Department of MSE
IIT Kanpur

Machine learning-driven optimization in powder manufacturing of Ni-Co based superalloy

MSE643 (2022-23-II)

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Problem Statement

To optimize the process parameters in powder manufacturing to produce high-quality powders with desired sizes depending on the use.

Using Bayesian optimization technique to find optimum melt temperature and pressure to maximize % yield and minimize production cost

Motivation

Recent advances in powder metallurgy (PM) have accelerated the design and manufacturing cycle of high-temperature structural mate-rials for aerospace engineering

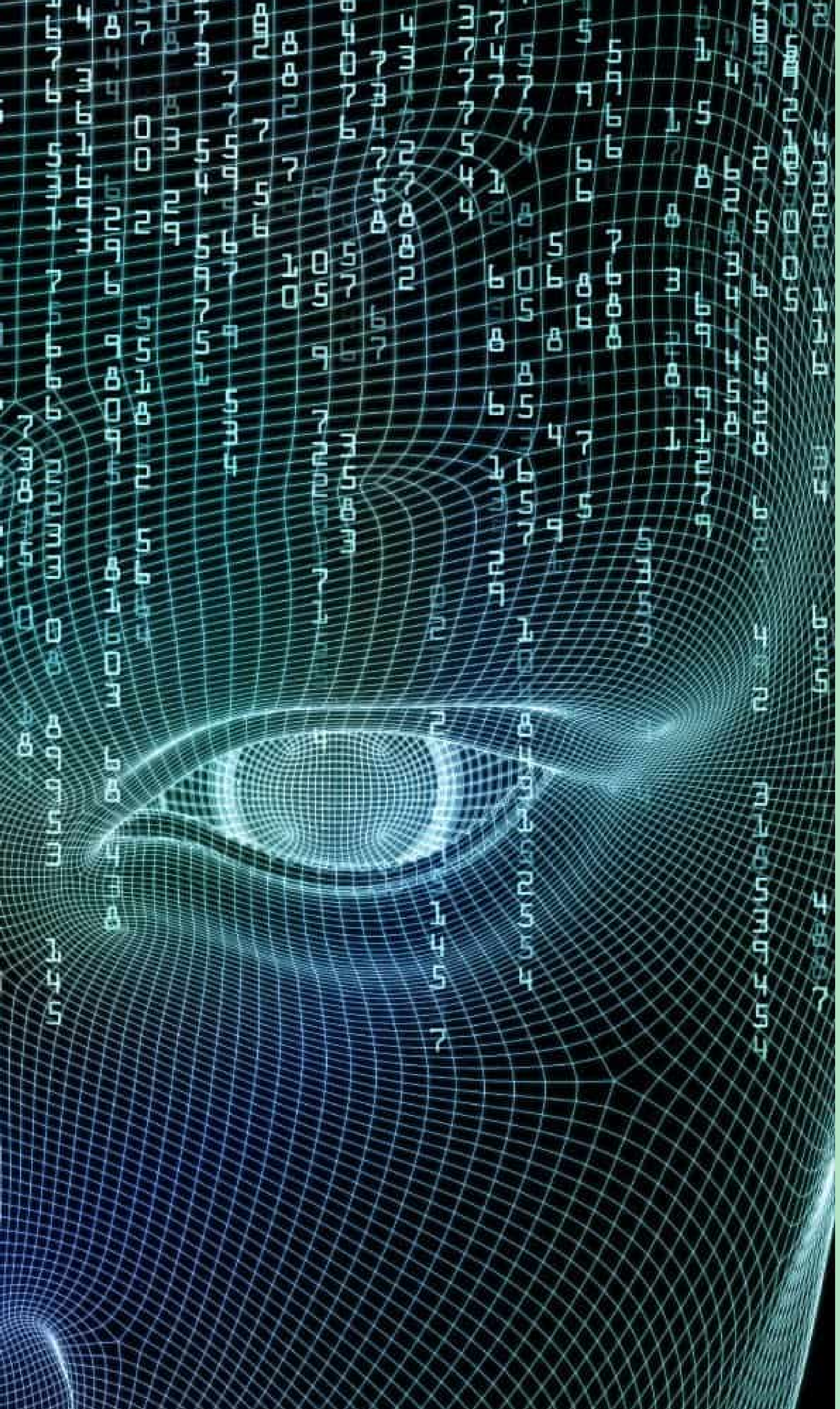
PM strongly contributes to improved performance, even for high-pressure turbine disks that utilize life-limited parts with high-level safety requirements

Hence, the production of parts using PM necessitates the manufacture and supply of high-quality and low-cost superalloy powders

Our group aims to find the optimum PM parameters that maximize the yield % of Ni-Co superalloy powder production

Why Bayesian Optimization?

