Inverse design of nanophotonic structures using complementary convex optimization

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Abstract: A computationally-fast inverse design method for nanophotonic structures is presented. The method is based on two complementary convex optimization problems which modify the dielectric structure and resonant field respectively. The design of one- and two-dimensional nanophotonic resonators is demonstrated and is shown to require minimal computational resources.

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References and links
11. CHOLMOD software package, accessed via Matlab.
12. Intel Core 2 Quad 2.5GHz, 8Gb RAM.
1. Introduction

Numerous numerical methods have been devised to solve Maxwell’s equations in both time[1] and frequency[2, 3] domains. We refer to these schemes as direct solvers, since they compute the electric and magnetic fields based on current sources, charge distributions and surrounding dielectric and/or metallic structures. While extremely useful in simulating optical components, using direct methods to design optical components, especially in two or three dimensions, typically requires an extremely time-consuming direct search in a large parameter space[4, 5, 6, 7, 8].

On the other hand, an inverse solver would be much more adept in such design and optimization problems[9, 10]. In this work, we define the inverse problem as that where the electromagnetic field is known, but the surrounding structure is not known. The goal in the inverse problem is, then, to find a dielectric structure that will produce that specific electromagnetic field profile.

We show that one can design nanophotonic resonators by specifying the electromagnetic field and its desirable characteristics (such as cavity quality (Q) factor and/or mode volume) and then using an inverse solver to find the corresponding dielectric structure. We show that the inverse method used is not only computationally-fast, but is also able to optimize for multiple device characteristics and produce multiple resonances, both of which are very difficult using direct methods.

2. Numerical setup

We start from the time-harmonic eigenvalue equation

\[
\nabla \times \epsilon^{-1} \nabla \times H = \left(\frac{\omega}{c}\right)^2 H
\]

where \(H, \epsilon, \omega\) and \(c\) are the magnetic field, relative permittivity, resonance frequency and speed of light respectively. To solve the problem numerically, \(H\) and \(\epsilon\) are discretized in space using the standard Yee cell used in finite difference methods[1]. Also, the curl operators, since they are linear, are represented by the matrix \(A\). Equation (1) can now be written as

\[
AYAx = \xi x
\]

where

\[
A = \text{discretized curl operator}, \quad Y = \text{diag}(\epsilon^{-1})\text{ is the diagonal matrix representing the dielectric structure}, \quad x = \text{a vector representing } H, \text{ and } \xi = \left(\frac{\omega}{c}\right)^2.
\]

In this form, given \(Y\), we can solve the direct problem by computing \(x\) using an eigenvalue solver[13]. However, we note that Eq. (2) is also linear in \(Y\), which allows us, if \(x\) is held constant, to solve the inverse problem by expressing Eq. (1) as

\[
By = d
\]
where
\[ B = A \cdot \text{diag}(Ax), \]
\[ d = \xi x, \text{ and} \]
\[ y = \begin{bmatrix} \epsilon_1^{-1} \\ \epsilon_2^{-1} \\ \vdots \end{bmatrix} \] the variable for which we solve.

Here, \( \text{diag}(Ax) \) is the matrix with the values of \( Ax \) along the main diagonal and zeros elsewhere.

3. Least-squares method in 1D

3.1. Least-Squares

Fig. 1. Inverse design of a one-dimensional structure using the unmodified least-squares method. The target field is a sinusoid within a Gaussian envelope. The computed dielectric structure (green area) supports a field (red circles) that exactly matches the target field (blue line). The entire design process is also extremely fast and takes less than 1 second to complete on a generic desktop computer [12]. The periodic singularities in the dielectric structure are non-physical and will be addressed later in the article.

The result of applying this method to a simple one-dimensional problem is shown in Fig. 1. A generic least-squares solver [11] was used to find the dielectric structure, \( y \) (green region), that exactly produces the target field, \( x \) (blue line), using Eq. (2). Using a generic desktop computer, the solution was obtained in less than a second. Then a finite-difference time-domain (FDTD) solver was used to obtain the actual field (red circles) produced by the structure and to verify the accuracy of \( y \).

As expected, Fig. 1 shows that the target field is reproduced exactly by the dielectric structure. However, the resulting structure is full of undesirable singularities. The rest of the section focuses on producing a well-behaved dielectric structure that still reproduces the target field accurately.

