Machine Learning for Global Optimization of Black-box Functions

SPE Stavanger Student Chapter Lecture Series, UiS

Peyman Kor

2021-10-18

Who is this guy?

Introduction: Peyman Kor

🇮🇷 **B.Sc in Petroleum Engineering , Petroleum University of Technology (2011-2016)**

🇳🇴 **M.Sc in Reservoir Engineering, University of Stavanger (2017-2019)**

Decision-Driven Data Analytics for Well Placement Optimization in Field Development Scenario - Powered by Machine Learning

M.Sc Thesis

Peyman Kor

June 2019

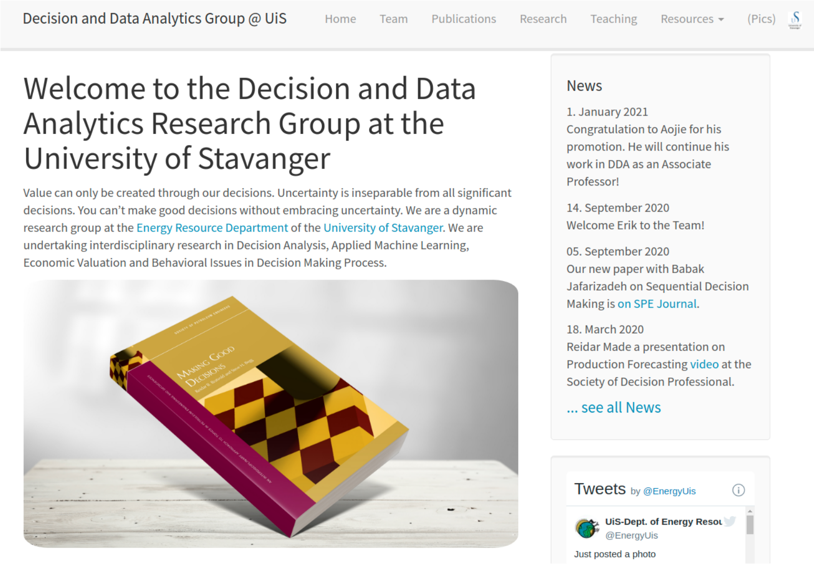
🇩🇰 **M.Sc in Applied Mathematics and Computation, Technical University of Denmark (2019 - 2020)**

Introduction: Peyman Kor

🇳🇴 Ph.D. Student in Computational Engineering, University of Stavanger, Dec 2020 - Ongoing

- Decision Analysis, Optimization, and Reinforcement Learning.
- Supervisors: Reidar B. Bratvold and Aojie Hong

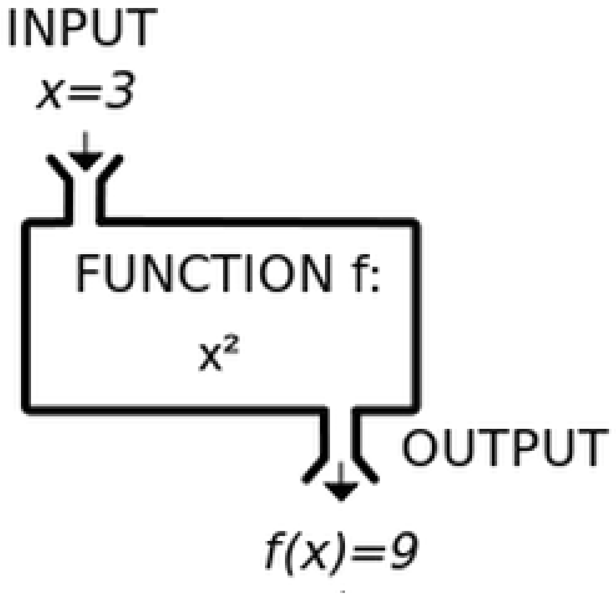
- Decision and Data Analytics (DDA) Research Group at the University of Stavanger



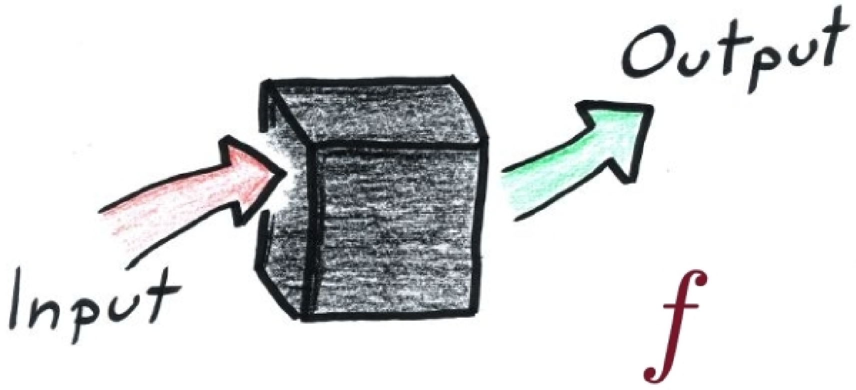
Black-Box Function Optimization?

What is Black-box Function?

