NOLOSS
Lossless photon management
Optical design for manufacture at different length scales

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OPTIMIZATION OF NANOPHOTONIC STRUCTURES USING GAUSSIAN PROCESSES

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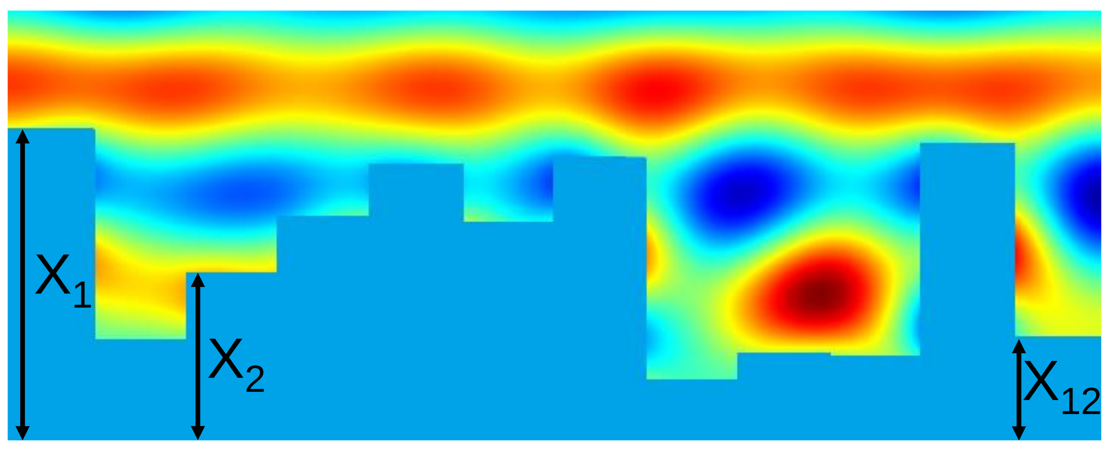
Project objective

Nanophotonic devices with high performance normally requires the use of complex structures. The search for their optimal shapes is normally a high dimensional global optimization problem hard to compute. We present a Bayesian optimization algorithm based on Gaussian processes in order to optimize nanophotonic strucutres. This method demonstrates to be very efficient in high dimensional problems where relatively high computational times are required for each simulation .

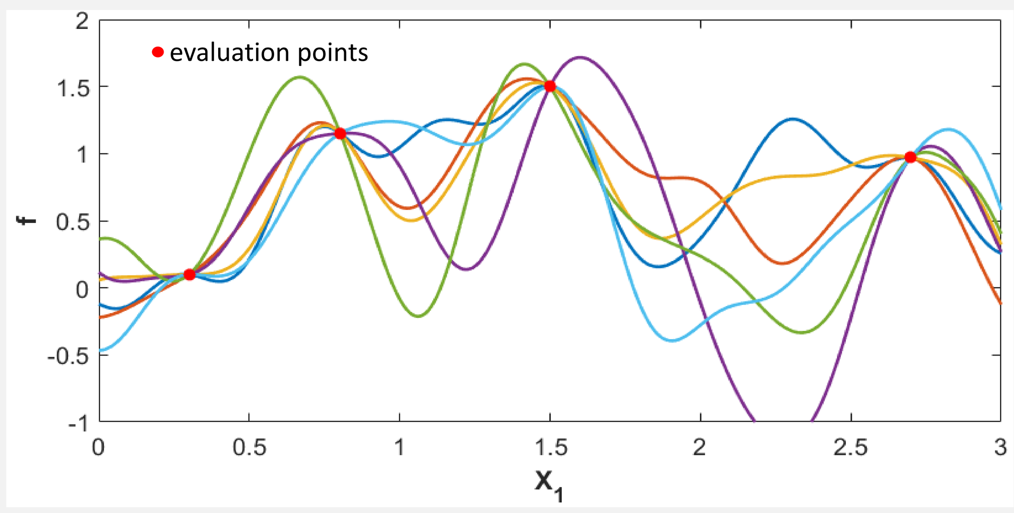
Optimizing photonic structures



- Length scales in the order of λ
- Complex structures
- High dimensional parameter spaces
- Maxwell's equations rigorously solved
- Interference effects leading to global optimization problems

