A simple algorithm to generate small geostatistical ensembles for subsurface flow simulation

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Abstract
This note describes the theory behind a simple Matlab program to generate ensembles of geological realizations of relatively small-scale reservoir models (permeability fields) for subsurface flow simulation. The algorithm makes use of Principal Component Analysis (PCA) to parameterize the spatial covariance of a reference image, and a Bayesian optimization approach to condition the realizations to well data. The method is limited to relatively small images, mainly because of memory requirements, and only uses two-point statistics. However, it does not require iteration or rejection of ensembles and is computationally efficient because of the use of vectorized Matlab operations.

Geostatistical procedure
Principal Component Analysis
Principal Component Analysis (PCA), also known as Karhunen-Loève decomposition, is a technique used in image compression to decompose the spatial statistics of an image, as expressed in a covariance matrix of the pixel values, in a number of orthogonal basis functions; see e.g. Dony, 2001. A reduced, approximate, representation of the image can then be obtained by discarding those basis functions that contain the least information. Reynolds et al. (1996) and Sarma et al. (2006) applied PCA to represent permeability fields in geological realizations with a limited number of basis functions. This was done to reduce the number of parameters for permeability estimation in ‘computer-assisted history matching’ of an oil reservoir using measured data in the wells. Here, we describe the use of PCA to capture the two-point spatial statistics (i.e. the mean and the covariance) of a single geological ‘reference image’ with \( n \) cells (pixels) with a limited number of basis functions. This method is a simplified implementation of the ‘Kernel PCA’ method described by Sarma et al. (2008) to create reduced-order representations of geological images honoring higher-order statistics. Following the route taken in image compression, we collect an ensemble of \( \kappa \) spatial samples of a geological reference image, where the samples size \( m \) (i.e. the number of cells in the sample) is equal or smaller than \( n \). The samples can be taken regularly, such that the entire image can be covered exactly if the sample dimensions (length and width for a 2D image, or length, width and depth for a 3D image) are an integer fraction of the image dimension. Otherwise a small overlap of the samples is required. Alternatively, the samples can be taken at random. In all cases, the samples can be represented as \( m \times 1 \) column vectors \( \mathbf{k}(i), i = 1 \ldots \kappa \), where the \( m \) elements of \( \mathbf{k} \) are the permeabilities, or, in our case, the base-10 logarithms of the permeabilities, in the sample cells, and where usually, although not necessarily, \( \kappa \ll m \). We collect all snapshots in an \( m \times \kappa \) sample matrix

\[
\mathbf{K} = \begin{bmatrix} k(1) - \bar{k} & k(2) - \bar{k} & \ldots & k(\kappa) - \bar{k} \end{bmatrix},
\]

where

\[
\bar{k} = (1/\kappa) \sum_{i=1}^{\kappa} k(i)
\]

is the ensemble average. The \( m \times m \) matrix

\[
\mathbf{R}_m = \mathbf{K} \mathbf{K}^T / (\kappa - 1)
\]

is the covariance matrix of the ensemble. The covariance matrix of a simplified ensemble is

\[
\mathbf{R}_r = (1/\kappa) \mathbf{R}_m
\]
is the co-variance matrix of (the logarithms of) the permeability values as captured by the samples. It can be shown that the eigenvectors of the eigenvalue problem

\[ R_m \varphi = \varphi \lambda \] (4)

determine principal directions in a projected space that best fit the collected samples, measured in terms of the relative ‘energy’, i.e. mean square fluctuations, associated with particular directions in the projected space. Because generally \( \kappa < m \), the rank of \( R_m \) can be at most \( \kappa - 1 \) and therefore it is sufficient to solve the smaller eigenvalue problem

\[ \psi^T R_\kappa = \lambda \psi^T \] , (5)

where \( R_\kappa = K^T K / (\kappa - 1) \) is a \( \kappa \times \kappa \) matrix. Note: the maximum rank is \( \kappa - 1 \) and not \( \kappa \) because we have subtracted the mean, which is a linear combination of all snapshots, from each snapshot. We can decompose the covariance matrices \( R_m \) and \( R_\kappa \) according to

\[ R_m = \Phi \Lambda_m \Phi^T \] and \[ R_\kappa = \Psi \Lambda_\kappa \Psi^T \] , (6, 7)

