Bayesian optimization for polymer translocation

GitHub: https://github.com/Nina-Konovalova/bayes_experiment

Некоторые параметры для аппроксимации (для гаусса)

Aq functions:

- MPI
- EI

Num opt steps

- 70
- 100
- 200

Space

mu: [0; 100]

sigma: (0;400)

Amplitude: (-100;100)

GP

- exact feval: True
- num restarts: 3
- normalize: False

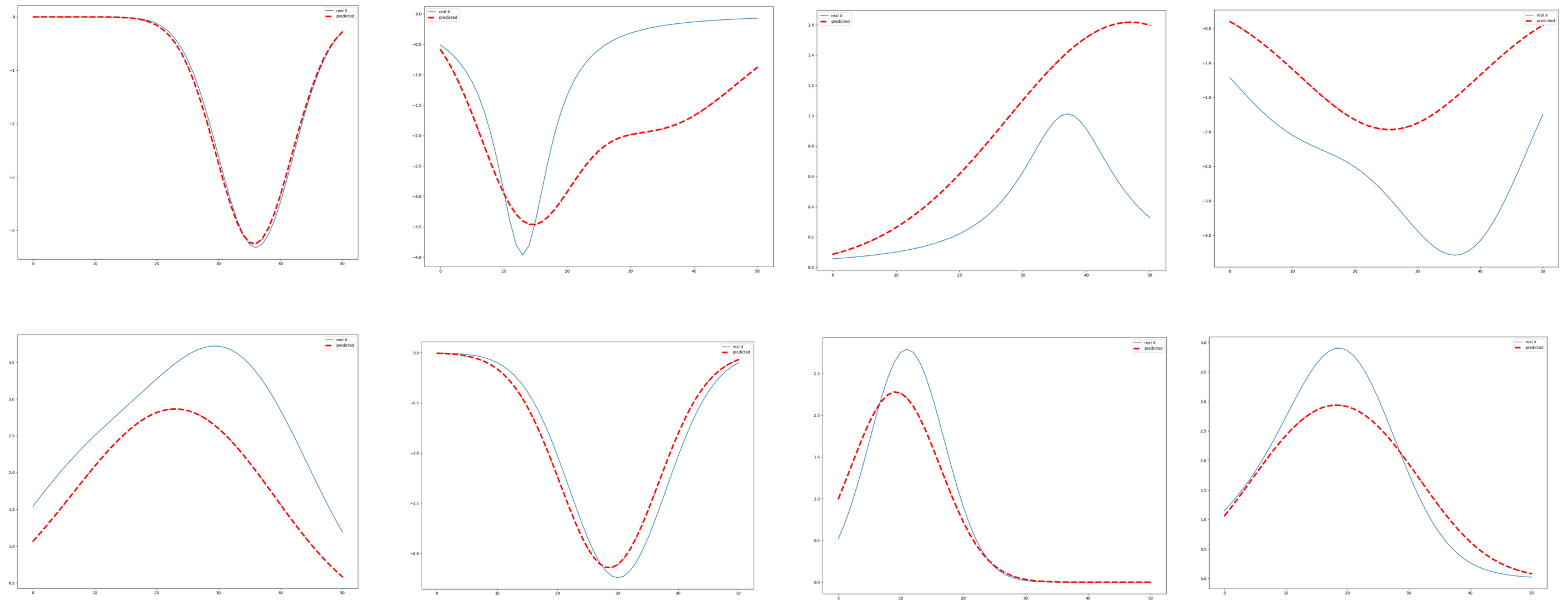
Kernels:

