But what is a Gaussian process?

Regression while knowing how certain you are

Quan Nguyen

Who am I?

- **Quan Nguyen**
- Ph.D. student – Bayesian machine learning, decision-making under uncertainty

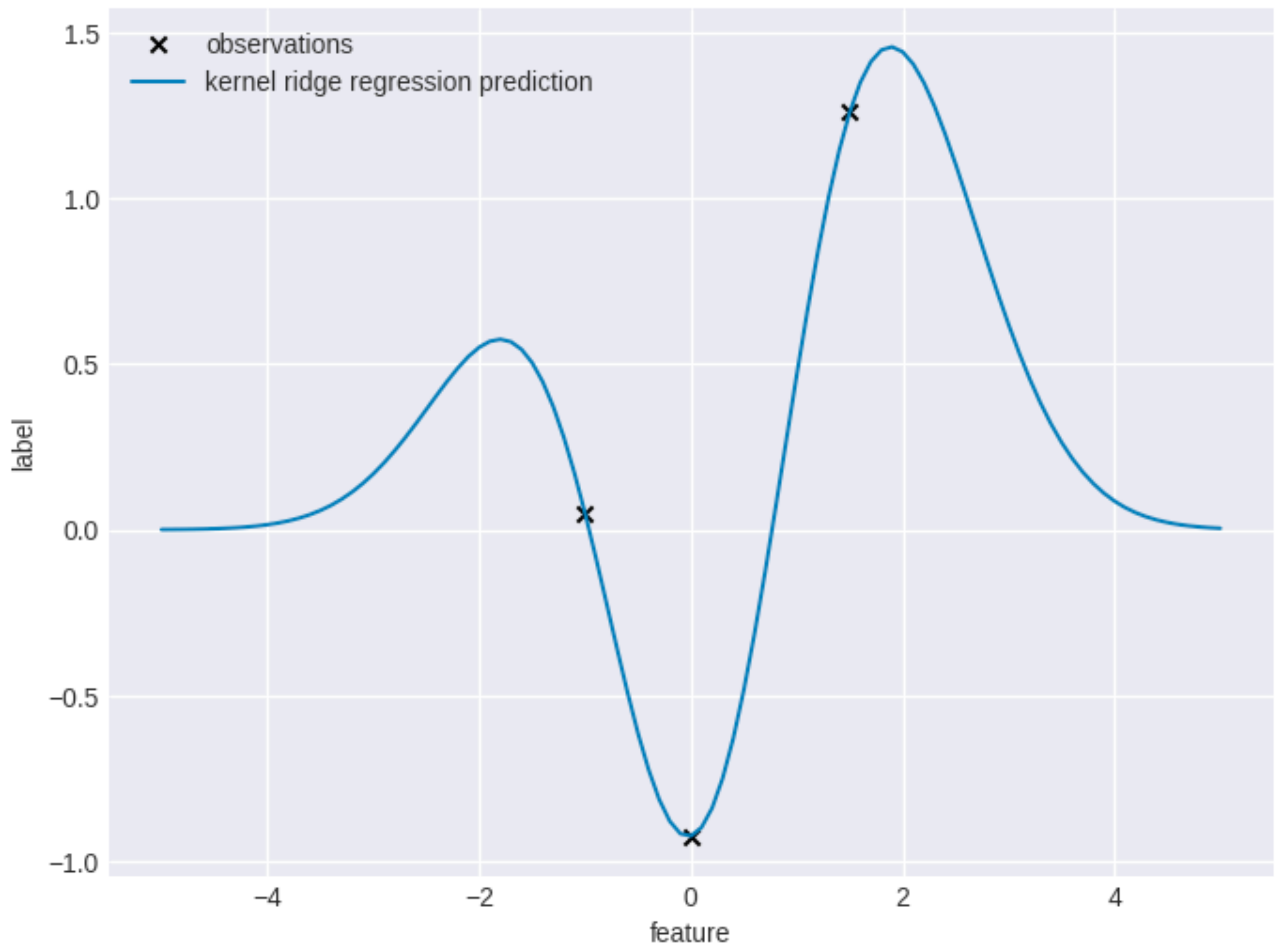
krisnguyen135.github.io

github.com/KrisNguyen135/Talks

@the_subtrahend

Interpolation vs. extrapolation

quantifying what we do and don’t know



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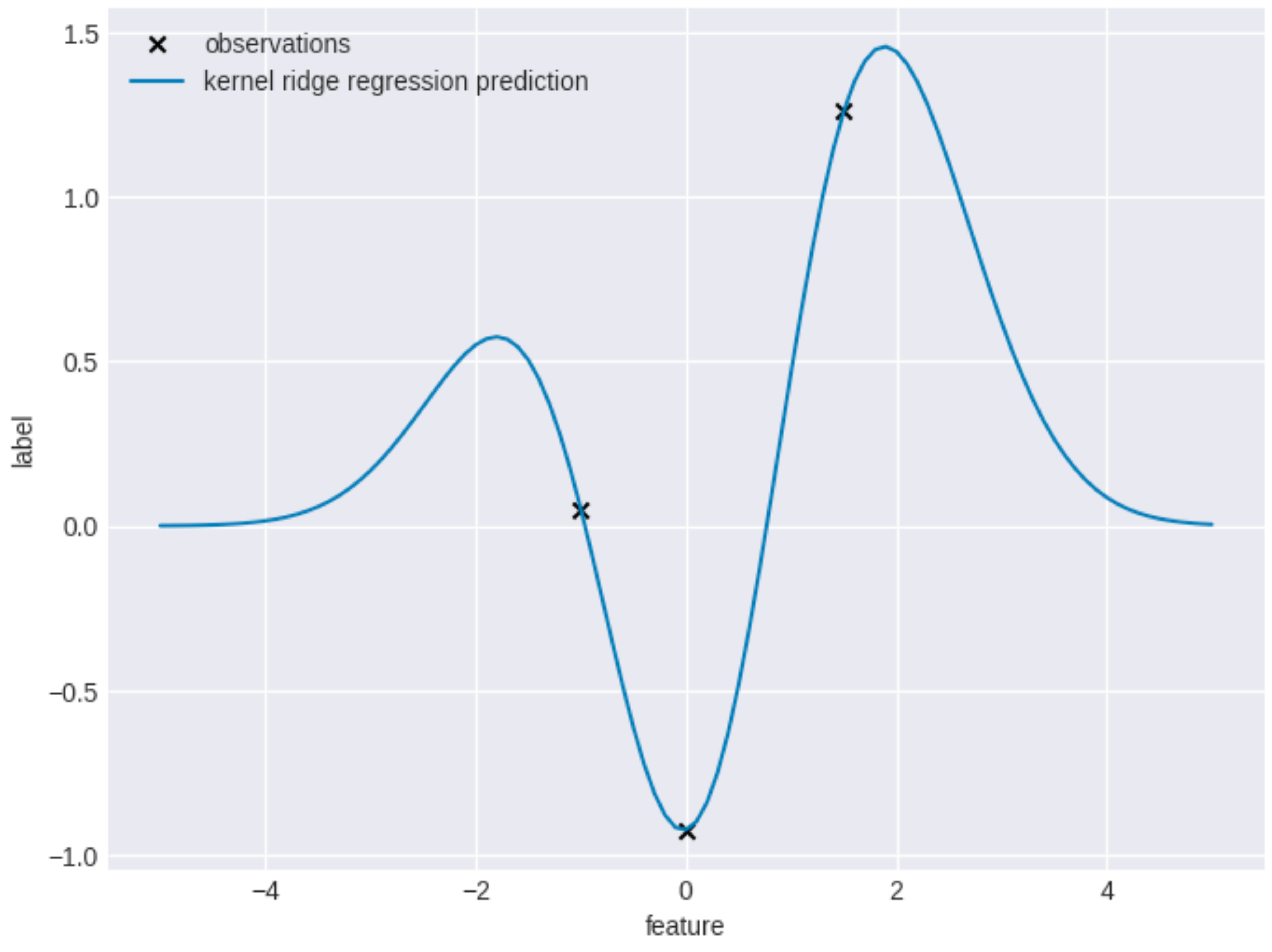
- **Typical ML models**: *single-valued* numbers as predictions



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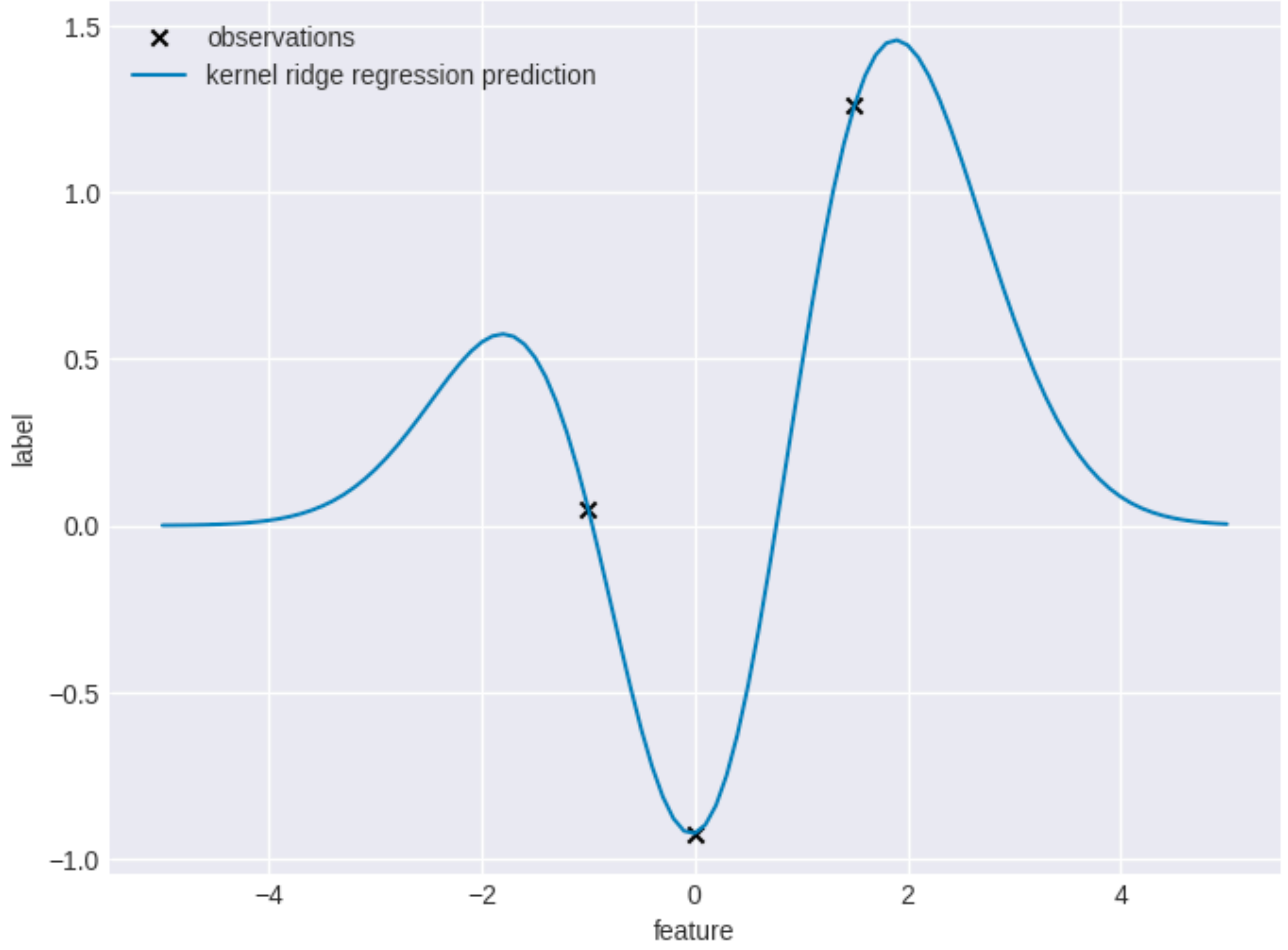