Gaussian Processes (GP)

- We use a stochastic model for the objective function based on GP [1]
- The regions where the objective function is unknown follow a probability distribution
- The model is updated after each evaluation performed (Regression)
- The hyper-parameters (μ, σ) of the GP determine the most likely behaviour in the full parameter space
- The hyper-parameters, i.e. the stochastic model, are also updated after every iteration (learning process)



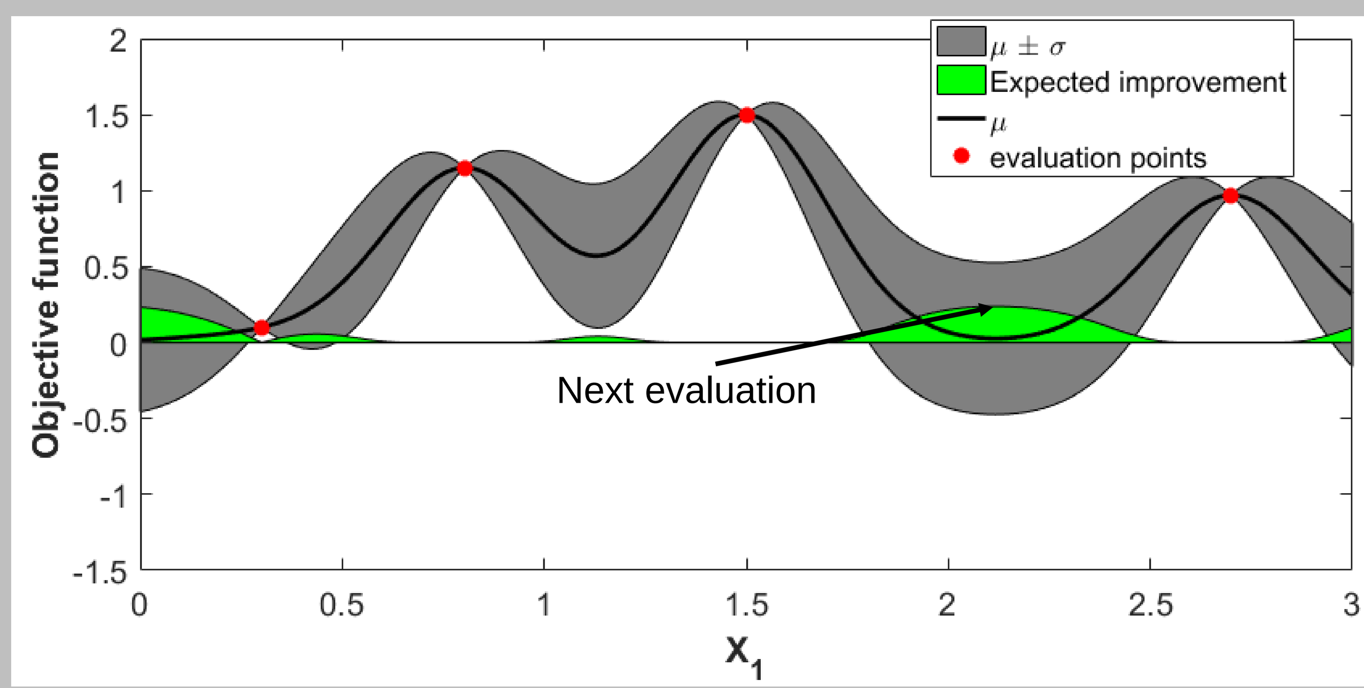
$$P(\boldsymbol{Y}) = \frac{1}{(2\pi)^{\frac{N}{2}}|\Sigma_{\text{p}}|^{\frac{1}{2}}} e^{-\frac{1}{2}(\boldsymbol{Y}-\boldsymbol{\mu}_{\boldsymbol{p}})^T \Sigma_p^{-1}(\boldsymbol{Y}-\boldsymbol{\mu}_{\boldsymbol{p}})}$$

