Robust Design of Multilayer Optical Coatings by Means of Evolution Strategies

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March 31, 1998

Abstract

Robustness is an important requirement for almost all kinds of products. In this article we show how evolutionary algorithms can be applied for robust design based on the approach of Taguchi. As an example we consider the design of multilayer optical coatings most frequently used for optical filters.

1   Introduction

Robustness is an important requirement for almost all kinds of products, i.e. they should keep a good performance under varying conditions (temperature or humidity). Furthermore, the impact of wear, as well as manufacturing tolerances, should be limited as much as possible. Consequently, the production process itself as well as the environmental influences after the product is put to use have to be regarded during the product design.

In this paper we focus on multilayer optical coatings (MOCs) as an example of how to achieve robust designs using evolutionary algorithms. MOCs are used to guarantee specific transmission and/or reflection characteristics of optical devices. The objective of MOC designs is to find sequences of layers of particular materials with specific thicknesses showing the desired characteristics as closely as possible. Since in general the MOC design problem is not analytically solvable, simplifications are introduced in practice. In many cases however this leads to suboptimal designs.

Here we follow the approach of Greiner [Gre94, Gre96] who replaces the design parameters x_i by stochastic variables of the form $x_i + \delta_i$, where δ_i resembles the stochastic influence of the manufacturing tolerances. Instead of the objective function $f(\vec{x})$ an *expected loss* L based on the expectation of a function of $f(\vec{x} + \vec{\delta})$ is used. Greiners' approach which is largely motivated by Taguchis' work on quality engineering [Tag89, Kac90] has two difficulties. First, as we will show in section 3, an optimal point of L does not necessarily correspond to an optimal point of f. The consequences of this fact have to be clarified. Secondly, given that in most cases L can only be approximated by the mean of a limited number of evaluations the optimization algorithm has to deal with a stochastic objective function.

Various instances of evolutionary algorithms have proven to be robust in the case of stochastic objective functions [FG88, Bey93, BH94, HB94]. In section 4 we show that evolutionary algorithms can be successfully applied to the robust design problem by investigating the example of multilayer optical coatings.

2 Robust Design

Let $\vec{x} = (x_1, \ldots, x_n)$ be a vector of parameters of a given design problem, e.g., the refraction indices and thickness of the optical layers. Given a function $f(\vec{x})$ describing the merit of a design feature, e.g. the color perception of the reflected light, and τ being a target value for $f(\vec{x})$, then if disturbances are neglected the task is to find such an $\vec{x}^*$ that the difference between $f(\vec{x}^*)$ and τ is minimized.

On the other hand the usability of two products although manufactured under almost identical conditions might differ significantly, due to external conditions such as temperature and humidity, or internal factors such as wear as well as manufacturing tolerances. Some of these factors are not controllable at all. Others can only be reduced with unjustifiable effort. Thus they are regarded as disturbances, and it is desired to reduce their influence as much as possible. In this paper our focus is on manufacturing tolerances, but the approach could easily be extended.

The disturbances are represented by a vector of random numbers $\vec{\delta} = (\delta_1, \ldots, \delta_n)$. If the probability distribution of the δ_i are known as well as their influence on f we might rewrite $f(\vec{x})$ as $\tilde{f}(\vec{x}, \vec{\delta})$. In our example the disturbances are assumed to be normally distributed with zero mean and will have an additive influence on the parameter values. Thus, we define

$$\tilde{f}(\vec{x}, \vec{\delta}) = f(x_1 + \delta_1, \ldots, x_n + \delta_n). \tag{1}$$

The task is now to minimize the deviations of $\tilde{f}(\vec{x}, \vec{\delta})$ from τ.

This leads to the question of how to assess these deviations. The traditional approach regards all products with $|\tilde{f}(\vec{x}, \vec{\delta}) - \tau| \leq \epsilon$ as equally good for some predefined ϵ and all others as off-cuts. But this approach is somewhat unrealistic, since if such products are assembled to larger units such as devices on electronic boards malfunctions might occur due to aggregations of deviations of single elements.

