Numerically Optimizing Solar Cell Design

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With solar energy becoming an increasingly popular and widespread power source, optimizing the design of solar cells to absorb as much as light as possible has surfaced as an important and vital area of interdisciplinary research. This study describes a three-phase numerical approach to designing optimized solar cells given any sequence of pre-existing materials.

In the first phase, we investigate light’s behavior as it moves from layer to layer in any given structure. Using electromagnetic principles, we apply the transfer-matrix method to derive a system of equations that describe the wave and amplitude of light in any layer. These equations also provide reflectivity and transmission coefficients ($r$ and $t$), which denote how much light is being reflected out or travelling through each layer, respectively.

After slight manipulation, the model of light in the second phase outputs only the reflectivity coefficient, and since the reflectivity and transmission coefficients have the convenient relation $r^2 + t^2 = 1$, by minimizing the output $r^2$, we equivalently maximize the light travelling through the structure. Our minimization problem, then, can be expressed as:

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\begin{align*}
\text{min} & \quad r^2, \\
\text{subject to} & \quad w_i(x) \geq 0, \quad i \in [1, n], \\
& \quad 0 \leq t \leq L,
\end{align*}
\]

where $w_i$ is the width of layer $i$ for all layers 1 through $n$, $t$ is the total width, and $L$ is the maximum structure width.

In phase three, we solve the optimization problem (A) by adapting a Sequential Quadratic Programming (SQP) algorithm. To do this, we first create a quadratic approximation of our original function (by estimating the multi-variable light model as a function in the form $f(x) = \frac{1}{2} x^T G x + x c$) at an educated starting point. Then, we develop a quadratic program to minimize this localized approximate function. After a minimum is found, the SQP input is updated to have a new starting point with a new approximated quadratic function. This new function is next minimized, and the process is repeated until a universal minimum is reached. After altering the typical SQP algorithm to account for specific difficulties arising from the nature of our model, such as its non-universally positive-definite Hessian, we arrive at a program that efficiently minimizes the percentage of light reflected.

While the algorithm is scalable to any $n$ number of layers, we provide an example in Figure 1 of the program’s results on a three-layer structure. As shown, in just a few algorithmic iterations, the amount of reflected light decreases dramatically; by the tenth iteration, $r^2$ is reduced from an initial value of 0.199 to 0.002. Though the given maximum structure width in this example is 6 units, the width of the three layers after the tenth iteration is 4.71 units, which is important to note, as the algorithm does not simply reduce the total sum to zero nor cling to the maximum, but rather finds the truly optimal structure.

The key impact of this research is the application of an advanced, purely numerical optimization method to the design of solar cells that provides large increases in light absorption efficiency with minimal impact to the cell structure.

![Figure 1: Results of sequential quadratic programming (SQP) optimization algorithm on reflected light. By the tenth iteration, the squared reflection value is reduced from .199 to .002.](image)
Statement of Research Advisor

Nathan’s research seeks to develop computational approaches to model and design the multi-layered solar cells. He applied the so-called transfer matrix method to solve the differential equation model for optical light propagation in the multi-layered media and developed the sequential programming method to solve the underlying optimization problem. His study for the specific optical structure demonstrates that the computational methods are useful in guiding the design of the solar cells for realistic applications. It also sheds light on how one can increase the light absorption for more complicated solar cell structures.

-Junshan Lin, Mathematics and Statistics