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► To cite this version:

Pauline Bennet, Emmanuel Centeno, Jérémy Rapin, Olivier Teytaud, Antoine Moreau. The photonics and ARCoating testbeds in Nevergrad. 2020. hal-02613161

HAL Id: hal-02613161 https://hal.science/hal-02613161

Preprint submitted on 19 May 2020

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The photonics and ARCoating testbeds in Nevergrad

Pauline Bennet¹, Emmanuel Centeno¹, Jérémy Rapin², Olivier Teytaud², Antoine Moreau^{1*}

Abstract

We detail the testbeds which can be found in the photonics and ARCoating test cases in Nevergrad [1]. These testbeds, beyond their practical importance, are especially modular - and like all problems in photonics, possess a very high number of local minima. They constitute simple but crucial design challenges: designing a multilayered structure which can reflect light at a given frequency, reflect light on a whole range of frequencies or cancel the reflectivity ; designing a complex structure able to diffract the blue part of the spectrum and to cancel the reflectivity at any other wavelength.

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1. Photonics

The test cases regarding photonics which are included in Nevergrad are inspired by the structures which can be found on the back or on the wings of insects. These structures have been obtained after millions of years of natural evolution and seem to be close to an optical optimum. It has been shown that such structures could be retrieved through optimization with evolutionary algorithms[2].

1.1 Bragg

Bragg mirrors are the first known example of a photonic crystal. They are widely used in technology to reflect light and are quite ubiquitous in nature on the back of insects. Such dielectric mirrors are multilayered structures where each layer is actually transparent, characterized by a thickness (here in nm) and a refractive index (or a permittivity). The interference between all the waves reflected and transmitted by each interface between two different media produces a strong reflection.

Such structures typically emerge when the reflection coefficient of the multilayered structure is maximized and when bounds for the refractive index are imposed. Here the cost function is thus 1 - R where R is the reflectance of the structure at a fixed wavelength (here $\lambda = 600$ nm).

The advantage of this testbed is that, contrarily to others, the theoretical structure producing the minimum is known, and thus the lowest reachable value for the cost function can be determined very precisely (see Table 1).

Instantiation. Once Nevergrad is installed, the cost function can be very easily instantiated using the following lines in Python:

from nevergrad.functions.photonics import Photonics
func = Photonics("bragg", 4)
func([3, 2, 86, 106])
>>>0.8027533239625988

The other functions can all be instantiated in the same way.

Speed. The cost function, based on the technique of the admittances and with a reflectance computed for only one wavelength, is extremely fast to run.

Space dimension. A structure is defined by a vector with an <u>even</u> number of components. The first half corresponds to the permittivity of each layer, and the second to the heights in nanometers. The number of dimensions of the parameter space can thus be chosen arbitrarily as long as it is even and the complexity of the problem increases of course with the number of dimensions.

Bounds. The bounds of the permittivity (and thus the first half of the vector) should be 2 for the lower and 3 for the higher. The bounds for the thicknesses (and thus the second half of the vector) should be 30 for the lower and 180 for the higher. With these constraints, it has been shown that Bragg mirrors are the optimal way to reflect light at a given wavelength [2].

Best solution. This problem is the only one for which the solution is unique and known with almost perfect certainty. The optimal solution should be alternating layers with a permittivity of 3 and a thickness of 86.603 nm and layers with a permittivity of 2 and a thickness of 106.07 nm. The vector provided in that case to the cost function should look like

 $[3, 2, \ldots, 2, 86.603, 106.07, 86.603, 106.07, \ldots, 106.07].$

The value of the minimum cost function depends on the size of the parameter space, but it will gradually tend towards zero when the size is increased, as shown Tab. 1. These minimum have been computed using the theoretical formulas for the Bragg mirrors, which are more precise than the values given above for the thicknesses.

Number of layers	Theoretical minimum	
5	0.262660386845925	
10	0.0392584897236201	
15	0.00526000338118893	
20	0.000694261986326494	
25	0.0000914530150757376	

Table 1. Lowest cost function theoretically reachable fordifferent numbers of layers, obtained for Bragg mirrors.The leaderboard of Nevegrad can be found here.