- RBF
- Matern32
- Matern52
- RatQuad

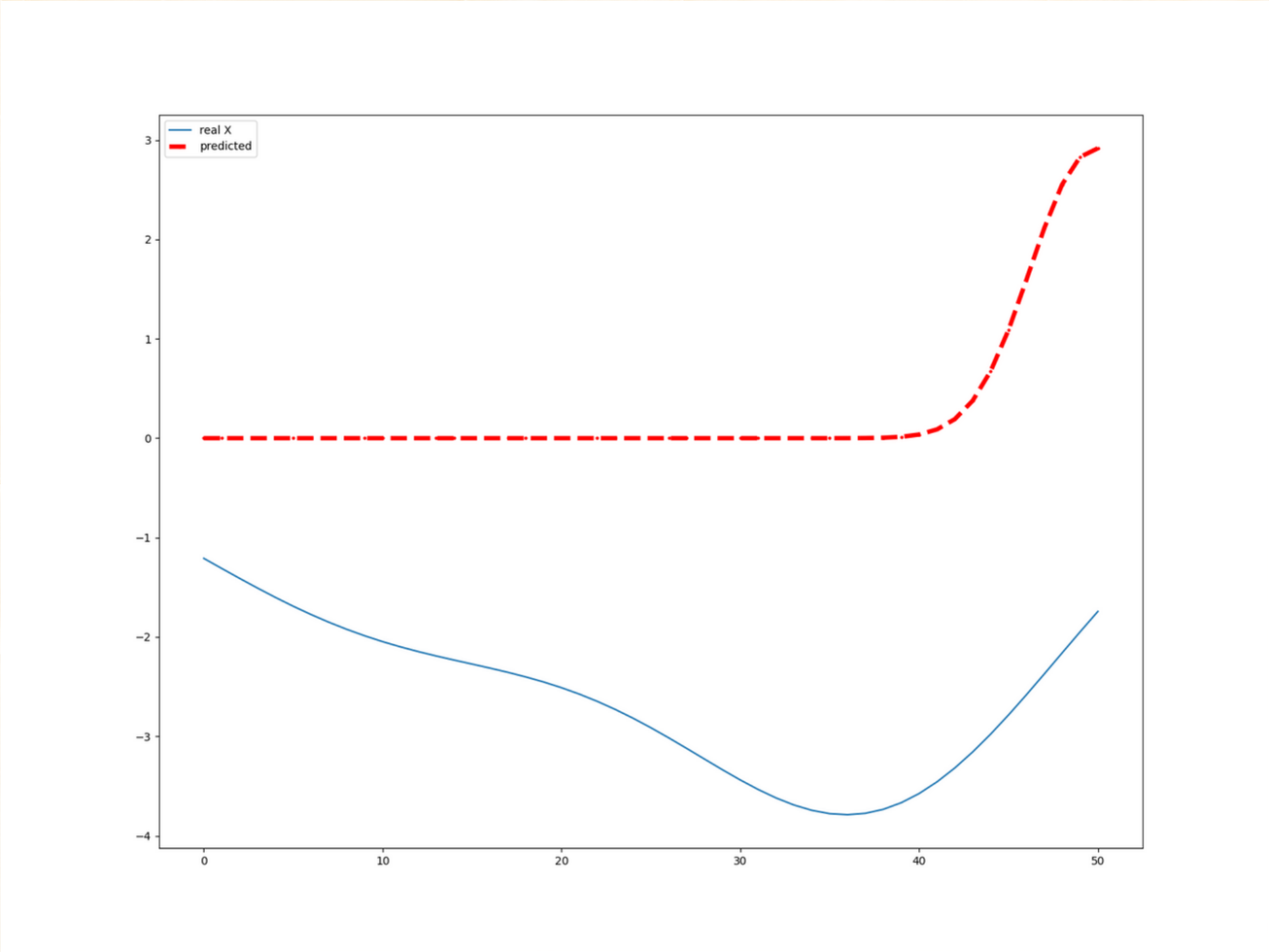
Constraints

A - 4sqrt(2pi*e)*sigma <=0

Аппроксимация нефиксированными гауссианами



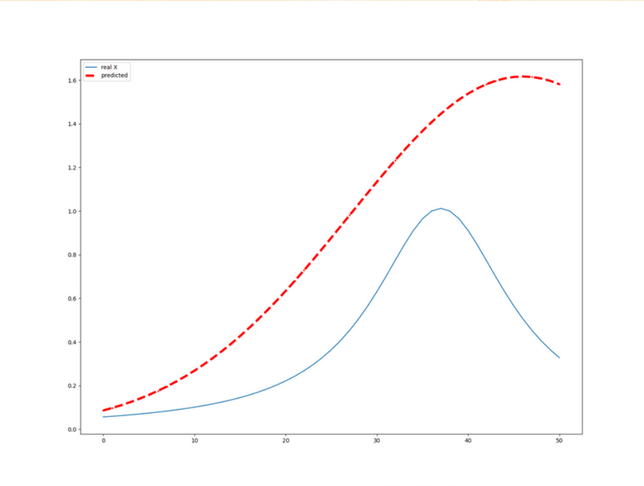
Проблемы: если делать нормализацию

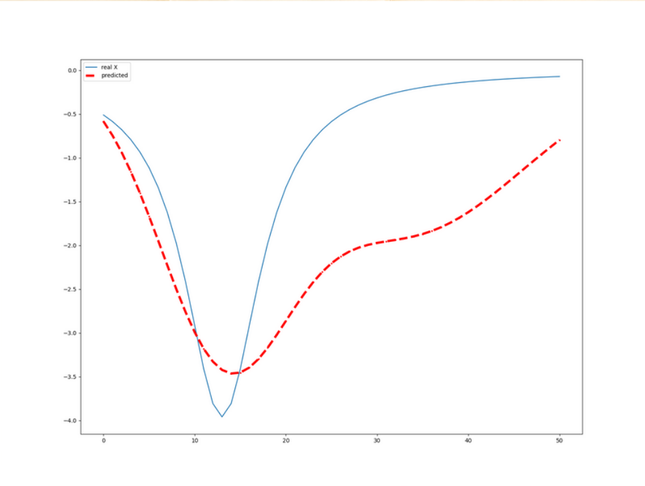