Blackbox target function	Minimum evaluations required	Domain specific knowledge	Fewer iterations	Small dataset
Bayesian optimization is an efficient algorithm for global optimization in black-box settings.	It is well-suited for expensive optimization problems where evaluations of the objective function are costly.	Bayesian optimization is an iterative process that can easily be modified to incorporate prior knowledge, such as domain-specific knowledge or user-specified constraints.	As it is based on a probabilistic model, it has the potential to obtain better solutions in fewer iterations thereby saving time and resources	The Bayesian optimization algorithm does not require a large amount of data to begin the optimization process, making it suitable for problems where data is limited.



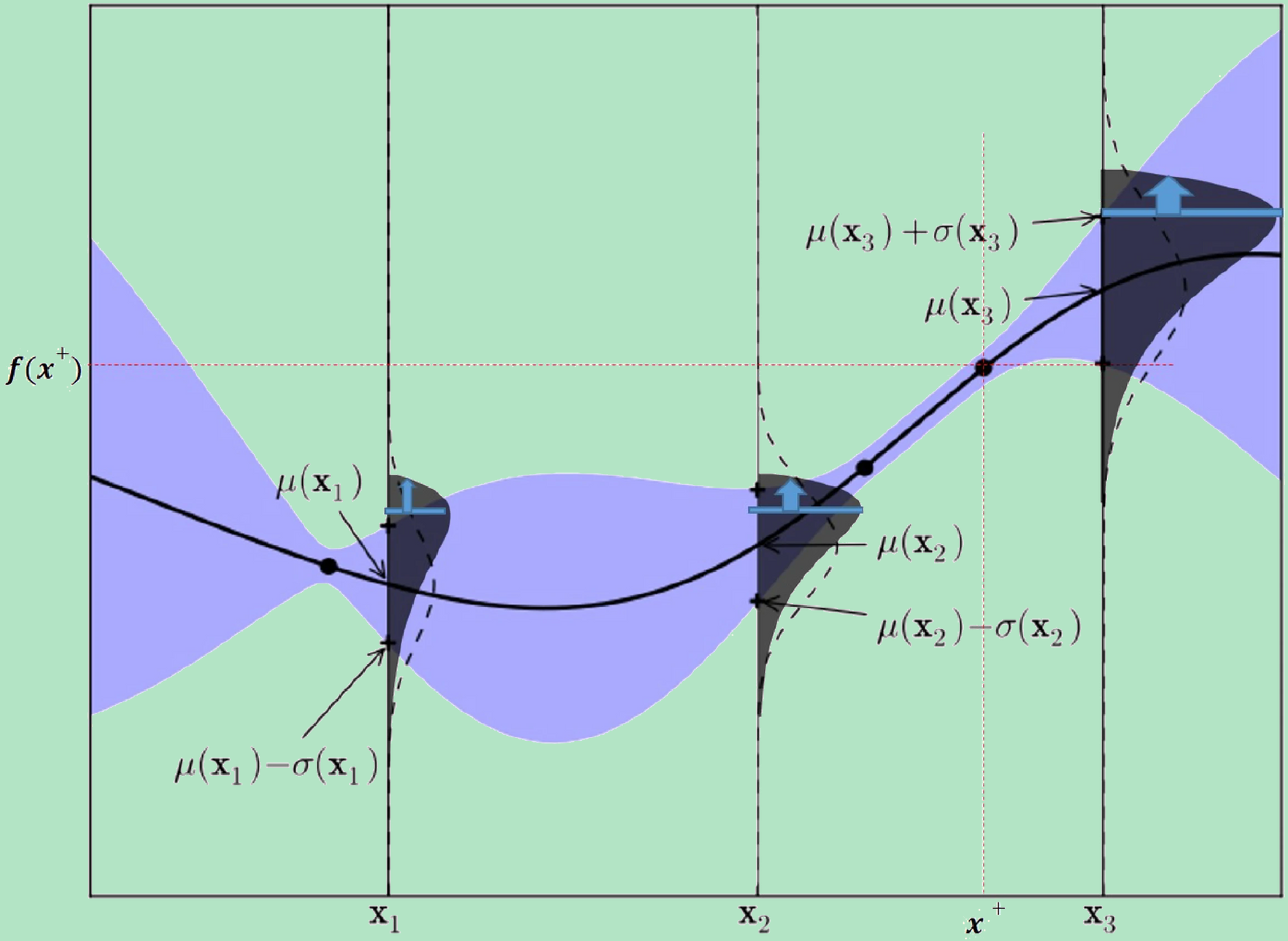
Bayesian Optimization

Overview

- We have to find the global maximum of an unknown, costly, and possibly noisy objective function f(x).
- To find the maximum value, we fit a Gaussian Process to our observed points and pick our next best point where we believe the maximum will be.
- This next point is determined by an acquisition function - that trades of exploration and exploitation.

