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Bounds on Efficiency Metrics in Photonics

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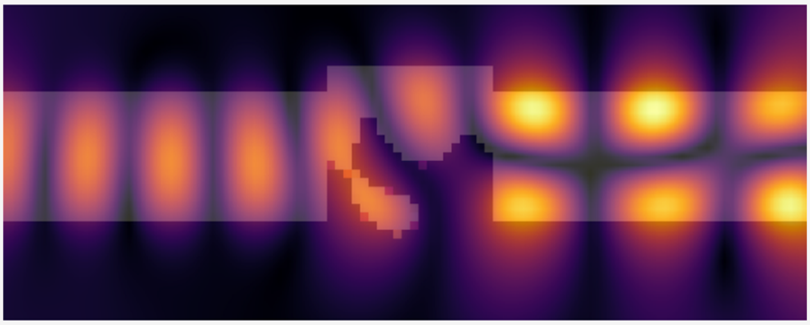

ABSTRACT: In this paper, we present a method for computing bounds for a variety of efficiency metrics in photonics, such as the focusing efficiency or the mode purity. We focus on the special case where the objective function can be written as the ratio of two quadratic functions of the field and show that there exists a simple semidefinite programming relaxation for this problem. We provide a numerical example of bounding the maximal mode conversion purity for a device of given size. This paper is accompanied by an open source Julia package for basic simulations and bounds.

KEYWORDS: *computational bounds, impossibility results, Lagrange duality, inverse design, nanophotonic optimization, optical devices*

■ INTRODUCTION

Traditionally, photonic devices were designed by a scientist or engineer (whom we will call a designer) for a specific application. This designer would piece together components from a library to create a device for the desired task. While effective in practice, this process is time consuming, possibly irrelevant to the final application of the design itself, and may produce designs that are far from optimal. In an alternative approach to constructing devices, a designer specifies what they want while forfeiting control of how the device is constructed to an optimization algorithm. This optimization algorithm then attempts to find a device that maximizes the designer-specified performance metric—a mathematical objective function that outputs a number representing how well the design matches the desired specifications. In photonics, this approach is called "inverse design."

Inverse Design. Photonic inverse design[1−6] has been extremely successful in finding photonic chip designs with very good practical performance when compared to designs generated by traditional methods. Still, there is an outstanding question of whether there exist designs with much better performance. For simple devices, such as spherical lenses, a designer can find the optimal design with basic algebra and ray optics. However, for more complicated devices, finding the optimal design with respect to some performance metric is an open research problem. As a result, designs are usually found using heuristic methods in practice.[7,8]

Bounds. Given a design generated using a heuristic, it is natural to wonder how much better one could have done. To answer this question, we need to determine a design's suboptimality with respect to some performance metric. Recently, there has been a large amount of work in this area, attempting to find bounds of this form for a variety of metrics, including mode volume,[9] free-space concentration,[10] integral overlap,[11,12] among many others.[13−20] Additionally, the focusing objectives shown in ref 21, released well after the preprint of this article, are included as a special case of the formulation presented here.

This Paper. In this paper, we extend the current bound formulations to include objective functions that can be expressed as the ratio of two quadratic functions of the field. This type of objective includes several efficiency metrics such as the focusing efficiency, the mode purity, among many others. We show a numerical example of these bounds and also provide a set of simple open source packages that can be used to compute bounds for many inverse design problems whose

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objectives can be phrased as quadratics or the ratio of quadratics.

THE PROBLEM OF MAXIMIZING EFFICIENCY

In the general photonic design problem, a designer must design a device that maximizes some objective function f of the fields z by choosing from a range of possible permittivities θ of a device at each point in space. (For example, this might mean that the designer is only able to choose some permittivity between that of air and silicon at each point in the design domain.)

We will assume that the fields z must satisfy the *electromagnetic wave equation*, which can be written as

$$Az + \mathbf{diag}(\theta)z = b \tag{1}$$

for some linear operator A and excitation b. In general, we will work with a discretization of the fields and permittivities, such that $\theta, z, b \in \mathbf{R}^n$ are represented as real-valued n-vectors, that $f : \mathbf{R}^n \to \mathbf{R}$ is a function mapping z to a real number, while $A \in \mathbf{R}^{n\times n}$ is a real $n \times n$ matrix. We have assumed that A, z, and b are real in this case, but the complex case can be reduced to the real one by separating it into its real and imaginary parts. (We will see an explicit example of how to do this later in this paper.) As a rough guideline, we may view eq 1 as the linear-algebraic generalization of

$$-\underbrace{\nabla \times \nabla \times}_{A} \underbrace{E}_{z} + \underbrace{\omega^2 \mu_0 \varepsilon E}_{\mathbf{diag}(\theta)z} = \underbrace{-\mathbf{i}\omega\mu_0 J}_{b}$$

where the linear operator A corresponds to a discretization of $-\nabla \times \nabla \times \cdot$; the design parameters θ correspond to a (scaled) discretization of the permittivities ε; the fields z, of course, correspond to the field E; and the excitation b corresponds to the current $-\mathbf{i}\omega\mu_0 J$.

Because the designer is only allowed to choose materials whose parameters range within some interval, we will write $\theta_i^{\min} \le \theta \le \theta_i^{\max}$ for $i = 1, \cdots, n$. Without loss of generality, we will assume that $\theta^{\max} = -\theta^{\min} = \mathbf{1}$ since eq 1 can always be rescaled such that this is true. (See, *e.g.*, Section 2.2 of ref 8 for more details.) The general optimization problem the designer wishes to solve is then

$$\begin{aligned} &\text{maximize} && f(z) \\ &\text{subject to} && Az + \mathbf{diag}(\theta)z = b \\ &&& -\mathbf{1} \le \theta \le \mathbf{1} \end{aligned} \tag{2}$$

Here the variables are the fields $z \in \mathbf{R}^n$ and the permittivities $\theta \in \mathbf{R}^n$, while the problem data are the matrix $A \in \mathbf{R}^{n\times n}$ and the excitation $b \in \mathbf{R}^n$. Note that this problem, as stated, is NP-hard (see Section 2.3 of 8), so finding its optimal value, which we will call p^*, is likely to be computationally infeasible except for very small problems.