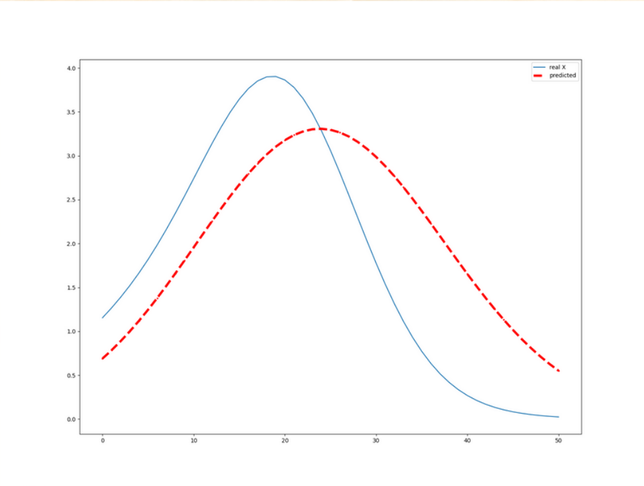
Некоторые выводы

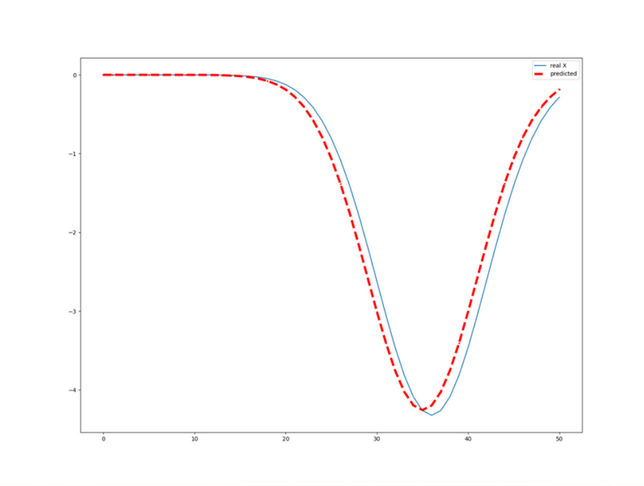
1. Некоторые случаи хорошо аппроксимирует
2. Не зависит от кернела
3. Не замечала сильных изменений при увеличении числа итераций

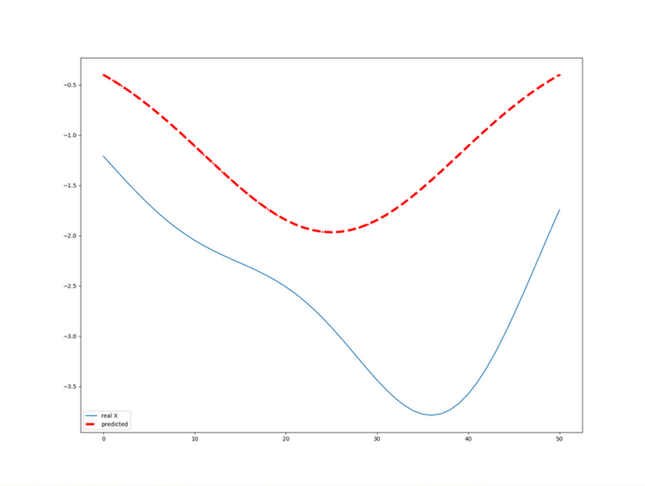
Аппроксимация гауссианами с фиксированными mean value

