Generating saddle points in the merit function landscape of optical systems

Florian Bociort and Maarten van Turnhout*
Optics Research Group, Delft University of Technology
Lorentzweg 1, 2628 CJ Delft, The Netherlands

ABSTRACT

Finding multiple local minima in the merit function landscape of optical system optimization is a difficult task, especially for complex designs that have a large number of variables. We discuss here a method that enables a rapid generation of new local minima for optical systems of arbitrary complexity. We have recently shown that saddle points known in mathematics as Morse index 1 saddle points can be useful for global optical system optimization. In this work we show that by inserting a thin meniscus lens (or two mirror surfaces) into an optical design with N surfaces that is a local minimum, we obtain a system with $N+2$ surfaces that is a Morse index 1 saddle point. A simple method to compute the required meniscus curvatures will be discussed. Then, letting the optimization roll down on both sides of the saddle leads to two different local minima. Often, one of them has interesting special properties.

Keywords: saddle point, optimization, optical system design, lithography

1. INTRODUCTION

The impressive progress in the global optimization of optical systems over the past two decades has resulted in powerful software tools¹⁻⁴. For optical designs for which the complexity is not too high, present-day global optimization algorithms are valuable tools for finding a good (perhaps even the best) solution among the many local minima that are found in the merit function landscape. Recent results showing that these local minima form a connected network have also provided new insight in the topography of the merit function landscape for such systems⁵⁻⁹. However, if the number of components is large, even local optimization is time consuming, and it is difficult to apply such tools straightforwardly. In this case, local minima that differ from the known ones must be found with methods that use only a small number of local optimizations to achieve their goal. In this work, we present a method that enables a rapid generation of new local minima for optical systems of arbitrary complexity. Here we discuss the basic new ideas and give simple examples of their application. The results obtained with this method for lithographic systems will be discussed in an accompanying article in this volume¹⁰.

Our studies of the network structure of the set of local minima have shown that we have a certain degree of order in the merit function landscape of optical systems and that this order is best understood if one focuses not only on local minima, but on saddle points as well. Minima, saddle points and maxima are all critical points, i.e. the gradient of the merit function vanishes at these points. An important property of (non-degenerate) critical points is the so-called Morse index. (When critical points "merge" we call them degenerate. A more rigorous discussion of the Morse index and of the related properties is given in our earlier papers.) Intuitively, one can think about a two-dimensional saddle point (a horse saddle for example), which is a minimum along a certain direction and a maximum along the perpendicular direction. Similarly, critical points in an N -dimensional optimization problem have a set of mutually orthogonal directions; along some of these directions the critical points are minima, along the other ones (called downward directions) they are maxima. The Morse index is the number of downward directions. Thus, for minima and maxima the Morse index is 0 and N , respectively, and saddle points have a Morse index between 1 and $N-1$.

* m.vanturnhout@tnw.tudelft.nl; phone: +31 15 278 8109; fax +31 15 278 8105;
<http://www.optica.tn.tudelft.nl/users/bociort/networks.html>

For our problem, saddle points with Morse index 1 are of special interest. They are maxima in one direction, which one can visualize as the downward direction of a two-dimensional saddle point, and they are minima in the remaining $N-1$ directions, which are all very similar to the upward direction in the two-dimensional case. As in a two-dimensional situation, choosing two points close to each other, but on opposite sides of the saddle and starting local optimizations at those points will lead to two distinct minima. (In most cases, which minima are reached is determined by the merit function landscape and not by the implementation details of the local optimization algorithm. Otherwise, the two paths down the gradient from the saddle point can be determined, more accurately but at the cost of extra computer time, with a differential equation.) Together with the saddle point, the two downward paths form a link in the variable space between the two local minima.

Detecting Morse index 1 saddle points without a-priori information about them is computationally more expensive than finding local minima and the method described in Ref. 7 is not applicable for systems with many variables such as lithographic lenses. However, the analysis of the networks corresponding to less complex systems shows recurring properties that facilitate the task, at least for a certain type of saddle points.