where \( \Lambda_m \) and \( \Lambda_\kappa \) are \( m \times m \) and \( \kappa \times \kappa \) diagonal matrices with ordered eigenvalues on the diagonal, \( \Phi \) and \( \Psi \) are \( m \times m \) and \( \kappa \times \kappa \) orthogonal matrices containing the eigenvectors \( \varphi \) and \( \psi \) as columns and rows respectively, and where we have used the transpose instead of the inverse because \( R_m \) and \( R_\kappa \) are symmetric and therefore the eigenvectors are orthogonal. Alternatively, the eigenvector matrices \( \Phi \) and \( \Psi \) can be computed with the aid of a singular value decomposition (SVD) of the snapshot matrix (Golub and Van Loan, 1983):

\[ K = \Phi \Sigma \Psi^T \] , (8)

where the \( m \times \kappa \) matrix \( \Sigma \) is given by

\[ \Sigma = \begin{bmatrix} \sigma_1 & 0 & \ldots & 0 & 0 \\ 0 & \sigma_2 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & \sigma_{\kappa-1} & 0 \\ 0 & 0 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 0 & 0 \end{bmatrix} \] . (9)

Here \( \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{\kappa-1} \geq 0 \) are the singular values of \( K \), i.e. the square roots of the eigenvalues \( \lambda_i, i = 1, 2, \ldots, \kappa - 1 \), while we have tacitly assumed that \( \kappa < m \) as is normally the case. It can be simply verified that equations (6) and (7) are obtained from equation (8), by working out the matrix products \( K K^T \) and \( K^T K \). Each of the samples \( k_j \) can now be represented as

\[ k_i - \bar{k} = \Phi_\kappa z_i \] , (10)

where \( z_i \) is a \((\kappa - 1) \times 1\) vector, and \( \Phi_\kappa \) is an orthogonal \( m \times (\kappa - 1) \) matrix consisting of the first \( \kappa - 1 \) left eigenvectors corresponding the \( \kappa - 1 \) non-zero singular values. A further reduction can often be obtained if we use a ‘truncated’ \( m \times \ell \) transformation matrix \( \Phi_\ell \), where \( \ell < \kappa \), which is defined as the first \( \ell \) columns of \( \Phi \). The cut-off point \( \ell \) depends on the magnitude of the singular values, and an often followed approach is to choose an \( \ell \) for which
where $\alpha$ is close to one. These $\ell$ eigenvectors (or $\kappa$–1 eigenvectors if $\alpha = 1$) form the basis functions for the reduced-order description of the permeability field:

$$\begin{align*}
(k - \bar{k}) & \approx \Phi_\ell \zeta \quad \text{or} \quad \zeta = \Phi_\ell^T (k - \bar{k}),
\end{align*}$$

where $\zeta$ is now an $\ell \times 1$ vector. This reduced-order representation of the permeability field using basis functions obtained by PCA is ‘optimal’ in the sense that it has a smaller mean square error than a representation by any other basis of the same dimension.

**Unconditioned realizations**

Instead of using PCA to create a low-order representation of a permeability field, we use it to create new realizations with similar second-order spatial statistics (i.e. mean and covariance) as the permeability field of a reference image. As a first step, we describe the generation of new, sample-sized and unconditioned, realizations. This could be done, in theory, by first transforming all samples $k_i$, $i = 1, \ldots, \kappa$, to reduced representations $\zeta_i$ with the aid of equation (13). We could then collect all $\kappa$ vectors $\zeta_i$ in an $\ell \times \kappa$ matrix

$$Z = \begin{bmatrix} z(1) & z(2) & \ldots & z(\kappa) \end{bmatrix},$$

such that the $\ell \times \ell$ matrix

$$R_\ell = \frac{Z Z^T}{\ell}$$

is the covariance matrix of the ensemble of vectors $\zeta_i$. (Note that $\bar{Z} = 0$.) However, we don’t have to compute $R_\ell$ in this way because the statistics are already available from the SVD of $K$ according to:

$$R_\ell = \Phi_\ell^T K K^T \Phi_\ell = \Phi_\ell^T \Phi_\ell \Sigma_\ell \Psi^T \Psi \Sigma_\ell^T \Phi_\ell = \Sigma_\ell^2,$$

where $\Sigma_\ell$ is the $\ell \times \ell$ diagonal matrix consisting of the $\ell$ top rows of $\Sigma$, and where we used the orthogonality of $\Phi_\ell$ and $\Psi$ to eliminate the products $\Phi_\ell^T \Phi_\ell$ and $\Psi^T \Psi$. The $\ell \times \ell$ covariance matrix $R_\ell$ is therefore diagonal and can simply be computed as