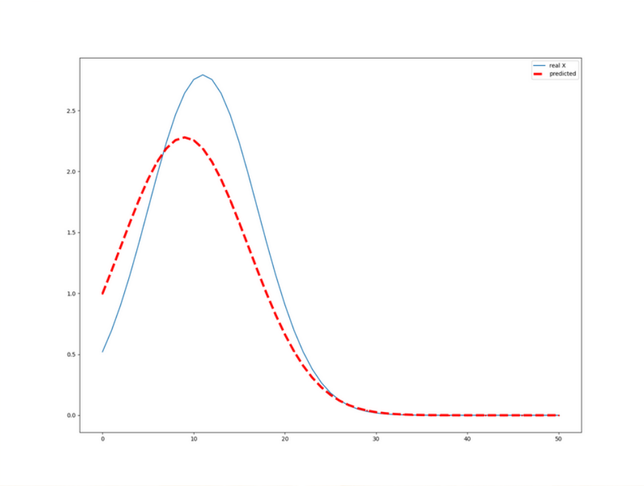




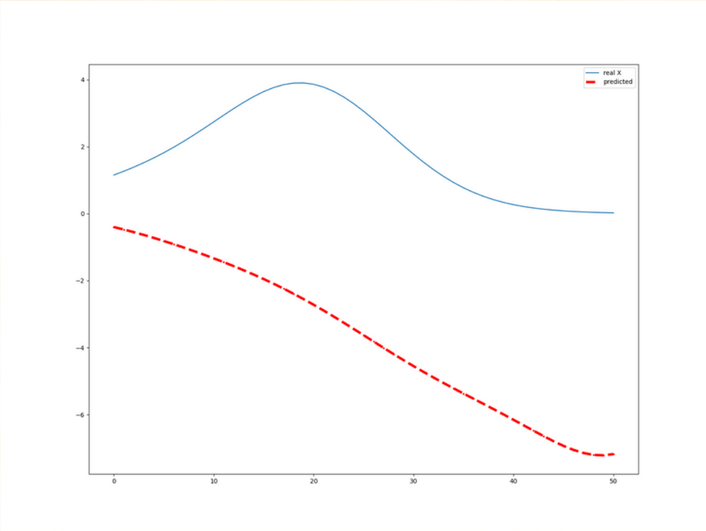


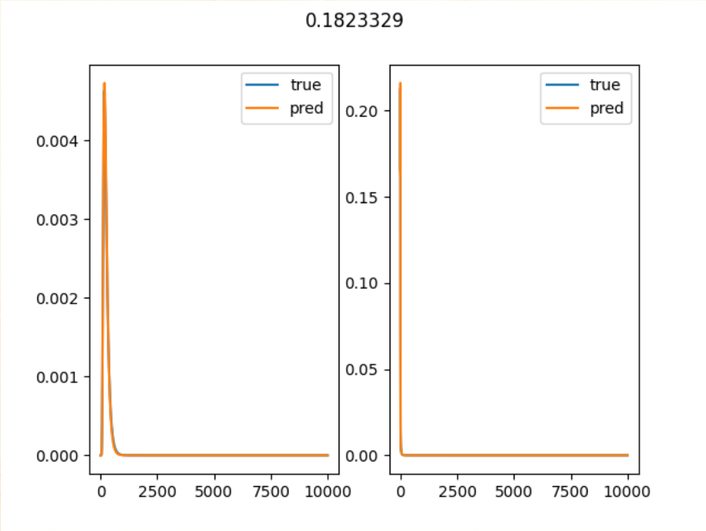






Проблемы



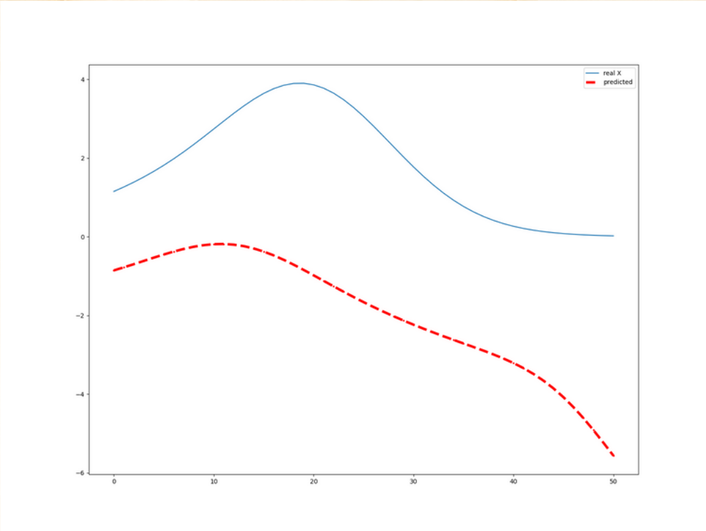


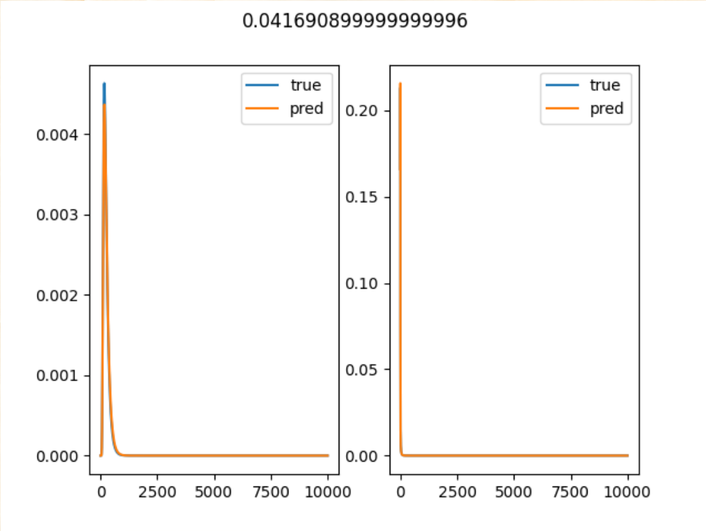
Matern32 10 gauss 200 steps

MSE_pos: 5.61e-10

MSE_neg: 2.18e-09

Difference between rates: 0.01 0.19 0.18





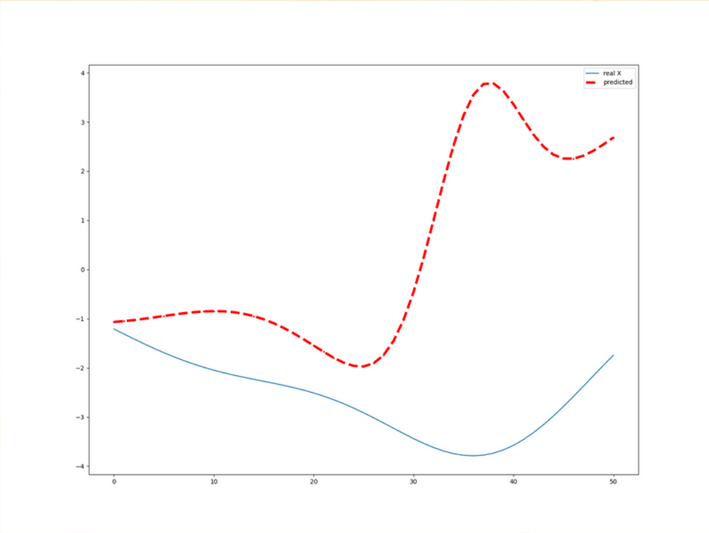
Matern32 15 gauss 200 steps

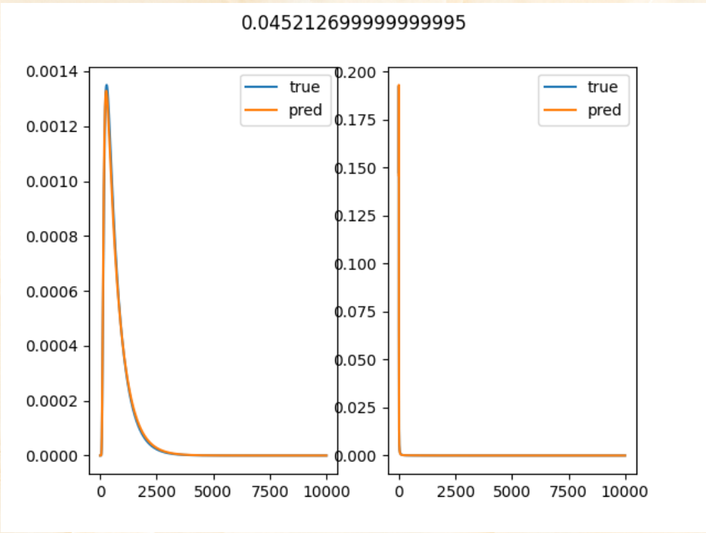
MSE_pos: 9.39e-10

MSE_neg: 9.69e-09

Difference between rates: 0.01 0.05 0.04

Проблемы