1.2 Chirped

Chirped dielectric mirrors are like Bragg mirrors, except that they reflect a whole part of the optical spectrum and not some values centered around a given wavelength. Such structures are not periodic but the thicknesses of the different layers change gradually. They can increase or decrease. This problem is particularly modular, as certain parts of the structures are devoted to the reflection of certain parts of the optical spectrum.

Speed. Since a whole spectrum has to be computed for each cost function, much more computational time is needed here (roughly 50 times more than Bragg). Compared to the precedent test case, the refractive index of each layer is fixed, only the thicknesses are left to vary – so that all the parameters are layer thicknesses and have the same bounds.

Space dimension. The dimension of the space can be chosen arbitrarily, but it must be **even** in all cases.

Bounds. The same bounds as for Bragg can be chosen. A minimum of 30 (nm) and a maximum of 180 (nm).

Best solution. The best solution depends on the number of layers. For relatively low numbers (below 20) the structure (and thus the parameters) may not seem regular. When the dimension increases, the change from one period to another is more gradual (see Fig. 1). Contrarily to the previous case, the best solution is not known with certainty, but all the optimization point towards the kind of structure shown Fig. 1. This document may thus be updated in the future with even better results.

Number of layers	Minimum cost function	Obtained by
10	0.59057	P. Bennet
20	0.3860	P. Bennet
30	0.26599	P. Bennet
40	0.17102	P. Bennet
50	0.11656	J. Rapin

Table 2. Best results obtained so far on the chirped problem. Ask antoine.moreau@uca.fr if you have obtained a lower cost function and want to be included in this hall of fame, or if you want to know which structures are the best to date. The leaderboard of Nevegrad can be found here.

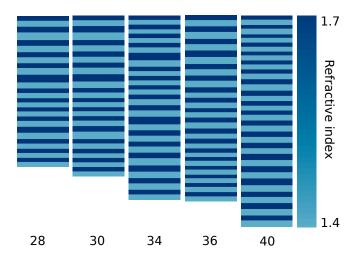


Figure 1. Typical results for different number of layers.

1.3 Morpho

The Morpho testbed is inspired directly by the structures which can be found on the wings of the Morpho butterfly. The purpose of these complex structures is to maximize the reflectivity for one wavelength in the blue part of the spectrum, but not in the 0-th order (the specular reflection), while keeping it extremely low for any other wavelength and diffraction order. The results of the optimization should not be strictly speaking the naturally occurring structure, which is not optimal from an optical point of view - and is thus the result of other constraints of a different nature.

The structure is naturally periodical in the horizontal direction with a periodicity of 600 nm. It is constituted of a given number of layers. Each layer is a block characterized by a width (from 30 to 600 nm, smallest values than 30 can actually cause numerical stability issues), a thickness (from 30 to 300 nm), a position in the period (from 0 to 600 nm) and is above a layer of air (from 0 to 300 nm).

Speed. The optical response of the structure is computed using RCWA, a way to compute the solution of

Maxwell's equations in such a case. This is considerably more resource consuming than the technique of impedances used in all the other test cases for multilayered structures.

Space dimension. Input vector describes the structure and its dimension must be a multiple of 4.

Bounds. This first fourth gives the thickness of each block. It should be chosen between 30 and 300 (nm). The second fourth of the vector is comprised between 0 and 600 and corresponds to the position of the beginning of the block in the horizontal period. The third fourth is the width of each block and should thus be chosen between 30 and 600. The last fourth is the thickness of the air layer immediately below the block and should be chosen between 0 and 300 nm.

Best solutions. Some very good solutions are represented Fig. 2, see [2] for more explanations. We keep a track of the lowest cost function values reached in Table 3.

Number of layers	Cost function	Obtained by
5	0.732584428839321	V. Berthier
6	0.661822146354456	V. Berthier
9	0.561513047787714	V. Berthier
12	0.520506426722375	V. Berthier
15	0.50613155963	J. Rapin

Table 3. Best results obtained so far on the morpho problem. Ask antoine.moreau@uca.fr if you have obtained a lower cost function and want to be included in this hall of fame, or if you want to know which structures are the best to date. The leaderboard of Nevegrad can be found here.

