Heuristics and Bounds For Photonic Design

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Outline

(Very) high level overview

Problem set up

Sign flip descent

Performance bounds

Example

Optical devices

- Optical devices are everywhere !

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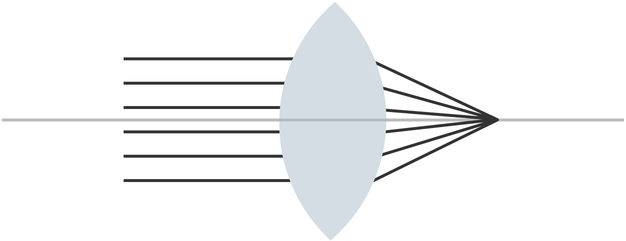
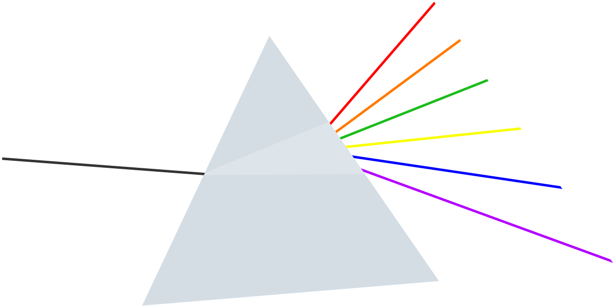
- Lenses



Optical devices

- Optical devices are everywhere !
- Prisms



More complicated optical devices

- Many more ‘simple’ devices (mirrors, filters, *etc.*)
- Can be combined to make more complex devices

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More complicated optical devices

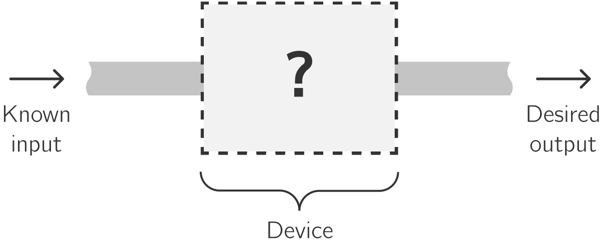
- Many more ‘simple’ devices (mirrors, filters, *etc.*)
- Can be combined to make more complex devices
- We (as designers) generally have a specific goal
- But: usually not obvious how to achieve goal by combining ‘simple’ components

A weird idea

- Given a device and an input, we can simulate its behavior
- Can ‘experiment’ as much as we want until we find a good design
- Possible to automate this?

The 'experimental' set up

- A typical set up looks like the following:



What is ‘good’ anyways

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- What does it mean for a design to be ‘good’?

What is ‘good’ anyways

- The first question:
- What does it mean for a design to be ‘good’?
- We write this as an *objective function*
- This function takes in a device’s output and gives a number
- The lower the number, the better the design

Parametrizations

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Parametrizations

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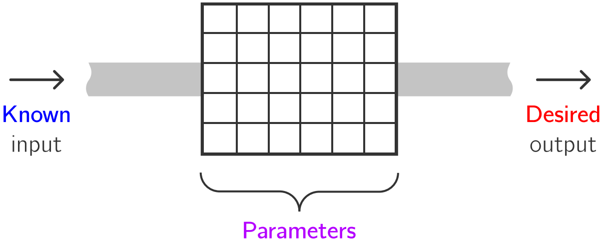
- How do we turn ‘design something’ into a (simple) mathematical problem?

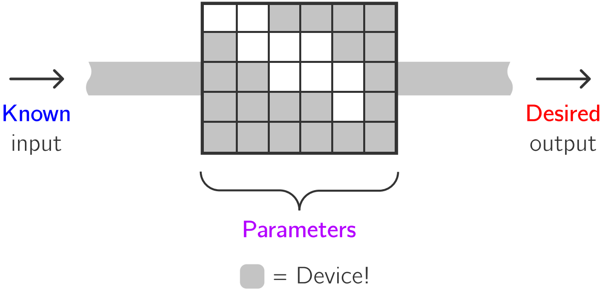
Parametrizations

- The second question:
- How do we turn 'design something' into a (simple) mathematical problem?
- Many possibilities! We will choose a simple *parametrization*:



Parametrizations

- Computer proposes a *design* (-1 or 1 at each square)
- Receives a score (or objective value); lower is better:



- The 'best' design has the lowest possible score

What are the questions?