3.2. Regularized least-squares

The simplest way to produce a well-behaved dielectric structure is to add a regularization term to our least-squares problem, which is equivalent to solving the following optimization problem

\[
\text{minimize} \quad \|By - d\|^2 + \eta \|y - y_0\|^2.
\]
Here \( y_0 \) represents some initial guess for the dielectric structure, which we want the values of \( y \) to stay close to, and \( \eta > 0 \) is a parameter used to trade off fit, i.e. \( \| B y - d \|_2 \), and deviation from \( y_0 \), i.e. \( \| y - y_0 \|_2 \).

We chose to constrain \( \epsilon \) around a constant value of \( \epsilon_0 = 10 \) and solved the least-squares system for \( \eta = 10^{-8} \), \( 10^{-6} \), and \( 10^{-4} \). The results, each still obtained in under a second, are shown in Fig. 2 and illustrate the trade-off between constraining \( \epsilon \) and accurately reproducing \( H \).

![Fig. 2. Inverse design of one-dimensional structures using the regularized least-squares method. The same target field is used as in Fig. 1, and the computation time remains below 1 second. As the regularization parameter, \( \eta \), is increased, \( \epsilon \) is increasingly constrained to a chosen constant value of 10. At the same time, the mismatch between target and actual fields increases markedly. This illustrates the apparent trade-off between producing reasonable structures and accurately reproducing a fixed target field.](image)

4. Complementary optimization in 1D

4.1. Motivation for a Complementary Optimization Strategy

The fundamental problem in the previous examples is actually not in the methods themselves, but in the improper selection of a target field. In fact, it is very difficult to select a suitable
target resonant field because not every resonant mode even has a corresponding dielectric structure that is able to reproduce it. Furthermore, it is nearly impossible to select a multi-dimensional field which corresponds to a well-behaved, isotropic and discretely-valued $\varepsilon$, as would be needed for practical structures.

For this reason, a successful method must be allowed to either modify the target field, or specify it completely, in which case the user would only determine certain characteristics (e.g. mode-volume, Q-factor) that the target field should have. The former strategy is developed in both one and two dimensions, while the latter strategy is implemented in Section 6 in order to design two-dimensional resonators with discrete values of $\varepsilon$.

4.2. Complementary optimization

We start with the same target field as in the previous examples but we now formulate a method that allows for it to be modified during the design process. The formulation chosen is a complementary optimization routine, where we continually alternate between modifying $\varepsilon$ to better fit the field, and then modifying the field to better fit $\varepsilon$. Here, we use the term “fit” to mean that either $\varepsilon$ or $H$ is solved so that the residual error from Eq. (1) is minimized. Additionally, both iterations are regularized in order to stably approach a solution. This algorithm can be summarized as follows,

choose $x_0$ and $y_0$
for $i = 1, 2, \ldots$
\begin{align*}
\text{minimize } & \|B_{i-1}y_i - d_{i-1}\|^2 + \eta_1 \|y_i - y_{i-1}\|^2 \quad (5) \\
\text{minimize } & \|AY_iA_{x_i} - \xi x_{i-1}\|^2 + \eta_2 \|x_i - x_{i-1}\|^2 \quad (6)
\end{align*}

where $Y_i = \text{diag}(y_i)$, $B_i = A \cdot \text{diag}(A_{x_i})$ and $d_i = \xi x_i$. $\|AY_iA_{x_i} - \xi x_{i-1}\|^2$ is used instead of $\|AY_iA_{x_i} - \xi x_i\|^2$ to avoid the trivial $x_i = 0$ solution and does not affect the overall accuracy since $x$ changes very slowly.

Fig. 3. Inverse design of a one-dimensional structure using the complementary optimization method. The target field in Figs. 1 and 2 is used as the initial target field. The rates of change for both $\varepsilon$ and $H$ are controlled by regularization parameters $\eta_1 = 10^{-4}$ and $\eta_2 = 10^{-3}$ respectively. The 400 iterations used to achieve this result took 60 seconds to compute. This method results in a well-behaved $\varepsilon$ that actually produces a field very similar to the original target field. Interestingly, the formation of a “steady-state” periodic structure toward the sides of the structure has emerged.