Efficiency Metrics. A common problem in photonic design (and, more generally, in physical design) is the problem of maximizing an efficiency metric. We say an objective is an *efficiency metric* whenever, for any $z \in \mathbf{dom}\, f$, we have that

$$0 \le f(z) \le 1 \tag{3}$$

or, in other words, that the objective value for a feasible field z is always a number between 0 and 1. (We may, of course, replace the upper bound of 1 with any finite number, say v, but this is the same as defining a new objective function $\tilde{f} = (1/v) f$ which satisfies eq 3.) Note that there are some cases in which the function f might be unbounded from above (or below) and are therefore not “efficiency metrics” in the sense specified here. Even in these cases, the relaxation method we present will hold, but it is not guaranteed to return points that are “reasonable”; *i.e.*, the relaxation might give bounds which are trivial. (We note that, in practice, we still expect the results to be relatively tight, even without these guarantees.)

Ratio of Quadratics. In many important cases in photonic design, efficiency metrics can be written as the ratio of two quadratics in z, *i.e.*

$$f(z) = \frac{z^T P z + 2p^T z + r}{z^T Q z + 2q^T z + s} \tag{4}$$

where $P, Q \in \mathbf{S}^n$ are two symmetric matrices, while $p, q \in \mathbf{R}^n$ and $r, s \in \mathbf{R}$, whenever $z^T Q z + 2q^T z + s > 0$ and is $-\infty$ otherwise. Note that this function f is, in general, nonconvex. (We will see some examples of such objective functions soon.) In order for f to be an efficiency metric (see eq 3), the numerator and denominator must satisfy

$$0 \le z^T P z + 2p^T z + r \le z^T Q z + 2q^T z + s$$

for all $z \in \mathbf{R}^n$. By minimizing over z, this is true whenever

$$0 \le \begin{bmatrix} P & p \\ p^T & r \end{bmatrix} \le \begin{bmatrix} Q & q \\ q^T & s \end{bmatrix} \tag{5}$$

where the inequalities are semidefinite inequalities (see Section 2.4.1 of ref 22). The inequalities of eq 5 imply that P and Q satisfy $0 \le P \le Q$, while r and s must satisfy $0 \le r \le s$.

Optimization Problem. The resulting optimization problem, when f is the ratio of two quadratics, is

$$\begin{aligned} &\text{maximize} && \frac{z^T P z + 2p^T z + r}{z^T Q z + 2q^T z + s} \\ &\text{subject to} && Az + \mathbf{diag}(\theta)z = b \\ &&& -\mathbf{1} \le \theta \le \mathbf{1} \end{aligned} \tag{6}$$

The variables in this problem are the fields $z \in \mathbf{R}^n$ and the design parameters $\theta \in \mathbf{R}^n$, while the data are the matrices $A \in \mathbf{R}^{n\times n}$ and $P, Q \in \mathbf{S}^n$; the vectors $p, q \in \mathbf{R}^n$; and the scalars $r, s \in \mathbf{R}$. From the previous discussion, if the objective is an efficiency metric, then the optimal value of problem 6, p^*, will also satisfy $0 \le p^* \le 1$. Finding an upper bound to this optimal value p^* would then give us an upper bound on the maximal efficiency of the best possible design.

Example: Normalized Overlap. One important special case of an efficiency metric is sometimes known as the *normalized overlap*. The normalized overlap is defined as

$$f(z) = \frac{(c^T z)^2}{\|z\|_2^2}$$

where $c \in \mathbf{R}^n$ is a normalized vector with $\|c\|_2^2 = 1$. This is a special case of eq 4 where $P = cc^T$, $Q = I$, and $p = q = 0$, while $r = s = 0$.

It is easy to verify that this is indeed an efficiency metric since $f(z) \ge 0$ as it is the ratio of two nonnegative quantities, while

$$f(z) = \frac{(c^T z)^2}{\|z\|_2^2} \le \frac{\|c\|_2^2 \|z\|_2^2}{\|z\|_2^2} = \|c\|_2^2 = 1$$

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where the first inequality follows from Cauchy−Schwarz (see Section 3.4 of ref 23). Whenever c is a mode of the system, this objective is sometimes called the normalized mode overlap, or the mode purity, and can be interpreted as the fraction of power that is coupled into the mode specified by c, compared to the total fraction of power going to all possible output modes.

In the case we wish to measure the normalized overlap only over some region specified by indices $S \subseteq \{1, ..., n\}$, we can instead write

$$f(z) = \frac{(c^T R z)^2}{\|Rz\|_2^2} \tag{7}$$

where the matrix $R \in \mathbf{R}^{n\times n}$ is a diagonal matrix with diagonal entries

$$R_{ii} = \begin{cases} 1 & i \in S \\ 0 & \text{otherwise} \end{cases} \tag{8}$$

for $i = 1, ..., n$. The resulting objective can be written in as the special case of eq 4 where $P = Rcc^T R$ and $Q = R^2 = R$, while $q = p = 0$ and $r = s = 0$, and is also easily shown to be an efficiency metric.

