Objective-First Nanophotonic Design Plan

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Chapter 1

Introduction

1.1 Problem statement

Our goal is to create a software package to enable the design of nanophotonic devices. Presently, almost all nanophotonic devices are designed by guessing what a good design might look like, based on intuition and experience, and then optimizing it by trial-and-error. In contrast, we want to enable the *inverse design* of nanophotonic devices; that is, to design devices by simply describing the desired performance that it must achieve.

To put things mathematically, we want to create software to solve the following problem,

$$\begin{aligned} \text{minimize} \quad & f(x) + g(z) && \text{(1.1a)} \\ \text{subject to} \quad & A(z)x - b(z) = 0 && \text{(1.1b)} \end{aligned}$$

where

- x and z are the variables representing the *field* our device produces and the *structure* of the device respectively,
- $f(x)$ and $g(z)$ are our *design objectives*, which tell us the desirable properties that we would like our device to achieve, and
- $A(z)x - b(z)$ is the *physics residual*, the underlying physical laws which must be met.

In general, we need to consider multiple fields produced by the device. Our problem statement is then

$$\begin{aligned} \text{minimize} \quad & \sum_{i}^{N} f_i(x_i) + g(z) && \text{(1.2a)} \\ \text{subject to} \quad & A_i(z)x_i - b_i(z) = 0, \quad \text{for } i = 1, \ldots, N. && \text{(1.2b)} \end{aligned}$$

1.2 Capabilities of our software

We have implemented various *optimization paradigms* and *structure parameterizations* which a user can arbitrarily combine in order to to solve (1.2).

Specifically, the user can choose to work in either a *local* or *global* optimization paradigm:

- the local paradigm uses the adjoint method to find small changes in the structure which will decrease the design objective;
- the global paradigm uses the objective-first method to arrive at a structure by forcing the design objective to be met from the start.

Also, the user can choose between the various structure parameterizations which include density, boundary, continuous, and combinatoric parameterizations. These parameterizations describe the structure as either

- a material density at every point in space;
- a boundary between objects of different materials;
- a set of continuously variable user-defined parameters; or
- a selective combination of user-defined objects.

Chapter 2

Theory

2.1 Mathematically rigorous statement of the problem

As previously stated, the problem we want to solve is

$$\text{minimize} \quad \sum_{i}^{N} f_i(x_i) + g(z) \tag{2.1a}$$

$$\text{subject to} \quad A_i(z)x_i - b_i(z) = 0, \quad \text{for } i = 1, \ldots, N. \tag{2.1b}$$

To now be more precise,

- $x_i \in \mathbf{C}^m$ are the field variables,
- $z \in \mathbf{R}^n$ is the structure variable,
- $f_i(x_i) \in \mathbf{C}^m \to \mathbf{R}$ are the field design objectives,
- $g(z) \in \mathbf{R}^n \to \mathbf{R}$ is the structure design objective,
- $A_i(z)x_i - b_i(z)$ are the physics residuals, with
- $A_i(z) \in \mathbf{C}^{m \times m}$ and
- $b_i(z) \in \mathbf{C}^m$.

2.1.1 Definition of physics residual

The physics residual corresponds to the electromagnetic wave equation

$$(\nabla \times \mu^{-1} \nabla \times -\omega^2 \epsilon)E = -i\omega J \tag{2.2}$$

which is described as $A_i(z)x_i - b_i(z)$ via

- $\nabla \times \mu^{-1}\nabla \times -\omega^2\epsilon \rightarrow A_i(z)$,
- $\epsilon \rightarrow z$,
- $E \rightarrow x_i$, and
- $-i\omega J \rightarrow b_i(z)$.

2.1.2 Bi-affine property of the physics residual

Critically, (2.2) is not only linear in E, but is also affine in ϵ. This allows us to form the extremely useful relationship,

$$A_i(z)x_i - b_i(z) = B(x_i)z - d(x_i) = 0, \tag{2.3}$$

where $B(x_i) \in \mathbf{C}^{n\times n}$ and $d(x_i) \in \mathbf{C}^n$.

