Optimal distribution of resonators in acoustic/elastic metamaterials via Bayesian optimization

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Abstract

Acoustic/elastic metamaterials are materials where resonant inclusions are placed inside of a matrix. These types of material have a frequency bandgap where no waves can propagate. As such, these materials naturally lend themselves to applications in vibration control. The resonant inclusions themselves can be placed in the matrix at will to produce this attenuation effect. Experimentally, it has been found that random distributions outperform periodic arrangements. The subject of which particular random distribution has yet to receive much attention in the field. In this study, we use techniques from machine learning -namely Bayesian optimization to find the optimal arrangement of resonators.

Keywords: Acoustic/Elastic Metamaterials, Optimization, Gaussian Process Regression, Bayesian Optimization

1. Introduction

Recently, interest has grown in artificially constructed phononic media which can alter the propagation of acoustic and elastic waves. A phononic crystal is a heterogeneous material which possesses spatial periodicity in the arrangement of its constituents, its structure, or the boundary conditions applied to it. As a result of this special structure, it has been shown that there exist band gaps for which certain frequencies of waves cannot propagate. These frequency band gaps have been utilized in many engineering applications related to vibrations and the control of acoustic and elastic waves. In 2000, Liu et al [1] introduced a brand new class of phononic media that is of much interest today. These are called acoustic/elastic metamaterials

These metamaterials possess "local resonance" which is a different way for producing band gaps that is not seen in regular phononic crystals. The local resonance effect is produced by embedding resonant structures inside of a matrix. The included resonant structures do not need to be arranged periodically for a band gap to appear. Without this requirement, we are free to place the resonators inside of the matrix in any which way that we like. The question we seek to answer in this study is what is the best way to place resonators. In the recent literature, it has been found that randomly distributions seem to out perform periodic arrangements. This begs the question: what is the best kind of random? We seek to answer this question via topology optimization of an elastic metamaterial composed of an epoxy matrix with embedded lead spheres which are coated in rubber. Specifically, we will try to optimize the distribution of the resonators to best attenuate the propagation of waves. The approach we use is Bayesian optimization which allows us to sample the space of distributions efficiently. Drawing upon machine learning techniques is not common in mechanics and in the study of acoustic/elastic metamaterials which makes this study especially novel. Additionally, obtaining the optimal random distribution is of high importance to the field.

2. Acoustic/elastic metamaterials

There are two mechanisms which cause band gaps to form: 1) *Bragg scattering* which is dependent on the periodicity in the arrangement of the material phases or structure of the material [2] and 2)*Local resonance* where interactions occur at the resonant frequency of the resonator. These two mechanisms have predictable effects on the frequency band structure of phononic media. In the first case, the band gap is relatively wide, but is more than likely much high that the range of frequency you would like to operate at. This is due to size constraints and the required period of unit cells to block waves at low frequencies. Band gaps generated due to local resonance can much more easily be in the low frequency regime but are quite narrow. There is also the added advantage of not having to arrange the resonators in any particular periodic arrangement. The existence of frequency band gaps in these materials has resulted in many practical applications such as: vibration control acoustic/elastic waveguides [3], acoustic diodes [4], subwavelength imaging [5], and even cloaking [6].

We will focus on materials that generate bandgaps in the second manner.

Of particular interest is the fact that the resonators can be placed in a random manner. In a recent study by Gonella et al [7], it was found that a random arrangement of resonators of five different resonant frequencies produced a wider bandwidth bandgap than a layered, periodic arrangement. Additionally, Florescu et al [8] studied a particular type of random distribution for phononic crystals. Despite these examples, there has been little done in the literature when it comes to disorder. For this study, we seek to address this deficiency and find the optimal random distribution that attenuates waves (at the resonant frequency) most effectively.

3. Problem statement

We consider a fixed, rectangular domain in two dimensions that has been populated with a random arrangement of N spherical resonators. The rectangular domain has a width of 0.1143 m and height of 0.05715 m. The matrix phase is epoxy with Young's modulus $G = 1.59 \times 10^9$ Pa, density $\rho = 1180$ kg/m^3, and Poisson's ratio $\nu = 0.49$. For resonators we use lead spheres coated in a shell of soft rubber. The radius of the lead spheres is 0.001937 m. The inner radius of the rubber shell is 0.001937 m and the outer radius is 0.002391 m. The material properties of the lead are: $E = 210$ GPa, $\rho = 11850$ kg/m^3, and $\nu = 0.29$. For the rubber shell, the properties are $E = 4.0 \times 10^4$ Pa, $\rho = 1300$ kg/m^3, and $\nu = 0.49$. When we populate the resonators in the matrix, we don't let the boundaries of the resonators come any closer than 0.009525 m to the left and right boundaries of the matrix. The domain with a resonator at the center is pictured in Figure 1.