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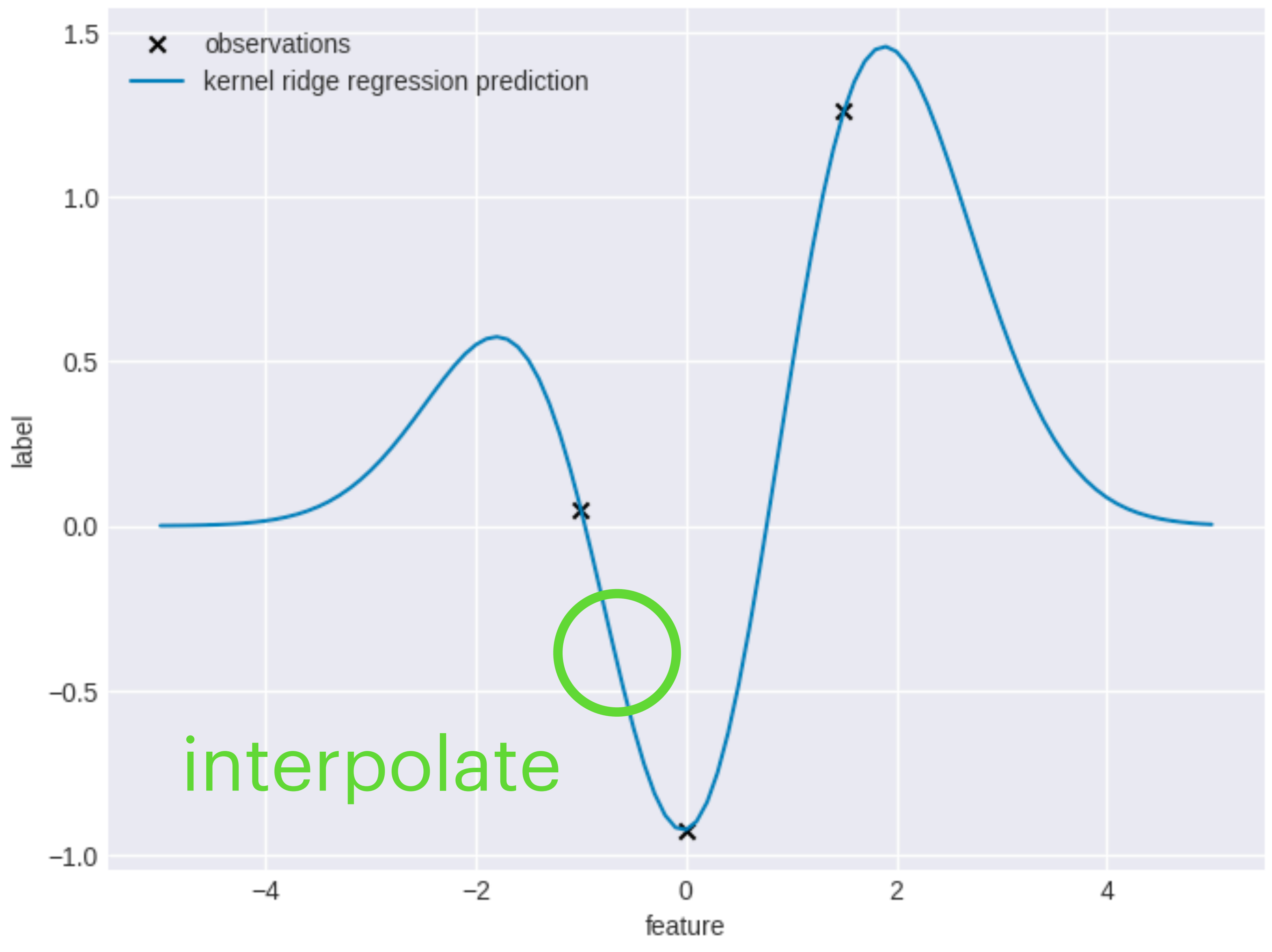

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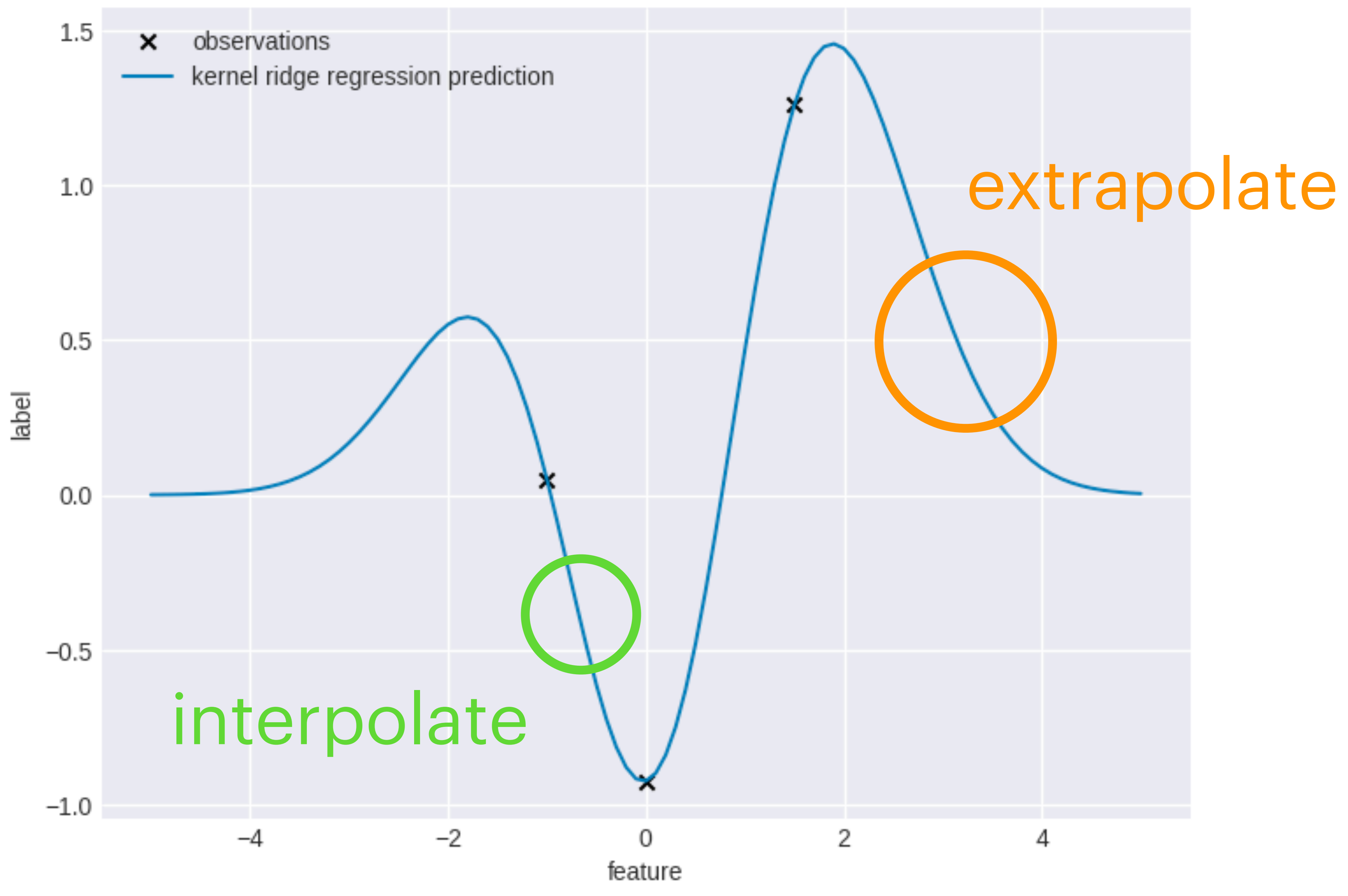