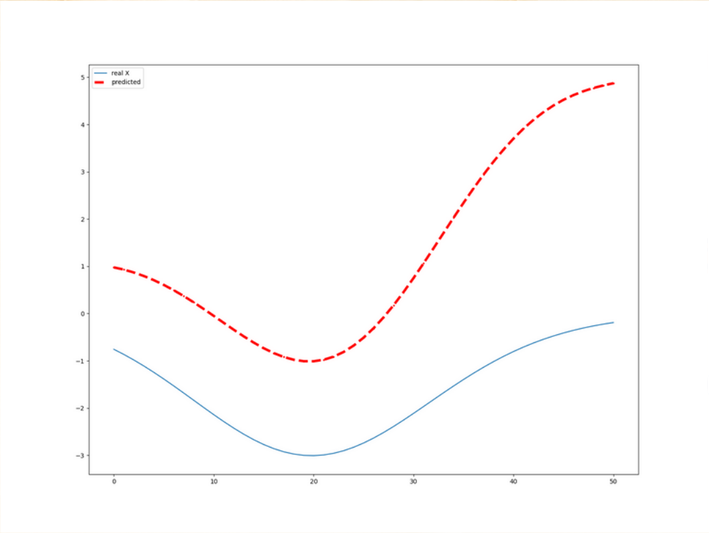


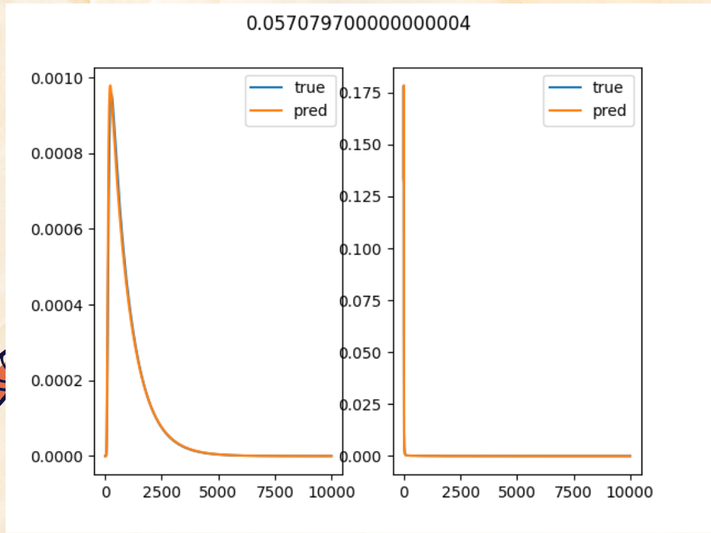
Matern32 20 gauss 200 steps

MSE_pos: 1.4e-10

MSE_neg: 1.13e-09

Difference between rates: 0.125 0.079 0.045





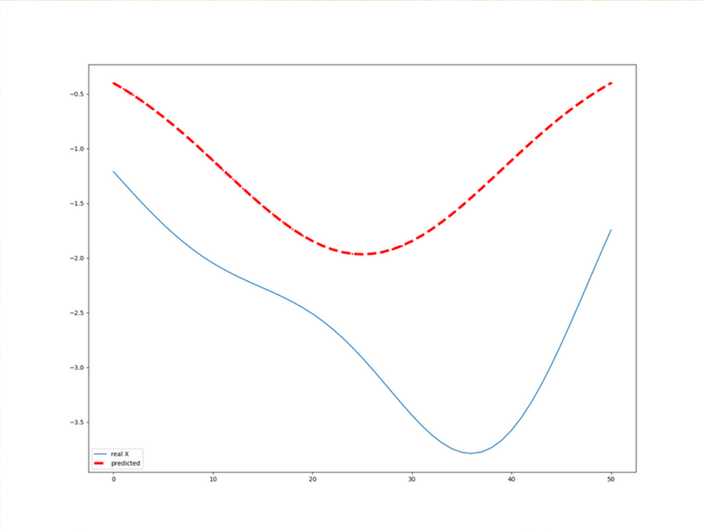
RBF 20 gauss 200 steps

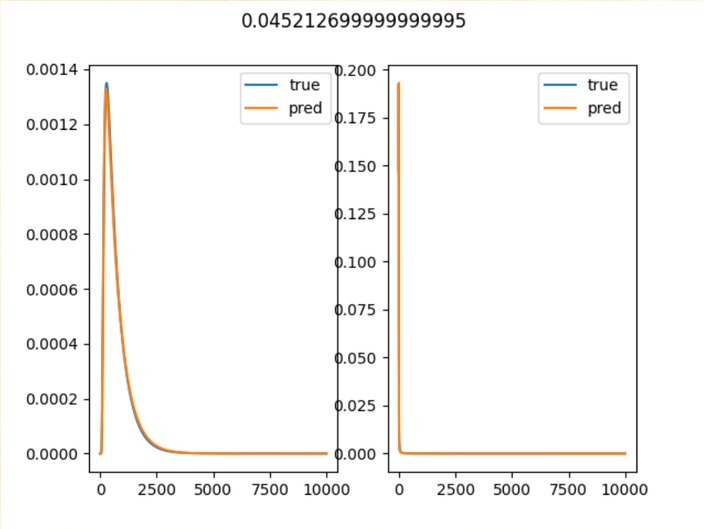
MSE_pos: 3.13e-10

MSE_neg: 2.27e-10

Difference between rates: 0.061 0.0046 0.057

Проблемы



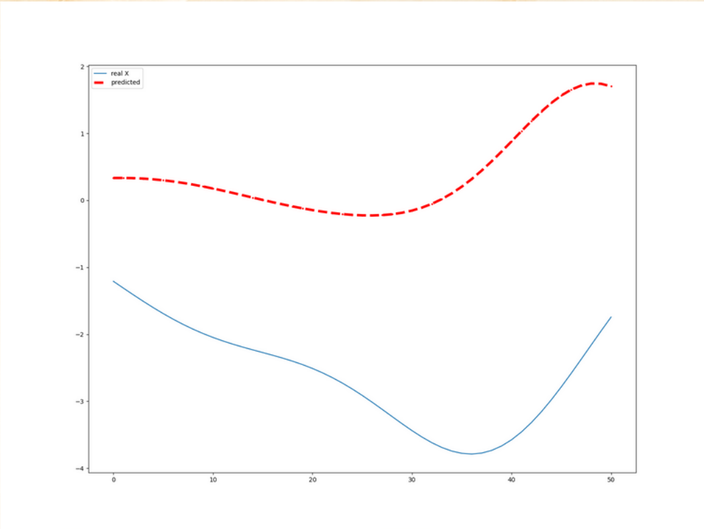


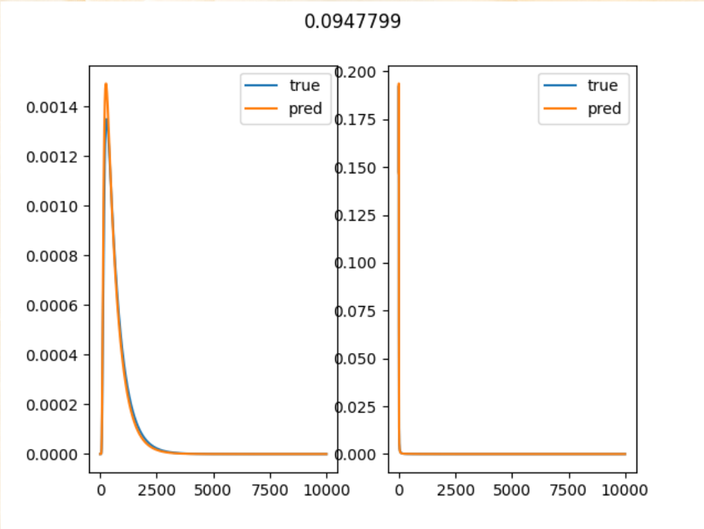
RatQuad 20 gauss 100 steps

MSE_pos: 1.4e-10

MSE_neg: 1.13e-09