The system is governed by the equations of elasticity. We have the equilibrium equation

$$\nabla \cdot \sigma + f = \rho \ddot{u} \tag{1}$$

where σ is the stress in the solid, f is the body force, ρ is the density and u is the displacement field. The stress is related to the strain by the constitutive equation

$$\sigma = C\epsilon \tag{2}$$

where C is the fourth order elasticity tensor and ϵ is the strain in the solid which can be calculated from the displacement field:

$$\varepsilon_{ij} = \frac{1}{2}\left[u_{i,j} + u_{j,i}\right] \tag{3}$$

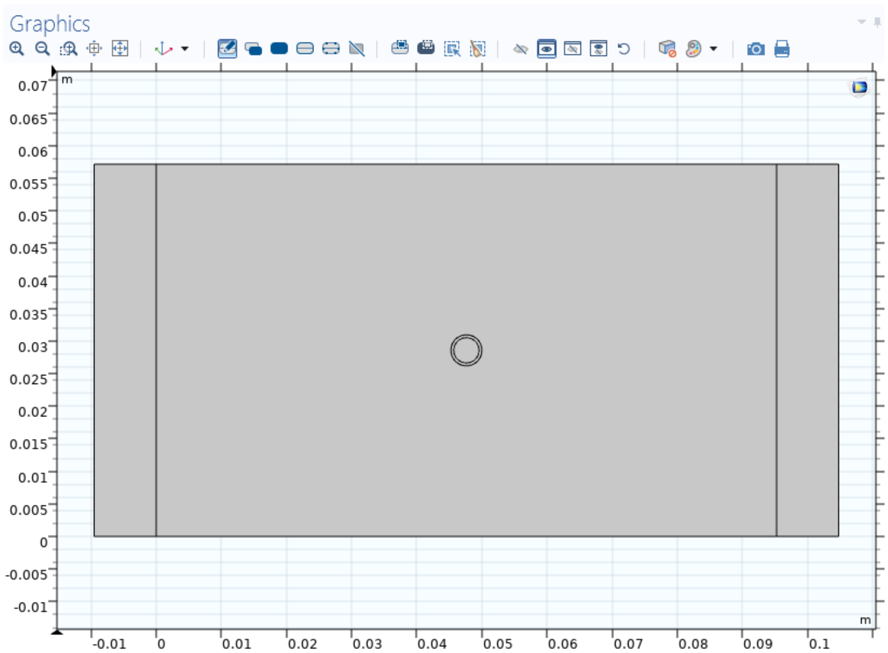

Figure 1: Geometry of the elastic metamaterial.

At the left end of the domain, we apply a sinusoidal forcing in the x-direction and, at the right end, we fix the displacement in the y-direction at a single point on the boundary. Free boundary conditions are applied to the remainder of the boundary. The frequency of sinusoidal forcing will be at the resonant frequency of the resonator such that the resulting wave will experience attenuation. We find the resonant frequency by placing a single resonator in the center of the domain and sweeping over a set of frequencies until we experience attenuation of the wave. For the specified geometry and material properties, this is 421.81 Hz. As shown in Figure , the resonator causes attenuation in the rest of the domain. 1.

The transmission loss (the attenuation), which we wish to optimize, is measured by picking two points: one point x_{tl} near where the sinusoidal forcing is applied and one point x_{tr} at the boundary opposite of where the sinusoidal forcing is applied. The attenuation is some function $\mathcal{A}$ of the position of the resonators $(x_1, x_2, ..., x_{2N-1}, x_{2N})$. We measure $\mathcal{A}$ in dB according to the following equation:

$$\mathcal{A}(x_1, x_2, ..., x_{2N-1}, x_{2N}) = 10 \log_{10} \left(\frac{u(x_{tl})}{u(x_{tr})} \right) \tag{4}$$

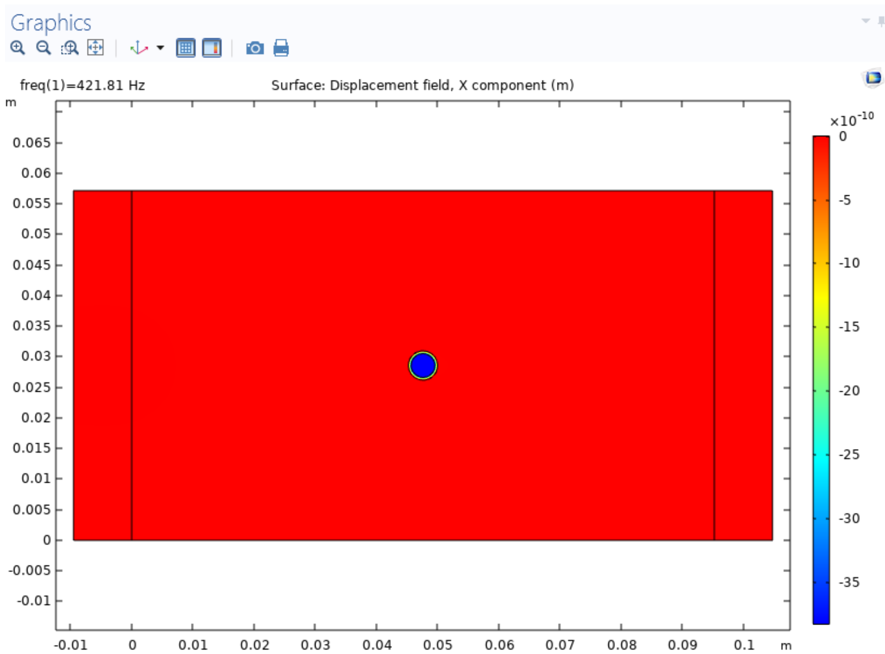

Figure 2: Attenuation due to the internal resonator.

The data will be generated using COMSOL Multiphysics for a variety of random arrangements of resonant inclusions.