The method of parameter design after Taguchi [Tag89, Kac90, Ros88] takes these effects into account by considering every deviation from the objective τ as a loss. In practical applications quadratic loss functions of the form

$$(\tilde{f}(\vec{x}, \vec{\delta}) - \tau))^2 \tag{2}$$

have proven to be well suited if no better alternative is known. The expected loss then becomes

$$L = k \cdot E((\tilde{f}(\vec{x}, \vec{\delta}) - \tau)^2) \tag{3}$$

where k is some constant and E denotes the expectation value of the quadratic deviation.

A naive approach to find minimal values for the expected loss would be to determine a set of (local) optima of the original problem $f(\vec{x})$ with the help of a suitable optimization method and to choose the one with a minimal loss function value. This approach has several drawbacks. First, optimal points of L do not necessarily correspond to optimal points of $|f(\vec{x}) - \tau|$ (see section 3). Furthermore, it would be much more efficient to avoid the exploration of sensitive regions of the search space during the search process.

In our work we follow the approach of Greiner [Gre94, Gre96] who defines the objective function as

$$E_{(\tau - \tilde{f})^2}(\vec{x}) = k \cdot \int (\tau - \tilde{f}(\vec{x}, \vec{\delta}))^2 \cdot P(\vec{\delta})d\vec{\delta} \qquad , \tag{4}$$

where $P(\vec{\delta})$ denotes the the joint probability distribution of the distrubances. Since in most applications the expectation value E cannot be calculated analytically it must be approximated. Here we use

$$\frac{1}{t} \cdot \sum_{i=1}^{t}(\tau - \tilde{f}(\vec{x}, \vec{\delta}_i))^2 \tag{5}$$

as an estimate, where $\vec{\delta}_i, i = 1, \ldots, t$, are vectors of normally distributed random numbers with mean zero and standard deviation σ. The estimation error scales proportional to $\sqrt{t}$, and since in most applications the possible number of evaluations is very limited this approach yields a stochastic optimization problem. As evolutionary algorithms have proven their robustness in case of noisy objective functions [FG88, Bey93, BH94, HB94] they are promising candidates here. But before turning to a concrete case study of optimal MOC designs we try to get deeper insights into the consequences of this approach by some analytical considerations.

3 Analysis of a Simple Example

In order to clarify the relationship between the original merit function f and the expected loss L we investigate the simple rectangular function $f_{c,b,h} : R \to R$ with height $h \in R_+$, width $b \in R_+$ and center $c \in R$:

$$f_{c,b,h}(x) = \begin{cases} h & \text{if } c - \frac{1}{2}b \leq x \leq c + \frac{1}{2}b \\ 0 & \text{else.} \end{cases} \tag{6}$$

The analysis follows the previous work of Tsutsui, Ghosh and Fujimoto [TGF96] for the expectation

$$E_{\tilde{f}}(\vec{x}) = \int \tilde{f}(\vec{x}, \vec{\delta}) \cdot P(\vec{\delta}) d\vec{\delta}. \tag{7}$$

and a similar rectangular function. If the disturbances are assumed to be normal distributed with zero mean and standard deviation σ then the expected quadratic loss can be calculated as

$$
\begin{aligned}
F(x) &= E_{(\tau - f_{c,b,h})^2}(x) \\
&= \frac{1}{\sigma} \cdot \int_{-\infty}^{+\infty} (\tau - f_{c,b,h}(x + \delta))^2 \varphi(\frac{\delta}{\sigma}) d\delta \tag{8} \\
&= \tau^2 - \frac{2\tau h b}{\sigma} \cdot \int_{c-\frac{1}{2}b}^{c+\frac{1}{2}b} \varphi(\frac{z-x}{\sigma}) dz \\
&\quad + \frac{(hb)^2}{\sigma} \cdot \int_{c-\frac{1}{2}b}^{c+\frac{1}{2}b} \varphi(\frac{z-x}{\sigma}) dz \tag{9} \\
&= \tau^2 - (2\tau h b - (hb)^2) \\
&\quad \cdot \left[\Phi\left(\frac{(c+\frac{1}{2}b)-x}{\sigma}\right) - \Phi\left(\frac{(c-\frac{1}{2}b)-x}{\sigma}\right) \right]
\end{aligned}
$$

where $z = x + \delta$. Φ and φ denote the Gaussian distribution and the corresponding density function, respectively. $F(x)$ has its global minimum at $x = c$ and therefore

$$
\begin{aligned}
\min_{x \in M} F(x) &= F(c) = \tau^2 - (2\tau h b - (hb)^2) \\
&\quad \cdot \left[2 \cdot \Phi\left(\frac{(c+\frac{1}{2}b)-c}{\sigma}\right) - 1 \right]. \tag{10}
\end{aligned}
$$