Difference between rates: 0.125 0.079 0.045





RatQuad 20 gauss 200 steps

MSE_pos: 8.56e-10

MSE_neg: 5.53e-10

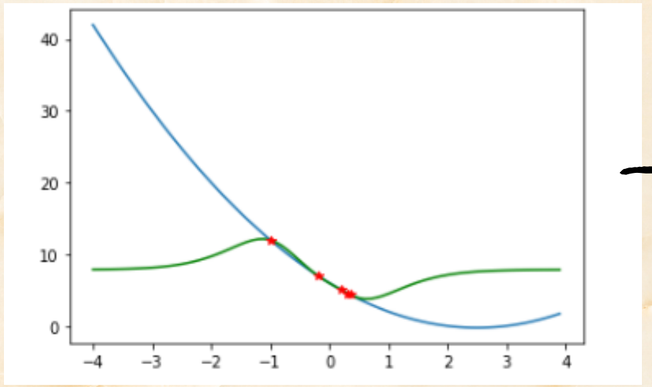
Difference between rates: 0.12 0.03 0.094

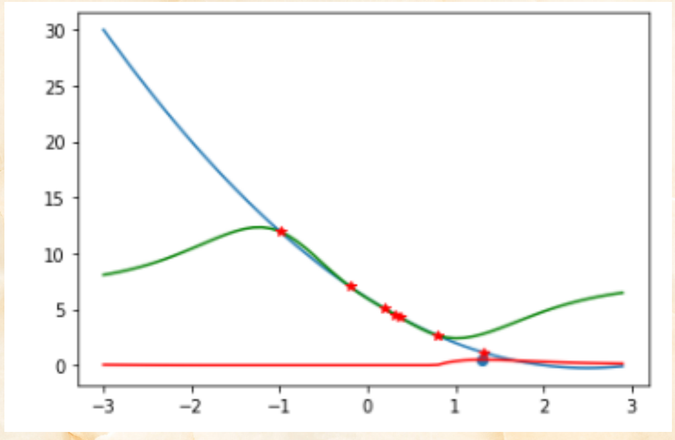
Некоторые выводы

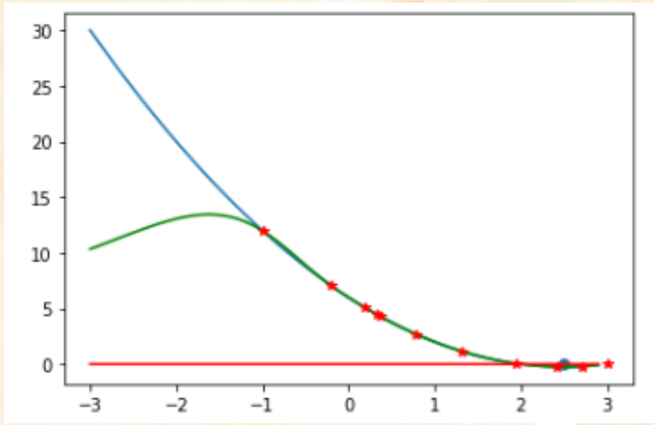
1. Не наблюдается улучшений по сравнению с нефиксированными гауссианами
2. Зависит от kernel
3. Не любой профиль фиттится количеством гауссиан меньше 15 (много параметров для оптимизации)
4. При увеличении количества итераций иногда уходит в не те значения (*)