Gaussian Processes

Model the data as a Gaussian distrubutiion, conditioned on the training points



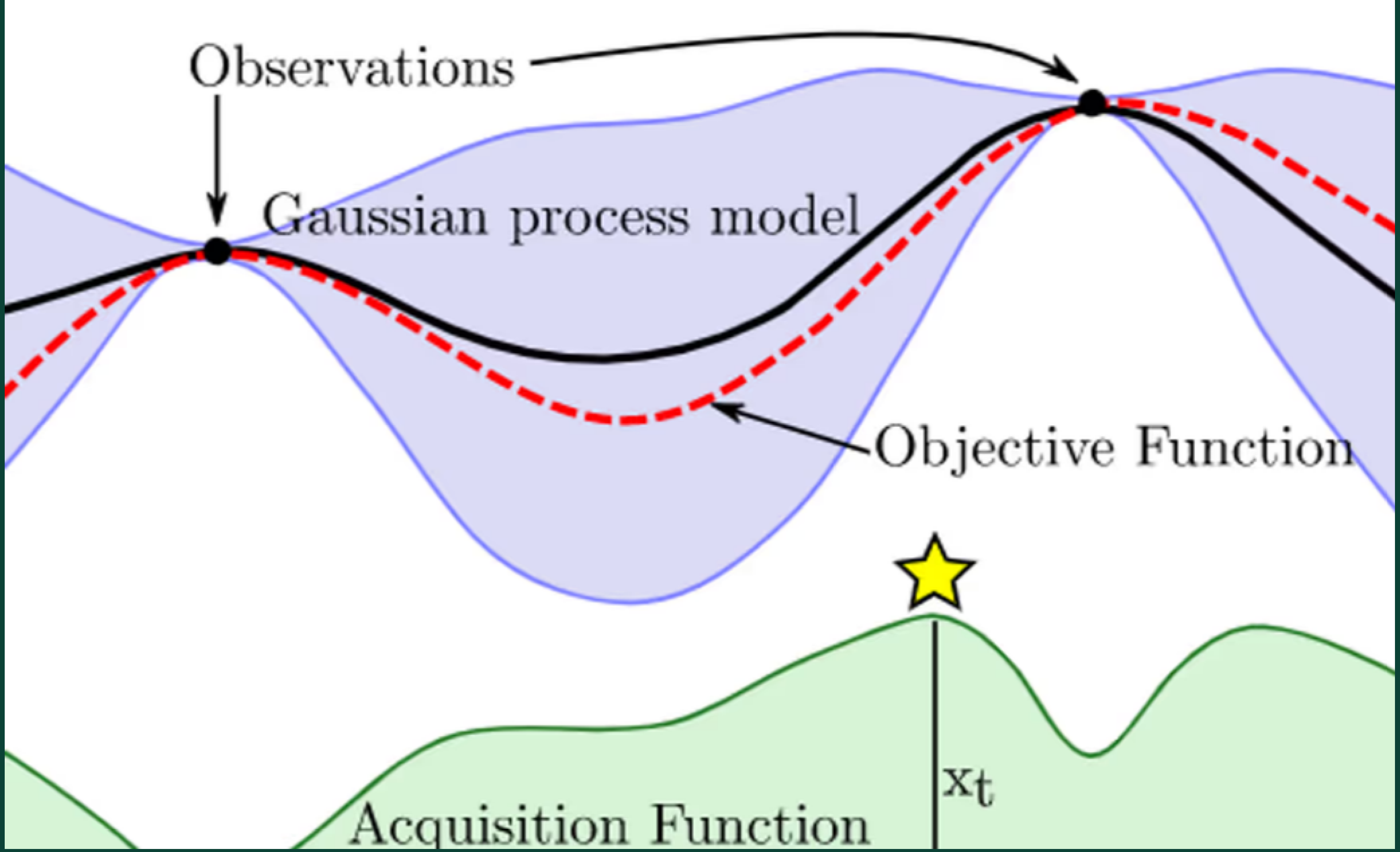
Surrogate function v/s Acquisition function