Figure 1 exemplifies the relationship of $f_{c,b,h}$ and $E_{(\tau - f_{c,b,h})^2}$ for the case of $f_{0,1,1}$ and $\tau = 1$.

For disturbances with $\sigma \geq 0.2$ the loss function takes values greater than zero for all values of x. As expected, the loss becomes minimal for $x = 0$. Thus, in this situation $x = 0$ is the optimal choice, independently of the magnitude of the disturbances.

Now consider the function

$$r_1(x) = f_{-1,0.5,1}(x) + f_{1,1,1}(x) \tag{11}$$

which has two peaks centered at $x = 1$ and $x = -1$. Since the peak at $x = 1$ is wider than the one at $x = -1$ the setting $x = 1$ should be a safe choice. From figure 2 which shows functions $r_1(x)$ and $E_{(1-r_1)^2}$ we conclude that this is true for small values of σ. But for increasing σ the minimum of the loss function moves to smaller values of x.

From this observation we can easily construct examples where the minimal loss does not fall within a peak of the merit function at all. This situation is shown in figure 3 for the function

$$r_2(x) = f_{-1,1,1}(x) + f_{1,1,1}(x) \tag{12}$$

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Tsutsui, Ghosh and Fujimoto [TGF96] consider this case as not desirable. They suggest that the optimal points of equation 7 should always correspond to optimal points of the original merit function
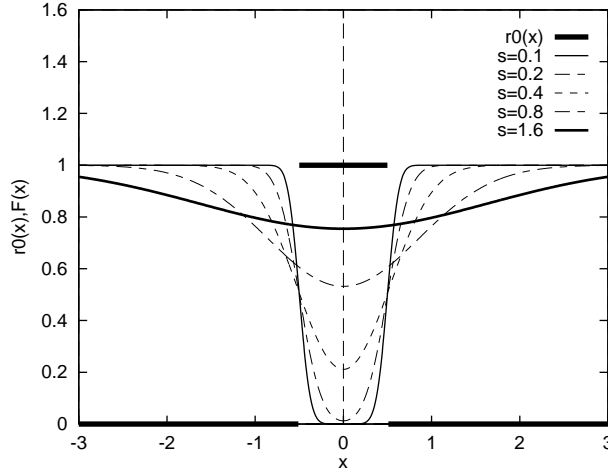
Figure 1: Function $f_{0,1,1}(x) = r_0(x)$ and the corresponding expected quadratic loss $F(x) = E_{(1-f_{0,1,1})^2}(x)$ for disturbances $s = \sigma \in \{0.1, 0.2, 0.4, 0.8, 1.6\}$ and $\tau = 1$.
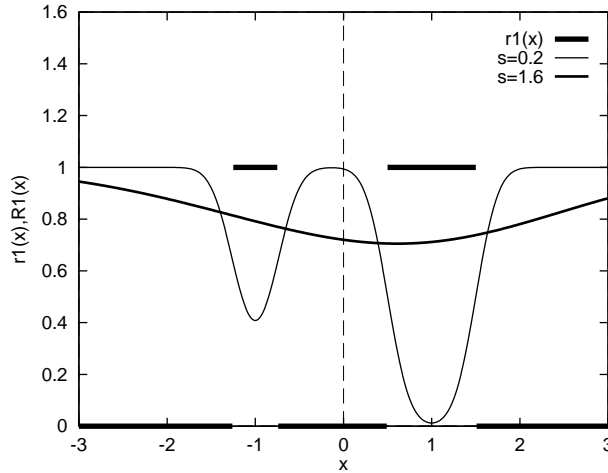

Figure 2: Function $r_1(x)$ and the corresponding quadratic loss function $R_1(x) = E_{(1-r_1)^2}(x)$ for disturbances $s = \sigma = 0.2$ and $s = \sigma = 1.6$, $\tau = 1$

f. We claim that this requirement is not useful in every situation. E.g., in the extreme case of function $r_2(x)$ and $\sigma = 1$, provided that the model (quadratic loss function, normally distributed disturbances, etc.) reflects the real situation close enough, then the average loss is minimal for $x = 0$, i.e., the gain for $x = 0$ is larger than for $x = 1$ or $x = -1$ even if those products for which $r_2(x) = 0$ are considered as off-cuts.