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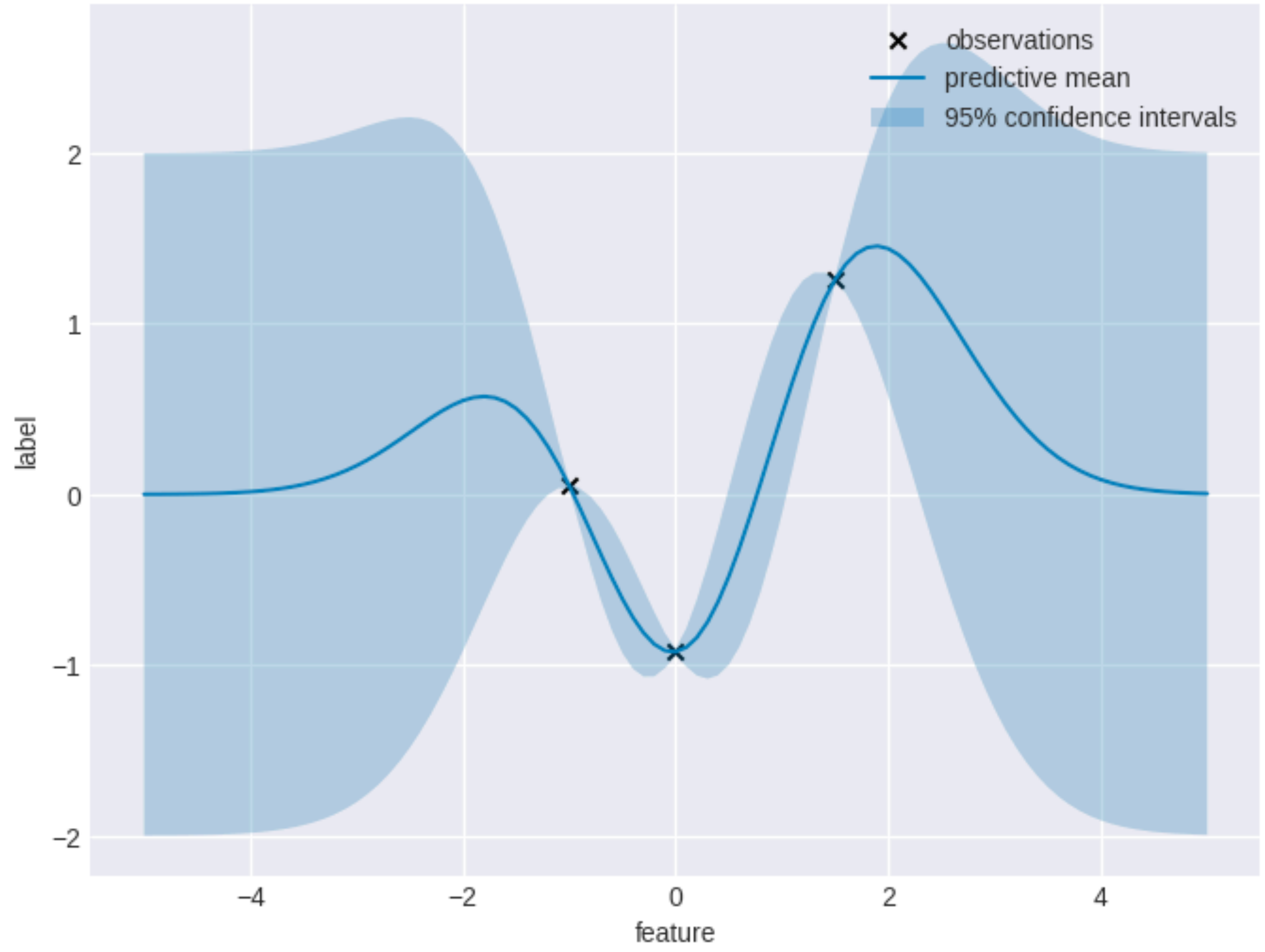

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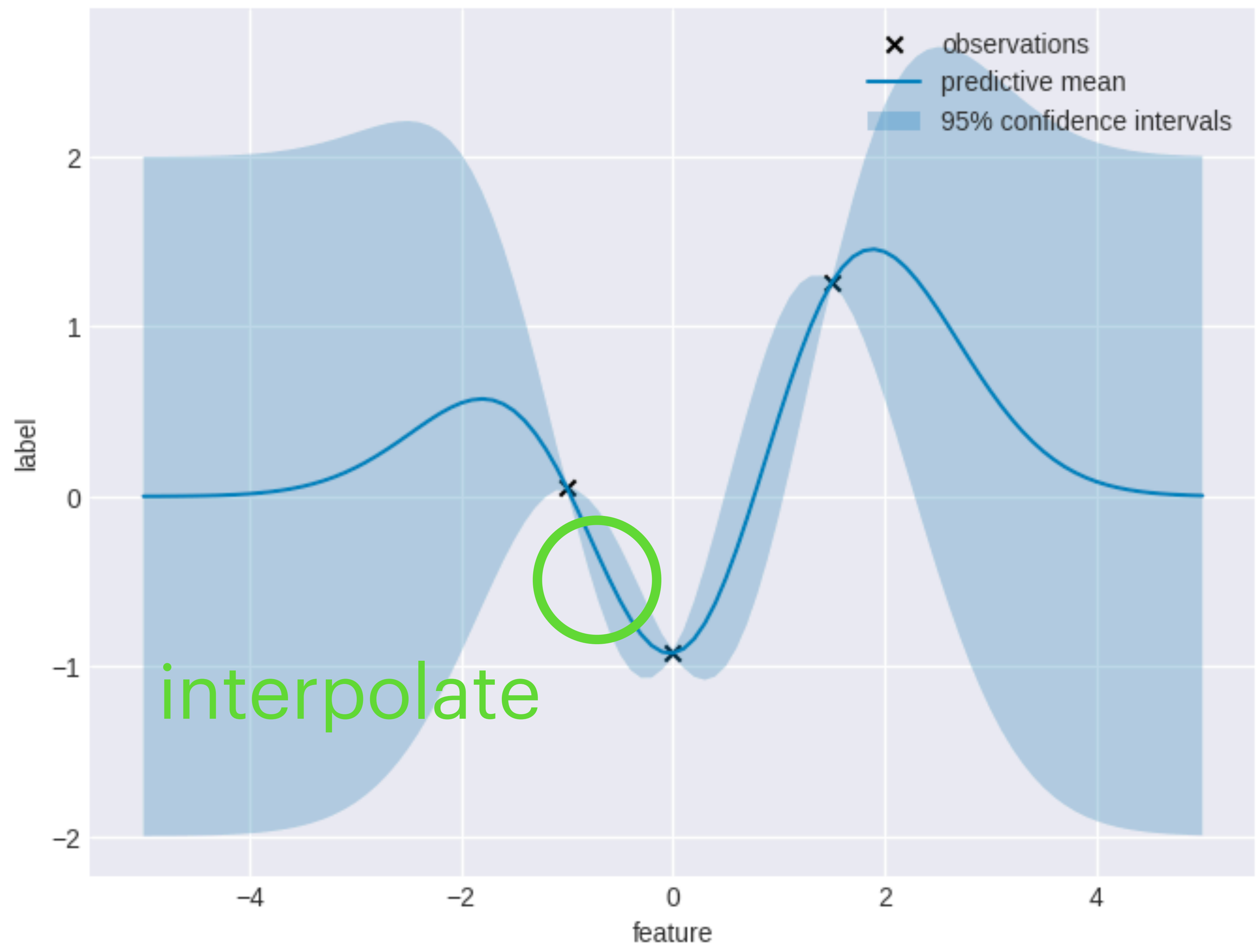

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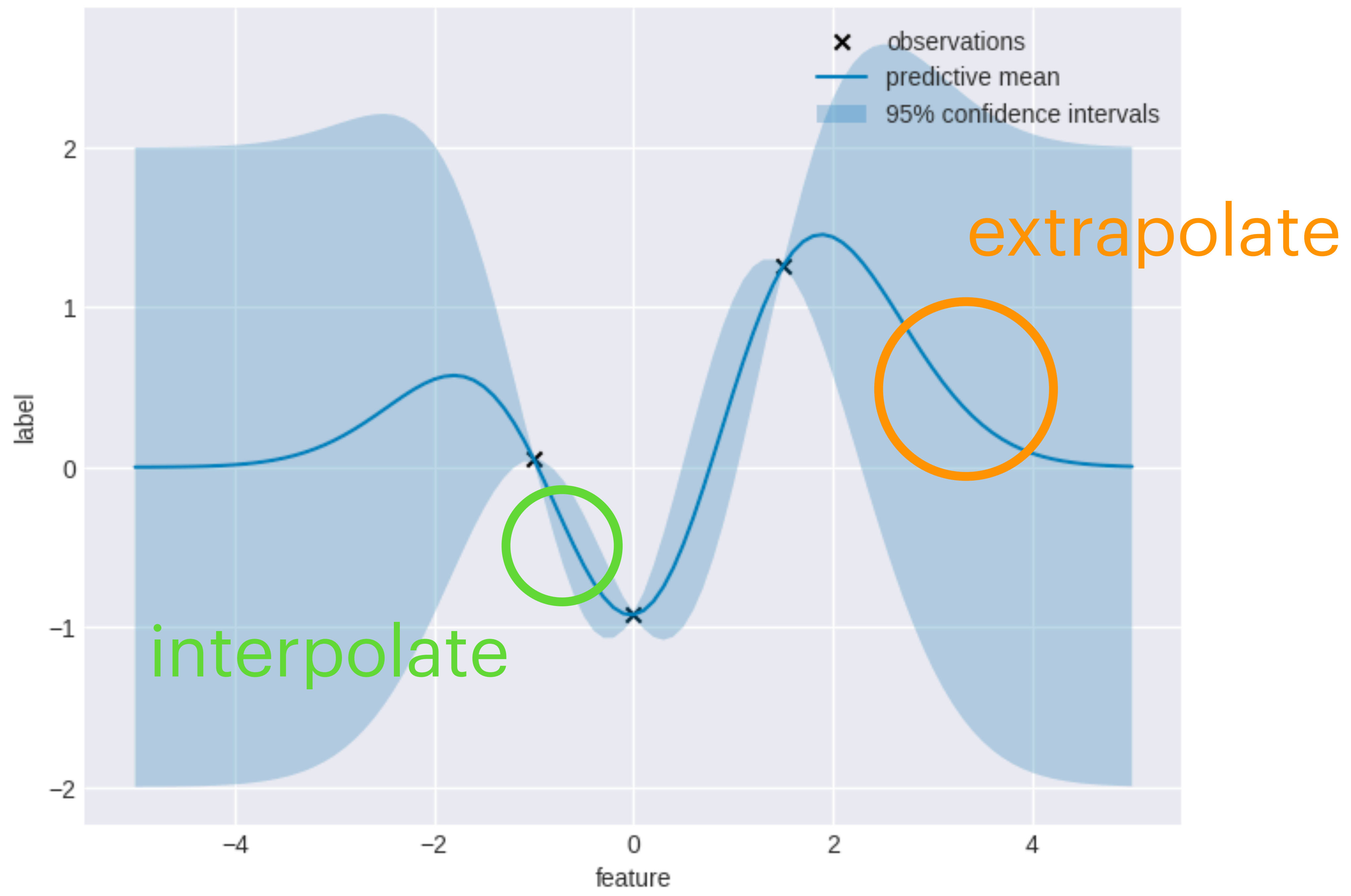