$$R_\ell = \frac{\Sigma_\ell^2}{\ell},$$

The spatial statistics of the ensemble of samples $k_i$ are now fully defined by $\Phi_\ell$, $\bar{k}$ and $\Sigma_\ell$. To create new ensembles, we can simply draw new vectors $\zeta$ from a multivariate Normal distribution with mean $0$ and covariance matrix $R_\ell$, and use equation (12) to create new realizations $k$. In general, random realizations of $z$ can be obtained from a vector $y$ of uncorrelated Normal distributed random variables mean $\bar{z}$ and unit variance according to

$$z = C y + \bar{z},$$

where

$$C = (R_\ell)^{\frac{1}{2}}$$
is the Choleski decomposition (symmetric LU decomposition) of $R_\ell$. In our case we have $z = 0$ and, from equation (17),

$$C = \frac{\Sigma}{\varphi}.$$  

(20)

Combining equations (12) and (18) we find that a new, unconditioned, realization $k_{unc}$ can be obtained from a random vector $y$ according to

$$k_{unc} = \Phi_\ell Cy + \kappa.$$  

(21)

A total of $\mu$ realizations can now be created in one vectorized Matlab operation according to

$$K_{unc} = \Phi_\ell CY.$$  

(22)

where $Y$ and $K_{unc}$ are $\mu \times m$ matrices of random vectors and mean-shifted unconditioned realizations respectively. If we choose $\mu = \kappa$, i.e. a number of new realizations equal to the number of snapshots we can verify that the covariance matrix of the new realizations is equal to that of the snapshots:

$$K_{unc}K_{unc}^T = \Phi_\ell CYY^T C^T \Phi_\ell^T = \Phi_\ell ZZ^T \Phi_\ell^T = \Phi_\ell \Phi_\ell^T KK^T \Phi_\ell \Phi_\ell^T = KK^T,$$  

(23)

where we have left out the scaling factor $1/(\kappa - 1)$ for clarity.

**Conditioned realizations**

As a next step we consider the generation of new, sample-sized, realizations conditioned by data in the form of $q$ measured well bore permeabilities where $q < \ell$. We assemble the measured permeabilities in a $(q \times 1)$ vector $k_{fix}$ such that

$$k_{fix} = Lk.$$  

(24)

where $L$ is an $(m \times q)$ selection matrix filled with zeros and ones in the appropriate places. Moreover, we assume that the permeabilities are measured with uncorrelated zero-mean Normally distributed measurement errors which can be described with a covariance matrix $R_q$. Conditioning on these well data will inevitably lead to a change in the grid block permeabilities in the neighborhood of the wells. However, we aim to minimize this change, whereas we also aim to bring the conditioned well data as close as possible to the measured data. This leads to the following optimization problem:

$$k_{con} = \arg\min_k J(k),$$  

(25)

where the objective function $J$ is defined as

$$J(k) = (k - k_{unc})^T R_m^{-1} (k - k_{unc}) + (k_{fix} - Lk)^T R_q^{-1} (k_{fix} - Lk).$$  

(26)

This is a Bayesian formulation which produces an optimal (minimal-variance) estimate of $k$, under the assumption of Normally distributed unconditioned realizations and measurement errors; see e.g. Oliver et al. (2008). A necessary condition for a minimum is the vanishing of the first derivatives of $J(k)$:

$$\frac{dJ}{dk} = 2\left[(k - k_{unc})^T R_m^{-1} - (k_{fix} - Lk)^T R_q^{-1} L\right] = 0^T,$$  

(27)
which can be transposed and simplified, resulting in
\[
\left( \mathbf{I} + \mathbf{R}_m \mathbf{L}^\top \mathbf{R}_q^{-1} \mathbf{L} \right) \mathbf{k} = \mathbf{k}_{unc} + \mathbf{R}_m \mathbf{L}^\top \mathbf{R}_q^{-1} \mathbf{k}_{fix}.
\] (28)

Equation (28) represents a linear system of equations of size \( m \) which can be solved for \( \mathbf{k} \). For \( \mathbf{k} \) to represent a minimum it is also necessary that the Jacobian of \( J(\mathbf{k}) \) (i.e. its matrix of second derivatives) is positive definite. The Jacobian follows as
\[
\frac{d^2 J(\mathbf{k})}{d\mathbf{k}^2} = 2 \left( \mathbf{R}_m^{-1} + \mathbf{L}^\top \mathbf{R}_q^{-1} \mathbf{L} \right).
\] (29)

The \( m \times m \) covariance matrix \( \mathbf{R}_m \) and the diagonal \( q \times q \) covariance matrix \( \mathbf{R}_q \) are positive definite (by definition) and so are therefore their inverses. The pre- and post-multiplication with selection matrices \( \mathbf{L}^\top \) and \( \mathbf{L} \) results in an \( m \times m \) semi-positive definite diagonal matrix, and the sum between the brackets in equation (29) remains therefore positive definite. As a result, the value of \( \mathbf{k} \) as obtained from equation (28) is the desired value \( \mathbf{k}_{con} \).

