Implementation-Robust Design:
Modeling, Theory, and Application to Photonic Crystal Design with Bandgaps

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\[ P(\varepsilon) : \quad f(\varepsilon) = \min_{x} c_{\varepsilon}^T x \quad \text{s.t.} \quad A_{\varepsilon} x = b_{\varepsilon}, \quad x \geq 0. \]

\[ D(\varepsilon) : \quad \max_{y} b_{\varepsilon}^T y \quad \text{s.t.} \quad A_{\varepsilon}^T y \leq c_{\varepsilon}, \]

**Sensitivity Analysis Theorem**

Suppose \((A_{\varepsilon}, b_{\varepsilon}, c_{\varepsilon}) = (A, b, c)_0 + \sum_{k=1}^{n} (A_k, b_k, c_k) \varepsilon_k\), where \(\varepsilon = (\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n)\) are parameters that determine the data \((A_{\varepsilon}, b_{\varepsilon}, c_{\varepsilon})\) of the LP pair \(P(\varepsilon), D(\varepsilon)\). For a given \(\hat{\varepsilon}\), if \(x^*, y^*\) are nondegenerate optimal solutions of \(P(\hat{\varepsilon})\) and \(D(\hat{\varepsilon})\), then

\[
\frac{\partial f(\varepsilon)}{\partial \varepsilon_k} \bigg|_{\varepsilon_k = \hat{\varepsilon}_k} = c_k^T x^* + b_k^T y^* - y^* A_k x^*.
\]
Wave Propagation in Periodic Media

For most $\lambda$, beam(s) propagate through crystal without scattering (scattering cancels coherently).

But for some $\lambda$ ($\sim 2a$), no light can propagate: a band gap

$E, H \sim e^{i(k \cdot x - \omega t)}$

$|k| = \frac{\omega}{c} = \frac{2\pi}{\lambda}$

(from S.G. Johnson)
**Photonic Crystals**

3D Crystals

Band Gap: Objective

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*S. G. Johnson et al., Appl. Phys. Lett. 77, 3490 (2000)*

**Applications**

By introducing “imperfections” one can develop:

- Waveguides
- Hyperlens
- Resonant cavities
- Switches
- Splitters
- …

*Mangan, et al., OFC 2004 PDP24*
The Optimal Design Problem for Photonic Crystals

A photonic crystal with optimized 7th band gap.
The Optimal Design Problem for Photonic Crystals

Exploit linearity and periodicity to formulate Maxwell’s equations as an eigenvalue problem

\[ A(\varepsilon(r, k))u = \lambda u \Rightarrow \lambda(\varepsilon(r), k) \]

\( \varepsilon(r) \) : dielectric function varying with the spatial position \( r \).
\( k \) : a parameterization of wave vector varying in the Brillouin zone \( \mathcal{B} \).
The gap-midgap ratio between $\lambda_m$ and $\lambda_{m+1}$ for $m \geq 1$ is defined as

$$J(\varepsilon(r)) = \frac{\min_{k \in B} \lambda_{m+1}(\varepsilon(r), k) - \max_{k \in B} \lambda_m(\varepsilon(r), k)}{\min_{k \in B} \lambda_{m+1}(\varepsilon(r), k) + \max_{k \in B} \lambda_m(\varepsilon(r), k)}$$
The design problem is to find an **optimal dielectric distribution** $\varepsilon_{opt}(r)$ that **maximizes** the gap-midgap ratio $J(\varepsilon(r))$.

This is in general a **non-convex, nonlinear, and infinite scale** optimization problem.
Previous Work

There are some approaches proposed for solving the band gap optimization problem:

- Cox and Dobson (2000) first considered the mathematical optimization of the band gap problem and proposed a projected generalized gradient ascent method.
- Sigmund and Jensen (2003) combined topology optimization with the method of moving asymptotes (Svanberg (1987)).
- Kao, Osher, and Yablonovith (2005) used “the level set” method with a generalized gradient ascent method.

However, these earlier proposals are gradient-based methods and use eigenvalues as explicit functions. They suffer from the low regularity of the problem due to eigenvalue multiplicity.
Optimization Formulation $P_0$

$$P_0: \max_{\varepsilon, \lambda^\ell, \lambda^u} \frac{\lambda^u - \lambda^\ell}{\lambda^u + \lambda^\ell}$$

s.t. $\lambda_m(\varepsilon, k) \leq \lambda^\ell, \; \lambda^u \leq \lambda_{m+1}(\varepsilon, k), \; \forall k \in \mathcal{B},$

$A(\varepsilon, k)u_m = \lambda_m M(\varepsilon)u_m, \; \forall k \in \mathcal{B},$

$A(\varepsilon, k)u_{m+1} = \lambda_{m+1} M(\varepsilon)u_{m+1}, \; \forall k \in \mathcal{B},$

$\varepsilon_{\min} \leq \varepsilon \leq \varepsilon_{\max},$

$\lambda^u, \lambda^\ell > 0.$

Typically,

- $n_k := |\mathcal{B}| = 10 \sim 20$
- $n_{\varepsilon} = 200 \sim 500$
- $\mathcal{N} = 2,000 \sim 4,000$
- $A, M$ are Hermitian, sparse, and banded
Results: Optimal Structures

Optimization of the band gap between $\lambda_{2}^{TE}$ and $\lambda_{3}^{TE}$.