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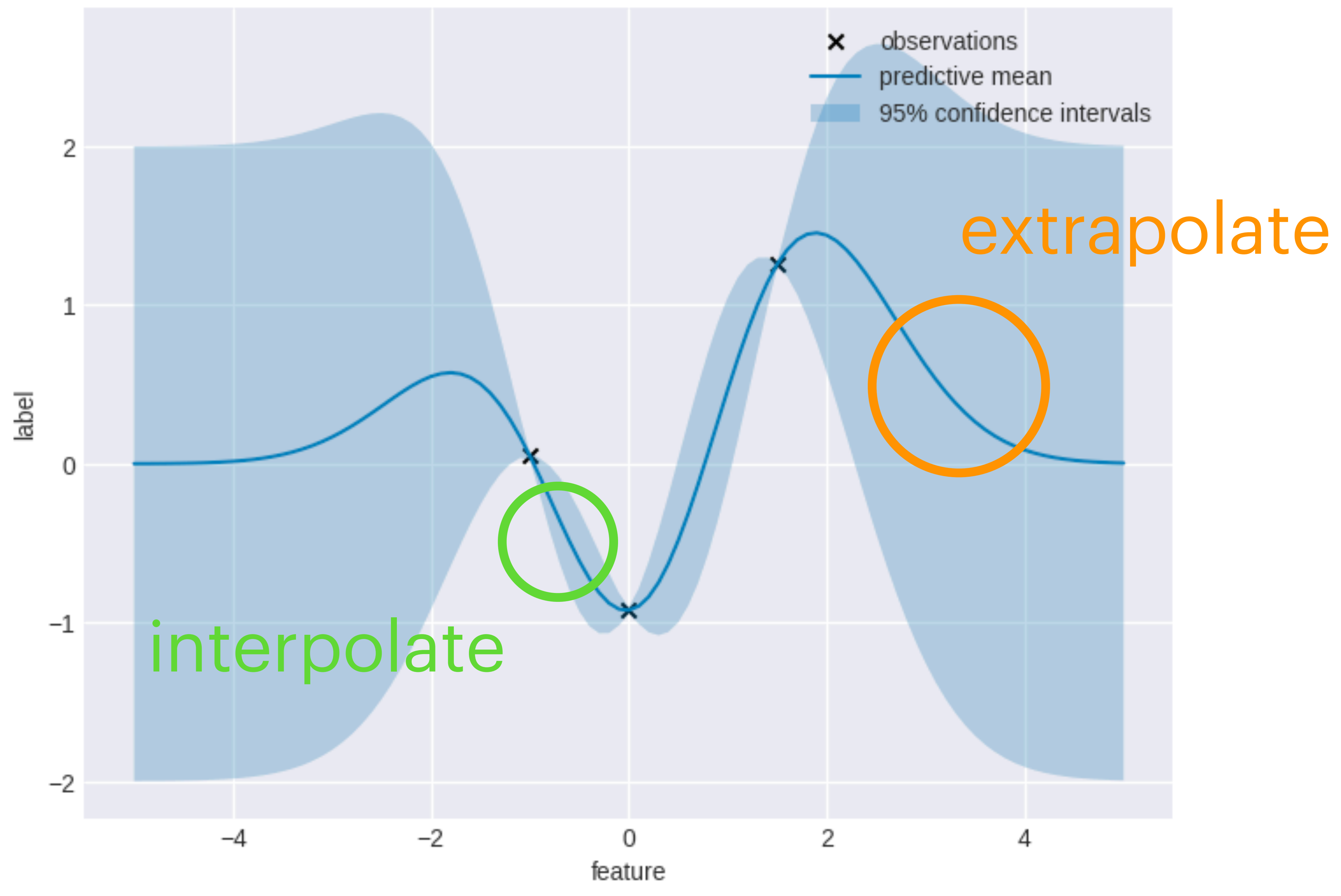
  - good for decision making under uncertainty



Multivariate Gaussian distributions

a statistician’ way of
accounting for
similarity & uncertainty

Looking to sell your house?

see how much others are selling theirs for

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training point 2: price of neighbor house
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the high-dimensional bell curve

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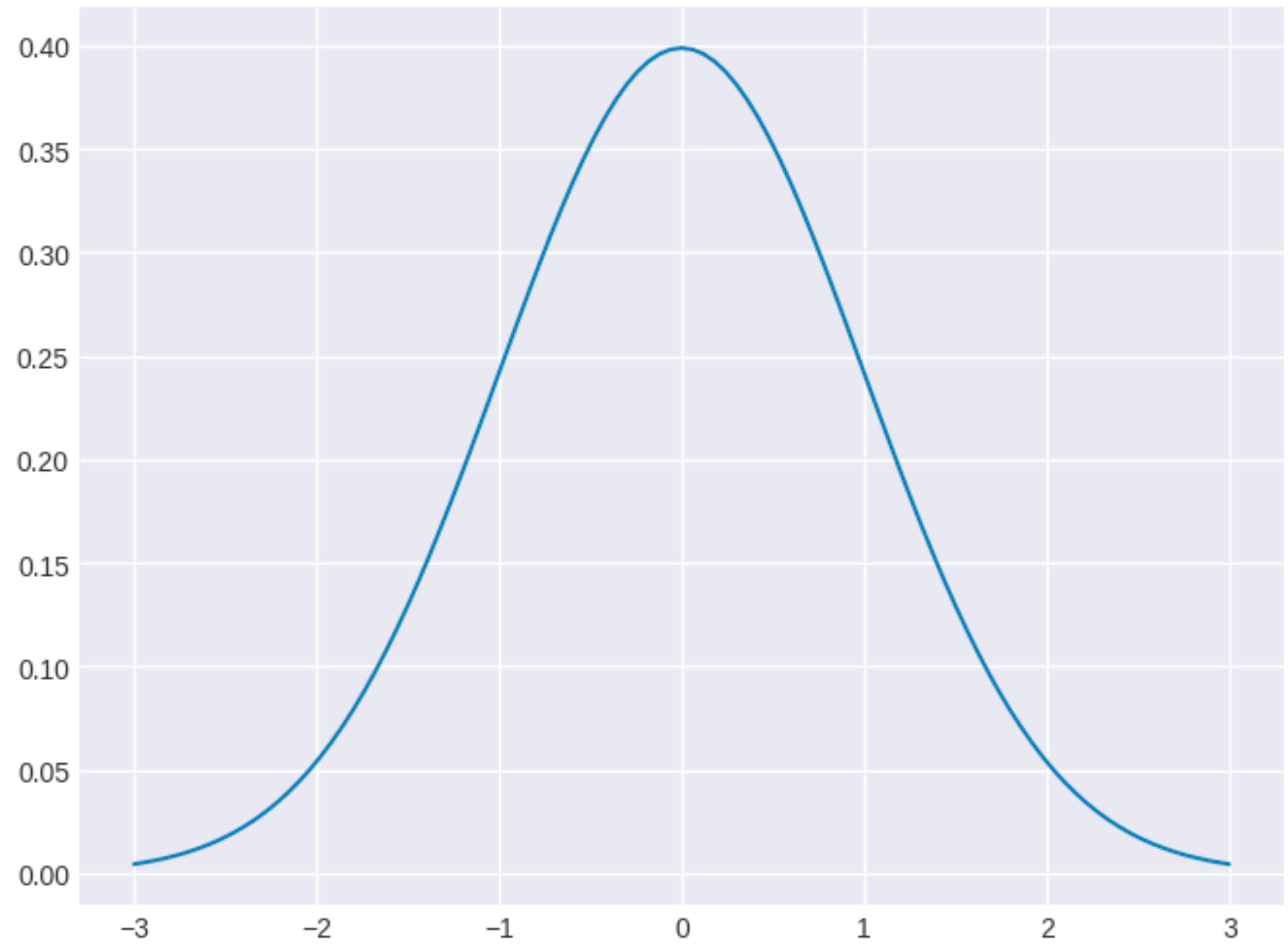

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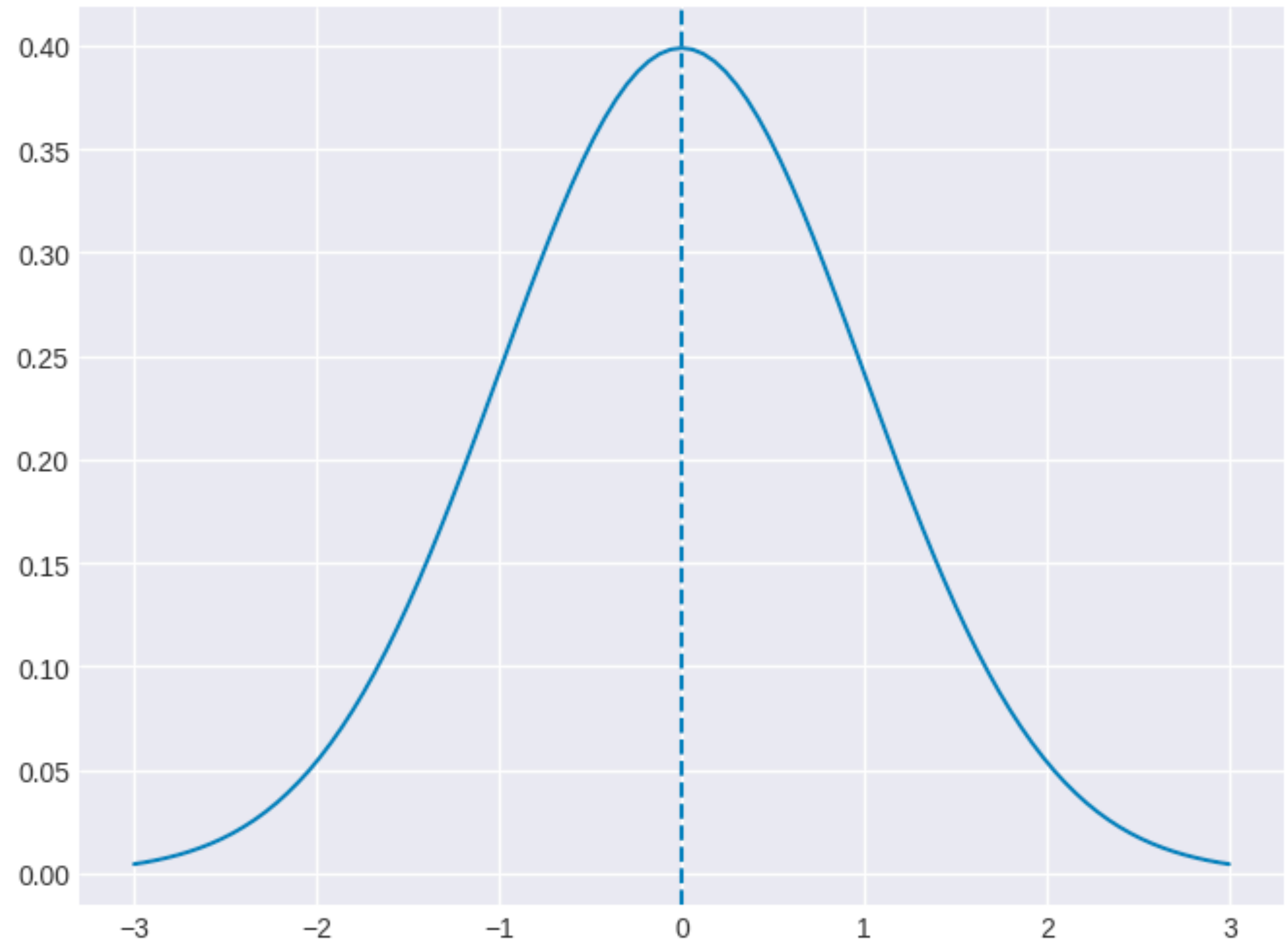