4. Computational approach

The computational approach employed here is *Bayesian optimization.* The function $\mathcal{A}$ is unknown and we need to run a finite element simulation each time we want to evaluate it for some distribution of resonators. For one resonator, the process of finding the minimum may not seem so cumbersome, but once we start probing all of the random arrangements of N number of resonators this can be computationally expensive. Bayesian optimization is an iterative optimization technique that allows us to intelligently pick the next point or distribution to evaluate $\mathcal{A}$ with the aim of finding it's minimum. Central to our Bayesian optimization are Gaussian processes which we'll use as a so called "surrogate model" to approximate $\mathcal{A}$. Bayesian optimization and Gaussian processes are discussed in the following subsections. Refer to references [9],[10],[11], and [12] from which the following subsections summarize for more details.

4.1. Gaussian process regression

Before discussing Bayesian optimization, we introduce Gaussian processes and Gaussian process regression which are central to our computational approach. Gaussian processes are best understood in the context of multivariate Gaussian distributions. These are described by a vector μ containing n mean values and an $n \times n$ covariance matrix Σ describing the variance and correlation between each dimension. The notation we use for the multivariate Gaussian distribution is $\mathcal{N}(\mu, \Sigma)$. Additionally, when X is a random variable drawn from $\mathcal{N}$ we write

$$P_X = X = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_n \end{bmatrix} \sim \mathcal{N}(\mu, \Sigma) \tag{5}$$

Closure under the operations of marginalization and condition are two important properties of Gaussian distributions that will allow us to interpolate our data later on. Consider two subsets X and Y that are drawn from the same multivariate Gaussian distribution. Written as a joint distribution,

$$P_{X,Y} = \begin{bmatrix} X \\ Y \end{bmatrix} \sim \mathcal{N}(\mu, \Sigma) = \mathcal{N}\left(\begin{bmatrix} \mu_X \\ \mu_Y \end{bmatrix}, \begin{bmatrix} \Sigma_{XX} & \Sigma_{XY} \\ \Sigma_{YX} & \Sigma_{YY} \end{bmatrix} \right) \tag{6}$$

Mathematically, the operation of marginalization is

$$p_X(x) = \int_y p_{X,Y}(x, y) dy = \int_y p_{X|Y} p_Y(y) dy \tag{7}$$

For Gaussian distributions, the marginalized probability distributions are also Gaussian distributions. For X and Y above, we have

$$X \sim \mathcal{N}(\mu_X, \Sigma_{XX}) \tag{8}$$

$$Y \sim \mathcal{N}(\mu_Y, \Sigma_{YY}) \tag{9}$$

Likewise, conditioning of a Gaussian distribution, where we find the distribution of one set of random variables after fixing another set of random variables, is also a closed operation with the following expressions.

$$X|Y \sim \mathcal{N}(\mu_X + \Sigma_{XY}\Sigma_{YY}^{-1}(Y - \mu_Y), \Sigma_{XX} - \Sigma_{XY}\Sigma_{YY}^{-1}\Sigma_{YX}) \tag{10}$$

$$Y|X \sim \mathcal{N}(\mu_Y + \Sigma_{YX}\Sigma_{XX}^{-1}(X - \mu_X), \Sigma_{YY} - \Sigma_{YX}\Sigma_{XX}^{-1}\Sigma_{XX}) \tag{11}$$

The above equations will be used to incorporate existing data into our model.

Gaussian processes model the joint distribution between some test points in a domain and existing/training data as a multivariate Gaussian distribution. Gaussian process regression is done in a Bayesian manner where we seek the distribution of the test points after conditioning with respect to the existing data. Now, to fully define our model lets explicitly write the joint distribution between the test points X and the existing data Y. For our joint distribution $P_{X,Y}$, we let $\mu = 0$ and Σ is calculated according to a specially chosen kernel function k. As in (14), we split Σ into four different blocks evaluated as

$$\Sigma_{XY} = Cov(X, Y) = \begin{bmatrix} k(X_1, Y_1) & \cdots & k(X_n, Y_1) \\ \vdots & \ddots & \vdots \\ k(X_1, Y_n) & \cdots & k(X_n, Y_n) \end{bmatrix} \tag{12}$$

with similar expressions for Σ_{XX}, Σ_{YX}, and Σ_{YY}. The kernel function we use in our implementation is the RBF kernel

$$k(x_p, x_q) = \sigma_f^2 \exp\left(-\frac{1}{2}(x_p - x_q)^T M (x_p - x_q)\right) \tag{13}$$

where $M = \text{diag}(l)^{-2}$ which is a $d \times d$ matrix. Note, that we introduce the parameters σ_f and l here. Thus, the joint distribution is

$$P_{X,Y} = \begin{bmatrix} X \\ Y \end{bmatrix} \sim \mathcal{N}(\mu, \Sigma) = \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \Sigma_{XX} & \Sigma_{XY} \\ \Sigma_{YX} & \Sigma_{YY} \end{bmatrix}\right) \tag{14}$$

with the blocks of the covariance matrix being calculated based on equation (12). Before drawing any predictions, we optimize the the model by maximizing the marginal likelihood

$$\log P_{y,X} = -\frac{1}{2} y \Sigma^{-1} y - \frac{1}{2} \log|\Sigma| - \frac{N}{2} \log(2\pi) \tag{15}$$

$|\Sigma|$ denotes the determinant of Σ and for the above equation y are known outputs and Σ is calculated using the corresponding inputs.

At this point, we condition the joint distribution in order to obtain the posterior distribution $P_{X|Y}$ The function that we wish to find based on existing data at certain test points is drawn from $P_{X|Y}$ i.e.

$$f \sim P_{X|Y} \tag{16}$$

Given the probabilistic nature of our inference, we can find the mean and variance of our prediction.