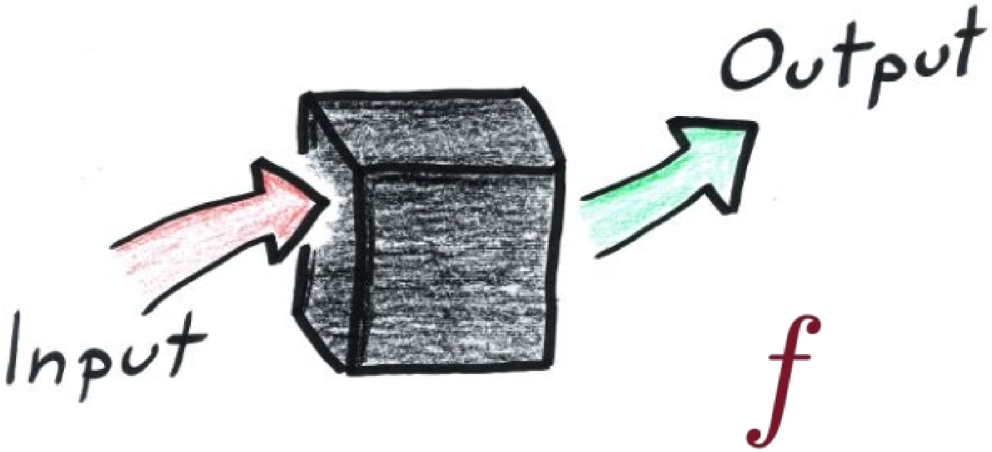
White-box function



Black-box function



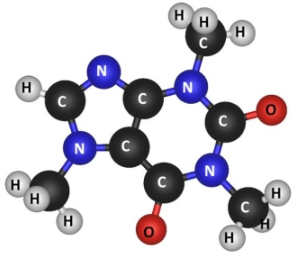
Black-box Function Optimization

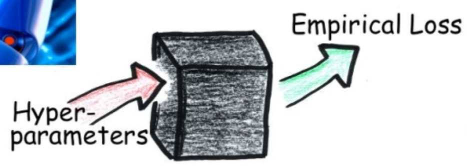


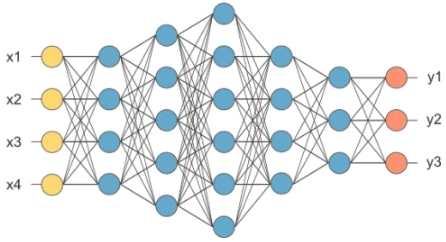
Goal:

$$x_* = \underset{\mathcal{X} \subset \mathbb{R}^d}{\operatorname{argmax}} \; f(x)$$

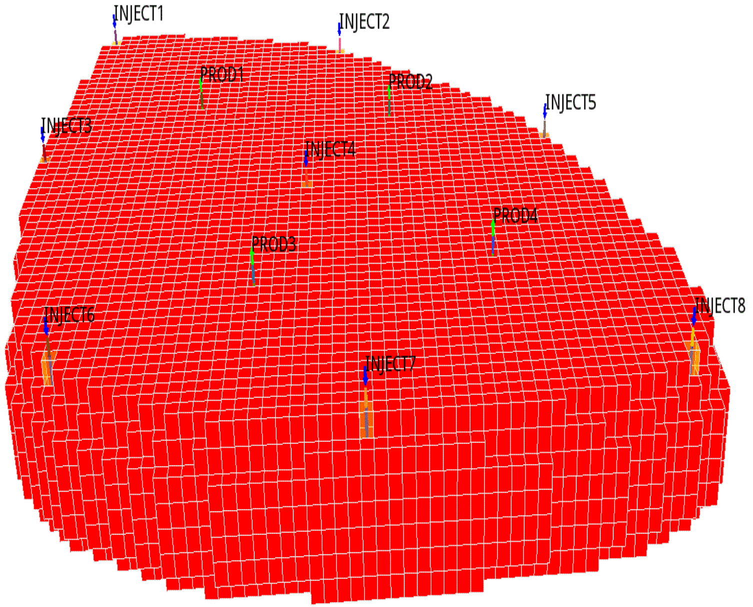
Black-box Function Optimization







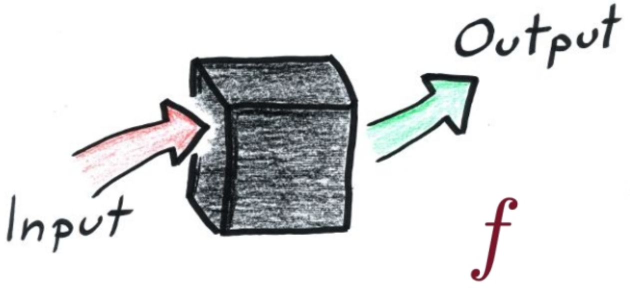
Output of Reservoir Simulation



Why Black-box Function Optimization is difficult?

Three main reasons: A, B, C

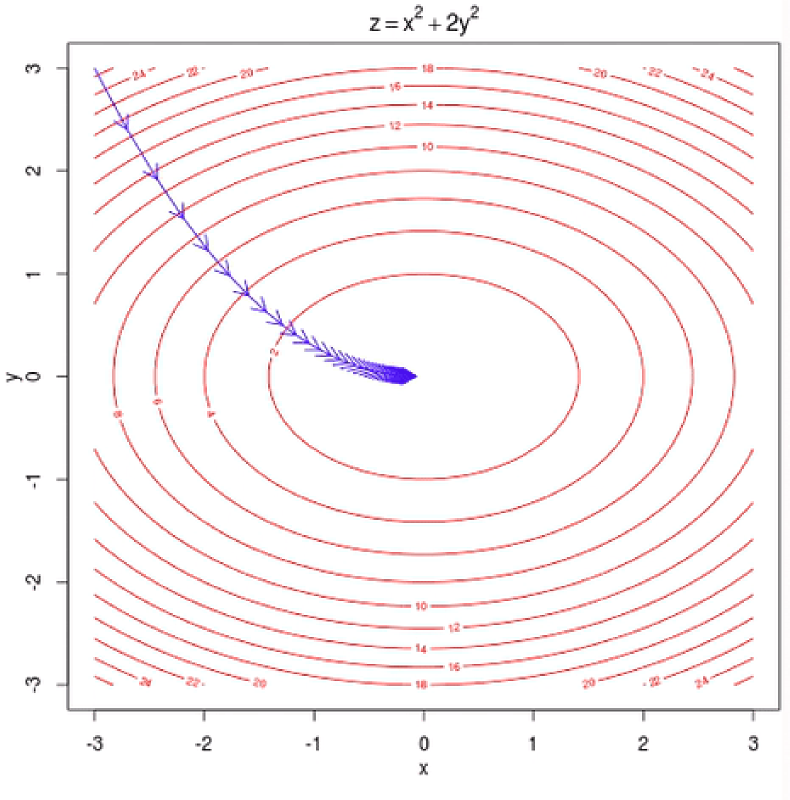
Why Black-box Function Optimization is difficult? (A)