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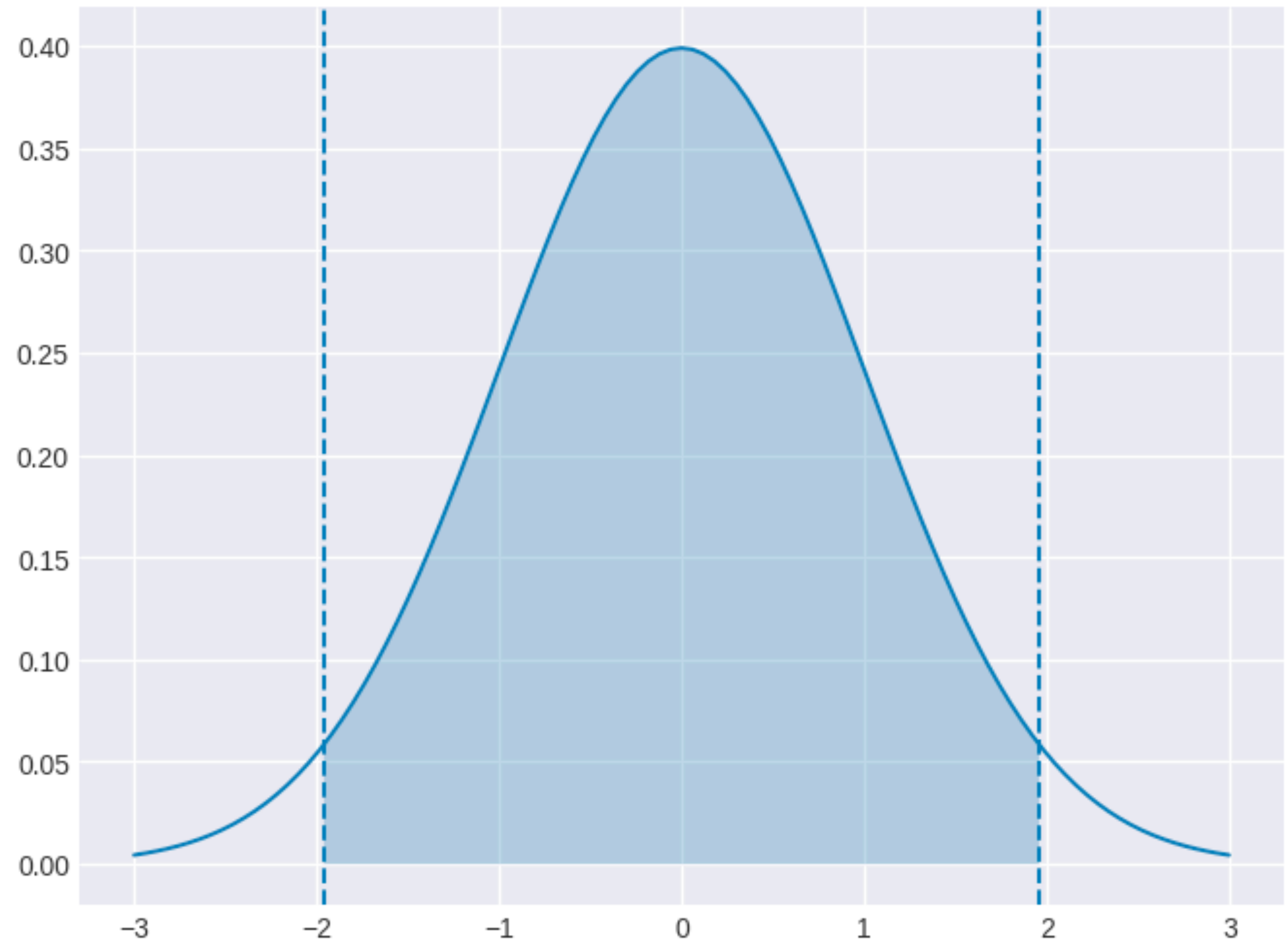

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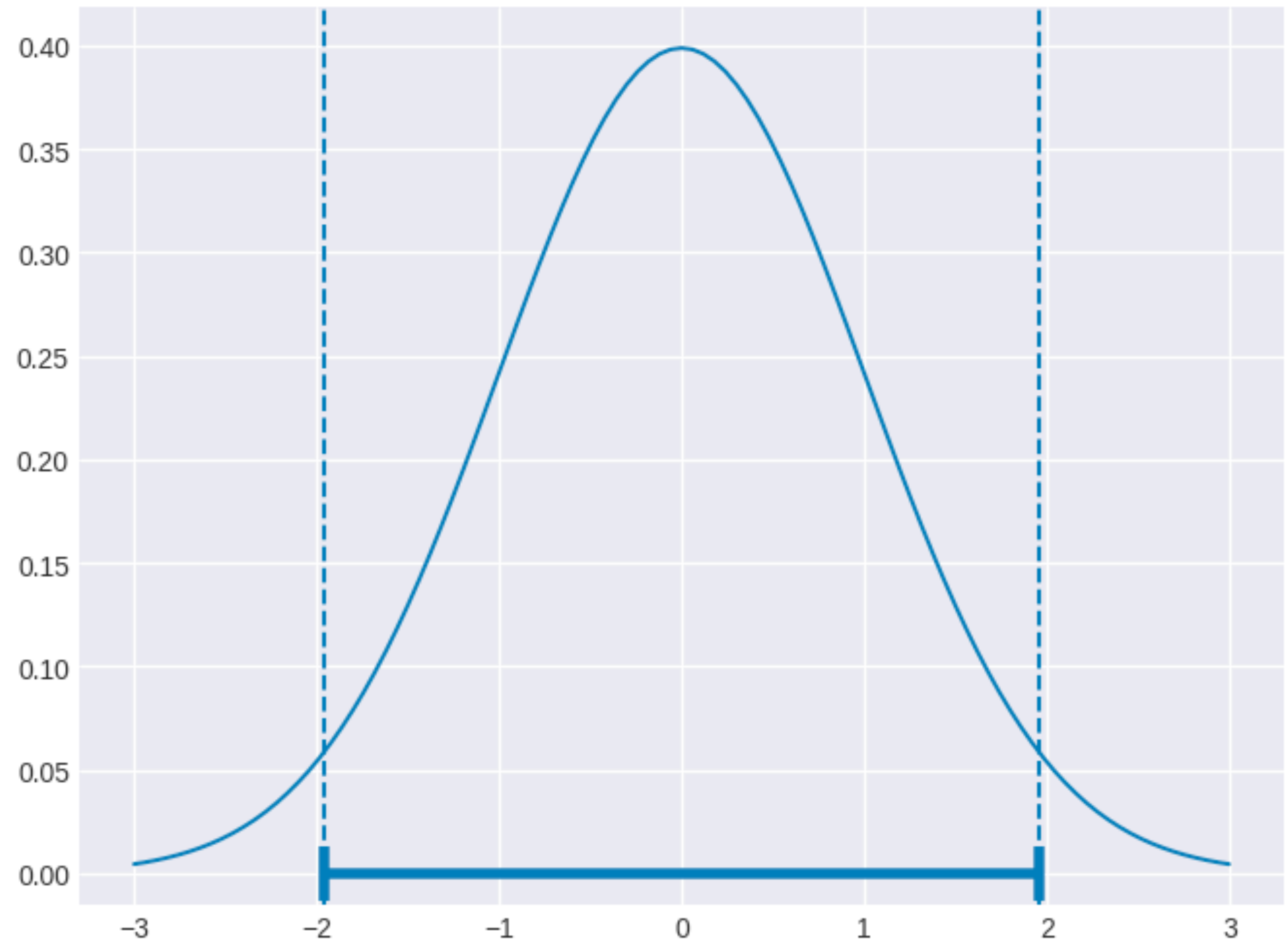

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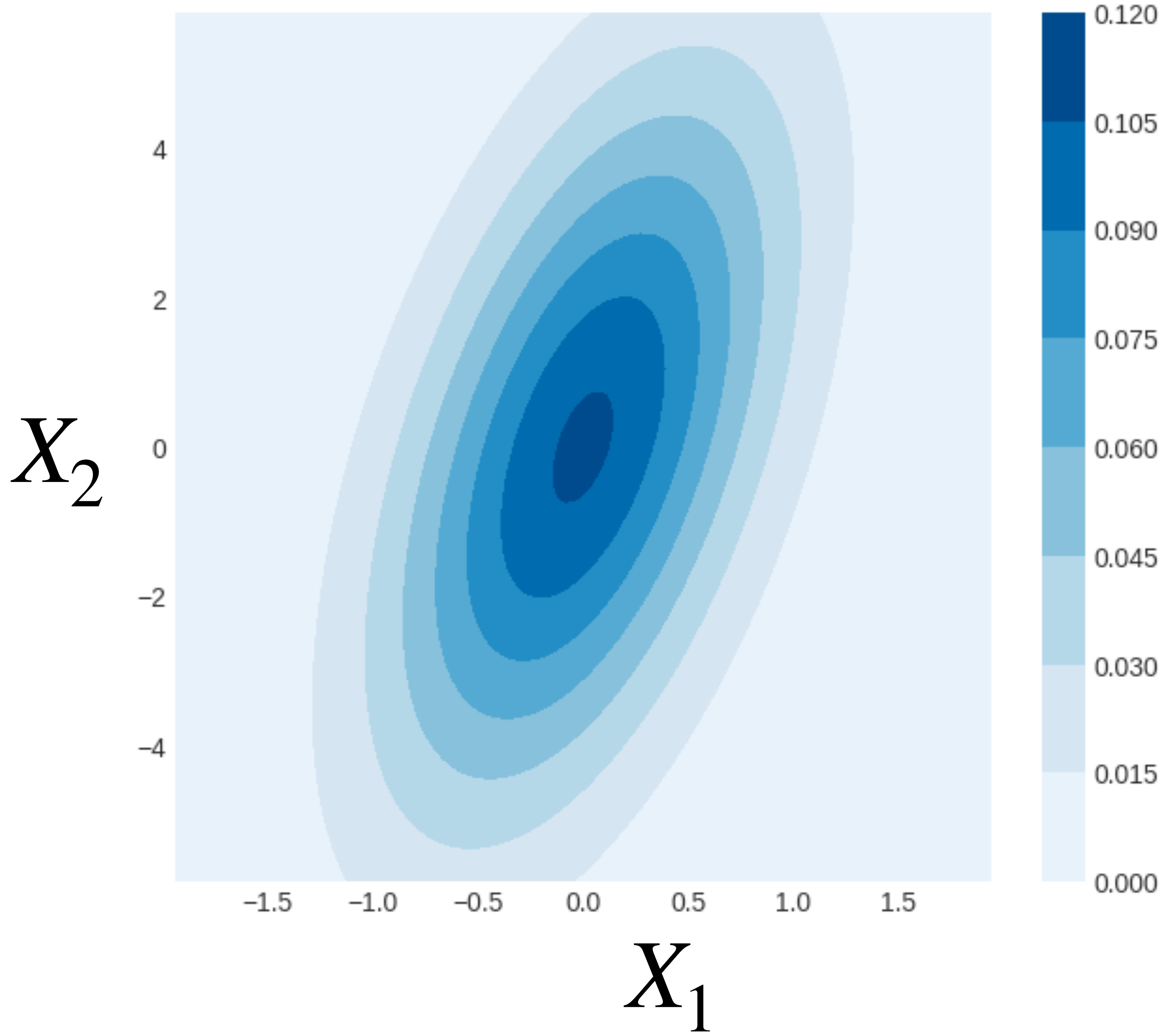