Surrogate Functionn

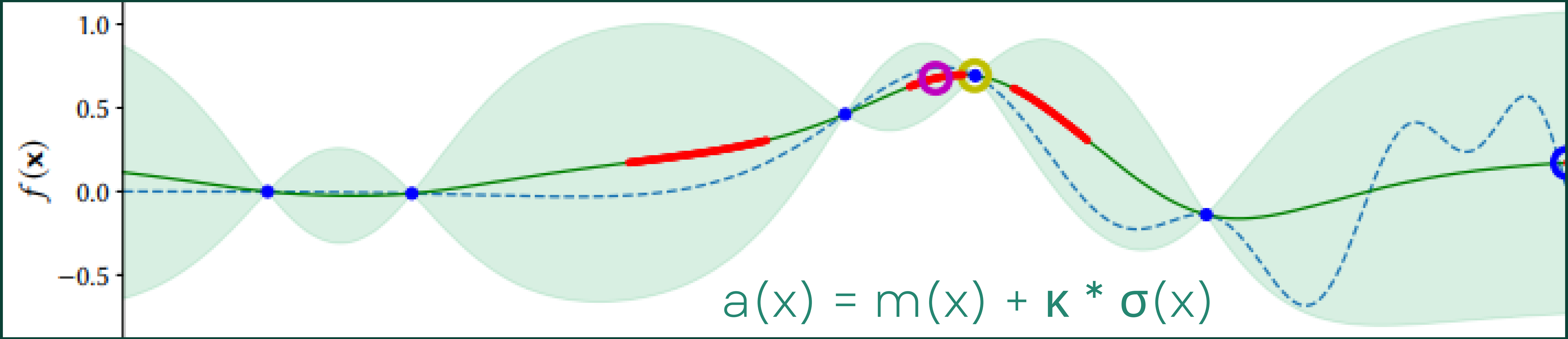
- Mathematical function that approximates the true objective function based on a set of observed data points

Acquisition function

- Mathematical function that guides the selection of the next point to evaluate in the search space, based on the information provided by the surrogate model.