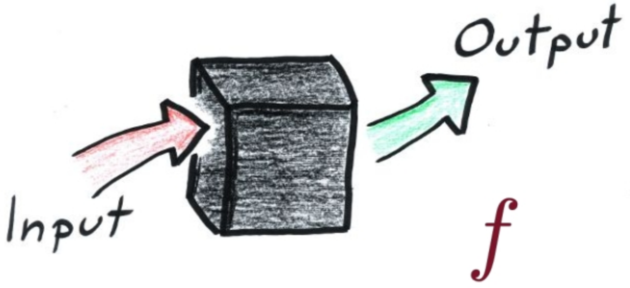
Goal:

$$x_* = \underset{\mathcal{X}\subset\mathbb{R}^d}{\operatorname{argmax}}\, f(x)$$

A) No grdaient information!



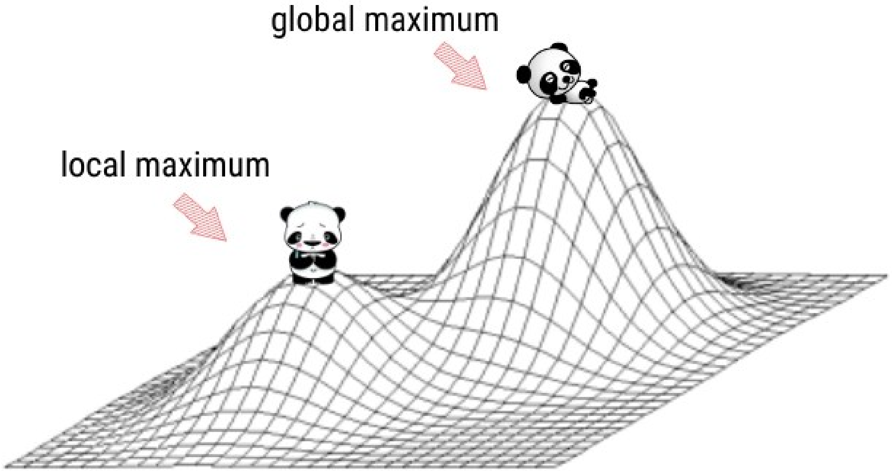
Why Black-box Function Optimization is difficult? (B)



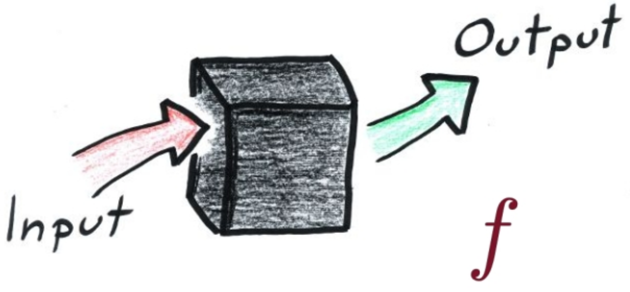
Goal:

$$x_* = \underset{\mathcal{X} \subset \mathbb{R}^d}{\operatorname{argmax}} f(x)$$

B) $f(x)$ is multi-peak!



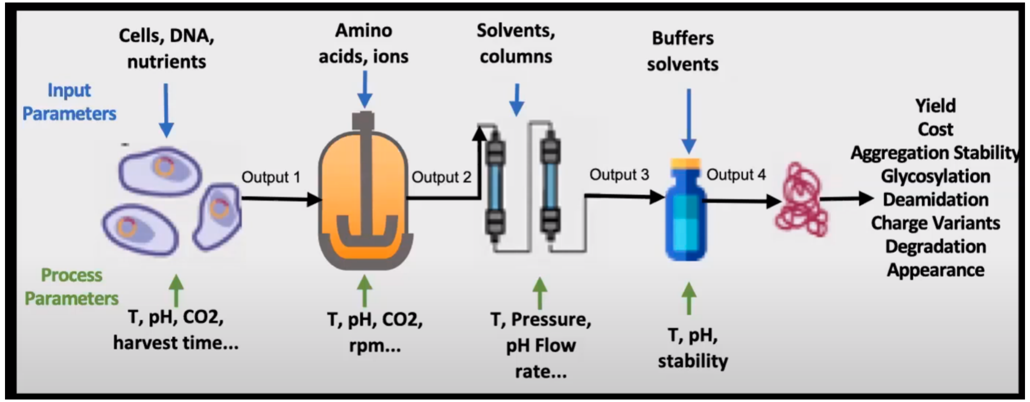
Why Black-box Function Optimization is difficult? (C)



Goal:

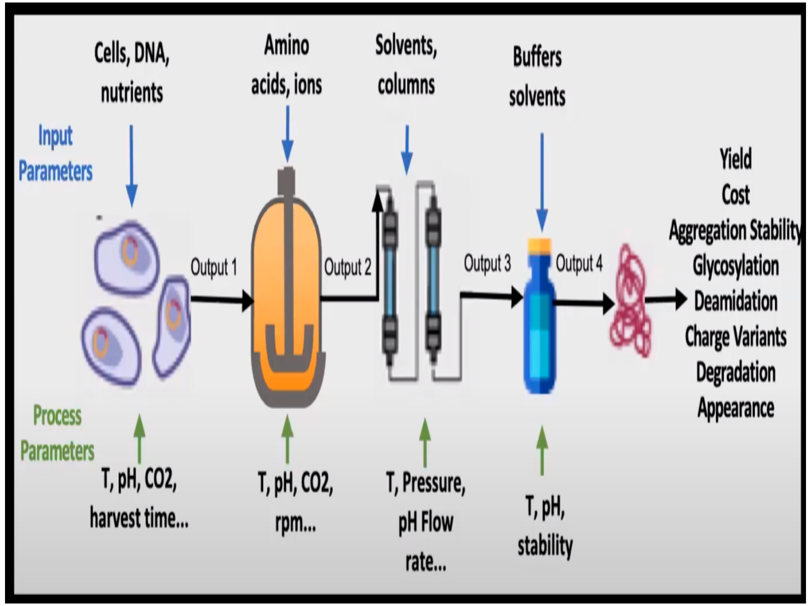
$$x_* = \underset{\mathcal{X} \subset \mathbb{R}^d}{\operatorname{argmax}} f(x)$$

B) forward evaluation of $f(x)$ is time-consuming!



Why Black-box Function Optimization is difficult? (C)

- Each forward evaluation of the experiments takes around $\sim 1\text{month}$



- Say the biochemical engineering team of company has identified 4 main process parameters.
  - 1)Temperature, 2)pH, 3)Co2 Concentration, 4)Harvest Time
- According to them, each of the process parameters can take 5 different value.
- Then total possible combinations are $5^4 = 625$
- Then total time to evaluate all possible combination of solution is

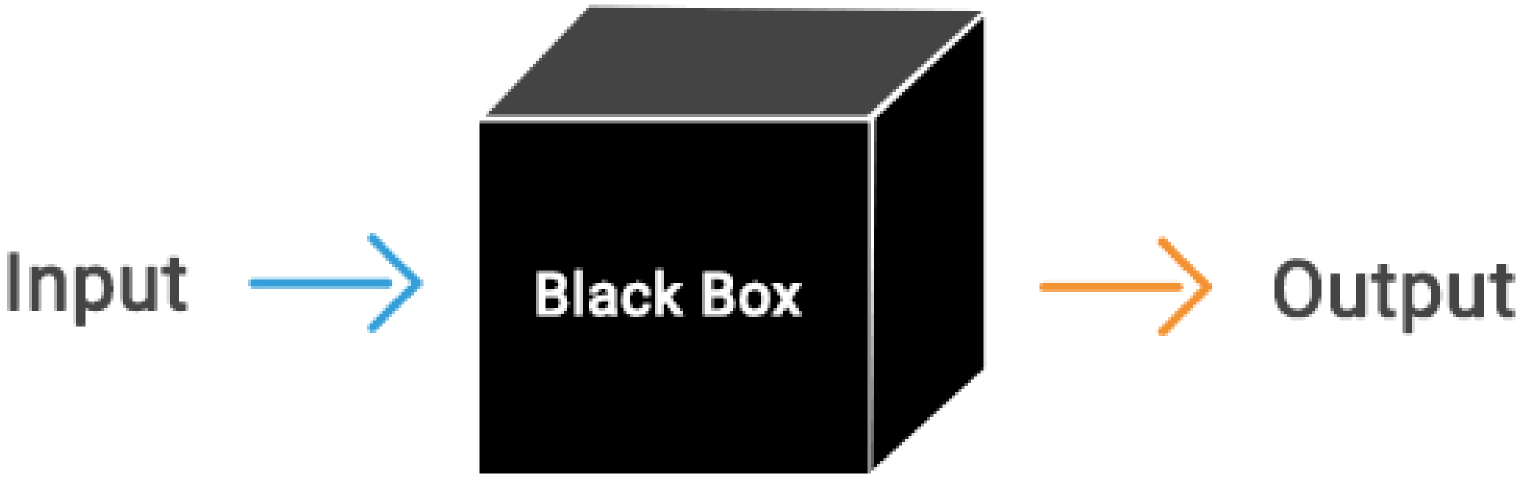
$$5^4 \times \text{month} = 625 \times \text{month} \sim 52 \text{ years!}$$

We need an optimization method that can handle all three difficulties!

Bayesian Optimization

Well-suited method for global optimization of black-box functions.