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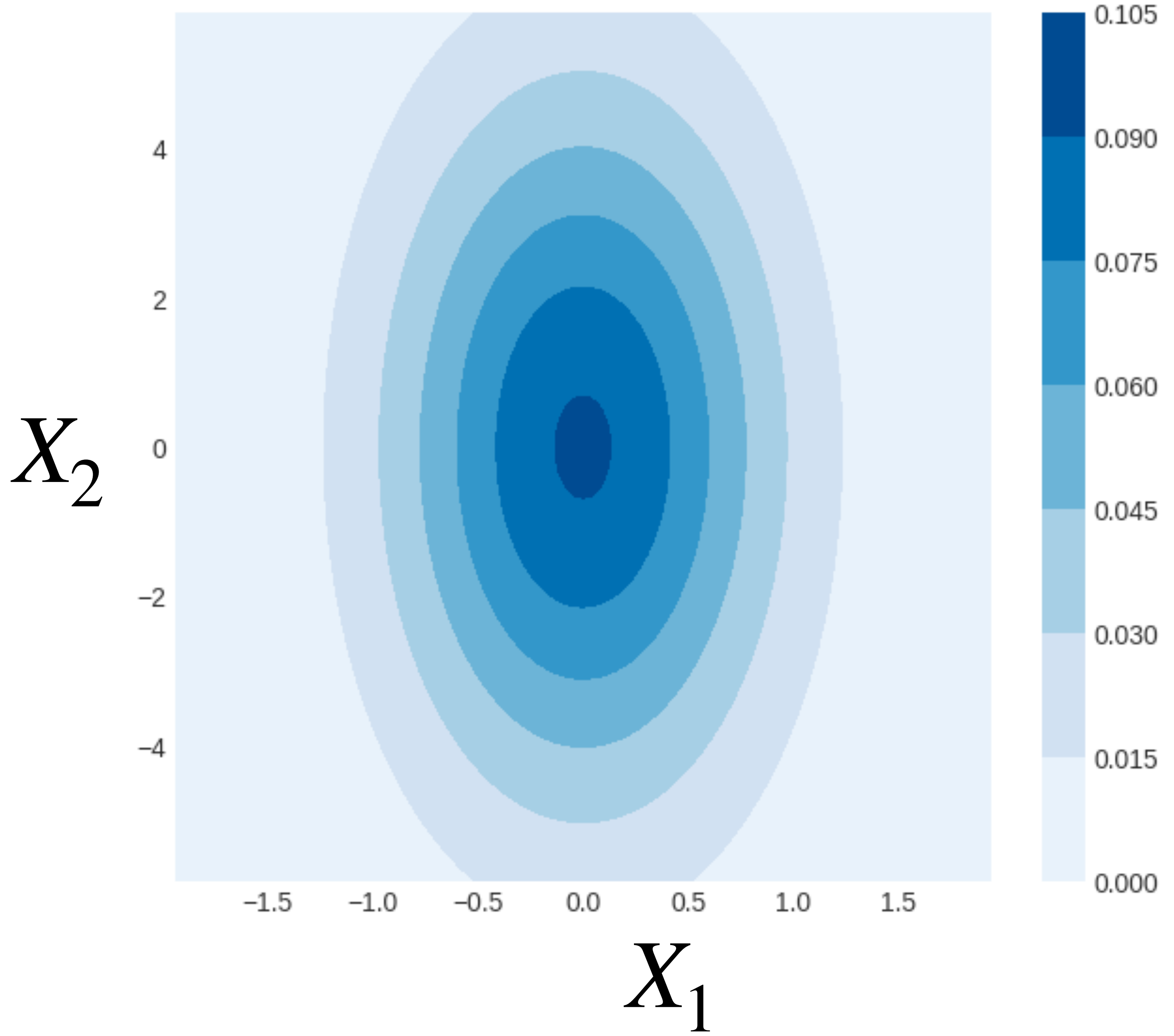

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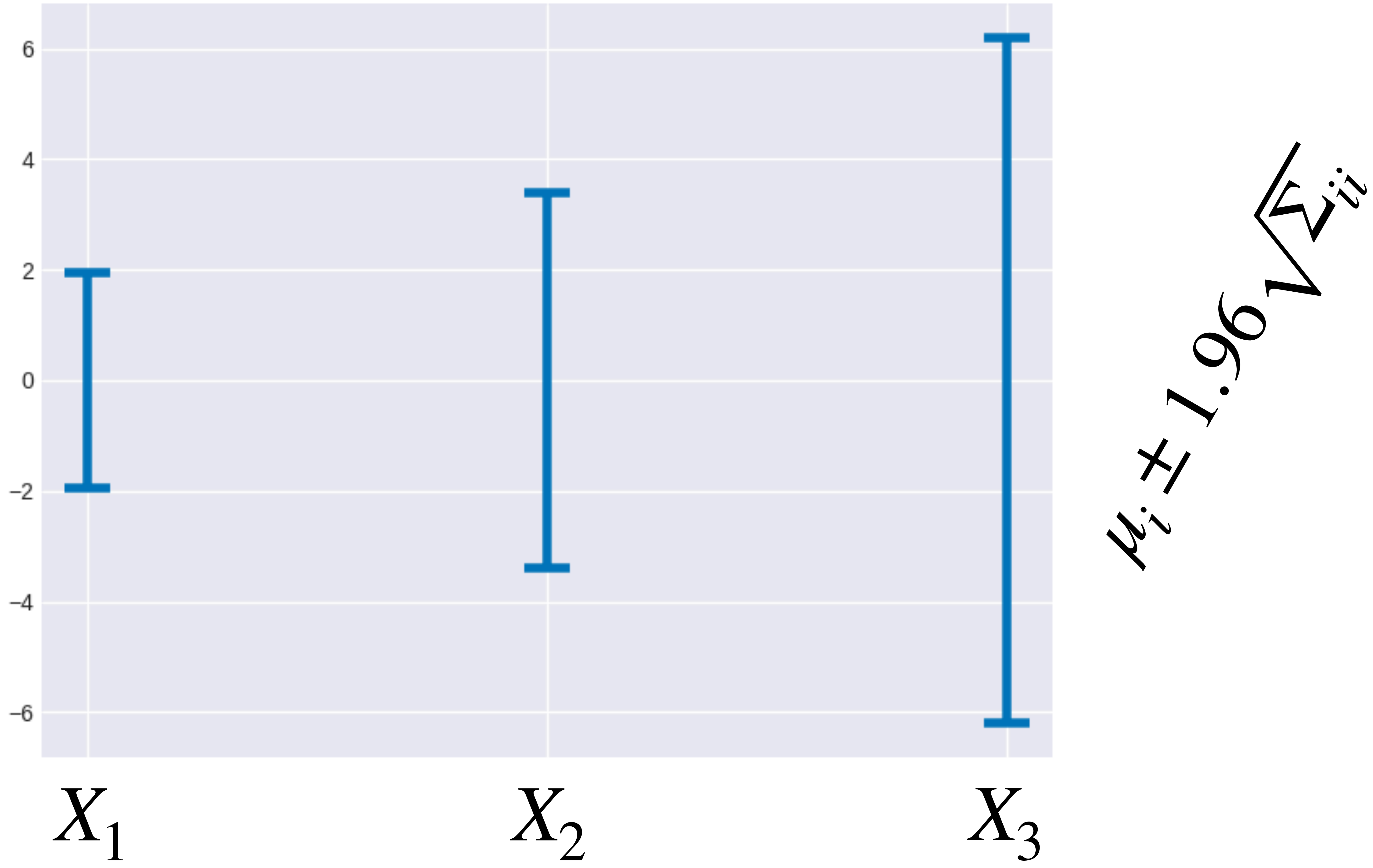