It is interesting to study how networks change when control parameters such as aperture, field or system parameters that have not been used for optimization are changed. In fact, saddle points with Morse index 1 can be further classified according to the way in which they appear in or disappear from the network when control parameters are changed. We mention without entering into many mathematical details that the classification can be made mathematically rigorous by using Catastrophe Theory¹¹. Some saddle points tend to appear in and disappear from the network more easily and are therefore in a certain sense less fundamental. We have already reported examples of such appearances and disappearances in the networks of EUV lithographic objectives⁹ (in that example we have the so called "fold" catastrophe) and of the Cooke Triplet⁶ (the "cusp" catastrophe). (A local minimum always appears/disappears together with the saddle point in these cases.)

In this paper we will focus on a more robust and therefore more fundamental type of Morse index 1 saddle point which will be called "curvature" saddle point. The name comes from the fact that such saddle points already exist in simple systems consisting of thin spherical lenses in contact, where the only variables are curvatures. Saddle points for these simple systems have already been studied in Ref. 8. In the next section we will continue the discussion of these systems with emphasis on a remarkable property that survives generalization. As shown in Sec. 3 in a special case and in Sec. 4 in the general case, curvature saddle points for arbitrary optical systems can be generated from local minima taken from a variable space with lower dimensionality.

2. SYSTEMS OF THIN LENSES IN CONTACT

Systems of thin spherical lenses, in which all lens thicknesses and air spaces between lenses are set equal to zero, and for which the merit function includes only spherical aberration, are simple enough to be studied analytically in detail. This model, which relies on third-order aberration theory, may seem oversimplified, but as will be seen below it enables us to understand a mechanism that is also present in systems having a much higher complexity.

Table 1 reproduces the exact values of the curvatures of several curvature saddle points of a monochromatic triplet with refractive index $n=1.5$, and object at infinity. (The first five curvatures were used as independent variables, the sixth one was used to keep the focal length unity. For more details see Ref. 8.)

c_1	c_2	c_3	c_4	c_5	c_6
$6/7$	$6/7$	$6/7$	$-1/7$	$11/7$	$4/7$
$6/7$	$-1/7$	$-1/7$	$-1/7$	$11/7$	$4/7$
$6/7$	$-1/7$	$11/7$	$11/7$	$11/7$	$4/7$
$6/7$	$-1/7$	$11/7$	$4/7$	$4/7$	$4/7$

Table 1. The curvatures of four of the six Morse index 1 saddle points of a thin-lens triplet.

With the same method, the values of the curvatures of certain local minima in these systems (called in Ref. 8 "hubs") can also be computed analytically. (Unlike most local minima, which have a small number of links in the network, the hubs have many links. For example, the hub in Fig. 8 of Ref. 8 has eight links.) The hub for a monochromatic doublet (focal length unity, $n=1.5$, object at infinity) has for instance

$$c_1=6/7, \quad c_2=-1/7, \quad c_3=11/7, \quad c_4=4/7. \quad (1)$$

Note that the curvatures of the triplet saddle points in Tab. 1 can be very simply derived from the parameters of the doublet local minimum given by (1). The triplet curvature values are those given by (1), but for each saddle point, one of these curvatures appears three times successively. Physically, this numerical property can be interpreted as follows: The four triplet saddle points are obtained by inserting successively one meniscus lens at the four surfaces of the doublet hub. In all cases, the meniscus lens has equal curvatures, and their common value is equal to the curvature of the original doublet surface where the meniscus is introduced. It results from general formulas for systems of thin lenses in contact that curvature saddle points with $N+2$ surfaces can be obtained in the same way from hubs with N surfaces. This happens when all curvatures are used as variables, and also when some of them are used as control parameters.