4.2. Bayesian optimization

Bayesian optimization encapsulates Gaussian process regression and uses it as a so called "surrogate model" to approximate some function that we seek the maximum/minimum of. Using the prediction of the posterior, Bayesian optimization evaluates an an acquisition function which is then used to suggest another point to sample our desired function -in this case $\mathcal{A}$. This type of iterative optimization technique is especially useful in this case because we do not know the explicit dependence of $\mathcal{A}$ on the positions of the resonators. Additionally, the hope is that using this Bayesian optimization approach we will be able to more efficiently sample the space of distribution of resonators and find the maximum attenuation more quickly.

Explicitly, the algorithm is as follows:

1. Compute $\mathcal{A}$ at some initial points
2. For sum number of desired iterations:
   (a) Update the posterior probability distribution the available data
   (b) Optimize the acquisition function (which depends on the prediction of the posterior probability) over the domain to find x_{next}
   (c) Evaluate $\mathcal{A}$ at x_{next}

The acquisition function we use is called the *expected improvement*. For a Gaussian process surrogate it has an analytical expression:

$$EI(x) = \begin{cases} (\mu(x) - f(x^+) - \xi)\Phi(Z) + \sigma(x)\phi(Z) & \text{if } \sigma(x) > 0 \\ 0 & \text{if } \sigma(x) = 0 \end{cases} \tag{17}$$

where

$$Z = \begin{cases} \frac{\mu(x) - f(x^+) - \xi}{\sigma(x)} & \text{if } \sigma(x) > 0 \\ 0 & \text{if } \sigma(x) = 0 \end{cases} \tag{18}$$

μ and σ are the mean and standard variance calculated from the posterior distribution. x^+ is the location that give the most optimal value of f the function we are trying to optimize. Φ and ϕ are the cumulative distribution function and the probability distribution function of the standard normal respectively.

5. Results

In the current iteration of the study, we were not able to use our computational approach on multiple resonators due to time constraints. As such we present the results for a single resonator

First we demonstrate the use of Gaussian process regression on data generated from COMSOL to interpolate the function $\mathcal{A}$. In Figure 3, we show the result of the Gaussian process regression of the attenuation $\mathcal{A}$ evaluated at 20 random points in the domain. On the right, we plot the variance of the prediction at each point and mark with a red 'x' the point suggested to be sampled next by our Bayesian optimization program.

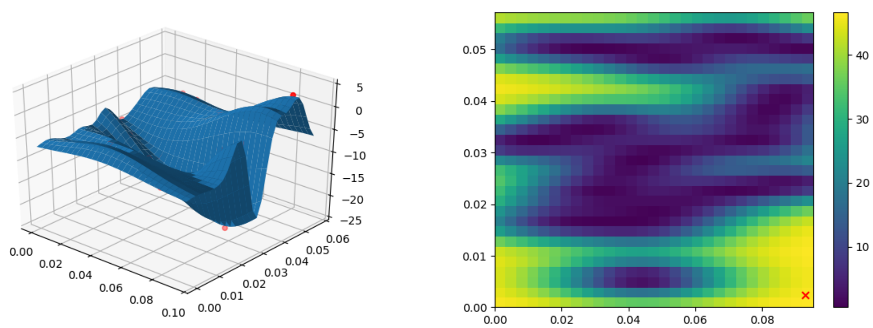

Figure 3: Gaussian process regression of $\mathcal{A}$ with 20 random points in the domain.

Next, we use Bayesian optimization to suggest new points to evaluate the COMSOL model. The next computation of $\mathcal{A}$ is done automatically via a Python script that runs an instance our model in COMSOL. We start with five initial points as shown in Figure 4 Then after 20 iterations we have the following result in Figure 5. For a complete progression, see Appendix A.

6. Discussion

In Figure 5, the minimum is $\mathcal{A} = -20.6$ dB at $x = (0.064265, 0.031395)$ m. This is less than the minimum found evaluating 20 random points which was -23.7 dB. Thus, it should be noted that this minimum is probably not *the* minimum of $\mathcal{A}$. The optimization algorithm will have to be run for more iterations to find the true minimum. We, however, note that the point does not reside on the center of the y-axis of the domain. Additionally, the

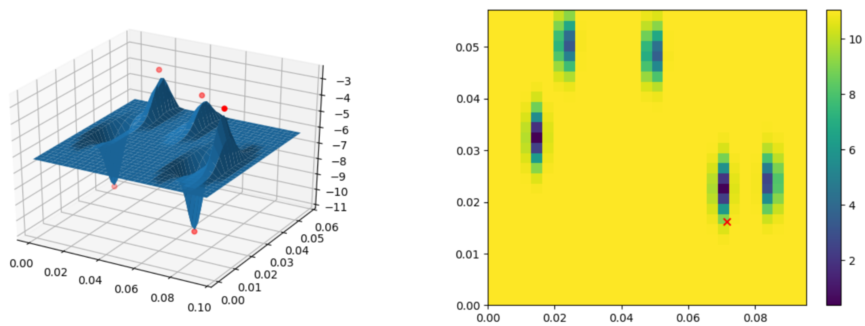

Figure 4: Gaussian process regression of $\mathcal{A}$ with 5 random points in the domain.