Optimization of the band gap between $\lambda_{2}^{TM}$ and $\lambda_{3}^{TM}$. 
### Results: Computation Time

#### TE polarization

<table>
<thead>
<tr>
<th>Execution time (min)</th>
<th>$\Delta \lambda_{TE}^{1,2}$</th>
<th>$\Delta \lambda_{TE}^{2,3}$</th>
<th>$\Delta \lambda_{TE}^{3,4}$</th>
<th>$\Delta \lambda_{TE}^{4,5}$</th>
<th>$\Delta \lambda_{TE}^{5,6}$</th>
<th>$\Delta \lambda_{TE}^{6,7}$</th>
<th>$\Delta \lambda_{TE}^{7,8}$</th>
<th>$\Delta \lambda_{TE}^{8,9}$</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>0.46</td>
<td>0.65</td>
<td>0.98</td>
<td>0.43</td>
<td>1.4</td>
<td>2.0</td>
<td>2.2</td>
<td>1.4</td>
</tr>
</tbody>
</table>

#### TM polarization

<table>
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<th>Execution time (min)</th>
<th>$\Delta \lambda_{TM}^{1,2}$</th>
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<tr>
<td></td>
<td>0.12</td>
<td>0.19</td>
<td>0.22</td>
<td>0.31</td>
<td>0.47</td>
<td>0.51</td>
<td>0.81</td>
<td>0.58</td>
</tr>
</tbody>
</table>

All computations performed on a Linux PC with dual core AMD Opteron 270, 1.99GHz.
Multiple Band Gap Optimization

Multiple band gap optimization is a natural extension of single band gap optimization, that seeks to maximize the (weighted) minimum of multiple gap-midgap ratios:

\[
\max_{\varepsilon \in S} \min_{1 \leq j \leq J} \sum_{k \in B} w_j \frac{\min_{k \in B} \lambda_{m_j+1}(\varepsilon, k) - \max_{k \in B} \lambda_{m_j}(\varepsilon, k)}{\min_{k \in B} \lambda_{m_j+1}(\varepsilon, k) + \max_{k \in B} \lambda_{m_j}(\varepsilon, k)},
\]

s.t.
\[
A(\varepsilon, k)u_m = \lambda_m M(\varepsilon)u_m, \\
m = m_j, m_j + 1, 1 \leq j \leq J, k \in B.
\]
Optimized Structures

- TE polarization,
- Triangular lattice,
- 1st and 3rd band gaps.

- TEM polarization,
- Square lattice,
- Complete band gaps,
- 3rd TE gap, 6th and 9th TM band gaps.
Need for Fabrication Robustness

Consider the optimized photonic crystal designs (PCDs):

These two PCDs cannot be easily fabricated due to
- small components, and
- the boundaries are too intricate for precise fabrication
Design Variables and Eigenvalues

Let $A_i \in \mathbb{C}^{N \times N}$, $0 = 1, \ldots, n$, and $M \in \mathbb{C}^{N \times N}$ and $M \succ 0$

Define $A(\epsilon) = A_0 + \sum_{i=1}^{n} A_i \epsilon_i$ where $\epsilon = (\epsilon_1, \ldots, \epsilon_n) \in \mathbb{R}^n$ are our design variables

Typically $\epsilon \in S$ and $S$ is a hypercube:
\[
\{ \epsilon \in \mathbb{R}^n : \epsilon_{\text{min}} \leq \epsilon \leq \epsilon_{\text{max}} \}
\]

Consider the generalized eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_N$ defined by:

$$A(\epsilon)u_j = \lambda_j Mu_j , \ j = 1, \ldots, N$$
Bandgap

\[ A(\varepsilon)u_j = \lambda_j Mu_j , \quad j = 1, \ldots, N \]

In many physics/engineering metamaterial applications one seeks to maximize the bandgap between two given consecutive eigenvalues:

\[ \max_{\varepsilon} \lambda_{m+1} - \lambda_m \]

s.t. \[ A(\varepsilon)u_j = \lambda_j Mu_j , \quad j = m, m + 1 \]

\[ \varepsilon \in S = \{ \varepsilon \in \mathbb{R}^n : \varepsilon_{\min e} \leq \varepsilon \leq \varepsilon_{\max e} \} \]
Relative Bandgap, Binary Model

One important refinement is to optimize the gap-midgap ratio:

$$\max_{\varepsilon} \frac{\lambda_{m+1} - \lambda_m}{\lambda_{m+1} + \lambda_m}$$

s.t. $$A(\varepsilon) u_j = \lambda_j M u_j, \quad j = m, m + 1$$

$$\varepsilon \in S = \{ \varepsilon \in \mathbb{R}^n : \varepsilon_{\min} e \leq \varepsilon \leq \varepsilon_{\max} e \}$$

Another refinement is to use the more realistic binary model of the design variables:

$$S = \{ \varepsilon \in \mathbb{R}^n : \varepsilon_i \in \{ \varepsilon_{\min}, \varepsilon_{\max} \}, \quad i = 1, \ldots, n \}$$

In our applications we fortunately obtain binary solutions “for free”
Tractability

\[
\max_{\varepsilon} \frac{\lambda_{m+1} - \lambda_m}{\lambda_{m+1} + \lambda_m}
\]

\[
s.t. \quad A(\varepsilon)u_j = \lambda_j M u_j, \quad j = m, m + 1
\]

\[
\varepsilon \in S
\]

Even when \( S \) is convex, this problem is nonconvex and nonlinear.

Traditional solution approaches build local models of the eigenvalue functions \( \lambda_j(\varepsilon) \) and take gradient or other first-order steps.

Methods suffer from low regularity due to eigenvalue multiplicities.
Reformulation

\[
\max_{\varepsilon, \lambda_\ell, \lambda_u} \frac{\lambda_u - \lambda_\ell}{\lambda_\ell + \lambda_u} \\
\text{s.t. } A(\varepsilon)u_j = \lambda_jMu_j, \quad j = m, m + 1 \\
\lambda_m \leq \lambda_\ell \leq \lambda_u \leq \lambda_{m+1} \\
\varepsilon \in S
\]