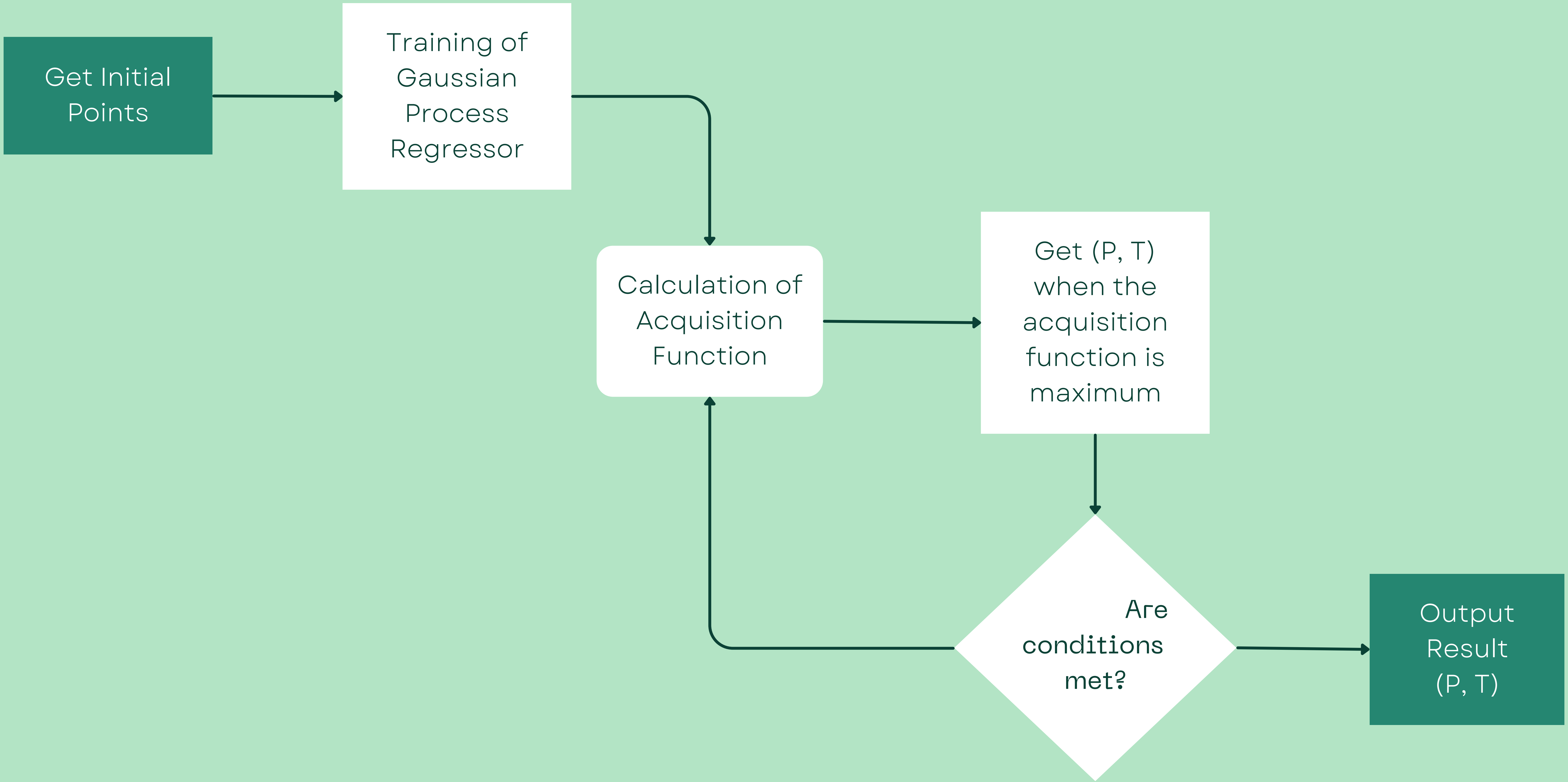
Tradeoff: Exploration v/s Exploitation

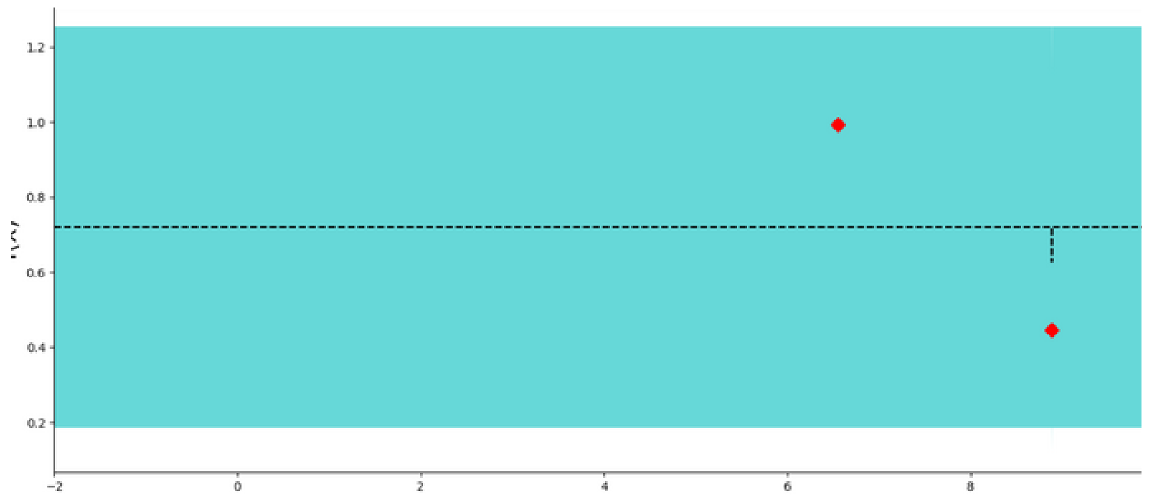


Exploitation	Exploration
Exploitation, on the other hand, refers to the selection of points that are expected to yield the highest value of the objective function based on the current knowledge of the search space, in order to improve the current best solution.	Exploration refers to the search for new points in the search space that have not been evaluated before, in order to gain more information about the objective function and reduce uncertainty.