Example: Focusing Efficiency. While there are many ways of defining the focusing efficiency of a lens, one practical definition is as the ratio of the sum of intensities over two regions, written

$$f(z) = \frac{\|R'z\|_2^2}{\|Rz\|_2^2}$$

Here, the matrices $R, R' \in \mathbf{R}^{n\times n}$ are defined as

$$R_{ii} = \begin{cases} 1 & i \in S \\ 0 & \text{otherwise,} \end{cases} \qquad R'_{ii} = \begin{cases} 1 & i \in S' \\ 0 & \text{otherwise} \end{cases}$$

where $S' \subseteq S \subseteq \{1, ..., n\}$ are sets of indices over which we sum the square of the field. In this case, we call S the focusing plane and S' the focusing region or focal spot, which is usually chosen to be approximately the full width at half maximum (FWHM) of the intensity along S.

This metric is nonnegative as it is the ratio of two nonnegative functions and satisfies $f(z) \le 1$ as $S' \subseteq S$. We can write this as the special case of eq 4, where $P = R'$ and $Q = R$, while $p = q = 0$ and $r = s = 0$.

■ HOMOGENIZATION AND BOUNDS

In this section, we will show a transformation of problem 6 which results in a quadratic objective with an additional quadratic constraint, by introducing a new variable. We will then show how to construct basic bounds using procedures similar to those of refs 8, 11, 12, and show a few simple extensions.

Homogenized Problem. The main difficulty of constructing bounds for problem 6 is that the fractional objective is difficult to deal with. We will first give a 'heuristic' derivation and show that it is always an upper bound to the original problem. We then show that the converse is true: this new problem is equivalent to the original when $A + \mathbf{diag}(\theta)$ is invertible for all $-\mathbf{1} \le \theta \le \mathbf{1}$.

The main idea behind this method is to dynamically scale the input excitation, b, by some factor $\alpha \in \mathbf{R}$, such that the denominator is always equal to 1. To do this, we replace eq 1 with one where the input b is scaled to get

$$Ay + \mathbf{diag}(\theta)y = \alpha b$$

Here y is a new variable we will call the *scaled field* as we can write $y = \alpha z$. Plugging this into the objective, assuming that z is feasible, we find that

$$f(z) = f(y/\alpha) = \frac{(1/\alpha)^2 y^T P y + 2(1/\alpha) p^T y + r}{(1/\alpha)^2 y^T Q y + 2(1/\alpha) q^T y + s} = \frac{y^T P y + 2\alpha p^T y + \alpha^2 r}{y^T Q y + 2\alpha q^T y + \alpha^2 s}$$

We will then constrain the denominator to equal 1, which results in the *homogenized* problem

$$\begin{array}{ll} \text{maximize} & y^T P y + 2\alpha p^T y + \alpha^2 r \\ \text{subject to} & y^T Q y + 2\alpha q^T y + \alpha^2 s = 1 \\ & Ay + \mathbf{diag}(\theta) y = \alpha b \\ & -\mathbf{1} \le \theta \le \mathbf{1}, \quad \alpha \ge 0 \end{array} \tag{9}$$

The variables in this problem are the scaled field $y \in \mathbf{R}^n$ and the scaling factor $\alpha \in \mathbf{R}$, while the problem data are the same as that of the original problem 6.

Upper Bound. We will now show that this new homogenized problem 9 is an upper bound to the original problem. More specifically, we will show that every feasible field z and design parameters θ for problem 6 have a feasible scaled field y, scaling factor $\alpha > 0$, using the same design parameters θ, with the same objective value.

First, note that z is feasible for 6, by definition, if $f(z) > -\infty$, *i.e.*, if z satisfies

$$z^T Q z + 2q^T z + s > 0, \ \ (A + \mathbf{diag}(\theta))z = b$$

for some $-\mathbf{1} \le \theta \le \mathbf{1}$. Based on this choice of z, we will set

$$\alpha = \frac{1}{\sqrt{z^T Q z + 2q^T z + s}}, \ \ y = \alpha z$$

and show that this choice of α and y satisfies the constraints of problem 9 with the same objective value. Plugging this value into the first constraint of problem 9, we see that

$$y^T Q y + 2\alpha q^T y + \alpha^2 s = \alpha^2 (z^T Q z + 2q^T z + s) = 1$$

while the second constraint has

$$(A + \mathbf{diag}(\theta))y = \alpha(A + \mathbf{diag}(\theta))z = \alpha b$$

Finally, the objective satisfies

$$y^T P y + 2\alpha p^T y + \alpha^2 r = \alpha^2 (z^T P z + 2p^T z + r) = \frac{z^T P z + 2p^T z + r}{z^T Q z + 2q^T z + s} = f(z)$$

so the objective value for y and α for problem 9 is the same as $f(z)$, the objective value for problem 6 with field z.

Equivalence. We will show that, in fact, problem 9 and problem 6 are equivalent in the special case where $A + \mathbf{diag}(\theta)$ is invertible for any choice of $-\mathbf{1} \le \theta \le \mathbf{1}$. (We note that the problems have the same optimal value even in the case where the physics equation is not always invertible, but invertibility usually holds in practice.) We have shown that every feasible field z and design parameters θ have a corresponding scaled

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fields y, scaling parameter α (with the same design parameters θ). We will now show the converse: every scaled field y with scaling parameter α that is feasible for problem 9 has some corresponding field z for problem 6 with the same objective value. We break this up into two cases, one in which $\alpha \neq 0$ and one in which $\alpha = 0$.