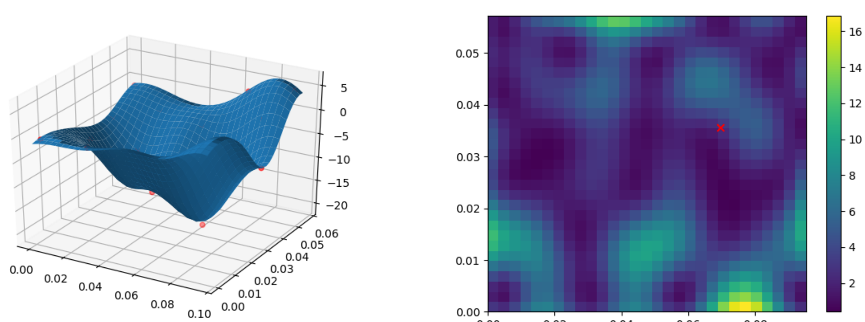

Figure 5: Gaussian process regression of $\mathcal{A}$ with 24 random points in the domain.

x-coordinate is to the right of the center of the domain which suggests it is more favorable to have the resonator closer to the point where $\mathcal{A}$ is measured rather that the location of the sinusoidal forcing.

As seen in the previous section, Bayesian optimization with a Gaussian process surrogate model is able to interpolate $\mathcal{A}$ well and find its minimum while also exploring the whole domain. This is a good indication of two things. One is that the RBF kernel is a good kernel to use when modeling the function $\mathcal{A}$. The second is that the acquisition function we use (Expected Improvement) balances exploitation and exploration well. Exploitation refers to suggesting points already near where a minimum is predicted. Exploration refers to suggesting points where the variance or uncertainty is high such that we explore the entire space.

At this stage in the study, we have a good proof-of-concept for using Bayesian optimisation to find the minimum of $\mathcal{A}$. This is a good sign as we will soon explore this computational approach for 2,3,4 and more resonators. Successful implementation of the Bayesian optimisation approach for several resonators would allow us to measure the radial distribution function or structure factor of the optimal array of resonators. Obtaining a definite answer to the question of optimal distribution of resonators would have far reaching impacts on future experiments and applications of acoustic and elastic resonant materials. Additionally, data driven approaches to solving problems in mechanics are not too popular as of today. This study would be a unique use of machine learning techniques in a field that largely relies on theoretical and experimental knowledge to generate results.

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Appendix A. Bayesian optimization