Ref: https://arxiv.org/pdf/1911.12809.pdf

Bayesian Optimization Workflow





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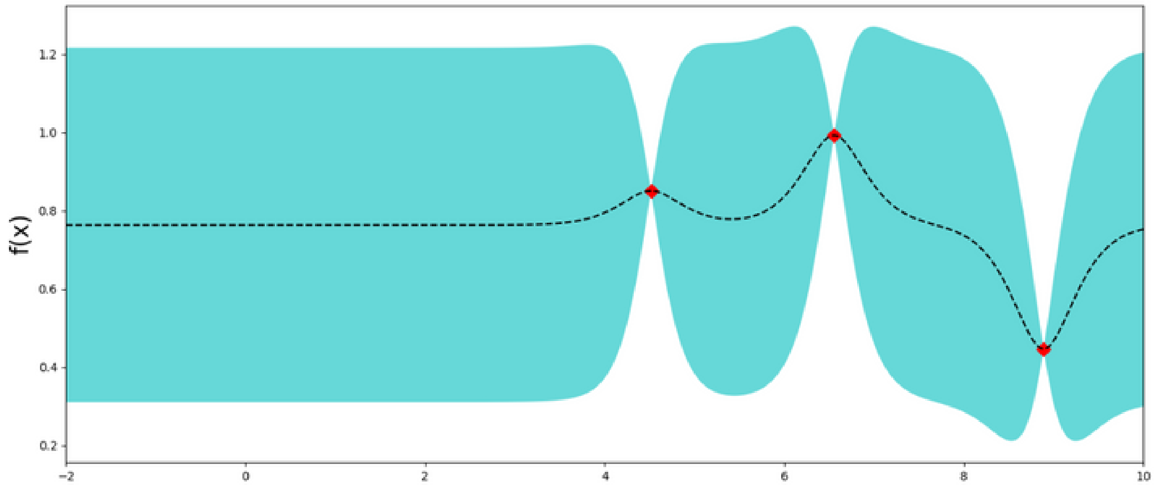

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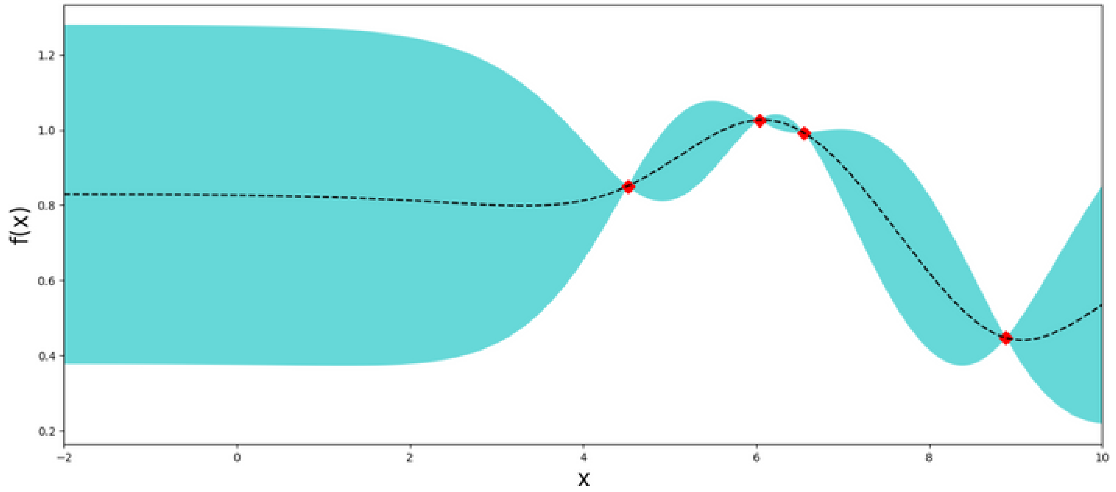

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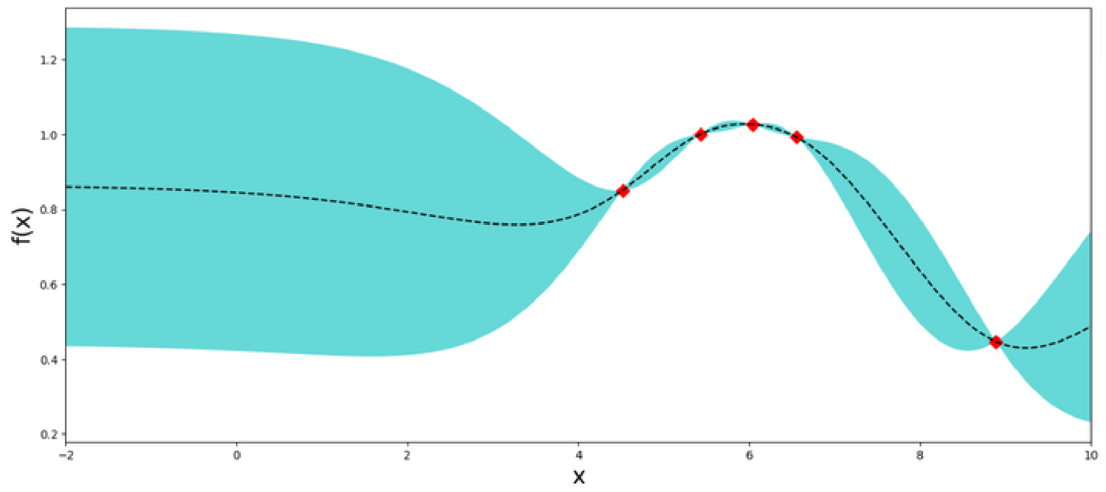