Updating Gaussian distributions

refining our beliefs with Bayes' rule

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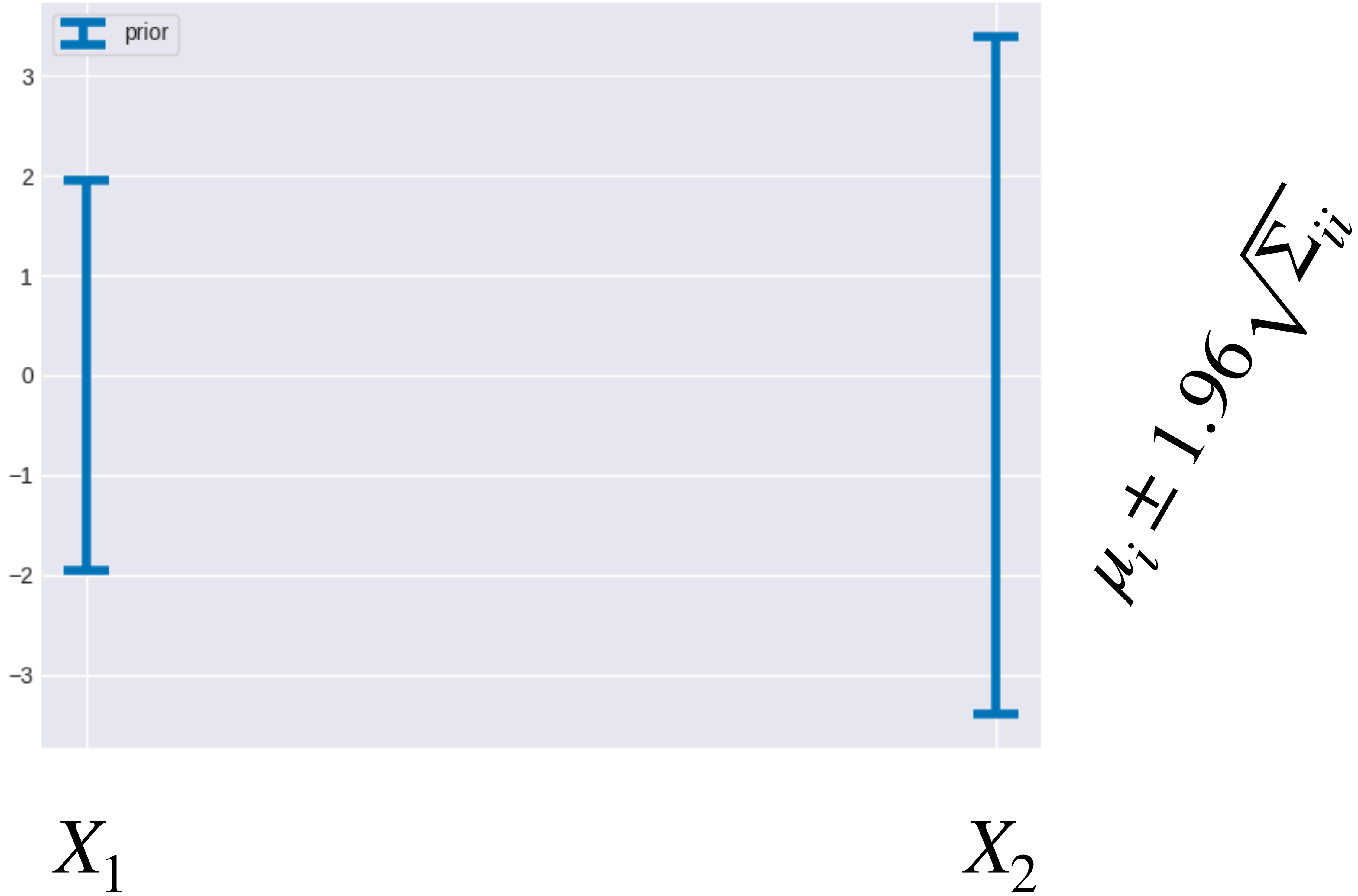

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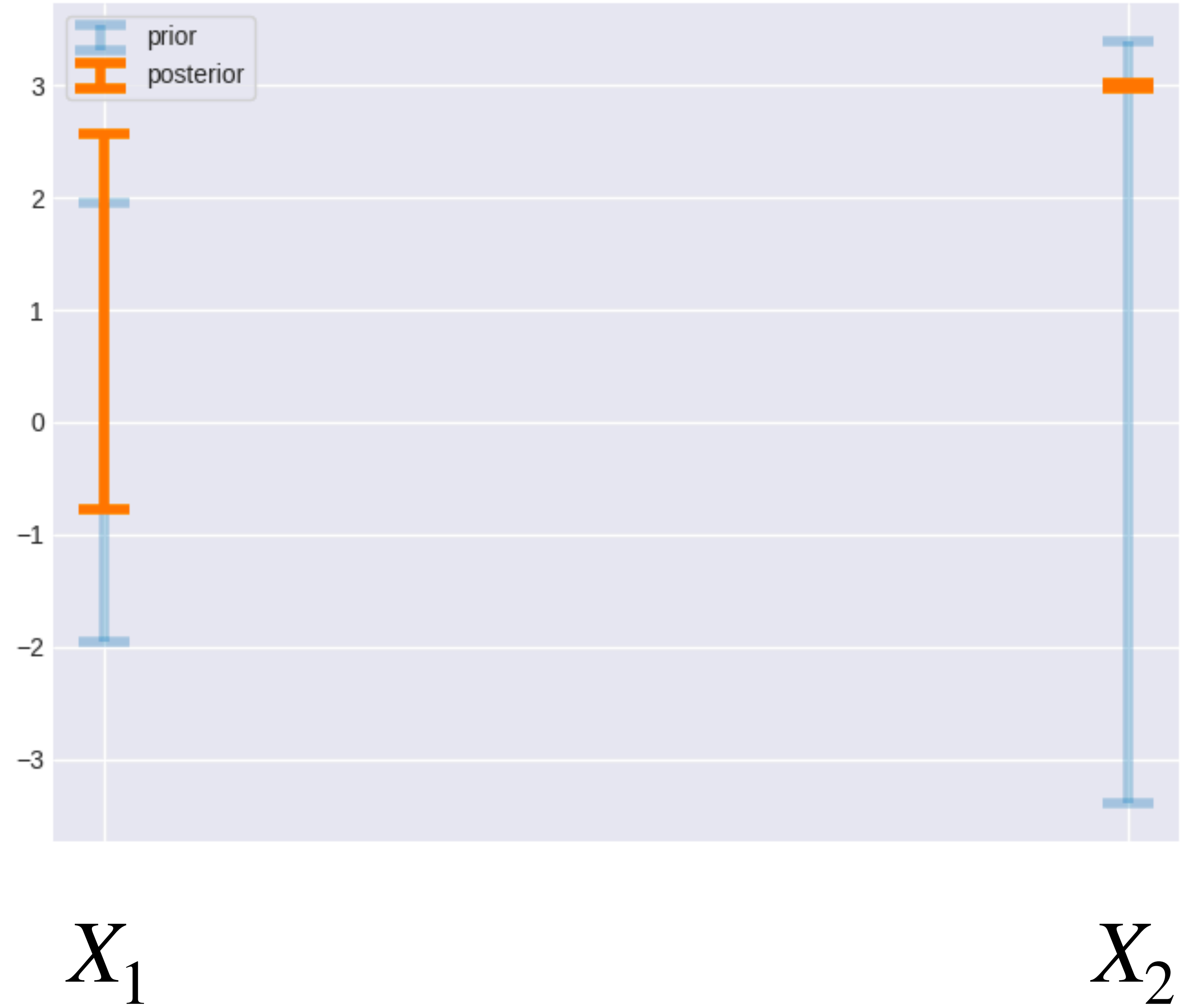

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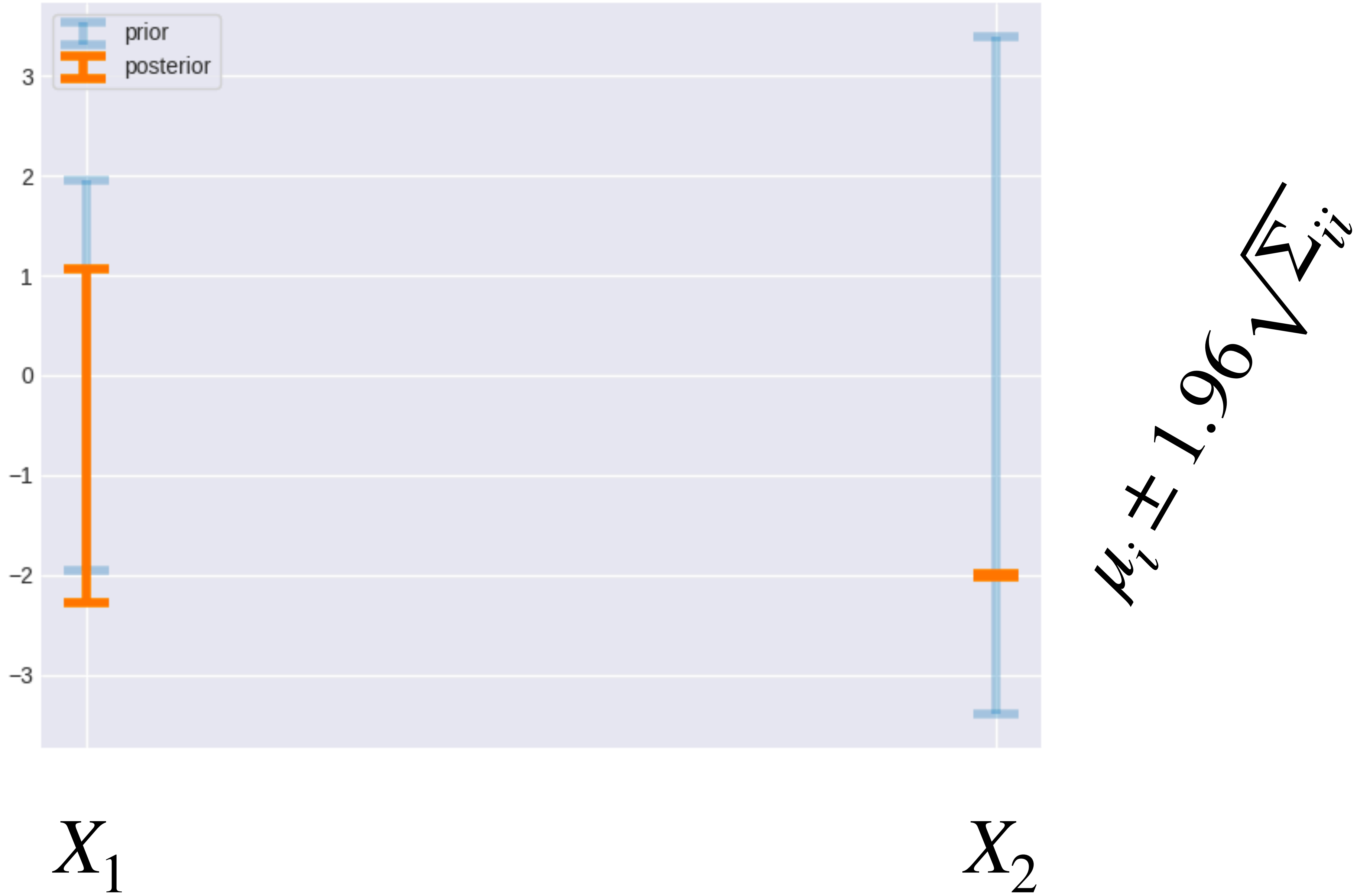
observation $X_2 = -2$