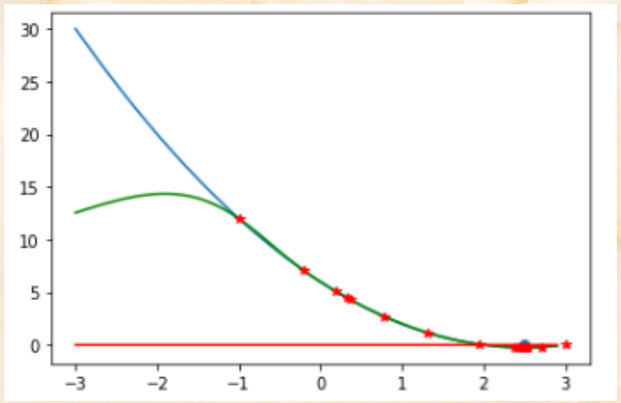
BoTorch

1D









x = 2.5007

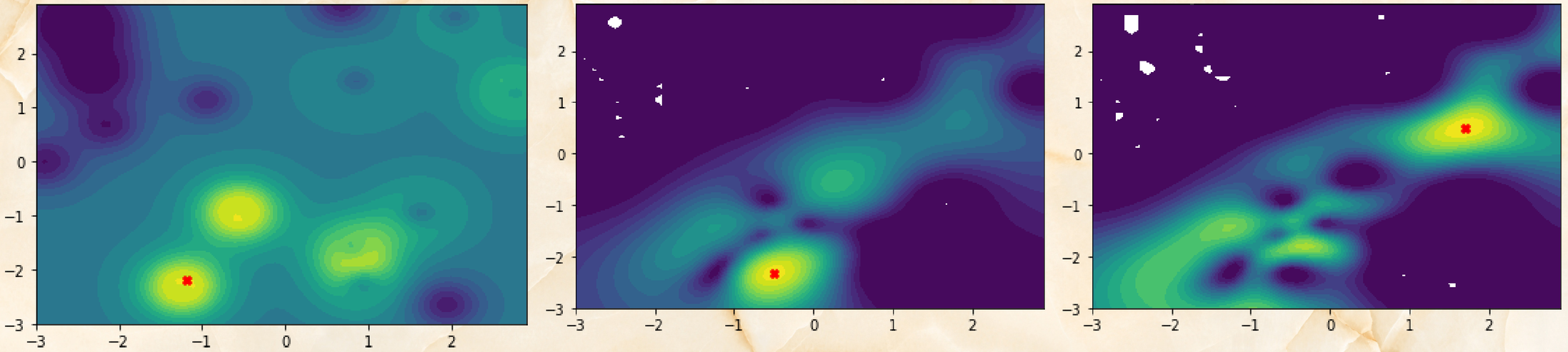
google colab

2D

МакКормика

$$f(x, y) = \sin(x + y) + (x - y)^2 - 1.5x + 2.5y + 1$$

$$f(-0.54719, -1.54719) = -1.9133$$

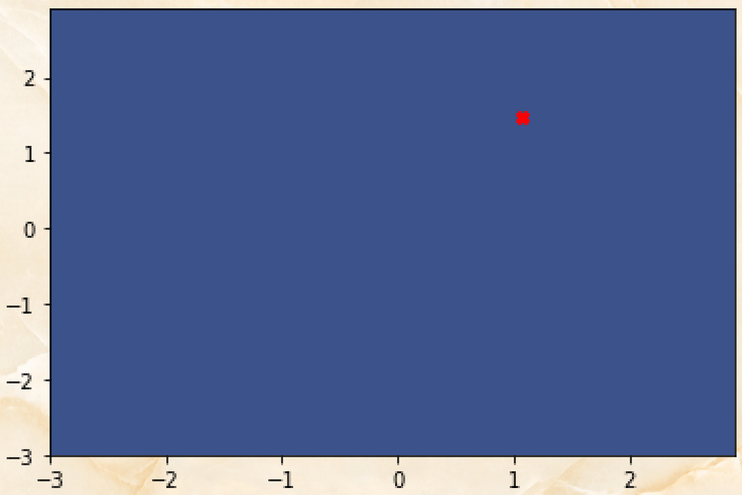


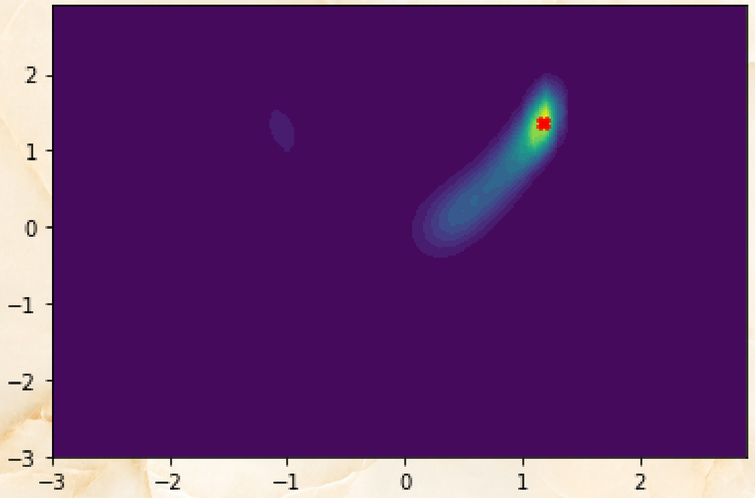