4   Multilayer Optical Coatings

Multilayer optical coatings (MOCs) consist of a sequence of single thin layers ($1nm - 1\mu m$) of different optical materials which in most cases are evaporated on a carrier substrate like glass. Most often MOCs are used as optical filters. If a beam of non-polarized light hits such a filter at each boundary surface it is partially reflected, transmitted or absorbed depending on the refraction indices of the layer material, the thickness of the layer and the wavelength. For most applications a perfect filter should cut off, i.e. reflect,
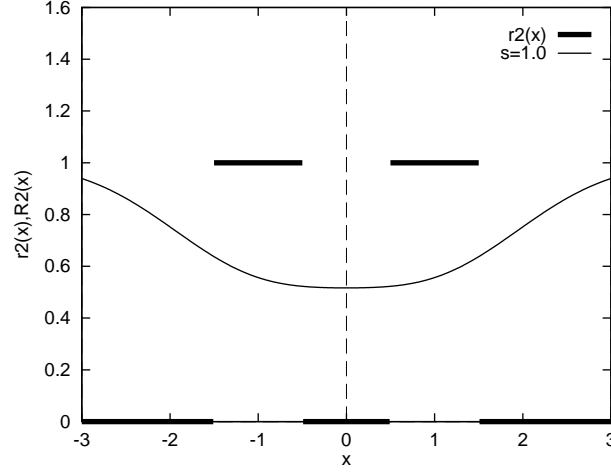
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Figure 3: Function $r_2(x)$ and the corresponding quadratic loss function $R_2(x) = E_{(1-r_2)^2}(x)$ for a disturbance of $s = \sigma = 1.0$, $\tau = 1$.

100% of the unwanted frequencies while passing the wanted frequencies without any reduction. But due to physical restrictions in practice only approximations of this ideal filter can be realized. The situation is depicted in figure 4. Commonly, up to five (up to three in our application) different optical materials
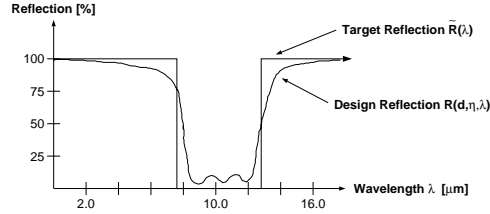

Figure 4: Profiles of an ideal coating and a real construction.

are used. Thus, each layer has a refraction index out of five possible values. Since the thickness of each layer is a real value and the number of layers may vary, the task can be described as a mixed-integer optimization problem with variable dimension.

The mathematical model for MOCs, the so-called *matrix method*, is based on the Maxwell equations, resulting in a formula for the reflectance R for a given wavelength λ that depends on a vector $\vec{d}$ of the thickness of the layers and the refractive indices $\vec{\eta}$ of the materials of the corresponding layers:

$$R(\vec{d}, \vec{\eta}, \lambda) \quad = \quad \frac{4\eta_a \eta_s}{|\eta_a B(\vec{d}, \vec{\eta}, \lambda) + C(\vec{d}, \vec{\eta}, \lambda)|^2} \tag{13}$$

where η_a and η_s describe the refractive index of the adjacent medium (e.g. air) and the substrate. B and C are non-linear terms of $\vec{d}, \vec{\eta}$ and λ according to the matrix method.

The quality of a design with respect to reflectance can be formulated as the average reflectance measured over the interesting interval of wavelengths

$$f(\vec{d}, \vec{\eta}) \quad = \quad 100 \cdot \sqrt{\frac{1}{m} \sum_{i=1}^{m} R(\vec{d}, \vec{\eta}, \lambda_i)^2} \tag{14}$$

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For practical purposes it is sufficient to average over $m = 81$ equidistant wavelengths. See [FT92] for details.