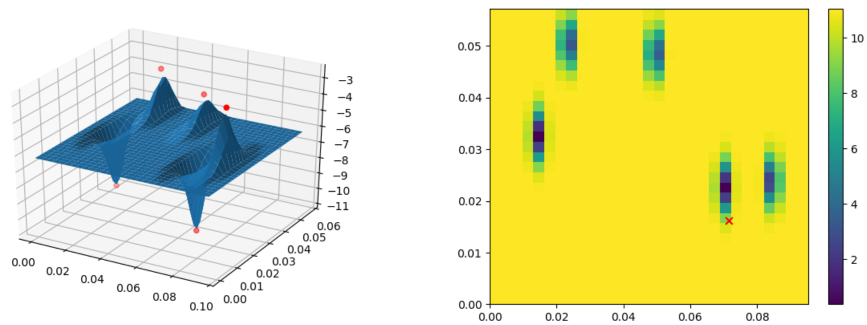

Figure A.6: Iteration 0

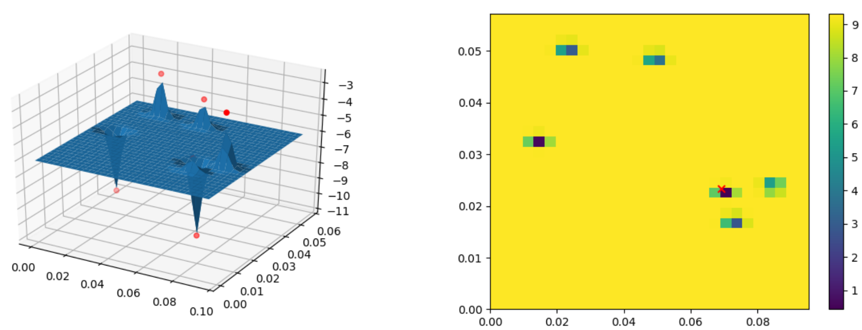

Figure A.7: Iteration 1

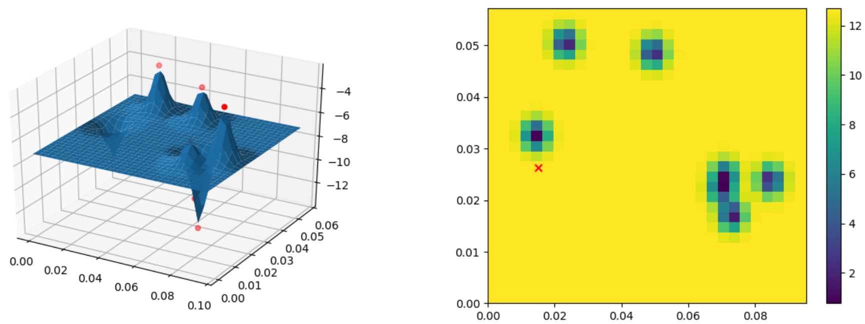

Figure A.8: Iteration 2

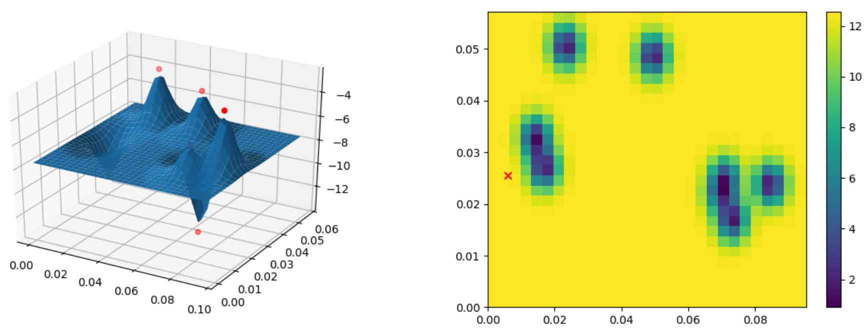

Figure A.9: Iteration 3

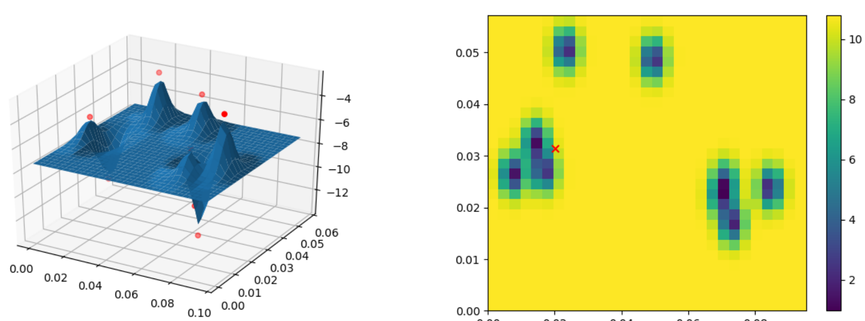

Figure A.10: Iteration 4

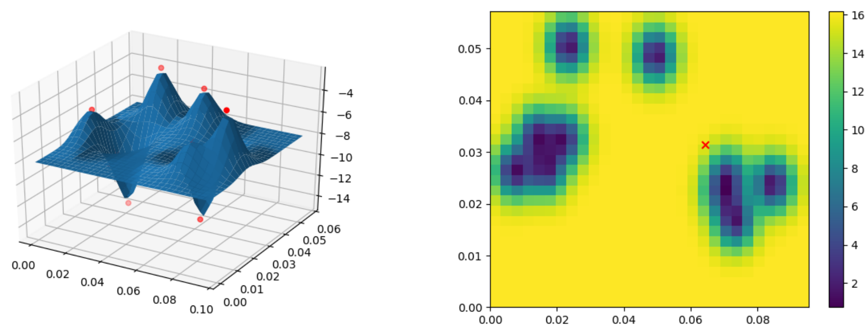

Figure A.11: Iteration 5

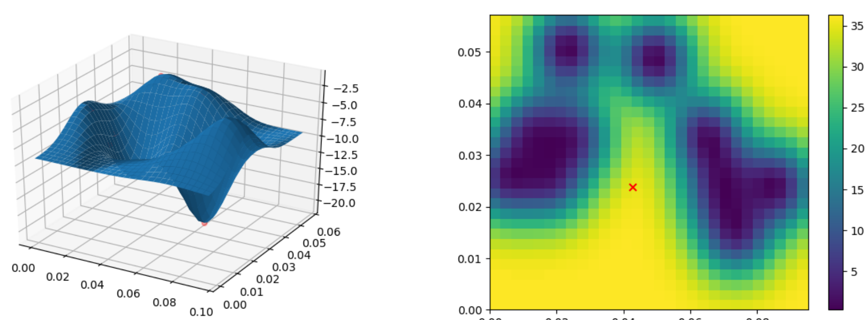