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- Given a good design... is it close to the best?
  (Or are there better designs we haven't found?)

The answers

- Can we find the best design? Probably not
- Can we quickly find a good design? Yes
- Given a good design... is it close to the best? Yes (in practice)
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- Can we quickly find a good design? Yes
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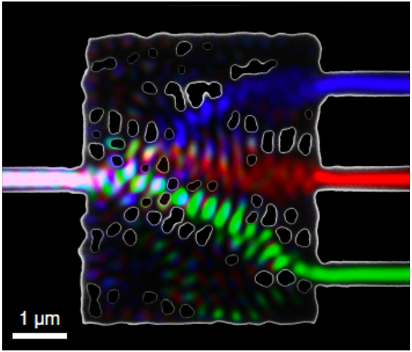
  (Or are there better designs we haven't found?)
- Bounds are (very!) common in physics
  (Wheeler, 1947), (Bohren, 1982), (Yu, Raman, Fan, 2012), (Miller 2019)
- *Computational* bounds are new

Examples

- Some designs:



(From Su, et al., 2018)

Examples

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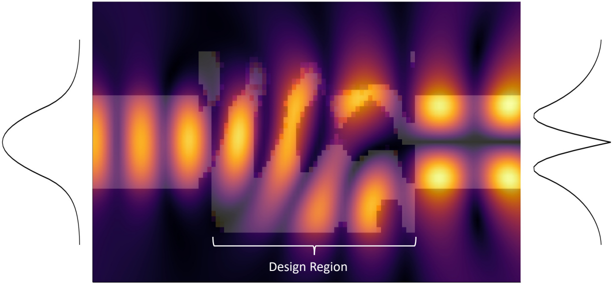

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Examples

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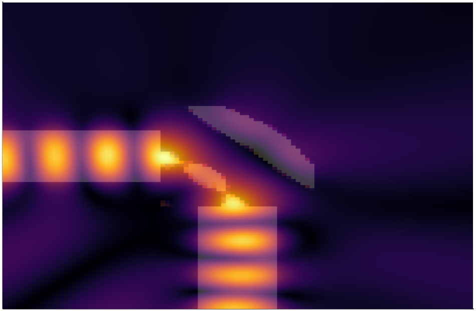

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Basic results

- In many cases, we find that optimized designs are usually quite close to optimal
- We can usually optimize large designs
- Usually, the designs found are no more than around 5-10 percent away from the best possible!

Here be dragons

- Onto the physics and math...

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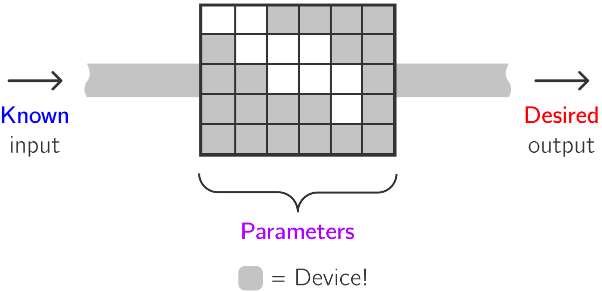
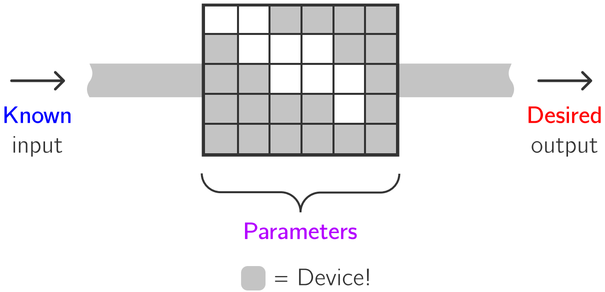
Physics equation

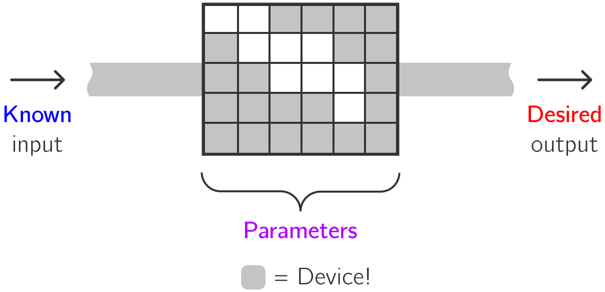


Physics equation



- We will call the *parameters* we control, $\theta \in [-1, 1]^n$
- The known input or *excitation* is $b \in \mathbf{R}^n$
- The *field* (including the output) is $z \in \mathbf{R}^n$

Physics equation



- In photonics, the equation connecting parameters to field is usually

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

where $A \in \mathbf{R}^{n \times n}$ is a matrix.

