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# Bayesian Optimisation of a Metasurface using a Penalised Objective Function

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**Mots-clés** : *Efficient Global Optimisation, Metasurface, Penalisation, Convolution*

## 1 Introduction

This study formulates the design of a metasurface as an unconstrained optimisation problem. The objective function is assumed to be expensive to evaluate and the performance of the optimisation process is assessed by the number of objective function evaluations. This characteristic of the problem motivates the use of a bayesian optimisation strategy called Efficient Global Optimisation (EGO). An undesirable modeling property of a natural objective function is solved by jointly minimising a necessary condition of optimality. We show numerically that penalising the objective improves the speed and robustness of the optimisation process.

## 2 Problem Formulation

Metasurfaces are planar arrangements of unitary elements [1]. When impinging on a periodic surface with unitary elements $\boldsymbol{x} \in \mathbb{R}^d$, an incident electromagnetic wave is reflected with a given magnitude $\boldsymbol{s}(\boldsymbol{x}) \in \mathbb{R}^F$, where $F$ is the number of frequencies at which Maxwell equations are solved. The bandpass filter proposed by [2] is presented in Figure 1 and used as a case of study to formulate the optimisation problem. We characterise an optimal response as any function $\boldsymbol{s}(\boldsymbol{x}^{opt}) \in \mathbb{R}^F$ satisfying $\boldsymbol{l} \leq \boldsymbol{s}(\boldsymbol{x}^{opt}) \leq \boldsymbol{u}$. The bounds $\boldsymbol{l}, \boldsymbol{u} \in \mathbb{R}^F$ are piece-wise constant functions of the frequency and presented in red and pink in Figure 2. An optimal frequency response $\boldsymbol{s}(\boldsymbol{x}^{opt})$ get close from zero at two resonant frequencies.

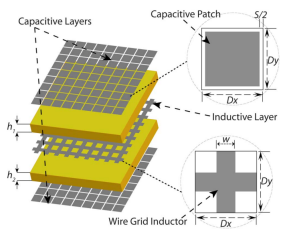



FIG. 1 – Multi-layer bandpass FSS

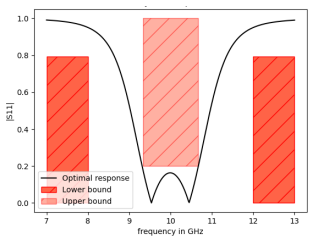



FIG. 2 – Optimal response $\boldsymbol{s}(\boldsymbol{x}^{opt})$ such that $\boldsymbol{l} \leq \boldsymbol{s}(\boldsymbol{x}^{opt}) \leq \boldsymbol{u}$.

The optimisation problem is formulated as :

$$\min_{x \in \mathbb{R}^d} f(\boldsymbol{x}) \tag{1}$$

The objective function takes the general form $f(\boldsymbol{x}) = g(\boldsymbol{s}(\boldsymbol{x}))$ where $\boldsymbol{s}(\boldsymbol{x}) : \mathbb{R}^d \mapsto \mathbb{R}^F$ is the response vector and $g(\boldsymbol{x}) : \mathbb{R}^F \mapsto \mathbb{R}$ is minimum when $\boldsymbol{l} \leq \boldsymbol{s}(\boldsymbol{x}) \leq \boldsymbol{u}$ holds.