Given $\alpha \neq 0$ and any y satisfying the constraints of problem 9, we set $z = y/\alpha$. This field z satisfies the physics constraint with the same design parameters θ as

$$(A + \mathbf{diag}(\theta))z = \frac{1}{\alpha}(A + \mathbf{diag}(\theta))y = \frac{1}{\alpha}(\alpha b) = b$$

On the other hand, the objective value for this choice of z is

$$\begin{aligned} f(z) = f(y/\alpha) &= \frac{y^T P y + 2\alpha p^T y + \alpha^2 r}{y^T Q y + 2\alpha q^T y + \alpha^2 s} \\ &= y^T P y + 2\alpha p^T y + \alpha^2 r \end{aligned}$$

So this z is also feasible with design parameters θ and the same objective value.

On the other hand, we will show that $\alpha = 0$ is never feasible for problem 9 for any choice of $-\mathbf{1} \leq \theta \leq \mathbf{1}$. If $\alpha = 0$, then $(A + \mathbf{diag}(\theta))\ y = \alpha b = 0$. Since $A + \mathbf{diag}(\theta)$ is invertible by assumption, then $y = 0$. This implies that

$$y^T Q y + 2\alpha q^T y + \alpha^2 s = 0 \neq 1$$

So, given any θ and $\alpha = 0$, there is no scaled field y that is feasible for problem 9. This shows that the problems are equivalent as any feasible point for one is feasible in the other, with the same objective value.

Semidefinite Relaxation. In general, problem 9 is still nonconvex and likely computationally difficult to solve. On the other hand, we can give a convex relaxation of the problem, yielding a new problem whose optimal value is guaranteed to be at least as large as that of problem 9 while also being computationally tractable.

Variable Elimination. As in refs 8, 24, we can eliminate the design variable θ from problem 9, giving the following equivalent problem over only the scaled field y and scaling parameter α

$$\begin{aligned} &\text{maximize} && y^T P y + 2\alpha p^T y + \alpha^2 r \\ &\text{subject to} && y^T Q y + 2\alpha q^T y + \alpha^2 s = 1 \\ &&& (a_i^T y - \alpha b_i)^2 \leq y_i^2, \quad i = 1, ..., n \end{aligned} \tag{10}$$

with variables $y \in \mathbf{R}^n$ and $\alpha \in \mathbf{R}$. Here, a_i^T denotes the ith row of the matrix A, and the problem data are otherwise identical to that of problem 9. Additionally, we note that this problem is equivalent to problem 9 by the same argument as that of ref 8 and therefore to problem 6.

Rewriting and Relaxation. The new problem 10 is a nonconvex quadratically constrained quadratic program (QCQP). We can write problem 10 in a slightly more compact form

$$\begin{aligned} &\text{maximize} && x^T \bar{P} x \\ &\text{subject to} && x^T \bar{Q} x = 1 \\ &&& x^T \bar{A}_i x \leq 0, \quad i = 1, ..., n \end{aligned} \tag{11}$$

Here, the variable is $x = (y, \alpha) \in \mathbf{R}^{n+1}$, while the problem data are the matrices

$$\bar{P} = \begin{bmatrix} P & p \\ p^T & r \end{bmatrix}, \quad \bar{Q} = \begin{bmatrix} Q & q \\ q^T & s \end{bmatrix},$$

$$\bar{A}_i = \begin{bmatrix} a_i a_i^T - e_i e_i^T & -b_i a_i \\ -b_i a_i^T & b_i^2 \end{bmatrix}, \quad i = 1, ..., n$$

Using this rewritten problem, we can then form a semidefinite relaxation in the following way

$$\begin{aligned} &\text{maximize} && \mathbf{tr}(\bar{P} X) \\ &\text{subject to} && \mathbf{tr}(\bar{Q} X) = 1 \\ &&& \mathbf{tr}(\bar{A}_i X) \leq 0, \quad i = 1, ..., n \\ &&& X \geq 0 \end{aligned} \tag{12}$$

where we are maximizing over the variable $X \in \mathbf{S}^n$. We will call d^* the optimal value of this problem. Problem 12 is a relaxation of problem 11 as any feasible point $x \in \mathbf{R}^n$ for problem 11 gives a feasible point $X = xx^T \geq 0$ for problem 12, since

$$\mathbf{tr}(\bar{Q} X) = \mathbf{tr}(\bar{Q} x x^T) = x^T \bar{Q} x = 1$$

with the same objective value, $\mathbf{tr}(\bar{P} X) = x^T\ \bar{P} x$. This implies that the optimal objective value of problem 6, p^*, is never larger than the optimal objective value of problem 12; *i.e.*, we always have $p^* \leq d^*$.

Properties. There are several interesting basic properties of the relaxation of problem 12. First, since $\bar{P} \geq 0$ by assumption eq 5, then $d^* \geq 0$ since we know that, for any feasible X

$$d^* \geq \mathbf{tr}(\bar{P} X) \geq 0$$

Since we also know from eq 5 that $\bar{P} \leq \bar{Q}$, then, for any optimal $X^* \geq 0$, we have

$$d^* = \mathbf{tr}(\bar{P} X^*) \leq \mathbf{tr}(\bar{Q} X^*) = 1$$

This implies that

$$0 \leq p^* \leq d^* \leq 1$$

so d^* can always be interpreted as a percentage upper bound of p^*, as expected. We note that, even if $\bar{P} \leq \bar{Q}$ does not hold, the resulting problem 12 still yields a bound on the optimal objective value p^*. The difference is that we lose the guarantees derived here that the resulting dual bound d^* satisfies $d^* \leq 1$. Additionally, given any $X \geq 0$ with $\mathbf{tr}(\bar{A}_i\ X) \leq 0$ for $i = 1, ..., n$, and $\mathbf{tr}(\bar{Q} X) > 0$, then

$$X^0 = \frac{1}{\mathbf{tr}(\bar{Q} X)} X$$

is a feasible point for problem 12.