Introduce \( \Phi^\varepsilon = [\Phi^\varepsilon_\ell | \Phi^\varepsilon_u] = [u^{1\varepsilon} | \cdots | u^{m\varepsilon} | u^{m+1\varepsilon} | \cdots | u^{N\varepsilon}] \)

\[
\max_{\varepsilon, \lambda_\ell, \lambda_u} \frac{\lambda_u - \lambda_\ell}{\lambda_\ell + \lambda_u} \\
\text{s.t. } (\Phi^\varepsilon_\ell)^* [A(\varepsilon) - \lambda_\ell M] \Phi^\varepsilon_\ell \preceq 0 \\
(\Phi^\varepsilon_u)^* [A(\varepsilon) - \lambda_u M] \Phi^\varepsilon_u \succeq 0 \\
\varepsilon \in S
\]
Approximation by Fixing Subspaces

\[
\begin{align*}
\max_{\varepsilon, \lambda_\ell, \lambda_u} & \quad \frac{\lambda_u - \lambda_\ell}{\lambda_u + \lambda_\ell} \\
\text{s.t.} & \quad (\Phi_\varepsilon^\ell)^* [A(\varepsilon) - \lambda_\ell M] \Phi_\varepsilon^\ell \preceq 0 \\
& \quad (\Phi_u^\varepsilon)^* [A(\varepsilon) - \lambda_u M] \Phi_u^\varepsilon \succeq 0 \\
& \quad \varepsilon \in S
\end{align*}
\]

Approximate this model by keeping the subspaces fixed based on the previous design variable value \( \hat{\varepsilon} \):

\[
\begin{align*}
\max_{\varepsilon, \lambda_\ell, \lambda_u} & \quad \frac{\lambda_u - \lambda_\ell}{\lambda_\ell + \lambda_u} \\
\text{s.t.} & \quad (\Phi_\varepsilon^\ell)^* [A(\varepsilon) - \lambda_\ell M] \Phi_\varepsilon^\ell \preceq 0 \\
& \quad (\Phi_u^\varepsilon)^* [A(\varepsilon) - \lambda_u M] \Phi_u^\varepsilon \succeq 0 \\
& \quad \varepsilon \in S
\end{align*}
\]

This is a linear fractional SDP, for which there is a standard conversion to a linear SDP.
Reducing the Scale

The SDP inclusions are large-scale (especially the 2nd set):
$N \approx 2000 - 4000$

We reduce the scale by only considering the “important” eigenvectors in the spirit of active-set methods:

$$\Phi^\varepsilon_\ell := [u_1^\varepsilon \cdots u_m^\varepsilon] \rightarrow [u_{m-b+1}^\varepsilon \cdots u_m^\varepsilon] =: \Phi^\varepsilon_b$$

$$\Phi^\varepsilon_u := [u_{m+1}^\varepsilon \cdots u_N^\varepsilon] \rightarrow [u_{m+1}^\varepsilon \cdots u_{m+a}^\varepsilon] =: \Phi^\varepsilon_a$$

where $a, b$ are small integers chosen heuristically, typically $a, b \sim 2, \ldots, 5$
The reduced-scale problem then is:

\[ P_{a,b}^\hat{\varepsilon} : \max_{\varepsilon, \lambda_\ell, \lambda_u} \frac{\lambda_u - \lambda_\ell}{\lambda_\ell + \lambda_u} \]

s.t. \[
\begin{align*}
(\Phi_{b}^\hat{\varepsilon})^* [A(\varepsilon) - \lambda_\ell M] \Phi_{b}^\hat{\varepsilon} & \preceq 0 \\
(\Phi_{a}^\hat{\varepsilon})^* [A(\varepsilon) - \lambda_u M] \Phi_{a}^\hat{\varepsilon} & \succeq 0 \\
\varepsilon & \in S
\end{align*}
\]

\( P_{a,b}^\hat{\varepsilon} \) has significantly smaller semidefinite inclusions than if the full subspaces were used.

\( P_{a,b}^\hat{\varepsilon} \) is a linear fractional SDP, and is amenable to solution by modern IPM software such as SDPT3.
Basic Solution Procedure

<table>
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<th>Basic Eigenvalue Separation Methodology</th>
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<td><strong>Step 1.</strong> Start with initial guess ( \hat{\varepsilon} := \varepsilon^0 ) and tolerance ( \varepsilon_{\text{tol}} )</td>
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| **Step 2.** Determine subspace dimensions \( a \) and \( b \)  
  Compute the subspaces \( \Phi_{\hat{\varepsilon}}^a \) and \( \Phi_{\hat{\varepsilon}}^b \) |
| **Step 3.** Form the convex SDP \( P_{\hat{\varepsilon}}^{a,b} \) |
| **Step 4.** Solve \( P_{\hat{\varepsilon}}^{a,b} \) for an optimal solution \( \varepsilon^* \) |
| **Step 5.** If \( \| \varepsilon^* - \hat{\varepsilon} \| \leq \varepsilon_{\text{tol}} \), stop.  
  Else update \( \hat{\varepsilon} \leftarrow \varepsilon^* \) and go to **Step 2.** |
Alternative Functional Forms for Eigensystem

In some applications we have:

\[ A(\varepsilon) = A_0 + \sum_{i=1}^{n} A_i (1/\varepsilon_i), \quad M \succ 0 \text{ is fixed.} \]

Define \( \tilde{\varepsilon}_i = 1/\varepsilon_i \), \( \tilde{S} := \{ \tilde{\varepsilon} \in \mathbb{R}^n : (1/\varepsilon_{\text{max}})e \leq \tilde{\varepsilon} \leq (1/\varepsilon_{\text{min}})e \} \) and proceed as before.