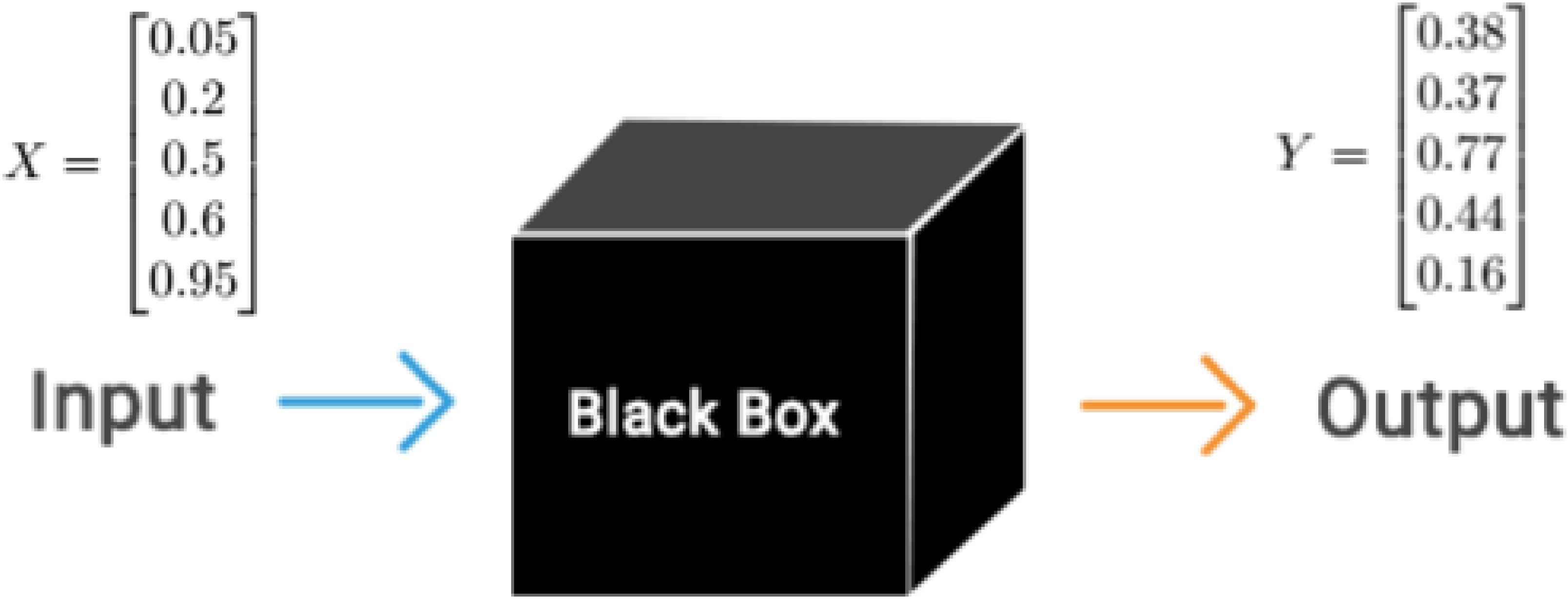
Example of Bayesian Optimization:



Question: What is the input that maximizes the output?

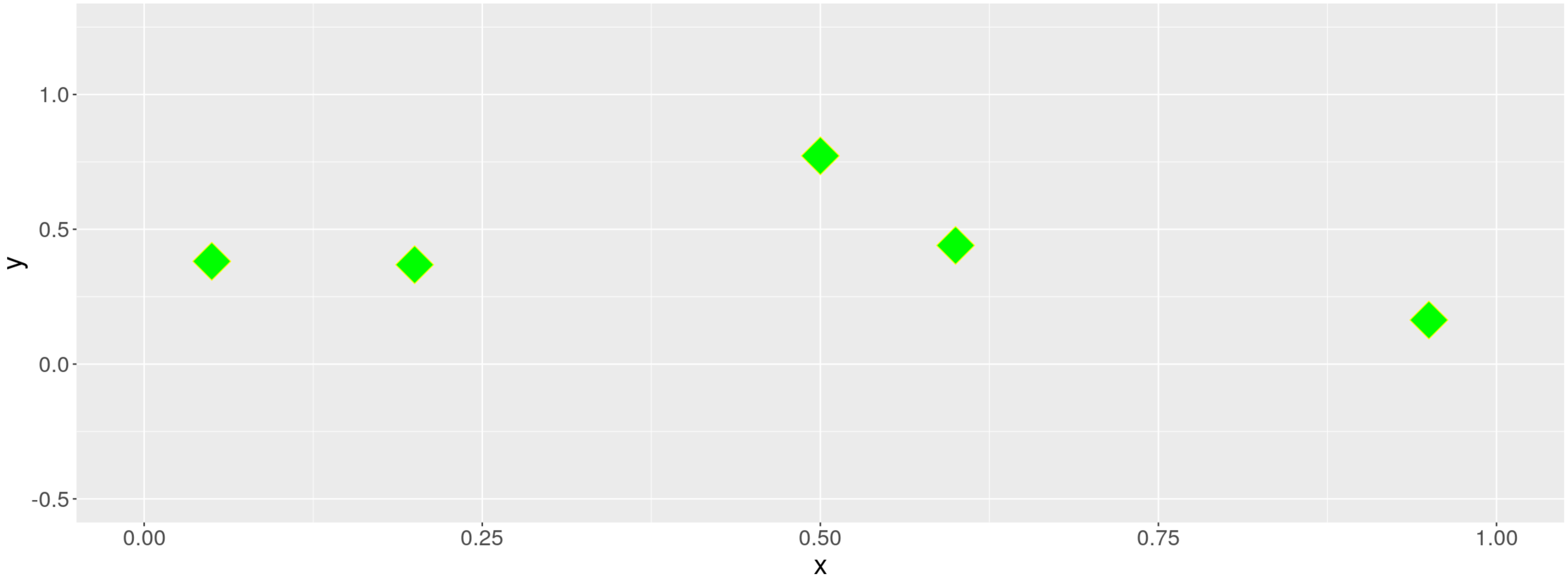
Example of Bayesian Optimization:

Step I) Initialization:



Example of Bayesian Optimization:

Step I) Plot of Initialization:



Example of Bayesian Optimization:

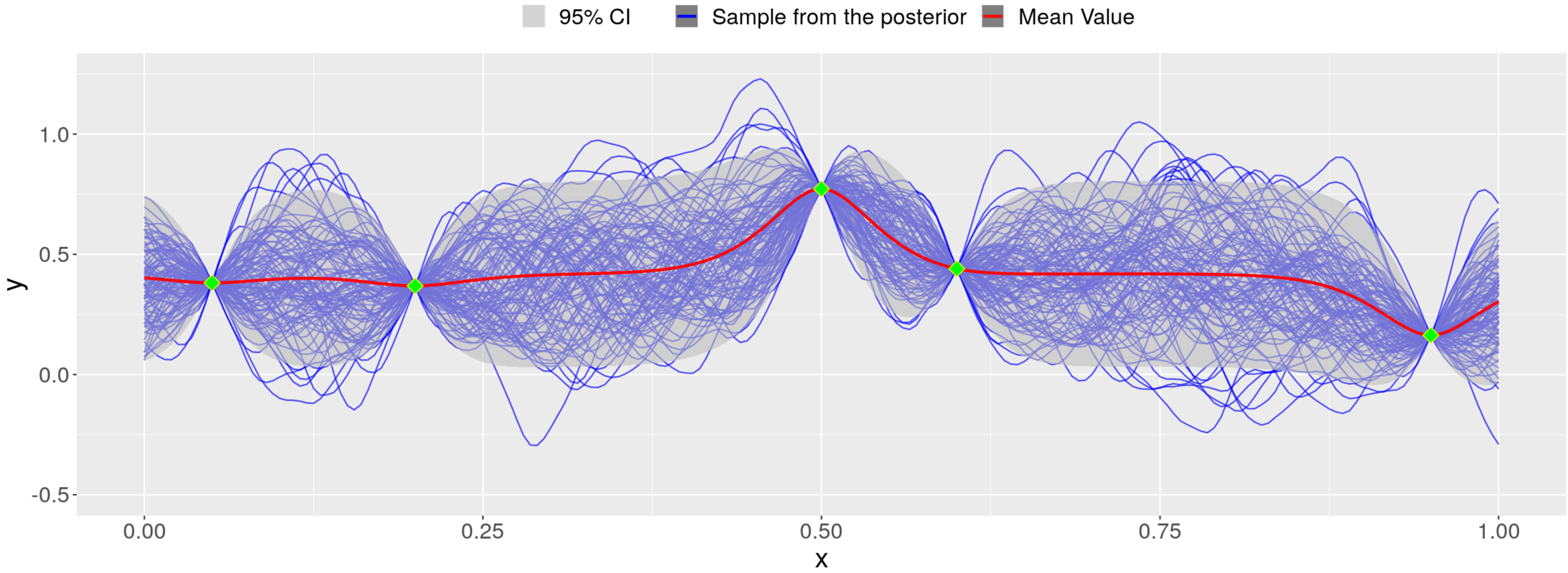
Step II) Build a probabilistic machine learning model

$$X = \begin{bmatrix} 0.05 \\ 0.2 \\ 0.5 \\ 0.6 \\ 0.95 \end{bmatrix}, Y = \begin{bmatrix} 0.38 \\ 0.37 \\ 0.77 \\ 0.44 \\ 0.16 \end{bmatrix}$$

- We use **Gaussian Process Regression** as a Machine Learning model.
- Gaussian Process Regression : Gives the **Mean** of this probability distribution at each test data x^*.
- Furthermore, Gaussian Process Regression gives the **Confidence Interval (CI)** at each test data x^*.

Example of Bayesian Optimization:

Step II) Build a probabilistic machine learning model.



Example of Bayesian Optimization:

Step III) How to find the next x^{next} from the expensive function?

Example of Bayesian Optimization:

Step III) How to find the x^{next} from the expensive function?

Example of Bayesian Optimization: (Three Iterations)

Final Solution of Bayesian Optimization (I):

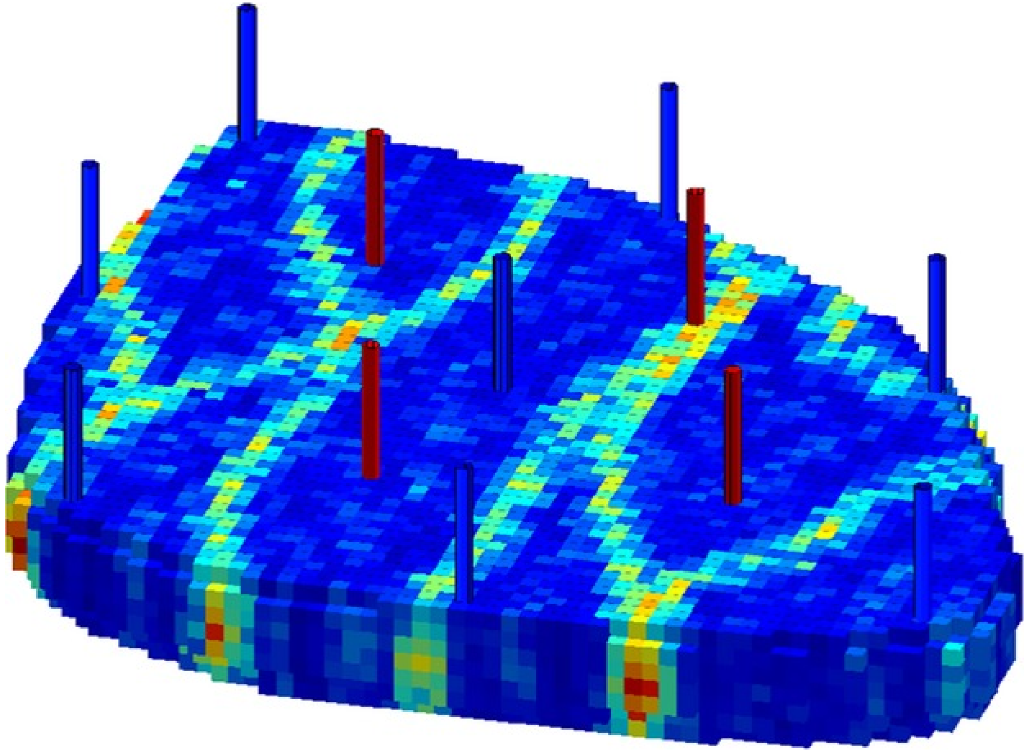
- The **True function** was:
- $y = 1 - \frac{1}{2}\left(\frac{\sin(12\mathbf{x})}{1+\mathbf{x}} + 2\cos(7\mathbf{x})\mathbf{x}^5 + 0.7\right)$
- The global optima of the function is $x_M = 0.39$
- After just two iterations, Bayesian Optimization solution is: 0.385
- Therefore, after two iteration, we are around $\frac{0.385}{0.390} = 98\%$
- Total number of function function has been evaluated is $size(D) + size(totaliteration) = 5 + 2 = 7$.