Bäck and Schütz [BS95] already reported above average results for MOC design problems using an extended evolution strategy (ES). Sprave and Schütz even outperformed these results by applying a massively parallel hybrid algorithm of GA and ES [SS96].

In this paper we focus on an extended MOC design problem where in addition to the reflectance the spectral composition of the reflected light is important, too. As a simple example consider the design of sun glasses where a specific color perception of the reflection is desired. Since the perception of color depends largely on individual sensitivities a suitable measure cannot be based solely on physical features like the spectral composition. Definitions of color perception are therefore based on extensive empirical investigations. The so called chromaticity diagram sketched in figure 5 is commonly used to express the relations of physical and empirical measures. X and Y are aggregations of some basic measures. The colors of the spectrum are located on a curve from 380 nm to 780 nm. All other positions denote secondary colors. E is the point of non-colors, i.e., black, white and any shade of gray. Since a complete description of the measures X and Y are beyond the scope of this article we have to refer to the literature, e.g., [NE93].

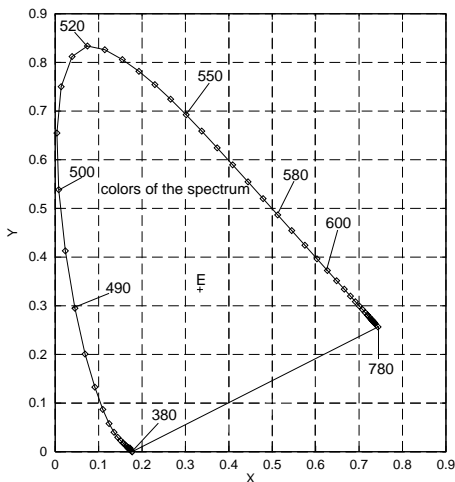Figure 5: Chromaticity diagram. The location of some spectral colors are labeld by their corresponding wavelength.

In our application a color located at (0.281,0.351) is desired. The merit function is based on the Euclidean distance in the chromaticity diagram [Gre96]:

$$G(\vec{d}, \vec{\eta}) = l \cdot \left[(x(\vec{d}, \vec{\eta}) - 0.281)^2 + (y(\vec{d}, \vec{\eta}) - 0.351)^2 \right]^{\frac{1}{2}} \tag{15}$$

where $(x(\vec{d}, \vec{\eta}), y(\vec{d}, \vec{\eta}))$ denote the coordinates in the chromaticity diagram of a k-layer filter with layer thicknesses $\vec{d} = (d_1, \ldots, d_k)$ and refractive indices $\vec{\eta} = (\eta_1, \cdots, \eta_k)$. For reasons of comparability we use $l = 100$.

During the production process the layer thickness can not be controlled with arbitrary precision. Additionally, the refraction indices vary slightly due to pollution of the optical materials. Thus, we might observe significant variances in the quality of single filters. A MOC-design which has to meet both objectives described in formulas (14) and (15) naturally leads to a multicriteria optimization problem. As a first approach, which already lead to above average designs we define the overall loss function F as:

$$F(\vec{d}, \vec{\eta}) = f^2(\vec{d} + \vec{\delta}_d, \vec{\eta} + \vec{\delta}_\eta) + G(\vec{d} + \vec{\delta}_d, \vec{\eta} + \vec{\delta}_\eta). \tag{16}$$

where $\vec{\delta}_d = (\delta_{d_1} \ldots \delta_{d_k})$ and $\vec{\delta}_\eta = (\delta_{\eta_1} \ldots \delta_{\eta_k})$ are vectors of normally distributed random numbers with zero mean denoting the disturbances of thickness and refraction indices, respectively. For both kinds of disturbances the standard deviations are set to 1% of the absolute values, which is reasonable for modern manufacturing processes [Gre96]. The expected loss is then approximated as

$$\frac{1}{t} \sum_{i=1}^{t} \left(f^2(\vec{d} + \vec{\delta}_d, \vec{\eta} + \vec{\delta}_\eta) + G(\vec{d} + \vec{\delta}_d, \vec{\eta} + \vec{\delta}_\eta) \right) \tag{17}$$