Using the first curvature in the system as a control parameter (and not as a variable) is useful for studying the relationship between the hubs and the curvature saddle points generated with the above mechanism. (In this analysis, we consider a hub that has the same number of lenses as the saddle points.) Our analytic results show that as long as the first curvature is lower than a certain critical value, all curvature saddle points are linked on one side with the same hub. (See for examples Ref. 8.) When the first curvature reaches the critical value, the hub, the surrounding Morse index 1 saddle points and, when they exist, also saddle points with a higher Morse index, merge into a single degenerate critical point. In the two-dimensional doublet example discussed in Figs. 4 and 6 of Ref. 8 this degenerate critical point is called the "monkey saddle"¹². Mathematically we encounter here the so-called "elliptic umbilic" catastrophe. In the spirit of Catastrophe Theory, it can be said that three non-degenerate curvature saddle points are "shaken loose" from the monkey saddle. Such degenerate critical points exist in higher dimensions as well. In the case of a triplet with four variable curvatures and a curvature used as control parameter, the higher-order equivalent of the monkey saddle is a critical point that is 16-fold degenerate. When the first curvature is below the critical value, this degenerate critical point splits into a local minimum (a hub), 5 curvature saddle points with Morse index 1 and 10 saddle points with Morse index 2.

For the monochromatic doublet, triplet and quartet, Fulcher has derived the curvatures of the minimum, which we call hub, several decades ago¹³. These systems turn out to be relaxed designs^{14,15}. While the hub doublet has a poor imaging quality, the Fulcher monochromatic quartet with $n=1.5$ is a remarkable system. By optimizing the thin-lens Fulcher specifications and adding adequate lens thicknesses, we obtain for axial imaging at a numerical aperture of 0.6 a Strehl Ratio of 0.999. Note in Fig.1 the smooth bending of the ray paths and the similarity with elements in designs of lithographic objectives. In fact, we have found that hubs exist also for high-quality lithographic designs¹⁰. It is worth investigating in detail whether, as it seems, there is a more general correlation between the hub structure and relaxation.

Figure 1. A Fulcher-type design.

3. GENERATING SADDLE POINTS FROM LOCAL MINIMA: THEORY

We have seen in the previous section that inserting concentric thin meniscus lenses into a local minimum of the third-order spherical aberration (in Sec. 2 these minima were hubs) transforms the given minimum into a curvature saddle point. Surprisingly, this relationship is valid more generally, for arbitrary rotationally symmetric systems. In this section we generalize this technique and show how curvature saddle points can be obtained from arbitrary local minima of arbitrary optical merit functions. A certain restriction (described below) on glass and axial thicknesses is needed in this section, but will be removed in the next one.

We consider the k -th surface of a system with N spherical surfaces that is a local minimum (Fig. 2a). The value of the merit function is MF_{ref} and the curvature of the surface is c_{ref} . After the surface we introduce a thin lens with zero axial thickness in contact with the k -th surface (i.e. the axial thickness of the airspace before the introduced lens is also zero). The thin lens has the same glass as the lens before it and the surfaces are also spherical. (In this paper we will discuss spherical lenses, but the technique can be generalized for mirror surfaces and for aspheric surfaces as well¹⁰.)

First, assume that the curvatures c_{k+1} and c_{k+2} of the thin lens are varied, but are kept equal. (Since a zero-thickness lens with identical surfaces disappears physically, we call it a "null" lens.) This "null" lens has no effect on ray propagation, and the merit function of the new system with $N+2$ surfaces remains equal to MF_{ref} (Fig. 2b). Similarly, if the curvatures c_k and c_{k+1} are varied, but are kept equal, the air space before the lens becomes a "null" lens. If in addition for the second curvature of the thin lens we have $c_{k+2} = c_{ref}$, the merit function of the new system remains again unchanged by the insertion and equal to MF_{ref} (Fig. 2c). (Note that, although the curvature c_k of the original minimum with N surfaces is varied, the second curvature of the new thin lens takes its role and ensures that MF_{ref} remains unchanged.)

