lanczos method soon lose bi-orthogonality if no measure is taken. This results in multiple eigenvalues and eigenvectors in the tri-diagonal matrix that are not multiples in the original matrix used in the eigenvalue method. Full re-orthogonalization results in a method that is more computationally expensive than Arnoldi’s method because of the two sets of vectors and because of the two matrix-vector products. Of course, if both right and left eigenvectors are needed, the cost of running the Bi-Lanczos method with full re-orthogonalization or running Arnoldi’s method twice is equally expensive. However, stability and robustness also play a role and are in general in favor of Arnoldi’s method. In practice, the Bi-Lanczos method is therefore more attractive than Arnoldi’s method only if partial re-orthogonalization is necessary occasionally.

Partial orthogonalization uses information about the bi-orthogonality situation found in the elements of matrix $W^T V$ constructed from the right and left iteration vectors. The new right and left iteration vectors are set explicitly orthogonal to the old left and right iteration vectors if the elements of $W^T V$ become larger than a threshold value.

To estimate when loss of bi-orthogonality can no longer be ignored, information about the elements of the matrix $\Omega_k = W_k^T V_k$ at iteration $k$ is needed without computing the matrix-matrix product $W_k^T V_k$ explicitly. The two Bi-Lanczos iterations are (Section 5.2.2, eqs. (5.27),(5.29)):

$$Kv_k = \beta_k v_{k+1} + \alpha_k v_k + \gamma_k v_{k-1}, \quad (5.36)$$

$$K^T w_k = \gamma_k w_{k+1} + \alpha_k w_k + \beta_k w_{k-1}. \quad (5.37)$$

Pre-multiplication with an old right iteration vector $v_l$ and left iteration vector $w_l$ and substituting the elements $\omega_{lm}$ of $\Omega_k$ wherever appropriate gives the recurrence relations:

$$w_l^T K v_k = \beta_k \omega_{l(k+1)} + \alpha_k \omega_{l(k)} + \gamma_k \omega_{l(k-1)}, \quad (5.38)$$

$$v_l^T K^T w_k = \gamma_k \omega_{l(k+1)} + \alpha_k \omega_{l(k)} + \beta_k \omega_{l(k-1)}. \quad (5.39)$$
Setting up the recurrence relations with $l$ and $k$ reversed gives:

\begin{align}
\mathbf{w}_l^T \mathbf{K} \mathbf{v}_l &= \beta_l \omega_{k(l+1)} + \alpha_l \omega_{kl} + \gamma_{l-1} \omega_{k(l-1)}, \\
\mathbf{v}_k^T \mathbf{K}^T \mathbf{w}_l &= \gamma_l \omega_{(l+1)k} + \alpha_l \omega_{lk} + \beta_{l-1} \omega_{(l-1)k},
\end{align}

and the terms with the matrix-vector product can be eliminated by subtracting the two related recurrence relations: (5.38) minus (5.41) and (5.39) minus (5.40). This results in:

\begin{align}
\beta_k \omega_{l(k+1)} &= \gamma_l \omega_{(l+1)k} + \alpha_l \omega_{lk} + \beta_{l-1} \omega_{(l-1)k} = \alpha_{k+1} \omega_{lk} - \gamma_{k-1} \omega_{l(k-1)}, \\
\gamma_k \omega_{(k+1)l} &= \beta_l \omega_{k(l+1)} + \alpha_l \omega_{kl} + \gamma_{l-1} \omega_{k(l-1)} = \alpha_{k+1} \omega_{kl} - \beta_{k-1} \omega_{(k-1)l}.
\end{align}

These recurrence relations are easy and cheap to update. To complete this method a value is necessary for starting the recurrence and a reset value whenever the orthogonality is set explicitly after a signal from this recurrence relation. Experiments showed that in both cases a value equal to the machine precision $\varepsilon$ was satisfactory. The threshold value for loss of orthogonality is set to $\sqrt{\varepsilon}$.

Whenever a serious loss of bi-orthogonality is signalled the new vectors as well as the vectors of the next iteration are orthogonalized against the appropriate set of old vectors, i.e. the right new vector and its successor against the old left vectors, and the left new vector and its successor against the old right vectors. It is necessary to perform this re-orthogonalization during two successive iterations because a new iteration vector is constructed from two previous iteration vectors. This method is referred to as the BILAPC method in the remainder of this research.

The method described in [11] follows roughly the above described procedure. However, the normalization of the Bi-Lanczos vectors is somewhat different as well as the signalling of loss of orthogonality. The Ph.D. thesis [10] preceding [11] includes a thorough error analysis of the BILAPC method and provides a sound theoretical basis.

5.3 Nonsymmetric eigenvalue methods in practice

A typical characteristic of the eigenvalues of the structural tangent stiffness matrix $\mathbf{K}$ is that they are strongly clustered around zero. These are exactly the eigenvalues that are needed for the perturbation methods that will be introduced in the next chapter. However, the convergence of eigenvalue iteration is
slow if they are clustered. This problem is eliminated by performing the inverse eigenvalue iteration. Instead of using $K$, $q_k = Kz$ is solved for $z$ in equation (5.23) for the Arnoldi method. In case of the Bi-Lanczos and BILAP0 methods, $v_k = Kz_1$ and $w_k = K^Tz_2$ are solved for $z_1$ and $z_2$ in equations (5.27) and (5.29). A decomposition of $K$ has already been set up in order to solve the equilibrium equations of the Newton-Raphson process and performing the inverse eigenvalue iteration is therefore not necessarily more expensive.

The difference between the respective eigenvalue methods regarding efficiency and accuracy is examined briefly in two different examples. The total cost is subdivided into the cost for a matrix-vector product and the cost of vector-dot products in case of the Arnoldi and BILAP0 methods. The examples discussed hereafter were introduced in Section 3.4.

For the example of biaxial compression with a coarse mesh, the plastic deformation begins after six millimeters prescribed displacement. This problem has 506 degrees of freedom of which 479 are free. The problem was analyzed with a zero dilatancy angle. For a given load level the results are the following. After thirty eigenvalue iterations the Arnoldi method produces nine converged eigenvalues with relative residual norms between $10^{-9}$ and $10^{-7}$ and the BILAP0 method also gives nine converged eigenvalues with norms between $10^{-8}$ and $10^{-5}$. The Bi-Lanczos method finds eight converged eigenvalues but only four of those are different. This is because of loss of bi-orthogonality so that converged eigenvalues start reappearing in later iterations. The norm of the converged eigenvalues is between $10^{-8}$ and $10^{-5}$.

Figure 5.1 presents a plot of the time consumed by each method. BILAP0 is the most expensive method. Orthogonalization of the iteration vectors was done at iterations 6,9,12,15,18,21,24,27,30. Because orthogonalization is reset during two successive iterations this means that once re-orthogonalization starts (in the sixth iteration) only one iteration passes before orthogonalization is necessary again. It is noted that the total amount of time consumed by the BILAP0 method is less than twice the consumed time with Arnoldi’s method, so that the BILAP0 method is more attractive than running Arnoldi’s method twice if both right and left eigenvectors are wanted.

As a next example the borehole stability problem is discussed. A total of 2000 triangles covers the area resulting in 8182 degrees of freedom of which 8100 are non-prescribed. The material parameters are: Young’s modulus 25MPa, Poisson’s ratio 0.2, $\sin \phi = 0.5$, $\sin \psi = 0.0$, cohesion 0.01 and some softening on the cohesion. When plasticity has spread through about a third of specimen, the BILAP0 method finds eight eigenvalues with relative residual norms less than $10^{-6}$. The norms of the eight eigenvalues found with Arnoldi’s method are better, namely less than $10^{-8}$. The Bi-Lanczos method finds nine converged
5.4 Evaluation of the eigenvalue methods

Arnoldi's method and the Bi-Lanczos and BILAPo methods were discussed and tested on some examples. These methods are specifically attractive for solving the nonsymmetric eigenvalue problem of large and sparse matrices that typically evolve from finite element computations.

If both right and left eigenvectors are wanted, the Bi-Lanczos method is the cheapest method as long as the vector-dot product dominates the matrix-vector multiplication, but it suffers from loss of orthogonality. The multiplicity brings in an uncertainty with respect to the total number of negative eigenvalues. Also, if two eigenvalues are close but one converges faster than the other,
Figure 5.2: Consumed time for borehole stability problem.

the other one may not be found. Therefore, this method was not used in the perturbation tests that will be discussed in the next chapter.

The BILAPo method is more expensive than Arnoldi’s method in both examples of the previous section, but at most equally expensive as performing Arnoldi twice. The new perturbation method developed in Section 6.2 uses both right and left eigenvectors and the BILAPo method was used to provide the necessary information.
Chapter 6

Perturbation techniques

In the previous chapter several methods were introduced that can be used to compute eigenvalues and eigenvectors of large and sparse matrices that typically evolve from a finite element discretization. The BILAPo method is used in this chapter to find eigenvectors associated to negative eigenvalues that are needed to perturb the solution and to excite a solution that describes a localized deformation mode.

First the idea of orthogonal perturbation is explained in Section 6.1 and then the method of deflation in Section 6.2. The different perturbation methods are tested on some examples in Section 6.3.

6.1 Orthogonal perturbation

This section introduces a generalization of the method first described by de Borst [4]. The original method is set up with only one eigenvector related to a negative eigenvalue and is recapitulated here briefly. It is then extended so that it can handle more than one negative eigenvalue.

A bifurcation point is defined by a system matrix with at least one zero eigenvalue (Section 3.3) while the load is not stationary. If, at this point, a right eigenvector associated to a zero eigenvalue is added to the incremental displacement vector, another solution is obtained for the same problem, because:

\[ K(\Delta u + \alpha x) = K\Delta u + 0, \]  

(6.1)

with \( x \) the right eigenvector related to the zero eigenvalue and \( \alpha \) a weight factor. In practice a zero eigenvalue is never found (Section 3.3). A bifurcation point is usually identified by the occurrence of negative eigenvalues in the tangent stiffness matrix. Using an eigenvector associated to a negative eigenvalue for
perturbing the solution \( \mathbf{u} \) may cause continuation on a secondary branch. This perturbation consists of adding the eigenvector to the solution multiplied by \( \alpha \):

\[
\tilde{\mathbf{u}} = \mathbf{u} + \alpha \mathbf{x},
\]

where \( \alpha \) is chosen such that \( \tilde{\mathbf{u}} \perp \mathbf{u} \). The orthogonal direction is chosen because the localization mode is often orthogonal to the homogeneous deformation mode. Parameter \( \alpha \) is then given by:

\[
\alpha = -\frac{\mathbf{u}^T \mathbf{u}}{\mathbf{x}^T \mathbf{u}}.
\]

For eigenvectors that are almost orthogonal to the displacement vector, the weight factor \( \alpha \) is very large. The shape of the eigenmode (the displacement field associated to the chosen eigenvector) influences the final deformation and the slope of the load-displacement curve. For more negative eigenvalues, the method can be extended by computing \( \alpha_l \) for every eigenvector that leads to \( \tilde{\mathbf{u}} \perp \mathbf{u} \):

\[
\tilde{\mathbf{u}} = k \mathbf{u} - \sum_{l=1}^{k} \frac{\mathbf{u}^T \mathbf{u}}{\mathbf{x}_l^T \mathbf{u}} \mathbf{x}_l.
\]

The number of negative eigenvalues \( k \) appears in the front of the right hand side of the equation, in order to guarantee the orthogonality condition \( \tilde{\mathbf{u}} \perp \mathbf{u} \) at the end of all eigenvector perturbations.