A computationally more efficient expression can be obtained with the aid of equation (12) and the identities
\[
\mathbf{R}_m = \frac{\mathbf{K}}{\kappa - 1} = \frac{\mathbf{\Phi}_z \mathbf{Z} \mathbf{\Phi}_z^\top}{\kappa - 1} = \frac{\mathbf{\Phi}_s \mathbf{R}_q \mathbf{\Phi}_s^\top}{\kappa - 1} = \frac{\mathbf{\Phi}_s \mathbf{\Sigma}^2 \mathbf{\Phi}_s^\top}{\kappa - 1}.
\] (30)

Substitution in equation (28) and reordering the results gives
\[
\left\{ \left. \mathbf{I} + \frac{\mathbf{\Phi}_s \mathbf{\Sigma}^2 \mathbf{\Phi}_s^\top \mathbf{L}^\top \mathbf{R}_q^{-1} \mathbf{L}}{\kappa - 1} \right\} \mathbf{\Phi}_s \mathbf{z} = \mathbf{\Phi}_s \mathbf{z}_{unc} + \frac{\mathbf{\Phi}_s \mathbf{\Sigma}^2 \mathbf{\Phi}_s^\top \mathbf{R}_q^{-1} \left( \mathbf{k}_{fix} - \mathbf{L} \mathbf{\bar{k}} \right)}{\kappa - 1},
\] (31)

which is an over-determined linear system of equations \( \mathbf{A} \mathbf{z} = \mathbf{b} \) where \( \mathbf{A} \) is an \( m \times \ell \) matrix whereas \( \mathbf{z} \) has only \( \ell \) elements. The system can be solved for \( \mathbf{z} = \mathbf{z}_{con} \) in least-squares sense according to
\[
\mathbf{A}^\top \mathbf{A} = \mathbf{A}^\top \mathbf{b},
\] (32)

just as in the unconditioned case, an ensemble of \( \mu \) realizations can now be created in one vectorized Matlab operation according to
\[
\mathbf{K}_{con} = \mathbf{\Phi} \left( \mathbf{A}^\top \mathbf{A} \backslash \mathbf{A}^\top \mathbf{B} \right).
\] (34)

The \( \ell \times \mu \) matrix \( \mathbf{Z}_{unc} \) is an ensemble of unconditioned realizations as computed with equation (22), the \( m \times m \) matrix \( \mathbf{\bar{K}} = \mathbf{\bar{k}} \mathbf{1}^\top \) consists of identical average vectors \( \mathbf{\bar{k}} \), and the
$m \times m$ matrix $K_{fix}$ is an ensemble of measured values $k_{fix}$, perturbed with zero-mean Normally distributed noise with covariance $R_q$ to represent the measurement error. (Note that the addition of noise is necessary to remain the statistical optimality.)

**Rank deficiency and bias**

The use of a (truncated) SVD of an $m \times \kappa$ snapshot matrix implies that the rank of the truncated matrix $\Phi_\ell$ is equal to the minimum of

- the number of pixels $m$,
- the number of snapshots $\kappa$ (assuming that all snapshots are different), or
- the number $\ell$ of remaining columns in $\Phi_\ell$,

where always $\ell \leq \kappa$ and usually $\kappa < m$. The number of independent new realizations can therefore never be larger than the rank of $\Phi_\ell$. If we choose $\kappa \geq m$ and apply no truncation the maximum number of independent realizations is therefore $m$, i.e. equal to the number of pixels in the snapshots. If we choose $\kappa < m$ it is possible to still obtain $m$ independent realizations by adding a small amount of zero-mean uncorrelated random noise to all pixels. However, this is mainly of theoretical interest because the images usually display a rapidly decaying eigenvalue spectrum (or singular value spectrum). The number of snapshots, $\kappa$, however, does influence the characteristics of the realizations. In general, a smaller number of snapshots results in larger spatial features, but also in less variety in the realizations.