Figure 2. a) The k -th surface with curvature c_{ref} of a system that is a local minimum. All rays pass undeviated through the thin lens with surfaces $k+1$ and $k+2$ if b) the thin lens has equal curvatures or c) the thin air meniscus before the thin lens has equal curvatures and the second thin-lens curvature is c_{ref} . d) Curvature saddle point in which three consecutive surfaces have the same curvature c_{ref} . For clarity, the thin lens and the air space before it are drawn with nonzero thickness.

The transformations

$$c_k = c_{ref}, c_{k+1} = c_{k+2} = u, \text{ all other variables of the minimum are kept unchanged,} \quad (2)$$

$$c_k = c_{k+1} = v, c_{k+2} = c_{ref}, \text{ all other variables of the minimum are kept unchanged,} \quad (3)$$

describe two lines in the variable space of the new system with $N+2$ surfaces. The position of individual points along these lines is given by the parameters u and v . As shown above, along both lines the merit function is invariant and equal to MF_{ref} . The two invariant lines intersect for $u = v = c_{ref}$, i.e.

$$c_k = c_{k+1} = c_{k+2} = c_{ref}, \text{ all other variables of the minimum are unchanged.} \quad (4)$$

In the above analysis we assumed that a thin lens with surfaces $k+1$ and $k+2$ is inserted *after* the k -th surface in an existing design that is a local minimum. However, (2-4) are also valid if a thin lens with surfaces k and $k+1$ is placed *before* the $k+2$ -th surface in an existing minimum. In this case, the invariant lines (2) and (3) are related to the "null" airspace lens and the "null" glass lens that are formed, respectively.

We will analyze below the properties of the intersection point (4) (see Fig. 2d) in the variable space of the new system with $N+2$ surfaces. It is sufficient for this purpose to examine the three-dimensional subspace of the variables c_k , c_{k+1} and c_{k+2} . The coordinate system in Fig. 3a has

$$x = c_k - c_{ref}, \quad y = c_{k+1} - c_{ref}, \quad z = c_{k+2} - c_{ref}. \quad (5)$$

In the unit cube in Fig. 3a, the invariant lines (3) and (2) are oriented along the vectors

$$\vec{OA} = (1, 1, 0), \quad \vec{OB} = (0, 1, 1), \quad (6)$$

respectively. It is convenient to rotate the coordinate system so that the points in the plane OAB can be parameterized by only two numbers (instead of three). Since $OA=OB=AB$, the angle between OA and OB is 60 degrees, and the two lines do not form a rectangular coordinate system. However, an orthogonal axis system in the plane OAB can be easily constructed. The new axes x' and y' are then oriented along the vectors

$$\vec{OP} = (\vec{OA} - \vec{OB})/2 = (1/2, 0, -1/2), \quad \vec{OQ} = (\vec{OA} + \vec{OB})/2 = (1/2, 1, 1/2) \quad (7)$$

(see Fig. 3a.). The axis z' orthogonal to the plane OAB (not shown in Fig. 3a) is then oriented along $(1,-1,1)$. By taking unit-length vectors along OP and OQ , the position of an arbitrary point in the plane OAB is given by

$$x', \frac{2}{\sqrt{2}} \vec{OP} + y', \frac{2}{\sqrt{6}} \vec{OQ} = \left(\frac{x'}{\sqrt{2}} + \frac{y'}{\sqrt{6}}, \sqrt{\frac{2}{3}} y', \frac{y'}{\sqrt{6}} - \frac{x'}{\sqrt{2}} \right). \quad (8)$$

The three curvatures for the points in the plane OAB are then given by

$$c_k = c_{ref} + \frac{x'}{\sqrt{2}} + \frac{y'}{\sqrt{6}}, \quad c_{k+1} = c_{ref} + \sqrt{\frac{2}{3}} y', \quad c_{k+2} = c_{ref} + \frac{y'}{\sqrt{6}} - \frac{x'}{\sqrt{2}}. \quad (9)$$

Figure 3. a) Plane OAB defined by the invariant lines (2) and (3) in the subspace defined by the variables c_k , c_{k+1} and c_{k+2} (hatched). Note that point P also belongs to this plane. b) The two invariant lines (continuous lines) and the orthogonal axes x' and y' (horizontal and vertical dashed lines) in the same plane. All these lines cross at the saddle point O .