The method described in this section will be referred to as orthogonal perturbation and will be denoted by \( \perp \). As a subscript will be added either a number corresponding to an eigenvector or the word 'all' if the perturbation is performed with all eigenvectors.

### 6.2 Deflation

It is assumed that a system matrix with negative eigenvalues indicates a passage beyond a bifurcation point. Once the path has been found that relates to the localization mode, the system matrix will again have only positive eigenvalues under displacement control (used consistently in this study). This property has been used in constructing a new, more general eigenvector perturbation method. All eigenvectors are considered related to negative eigenvalues, and the analysis is based on the right and the left eigenvectors. In this way the aspect of nonsymmetry in case of nonassociated plasticity problems is explicitly taken into account.

The original idea was to perturb the matrix with negative eigenvalues just after bifurcation with the associated eigenvectors such that the the negative
eigenvalues are replaced by positive eigenvalues. This can be done by applying the deflation technique used often to obtain several eigenvalues from a matrix, see for example [28]. If $\lambda_l$, $l = 1, \ldots, k$ are the negative eigenvalues of $K$, with associated right and left eigenvectors $x_l, y_l$, then the deflation of $K$ can be written as follows:

$$\tilde{K} = K - \sum_{l=1}^{k} \omega_l \lambda_l x_l y_l^T.$$

(6.5)

It is assumed that $x_l$ is normalized to Euclidean length one and that $|y_l^T x_l| = 1$. The deflation leaves all eigenvectors unchanged. This can be verified by post-multiplication with a right eigenvector. Also the positive eigenvalues are unperturbed. If $\omega_l = 1$ for all $l$ then zero eigenvalues replace the negative eigenvalues. If $\omega_l > 1$ the negative eigenvalues turn positive with magnitude $(1 - \omega_l)\lambda_l$ leaving the associated right and left eigenvectors unchanged. Thus, all eigenvalues of $\tilde{K}$ are again positive. For this reason $\omega_l$ is chosen larger than one.

Some first experiments were carried out, that perturbed the system matrix directly [39] with promising results. However, this method is computationally expensive. In general the system matrix is not assembled for the solution procedure, but all calculations are carried out on element level. However, to compute $\tilde{K}$ assembly of the element matrices is necessary. Moreover, the tangent stiffness matrix has a band structure that is destroyed by the perturbation. In [39] this was prevented by perturbing only the band, and hence introducing inaccuracies in the perturbation.

Due to the computational disadvantages of perturbing the system matrix directly, the method was further developed so that it would become more attractive. Next, it is shown how the perturbation can be rewritten as a multiple vector update.

In matrix form the deflation of (6.5) becomes:

$$\tilde{K} = K - XDY^T.$$

(6.6)

Here $D$ is a diagonal matrix with entries equal to:

$$d_l = \omega_l \lambda_l, \quad 1 \leq l \leq k,$$

$$d_l = 0, \quad k < l \leq n.$$  

(6.7)

Note that equation (6.6) includes all eigenvectors but this is only necessary for the derivation of the simplified formulation. The final method makes use only of eigenvectors associated to negative eigenvalues.

A solution is sought of the equation $\tilde{K}\Delta\tilde{u} = \Delta f$ (eq. (3.23)). This equation relates increments of displacement to increments of force, where the solution
is perturbed. In the following the \( \Delta s \) are left out of the equations for clarity. During this analysis it holds that \( \tilde{u} = K^{-1}f \). Of course, the inverse is never really computed in practice but a decomposition is made. The original and perturbed matrix can be decomposed in eigenvectors and eigenvalues as follows:

\[
K = X\Lambda Y^T, \quad \tilde{K} = X\tilde{\Lambda} Y^T, \quad \tilde{\Lambda} = \Lambda - D.
\] (6.8)

For the derivation of the computationally more attractive deflation method the theoretical inverse in \( \tilde{u} = \tilde{K}^{-1}f \) is split into two parts. One part is the known \( K^{-1} \) of the unperturbed problem. The inverse of \( \tilde{K} \) can be written as:

\[
\tilde{K}^{-1} = X\tilde{\Lambda}^{-1}Y^T = X\Lambda^{-1}Y^T - XDY^T = K^{-1} - XDY^T.
\] (6.9)

The elements of \( \tilde{D} \) (not the inverse of \( D \) but part of the inverse of the non-singular \( \tilde{\Lambda} \)), for \( 1 \leq l \leq k \), can be determined with equation (6.7) from:

\[
\frac{1}{\lambda_l - d_l} = \frac{1}{\lambda_l - \tilde{d}_l} \iff \tilde{d}_l = \frac{-\omega_l}{\lambda_l(1 - \omega_l)}.
\] (6.10)

For \( k < l \leq n \) the elements \( \tilde{d}_l \) are simply zero because \( d_l = 0 \). For the computation of \( \tilde{u} \), \( \tilde{K}^{-1}f \) is split as follows:

\[
\tilde{u} = \tilde{K}^{-1}f = K^{-1}f - XDY^Tf = u - XDY^Tf.
\] (6.11)

The last term can be written as a multiple vector update, leaving out the zero terms due to zero diagonal elements of \( \tilde{D} \):

\[
\tilde{u} = u - \sum_{l=1}^{k} \tilde{d}_l x_l y_l^T f = u + \sum_{l=1}^{k} \frac{\omega_l y_l^T u}{1 - \omega_l} x_l = u + \sum_{l=1}^{k} \alpha_{\omega_l} x_l,
\] (6.12)

with \( \alpha_{\omega_l} = \omega_l y_l^T u / (1 - \omega_l) \). In equation (6.12) the identity has been used that \( y_l^T f = y_l^T K u = \lambda_l y_l^T u \). The perturbation has been simplified to several vector updates of the displacement vector with the eigenvectors related to negative eigenvalues. Since \( \omega_l \) is larger than one, the weight factor \( \alpha_{\omega_l} \) of the vector updates falls in the range:

\[
\lim_{\omega_l \downarrow 1} \frac{\omega_l y_l^T u}{1 - \omega_l} = -\text{sign}(y_l^T u) \infty, \quad \lim_{\omega_l \rightarrow \infty} \frac{\omega_l y_l^T u}{1 - \omega_l} = -\text{sign}(y_l^T u) y_l^T u,
\] (6.13)

if the left eigenvector is not orthogonal to the displacement vector. If it is, the weight factor is zero and the perturbation cannot be used successfully.

The choice of \( \omega_l \) is free as long as it is larger than one. If \( \omega_l \) is taken constant, independent of the negative eigenvalue, a method arises denoted by \( \omega_c \). This method is referred to as constant deflation. If \( \omega_l \) is different for each
eigenvalue and such that the norm of the perturbation $\alpha_{\omega_l} \mathbf{x}_l$ for each $1 \leq l \leq k$ is equal to the norm of the unperturbed displacement vector $\mathbf{a}$, a method evolves that is denoted by $\omega_n$. The different $\omega_n$s for this normalized deflation method are determined according to:

$$
\| \mathbf{u} \| = \frac{\| \omega_n \mathbf{y}_l^T \mathbf{u} \|}{1 - \omega_n} \| \mathbf{x}_l \| \Leftrightarrow \omega_n = \frac{\| \mathbf{u} \|}{\| \mathbf{u} \| - \| \mathbf{y}_l^T \mathbf{u} \| \| \mathbf{x}_l \|},
$$

(6.14)

where $\| \mathbf{x}_l \| = 1$ and $\omega_n > 1$. If $\| \mathbf{u} \|$ is less than $| \mathbf{y}_l^T \mathbf{u} |$ the term on the right side of equation (6.14) assigns a value less than one to $\omega_n$ which is in contradiction to the assumption that $\omega_n > 1$. In practice this never happened. Note that $\alpha_{\omega_n}$ can be computed directly from the norm of $\mathbf{u}$ but then it would be impossible to verify $\omega_n > 1$. At the end of the summation of perturbations, $\mathbf{u}$ is renormalized to its original length. This method is referred to as normalized ($\omega_n$) deflation.

Relation between deflation and orthogonal perturbation

The deflation method as well as orthogonal perturbation can, for one negative eigenvalue, be written as $\tilde{\mathbf{u}} = \mathbf{u} + \alpha \mathbf{x}$. Each method determines $\alpha$ in a different manner:

$$
\begin{align*}
\omega & \Rightarrow \alpha_\omega = \frac{\omega \mathbf{y}_l^T \mathbf{u}}{1 - \omega}, \\
\perp & \Rightarrow \alpha_{\perp} = \frac{-\mathbf{u}_l^T \mathbf{u}}{\mathbf{u}_l^T \mathbf{x}}.
\end{align*}
$$

(6.15) (6.16)

Note that $\alpha_\omega$ and $\alpha_{\perp}$ are equal if:

$$
\frac{\omega \mathbf{y}_l^T \mathbf{u}}{1 - \omega} = -\frac{\mathbf{u}_l^T \mathbf{u}}{\mathbf{u}_l^T \mathbf{x}} \Leftrightarrow \omega = \frac{\mathbf{u}_l^T \mathbf{u}}{\mathbf{u}_l^T \mathbf{u} - (\mathbf{y}_l^T \mathbf{u})(\mathbf{u}_l^T \mathbf{x})}.
$$

(6.17)

The $\omega$ can therefore be chosen such that the deflation and the orthogonal perturbation methods are equal. However, the condition that $\omega > 1$ will not be satisfied if $(\mathbf{y}_l^T \mathbf{u})(\mathbf{u}_l^T \mathbf{x}) > \mathbf{u}_l^T \mathbf{u}$. This happened occasionally in the examples discussed in Section 6.3.

The deflation method includes right and left eigenvectors. With the BI-
LAPO method (see Chapter 5.2.3) these can both be computed easily. The perturbation itself (updating of the displacement vector) uses the same amount of CPU time and memory for all methods and is negligible compared to the cost of the Newton-Raphson iteration and the computation of the eigenvalues and eigenvectors.
<table>
<thead>
<tr>
<th>$\sin \psi$</th>
<th>$F_{\text{max}}$</th>
<th>$D_{\text{max}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>0.1359 N</td>
<td>6.0 mm</td>
</tr>
<tr>
<td>0.2</td>
<td>0.1334 N</td>
<td>7.8 mm</td>
</tr>
<tr>
<td>0.1</td>
<td>0.1284 N</td>
<td>6.6 mm</td>
</tr>
<tr>
<td>0.0</td>
<td>0.1224 N</td>
<td>1.2 mm</td>
</tr>
</tbody>
</table>

Table 6.1: Pure shear. Bifurcation load and displacement for different dilatancy angles.

### 6.3 Perturbation methods in practice

The orthogonal perturbation method with one or more eigenvectors and the constant or normalized deflation perturbation are now tested for the examples introduced in Section 3.4. All examples are loaded until negative pivots as well as negative eigenvalues arise. The algebraic set of equations (eq. (3.23)) is solved with the finite element package DIANA [41]. Any negative pivots encountered during the gaussian elimination process are part of the output of the package.

For symmetric matrices (associated plasticity) finding negative pivots or finding negative eigenvalues is an equivalent problem, but for nonsymmetric matrices this is not necessarily true. However, as the examples show, in most cases a check on the pivots gives the correct information, i.e. the solution is just beyond a bifurcation point if negative pivots appear.