Since we know that $\bar{P} \leq \bar{Q}$, then the equality constraint $\mathbf{tr}(\bar{Q} X) = 1$ in problem 12 can be relaxed to $\mathbf{tr}(\bar{Q} X) \leq 1$, with the same optimal objective value. Additionally, if we find a solution X^* whose rank is 1, then $X^* = xx^T$ for some x and therefore we have that $x = (y, \alpha)$ is a solution to the homogenized problem 9, which is easily turned into a solution of the original problem 6 by setting $z = y/\alpha$ and $\theta = (a_i^T z - b_i)/z_i$ when $z_i \neq 0$ and 0 otherwise.

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Dual Problem. The matrices $\bar{A}_i$ for $i = 1, ..., n$, $\bar{Q}$, and $\bar{P}$ are sometimes chordally sparse.[25] This structure can often be exploited to more quickly solve for the optimal value of problem 12 by considering the dual problem instead. Applying semidefinite duality (see Section 5.9 of ref 22) to problem 12 gives

$$\begin{aligned} \text{minimize} \quad & \lambda_{n+1} \\ \text{subject to} \quad & \sum_{i=1}^{n} \lambda_i \bar{A}_i + \lambda_{n+1}\bar{Q} \geq \bar{P} \\ & \lambda \geq 0 \end{aligned} \tag{13}$$

where $\lambda \in \mathbf{R}^{n+1}$ is our optimization variable. This problem can then be passed to solvers such as `COSMO.jl`,[26] which support chordal decompositions, for faster solution times.

Discussion. The transformation of variables used here is very similar to the transformation used in the reduction of linear fractional programs to linear programs in Section 4.3.2 of ref 22, and similar transformations have been used for computational physics bounds in ref 9 in the special case that $b = 0$ and $Q = e_ie_i^T$ (see, *e.g.*, Section 3.2 of ref 8). This family of variable transformations has been known in the optimization literature since the 1960s[27] for a specific subset of optimization problems known as 'fractional programming,' which include problems with objective functions of the form of eq 4. The variable transformation used on problem 6 to get the homogenized problem 9 is sometimes called the generalized Charnes−Cooper transformation.[28] We also note that the same methodology presented here can be applied to the formulation in refs[9,14,9], which is the special case where P and Q are diagonal with nonnegative entries.

Extensions. There are a few basic extensions for the bounds provided in problem 12.

Boolean Constraints. If we are allowed to choose only Boolean parameters, *i.e.*, if we have $\theta_i \in \{\pm 1\}$, instead of $-1 \leq \theta_i \leq 1$ for each $i = 1, ..., n$, we can write the bound as

$$\begin{aligned} \text{maximize} \quad & \mathbf{tr}(\bar{P}X) \\ \text{subject to} \quad & \mathbf{tr}(\bar{Q}X) = 1 \\ & \mathbf{tr}(\bar{A}_iX) = 0, \quad i = 1, ..., n \\ & X \geq 0 \end{aligned}$$

which follows from Section 3.2 of ref 8. All of the same properties for problem 12 also hold for the optimal value of this problem.

Rewriting the Physics Equation. In practice, it is sometimes the case that the physics eq 1 is better expressed in the following form

$$z + G\,\mathbf{diag}(\theta')z = b' \tag{14}$$

where $0 \leq \theta' \leq \mathbf{1}$, $b' \in \mathbf{R}^n$, and $G \in \mathbf{R}^{n\times n}$. This formulation is sometimes called the 'Green's formalism' or 'integral equation' in electromagnetism and is equivalent to that of eq 1, in that every (z, θ) that satisfies the physics eq 1 has a θ' such that (z, θ') satisfies eq 14, and vice versa. To see this in the case that A is invertible, we can map eqs 1−14 by setting $G = (2A - I)^{-1}$, $b' = Gb$, and $\theta' = (\theta + \mathbf{1})/2$.

Similar to refs 12,[8] we will reduce eq 14, which depends on both the field z and the design parameters θ', to an equation depending only on the *displacement field* $w = \mathbf{diag}(\theta')z$. To do this, we can write eq 14 in terms of w and z

$$z + Gw = b', \quad w = \mathbf{diag}(\theta')z$$

Multiplying both sides of the first equation elementwise by w gives

$$w_iz_i + w_ig_i^Tw = w_ib_i', \quad i = 1, ..., n$$

where g_i^T is the ith row of G. Finally, because $0 \leq \theta' \leq 1$, we get that $w_i^2 = \theta_iw_iz_i \leq w_iz_i$, which means that

$$w_i^2 + w_ig_i^Tw \leq w_ib_i', \quad i = 1, ..., n \tag{15}$$

The converse—that there exists a field z and design parameters θ' satisfying eq 14 and $w = \mathbf{diag}(\theta')z$, for any w satisfying eq 15—can be easily shown; *cf.*, App. A of ref 8.

Rewriting eq 14, we have that $z = b' - Gw$, and replacing the physics constraint in problem 6 with eq 15 gives a new problem over the displacement field w

$$\begin{aligned} \text{maximize} \quad & \frac{w^TP'w + 2p'^Tw + r'}{w^TQ'w + 2q'^Tw + s'} \\ \text{subject to} \quad & w_i^2 + w_ig_i^Tw \leq w_ib_i', \quad i = 1, ..., n \end{aligned}$$

with variable $w \in \mathbf{R}^n$ and problem data G, b, and

$$P' = G^TPG, \quad p' = -G^TP(p + b), \quad r' = b^TPb + 2p^Tb + r$$

while

$$Q' = G^TQG, \quad q' = -G^TQ(q + b), \quad s' = b^TQb + 2q^Tb + s$$

Applying the same homogenization procedure and semidefinite relaxation, this results in a problem identical to problem 12 with the following problem data

$$\bar{P} = \begin{bmatrix} P' & p' \\ p'^T & r' \end{bmatrix}, \quad \bar{Q} = \begin{bmatrix} Q' & q' \\ q'^T & s' \end{bmatrix},$$

$$\bar{A}_i = \begin{bmatrix} e_ie_i^T + (e_ig_i^T + g_ie_i^T)/2 & -b_i'e_i \\ -b_i'e_i^T & 0 \end{bmatrix}, \quad i = 1, ..., n$$