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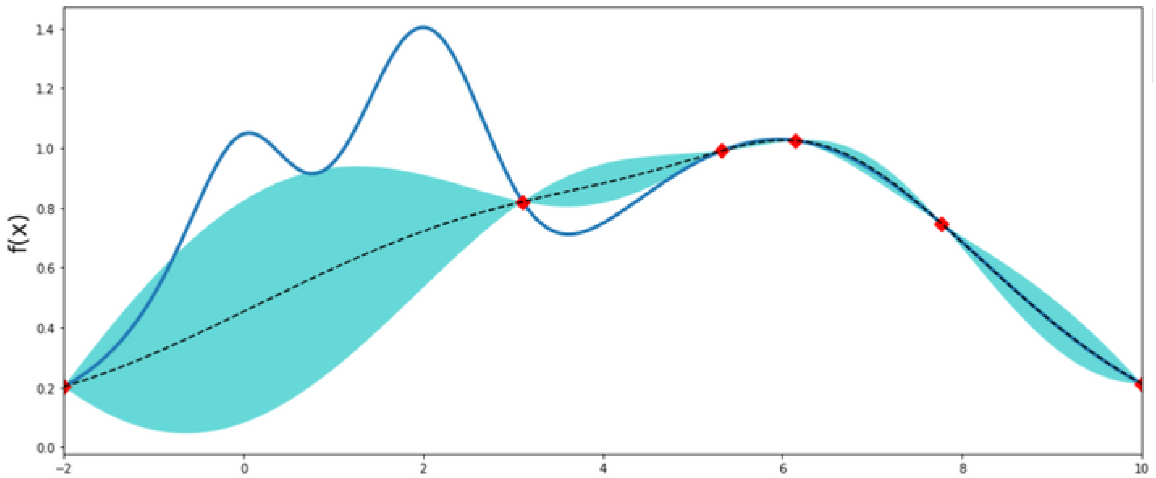

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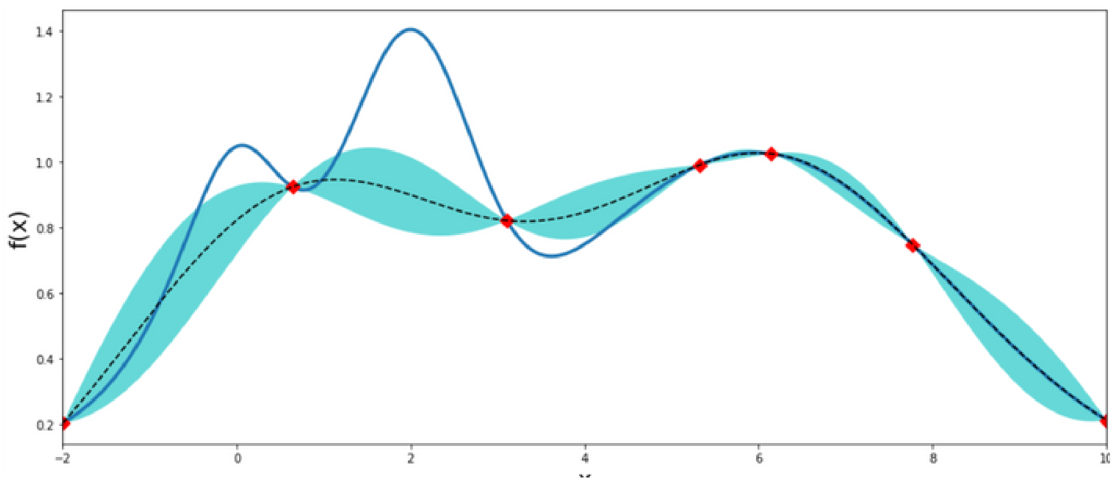