The columns of table 1 show the outcomes of the four most significant experiments of a series of approximately 50. Due to space limitations we restrict the presentation to this subset. The first column shows a reference design which was taken from [KHS90]. The reference design was generated in two steps. First a promising start design was derived by analytical means using a simplified model. The fine-tuning of the layer thicknesses are achieved by using a local hill-climbing algorithm. The reflectance for this design is shown in figures 6 where the solid line shows the reflected fraction for the interesting interval of wavelengths of the ideal filter manufactured without disturbances. The other curves are outcomes of experiments where disturbances are added according to $R(\vec{d} + \vec{\delta}_d, \vec{\eta} + \vec{\delta}_\eta, \lambda)$. The chromaticity distribution
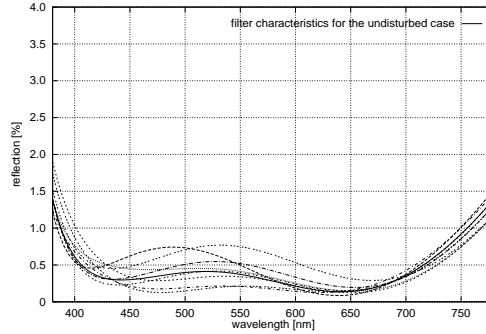

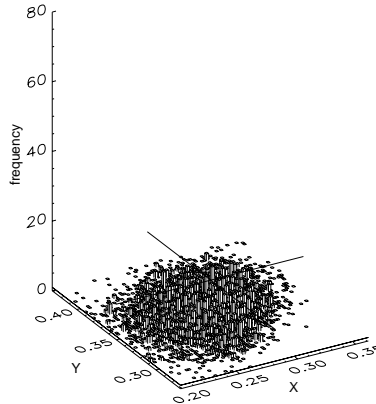Figure 6: Reflectance of the reference design 1

Figure 7: Chromaticity distribution of reference design 1

of this filter design is shown in figure 7 for 1000 simulations according to $(x(\vec{d} + \vec{\delta}_d, \vec{\eta} + \vec{\delta}_\eta), y(\vec{d} + \vec{\delta}_d, \vec{\eta} + \vec{\delta}_\eta))$.

The first row of table 1 denotes the Algorithm used. Basically, we applied two modified evolution strategies (ES). Algorithm 1 is a (25 + 50)-ES extended for mixed-integer optimization after [BS95]. Because of the stochastic nature of the objective function the plus-selection scheme requires a reevaluation

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Design	1	2	3	4	5
Alg.	-	1	1	2	2
Eval.	-	$8 \cdot 10^5$	$8 \cdot 10^5$	E	E
t	-	40	40	10	10
k_{max}	-	5	8	12	10
rms_i	0.54	0.98	0.81	0.64	0.84
rms_r	0.57	0.99	0.84	0.66	0.85
col_i	0.0005	0.0137	0.0012	0.0043	0.0020
col_r	0.0381	0.0191	0.0166	0.0184	0.0166
η_{air}	1.0	1.0	1.0	1.0	1.0
d_1	107.3	95.50	102.42	95.70	120.04
η_1	1.38	1.38	1.38	1.38	1.38
d_2	24.6	151.8	10.90	15.04	14.57
η_2	2.12	1.63	2.12	2.12	2.12
d_3	45.9	-	64.93	8.24	15.44
η_3	1.63	-	1.63	1.38	1.63
d_4	22.7	-	6.87	5.36	42.04
η_4	2.12	-	2.12	1.63	1.38
d_5	83.5	-	63.11	109.47	14.58
η_5	1.63	-	1.63	2.12	2.12
d_6	-	-	-	30.38	-
η_6	-	-	-	1.38	-
d_7	-	-	-	14.54	-
η_7	-	-	-	2.12	-
η_{sub}	1.52	1.52	1.52	1.52	1.52

Table 1: Comparison of the reference design (1) and designs generated by different ES-variants (2-5) . ($E = 2.25 \cdot 10^8$)

of the parent population during each iteration. Mutation is applied with n self-adapting step sizes and recombination is performed discrete on object variables and intermediate for step sizes. For details see [BS95]. Algorithm 2 is a parallel diffusion model after [SS96], where the individuals are located on a regular grid. We used 15 subpopulations with a size of 20x25, a neighborhood size of 7x7 and an isolation time of 30 generations.