Convex Constraints. We can also allow convex constraints in the SDP relaxation problem 12. If we have several convex constraints on the field $z = y/\alpha$ given by f_j: $\mathbf{R}^n \to \mathbf{R}$ for $j = 1, ..., m$, we can write

$$\begin{aligned} \text{maximize} \quad & \mathbf{tr}(\bar{P}X) \\ \text{subject to} \quad & \mathbf{tr}(\bar{Q}X) = 1 \\ & \mathbf{tr}(\bar{A}_iX) = 0, \quad i = 1, ..., n \\ & \alpha f_j\left(\frac{y}{\alpha}\right) \leq 0, \quad j = 1, ..., m \\ & X = \begin{bmatrix} Y & y \\ y^T & \alpha \end{bmatrix} \geq 0 \end{aligned}$$

The variables in this problem are the matrices $X \in \mathbf{S}^{n+1}$, $Y \in \mathbf{S}^n$, the vector $y \in \mathbf{R}^n$, and scalar $\alpha \in \mathbf{R}$, while the problem data are identical to that of problem 12. This new problem is again a convex optimization problem since the functions $\alpha f_j(y/\alpha)$ over

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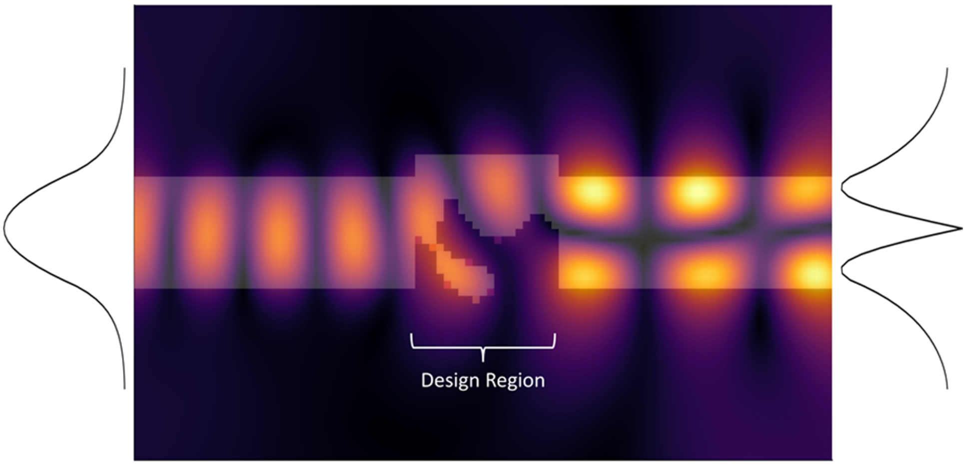

Figure 1. Designer wishes to choose materials in the design region to maximize the mode purity, measured at the output of the waveguide.

the variable (y, α) are convex if the original functions f_j are convex. This transformation is known as the perspective transform and always preserves convexity (see Section 3.2.6 of ref 22). The resulting problem is then convex and can therefore be efficiently solved in most cases.

Additional Quadratic Constraints. Similar to the previous, we can include additional (potentially indefinite) quadratic constraints on the field z into the relaxation problem 12. More specifically, we wish to include several constraints on the field z

$$z^T U_j z + 2u_j^T z + t_j \leq 0$$

with matrices $U_j \in \mathbf{S}^n$, vectors $u_j \in \mathbf{R}^n$, and scalars $t_j \in \mathbf{R}$ for $j = 1, ..., m$. Using the fact that $z = y/\alpha$, we can write these as

$$y^T U_i y + 2\alpha u_j^T y + \alpha^2 t_j \leq 0, \quad j = 1, ..., m$$

or equivalently as

$$x^T \bar{U}_j x \leq 0, \quad i = 1, ..., m$$

where $x = (y, \alpha)$ as in problem 12 and

$$\bar{U}_j = \begin{bmatrix} U_j & u_j \\ u_j^T & t_j \end{bmatrix}, \quad j = 1, ..., m$$

Using the same relaxation method as in problem 12 with the additional quadratic inequalities, we get the following semi-definite problem:

$$\begin{array}{ll} \text{maximize} & \mathbf{tr}(\bar{P}X) \\ \text{subject to} & \mathbf{tr}(\bar{Q}X) = 1 \\ & \mathbf{tr}(\bar{A}_i X) = 0, \quad i = 1, ..., n \\ & \mathbf{tr}(\bar{U}_j X) \leq 0, \quad j = 1, ..., m \\ & X \geq 0 \end{array}$$

This problem has the same variables and problem data as problem 12, with the addition of the matrices $\bar{U}_j \in \mathbf{S}^{n+1}$, as defined above.

NUMERICAL EXPERIMENTS

In this section, we solve problem 12 for the the maximal mode purity of a small mode converter. We also find a design that approximately saturates the bound. To compute these bounds, we introduce two open source Julia[29] packages, `WaveOperators.jl` and `PhysicalBounds.jl`, that allow users to setup physical design problems and compute bounds in only a few lines of code.

Our packages setup the dual form of the SDP, problem 13, using JuMP[30,31] and solve it using any conic solver that supports semidefinite programming. We use `SCS`[32] for the experiments in this paper. The code can be found at

github.com/cvxgrp/WaveOperators.jl

github.com/cvxgrp/PhysicalBounds.jl

which can be used to generate the plots found in this paper.