Physics equation (continued)

- Where does this come from?

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- The EM wave equation can be written as

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

where A, θ, z and b are the discretized counterparts

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  where A, θ, z and b are the discretized counterparts
- Hence

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

- This equation is very general
- Includes EM, thermal design, Schrödinger equation, ...

Objective function

- Given the physics and parameter constraints, we now need to specify the objective
- The *objective function* is a function $f : \mathbf{R}^n \to \mathbf{R} \cup \{+\infty\}$
- The value $f(z)$ tells us how good the field z is
- (From before, lower is better)

Optimization problem

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- Formulated as an optimization problem, we want

$$\begin{array}{ll} \text{minimize} & f(z) \\ \text{subject to} & (A + \mathbf{diag}(\theta))z = b \\ & -\mathbf{1} \leq \theta \leq \mathbf{1} \end{array}$$

  with variables z and θ

- This is the only problem we will focus on

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Basic properties

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  (Angeris, Vučković, Boyd, 2021)

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- Finding a feasible point is NP-hard in general
  (Angeris, Vučković, Boyd, 2021)

- Biconvex in θ and z when f is convex, smooth if f is smooth

- Many heuristics exploit these facts
  e.g., (Lu, Vučković, 2010), (Jiang, Fan, 2020)

Interesting properties

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Interesting properties

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- Knowing only the signs of any optimal field $z^\star$ is enough to solve the problem
- Implies optimal designs can be made *extremal*, $\theta_i \in \{\pm 1\}$, for many i when the objective depends only on a few i (not obvious)
  (Angeris, Vučković, Boyd, 2021)

The signs are all you need

- To see this, note we can eliminate the design variable to get

$$\begin{array}{ll} \text{minimize} & f(z) \\ \text{subject to} & |Az - b| \leq |z| \end{array}$$

- Still nonconvex, but given any optimal signs, $\mathbf{sign}(z^\star)$, the following (convex!) problem has the same optimal value:

$$\begin{array}{ll} \text{minimize} & f(z) \\ \text{subject to} & |Az - b| \leq \mathbf{sign}(z^\star) \circ z \end{array}$$

where $\circ$ is the Hadamard (elementwise) product

Sign flip descent

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- Start with some set of signs $s \in \{\pm 1\}^n$ and solve the convex problem

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with variable z

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- If $z_i \approx 0$ then sign is (probably) wrong, so set $s'_i = -s_i$ and try again

- Do this until objective does not decrease anymore (or decreases slowly)

Results

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- (We will see an example soon!)

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Quadratically constrained quadratic programs

- We can start with the 'new' problem

$$\begin{array}{ll} \text{minimize} & f(z) \\ \text{subject to} & |Az - b| \leq |z| \end{array}$$

- And square both sides of the inequality to get

$$\begin{array}{ll} \text{minimize} & f(z) \\ \text{subject to} & (a_i^T z - b_i)^2 \leq z_i^2, \quad i = 1, \dots, n, \end{array}$$

  where a_i^T is the ith row of A
  (Kuang and Miller, 2020), (Molesky, Chao, Rodriguez, 2020)

- If f is a quadratic then this is a QCQP, which is a very special type of problem

QCQPs, continued

- If f is a quadratic then it can be written as

$$f(z) = z^T P z + 2p^T z + r,$$

  where $P \in \mathbf{S}^n_+$, $q \in \mathbf{R}^n$, $r \in \mathbf{R}$ are problem data

- So the problem becomes

$$\begin{array}{ll} \text{minimize} & z^T P z + 2q^T z + r \\ \text{subject to} & (a_i^T z - b_i)^2 \leq z_i^2, \quad i = 1, \ldots, n \end{array}$$