Bayes Optimization with Gaussian Processes

- The optimization strategy (where to evaluate next) is based on the GP model
- We use the expected improvement (α_{EI}) as acquisition function:

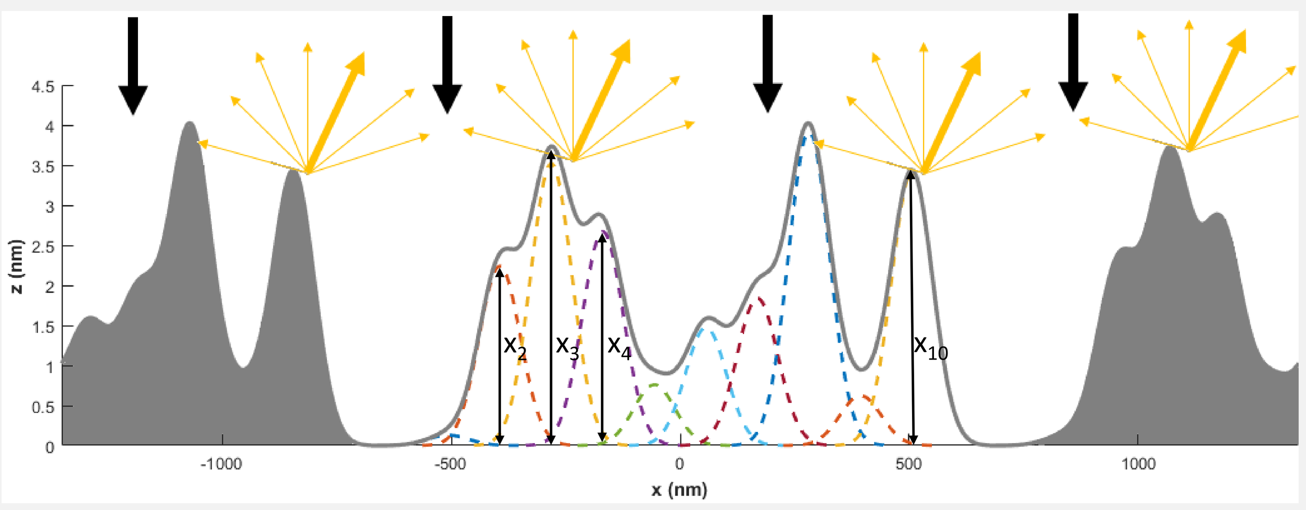
$$\alpha_{EI} = \mathbb{E}\left[\max\left(0, y_{min} - f(x)\right)\right]$$

- The parameter space is scanned based on where the GP expects a higher improvement of the objective function
- Efficient method for high dimensional parameter spaces with computationally expensive objective functions