Physics Equation. We assume that the EM wave equation is appropriately discretized and results in a problem of the form

$$Az + \mathbf{diag}(\theta)z = b$$

Here $z \in \mathbf{C}^n$ is the (complex) field while $\theta \in \mathbf{R}^n$ are the (real) parameters and $A \in \mathbf{C}^{n \times n}$, $b \in \mathbf{C}^n$. To turn this into a problem over real variables, we can separate the real and imaginary parts of the variables to get a new physics equation that is purely real

$$A'z' + \mathbf{diag}(\theta, \theta)z' = b'$$

Here, we define

$$A' = \begin{bmatrix} \mathbf{Re}(A) & -\mathbf{Im}(A) \\ \mathbf{Im}(A) & \mathbf{Re}(A) \end{bmatrix}, \quad b' = \begin{bmatrix} \mathbf{Re}(b) \\ \mathbf{Im}(b) \end{bmatrix}, \quad z' = \begin{bmatrix} \mathbf{Re}(z) \\ \mathbf{Im}(z) \end{bmatrix}$$

where $\mathbf{Re}(x)$ denotes the elementwise real part of x (where x is a vector or a matrix) while $\mathbf{Im}(x)$ denotes the imaginary part. Note that this results in a larger system with parameters $A' \in \mathbf{R}^{2n \times 2n}$, $b' \in \mathbf{R}^{2n}$, and field $z' \in \mathbf{R}^{2n}$, whose parameters are all real. Finally, note that we can write this system as

$$A'z' + \mathbf{diag}(\theta')z' = b', \quad \theta'_{n+i} = \theta'_i$$

where we have introduced a new, larger vector of parameters, $\theta' \in \mathbf{R}^{2n}$ with an additional constraint. Dropping this latter constraint over θ' leads to a relaxation of the original physics equation, in the following sense: any design and field that satisfies the original equation also satisfies this new 'relaxed' equation. This makes the final physics equation

$$Az + \mathbf{diag}(\theta)z = b \tag{16}$$

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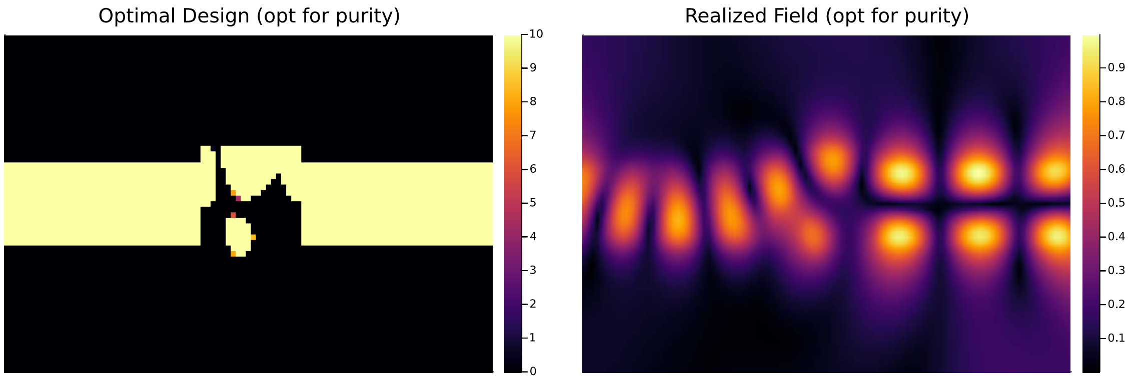

Figure 2. Design (left) is optimized for mode purity. The corresponding field (right) closely matches the target mode at the output.

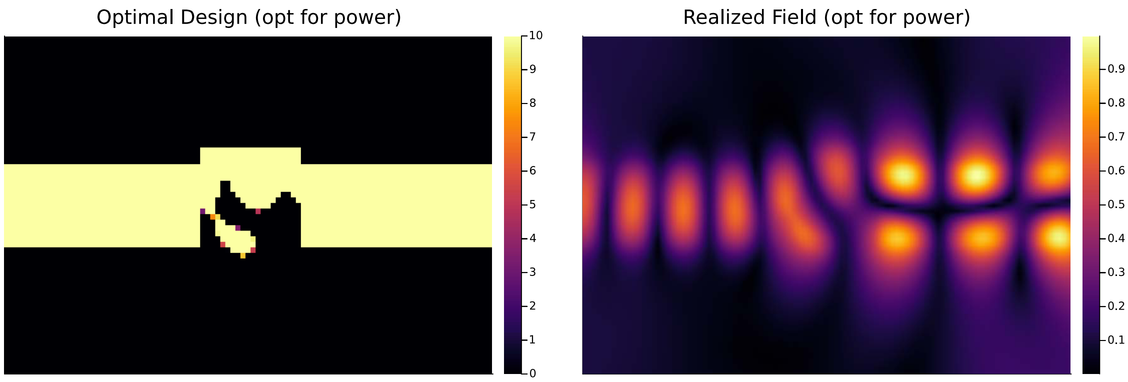

Figure 3. Design (left) is optimized for mode power. The corresponding field (right) has greater power at the output compared to that of the purity-optimized design, but it sacrifices some amount of purity.

where we have dropped the apostrophes for convenience. As a reminder we have the physics operator $A \in \mathbf{R}^{2n\times 2n}$, excitation $b \in \mathbf{R}^{2n}$, the field $z \in \mathbf{R}^{2n}$, and the permittivities $\theta \in \mathbf{R}^{2n}$. This relaxation corresponds to allowing the designer to vary both real and imaginary permittivities, where each component is box constrained, while the original problem only allows the designer to choose real permittivities. (We note that some solvers, including `Hypatia.jl`,[33] support complex variables, but we do not solve the problem over complex variables in this work.)