In other applications we have:

\[ A \succ 0 \text{ is fixed, and } M(\varepsilon) = M_0 + \sum_{i=1}^{n} M_i \varepsilon_i. \]

Define \( \tilde{\lambda}_j = 1/\lambda_j \) and work with reciprocal of eigenvalues:

\[ \tilde{\lambda}_j A u_j = M(\varepsilon) u_j , \quad j = 1, \ldots, N \]

Convenient arithmetic:

\[ \frac{\lambda_u - \lambda_{\ell}}{\lambda_{\ell} + \lambda_u} = \frac{\tilde{\lambda}_{\ell} - \tilde{\lambda}_u}{\tilde{\lambda}_u + \tilde{\lambda}_{\ell}} \]
Virtually all applications have simultaneous multiple eigensystems:

\[
\begin{align*}
\max_{\varepsilon} & \quad \frac{\min_k \in B \lambda_{m+1}(k) - \max_k \in B \lambda_m(k)}{\min_k \in B \lambda_{m+1}(k) + \max_k \in B \lambda_m(k)} \\
\text{s.t.} & \quad A(\varepsilon, k)u_j(k) = \lambda_j(k)M(k)u_j(k), \quad j = m, m+1, \quad k \in B \\
\varepsilon \in S & = \{ \varepsilon \in \mathbb{R}^n : \varepsilon_{\min} \leq \varepsilon \leq \varepsilon_{\max} \}
\end{align*}
\]

Let \( \Phi^\varepsilon(k) = [\Phi^\varepsilon(\ell)(k) | \Phi^\varepsilon_u(k)] = [u^1 \cdots u^m | u^{m+1} \cdots u^N](\varepsilon, k) \) for \( k \in B \)

Then reduce the scale as earlier:

\[
\Phi^\varepsilon_\ell(k) := [u^1 \cdots u^m](\varepsilon, k) \rightarrow [u^{m-b+1} \cdots u^m](\varepsilon, k) =: \Phi^\varepsilon_b(k)
\]

\[
\Phi^\varepsilon_u(k) := [u^{m+1} \cdots u^N](\varepsilon, k) \rightarrow [u^{m+1} \cdots u^{m+a}](\varepsilon, k) =: \Phi^\varepsilon_a(k)
\]

where \( a, b \) are small integers chosen heuristically, typically \( a, b \sim 2, \ldots, 5 \)
The reduced-scale multiple-system problem then is:

\[ P_{a,b}^\hat{\varepsilon} : \quad \max_{\varepsilon, \lambda_\ell, \lambda_u} \quad \frac{\lambda_u - \lambda_\ell}{\lambda_\ell + \lambda_u} \]

\[ \text{s.t. } \begin{align*}
(\Phi_b^\hat{\varepsilon}(k))^* [A(\varepsilon, k) - \lambda_\ell M(k)] \Phi_b^\hat{\varepsilon}(k) &\preceq 0 , \quad k \in B \\
(\Phi_a^\hat{\varepsilon}(k))^* [A(\varepsilon, k) - \lambda_u M(k)] \Phi_a^\hat{\varepsilon}(k) &\succeq 0 , \quad k \in B \\
\varepsilon &\in S
\end{align*} \]

\( P_{a,b}^\hat{\varepsilon} \) has significantly smaller semidefinite inclusions than if the full subspaces were used.

\( P_{a,b}^\hat{\varepsilon} \) is a linear fractional SDP, and is amenable to solution by modern IPM software such as SDPT3.
### Multiple Eigensystem Solution Procedure

#### Multiple Eigensystems Separation Methodology

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| **Step 2.** | For each $k \in \mathcal{B}$ do:  
Determine subspace dimensions $a$ and $b$  
Compute the subspaces $\Phi_{a}(k)$ and $\Phi_{b}(k)$ |
| **Step 3.** | Form the convex SDP $P_{a,b}^\hat{\epsilon}$ |
| **Step 4.** | Solve $P_{a,b}^\hat{\epsilon}$ for an optimal solution $\epsilon^*$ |
| **Step 5.** | If $\|\epsilon^* - \hat{\epsilon}\| \leq \epsilon_{\text{tol}}$, stop.  
Else update $\hat{\epsilon} \leftarrow \epsilon^*$ and go to **Step 2.** |
Recall the optimization formulation $P_0$ of the Photonic Crystal Design (PCD) problem:

$$P_0 : \max_{\varepsilon, \lambda_\ell, \lambda_u} \frac{\lambda_u - \lambda_\ell}{\lambda_u + \lambda_\ell}$$

s.t.

$$\lambda_m(\varepsilon, k) \leq \lambda_\ell, \quad \lambda_u \leq \lambda_{m+1}(\varepsilon, k), \quad \forall k \in B,$$

$$A(\varepsilon, k) u_m = \lambda_m M(k) u_m, \quad \forall k \in B,$$

$$A(\varepsilon, k) u_{m+1} = \lambda_{m+1} M(k) u_{m+1}, \quad \forall k \in B,$$

$$\varepsilon_{\min} e \leq \varepsilon \leq \varepsilon_{\max} e,$$

$$\lambda_u, \lambda_\ell > 0.$$
SDP Approximation of the Photonic Crystal Design Problem

The reduced-scale SDP approximation of $P_0$ at $\hat{\varepsilon}$ is:

$$\begin{align*}
P_{SDP}^\hat{\varepsilon} : \quad & \max_{\varepsilon, \lambda_\ell, \lambda_u} \frac{\lambda_u - \lambda_\ell}{\lambda_u + \lambda_\ell} \\
\text{s.t.} & \quad A_\ell(\varepsilon, k_t) \preceq \lambda_\ell M_\ell(\varepsilon, k_t), \quad t = 1, \ldots, n_k, \\
& \quad A_u(\varepsilon, k_t) \succeq \lambda_u M_u(\varepsilon, k_t), \quad t = 1, \ldots, n_k, \\
& \quad \varepsilon_{\min} \leq \varepsilon \leq \varepsilon_{\max}, \\
& \quad \lambda_\ell \geq 0, \quad \lambda_u \geq 0,
\end{align*}$$

where

$$\begin{align*}
\Phi_b^\hat{\varepsilon}(k_t) & := [u^{m-b+1} \cdots u^m](\hat{\varepsilon}, k_t) \\
M_\ell^\hat{\varepsilon}(k_t) & := [\Phi_b^\hat{\varepsilon}(k_t)]^* M(k_t) [\Phi_b^\hat{\varepsilon}(k_t)] \\
A_\ell^\hat{\varepsilon}(\varepsilon, k_t) & := [\Phi_b^\hat{\varepsilon}(k_t)]^* A(\varepsilon, k_t) [\Phi_b^\hat{\varepsilon}(k_t)] \\
\Phi_a^\hat{\varepsilon}(k_t) & := [u^{m+1} \cdots u^{m+a}](\hat{\varepsilon}, k_t) \\
M_u^\hat{\varepsilon}(k_t) & := [\Phi_a^\hat{\varepsilon}(k_t)]^* M(k_t) [\Phi_a^\hat{\varepsilon}(k_t)] \\
A_u^\hat{\varepsilon}(\varepsilon, k_t) & := [\Phi_a^\hat{\varepsilon}(k_t)]^* A(\varepsilon, k_t) [\Phi_a^\hat{\varepsilon}(k_t)]
\end{align*}$$
**Photonic Crystal Design Problem Solution Procedure**