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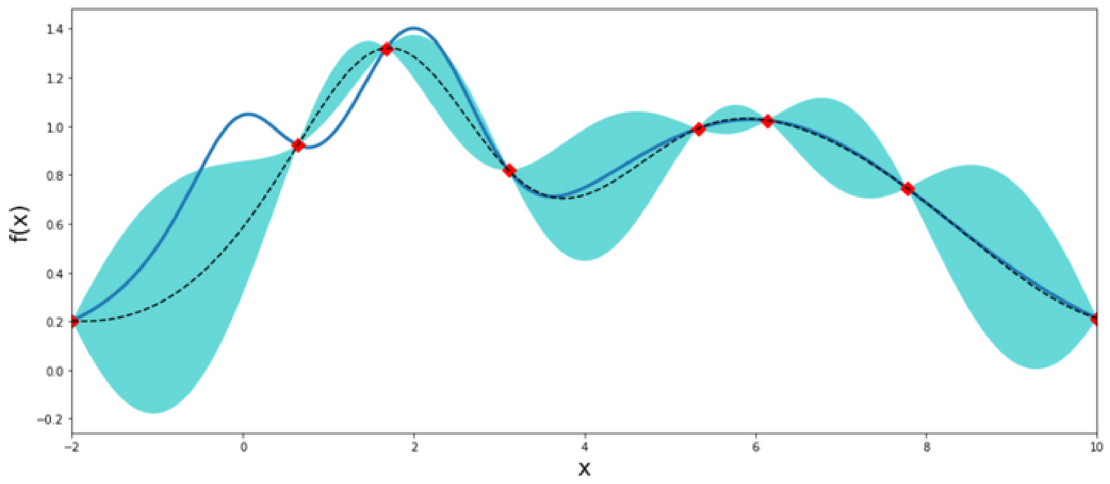

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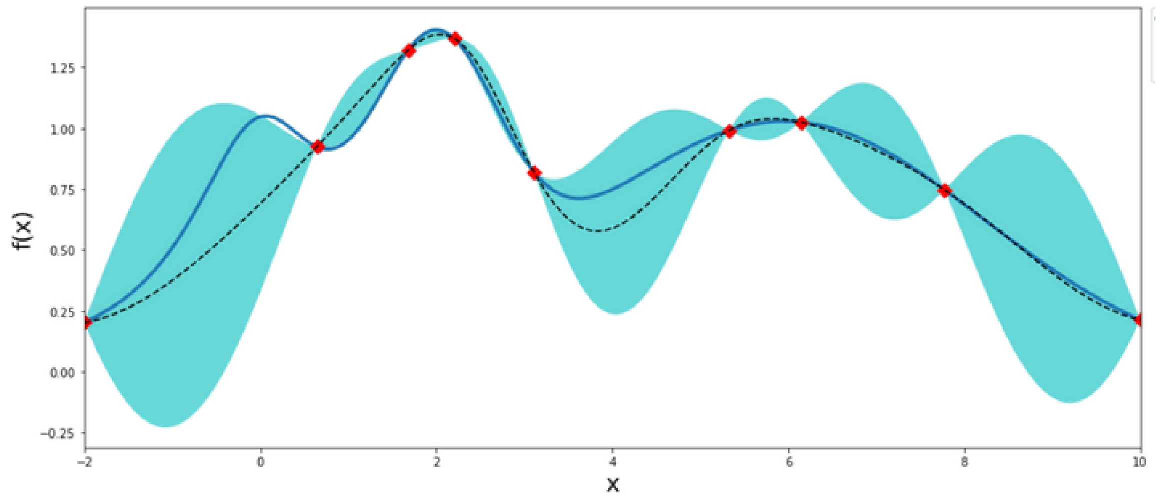

n = 9

Dataset

Temperature (C)	Pressure (MPa)	% Yield
1500	9.0	76.64815
1600	6.0	64.63658
1650	7.0	71.50594
⋮	⋮	⋮

https://doi.org/10.1016/j.matdes.2020.109290.

Results

Optimum process parameters	Production cost	Powder quality
We applied a machine learning-driven optimization approach to determine the promising process parameters for gas atomization of the Ni-Co based superalloy at TP = (1650 C, 9.0 MPa)	This improvement of yields contributed to the reduction of the powder manufacturing cost and successfully reduced the cost by approximately 72% compared to a commercial powder.	The powder quality was confirmed, from literature, to be extremely high, exhibiting higher circularity, higher homogeneity, and fewer satellites, as a result of the yield improvement by Bayesian optimization.

Future work

More features	Larger dataset
We only focused on the optimization of two process parameters, that is, melt temperature and gas pressure, but many other parameters should be controlled during gas atomization. Thus, the complete optimization of powder metallurgy by machine learning will be explored in the future.	A larger dataset based on state of the art techniques involved in domain of Material Informatics can be used to extend the dataset by extracting, cleaning and archiving experimental data for better model training.

References

- https://arxiv.org/pdf/1911.12809.pdf
- https://www.sciencedirect.com/science/article/pii/S0264127520308261
- https://ax.dev/docs/bayesopt.html
- https://doi.org/10.1016/j.matdes.2020.109290.

Thankyou