QCQPs, continued

- We will 'massage' it into one final form:

$$\begin{array}{ll} \text{minimize} & (z,1)^T \bar{P}(z,1) \\ \text{subject to} & (z,1)^T \bar{A}_i(z,1) \leq 0, \quad i=1,\ldots,n, \end{array}$$

  where

$$\bar{P} = \begin{bmatrix} P & q \\ q^T & r \end{bmatrix}, \quad \bar{A}_i = \begin{bmatrix} a_i a_i^T - E_{ii} & -b_i a_i \\ -b_i a_i^T & b_i^2 \end{bmatrix}, \quad i=1,\ldots,n,$$

  and E_{ii} is the all-zeros matrix except with a single 1 at the i,ith entry

- (The details are not super important; the fact we can do it is)

Finally, something

- Given the QCQP

$$
\begin{array}{ll}
\text{minimize} & (z,1)^T \bar{P}(z,1) \\
\text{subject to} & (z,1)^T \bar{A}_i(z,1) \leq 0, \quad i = 1,\ldots,n,
\end{array}
$$

  there is a standard 'relaxation' method

- This method gives a (semidefinite) convex problem:

$$
\begin{array}{ll}
\text{minimize} & \mathbf{tr}(\bar{P}Z) \\
\text{subject to} & \mathbf{tr}(\bar{A}_i Z) \leq 0, \quad i = 1,\ldots,n, \\
& Z_{n+1,n+1} = 1 \\
& Z \geq 0
\end{array}
$$

  with variable $Z \in \mathbf{S}^n_+$

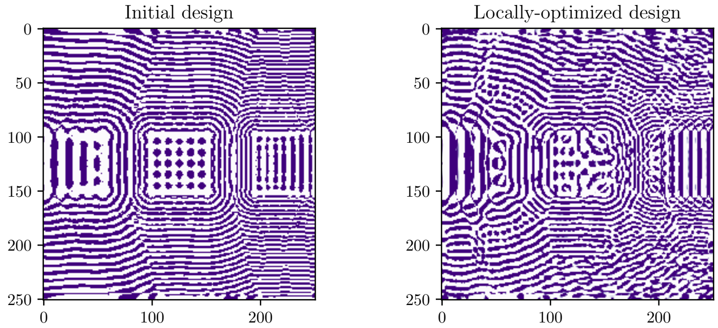
Some observations

- Always guaranteed to give a lower bound
- Solving can be done efficiently (in P)
- Solution gives reasonable initializations (!)
- This bound can be generalized to other objectives
  (Angeris, Diamandis, et al., 2022)

Results on bounds

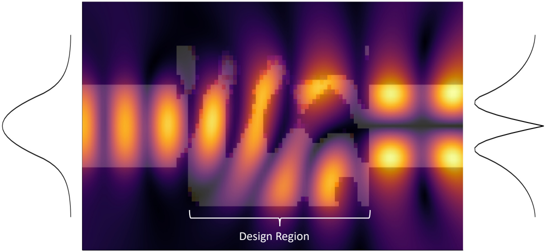
- There are many methods to get similar bounds
  (Angeris, Vučković, Boyd, 2019)

- Some suggest reasonable initializations



Results on bounds (continued)

- Similar bounds suggest that heuristics give nearly-optimal designs
- For example, mode converters are usually very close to optimal in both overlap and mode purity ($<$ 10% away)



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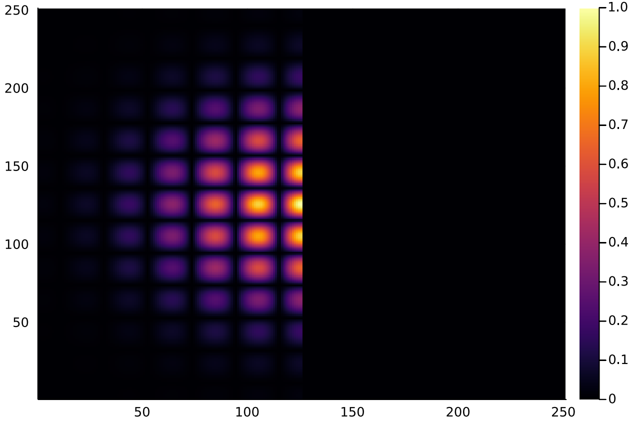
From start to end

- Let's see it in action
- Go from problem, to heuristic, to design, to bound!