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Determine subspace dimensions $a$ and $b$  
Compute the subspaces $\Phi_{\hat{a}}(k_t)$ and $\Phi_{\hat{b}}(k_t)$ |
| **Step 3.** | Form the convex SDP $P_{SDP}^{\hat{\varepsilon}}$ |
| **Step 4.** | Solve $P_{SDP}^{\hat{\varepsilon}}$ for an optimal solution $\varepsilon^*$ |
| **Step 5.** | If $\|\varepsilon^* - \hat{\varepsilon}\| \leq \varepsilon_{tol}$, stop.  
Else update $\hat{\varepsilon} \leftarrow \varepsilon^*$ and go to Step 2. |
Recall the reduced-scale SDP approximation of the PCD bandgap optimization problem at \( \hat{\epsilon} \): The reduced-scale SDP approximation of \( P_0 \) at \( \hat{\epsilon} \) is:

\[
P_{\text{SDP}}^{\hat{\epsilon}} : \max_{\epsilon, \lambda_\ell, \lambda_u} \frac{\lambda_u - \lambda_\ell}{\lambda_u + \lambda_\ell}
\]

s.t. \[
A_{\ell}(\epsilon, k_t) \leq \lambda_\ell M_{\ell}(k_t), \quad t = 1, \ldots, n_k, \\
A_{u}(\epsilon, k_t) \geq \lambda_u M_{u}(k_t), \quad t = 1, \ldots, n_k, \\
\epsilon_{\min} \leq \epsilon \leq \epsilon_{\max}, \\
\lambda_\ell \geq 0, \lambda_u \geq 0,
\]

where

\[
\Phi_{b}(k_t) := [u^{m-b+1} \ldots u^m](\hat{\epsilon}, k_t) \\
M_{\ell}(k_t) := [\Phi_{b}(k_t)]^* M(k_t) [\Phi_{b}(k_t)] \\
A_{\ell}(\epsilon, k_t) := [\Phi_{b}(k_t)]^* A(\epsilon, k_t) [\Phi_{b}(k_t)] \\
\Phi_{a}(k_t) := [u^{m+1} \ldots u^{m+a}](\hat{\epsilon}, k_t) \\
M_{u}(k_t) := [\Phi_{a}(k_t)]^* M(k_t) [\Phi_{a}(k_t)] \\
A_{u}(\epsilon, k_t) := [\Phi_{a}(k_t)]^* A(\epsilon, k_t) [\Phi_{a}(k_t)]
\]
LP Approximation of the SDP at $\hat{\varepsilon}$

$$P_{\text{SDP}}^{\hat{\varepsilon}} : \max_{\varepsilon, \lambda_\ell, \lambda_u} \frac{\lambda_u - \lambda_\ell}{\lambda_u + \lambda_\ell}$$

s.t.

$$A_\ell(\varepsilon, k_t) \preceq \lambda_\ell M_\ell^{\hat{\varepsilon}}(k_t), \quad t = 1, \ldots, n_k,$$

$$A_u(\varepsilon, k_t) \succeq \lambda_u M_u^{\hat{\varepsilon}}(k_t), \quad t = 1, \ldots, n_k,$$

$$\varepsilon_{\text{min}} \leq \varepsilon \leq \varepsilon_{\text{max}}$$

$$\lambda_\ell \geq 0, \; \lambda_u \geq 0,$$

Judiciously choose vectors $b^1, \ldots, b^{N_B}$ and $c^1, \ldots, c^{N_C}$ and replace the SDP inclusions with:

$$(b^i)^T[A_\ell(\varepsilon, k_t)](b^i) \leq (b^i)^T[\lambda_\ell M_\ell^{\hat{\varepsilon}}(k_t)](b^i), \quad t = 1, \ldots, n_k, \; j = 1, \ldots, N_B,$$

$$(c^i)^T[A_u(\varepsilon, k_t)](c^i) \geq (c^i)^T[\lambda_u M_u^{\hat{\varepsilon}}(k_t)](c^i), \quad t = 1, \ldots, n_k, \; i = 1, \ldots, N_C$$

Here $N_B \approx 100$, $N_C \approx 100$, and $n_\varepsilon \approx 200 - 500$
LP Approximation of SDP, continued

\[ P_{\hat{\text{SDP}}} : \max_{\varepsilon, \lambda_{\ell}, \lambda_u} \frac{\lambda_u - \lambda_{\ell}}{\lambda_u + \lambda_{\ell}} \]

s.t. \[ A_{\ell}(\varepsilon, k_t) \leq \lambda_{\ell} M_{\ell}(k_t), \quad t = 1, \ldots, n_k, \]
\[ A_u(\varepsilon, k_t) \geq \lambda_u M_u(k_t), \quad t = 1, \ldots, n_k, \]
\[ \varepsilon_{\min e} \leq \varepsilon \leq \varepsilon_{\max e} \]
\[ \lambda_{\ell} \geq 0, \quad \lambda_u \geq 0 \]

is approximated by:

\[ P_{\hat{\text{LFP}}} : \max_{\varepsilon, \lambda_{\ell}, \lambda_u} \frac{\lambda_u - \lambda_{\ell}}{\lambda_u + \lambda_{\ell}} \]

s.t. \[ B_{\ell} \varepsilon \leq e \lambda_{\ell} \]
\[ C_{\ell} \varepsilon \geq e \lambda_u \]
\[ \varepsilon_{\min e} \leq \varepsilon \leq \varepsilon_{\max e} \]
\[ \lambda_{\ell} \geq 0, \quad \lambda_u \geq 0 \]