x = (-0.6385, -1.5736) y = -1.90

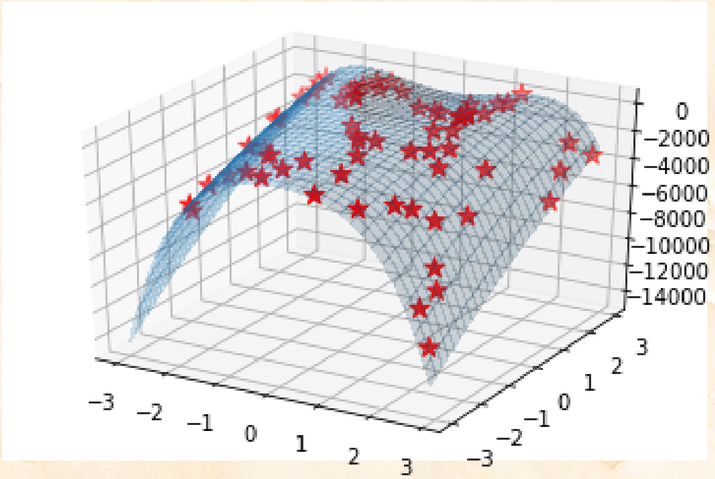
Розенброка

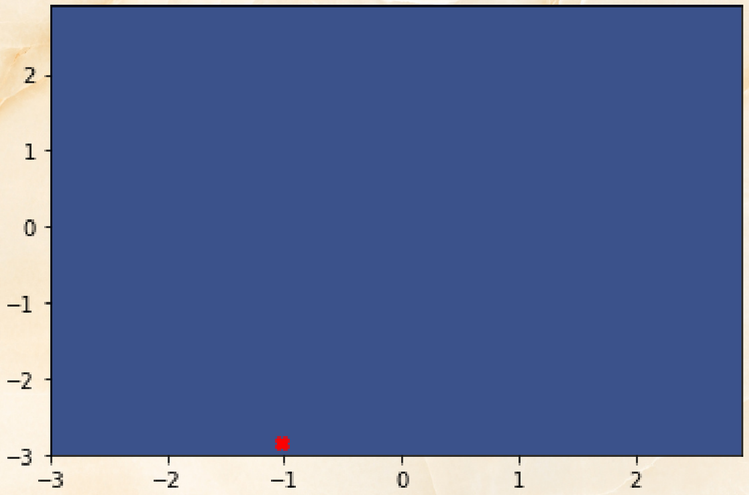
x = (1.0902, 1.1789) y = -0.0017

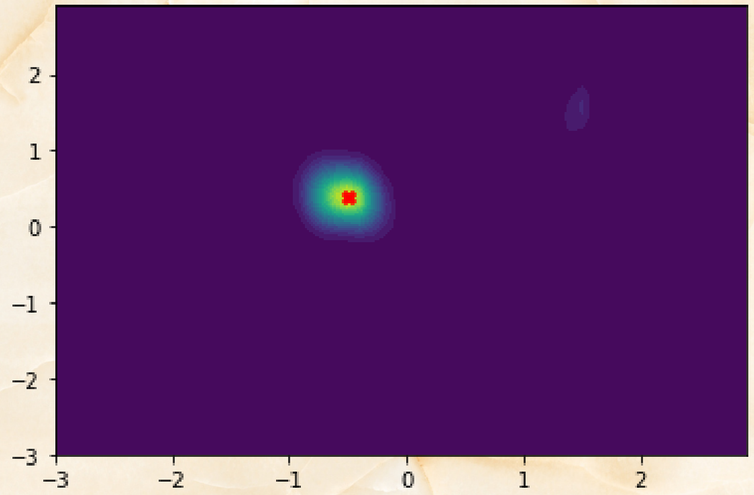
x = (1.5234, 2.20) y = -1.6

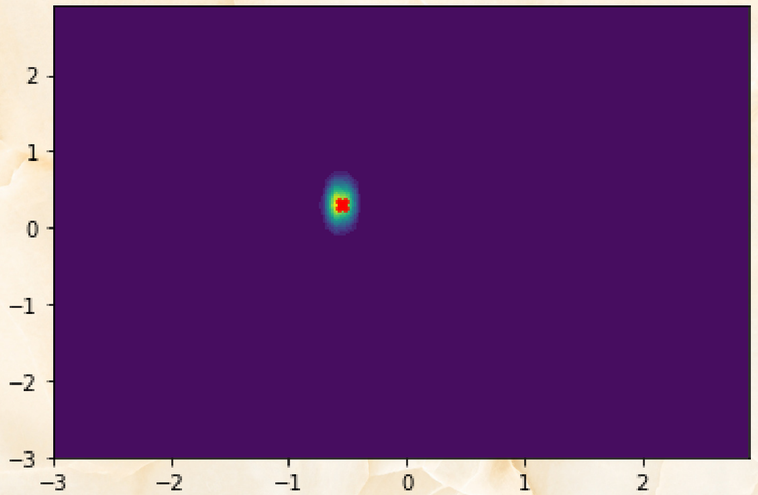












Полезная литература

Expected Hypervolume Improvement

Botorch