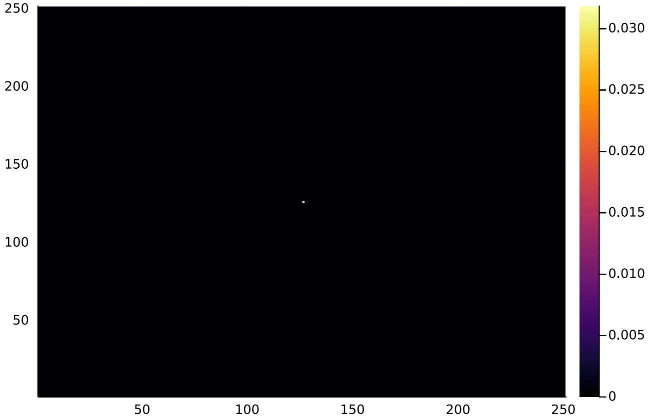
From start to end

- Goal: get a 'field' that looks like this



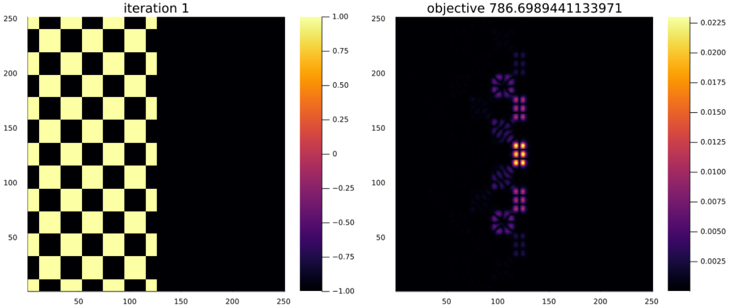
From start to end

- Given a single (tiny) excitation at the center:



From start to end

- Let's see what happens when we feed this to SFD!



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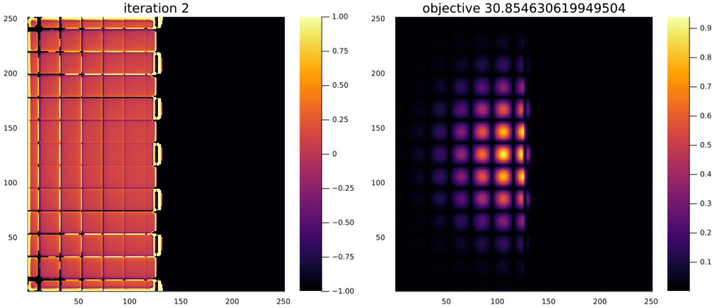

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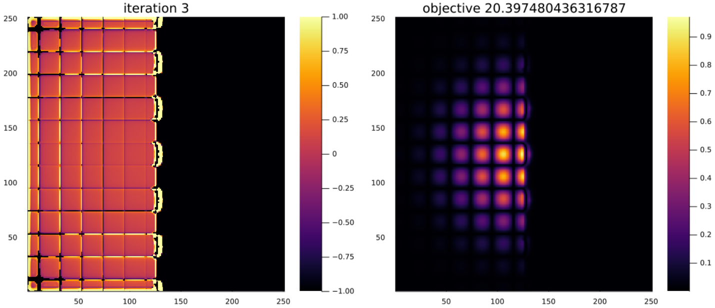

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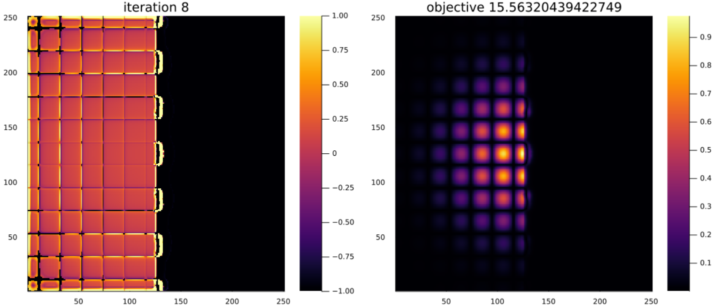