Note that the data for the LFP constraints depend (linearly) on the current point \( \hat{\varepsilon} \).
### Photonic Crystal Design Problem Solution Procedure via LP Approximation

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Quality of Solutions Produced by LP Approximation Method

We solved 10 trials of each problem using 10 different randomly chosen starting points:

**TE polarization**

<table>
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<tr>
<th>Average Outer Iterations / Number of Successful Solutions</th>
<th>$\Delta \lambda_{1,2}^{TE}$</th>
<th>$\Delta \lambda_{2,3}^{TE}$</th>
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<th>$\Delta \lambda_{9,10}^{TE}$</th>
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<tbody>
<tr>
<td><strong>SDP</strong></td>
<td>9.0/7</td>
<td>9.0/6</td>
<td>14.2/2</td>
<td>23.5/1</td>
</tr>
<tr>
<td><strong>LFP</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
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<td>$N_B, N_C \sim 10$ plus delayed constraint generation</td>
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Need for Fabrication Robustness

Consider the optimized photonic crystal designs (PCDs):

These two PCDs cannot be easily fabricated due to
- small components, and
- the boundaries are too intricate for precise fabrication.
We consider a very general optimization problem:

\[
\begin{align*}
    z^* &= \min_x f(x) \\
    \text{s.t.} & \quad x \in S
\end{align*}
\]

where \( S \subset \mathbb{R}^n \) is the feasible region. Let \( x^* \) be an optimal solution.

In many cases, it is not possible to fabricate/implement the optimal solution \( x^* \) due to any of the following reasons:

- deliberate simplification of the model to keep it tractable
- technological factors
- human factors
We anticipate that any solution $x$ can be easily converted to a fabricable solution $y$ that is within a distance $\delta$ of $x$. Replace $f(x)$ with the (conservative) fabrication robust (FR) counterpart function:

$$\tilde{f}(x) = \max_y f(y)$$

subject to

$$\|y - x\| \leq \delta$$

$y \in S$

where $\delta > 0$ is the FR parameter and $\| \cdot \|$ is some suitable norm, and instead solve:

$$\tilde{z}^* = \min_x \tilde{f}(x)$$

subject to

$x \in S$
Basic Results

\[ \tilde{f}(x) = \max_y f(y) \]
\[ \text{s.t. } \|y - x\| \leq \delta \]
\[ y \in S \]

\[ \tilde{z}^* = \min_x \tilde{f}(x) \]
\[ \text{s.t. } x \in S \]

**Theorem**

Suppose that \( S = \mathbb{R}^n \). Then:

- \( f(\cdot) \) is convex \( \Rightarrow \) \( \tilde{f}(\cdot) \) is convex.
- \( f(\cdot) \) is quasiconvex \( \Rightarrow \) \( \tilde{f}(\cdot) \) is quasiconvex.
Basic Results, continued

\[ \tilde{f}(x) = \max_y f(y) \]
\[ \text{s.t. } \|y - x\| \leq \delta \]
\[ y \in S \]

\[ \tilde{z}^* = \min_x \tilde{f}(x) \]
\[ \text{s.t. } x \in S \]

**Remark 1**

Unfortunately, when \( S \neq \mathbb{R}^n \), convex structure can be lost.

**Remark 2**

Generically, computing \( \tilde{z}^* \) is intractable. Indeed, simply computing \( \tilde{f}(x) \) is generally intractable as it involves maximizing a convex function.
Basic Results, continued

\[ \tilde{f}(x) = \max_y f(y) \]
\[ \text{s.t. } ||y - x|| \leq \delta \]
\[ y \in S \]

\[ \tilde{z}^* = \min_x \tilde{f}(x) \]
\[ \text{s.t. } x \in S \]

Remark 3
The computational viability of the FR model will therefore depend on special structure of \( f(\cdot) \), \( S \), and/or \( ||\cdot|| \).
Example 1: $S = \mathbb{R}^n$, $\| \cdot \|$ is any norm, $f(\cdot)$ is PL (piecewise linear) convex:

$$f(x) := \max_{i=1,\ldots,m} b_i + (a^i)^T x$$

Since $S = \mathbb{R}^n$, it is easy to derive that

$$\tilde{f}(x) = \max_{i=1,\ldots,m} (b_i + \delta \|a^i\|_*) + (a^i)^T x,$$

where $\| \cdot \|_*$ is the dual norm of $\| \cdot \|$.

Therefore $\tilde{f}(\cdot)$ retains the same properties of $f(\cdot)$ as PL convex, etc.
Computable FR Problems via Special Structure, continued

Example 2: $S$ is a polyhedon, $\| \cdot \|$ is $L_2$, $L_1$, or $L_\infty$-norm, $f(\cdot)$ is PL convex as before:

$$f(x) := \max_{i=1,...,m} b_i + (a_i)^T x$$

Then:

$$\tilde{f}(x) = \max_{y \in S, \|y-x\| \leq \delta} \max_{i=1,...,m} b_i + (a_i)^T y$$
$$= \max_{i=1,...,m} \max_{y \in S, \|y-x\| \leq \delta} b_i + (a_i)^T y$$
$$= \max_{i=1,...,m} b_i + c_i^*(x)$$

where, for $i = 1, \ldots, m$,

$$c_i^*(x) := \max_y (a_i)^T y$$
$$\text{s.t. } y \in S$$
$$\|y - x\| \leq \delta .$$

Computing $\tilde{f}(x)$ amounts to solving $m$ second-order cone optimization problems (when $\| \cdot \| = \| \cdot \|_2$) or linear programs (when $\| \cdot \| = \| \cdot \|_1$ or $\| \cdot \|_\infty$).
Example 2, continued:

\[ \tilde{f}(x) = \max_{i=1,...,m} b_i + c^*_i(x) \]

where, for \( i = 1, \ldots, m, \)

\[ c^*_i(x) := \max_y (a^i)^T y \]
\[ \text{s.t. } y \in S \]
\[ \|y - x\| \leq \delta. \]