Once negative eigenvalues have been found, the associated eigenvectors are computed and used in the perturbation. If the computation converges, the final deformation pattern is examined. The load-displacement branches related to a correct deformation are steeper than the homogeneous, non-localized branches and relate, under displacement control, to system matrices without negative eigenvalues.

#### 6.3.1 Pure shear

The bifurcation point is situated differently for every dilatancy angle, but the number of negative eigenvalues is constant, equal to five. The bifurcation points can be identified by the bifurcation load and displacement, Table 6.1. In this table $F_{\text{max}}$ stands for the maximum load and $D_{\text{max}}$ for the maximum displacement. The eigenmodes related to the five negative eigenvalues are the same for all the different dilatancy angles. In Figure 6.1 two of these eigenmodes are plotted for $\sin \psi = 0.1$. The magnitude of the eigenvalues closest to zero increases from $-0.16 \times 10^{-4}$ to $-0.17 \times 10^{-3}$ with descending dilatancy angle whereas the magnitude of the eigenvalues that are furthest from zero increase from $-0.22 \times 10^{-3}$ to $-0.24 \times 10^{-2}$. So the eigenvalues drift away from zero
6.3. PERTURBATION METHODS IN PRACTICE

Figure 6.1: Pure shear, \( \sin \psi = 0.1 \). To the left: the furthest and closest to zero negative eigenvalue. In the middle: two improper deformations, \( \perp_{all}, \perp_5 \). To the right: properly localized deformation, \( \omega_c \).

when \( \psi \) decreases. This type of behavior is typical for all examples.

In this example of pure shear only the constant deflation method worked properly. All other methods end up with one or more remaining negative pivots and an improper deformation mode is obtained with more than one localized element, see Figure 6.1. The branch of the constant deflation method is the steepest and the other branches are situated between the homogeneous branch and the properly localized branch in the load-displacement diagram where for more negative pivots the branch lies closer to the homogeneous branch, Figure 6.2. Note that for \( \sin \psi = 0.0 \) the bifurcation point is situated right at the onset of plasticity. For the other dilatancy angles the load-displacement graph follows a hardening/softening branch first.

6.3.2 Biaxial compression

In this section, four different variants of the biaxial compression test are discussed: first a coarse mesh, then a fine mesh and finally a triangular mesh is considered. The triangular mesh is used in combination with a standard as well as a Cosserat continuum (Section 3.4). With these examples the performance of the different perturbation methods is examined. In order to see if the perturbation yielded the desired results, the respective load-displacement graphs and post-bifurcation deformations are analyzed and the sign of the eigenvalues is examined.

Coarse mesh

The first example of biaxial compression is with a coarse mesh of \( 6 \times 12 \) quadratic rectangles.

All dilatancy angles give rise to two negative pivots and two negative eigenvalues, but after a different amount of force and displacement, see Table 6.2. When computing the two perturbation parameters \( \alpha \) for the orthogonal perturbation method (see Section 6.1, eq. (6.3)) it was noted that one parameter
Figure 6.2: Pure shear. Load-displacement diagram for different $\sin \psi$. For every dilatancy angle the flattest branch is found with $\perp_{all}$ and the steepest with $\omega_c$.

<table>
<thead>
<tr>
<th>$\sin \psi$</th>
<th>$F_{max}$</th>
<th>$D_{max}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>4.948 N</td>
<td>7.2 mm</td>
</tr>
<tr>
<td>0.2</td>
<td>4.912 N</td>
<td>9.6 mm</td>
</tr>
<tr>
<td>0.1</td>
<td>4.843 N</td>
<td>10.2 mm</td>
</tr>
<tr>
<td>0.0</td>
<td>4.759 N</td>
<td>5.8 mm</td>
</tr>
</tbody>
</table>

Table 6.2: Biaxial compression, coarse mesh. Bifurcation load and displacement for different dilatancy angles.
Figure 6.3: Biaxial compression, coarse mesh. To the left: two eigenmodes related to negative eigenvalues. To the right: single shear band deformation with $\perp_{all}, \sin \psi = 0.0$ and a reflected shear band with $\omega_n, \sin \psi = 0.3$.

<table>
<thead>
<tr>
<th>$\sin \psi$</th>
<th>$\perp_{all}$</th>
<th>$\perp_1$</th>
<th>$\perp_2$</th>
<th>$\omega_n$</th>
<th>$\omega_c$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>+</td>
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<td>+/-</td>
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<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 6.3: Biaxial compression, coarse mesh. Behavior of the different perturbation methods.

is much larger than the other, with a difference of the order $10^8$. This is because one eigenmode is symmetric and the other is anti-symmetric (Figure 6.3), whereas the homogeneous deformation mode is without any oscillations. Equation (6.3) shows that, since the dot product of an anti-symmetric mode with the deformation vector is small, a large perturbation parameter is computed.

Two types of localized deformation evolve that are considered physically reasonable, namely that of a reflected shear band (bulging mode) and that of a single shear band. The single shear band localization relates to a slightly flatter load-displacement graph and is found only when $\sin \psi = 0.0$, Figure 6.4. In Figure 6.3 the two deformation types are shown.

Some perturbations lead to bumps in the load-displacement diagram (Figure 6.4), but all finally resulted in a proper deformation mode except for the the constant deflation method when $\sin \psi = 0.0$. Table 6.3 summarizes the performance. In this table the plus sign indicates a successful perturbation, the minus sign an unsuccessful perturbation and '+' '-' a successful perturbation but with a bump in the load-displacement diagram.

Fine mesh

Upon refinement of the mesh to $12 \times 24$ quadratic rectangles, ten negative pivots were found for $\sin \psi$ equal to 0.3, 0.2 or 0.1. At the same time ten negative
Figure 6.4: Biaxial compression, coarse mesh. Load-displacement diagrams for different $\sin \psi$ with $\omega_n$. For $\sin \psi = 0.0$ the steepest graph is associated with a bulging mode ($\omega_n$) whereas the flatter graph is associated with a single shear band ($\perp_{alt}$).

eigenvalues were found for $\sin \psi = 0.3, 0.2$ but only eight for $\sin \psi = 0.1$. The numerical data are given in Table 6.4. Figure 6.5 shows some typical eigenmodes related to negative eigenvalues. All types of modes are represented: symmetric, anti-symmetric and nonsymmetric. For eigenvalues that are closer to zero, the associated eigenmode is less undulating. Two negative pivots appear before negative eigenvalues for $\sin \psi = 0.1$. The change from two to ten negative pivots coincides with the emergence of negative eigenvalues.

In the perturbation increment the Newton-Raphson process has difficulties to converge within ten iterations, but convergence is restored in subsequent steps. A bump around this point in the load-displacement graph relates to

<table>
<thead>
<tr>
<th>$\sin \psi$</th>
<th>$F_{max}$</th>
<th>$D_{max}$</th>
<th>$\lambda &lt; 0$</th>
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</thead>
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<td>0.3</td>
<td>4.972 N</td>
<td>18.428 mm</td>
<td>10</td>
</tr>
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<td>0.2</td>
<td>4.943 N</td>
<td>28.1 mm</td>
<td>10</td>
</tr>
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<td>0.1</td>
<td>4.871 N</td>
<td>32.46 mm</td>
<td>8</td>
</tr>
<tr>
<td>0.0</td>
<td>4.754 N</td>
<td>19.23 mm</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 6.4: Biaxial compression, fine mesh. Bifurcation load and displacement for different dilatancy angles.
6.3. PERTURBATION METHODS IN PRACTICE

Figure 6.5: Biaxial compression, fine mesh. To the left: typical eigenmodes associated to negative eigenvalues. In the middle: a spurious type eigenmode, \( \sin \psi = 0.0 \). To the right: improper \((\omega_c)\) and proper \((\omega_n)\) deformation, \( \sin \psi = 0.3 \).

<table>
<thead>
<tr>
<th>( \sin \psi )</th>
<th>( \perp_{all} )</th>
<th>( \perp_1 )</th>
<th>( \perp_2 )</th>
<th>( \omega_n )</th>
<th>( \omega_c )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( .3 )</td>
<td>+</td>
<td>+</td>
<td>-</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>( .2 )</td>
<td>+</td>
<td>-</td>
<td>+</td>
<td>+</td>
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</tr>
<tr>
<td>( .1 )</td>
<td>+</td>
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<td>+</td>
<td>+/-</td>
<td>-</td>
</tr>
<tr>
<td>( .0 )</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 6.5: Biaxial compression, fine mesh. Performance of the different perturbation methods.

such a non-converged increment, Figure 6.6. The orthogonal perturbation with all vectors as well as the normalized deflation method find proper localized deformations. If only one mode is used in the orthogonal perturbation or if the constant deflation method is chosen, double shear bands may evolve, Figure 6.5.

The example with a zero dilatancy angle is a special case. Again, negative pivots are present before the occurrence of negative eigenvalues. When the number changes from two to three, one negative eigenvalue is found which is associated with a strange eigenmode that looks more like an artifact of the model than like a physical mechanism, Figure 6.5. None of the methods converges when this single eigenmode is used.

The performance of the different methods is summarized in Table 6.5. Although the eigenmodes computed at bifurcation with \( \sin \psi = 0.3 \) and \( \sin \psi = 0.2 \) were similar, the ordering was different. This explains why for \( \sin \psi = 0.3 \) method \( \perp_1 \) worked well and \( \perp_2 \) did not, whereas for \( \sin \psi = 0.2 \) the results were reversed. Eigenmode two with \( \sin \psi = 0.3 \) is symmetric, giving rise to only a small perturbation parameter \( \alpha \). Eigenmode one is nonsymmetric, and results in a much larger perturbation parameter. The first eigenmode therefore has a much larger influence on the perturbation which may explain the successful perturbation.
Figure 6.6: Biaxial compression, fine mesh. Load-displacement diagrams for different \( \sin \psi \). Steepest branches relate to \( \omega_n \) and the less steep to \( \omega_n \) in case of double branches.

<table>
<thead>
<tr>
<th>( \sin \psi )</th>
<th>( F_{\text{max}} )</th>
<th>( D_{\text{max}} )</th>
<th>( \lambda &lt; 0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>4.948 N</td>
<td>7.4 mm</td>
<td>4</td>
</tr>
<tr>
<td>0.2</td>
<td>4.912 N</td>
<td>9.6 mm</td>
<td>1</td>
</tr>
<tr>
<td>0.1</td>
<td>4.843 N</td>
<td>10.0 mm</td>
<td>6</td>
</tr>
<tr>
<td>0.0</td>
<td>4.759 N</td>
<td>5.5 mm</td>
<td>5</td>
</tr>
</tbody>
</table>

Table 6.6: Biaxial compression, triangular mesh. Bifurcation loads and displacements for different dilatancy angles.

**Triangular mesh**

For the triangular mesh the bifurcation loads and the associated displacements for the different dilatancy angles are given in Table 6.6. The eigenmodes associated to negative eigenvalues are of the regular symmetric, anti-symmetric or nonsymmetric type. There is an exception for the case of a zero dilatancy angle when one real and four complex eigenvalues are found that are associated to modes that seem spurious, Figure 6.7. This is reflected in the perturbation procedure that works well until the dilatancy angle is reduced to zero. An occasional bump can be found in the load-displacement diagram whenever ten iterations were not enough for convergence. For the zero dilatancy angle, only the real eigenvalue was used in the perturbation. In Section 7.2.2 it is explained how complex eigenvectors can be incorporated in the perturbation.
Figure 6.7: Biaxial compression with triangular mesh. To the left: typical eigenmodes related to negative eigenvalues. In the middle: eigenmode associated to the single real negative eigenvalue for \( \sin \psi = 0.0 \). To the right: reflected and single shear band deformation with \( \perp_{\text{all}} \) and \( \perp_{1} \) respectively.