Mode Converter. The setup is shown in Figure 1. In this problem, the designer is attempting to design a mode converter with the maximum mode purity, by choosing the permittivities in the region shown. The input to this device is the first-order mode of the waveguide on the left-hand side. The desired output is a field whose normalized overlap with the second-order mode of the waveguide is maximized. In this problem, the designer is allowed to choose the permittivities within the design region, so long as the permittivities lie in a given interval. More information about the problem setup is given in appendix and the documentation of the corresponding packages.

Problem Data. In our specific problem setup, as shown in Figure 1, we have a source that is a distance of about one wavelength from the design region. The simulation region is a rectangle that is one wavelength tall and 1.6 wavelengths wide. The design region is a centered square with side length 1/3 of a wavelength. In this approximation, we assume that the grid is a 60×96 grid; *i.e.*, the side length of a pixel in this simulation is roughly 1/60th of a free-space wavelength, so $h = 1/60$. The material contrast (see appendix) is set to $\delta = 10$ while the free-space wavenumber is $k = 2\pi$.

Optimization Problem. In this experiment, we attempt to maximize the normalized overlap as defined in eq 7

$$\begin{array}{ll} \text{maximize} & \dfrac{(c^T R z)^2}{\|Rz\|_2^2} \\ \text{subject to} & Az + \mathbf{diag}(\theta)z = b \\ & -\mathbf{1} \le \theta \le \mathbf{1} \end{array}$$

Here, the variables and problem data are similar to those of problem 6. More specifically, the problem variables are $z \in \mathbf{R}^{2n}$, $\theta \in \mathbf{R}^{2n}$, while the problem data are the physics matrix $A \in \mathbf{R}^{2n\times 2n}$, the excitation $b \in \mathbf{R}^{2n}$, the vector $c \in \mathbf{R}^{2n}$ specifying the desired output mode, and the matrix $R \in \mathbf{R}^{2n\times 2n}$, defined in eq 8, where the region S is the rightmost column of pixels. The resulting semidefinite upper bound for this problem is given in problem 12 with

$$P = Rcc^T R, \quad Q = R, \quad p = 0, \quad q = 0, \quad r = 0, \quad s = 0$$

Results. The resulting upper bound on the mode purity, which no design can exceed, is .981. We also find an (approximately) optimal design with $\theta_i = \theta_{i+n}$ (*i.e.*, with real permittivities). This design and its corresponding field are shown in Figure 2. The mode purity this design achieves is .966, which is $(.981 - .966)/.981 \approx 1.5\%$ percent from the upper bound. We note that this design, while very close to the optimal value for the mode purity, is not very good in a practical sense: most of the power in the input waveguide is actually scattered out to space. In general, we find that simply

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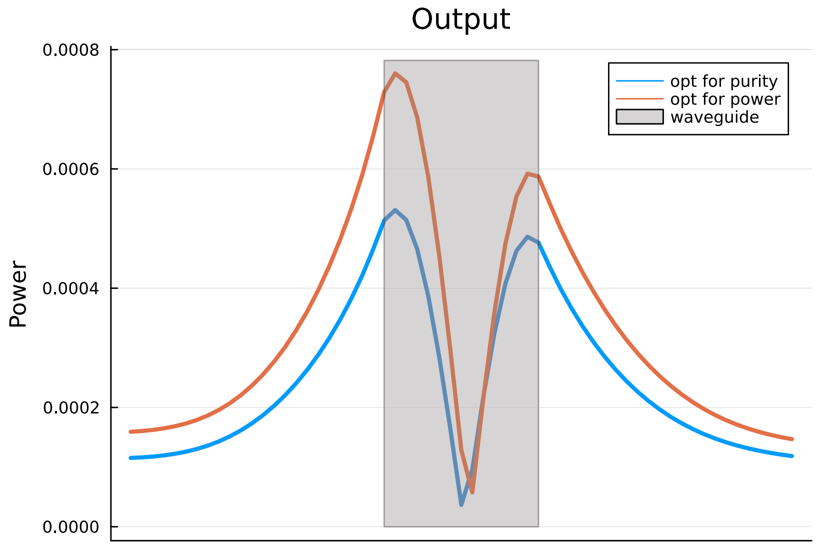

Figure 4. Design optimized for mode purity better matches the target mode waveform but has lower output power.

optimizing for the numerator, as is usually done in practice, yields designs that are relatively efficient and have reasonable mode purity. In this case, simply maximizing the numerator of the objective results in a design that achieves a mode purity of .933, with an output power that is approximately 76% greater. (This design, and its corresponding field, is shown in Figure 3.) This difference is highlighted in Figure 4.

CONCLUSIONS AND FUTURE WORK

In this paper, we have presented a simple method to compute bounds on several efficiency metrics for physical design problems, by solving a semidefinite program. In particular, we focused on the common case where the efficiency metric can be written as a ratio of two quadratics, which includes metrics such as the focusing efficiency and the mode conversion efficiency. We present a small example, but note that while larger numerical examples are possible, the resulting semidefinite programs are large; computing bounds on designs of larger sizes in reasonable time will likely require more sophisticated solvers (or larger computers). While the designs shown here are also somewhat reasonable, they are still very far from the three dimensional designs that are useful in practice. Future work would focus on creating faster solvers that can exploit the special structure of these problems, along with simple interfaces that are user-friendly and can be used to easily setup and solve these bounds.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsphotonics.3c00023.

Supporting Information, including derivations of the integral formalism and a plot showing the tradeoff between power and mode purity, is available for this paper (PDF)

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Notes

The authors declare no competing financial interest.

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