2. ARCoating

The ARCoating problem[3] corresponds to the maximization of the transmission between air and a silicon layer considered as a high refractive index medium (with a value of 3). Two parameters set up the problem: the overall thickness of the multilayer and the number of layers which constitute the Anti-Reflective (AR) coating. All the layers have the same thickness (the overall thickness divided by the number of "pixels"). The permittivities of the different layers are the parameters to be optimized.

For very large pixel numbers and a thick enough structure, a classical gaussian refractive index profile can be retrieved as the best solution (see Fig. 3). This kind of solution is classically considered in the literature as a very good solution.

Speed. The reflectivity is computed for 100 different wavelength using an impedance technique. The computation time required by ARCoating should be around 100 times larger than Bragg.

Space dimension. The space dimension is given by the number of pixels/layers.

Bounds. The permittivity of each layer must be comprised between 1 and 9.

Best solution. The best solution really depends on the number of layers. For 10 layers, the solution provided by the algorithms is a slowly growing index profile, different from the Gaussian profile usually expected to give the best results for a continuous profile. For a larger number of layers, a zone with a high refractive index systematically appears, as shown Fig. 4. Beyond 20 layers, the problems seems much more difficult to solve.

Numb	er of layers	Cost function	Obtained by
	10	$1.755505734 \times 10^{-4}$	P. Bennet
	20	$2.993172772 \times 10^{-6}$	P. Bennet
	30	$2.062801631 \times 10^{-5}$	P. Bennet
	40	$2.993172772 \times 10^{-6}$	P. Bennet
T.I.I. 4	D + 1+ -	-1.4. :	ADC

Table 4. Best results obtained so far on the ARCoating problem, for an overall thickness of 700 nm. Ask antoine.moreau@uca.fr if you have obtained a lower cost function and want to be included in this hall of fame, or if you want to know which structures are the best to date. The leaderboard of Nevegrad can be found here.

Funding

Antoine Moreau is an Academy CAP 20-25 chair holder. He (She) acknowledges the support received from the Agence Nationale de la Recherche of the French government through the program "Investissements d'Avenir" (16-IDEX-0001 CAP 20-25).

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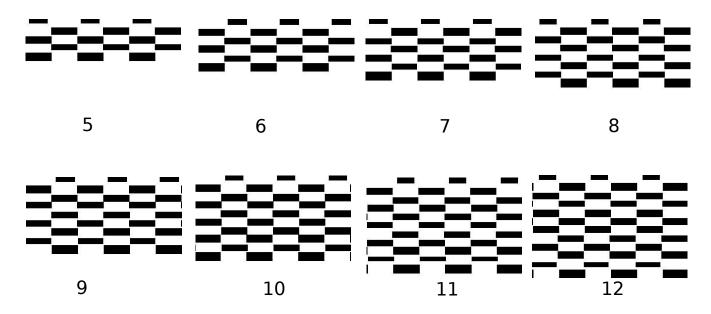


Figure 2. The best structures so far obtained on the Morpho problem for different numbers of layers. Three horizontal periods are actually represented here. The thicknesses of the blocks should be around 72 nm, the thickness of the air layers around 40 nm, the width of each block around 300 nm and the shift in the period should be either 0 or 300, or any other numbers as long as the difference is around 300 nm.

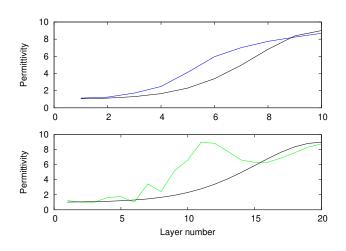


Figure 3. Refractive index profile obtained for an overall thickness of 700 nm and 10 (up) resp. 20 (below) layers. The curve in black represents a Gaussian profile, which is often presented as optimal for a continuous change of the refractive index in the literature. The index profiles shown here are clearly more efficient than a Gaussian profile (we have taken the standard deviation producing the lowest cost function and it proves difficult to beat).