<table>
<thead>
<tr>
<th>( \sin \psi )</th>
<th>( \perp_{\text{all}} )</th>
<th>( \perp_{1} )</th>
<th>( \omega_{n} )</th>
<th>( \omega_{c} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>.3</td>
<td>+/-</td>
<td>+</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>.2</td>
<td>+</td>
<td></td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>.1</td>
<td>+</td>
<td>+</td>
<td>+/-</td>
<td>-</td>
</tr>
<tr>
<td>.0</td>
<td>-</td>
<td></td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 6.7: Biaxial compression, triangular mesh. Performance of the different perturbation methods.

The deformation pattern is of a bulging type or a reflected shear band for \( \sin \psi \) ranging from 0.3 to 0.1. Only once a single shear band was found namely with \( \perp_{1}, \sin \psi = 0.1 \), Figure 6.7, and the associated load-displacement branch is somewhat less steep, see Figure 6.8. The overall performance of the methods is summarized in Table 6.7. None of the methods performed well for the problem with dilatancy angle equal to zero.

A Cosserat continuum includes a rotational degree of freedom for the nodes and helps to eliminate mesh dependence in softening and nonassociated plasticity [5]. Therefore, going from a coarser mesh to a finer mesh the width of the shear bands is unchanged, provided that the discretization of the coarse mesh is fine enough. In Groen [17] an example of biaxial compression is discussed based on a Cosserat continuum. In his example the post-peak response is obtained by weakening one of the elements. Here, eigenvector perturbations are applied in order to obtain a localized deformation mode.

To analyze the performance of eigenvector perturbations for the problem described in [17] the same triangular mesh is chosen as in the previous example, but with different material parameters. The combination of the dilatancy angle and the friction angle is taken from [17], that is \( \sin \phi = 0.38 \) and \( \sin \psi = 0.0 \). After a prescribed displacement of 16.5 mm, that corresponds to a load of 47.21N, the number of negative pivots jumps from two to fourteen and at this
Figure 6.8: Biaxial compression, triangular mesh. Load-displacement diagrams for different $\sin \psi$, $\perp_{\alpha H}$. For $\sin \psi = 0.1$ the less steep branch corresponds to the $\perp_1$ single shear band instead of a reflected shear band.

point eighteen negative eigenvalues are found, some of which are complex. Perturbation with the real vectors resulted in a single (reflected) shearband mode only for the orthogonal perturbation with the second, symmetric, eigenvector. The other methods converged to double shear bands, Figure 6.9.

The Cosserat model has a clear influence on the load-displacement paths, see Figure 6.10. The graph has a broad, almost horizontal top and flattens out at the end, a behavior not seen in the examples without the Cosserat continuum.

Figure 6.9: Biaxial compression, triangular mesh with a Cosserat continuum. To the left: two eigenmodes related to real negative eigenvalues. To the right: double shear band and reflected shearband with $\perp_{\alpha H}$ and $\perp_2$ respectively.
6.3.3 The borehole stability problem

The borehole stability problem is a difficult case. During the deformation plasticity develops from the inside boundary to the outer parts. In [19] the problem of removing the bore from the hole was modelled by pulling the inner boundary towards the center and fixing the outer boundary. In [24] the approach was adopted of a free inner boundary and a force or prescribed displacement on the outer boundary. In the latter publication a Cosserat continuum model is used while in [19] a standard Mohr-Coulomb material was chosen. According to Vardoulakis and Sulem [37] a numerical model without rotational degrees of freedom (standard continuum) is not sufficient for describing a post-bifurcation deformation.

Here, both types of loading were tried with Mohr-Coulomb and Drucker-Prager plasticity, but no post-bifurcation deformation could be obtained although in some cases one negative eigenvalue appeared. This negative eigenvalue corresponded to a wiggle around the center, but perturbation with it was unsuccessful.
6.4 Summary

In the example of pure shear only the constant deflation was successful. For the biaxial compression at least one of the methods worked satisfactorily, except for $\psi = 0.0$, when only with the coarse mesh a localized deformation mode was obtained. The idea of eigenvector perturbation was shown to be valuable and since the methods can be complementary it is best to consider all within a research framework.

The example of pure shear differs from the biaxial compression problem in that the perturbation parameters were of the same order. For biaxial compression the perturbation parameters constructed from a symmetric eigenmode were much smaller than those constructed from a nonsymmetric mode.

The general tendency is that the negative eigenvalues become larger in an absolute sense if the dilantancy angles becomes smaller. Also, the order of the negative eigenvalues is such that the most strongly undulating eigenvectors are related to the negative eigenvalues furthest from zero.

Negative pivots almost always appeared at the same time as negative eigenvalues. For a small number of examples, two negative pivots appeared before the occurrence of negative eigenvalues. In these cases the increase of negative pivots from two to three or more was used to signal the passage beyond a bifurcation point. The theory of potential energy (see Section 3.3) indicates that the solution may be unstable as soon as some of the pivots become negative. In the next chapter this problem is addressed in more detail.

The performance of all methods in the case of biaxial compression became less with decreasing dilatancy angle. A decrease of the dilatancy angle is related to an increase of the nonsymmetry which may cause a less accurate calculation of eigenvectors. The case of a zero dilatancy angle was particularly difficult. Eigennodes are often totally different from those found with other dilatancy angles. Loss of normality may influence the stability of perturbation methods in these examples where negative pivots appear before negative eigenvalues because the solution is then already unstable. This problem is again discussed in the next chapter.

In the examples of biaxial compression, the shape of the eigenmodes plays a significant role. Some eigenmodes lead to unstable paths, other to stable paths. The orthogonal perturbation method based on one eigenvector therefore depends on which particular eigenvector is chosen and is consequently less reliable than the other methods.
Chapter 7

Further analysis of the perturbation techniques

In the perturbation analysis of the previous chapter, computational difficulties arose in some examples. A further analysis of the perturbation techniques and the results of the different branches of investigation are described in this chapter. In Section 7.1 alternative approaches to the eigenvalue analysis and the bifurcation signalling are investigated. In Section 7.2 the convergence problems of the eigenvalue methods and of the perturbation itself are addressed.

7.1 Alternative approaches

In Section 7.1.1 an alternative approach to the eigenvalue analysis and eigenvector perturbation is presented in the form of Schur vectors [15]. Furthermore, the aspect of efficient signalling of the bifurcation point is considered. For this purpose, the development of the eigenmodes is investigated (Section 7.1.2) and the symmetric part of the tangent stiffness matrix is analyzed (Section 7.1.3).

7.1.1 Schur vectors

For some dilatancy angles (in particular $\psi = 0$, i.e. strong nonsymmetry), convergence of the perturbation method was poor or even unsuccessful. Possibly, badly converged eigenvalues and eigenvectors used in the perturbation are the cause. Instead of eigenvectors it may then be attractive to use Schur vectors. With Schur vectors an orthogonal reduction of $\mathbf{K}$ can be obtained as follows:

$$\mathbf{K}_S = \mathbf{S}\mathbf{R},$$  \hspace{1cm} (7.1)
with $R$ an upper triangular matrix, $S^T S = I$ and $I$ the identity matrix. All matrices are of the same dimensions. The eigenvalues of $K$ are found on the diagonal of $R$. If $K$ is normal ($KK^T = K^T K$) then $R$ equals the matrix of eigenvalues and $S$ the eigenvector matrix. A partial Schur decomposition is a decomposition with a Schur matrix that has less columns than rows to an upper triangular matrix that is accordingly of smaller dimension than $K$. Of course, the eigenvalues of this upper triangular matrix approximate the eigenvalues of $K$ better if the decomposition is more complete.

Schur vectors are mutually orthogonal and the ordinary deflation used to obtain more than one eigenvalue is often more stable if performed with Schur vectors [28]. This is similar to the fact that Arnoldi’s method is often more robust than the Bi-Lanczos method due to the orthogonality of the reduction [40].

To compute Schur vectors instead of eigenvectors the Arnoldi method (Section 5.2.1) can be used. A partial Schur decomposition of $K$ can be obtained from the Arnoldi iteration vectors $q$ by computing the full Schur decomposition (eq. (7.1)) of the Hessenberg matrix $H$. Suppose $k + 1$ iterations of Arnoldi’s method have been performed. The Arnoldi iteration can then be summarized by:

$$KQ_k = Q_k H_k + \beta_k q_{k+1} e_k^T, \quad \text{and} \quad H_k S_k = S_k R_k,$$

(7.2)

with $S_k, R_k, H_k \in \mathbb{R}^{k \times k}$. The Schur vectors are the columns of $S_k$ and thus $S^T S = I$ and $R_k$ is an upper triangular matrix. The complete Schur decomposition $H_k S_k = S_k R_k$ needs to be recomputed every time new approximated eigenvalues and vectors are wanted just like the eigenvalue and eigenvector computation of the Hessenberg matrix described in Section 5.2.1. Schur vectors of $K$ from the partial decomposition can be found by post-multiplication of the Arnoldi recurrence relation with $S_k$:

$$KQ_k S_k = Q_k H_k S_k + \beta_k q_{k+1} e_k^T S_k = Q_k S_k R_k + \beta_k q_{k+1} e_k^T S_k,$$

(7.3)

and thus:

$$KZ_k = Z_k R_k + \beta_k q_{k+1} e_k^T S_k, \quad \text{with} \quad Z_k = Q_k S_k.$$

(7.4)

Since $Z_k^T Z_k = I_k$, the columns of $Z_k$ are an orthonormal set of vectors. The accuracy of a particular Schur vector $z_l$ of $K$ can be computed by comparing the $l^{th}$ column of each of the matrices of equation (7.4):

$$\| Kz_l - \sum_{j=1}^{l} r_{jl} z_j \| = | \beta_k | \| q_{k+1} e_k^T s_l \| = | \beta_k s_{kl} | \| q_{k+1} \|,$$

(7.5)
with $s_{kl}$ the $k^{th}$ (last) entry of the $l^{th}$ Schur vector $s_l$ of the Hessenberg matrix $H_k$. Note that this is the same kind of bound that can be obtained when the right eigenvectors are computed (see Section 5.2.1). Instead of Arnoldi's method a variant of the Jacobi-Davidson method called JDQR [14] can also be used to generate a partial Schur decomposition.

Deflation with Schur vectors is similar to deflation with eigenvectors. For $m$ negative eigenvalues it can be summarized as:

$$
\tilde{K} = K - \sum_{l=1}^{m} \omega_l \lambda_l z_l z_l^T,
$$

(7.6)

cf. equation (6.12) of Section 6.2. Similarly, a Schur vector of $K$ is still a Schur vector of $\tilde{K}$. Because $z_l = Z_k e_k$ and $z_l^T Z_k = e_k^T$ it follows that for one particular eigenvalue $\lambda_l$:

$$
\tilde{K}Z_k = KZ_k - \omega_l \lambda_l z_l z_l^T Z_k = Z_k R - \omega_l \lambda_l e_k e_k^T
$$

(7.7)

and that eigenvalue $\lambda_l$ is replaced by $(1 - \omega_l)\lambda_l$. The eigenvalues thus become positive if they were negative before the deflation if $\omega > 1$. Following the analysis of Section 6.2 the matrix perturbation can be rewritten as a much cheaper vector perturbation. In practice the inverse iteration is performed but the Schur vectors of $K$ and its inverse are the same:

$$
K^{-1} = Z_k R Z_k^T \quad \Rightarrow \quad K = Z_k^{T^{-1}} R^{-1} Z_k^{-1} = Z_k R^{-1} Z_k^T.
$$

(7.8)

If the inverse iteration is performed, the eigenvalues of $K$ are the inverse of the diagonal elements of $R$. Of course the inverses are never really computed during the eigenvalue analysis (Section 5.3).