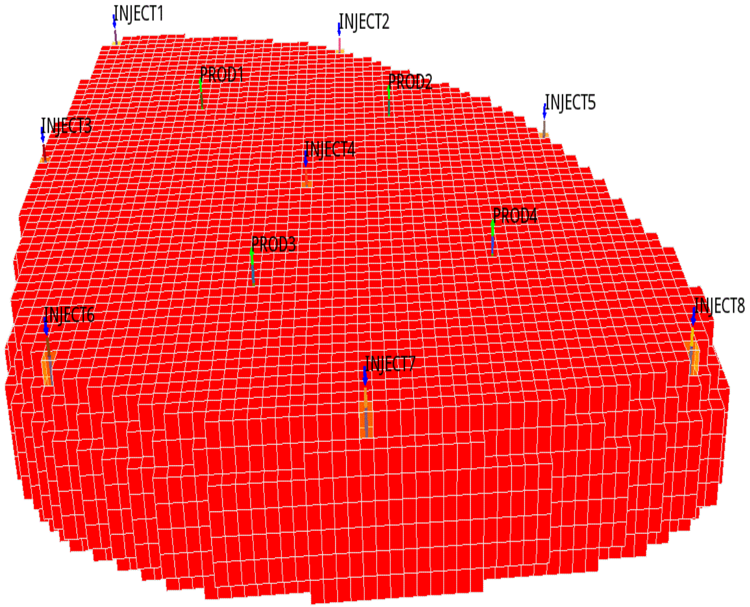
Final Solution of Bayesian Optimization (II)

Application of Bayesian Optimization for Management of Water flooding in Reservoir

Problem Definition:

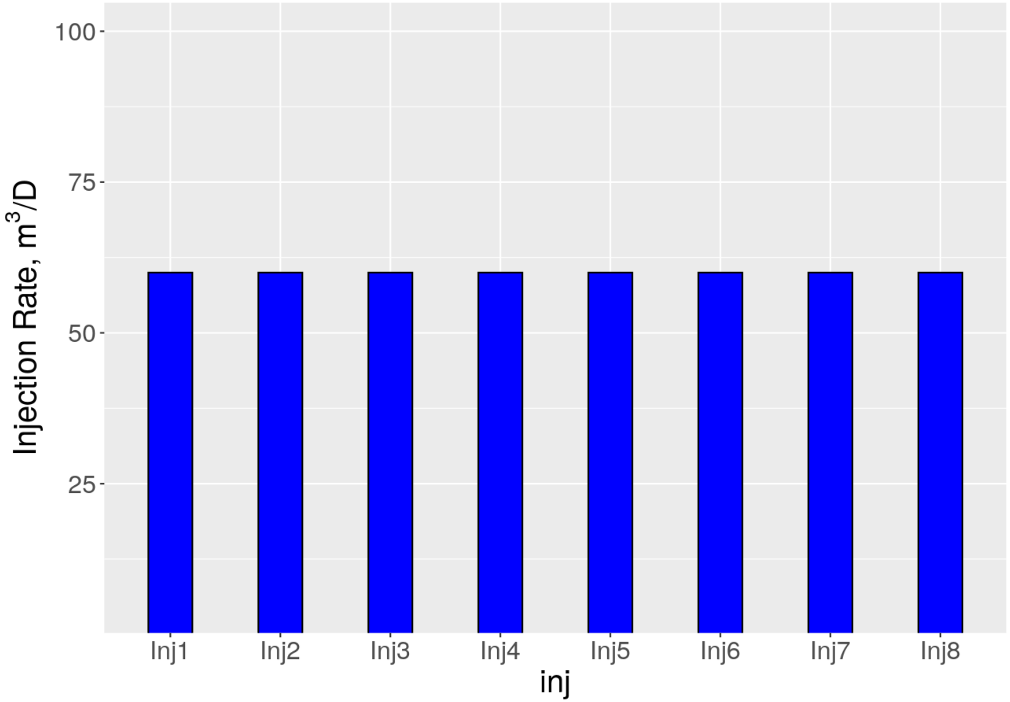
What are optimum wtaer injection rate for eight injection wells?





Improvemnet in profit compared to Base-case?

