Inverse Design of a Dispersive Graded-Index Device for Photovoltaics

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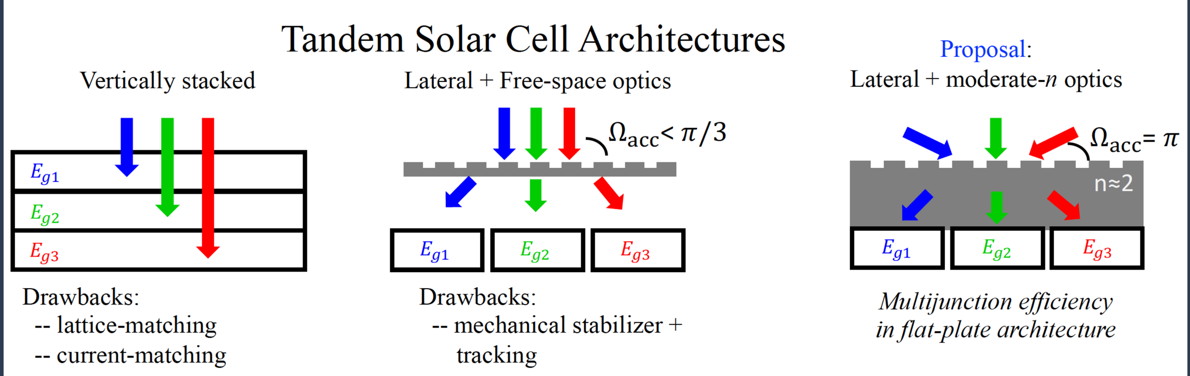
Introduction



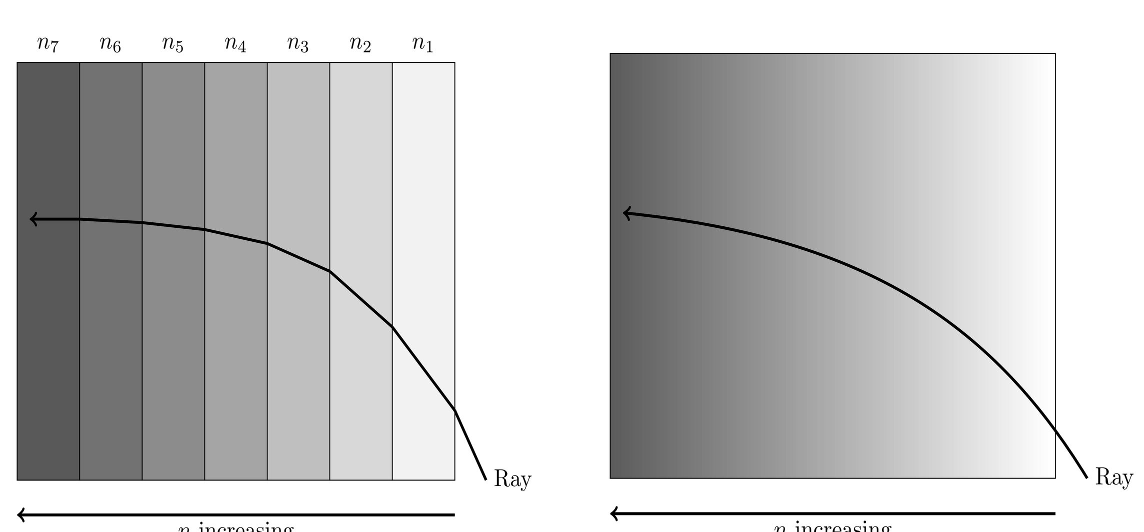
Solar cell design must balance financial cost, energy efficiency, and physical complexity.
Multi-junction photovoltaic (PV) cells may increase efficiency, but have shortcomings:

- Vertical PVs: high cost and complex manufacturing requirements
- Lateral PVs: require mechanical tracking of the sun

Proposal: lateral PV with a dispersive graded-index device

Theory

- When refractive index changes discretely, light travels in a piecewise linear path
- With graded-index (GRIN), differences in refractive index constantly alter light's path.
  - Light smoothly curves toward higher index