In practice there is no visual difference between the Schur vectors and the eigenvectors when both are plotted as deformation modes. No serious improvement is therefore expected from this approach. However, an advantage of the Schur decomposition is that there is no difference between right and left vectors. The information needed for the perturbation can therefore be obtained by running the Arnoldi method just once, whereas to obtain right and left eigenvectors, Arnoldi must be run twice. Instead of running Arnoldi twice, the BILAPRO method could be used, but this is often almost as expensive (Section 5.4).

If $K$ is symmetric $R$ is diagonal. For more nonsymmetric $K$ the values above the diagonal of $R$ are larger. For the problem of biaxial compression with fine mesh and $\psi = 0.1$, this is particularly the case from the twentieth iteration on, see Figure 7.1. This means that the nonsymmetry is quite pronounced which may be the cause of the convergence problems of the BILAPRO method. This is addressed in more detail in Section 7.2.1.
7.1.2 Evaluation of the eigenvectors during homogeneous deformation

The deformation before bifurcation is homogeneous. At first sight, it would therefore seem logical that the set of eigenvectors remains unaltered. The signalling of bifurcation could then be done with eigenvalues without too much cost. Suppose that the eigenvalues and eigenvectors have been computed at Newton-Raphson iteration \(i\), then the eigenvalues at iteration \(i + 1\) can be computed from the old eigenvectors as follows:

\[
Y_i^T K_{i+1} X_i \approx \Lambda_{i+1},
\]

if \(Y_i^T X_i = 1\). Whenever Schur vectors and not eigenvectors are available (see Section 7.1.1) the Schur matrix \(R_{i+1}\) can be set up with the Schur vectors from iteration \(i\):

\[
Z_i^T K_{i+1} Z_i \approx R_{i+1}.
\]

The diagonal elements of \(R_{i+1}\) are now the approximate new eigenvalues.

The results of the biaxial compression test were analyzed in order to verify the proposition that the eigenvectors or Schur vectors do not change noticeably during homogeneous deformation. It was found that the eigenmodes for homogeneous elastic deformation are different from those during homogeneous plastic deformation, see Figure 7.2. However, from the onset of plasticity until the bifurcation point the eigenmodes show no visual change. All elements become plastic at once and it is therefore possible that a change of eigenmodes occurs in
Figure 7.2: Biaxial compression, coarse mesh with associated plasticity. First row: Eigenmodes during homogeneous elastic deformation. Second row: Eigenmodes during homogeneous plastic deformation.

applications like the borehole stability problem where plasticity spreads more gradually.

Unfortunately, the proposition that eigenmodes remain unchanged during homogeneous plastic deformation does not hold in practice. For the pure shear test with $\sin \phi = \sin \psi = 0.3$ (associated plasticity), eigenvectors were computed at the onset of plasticity (step $i$) and used in the next step (step $i + 1$) of the deformation process to compute new approximate eigenvalues. The choice of associated plasticity results in a symmetric $K$ with equal eigenvectors and Schur vectors. As it turns out, the norm of the eigenvalues computed with equation (7.9) is larger than one and the approximation is useless. In Figure 7.3 the size of the entries of the matrix $Y_i^T K_{i+1} X_i$ ($X_i = Y_i$) is plotted. If the eigenvectors had been properly approximated, $Y_i^T K_{i+1} X_i$ would have been diagonal, with new approximate eigenvalues on the diagonal.

For the biaxial compression test with a coarse mesh and associated plasticity a checker board pattern evolves if $Y_i^T K_{i+1} X_i$ is computed. The pattern is probably due to the fact that some eigenmodes are symmetric and others are unsymmetric. The biaxial compression test with the fine mesh yields similar results. The approximation of the eigenvalues may just be good enough to yield almost zero inner products for symmetric modes with nonsymmetric modes.

The eigenvalues computed with the proposed method at the bifurcation point (biaxial compression with fine mesh and associated plasticity) are positive and this finding confirms the non-applicability of the proposition.
Figure 7.3: Logarithm of $\mathbf{Y}_{i+1}^T \mathbf{K}_i \mathbf{X}_{i+1}$, associated plasticity. On the left: Pure shear. On the right: Biaxial compression with fine mesh.

7.1.3 Positive definiteness and negative eigenvalues

According to Hill’s assumption, (see Section 3.3), a mechanical system is unstable if the associated system matrix is not positive definite. Visually there is not much difference between eigenvectors related to a symmetric and those related to a nonsymmetric matrix, but negative eigenvalues and loss of positive definiteness do not necessarily occur at the same time if the matrix is nonsymmetric. For stability, the eigenvalues of the symmetric part of the matrix should be examined. For a symmetric matrix it holds that at least one eigenvalue is negative if the matrix is indefinite. The sign of the eigenvalues of the symmetric part of $\mathbf{K}$ can therefore be used to investigate the positive definiteness of the nonsymmetric problem, since:

$$z^T \mathbf{K} z = z^T (\mathbf{K} + \mathbf{K}^T) z / 2,$$

and therefore:

$$z^T \mathbf{K} z > 0 \Leftrightarrow z^T (\mathbf{K} + \mathbf{K}^T) z > 0.$$  \hspace{1cm} (7.12)

This shows that if the symmetric part of $\mathbf{K}$ has negative eigenvalues and is thus indefinite, the nonsymmetric $\mathbf{K}$ itself is also indefinite.

Deflation of the tangent stiffness matrix so that it becomes positive definite (see Section 6.2) can be performed with an eigenvector of the symmetric problem. If the eigenvalue problem of the symmetric part of $\mathbf{K}$ is given by $(\mathbf{K} + \mathbf{K}^T) \mathbf{x}_i / 2 = \lambda_i \mathbf{x}_i$ with $\lambda_i$ a negative eigenvalue and the perturbation by
\[ \hat{K} = K - \omega_l \lambda_l x_l x_l^T \]
then:

\[ z^T \hat{K} z = z^T \left\{ (K + K^T)/2 + (K - K^T)/2 - \omega_l \lambda_l x_l x_l^T \right\} z \]
\[ = z^T \left\{ (K + K^T)/2 - \omega_l \lambda_l x_l x_l^T \right\} z + z^T (K - K^T)z/2 \]
\[ = z^T \left\{ (K + K^T)/2 - \omega_l \lambda_l x_l x_l^T \right\} z. \] (7.13)

If the symmetric part of \( K \) was initially indefinite, then deflation with \( \omega_l > 1 \)
and the eigenvalues and eigenvectors of the symmetric part of \( K \) results in a
positive definite matrix, see also Section 6.2. This idea can easily be extended
to more negative eigenvalues (compare Section 6.2, eq. (6.12)). Although it is
possible to perform the Bi-Lanczos method and then to compute the eigenvectors
of the symmetric part of the tri-diagonal matrix, it is better for convergence
and cheaper, to perform the iteration with the symmetric part of \( K \) only (i.e.
\( K + K^T \)). Naturally the Arnoldi and Bi-Lanczos methods then reduce to the
symmetric Lanczos method.

**An eigenvalue analysis of the symmetric part of \( K \) in practice**

In the following several tests are described in which the relation between loss
of positive definiteness and various material parameters is analyzed. The tests
include specimens with and without softening and dilatancy angles close to and
far away from the friction angle. Loss of positive definiteness is characterized
by the minimum load and minimum displacement for which the symmetric part
of \( K \) has negative eigenvalues. These minimum values are compared to the bi-
furcation values. Note that for the problems without softening bifurcation does
not occur. The values for the bifurcation load are taken from the experiments
described in Chapter 6. A detailed description of the test characteristics has
been given in Section 3.4.

For the biaxial compression test with a coarse mesh, Figure 7.4 shows the
relation between \( \sin \psi \) and the minimum load and displacement. Apparently
the specimen becomes unstable and loses uniqueness at an earlier load level for
lower \( \psi \).

For \( \sin \phi = 0.3 \) and \( \sin \psi \) ranging from 0.3, 0.29, 0.25, 0.2, 0.1 to 0.0 the
number of negative eigenvalues of the symmetric part of \( K \) is 2, 2, 2, 6, 10, 9.
The magnitude of the negative eigenvalues is in the range of \( 10^{-5} \) to \( 1 \)
for the eigenvalue that is farthest from zero and between \( 10^{-6} \) to \( 10^{-1} \) for the
eigenvalue that is the closest to zero. In other words, the eigenvalues drift away
from zero when the dilatancy angle decreases. In Figure 7.5 some eigenvectors
associated to negative eigenvalues are shown as deformation modes. For the
smaller dilatancy angles these modes relate less to the nonsymmetric physical
problem.
Figure 7.4: Biaxial compression coarse mesh with and without softening. Minimum load and displacement for loss of stability and for bifurcation.

Figure 7.5: Biaxial compression, coarse mesh, with softening. Eigenmodes associated to negative eigenvalues of the symmetric part of $\mathbf{K}$. First two modes: $\sin \psi = 0.2$, third and fourth: $\sin \psi = 0.1$, fifth and sixth: $\sin \psi = 0.0$. 
7.1. ALTERNATIVE APPROACHES

Figure 7.6: Biaxial compression, fine mesh, with softening. Eigenmodes associated to negative eigenvalues of the symmetric part of $K$. First two modes: $\sin \psi = 0.2$, third and fourth: $\sin \psi = 0.1$, fifth and sixth: $\sin \psi = 0.0$.

Figure 7.7: Biaxial compression, fine mesh, with and without softening. Minimum load and displacement for loss of stability and for bifurcation.

For the fine mesh the number of negative eigenvalues of the symmetric part of $K$ is, in order of decreasing dilatancy angle, 14, 14, 20, 26, 14, 13 ranging from $10^{-4}$ to $10^{-2}$ for the negative eigenvalues farthest from zero and ranging from $10^{-6}$ to $10^{-4}$ for the negative eigenvalues closest to zero. Some eigenmodes associated to negative eigenvalues are shown in Figure 7.6. Again a general pattern of a drift away from zero is noted.

The negative eigenvalues related to the nonsymmetric eigenvalue problem appeared later than the negative eigenvalues in the symmetric part, with an exception of $\sin \psi = 0.29$, with softening. In this test case ten negative eigenvalues were found, closer to zero than those of the eigenproblem associated to the symmetric part of $K$. A finer division of the step size would probably have led to the observation that also in this case loss of stability precedes loss of uniqueness.

The relation between the dilatancy angle and the minimum load and displacement for this example is visualized in Figure 7.7. Again the minimum load and displacement become smaller when the dilatancy angle decreases. The re-
lation is smoother than with the coarse mesh, probably due to the increased precision of the solution as a result of the mesh refinement. The same problem without softening gives results that are similar.

The results found with the example of pure shear are rather similar. The number of negative eigenvalues is constant (five) for all of the different dilatancy angles. But again, for smaller dilatancy angles the negative eigenvalues appear earlier in the symmetric part of the matrix. Also, the negative eigenvalues become larger for a decreasing dilatancy angle.