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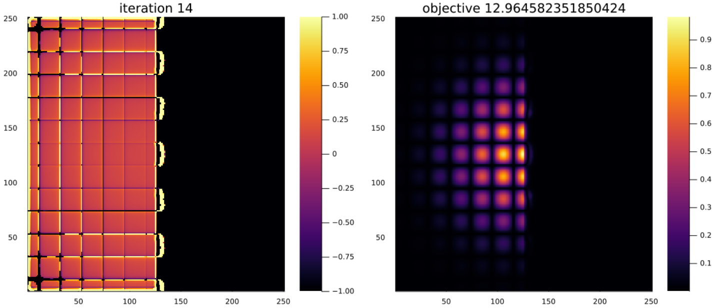

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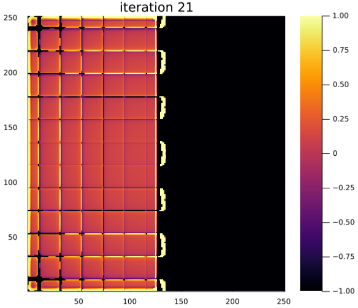

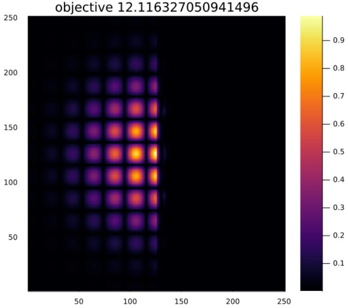

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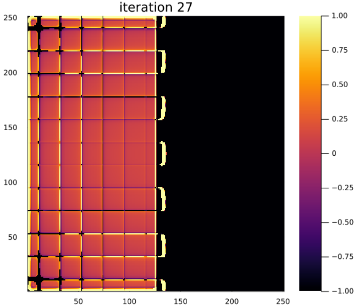

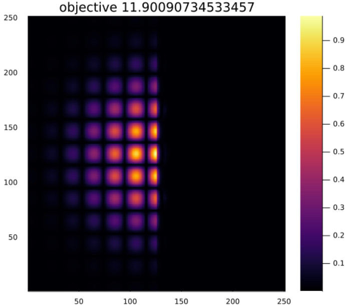

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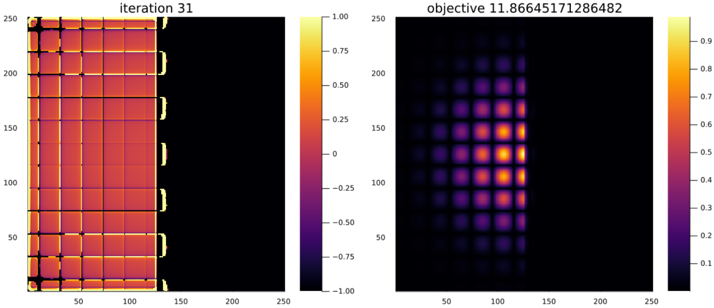

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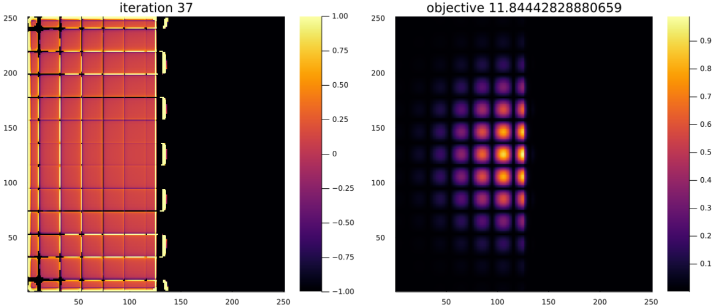

- And the algorithm terminates here!

From start to end

- SFD terminates with an objective value of 11.84
- What does the bound say is possible?

From start to end

- SFD terminates with an objective value of 11.84
- What does the bound say is possible? 11.69 (!)
- In other words, the design is no more than

$$\frac{11.84 - 11.69}{11.69} \approx 1.3\%$$

  suboptimal
- (We are essentially globally optimal!)

Conclusion

- Inverse design is *really* good at finding designs
- The photonic design problem is very structured, even though it is nonconvex and hard to solve exactly
- In general, bounds give us a good 'view of the land': can we even achieve a desired goal?
- Results suggest that the photonic design problem has more properties that can be exploited for faster solving

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- Coauthors: Theo, Alex, Tarun, Akshay, Shane, Kunal

Acknowledgements

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- And *you*!