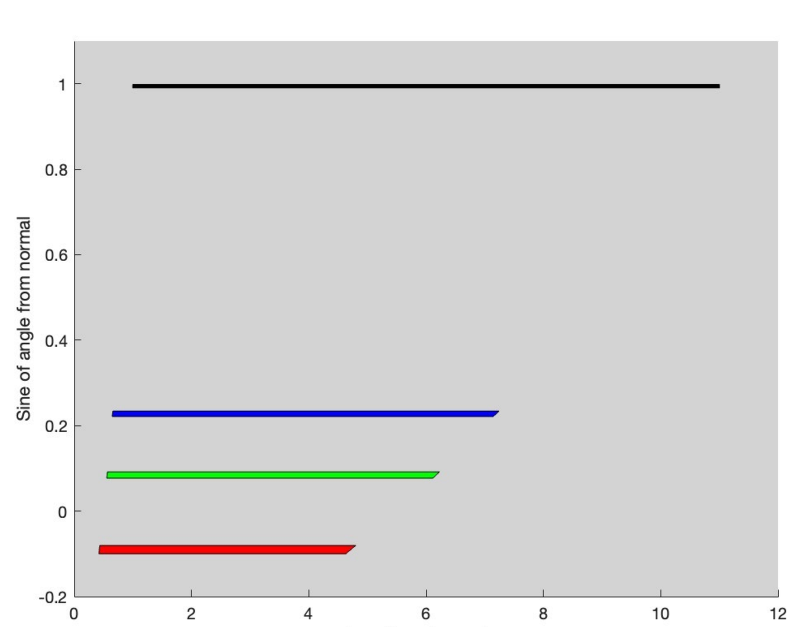
Etendue is an important tool in nonimaging optics:

$$dE = dx\,dy\,dp\,dq$$

- This is a volume in 4D phase space.
- For 2D geometry (rays exist in a plane), etendue can also be defined:

$$dE = n\,dx\,dL$$

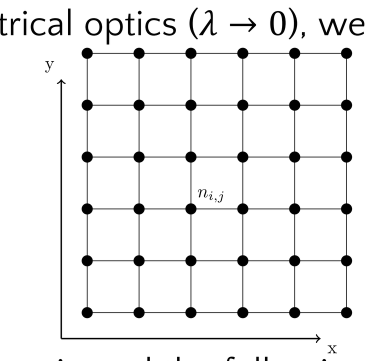
This phase space plot for the light entering and exiting a prism shows phase space separation persists across refractive boundaries.



Adjoint gradients for ray-tracing

From Maxwell's Equations in the limit of geometrical optics ($\lambda \to 0$), we can derive the ray equation

$$\frac{d}{ds}\left[n(\boldsymbol{r})\frac{d\boldsymbol{r}}{ds}\right] = \nabla n(\boldsymbol{r})$$



Define $dt = \frac{ds}{n}$ (optical path length) to get

$$\frac{d^2\boldsymbol{r}}{dt^2} = n(\boldsymbol{r})\nabla n(\boldsymbol{r})$$

This is solved numerically using a discretized domain and the following equations:

$$-\frac{d\boldsymbol{r}}{dt} + \boldsymbol{T} = 0$$
$$-\frac{d\boldsymbol{T}}{dt} + n(\boldsymbol{r})\nabla n(\boldsymbol{r}) = 0$$
$$\boldsymbol{R}(0) = \boldsymbol{R_0}$$
$$\boldsymbol{T}(0) = \boldsymbol{T_0}$$

Which are obtained by the substitution $\boldsymbol{T} = \frac{d\boldsymbol{r}}{dt} = \langle n\frac{dx}{ds}, n\frac{dy}{ds}, n\frac{dz}{ds}\rangle$, the optical ray vector.
Such a simulation scheme is well-suited to inverse design.