Evaluation

Evidently, loss of positive definiteness (negative eigenvalues in the symmetric part of the matrix) does not always occur at the same time as loss of uniqueness (bifurcation) [9], see also Section 3.3. An effort to perform the branch switch procedure with negative eigenvalues of the symmetric part of $K$ as soon as they appear was not successful. It led to divergence of the Newton-Raphson iteration or to convergence to the old solution within the perturbation increment.

At the moment of loss of stability a carefully chosen load case or prescribed displacement might cause uncontrollability, but in the examples discussed here, an increase of downward displacement does not result in unstable behavior.

7.2 Investigation of convergence problems

Convergence problems can be divided into two classes: problems with eigenvalue methods and problems with the Newton-Raphson iteration. Section 7.2.1 discusses problems of convergence with the Bi-Lanczos method with partial orthogonalization (BILAPo) whereas Section 7.2.2 considers the convergence problems of the Newton-Raphson procedure in the perturbed increment by analyzing the eigenmodes corresponding to negative eigenvalues that seem to have no physical meaning.

7.2.1 Poor convergence of the BILAPo method

Convergence of the BILAPo method (Section 5.2.3) is poor in some applications. The key to this problem lies in the bi-orthogonality or the loss thereof. The BILAPo method is constructed from the Bi-Lanczos method by extending this method with partial orthogonalization. Every now and then the iteration is stopped to set a new iteration vector and its successor explicitly orthogonal to the previous vectors. In some (rare) cases this is not sufficient to guarantee proper convergence of the eigenvalues and eigenvectors.
7.2. INVESTIGATION OF CONVERGENCE PROBLEMS

If the BILAP0 (or Bi-Lanczos) method is used to solve a symmetric matrix, the iteration reduces to the Lanczos method. Right and left iteration vectors are then the same and form an orthogonal set of vectors. In contrast, the right and left iteration vectors become less and less orthogonal with respect to each other for an increasing degree of nonsymmetry of the matrix. The example of biaxial compression for the fine mesh with \( \sin \psi = 0.1 \) suffers from lack of convergence of the BILAP0 method around the bifurcation point. At the first stage of the analysis it was investigated how far the right and left iteration vectors are from orthogonality. Figure 7.8 is an image of the matrices \( V^T V \) and \( W^T W \). The first column of both matrices is not included because it contained values much smaller than the other values. Clearly, the vectors are not orthogonal. Whether iteration vectors may even be dependent is much harder to investigate due to the size of the problem \( \text{(1825 \times 25)} \) and roundoff errors.

The BILAP0 method includes partial re-orthogonalization of the iteration vectors. Evidently, as the experiments show, it is not always sufficient to guarantee convergence of eigenvalues and vectors. A plot of \( W^T V \) clearly shows that loss of orthogonality is not cured in the example considered. Figure 7.9 presents a plot of \( \log | w_l^T v_m | \), the elements of \( W_k^T V_k \), for \( l, m \leq k \). Note that the Modified Gram-Schmidt procedure is performed from the oldest to the more recent iteration vectors (columns are darker near the diagonal). The iteration at which duality is reestablished can be recognized by a light first element of a row or column. Two successive iterations are re-orthogonalized (see Section 5.2.3).

If Modified Gram-Schmidt is performed from the most recent iteration vectors to the first ones (from the diagonal to the sides in Figure 7.9) the convergence of Bi-Lanczos with partial orthogonalization is equally bad and a plot similar to Figure 7.9 evolves. Next, it is explained why the Gram-Schmidt
Figure 7.9: Biaxial compression, fine mesh, sin $\psi = 0.1$. Logarithm of the entries in absolute value of the matrix $W^T V$.

process may not be sufficient for reestablishing orthogonality.

**Gram-Schmidt revisited**

Suppose that the right and left iteration vectors $v_{k+1}$ and $w_{k+1}$ have drifted too far from orthogonality with respect to the older iteration vectors. Re-orthogonalization is then performed with the Modified Gram-Schmidt procedure. This means that at eigenvector iteration $k+1$ the following vector updates are computed for $l = 1$ to $k$:

$$v_{k+1} = v_{k+1} - (v_{k+1}^T w_l)v_l, \quad (7.14)$$

$$w_{k+1} = w_{k+1} - (w_{k+1}^T v_l)v_l,$$

where it is supposed that $v_l^T w_l = 1$. The BILAPL method allows for some loss of orthogonality which may introduce unwanted inaccuracies if loss of orthogonality is rapid. This is most easily explained by going through the recurrence relation (7.14). The first two corrections of iteration vectors $v_{k+1}$ read:

$$v_{k+1}^1 = v_{k+1} - (v_{k+1}^T w_1)v_1, \quad (7.15)$$

$$v_{k+1}^2 = v_{k+1}^1 - (v_{k+1}^1)^T w_2)v_2.$$

After the first update, $v_{k+1}^1$ is orthogonal to $w_1$. After the second update $v_{k+1}^2$ is orthogonal to $w_2$, but it may no longer be orthogonal to $w_1$. The inner product of $v_{k+1}^2$ and $w_1$ reads:

$$w_1^T v_{k+1}^2 = w_1^T v_{k+1}^1 - (v_{k+1}^1)^T w_2 w_1^T v_2. \quad (7.16)$$
7.2. INVESTIGATION OF CONVERGENCE PROBLEMS

The product \( w_1^T v_{k+1} \) is zero as a result from the first correction, but \( w_1^T v_2 \) is only as small as the maximum allowed loss of orthogonality (i.e. \( \sqrt{\epsilon} \) with \( \epsilon \) the machine precision). This inaccuracy may spoil the Gram-Schmidt procedure as Figure 7.9 shows.

Another way to look at the failure of the Modified Gram-Schmidt process is by considering the ordinary Gram-Schmidt procedure:

\[
\begin{align*}
\tilde{v}_{k+1} &= (I - V_k W_k^T) v_{k+1}, \\
\tilde{w}_{k+1}^T &= w_{k+1}^T (I - V_k W_k^T).
\end{align*}
\] (7.17)

The identity matrix \( I_n \) is of dimension \( n \times n \) and \( V_k, W_k \in \mathbb{R}^{n \times k} \). It then holds that the re-orthogonalization improves the orthogonality if the norm of the inner product of the old iteration vectors \( w_l, v_l \) for \( l \leq k \) minus the identity matrix is less than one:

\[
W_k^T \tilde{v}_{k+1} = W_k^T (I - V_k W_k^T) v_{k+1} = (I - W_k^T V_k) W_k^T v_{k+1},
\] (7.18)

so that:

\[
\| I_n - W_k^T V_k \|_2 < 1 \quad \text{implies} \quad \| W_k^T \tilde{v}_{k+1} \|_2 \leq \| W_k^T v_{k+1} \|_2.
\] (7.19)

This problem has also been addressed in [10, 11], but no remedy has been found so far. If Modified Gram-Schmidt is used then the bound may be too strict because, although theoretically the same results should evolve, the modification yields a more stable algorithm in practice. The bound seems easy to fulfill but the next example shows that it can be violated.

Again the example of biaxial compression with a fine mesh and \( \psi = 0.1 \) was analyzed. The norm \( \| I_n - W_k^T V_k \|_2 \), see equation (7.18), was computed for each of the twenty five eigenvalue iterations, i.e. \( k = 1, \ldots, 25 \). This value should remain below one. During the BILAPo iterations this norm increased from far below one to more than one, see Figure 7.10, to the left. The final results were therefore of poor quality. Stopping the iteration before is not possible. After twenty-five iterations only one negative eigenvalue had converged.

Figure 7.10, to the right, shows the logarithm of the relative residual norm \( \| Kx - \lambda x \|_2 / \| \lambda x \|_2 \) of this negative eigenvalue. The norm of the other eigenvalues is around one.

Full re-orthogonalization was attempted as well, but unfortunately, the results are not satisfactory either. Although the norm of \( I_n - W_k^T V_k \) is always less than \( 9 \times 10^{-9} \), the relative residual norm of the negative eigenvalues does not become smaller than \( 10^{-3} \). Figure 7.11 shows a plot of the norm of the four negative eigenvalues closest to zero. The smallest eigenvalue is of the order \( 10^{-10} \) and the absolute residual norm of the eigenvalue \( \| Kx - \lambda x \|_2 \), is evidently satisfactory long before the 25th iteration.
Figure 7.10: Biaxial compression, fine mesh with \( \sin \psi = 0.1 \). To the left: \( \| I_n - W_k^T V_k \|_2 \) for every iteration \( k \) from 1 to 25 just after the bifurcation point. To the right: The relative residual norm of the only converged negative eigenvalue.

Figure 7.11: Biaxial compression, fine mesh, \( \sin \psi = 0.1 \). Bi-Lanczos with full re-orthogonalization. Logarithm of the relative residual norm of the four negative eigenvalues closest to zero.
7.2. INVESTIGATION OF CONVERGENCE PROBLEMS

Performance of other eigenvalue methods

The convergence of eigenvalues is much better with Arnoldi's method for the
problem of biaxial compression with a fine mesh and \( \sin \psi = 0.1 \). This is probably because the reduction is performed with orthogonal vectors which is known to be more stable. In order to obtain both right and left eigenvectors for the
deflation type of eigenvector perturbation, Arnoldi's method could be executed
twice, once with \( \mathbf{K} \) and once with \( \mathbf{K}^T \). This is expensive, but the accuracy is better, and therefore the perturbation might go smoother. The results of
Chapter 6 show that the normalized deflation procedure finally converges but
shifts away from the proper solution during the perturbation increment. This is still the case if the perturbation is performed with the eigenvectors found with Arnoldi's method.

If Schur vectors are used instead of eigenvectors (Section 7.1.1) then only one
set of vectors needs to be computed. Moreover, the advantage of an orthogonal
reduction is used.

Day [10] (see also Section 5.2.3) has proposed another scaling of the iteration
vectors than that chosen for the BILAPo method. Instead of scaling the inner
product of the right and left iteration vectors to one, each iteration vector is
scaled to one. Investigation of the inner product values (no longer equal to
one) reveals no particular problems, i.e. no really small or large values that
previously might have caused inaccuracies in the BILAPo iteration are found.
The values are somewhere between plus and minus one. It is therefore logical
that this scaling results in equally badly converged eigenvectors and eigenvalues.
Only one eigenvalue (the negative eigenvalue closest to zero) has a relative
residual norm that drops to \( 10^{-6} \). All other norms remain around one, similar
to the results obtained with the BILAPo method.

It is noted that the updating recurrence for signalling loss of orthogonality that is used in the program is not the same as proposed by Day, but that it is the one discussed in Section 5.2.3. In this case the result of the recurrence
procedure is that every four iterations re-orthogonalization takes place. With
the BILAPo method re-orthogonalization took place every five iterations. This
difference is mainly caused by the stop criterion in the adjusted method that is set a little stricter following the analysis of Day [10].

Full re-orthogonalization with scaling according to Day [10], gives similar
results, with norms dropping to \( 10^{-3} \) on average for the positive eigenvalues and to only \( 10^{-2} \) for the negative eigenvalues. This is comparable with the results found with the BILAPo method.
Figure 7.12: Biaxial compression, fine mesh, sin $\psi = 0.0$. Eigenmodes 1, 2, 5, 7 and 8 after 12mm of prescribed displacement.