Remark

Each \( c^*_i(\cdot) \) is concave in \( x \), whereby \( \tilde{f}(\cdot) \) is the pointwise maximum of \( m \) concave functions.
Example 3: Consider the largest eigenvalue of a symmetric matrix that is a linear function of the design variables $x \in S := [x_{\text{min}}, x_{\text{max}}]^n$ and $\| \cdot \| := \| \cdot \|_1$

$$f(x) := \lambda_{\text{max}} \left( A_0 + \sum_{j=1}^{n} A_j x_j \right)$$

The FR model is:

$$\tilde{f}(x) := \max_{y \in S, \|y-x\|_1 \leq \delta} \lambda_{\text{max}} \left( A_0 + \sum_{j=1}^{n} A_j y_j \right)$$

Considering the special case when $x_{\text{min}} = 0$, $x_{\text{max}} = 1$, and $x = 0$ yields:

$$\tilde{f}(x) = \max_{v^T v \leq 1} v^T A_0 v + \|(v^T A_1 v)^+ + (v^T A_2 v)^+ + \ldots + (v^T A_n v)^+\|_{50}^{\diamondsuit}$$

where $(\gamma)^+$ denotes the positive part of the scalar $\gamma$, and $\|v\|_{50}^{\diamondsuit}$ is the sum of the 50 largest coefficients of $v$.

Remark

Although $f(x)$ is a computable convex function of $x$, the problem of computing $\tilde{f}(x)$ appears to be intractable. This is unfortunate, as modeling largest (and smallest) eigenvalues arises of necessity in photonic crystal design problems.
Here $x \in S := [x_{\text{min}}, x_{\text{max}}]^n$. Assume we anticipate the ability to modify $x$ to a fabricable solution $y = x + d$, where

$$x_{\text{min}} e \leq y \leq x_{\text{max}} e \quad \iff \quad x_{\text{min}} e - x \leq d \leq x_{\text{max}} e - x$$

$$\|y - x\|_1 \leq \delta \quad \iff \quad \|d\|_1 \leq \delta$$

Typically $\delta \ll n(x_{\text{max}} - x_{\text{min}})$. 
If $S = [x_{\text{min}}, x_{\text{max}}]^n$, $\| \cdot \| = \| \cdot \|_1$, and $f(\cdot)$ is PL convex:

$$f(x) := \max_{i=1,\ldots,m} b_i + (a^i)^T x,$$

then

$$\tilde{f}(x) := \max_y f(y) \quad \text{s.t.} \quad \|y - x\|_1 \leq \delta$$

$$x_{\text{min}} e \leq y \leq x_{\text{max}} e,$$

By the change of variable $d = y - x$ we can write:

$$\tilde{f}(x) = \max_{i=1,\ldots,m} \left( b_i + (a^i)^T x + \max_{x_{\text{min}} e - x \leq d \leq x_{\text{max}} e - x, \|d\|_1 \leq \delta} (a^i)^T d \right).$$

**Remark**

Note that the maximization problem in the right-most expression above is a very simple LP that can be solved in $O(n \ln(n))$ operations by ordering the components $|a_i|$. This suggests we try to model photonic crystal design with a PL function (approximations) of the eigenvalues.
Recall the LFP approximation of bandgap problem at $\hat{\varepsilon}$:

$$P_{LFP}^{\hat{\varepsilon}} : \max_{\varepsilon, \lambda_\ell, \lambda_u} \frac{\lambda_u - \lambda_\ell}{\lambda_u + \lambda_\ell}$$

s.t.  
$$B^{\hat{\varepsilon}\varepsilon} \leq e \lambda_\ell$$

$$C^{\hat{\varepsilon}\varepsilon} \geq e \lambda_u$$

$$\varepsilon_{\text{min}} e \leq \varepsilon \leq \varepsilon_{\text{max}} e$$

$$\lambda_\ell \geq 0, \lambda_u \geq 0$$

Re-write as:

$$P_{LFP}^{\hat{\varepsilon}} : \max_{\varepsilon, \lambda_\ell, \lambda_u} f^{\hat{\varepsilon}}(\varepsilon) := \frac{\min_i (C^{\hat{\varepsilon}\varepsilon})_i - \max_j (B^{\hat{\varepsilon}\varepsilon})_j}{\min_i (C^{\hat{\varepsilon}\varepsilon})_i + \max_j (B^{\hat{\varepsilon}\varepsilon})_j}$$

s.t.  
$$\varepsilon_{\text{min}} e \leq \varepsilon \leq \varepsilon_{\text{max}} e$$
Fabrication Robust Model for Bandgap Optimization, continued

\[ P_{LFP}^{\hat{\varepsilon}} : \max_{\varepsilon, \lambda_{\ell}, \lambda_{u}} f^{\hat{\varepsilon}}(\varepsilon) := \frac{\min_i (C^{\hat{\varepsilon}} \varepsilon)_i - \max_j (B^{\hat{\varepsilon}} \varepsilon)_j}{\min_i (C^{\hat{\varepsilon}} \varepsilon)_i + \max_j (B^{\hat{\varepsilon}} \varepsilon)_j} \]

\[ \text{s.t. } \varepsilon_{\min e} \leq \varepsilon \leq \varepsilon_{\max e} \]

Define \( f_{i,j}^{\hat{\varepsilon}}(\varepsilon) := \frac{(C^{\hat{\varepsilon}} \varepsilon)_i - (B^{\hat{\varepsilon}} \varepsilon)_j}{(C^{\hat{\varepsilon}} \varepsilon)_i + (B^{\hat{\varepsilon}} \varepsilon)_j} \)