Now, let $\boldsymbol{p}$ be the state variables, θ the control variables, $C(\boldsymbol{p})$ the cost function, and $\boldsymbol{S}(\boldsymbol{p};\theta)$ the ray-tracing differential equations. Then we want

$$\min_{\theta} C(\boldsymbol{p}) \quad \text{s.t. } \boldsymbol{S}(\boldsymbol{p};\theta) = 0$$

Define a Lagrangian $\mathcal{L}(\boldsymbol{p},\theta,\boldsymbol{\lambda}) = C(\boldsymbol{p}) - \langle \boldsymbol{\lambda}, \boldsymbol{S}(\boldsymbol{p};\theta)\rangle$

Our objective is now unconstrained and given by

$$\min_{\theta,\boldsymbol{p},\boldsymbol{\lambda}} \mathcal{L}(\boldsymbol{p},\theta,\boldsymbol{\lambda})$$

For an arbitrary cost function, $C(\boldsymbol{p})$, we can write

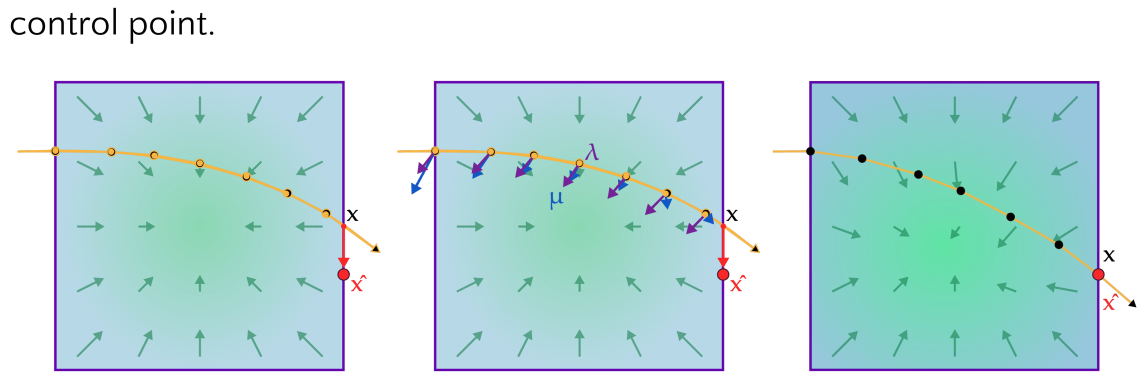
$$\mathcal{L} = C\left(\boldsymbol{R}(t_f), \boldsymbol{T}(t_f)\right) - \int_0^{t_f} \boldsymbol{\lambda}^T(\boldsymbol{R}' - \boldsymbol{T})\,dt - \int_0^{t_f} \boldsymbol{\mu}^T(\boldsymbol{T}' - n\nabla n)\,dt$$

With the Lagrange multipliers $\boldsymbol{\lambda}$ and $\boldsymbol{\mu}$ given by the critical points.

The gradient of this unconstrained objective with respect to $n(\boldsymbol{R})$ is

$$d_n\mathcal{L} = \int_0^{t_f} (n\nabla(dn) + dn\nabla n)^T \boldsymbol{\mu}\,dt$$

This gradient dictates the updates made to the refractive index at each control point.



The optimization procedure is implemented in MATLAB:

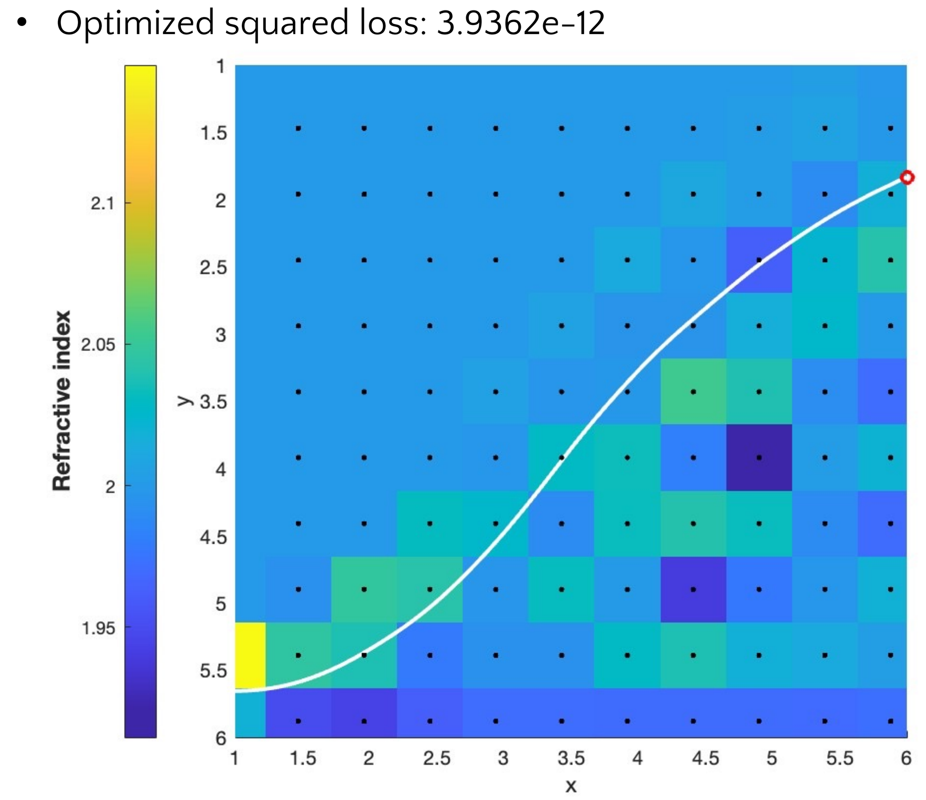
1. Discretize domain and define initial ray positions and velocities.
2. Trace all rays forward in time until they exit the optimization region.
3. Initialize the adjoint state variables, $\boldsymbol{\lambda}$ and $\boldsymbol{\mu}$, at the region boundary.
4. Trace the rays backward through the region to the starting point, updating $\boldsymbol{\lambda}$ and $\boldsymbol{\mu}$ at each step.
5. Calculate $d_n\mathcal{L}$
6. Update the refractive index at each control point.
7. Repeat until convergence.

The adjoint gradients are then fed to standard nonlinear optimization algorithms implemented by MATLAB's fmincon function.

Preliminary results: ray-tracing optimizations

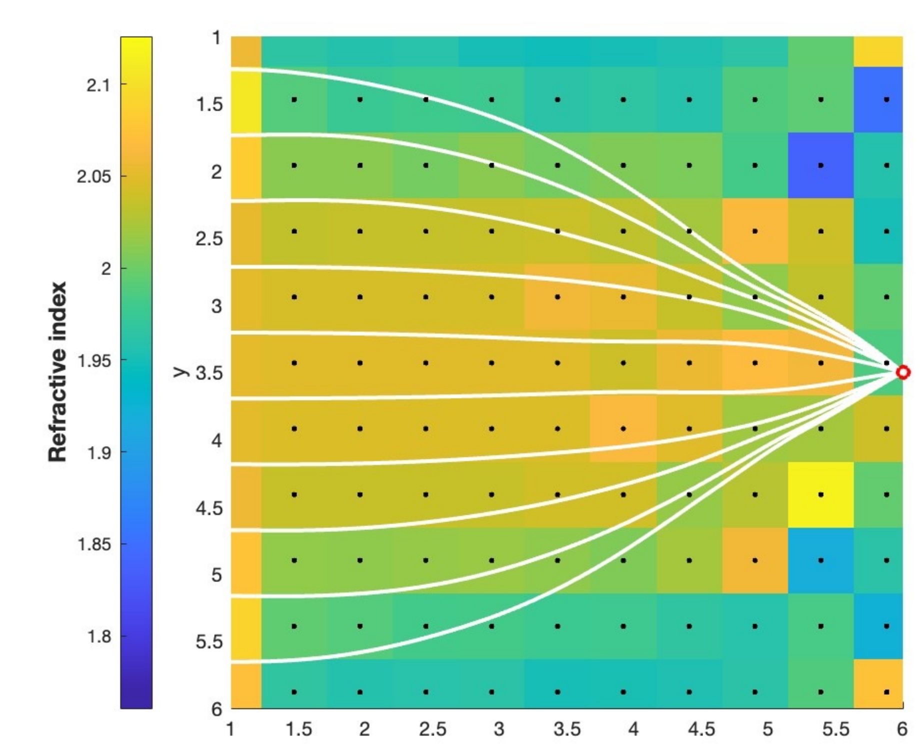
Path of a ray through an optimized refractive index field.