Figure A.12: Iteration 6

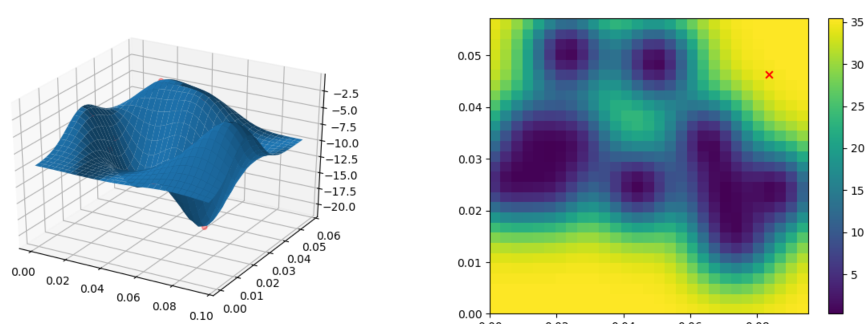

Figure A.13: Iteration 7

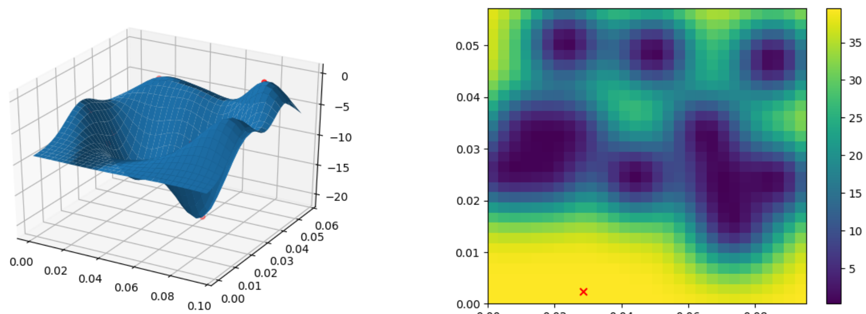

Figure A.14: Iteration 8

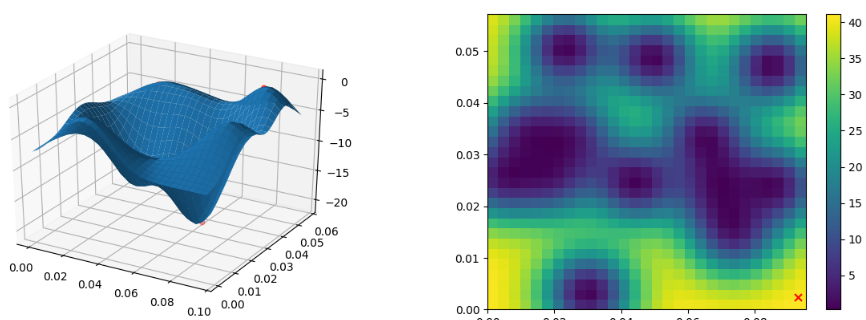

Figure A.15: Iteration 9

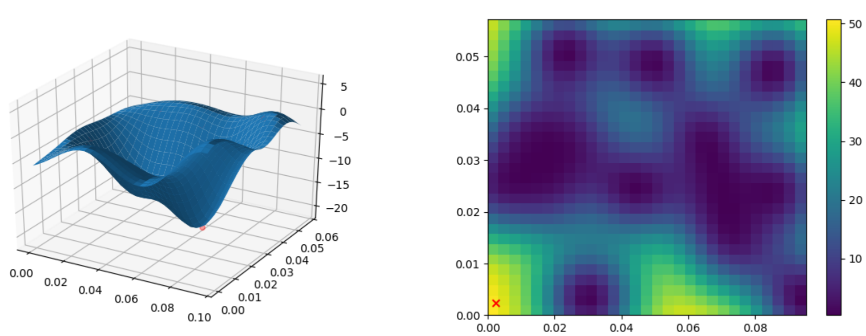

Figure A.16: Iteration 10

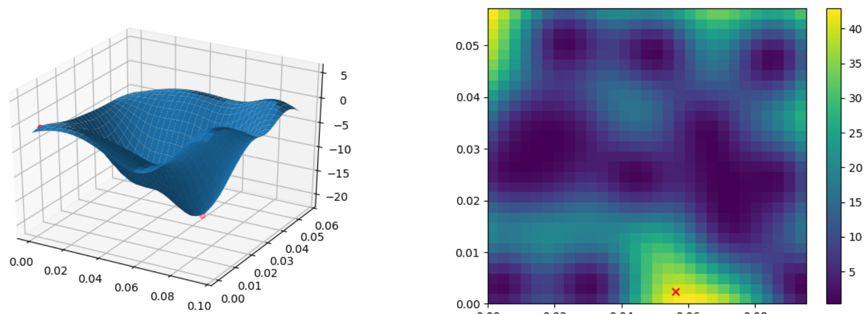

Figure A.17: Iteration 11

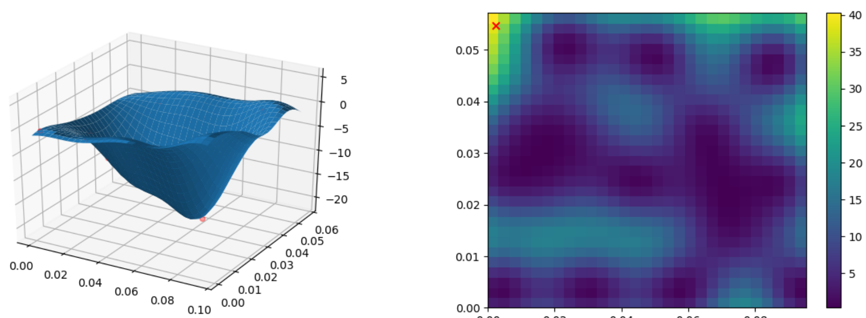

Figure A.18: Iteration 12

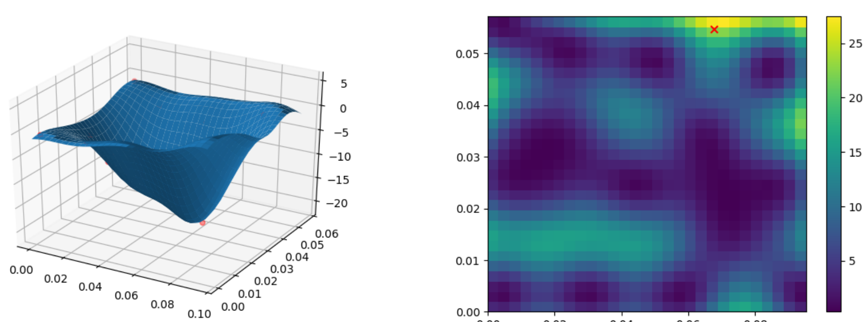