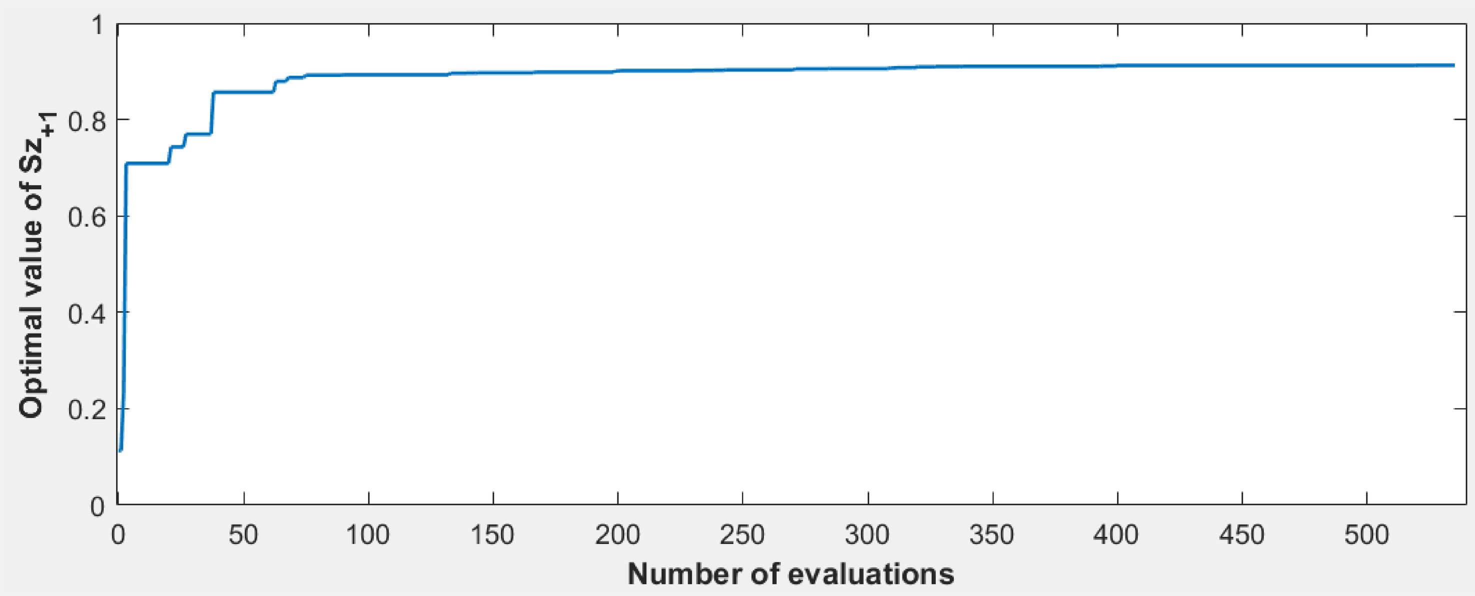


Example: Optimization of a reflective nanostructure [2]

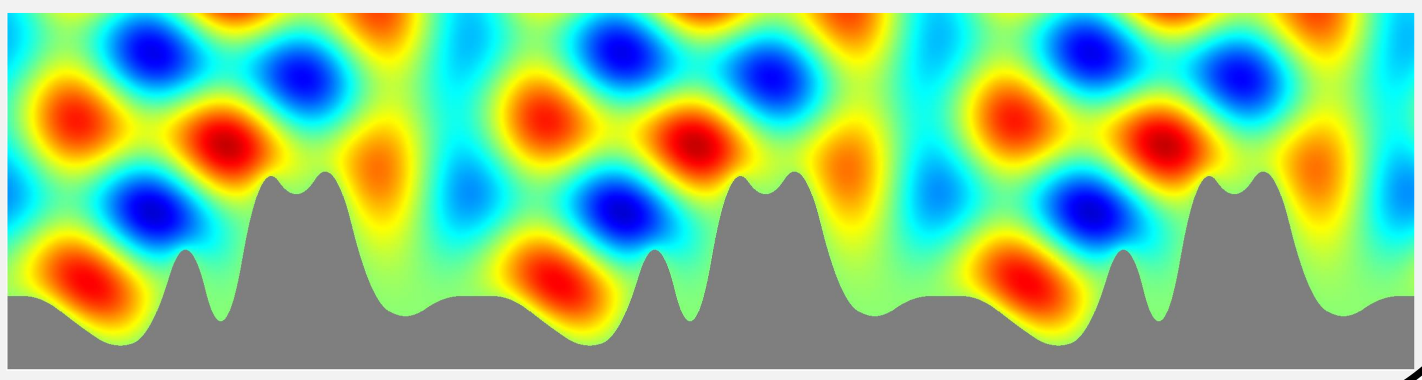
- **Objective**: Maximize reflectivity into the 1st diffraction order



$$f = \frac{Sz_{+1}}{Sz_{inc}} = Sz_{+1}$$



Optimal shape: Efficiency 0.91



- **Shape parametrization**: The periodic unit cell is parametrized with 10 b-splines
- **Convergence**: Maximum of 0.91 reached after 530 evaluations, which means less than 2 samples per dimension.

References

[1] Schneider P I, Garcia-Santiago X, Rockstuhl C and Burger S 2017 Proc. SPIE 10335 103350O
[2] Garcia-Santiago S, Schneider P-I , Rockstuhl C and Burger S 2017 Proc. AIP IWMbD2017

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