## 3 Necessary Condition of Optimality

With the notations $(\boldsymbol{z})^+ = \max(\boldsymbol{0}, \boldsymbol{z})$, the vector of infractions of the bounds by the response is defined as $\boldsymbol{h}(\boldsymbol{x}) = (\boldsymbol{l} - \boldsymbol{s}(\boldsymbol{x}))^+ + (\boldsymbol{s}(\boldsymbol{x}) - \boldsymbol{u}))^+ \in \mathbb{R}^F$. Since $||\boldsymbol{h}(\boldsymbol{x})|| = 0 \iff \boldsymbol{l} \leq \boldsymbol{s}(\boldsymbol{x}) \leq \boldsymbol{u}$, a natural objective function is $\mathcal{M}(\boldsymbol{x}) = ||\boldsymbol{h}(\boldsymbol{x})||$. Assume that a response $\boldsymbol{s}(\boldsymbol{x})$ vanishes at a frequency $i$ but we have $\boldsymbol{l}_i \geq \boldsymbol{s}_i(\boldsymbol{x})$. The design $\boldsymbol{x}$ might be close from the optimum but is highly penalised by $||\boldsymbol{h}(\boldsymbol{x})||$.

To better assess the filtering properties of the surface, we propose to apply autoconvolution on the response and the bounds before measuring the infraction. We define the infraction of the convolved response as $\boldsymbol{\mathcal{H}}(\boldsymbol{x}) = (\boldsymbol{\mathcal{S}}(\boldsymbol{x}) - \boldsymbol{\mathcal{U}})_+ + (\boldsymbol{\mathcal{L}} - \boldsymbol{\mathcal{S}}(\boldsymbol{x}))_+ \in \mathbb{R}^{2F-1}$, where the caligraphed letters stand for the autoconvolution of the response $\boldsymbol{\mathcal{S}}(\boldsymbol{x}) = \boldsymbol{s}(\boldsymbol{x}) * \boldsymbol{s}(\boldsymbol{x})$ and the bounds $\boldsymbol{\mathcal{U}} = \boldsymbol{u} * \boldsymbol{u}$ and $\boldsymbol{\mathcal{L}} = \boldsymbol{l} * \boldsymbol{l}$. Note that we have $||\boldsymbol{h}(\boldsymbol{x})|| = 0 \implies ||\boldsymbol{\mathcal{H}}(\boldsymbol{x})|| = 0$.

## 4 Numerical Results

We apply the Efficient Global Optimisation [3] algorithm on problem (1), starting with 100 different initial design of experiments to train the gaussian process [4]. Three objective functions are first minimised : $||\boldsymbol{h}(\boldsymbol{x})||_1$, $||\boldsymbol{h}(\boldsymbol{x})||_2$ and $||\boldsymbol{h}(\boldsymbol{x})||_\infty$. Naturally, the choice of objective function impacts the optimisation process. The mean minimum value of the objective obtained at each iteration is presented in Figure 3. We present the data profiles in Figure 4 where we plot the percentage of converged runs given a budget of iterations. The least performing objective function is the minimax $||\boldsymbol{h}(\boldsymbol{x})||_\infty$ with 20% runs not converging with a budget of 200 evaluations. Since $||\boldsymbol{h}(\boldsymbol{x})||_1$ is the best performing objective function, we penalise it with the proposed necessary condition of optimality and minimise $||\boldsymbol{h}(\boldsymbol{x})||_1 + ||\boldsymbol{\mathcal{H}}(\boldsymbol{x})||_1$. We observe a significant improvement when using the penalisation.

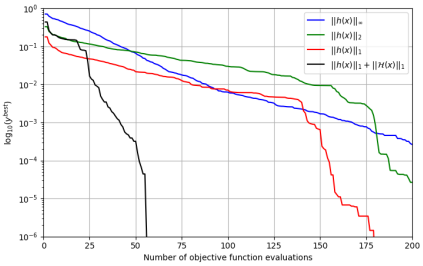



FIG. 3 – Average minimum value of the objective function through the iterations.

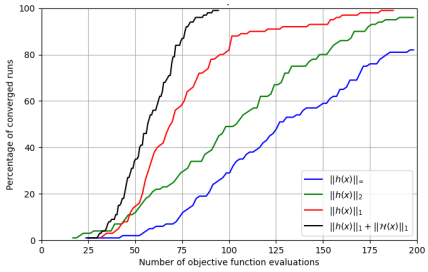



FIG. 4 – Percentage of converged runs for a given budget of evaluations

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