Figure A.19: Iteration 13

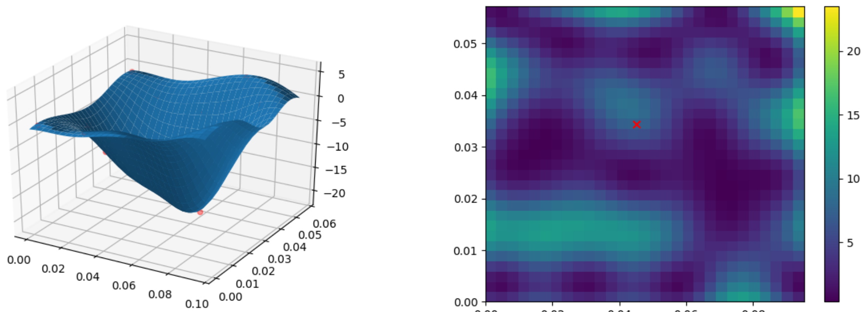

Figure A.20: Iteration 14

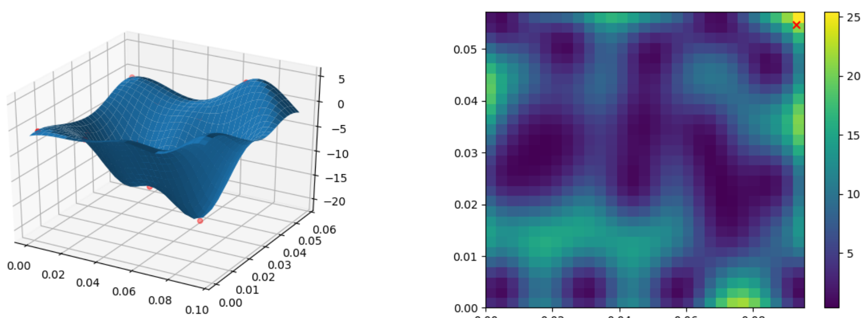

Figure A.21: Iteration 15

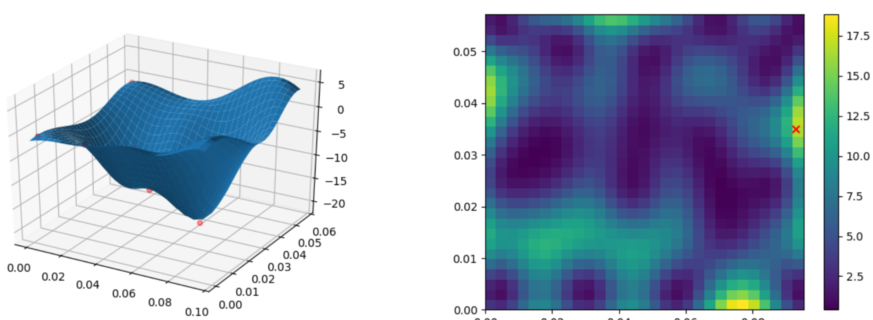

Figure A.22: Iteration 16

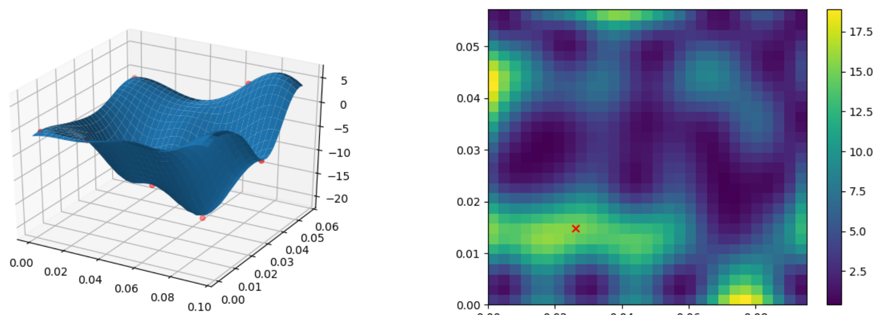

Figure A.23: Iteration 17

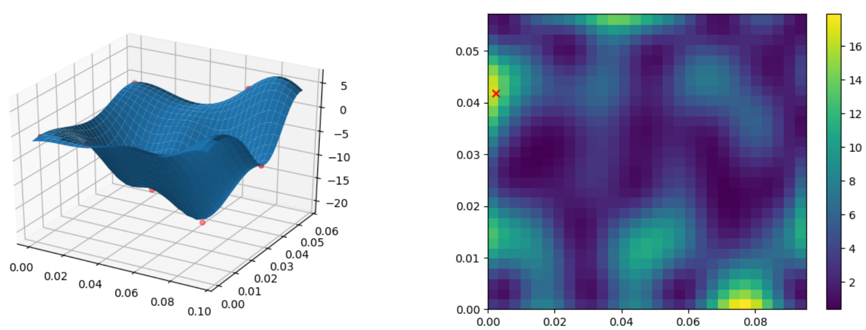

Figure A.24: Iteration 18

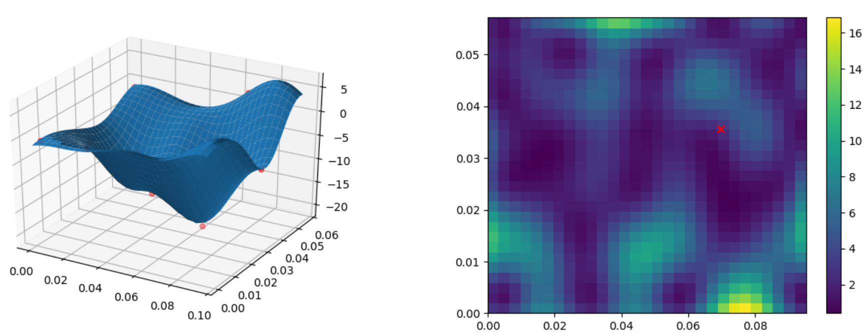

Figure A.25: Iteration 19