### 7.2.2 Spurious eigenmodes and poor convergence of the perturbation process

During the deformation process of the specimen computed with a Newton-Raphson iteration (Section 3.2.2) the eigenvectors of the structural matrix can be interpreted physically and related to deformation modes. For some problems however, eigenvectors were computed that seemed to have no relation with the deformation process. These modes were occasionally related to complex eigenvalues. In this section the occurrence of physically spurious eigenmodes as well as complex modes is investigated in greater detail. The reduction of the step size of the Newton-Raphson iteration is also considered.

**Real eigenmodes**

In some applications eigenmodes are found that seem to have no physical relevance, i.e. that look like spurious modes. In this section it is investigated whether these modes disappear upon setting stricter threshold values and a detailed analysis is performed of the Newton-Raphson iteration in order to find as accurate as possible the moment that these modes evolve. The results are then related to the eigenvalues of the symmetric part of the structural matrix (see also Section 7.1.3).

In the problem of biaxial compression with a fine mesh and nonassociated plasticity with $\sin \psi = 0.0$, peculiar looking eigenmodes are found at bifurcation (Section 6.3.2). The eigenmodes change slightly during plastic deformation but at the onset of plasticity the modes are basically the same as the elastic eigenmodes (Section 7.1.2, Fig. 7.2). After 12 mm of prescribed displacement (bifurcation takes place after 32.46 mm) some of the nonsymmetric modes show a beginning bulging shape, Figure 7.12. Perturbation with some or all of the modes presented in Figure 7.12 led to divergence. The eigenvalue problem of the symmetric part of the system matrix has eleven negative eigenvalues. With these modes the perturbation did not succeed either.
After applying 14 mm of prescribed displacement in several steps two negative pivots appear. The nonsymmetric eigenproblem does not yet have negative eigenvalues at this point but some eigenmodes (the nonsymmetric ones) seem to have lost physical meaning. The symmetric modes (similar to the symmetric elastic eigenmodes) are still present. In Figure 7.13 five modes (two symmetric and three nonsymmetric) are plotted.

The eigenvalue problem of the symmetric part of the tangent stiffness matrix has fourteen negative eigenvalues at this stage, including some that seem to be spurious, see Figure 7.14. Perturbation was not successful, neither with all nor with only the symmetric modes of the original problem, nor with the eigenvectors associated to negative eigenvalues of the symmetric part of $K$. The results do not change if the accuracy of the eigenmodes as well as the Newton-Raphson iteration is set to $10^{-6}$.

If the last increment of two millimeters of the fourteen is subdivided into ten sub increments, two negative pivots appear after three of the sub increments. The two negative pivots remain and after the seventh sub iteration the wavy pattern returns in the eigenmode without any appearance of negative eigenvalues in the nonsymmetric tangent stiffness matrix. The symmetric part of the matrix has eight negative eigenvalues. Perturbation with all modes or with only
the symmetric modes eventually resulted in divergence after initiating several shear bands in the material.

After nine sub increments the nonsymmetric eigenvalue problem has a negative eigenvalue associated to a strongly undulating eigenmode. As before, perturbation with this eigenvector did not result in a properly converged solution.

The experiments suggest that the instability is not a result of insufficient accuracy of the eigenvalue method or of the Newton-Raphson iteration. Neither more accurate eigenvectors, nor smaller and more accurate Newton-Raphson steps could eliminate the spurious modes or make the perturbation procedure succeed. In Section 7.1.3 the discrepancy between negative eigenvalues of $K$ and negative eigenvalues of $K + K^T$ has been analyzed in more detail.

Complex eigenmodes

In theory a nonsymmetric eigenproblem may have a complex solution. The deformation is a weighted sum of all eigenvectors and since for a real matrix a complex eigenvector and its complex conjugate are both present, the complexity of eigenvectors is not reflected in the deformation. However, the mode itself does not have a physical meaning and it is not often that complex eigenvalues and eigenvectors appear. In the examples described in the previous chapter, they were found in the biaxial compression with triangular mesh and sin $\psi = 0.0$ and with the Cosserat continuum. Specifically, these modes appear at the same time that spurious modes (see the previous section) are found and may be a sign of instability.

The perturbation of Chapter 6 was done with the real eigenvectors only because the complex modes seem to have no meaning and can therefore result in a meaningless perturbation only. Now, the perturbation with complex eigenvectors is investigated and it is analyzed if the complexity can be eliminated by taking smaller Newton-Raphson iteration steps.

Perturbation with complex eigenmodes

It is possible to perturb with a complex eigenvector such that the solution vector remains real. If an eigenvalue is complex with negative real part ($\lambda = a + ib$, $i^2 = -1$ and $a < 0$) but if the matrix is real, then the complex conjugate of this eigenvalue ($a - ib$) is also present. The two associated pairs of right and left eigenvectors are denoted by $x^r + ix^l, y^r + iy^l$ and $x^l - ix^r, y^l - iy^l$. Suppose that only two eigenvalues have become complex: $\lambda_1 = a + ib$ and the associated complex conjugate $\lambda_2 = a - ib$. The orthogonal perturbation (Section 6.1, eq.
(6.4)) then reads:

\[ \hat{u} = 2u - \frac{u^T u}{(x^r + ix^i)^T u} (x^r + ix^i) - \frac{u^T u}{(x^r - ix^i)^T u} (x^r - ix^i) \]

\[ = 2u - \frac{u^T u (x^r - ix^i)^T u (x^r + ix^i) + u^T u (x^r + ix^i)^T u (x^r - ix^i)}{(x^r + ix^i)^T u (x^r - ix^i)^T u} \]

\[ = 2u - \frac{2u^T u x^r x^r u x^r + 2u^T u x^i x^i u x^i}{(x^r u)^2 + (x^i u)^2}. \]

(7.20)

The cross products with imaginary terms cancel. A similar simplification occurs in the deflation type of perturbation (Section 6.2, eq. (6.12)):

\[ \hat{u} = u + \frac{\omega_1 (y^r + iy^i)^T u}{1 - \omega_1} (x^r + ix^i) + \frac{\omega_2 (y^r - iy^i)^T u}{1 - \omega_2} (x^r - ix^i) \]

\[ = u + \left\{ \frac{\omega_1}{1 - \omega_1} + \frac{\omega_2}{1 - \omega_2} \right\} (y^r u) x^r - \left\{ \frac{\omega_1}{1 - \omega_1} + \frac{\omega_2}{1 - \omega_2} \right\} (y^i u) x^i \]

\[ + \left\{ \frac{i\omega_1}{1 - \omega_1} - \frac{i\omega_2}{1 - \omega_2} \right\} (y^r u) x^i + \left\{ \frac{i\omega_1}{1 - \omega_1} - \frac{i\omega_2}{1 - \omega_2} \right\} (y^i u) x^r. \]

(7.21)

The imaginary cross products disappear if \( \omega_1 = \omega_2 \). For the constant deflation this is so by definition. Parameter \( \omega_i \) for the normalized deflation is determined by the norm of the eigenvectors (eq. (6.14) on page 63) and is therefore the same for the first eigenvalue and for the second eigenvalue that is the complex conjugate of the first. The deflation perturbation with complex eigenvectors thus becomes:

\[ \hat{u} = u + \frac{2\omega y^r u}{1 - \omega} x^r - \frac{2\omega y^i u}{1 - \omega} x^i. \]

(7.22)

Extension of the complex eigenvector perturbation to more eigenvectors, complex or not, is straightforward.

The biaxial compression test with a triangular mesh and \( \sin \phi = 0.0 \) exhibits complex eigenmodes just after the bifurcation point (Section 6.3.2). Perturbation using the above described parameters was unsuccessful. It is not clear if this failure is a problem of the complexity, or simply of the possible spurious character of the modes.
Elimination of complex eigenmodes

The biaxial compression test with a triangular mesh and \( \sin \psi = 0.0 \) was investigated somewhat further to establish whether the complexity could be eliminated. In this example the negative eigenvalues and the plasticity occurred simultaneously. The steps were subdivided and the stop criterion of the Newton-Raphson iteration based on the energy was set to \( 10^{-9} \). The first step size was two millimeters and the last step size, the one that triggered the negative eigenvalues, was \( 2 \times 10^{-5} \) millimeters. The number of negative eigenvalues is still eighteen and plastic deformation starts in the very last iteration only. The complex eigenvalues are still there, and the modes seem nonphysical.

The other example where complex eigenvalues were found was that of biaxial compression with triangular mesh and a Cosserat [6] continuum (Section 3.4). If a stricter convergence criterion is applied in this problem, another problem arises, namely that no negative pivots emerge at all. The descending homogeneous deformation branch is followed automatically. Remarkably, the eigenproblem of the symmetric part of the tangent stiffness matrix does not possess negative eigenvalues once the slope starts descending, i.e. the ascending and descending slopes that correspond to homogeneous deformation are stable according to Hill's criterion [18].

It is concluded that the complexity of the eigenvalues and vectors is a problem of the underlying physical model and not of the numerical procedures, neither the Newton-Raphson iteration nor the eigenvalue iteration. The complex eigenmodes investigated seem to be spurious of character and do not disappear upon refinement of the Newton-Raphson step size.
Chapter 8

Evaluation

The investigation of typical models for soil deformation was divided into a material analysis and a numerical analysis. The material analysis was aimed at identifying possible causes of problems due to nonphysical features of the model. The numerical analysis focused on the eigenvector branch switch procedure. Related to the branch switching is the connection between stability, uniqueness and positive definiteness of the tangent stiffness matrix.

Conclusions

The eigenvalues of the elasto-plastic material matrix were analyzed for isotropic and orthotropic plane-stress and plane-strain configurations. It was shown that for an isotropic elasto-plastic material with a Drucker-Prager yield function, the elasto-plastic material matrix has only real eigenvalues. However, orthotropic material models may exhibit complex eigenvalues for some stress combinations in case of nonassociated plasticity, as was demonstrated. The difference between the friction angle and the dilatancy angle is decisive for the range of stresses that yield complex eigenvalues.

Some stress distributions found with numerical examples were compared to the eigenvalue analysis of the material matrix set up with the stresses on the Drucker-Prager yield surface. It was shown that the stress path followed by these tests did not coincide with the stresses that yield complex eigenvalues of the material matrix. In theory the complex eigenvalues can cause instabilities in the numerical computations. However, because stress combinations associated to complex eigenvalues were not present in the tests, this nonphysical feature of the material model did not influence the numerical computations.

The Bi-Lanczos method computes right and left eigenvectors at the same time and both are needed for branch switching using the deflation perturbation
method. However, the Bi-Lanczos method suffers from loss of orthogonality and therefore it was further developed resulting in the BILAPO method. This method was shown to be at most twice as time consuming as Arnoldi’s method for a fixed number of iterations.

The number of negative eigenvalues is only a small subset of the total. Therefore, to compute all negative eigenvalues the number of iterations necessary is much less than the number of nodal degrees of freedom, i.e. the total number of eigenvalues. The iteration is further accelerated by performing an inverse eigenvalue iteration. In every step of the Newton-Raphson iteration a decomposition is made of the tangent stiffness matrix that can be used for the inverse eigenvalue iteration. The cost of the eigenvalue analysis is consequently small compared to the cost of the Newton-Raphson iteration.