The conditioning of the realizations to known permeability values in the wells results in a change in the spatial statistics of the ensemble. The wells are usually located in zones of high permeability, which means that the conditioned ensemble will have a higher mean than the reference image. If this bias is deemed to be a problem it can be simply corrected by subtracting the bias from all values.

Finally, it should be checked if there are realizations with permeability values equal to or below zero, or, correspondingly, log-permeability values equal to or below one. If so, they should be discarded, which implies that the (log-)normal distribution is replaced by a truncated (log-)normal distribution. Alternatively, the occasional ‘unphysical’ pixel value may be reset to a small value.

**Correlated porosities and permeabilities**

Corresponding ensembles of porosity realizations can be generated through the use of a linear correlation with Normally distributed random coefficients. For each pixel the porosity can e.g. be computed as:

$$
\phi = \phi_{min} + \left(\alpha k_{scaled} + (1-\alpha) \times \text{rand}[0,1]\right) \times (\phi_{max} - \phi_{min}),
$$

where

$$
k_{scaled} = \frac{\ln k - \min\left(\ln k\right)}{\max\left(\ln k\right) - \min\left(\ln k\right)},
$$

with minimum and maximum values of $\ln k$ taken over the entire ensemble.

**Example**

Figure 1 depicts a two-dimensional (2D) reference image. It represents a horizontal heterogeneous permeability field with a contrast between pixel values of somewhat more than...
three orders of magnitude. The image displays spatial features that would be extremely unlikely to be generated by sampling from a multivariate Normal distribution. However, as discussed above, the method used to generate the ensembles is based on just the first two moments (mean and covariance) as determined from the reference image, and the realizations will therefore display much smoother heterogeneities.

Figure 1: Reference image of a heterogeneous permeability field (10201 pixels). The permeability units are expressed in m² on a natural-log scale.

Figure 2 depicts the first 9 snapshots, and Figure 3 the singular values for a total of 561 snapshots (i.e. just equal to the number of pixels). Figure 4 depicts the first eight realizations of the permeability ensemble plus the ‘truth case’ (chosen as snapshot nr. 25). Figures 2 and 4 also display the four wells that have been used to condition the realizations to data at the well locations. We used a standard deviation of 0.05 times the known permeability values in the wells to represent zero-mean Normally distributed measurement noise. To generate the porosity realizations we used \( \phi_{\min} = 0.175 \), \( \phi_{\max} = 0.325 \) and \( \alpha = 0.8 \). The porosity realizations display similar spatial heterogeneity patterns as the permeability realizations, but over a much smaller range. Examples of the probability density functions (pdfs) of grid block permeabilities and porosities are displayed in the Figure 3 and illustrate the approximately log-Normal and Normal distributions of permeability and porosity respectively.

We performed water flooding simulations for all 1000 realizations with parameters given in Table 1. Typical ‘fans’ of the resulting bottom hole pressures and oil- and water rates for the last 20 realizations are shown in Figure 7, while Figure 8 displays the pdfs of the total oil and water production for the entire ensemble illustrating that the geological uncertainty implies that there is also a significant uncertainty in the production figures.
Figure 2: Nine snapshots (561 pixels each). The snapshot number is displayed above the figures. The two crossed circles represent water injection wells, and the two dotted circles represent oil production wells. Scale as in Figure 1.

Figure 3: Singular values for 561 snapshots.
Figure 4: Snapshot average values and first eight basis functions (561 pixels each). Scale for average as in Figure 1. Scales for basis functions are varying (not displayed).

Figure 5: Eight conditioned permeability realizations, and truth case (i.e. 25\textsuperscript{th} snapshot) (561 pixels each). The realization number is displayed above the figures. The two crossed circles represent water injection wells, and the two dotted circles represent oil production wells. Scale as in Figure 1.
Figure 6: Probability density functions of natural-log permeability and porosity for grid block nr. 281 (the center grid block in the images).

Figure 7: Top: bottom-hole pressures; dark and light blue: injection wells; red and green (covered): production wells (constant pressure); black: truth case. Bottom: oil- and water rates; solid lines: oil production rates; dotted lines: water production or injection rates; red and green (covered): production wells; dark and light blue (hardly visible): injection wells (constant rates); black: truth case. The results correspond to the last 20 ensemble members out of an ensemble of 1000.
Figure 8: Probability density functions of cumulative oil and water production for 1000 ensemble members.
Table 1: Reservoir and fluid properties

<table>
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<tr>
<th>Symbol</th>
<th>Variable</th>
<th>Value</th>
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References