If in a plane two lines, along which a function is constant, cross, then the crossing point is a two-dimensional saddle point of that function. In the plane OAB the two invariant lines intersect in O (Fig. 3b). We show now that O is a critical point. It is well known that the direction of the most rapid variation of a function is orthogonal to the direction along which the function is constant. Therefore, at each point along the invariant lines, the projection on OAB of the gradient of the merit function is orthogonal to the invariant lines. At the intersection point, the projection of the gradient must be zero, because it cannot point in two different directions. Therefore, in the plane OAB the point O is a two-dimensional saddle point. (It cannot be a two-dimensional maximum or minimum, because in these cases the equimagnitude contours are ellipses, not straight lines.) Along one of the orthogonal axes in the plane OAB the point O is a minimum, along the other one it is a maximum. Because for the original local minimum the merit function derivative with respect to c_k was already zero, the point O is also a minimum along the direction of Ox , outside OAB . Consequently, the merit function derivatives with respect to x , y and z must all be zero at O . Because the variables of the original local minimum other than c_k are kept unchanged, the merit function derivatives with respect to them remain zero. Thus, all components of the gradient of the merit function are zero at O .

We have shown that O is a maximum in one direction in the plane OAB , that it is a minimum in the orthogonal direction in that plane and that it is also a minimum with respect to the variables of the original local minimum other than c_k . The only direction that remains to be studied is that of Oz' . In the cases we have examined, numerical tests indicated that along $(1,-1,1)$ O was also a minimum. (This is plausible because along Ox , which is also outside the plane OAB , we know that O must be a minimum.) Thus, typically the curvature saddle point O is a Morse index 1 saddle point. (If counterexamples with O a maximum along Oz' will be found, then in those cases the Morse index will be 2 and the procedure described in the next section for generating local minima from the saddle point must be adapted.)

In the examples shown in this paper we use the optical design software CODE V and our merit function is the default merit function based on transverse aberrations of this program. The local optimization variables are the surface curvatures, the object is at infinity and the last curvature has a solve to keep the effective focal length constant. Figure 4 shows for two different systems equimagnitude contours (i.e. the contours along which the function is constant) computed numerically with Eqs. (9) for points in the plane OAB . The merit function is shown in black and in addition, the third-order spherical aberration is shown in gray. While general equimagnitude contours are curved, note the crossing straight lines that generate the curvature saddle point (4). Since the lines (2) and (3) do not depend on the nature of the optical function used, their plots for the third-order spherical aberration and for the merit function are fully superimposed. Note for the third-order spherical aberration the presence of a third line. The resulting triangle, which is similar with the one analyzed in detail in Ref. 8, shows that the mathematical origin of these saddle points is related to the elliptic umbilic catastrophe.

Figure 4. Equimagnitude contours (with function values close to that of the saddle point) in the plane OAB . A zero-thickness lens is inserted at zero distance a) before the third surface of a thin-lens monochromatic triplet minimum in which all glasses are identical, $n=1.5$, $F/5$, half-field 3 degrees, b) before the third surface of a polychromatic Double Gauss system with different glasses, $F/2$, half-field 14 degrees. The glass of the thin lens is the same as the glass of the next lens. c) Region around the saddle point O in Fig. 4b, enlarged.

