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 device 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 design nanophotonic devices.

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.

And the user can also 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 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

$$\begin{aligned} \text{minimize} \quad & \sum_i^N f_i(x_i) + g(z) && (2.1a) \\ \text{subject to} \quad & A_i(z)x_i - b_i(z) = 0, \quad \text{for } i = 1, \ldots, N. && (2.1b) \end{aligned}$$

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

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

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

- $\nabla \times \mu^{-1} \nabla \times -\omega^2 \epsilon \rightarrow A_i(z)$,
- $\epsilon \in z$,
- $E \rightarrow x_i$, 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 following relationship,

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

which will prove to be very useful.

2.1.3 Definition of the field design objective

Although $f_i(x_i)$ 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

2.2.1 nonconvexity

2.2.2 optimality condition

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?

2.3.2 Structure update