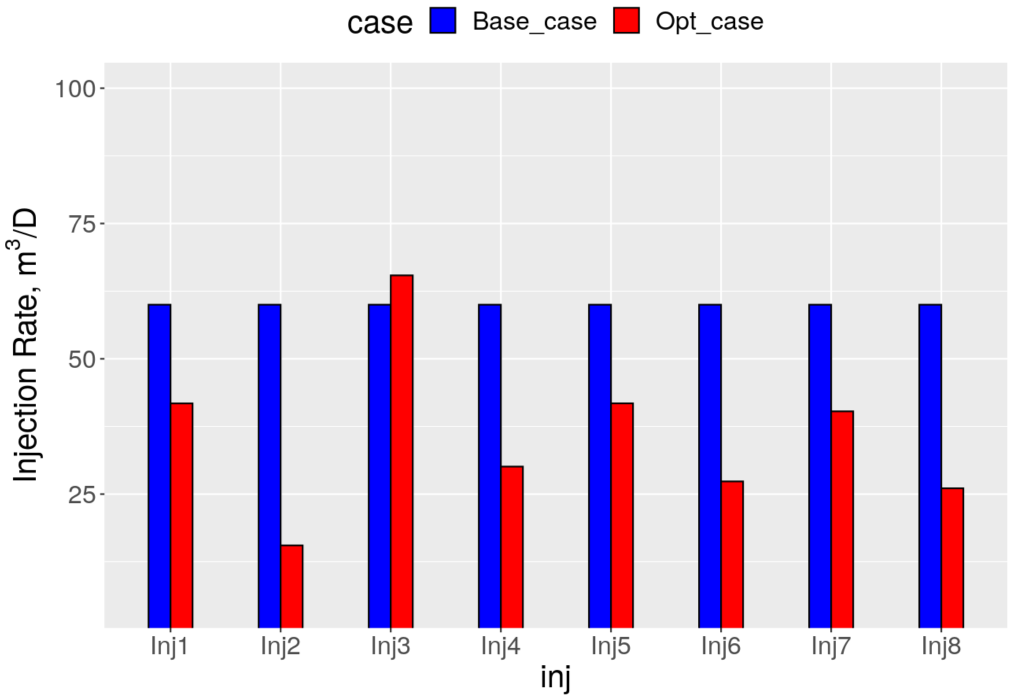
- **Base Case:**



- Objective Function: Net Present Value (NPV)=

$\sim$ 34.5 MM USD

- **Optimum Case:**



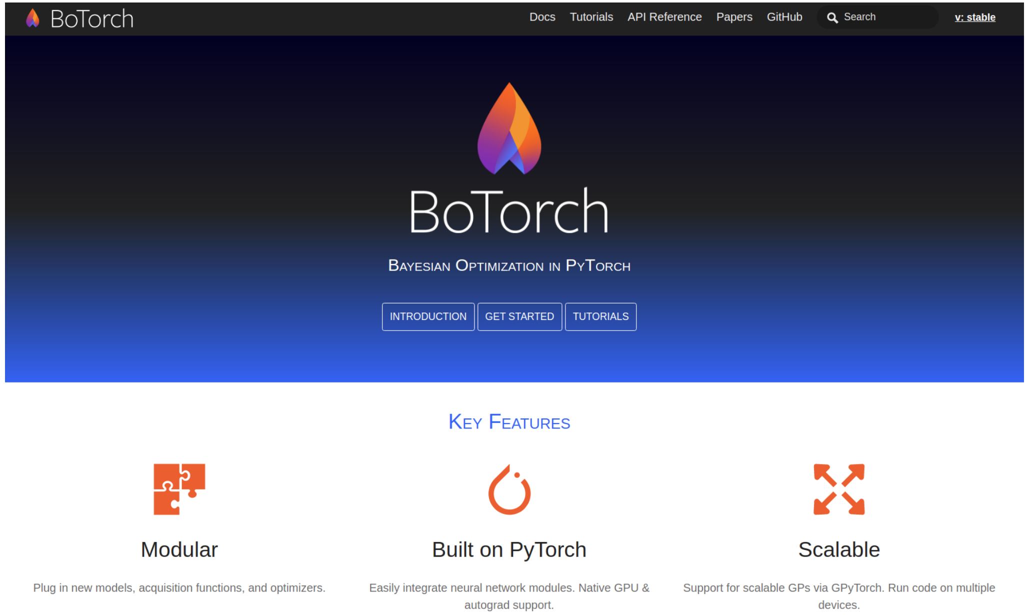
- Objective Function: Net Present Value (NPV)=

$\sim$ 36.8 MM USD

Big Tech Company working on Bayesian Optimization?

Facebook:

Python Package:



Research Team:

More detail about Bayesian Optimization:

Draft Title: Bayesian Optimization for Production Optimization under Uncertainty

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Abstract

An underlying challenge in well-control (production) optimization is that full-physic flow simulation of a 3D; rich grid-based model is computationally prohibitive. In a robust optimization (RO) setting, where flow simulation has to be repeated over a hundred(s) of geological realizations, conducting the RO becomes impractical in many field-scale cases. In this work, to alleviate this computational burden, a new computationally efficient optimization workflow is presented. In this context, computational efficiency means that the workflow needs a minimum number of forward model (flow-simulation) evaluations while still being able to capture the near-global optimum of the pre-defined objective function. Moreover, the workflow can handle cases where precise analytical expression of the objective function is nonexistent. Such situations typically arise when the objective function requires the result of solving a large number of PDE(s), such as in reservoir-flow simulation. In this workflow, referred to as 'Bayesian Optimization,' the objective function for samples of decision (control) variables is first computed using a proper design experiment. Then, given the samples, a Gaussian Process Regression (GPR) is trained to mimic the surface of the objective function as a surrogate model. While balancing the dilemma to select the next point between high mean, low uncertainty (exploitation) or low mean, high uncertainty (exploration), a new control variable is selected, and flow simulation is run for this new point. Later, the GPR is updated, given the output of the flow simulation. This process continues sequentially until termination criteria are reached. To validate the workflow and get better insight into the details of steps, we first optimize a 1D problem. Then, the workflow is implemented for a 3D synthetic reservoir model to perform robust optimization in a realistic field scenario. Finally, a comparison of the workflow with two other commonly used gradient-free algorithms in the literature, namely Particle Swarm Optimization (PSO) and Genetic Algorithm (GA), is performed. The comparison shows that the workflow presented here will reach the same near-optimal solution achieved with GA and PSO, yet reduce computational time of the optimization 5X (times). We conclude that the method presented here significantly speeds up the optimization process leveraging a faster workflow for real-world 3D optimization tasks, potentially reducing CPU times by days or months, yet giving robust results that lead to a near-optimal solution.

Key words: Optimization, Gaussian Process, Probabilistic Modeling, Bayesian

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Preprint submitted to Journal of Petroleum Science And Engineering *October 13, 2021*

Thank you for your time and

Thanks to SPE Stavanger Student Chapter, for Invitation!