Due to nonnegativity of all terms it holds that:

\[ P_{LFP}^{\hat{\varepsilon}} : \max_{\varepsilon, \lambda_{\ell}, \lambda_{u}} f^{\hat{\varepsilon}}(\varepsilon) = \min_{i,j} f_{i,j}^{\hat{\varepsilon}}(\varepsilon) \]

\[ \text{s.t. } \varepsilon_{\min e} \leq \varepsilon \leq \varepsilon_{\max e} \]
Fabrication Robust Model for Bandgap Optimization, continued

\[ P_{LFP}^{\hat{\epsilon}} : \max_{\epsilon, \lambda_l, \lambda_u} f^{\hat{\epsilon}}(\epsilon) = \min_{i,j} f^{\hat{\epsilon}}_{i,j}(\epsilon) \]

s.t. \( \epsilon_{\min e} \leq \epsilon \leq \epsilon_{\max e} \)

The Fabrication Robust counterpart function \( \tilde{f}^{\hat{\epsilon}}(\epsilon) \) can be written as:

\[ \tilde{f}^{\hat{\epsilon}}(\epsilon) := \min_{d \in S - \epsilon} \min_{i,j} f^{\hat{\epsilon}}_{i,j}(\epsilon + d) \]

where \( S \) is the hypercube \( S := \{ \epsilon : \epsilon_{\min e} \leq \epsilon \leq \epsilon_{\max e} \} \).
The Fabrication Robust counterpart function $\tilde{f}^\hat{\epsilon}(\epsilon)$ is:

$$
\tilde{f}^\hat{\epsilon}(\epsilon) = \min_{d \in S - \epsilon} \min_{i,j} f_{i,j}^\hat{\epsilon}(\epsilon + d)
$$

$$
= \min_{i,j} \min_{d \in S - \epsilon} f_{i,j}^\hat{\epsilon}(\epsilon + d)
$$

$$
= \min_{i,j} \min_{d \in S - \epsilon} \frac{(C^\hat{\epsilon}(\epsilon + d))_i - (B^\hat{\epsilon}(\epsilon + d))_j}{(C^\hat{\epsilon}(\epsilon + d))_i + (B^\hat{\epsilon}(\epsilon + d))_j}
$$

Therefore $\tilde{f}^\hat{\epsilon}(\hat{\epsilon})$ is computable as $N_B \times N_C$ linear fractional programs on the hypercube. ($N_B \times N_C \approx 10000$. But each LFP is very simple.)

Furthermore, using Sensitivity Analysis Theorem, we can obtain

$$
g_{i,j}(\hat{\epsilon}) = \nabla \tilde{f}_{i,j}^\hat{\epsilon}(\hat{\epsilon})$$

(otherwise other local first-order estimate) when the linear fractional program has a nondegenerate solution (or otherwise).
Fabrication Robust Model for Bandgap Optimization, continued

Fabrication Robust counterpart function $\tilde{f}^\hat{\varepsilon}(\varepsilon)$:

$$
\tilde{f}^\hat{\varepsilon}(\varepsilon) = \min_{i,j} \min_{d \in S-\varepsilon} f_{i,j}^\hat{\varepsilon}(\varepsilon) := \frac{(C^\hat{\varepsilon}(\varepsilon + d))_i - (B^\hat{\varepsilon}(\varepsilon + d))_j}{(C^\hat{\varepsilon}(\varepsilon + d))_i + (B^\hat{\varepsilon}(\varepsilon + d))_j}
$$

Compute $\tilde{f}_{i,j}^\hat{\varepsilon}(\hat{\varepsilon})$ and $g_{i,j}(\hat{\varepsilon}) := \nabla \tilde{f}_{i,j}^\hat{\varepsilon}(\hat{\varepsilon})$ for all $N_B \times N_C$ pairs $(i,j)$

Construct the following concave local representation of the Fabrication Robustness optimization problem:

$$
P_{FR}^\hat{\varepsilon} : \max_{\varepsilon} \min_{i,j} \tilde{f}_{i,j}^\hat{\varepsilon}(\hat{\varepsilon}) + [g_{i,j}(\hat{\varepsilon})]^T (\varepsilon - \hat{\varepsilon})
$$

s.t. $\varepsilon_{\min} \leq \varepsilon \leq \varepsilon_{\max}$

Note that $P_{FR}^\hat{\varepsilon}$ is solvable as an LP in $N_B \times N_C \approx 10000$ constraints and $n_\varepsilon \approx 200 - 500$ variables
Solution Procedure Fabrication Robust Bandgap Optimization

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Some Results

Design for optimal $1^{\text{st}}$ TE bandgap in triangular lattice. Here $\delta = 10\%$ of pixels.

(a) Nominal solution, bandgap = 96.8%
(b) Fabrication Robust solution, bandgap = 84.7%
(c) Worst-case FR solution, bandgap = 40.8%
(d) Manual solution from FR solution, bandgap = 83.1%
Some Results

Design for optimal 2\textsuperscript{nd} TE bandgap in square lattice. Here $\delta = 5\%$ of pixels.

(a) Nominal solution, bandgap = 65.5\%
(b) Fabrication Robust solution, bandgap = 37.2\%
(c) Worst-case FR solution, bandgap = 21.9\%
(d) Manual solution from FR solution, bandgap = 36.1\%
Some Results

Design for optimal 1\textsuperscript{st} TE and 2\textsuperscript{nd} TM bandgaps in triangular lattice. Here $\delta = 5\%$ of pixels.

(a) Nominal solution, bandgap = 33.1%
(b) Fabrication Robust solution, bandgap = 29.2%
(c) Worst-case FR solution, bandgap = 23.5%
(d) Manual solution from FR solution (modifying $\tilde{\delta} = 27\%$ of pixels), bandgap = 30.7%
Conclusions

1. Fabrication Robust optimization is not straightforward

2. Fabrication Robust optimization works reasonably well for PCD bandgap optimization

3. “Simple” optimization in metamaterial and other optical/phononic problems often produce non-fabricable designs

4. Many other design problems that can benefit from fabrication robust optimization include:
   - Photonic crystal (optical) cavity
   - Waveguide taper
   - …