Figure 3 shows that the complementary optimization algorithm, after 400 iterations and with the correct choice of regularization parameters $\eta_1$ and $\eta_2$, results in a well-behaved structure.
that is able to closely reproduce the modified target field. Numerically, the least-squares problem must now be solved numerous times, which increases the computational time needed to around 60 seconds.

4.3. Complementary optimization with bounded $\varepsilon$

In order to achieve a more practical, discretely-valued dielectric structure, we can impose strict upper- and lower-bounds on $\varepsilon$. To this end, we modify our algorithm as such,

\begin{align*}
\text{choose } x_0 \text{ and } y_0 \\
\text{for } i = 1, 2, \ldots \\
\text{minimize } & B_i y_i - d_{i-1} \quad \text{subject to } \\
\epsilon_{\text{max}}^{-1} \leq y_i \leq \epsilon_{\text{min}}^{-1} \\
\text{minimize } & A Y_i A x_i - \xi x_{i-1} \quad \text{subject to } \\
\eta_2 \| x_i - x_{i-1} \|^2.
\end{align*}

In this algorithm, Eq. (7) is a convex optimization problem[14]. This allows us to impose hard constraints on $\varepsilon$, which in turn allows us to remove the regularization term present in Eq. (5). The CVX package[15], a Matlab-based modeling system for convex optimization, is used to solve Eq. (7), with each iteration of the algorithm now requiring roughly 1 second of computation time.

![Fig. 4. Inverse design of a one-dimensional structure using the complementary optimization method with bounded $\varepsilon$. The parameters are identical to those used to produce Fig. 3 with the exception that only one regularization term is now needed ($\eta_2 = 10^{-3}$). The algorithm was run for 100 iterations, which took 100 seconds. The structure turns out to be almost completely binary-valued and looks like a periodic structure with tapered duty cycle. It produces an actual field which very closely matches the final target field.](image)

A nearly binary-valued dielectric structure is obtained in Fig. 4, which accurately produces the final target field. This is very useful for the design of practical structures, since they usually consist of two or three different materials at most. Interestingly, although the directly discreteness of $\varepsilon$ was not enforced (since that would make the problem non-convex), a discrete, binary-valued structure has still arisen.
Fig. 5. Inverse design of an “S” resonator using the complementary optimization method without bounds on $\varepsilon$. The design was initialized by specifying an initial dielectric structure ($\varepsilon = 1$ everywhere) and a resonant field in the shape of an “S”. The final dielectric structure was produced after 50 iterations which took 90 seconds to complete in total. The grid size was $80 \times 120$. The final dielectric structure is quite unintuitive, and yet reproduces the target field surprisingly well. This example demonstrates the versatility of the complementary optimization method in producing designs, from very simple specifications, which otherwise could be attained only with considerable difficulty.

5. Complementary optimization in 2D

5.1. “S” Resonator

We now demonstrate that the complementary optimization method is versatile and can be scaled to multiple dimensions. To ensure that $\varepsilon$ is well-behaved we use a point-spread function which does not allow $\varepsilon$ to change at a certain point in space without affecting the values surrounding it.

In order to show that our method can produce complex designs, we choose an S-shaped target field which is non-trivial to reproduce. The optimization results, using the complementary optimization method from Section 4.2, are shown in Fig. 5. The resulting dielectric structure is continuous, unbounded and contains some singularities (white dots), but the final target and actual fields match up well. Also, the computational cost remains quite reasonable; the 50 iterations needed required only 5 minutes of computation time. The resulting structure is completely unintuitive, and illustrates the kind of new capabilities offered by the inverse design strategy. Specifically, that a complex, intricate structure can be designed just by specifying the shape and frequency of a rather simple electromagnetic mode.

5.2. Multi-mode inverse design

The complementary optimization method can also be extended to produce dielectric structures with multiple resonances. To do so, multiple initial target fields are specified. The dielectric structure is first modified to simultaneously fit all target fields using a multi-objective least-squares method. Then each target field is individually modified to fit the structure; and we continue alternating between optimizing $\varepsilon$ and $H^{(j)}$ in this way. A benefit of this scheme is that only the $\varepsilon$ optimization increases in size, so the design process remains computationally...