When enforcing branch switching according to the classical orthogonal perturbation method one eigenvector is used to perturb the solution vector and to set up a trial solution orthogonal to the original one. The outcome of this perturbation depends on the eigenvector chosen and the method can therefore be unpredictable if the set of negative eigenvalues is larger than one. The orthogonal perturbation method was generalized to include all eigenvectors associated to negative eigenvalues. This method worked well and is more robust than the single eigenvector perturbation.

The orthogonal perturbation uses only right eigenvectors. Also, the orthogonality requirement may be disadvantageous. Therefore a new perturbation technique was developed that is more general. It is based on the idea that under displacement control a tangent stiffness matrix associated with a properly localized solution possesses no negative eigenvalues. This eigenvector perturbation method is called deflation and performs as well as the orthogonal perturbation. For the more difficult experiments it appeared that the methods were complementary and it is therefore advised to have both methods available.

In some rare cases the BILAPO method did not converge, in particular for those problems which were strongly nonsymmetric. The partial re-orthogonalization procedure of BILAPO may then break down. Arnoldi’s method converged, but to extract both right and left eigenvectors Arnoldi’s method would have to be executed twice. As an alternative it was proposed to perform the eigenvector perturbation with Schur vectors.

Another difficulty that was encountered occasionally in the perturbation procedure, was divergence or non-convergence of the Newton-Raphson iteration. This often coincided with eigenvectors, sometimes associated to negative eigenvalues, that seemed to have no physical meaning. A more detailed investigation of the Newton-Raphson iteration with respect to the eigenmodes suggested that
the nonphysical modes seem to appear ahead of the probable bifurcation point. Refinement of the Newton-Raphson steps did not remove the nonphysical behavior and it is believed that the spurious modes are an artifact of the numerical model.

Hill's [18] assumption relates stability to positive definiteness. However, no link is made to loss of uniqueness. It was shown that loss of stability may indeed occur before loss of uniqueness. The difference between loss of positive definiteness and loss of uniqueness is influenced by the difference between the dilatancy angle and the friction angle of the material. A large difference between these angles results in a large difference between loss of stability and loss of uniqueness. Softening of the material has only little influence on this behavior.

It is noteworthy that the signalling of bifurcation by negative eigenvalues of the nonsymmetric tangent stiffness matrix $K$ was quite accurate. The negative eigenvalues of $K$ appeared after negative eigenvalues were found in the symmetric part. In other words, the tangent stiffness matrix became indefinite and stability was lost before bifurcation occurred. In a few examples, where nonsymmetry was very pronounced, one or two negative pivots would appear before the solution could be steered onto another branch. A sudden increase of negative pivots indicated a passage beyond a bifurcation point and the presence of negative eigenvalues. The solution could then be steered onto another stable path with help of eigenvectors associated to negative eigenvalues.

Reflections

The eigenvalue analysis on a material level was shown to relate to all possible stress combinations on a Drucker-Prager yield surface. The algebraic elaboration of the eigenvalue problem of the elasto-plastic material matrix combined with a yield surface therefore provides a useful tool for evaluation of a material model and for signalling problems in a numerical analysis. In this research only the Drucker-Prager yield function was used and analyzed by studying the eigenvalues of the elasto-plastic material matrix. However, this analysis can also be used for other material models.

The numerical examples investigated were of the same loading type. Different loadings and different geometrical configurations will lead to more complex bifurcation patterns. However, the perturbation techniques developed here do not depend on the geometry or material and can be used in more complex situations too.
Bibliography


Summary in English and Dutch

Summary: The significance and use of eigenvalues and eigenvectors in the numerical analysis of elasto-plastic soils

The modeling of soil finds its application in a variety of fields. When dikes or slopes are considered, typical deformation is sliding due to top loads. For tunnels and boreholes the problem is characterized by a movement of the soil towards a cavity. In the transition from an application to a numerical model the simplification of a two-dimensional response has been introduced. In particular, plane-strain material models are considered. In this study the significance and use of eigenvalues and eigenvectors in soil modeling was explored on a material and structural level.

On a material level the Drucker-Prager yield function was used as separation surface between elastic and plastic response. With this yield function an elasto-plastic material matrix was set up. This elasto-plastic material matrix relates stress rates to strain rates and can be nonsymmetric. If the direction of flow is equal to the normal to the yield surface, the material response is called associated and if these two vectors are unequal it is called nonassociated. For nonassociated plasticity the elasto-plastic matrix is nonsymmetric giving rise to possibly complex eigenvalues. Complex eigenvalues have no physical meaning and it was therefore investigated if complex eigenvalues were present within the range of possible stresses defined by the yield function.

For the eigenvalue analysis of the elasto-plastic material matrix, all stresses related to plane-strain and plane-stress conditions were considered for isotropic and orthotropic materials. It was shown that the elasto-plastic material matrix related to isotropy does not possess complex eigenvalues. However, for orthotropic plane-stress and plane-strain configurations complex eigenvalues are found if the direction of plastic flow does not coincide with the normal to the yield surface.
In order to compare the stresses leading to complex eigenvalues of the material matrix to the stresses of numerical examples a computational analysis was set up. With this setup any stress on the three-dimensional yield surface can be mapped onto a two-dimensional reference configuration. In this fashion the stress distributions of some numerical tests were compared to results of the eigenvalue analyses and it was shown that the stress distributions of these tests did not lead to complex eigenvalues of the material matrix.

After discretization of the continuum problem with the finite element method a numerical model evolves. At a certain level of loading the solution reaches a point where another deformation mode becomes possible apart from the homogeneous deformation. Eigenvector based branch switch procedures were developed to excite a solution associated to a localized deformation mode. Eigenvectors related to negative eigenvalues are used for this purpose. The already known orthogonal perturbation was extended so that it uses all eigenvectors associated to negative eigenvalues. Also, an alternative to the orthogonal perturbation called deflation was constructed that uses both right and left eigenvectors.

The significance of negative eigenvalues and pivots for loss of stability and loss of uniqueness has been analyzed. In the examples considered, negative pivots implied negative eigenvalues as well as a bifurcation point. Even though loss of stability occurred before bifurcation the material behaved stable under the applied loading and the computations could be continued until a bifurcation point was reached.

For some numerical tests the computed eigenvectors were of a spurious nature, sometimes even complex. Using these eigenvectors, none of the perturbation methods was succesful. Unfortunately, the spurious vectors could not be eliminated by step refinement or more critical termination criteria.

The BILAPo method was used in numerical tests to obtain eigenvalues and eigenvectors. Very occasionally, BILAPo did not converge properly and Arnoldi's method had to be applied. Since Arnoldi's method only computes one set of eigenvectors, the method had to be run twice for the deflation perturbation in which right and left eigenvectors are used. Instead of eigenvectors, Schur vectors can be used. For Schur vectors there is no difference between left and right and the cost of computing Schur vectors is therefore only as time consuming as running Arnoldi's method once.

Hilda van der Veen
Samenvatting: De betekenis en het nut van eigenwaarden en eigenvectoren in de numerieke analyse van elasto-plastische grond

Het modelleren van grond is nodig voor verschillende toepassingen. Bij hellingen wordt de vervorming gedomineerd door afschuiving van grond, terwijl het vervormingsprobleem bij tunnels en boorgaten wordt gekarakteriseerd door drukopbouw rond een opening. Tijdens de overgang van de toepassing naar een numeriek model wordt twee-dimensionaal gedrag verondersteld. In het bijzonder wordt een vlakke-rek configuratie beschouwd. In dit onderzoek is de betekenis en waarde van eigenwaarden en eigenvectoren onderzocht voor het modelleren van grond op materiaal en structuur niveau.

De Drucker-Prager vloefunctie is gebruikt op materiaal niveau om elastisch en plastisch gedrag te onderscheiden. Deze vloefunctie is gebruikt om de elasto-plastische materiaal matrix op te zetten die rek aan spanning relateert. Als de plastische vloeiingsrichting gelijk is aan de normaal aan het vloeioppervlak dan is er sprake van associatieve plasticiteit en als deze twee vectoren ongelijk zijn is er sprake van niet-associatieve plasticiteit. In het geval van niet-associatieve plasticiteit is de elasto-plastische materiaal matrix niet symmetrisch wat mogelijk kan leiden tot complexe eigenwaarden. Complex eigenwaarden hebben geen fysische betekenis en er is daarom onderzocht of ze voor komen voor de spanningen die op het vloeioppervlak liggen.

Voor de eigenwaarde analyse van de elasto-plastische materiaal matrix zijn alle spanningen voor vlakke-rek en vlakke-spanningsverdelingen bekeken voor isotrope en orthotrope materialen. Er is aangetoond dat de isotrope materiaal matrix geen complexe eigenwaarden bezit. Echter, de orthotrope materiaal matrix bezit complexe eigenwaarden indien de richting van plastische vloei ongelijk is aan de normaal aan het vloeioppervlak.

Om de spanningen die aanleiding geven tot complexe eigenwaarden te kunnen vergelijken met de spanningen van numerieke testen, is een wiskundig kader opgezet waarbinnen elke willekeurige drie-dimensionale spanningsverdeling kan worden gerelateerd aan een twee-dimensionale configuratie. Op deze manier zijn enkele numerieke testen geïntegreerd in de hierboven beschreven eigenwaarde analyse. Geen van de berekende spanningsverdelingen viel in de gebieden die aanleiding geven tot complexe eigenwaarden in de elasto-plastische materiaal matrix.

Uit discretisatie van het continuum probleem met de eindige elementenmethode volgt een numeriek model. Na een bepaalde hoeveelheid belasting wordt een punt bereikt waar meerdere oplossingen mogelijk zijn naast de homogene vervorming. Padverwisselmethoden gebaseerd op eigenvectoren zijn ontwikkeld om oplossingen gerelateerd aan een gelokaliseerde vervorming te verkrijgen. Hiervoor zijn eigenvectoren horende bij negatieve eigenwaarden gebruikt. De
bestaande orthogonale perturbatie is verder ontwikkeld zodat alle eigenvectoren horende bij negatieve eigenwaarden worden meegenomen. Daarnaast is een methode ontwikkeld die deflatie is genoemd en die zowel rechter als linker eigenvectoren gebruikt.

De betekenis van negatieve eigenwaarden en pivots voor verlies van stabiliteit is eveneens onderzocht. Voor de beschouwde problemen duidden negatieve pivots op negatieve eigenwaarden evenals op een bifurcatiepunt. Hoewel verlies van stabiliteit al eerder in het Newton-Raphson proces werd geconstateerd, kon de opgelegde kracht zonder problemen toenemen tot aan het niveau van bifurcatie.

Voor een enkel probleem waren de berekende eigenvectoren ongewoon of zelfs complex. Helaas waren deze vectoren ongevoelig voor stapgrootte verfijning of strengere stopcriteria, en kunnen ze worden aangeduid als artefacten van het numerieke model.

De BILAPo methode is gebruikt voor de berekening van eigenwaarden en eigenvectoren in de numerieke testen. Een enkele keer convergeerde de BILAPo methode niet en moest de methode van Arnoldi worden gebruikt. Gezien het feit dat Arnoldi's methode maar één set eigenvectoren per keer berekent moet de methode twee keer worden uitgevoerd om alle benodigde informatie te verkrijgen voor de deflatie die gebruikt maakt van zowel de rechter als de linker eigenvectoren. In plaats van eigenvectoren is het mogelijk om Schur vectoren te gebruiken. Voor Schur vectoren is er geen onderscheid tussen links en rechts, en de kosten voor het berekenen van Schur vectoren zijn daarom even hoog als voor een enkele Arnoldi procedure.

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Publications


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