In the second row the total number of evaluations of function (16) is given. The third row contains the sample size t. k_{max} is the maximum number of layers allowed for that simulation run. The last 16 rows show the sequence of layers (thickness d and refraction index η) for the best filter found in each experiment. For this filter $rms_i = f(\vec{d}, \vec{\eta})$ and $col_i = G(\vec{d}, \vec{\eta})$ (where l is set to 1) denote the reflectance and the chromaticity for the undisturbed case. rms_r and col_r denote the average reflectance and chromaticity of a sample of 500 simulations if disturbances are added.

The reflectance and the chromaticity distribution for the best MOC design 5, (table 1) found by the ES are shown in figure 8 and 9, which demonstrates that filters manufactured acording to design 5 will in the average case show chromaticity characteristics much closer to the optimum (0.281,0.351) compared to the reference design 1 (figure 7).

To summarize, with respect to chromaticity the MOC designs found by the evolution strategy are substantially more robust to parameter variations than the reference design 1, (table 1) and therefore perform much better in the average case, although for the undisturbed case the reference design is significantly better. This observation was expected, since sensitivity analysis shows that many local optima are not robust under parameter variations. In most cases this advantage has to be paid by a reduction in the average reflectance. Only in the case of experiment 4 the ES was able to locate a design which could compete with the reference design 1 in this respect. Additional experiments suggest that this is due to a biased design of function 16 where the influence of $G(\vec{d} + \vec{\delta}_d, \vec{\eta} + \vec{\delta}_\eta)$ seems to dominate $f^2(\vec{d} + \vec{\delta}_d, \vec{\eta} + \vec{\delta}_\eta)$. Furthermore it seems promising to integrate other characteristics of the resulting distribution of function (16), e.g., the skewness.
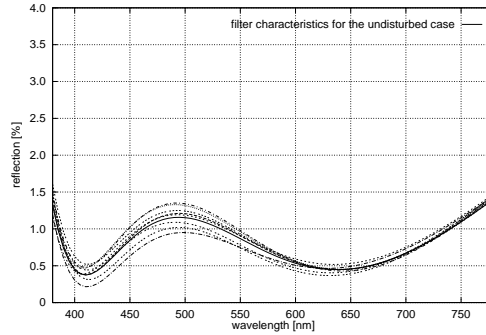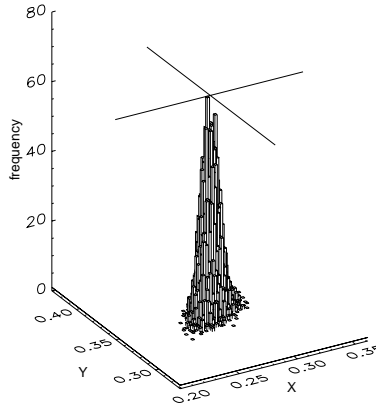
Figure 8: Reflectance of filter design 5, table 1

Figure 9: Chromaticity distribution of the design 5, table 1.

5   Summary and Outlook

It was shown that evolutionary algorithms can compete with or even outperform traditional methods of robust MOC-design. It has to be emphasized that no domain specific knowledge was incorporated into the search strategy and that all start designs were chosen with equal probability from the feasible region, i.e., there is no need to develop high quality start designs manually. In contrast, traditional MOC-design is a laborious task. The robust design approach outlined in this paper should easily be adopted to other application domains.

Future work will focus on improving the objective function as already mentioned in the previous section. Furthermore, the potential of EAs for multicriteria optimization will be evaluated for this application domain, i.e., the exploration of the Pareto set. Since the experiments are very time consuming due to the fact that a sample of t experiments have to be performed for each single individual we are much interested to reduce this overhead. A promising approach is to let t vary through the course of evolution either by an external schedule or by some self-adaptation mechanism. Finally, there seems to be some potential to improve the algorithm itself, especially the interplay between modifications of the integer and real values as well as the handling of variable dimensions.

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