4. GENERATING SADDLE POINTS FROM LOCAL MINIMA: PRACTICE

Generating saddle points by inserting at certain surfaces concentric meniscus lenses as shown in Fig. 2d can be very useful for practical purposes¹⁰. First, we take two points close to each other, but on both sides of the saddle. This can be done for instance by setting in (2) $u = c_{ref} \pm \varepsilon$ (the points P_1 and P_2 in Fig. 3b) or by setting in (3) $v = c_{ref} \pm \varepsilon$ (the points P_3 and P_4), where ε indicates a small curvature change. Then, two different local minima result from the optimization of these points. Finally, in these solutions the zero distances between surfaces can be increased to the desired values.

Often, (but not always) one of the minima resulting from curvature saddle points generated in this way is a hub. Figure 5a shows a local minimum for a monochromatic quartet, in which the lenses have identical glasses. To facilitate the analysis, the thicknesses of the first two lenses are made equal, and the airspace between them is zero. (For obtaining practical results, this is not necessary.) Four saddle points have been generated by inserting successively at the first four surfaces thin meniscus lenses of the same glass, concentric with the corresponding surface. In the eight local minima that resulted, the thickness of the inserted lens has been increased to the same value as that for the neighboring lenses. Remarkably, four of these minima, one resulting from each saddle point, turned out to be identical (the configuration shown in Fig. 5b).

For practical purposes, it is easier to increase thicknesses in the two resulting minima than in the saddle point itself. However, the four curvature saddle points continue to exist in the merit function landscape of the system shown in Fig. 5b when in them the thin-lens thickness is increased to the same value as that for the neighboring lenses. The system shown in Fig. 5b is connected to all of them. Since this system is connected to several saddle points, we call it a hub.

Figure 5. a) Starting system. b) Hub resulting from the saddle points generated at the surfaces 1, 2, 3 and 4 in Fig. 5a.

In the discussion above, we have analyzed the special situation when the thin meniscus was introduced in contact with another lens with the same glass. However, in practice these restrictions can be removed. If in the final design the glass of the new lens must be different and/or the lens must be placed at a certain distance from a given surface of an existing minimum, then the curvatures of the lens to be inserted can be computed numerically. The difference in glass properties and the distance to the existing surface can be interpreted as a "perturbation" of the previous "ideal" situation, and as long as this "perturbation" is not too large, it can be shown mathematically that the saddle point continues to exist and that it will keep the same Morse index. In the neighborhood of a Morse index 1 saddle point, the equimagnitude (hyper)surface passing through the saddle point in the multidimensional variable space is a (hyper) conical surface with the top at the saddle point. (In three dimensions, think about two cones, opposite to each other, with common top and axis.) We can still begin by inserting a zero-thickness meniscus with equal curvatures as shown in Fig. 2b. Then, only one of the two invariant lines (2) and (3) will exist, but since it must be contained in the hypercone mentioned above, this line passes through the saddle point. (No straight line can be contained in only one half of the hyperconical surface.) If the invariant line is (2) (the situation for (3) is similar), the value of the parameter u for the saddle point is the value for which $\partial f / \partial c_{k+1} = 0$, where f is the merit function. (It can be easily shown that along the invariant line (2) we have $\partial f / \partial c_{k+2} = - \partial f / \partial c_{k+1}$ and therefore it is sufficient to consider only one of the partial derivatives.) Interestingly, this

equation has typically more than one solution and several saddle points are obtained. We have implemented this method in the macro language of CODE V and have tested it in several cases. Once the saddle point is found, the remaining steps are the same as those described at the beginning of this section.

5. CONCLUSIONS

One of the major difficulties in present-day global optimization is that the computing time increases significantly if the dimensionality of the optimization problem is increased. The method discussed here for finding new local minima suffers much less from this drawback. By inserting a meniscus lens at different positions in a design that is a local minimum, saddle points are created and new local minima result from these saddle points. If the number of surfaces must be restored, a pair of surfaces can be removed from the resulting local minima. In common practice, inserting a lens in a system usually leads after optimization to a single local minimum. If however a lens is inserted so that a saddle point is created, two minima result after optimization and for further design we can choose the best of them.

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