- Ray begins parallel to the x-axis.
- The target is the red dot in the upper right.
- Optimized squared loss: 3.9362e-12



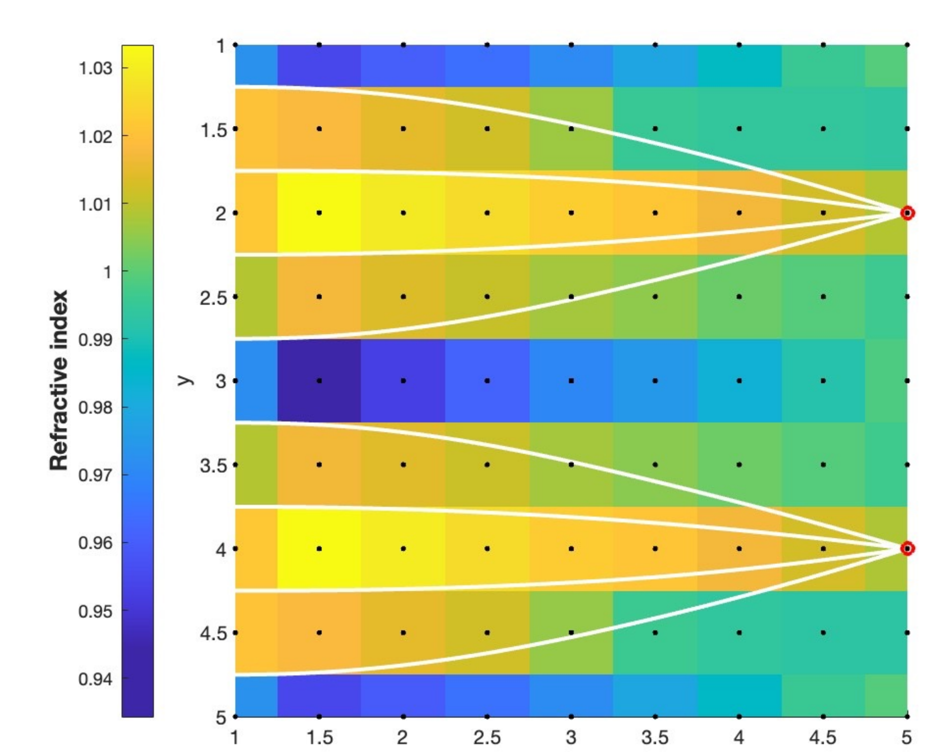
Path of 10 rays through an optimized refractive index field.

- Rays begin evenly spaced, parallel to the x-axis.
- The target is the red dot in the center right.
- Optimized squared loss: 1.4688e-06



Path of 8 rays through an optimized refractive index field.

- Rays begin evenly spaced, parallel to the x-axis.
- The upper 4 and lower 4 rays have separate targets.
- Optimized squared loss: 8.7085e-09



Conclusion and Outlook

Accomplishments:

1. Showed that phase space separation persists across media boundaries.
2. Implemented a ray tracing procedure in MATLAB.
3. Implemented a refractive index optimization scheme.

Next steps:

1. Improve optimization performance in low-symmetry scenarios.
   - Currently, multi-ray convergence is strongest for a centered target, whereas single-ray convergence is symmetry agnostic.

2. Introduce a model of dispersion.
   - The medium being optimized is not yet dispersive—all rays are treated identically by the device.
   - Most realistically, exogenously define a level of dispersiveness, and add another degree of freedom to the optimization that determines the coefficient on the dispersiveness at each control point.
     - Coefficient between 0 and 1.
     - This corresponds to adding air pockets to a dispersive medium.
   - Another possibility is simply imposing normal dispersion.
     - i.e., $n_{\text{red}} < n_{\text{green}} < n_{\text{blue}}$
     - By assuming no further material constraints, the optimizer could then produce the best possible device.

3. Introduce physical constraints to the optimization.
   - There is not yet a model of scattering or other material losses, but such considerations will be useful in assessing the efficacy of the light splitter.

4. Optimize over multiple angles of light.
   - From etendue conservation, we know there is no such thing as a perfectly collimated beam.
   - Sunlight is not perfectly collimated.
   - Must design the light splitter for numerous beam directions and large angular spread.

Ultimate objective:
Determine the optimal refractive index distribution to predictably split sunlight regardless of incident angle and position. This device would enable a lateral-tandem solar cell without tracking.

Citations

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