2.1.3 Definition of the field design objective

Although the field design objective $f_i(x_i)$ can take on virtually any form, we choose to define it very specifically as

$$f_i(x_i) = \sum_j I_+(|c_{ij}^\dagger x_i| - \alpha_{ij}) + I_+(\beta_{ij} - |c_{ij}^\dagger x_i|), \tag{2.4}$$

where $c_{ij} \in \mathbf{C}^m$ and I_+ is the indicator function on nonnegative reals,

$$I_+(u) = \begin{cases} 0 & u \geq 0, \\ \infty & u < 0. \end{cases} \tag{2.5}$$

Such a design objective implements the constraints $\alpha_{ij} \leq |c_{ij}^\dagger x_i| \leq \beta_{ij}$ which can be interpreted physically as constraining the power emitted into the optical modes represented by c_{ij}.

2.1.4 Choice of the structure design objective

In contrast to the narrow definition of the field design objective, the structure design objective is relatively unconstrained; taking on various forms to best suit the needs of the structure parameterization in use.

2.2 Properties of the problem

We now examine the general mathematical properties of the stated problem (2.1).

2.2.1 Convexity analysis

First we note that, as presented, (2.1) is non-convex in the variables x_i and z. Not only are the physics residuals $A_i(z)x_i - b_i(z)$ non-convex, but the field design objective, in that it implements the $\alpha_{ij} \leq |c_{ij}^\dagger x_i|$ constraint, is non-convex as well.

That our problem is non-convex means that it is fundamentally hard to solve because of the existence of multiple local minima. Additionally, even if we were to arrive at the global maxima, we would not have a straightforward way to verify global optimality. Lastly, fast convergence even to local minima may be difficult because methods such as Newton's method can not be directly applied to non-convex problems.

That said, (2.1) is *separably convex* in x_i and z if we ignore the non-convexity in the field design objectives, $f_i(x_i)$, and assume that the structure design objective, $g(z)$, is convex as well. This is given because of the bi-affine property of the physics residual, as shown in (2.3).

The separably convex, or *bi-convex*, properties of our problem open the door for the use of alternating direction algorithms, and specifically the alternating directions methods of multipliers (ADMM), for the implementation of a global optimization paradigm, as referred to in section 1.2. Of course, in this context we do not use the term "global" rigorously, but only to differentiate it from strategies that rely purely on local information.

Lastly, since our problem is not bi-convex in the case of non-convex field or structure design objectives, simple extensions to alternating direction algorithms are employed.

2.2.2 Optimality condition

Based on the problem definition in (2.1), we can write down a set of equations that, when met, signal that we have arrived at a locally optimal point. Otherwise known as the Karush-Kuhn-Tucker (KKT) conditions, these are, for (2.1),

$$|c_{ij}^\dagger x_i| - \beta_{ij} \leq 0, \tag{2.6a}$$

$$\alpha_{ij} - |c_{ij}^\dagger x_i| \leq 0, \tag{2.6b}$$

$$A_i(z)x_i - b_i(z) = 0, \tag{2.6c}$$

$$\nabla_z g(z) + \sum_i B(x_i)^\dagger \nu_i = 0, \tag{2.6d}$$

where $\nu_i \in \mathbf{C}^n$ are dual variables.

2.3 General strategy to solve the problem

2.3.1 Field update

Give the *specific* interfaces here. What exactly gets input and what does each update output?

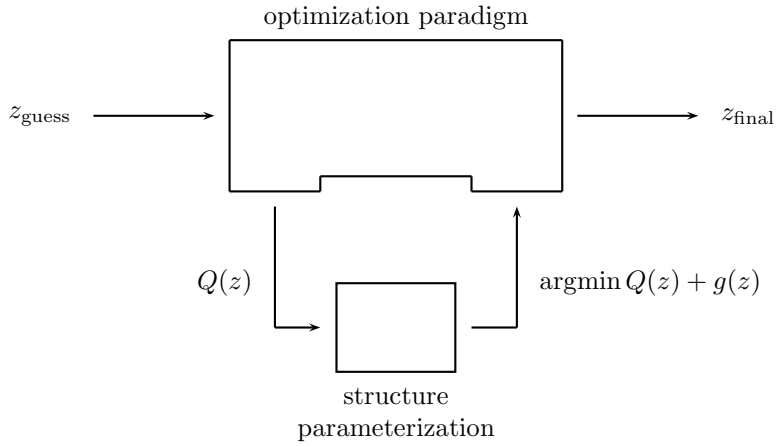

Figure 2.1: Basic layout of our software. At the most basic level, the chosen optimization paradigm accepts an initial structure z_{guess} and returns a final, optimized structure z_{final}. This is accomplished by repeatedly passing quadratic functions $Q(z)$ to the structure parameterization, which returns an updated structure z which minimizes $Q(z) + g(z)$.

2.3.2 Structure update