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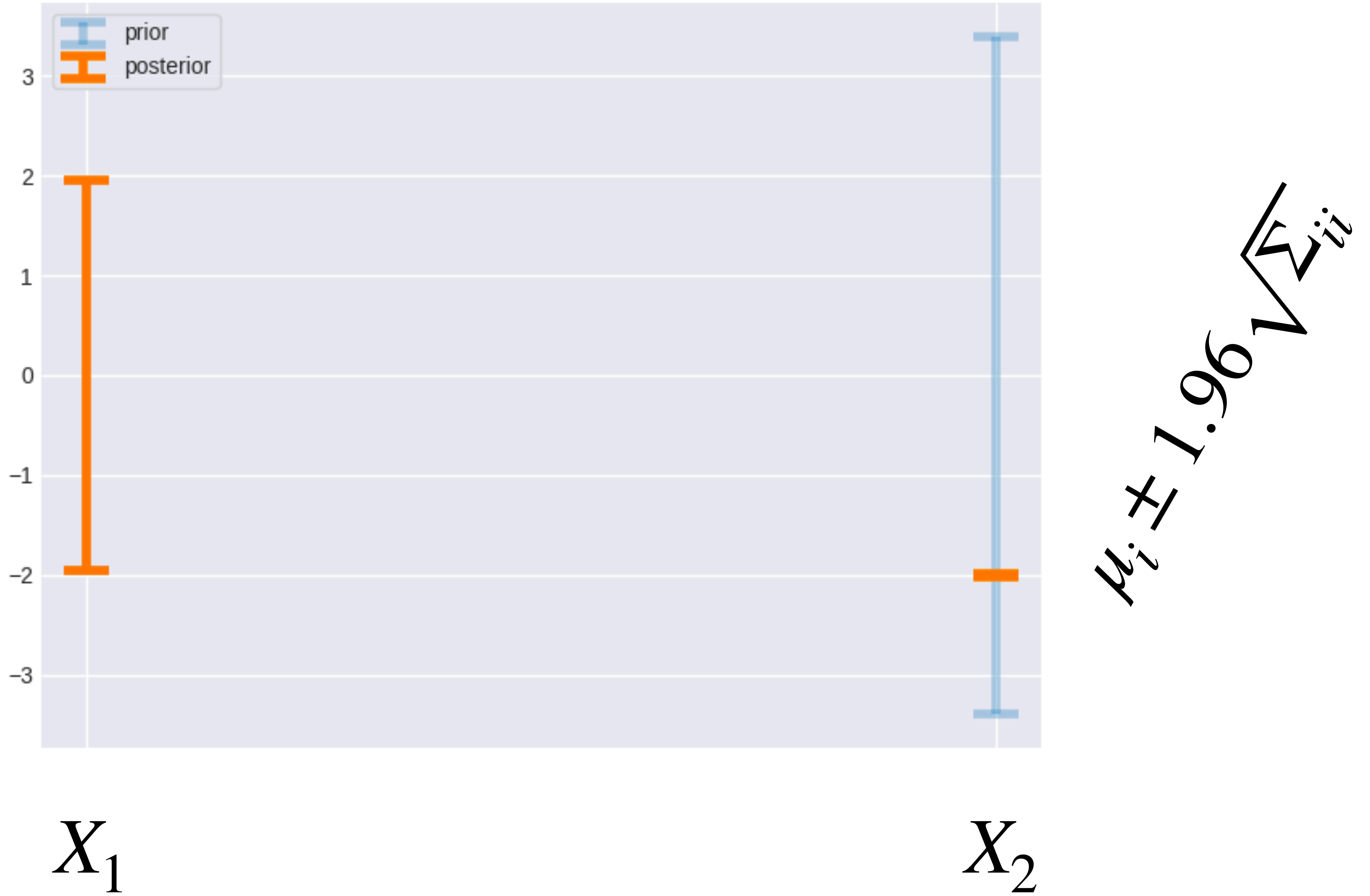

Setting house prices, the Bayesian way

updating our Gaussian beliefs

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x $100,000

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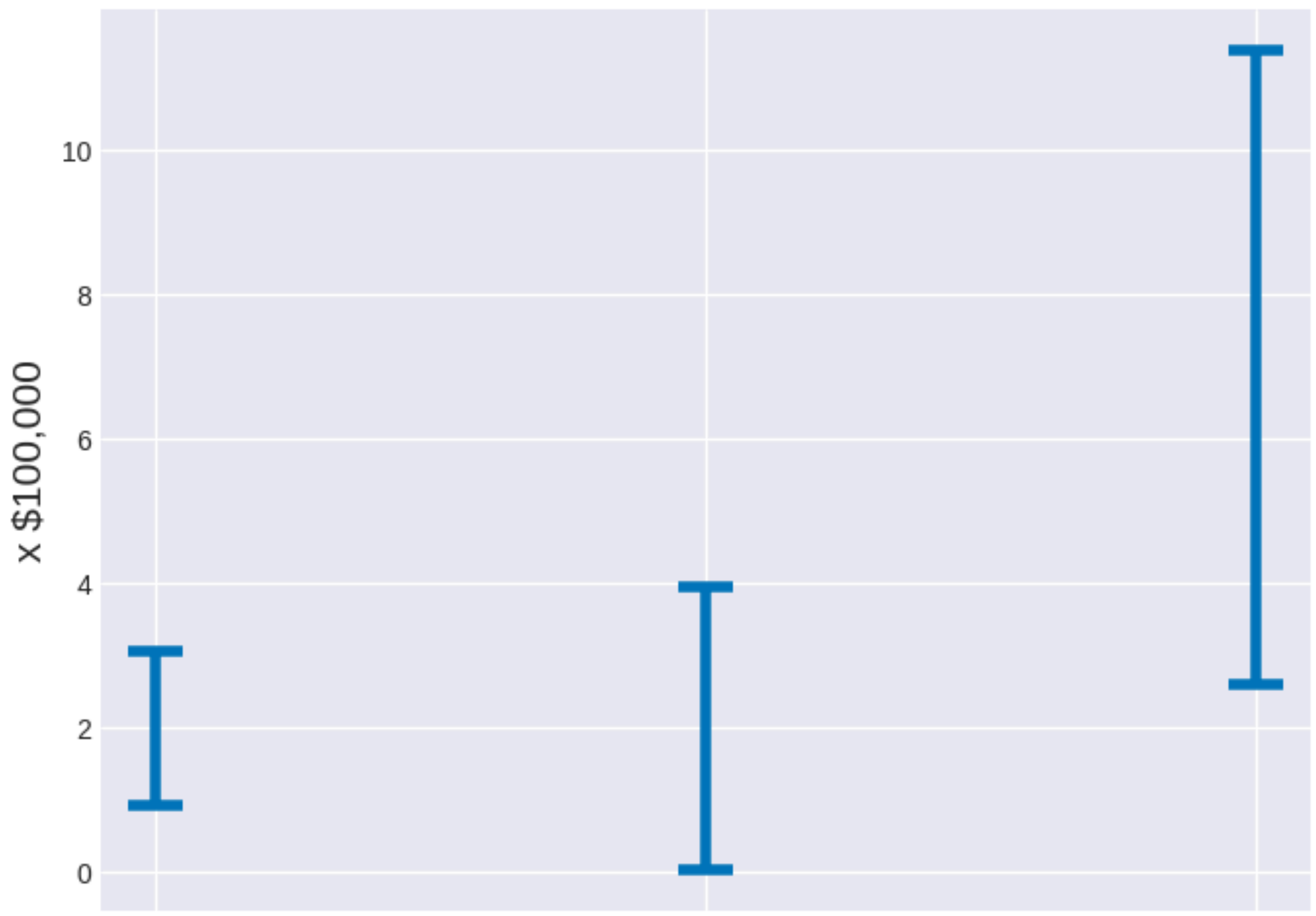

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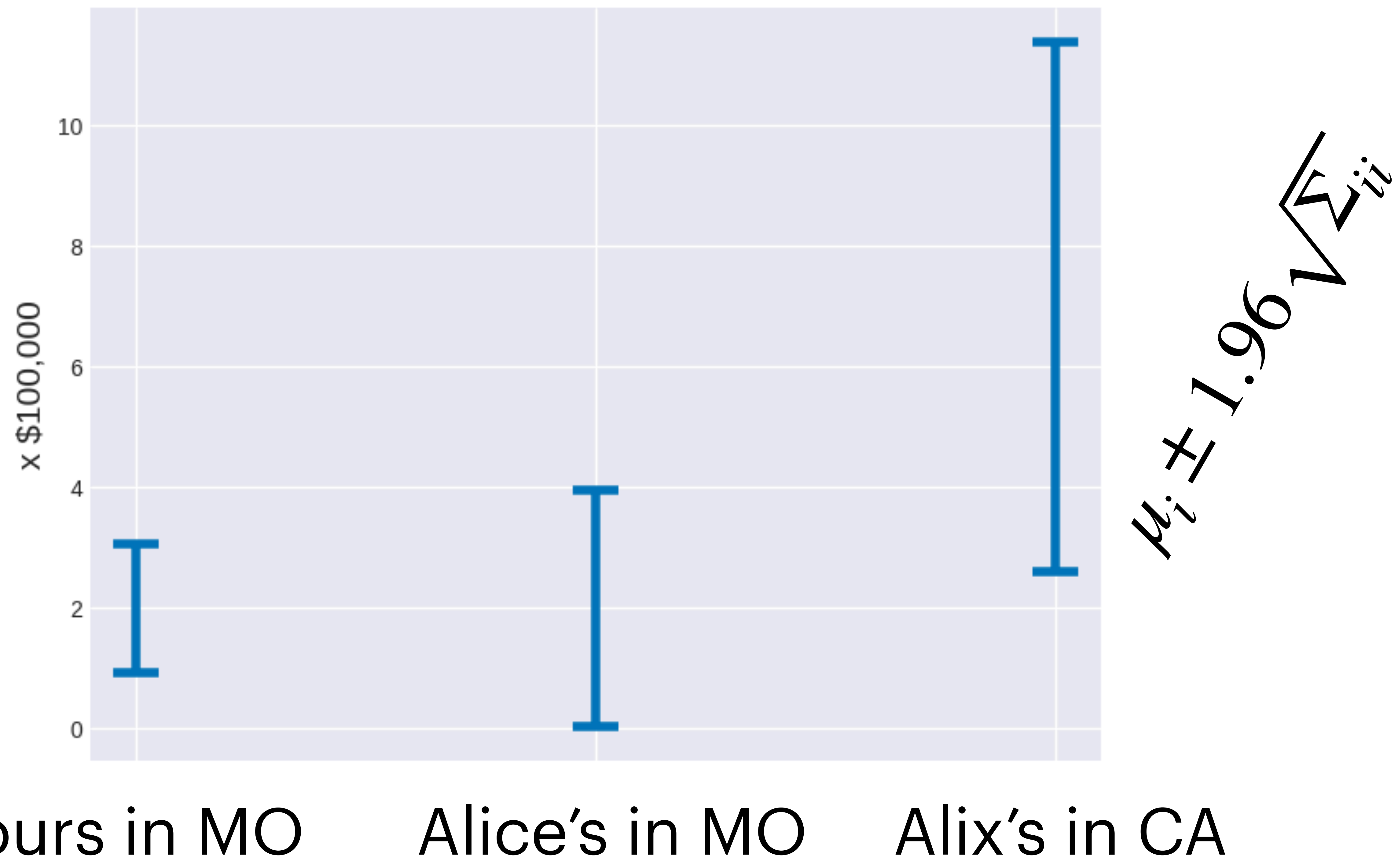

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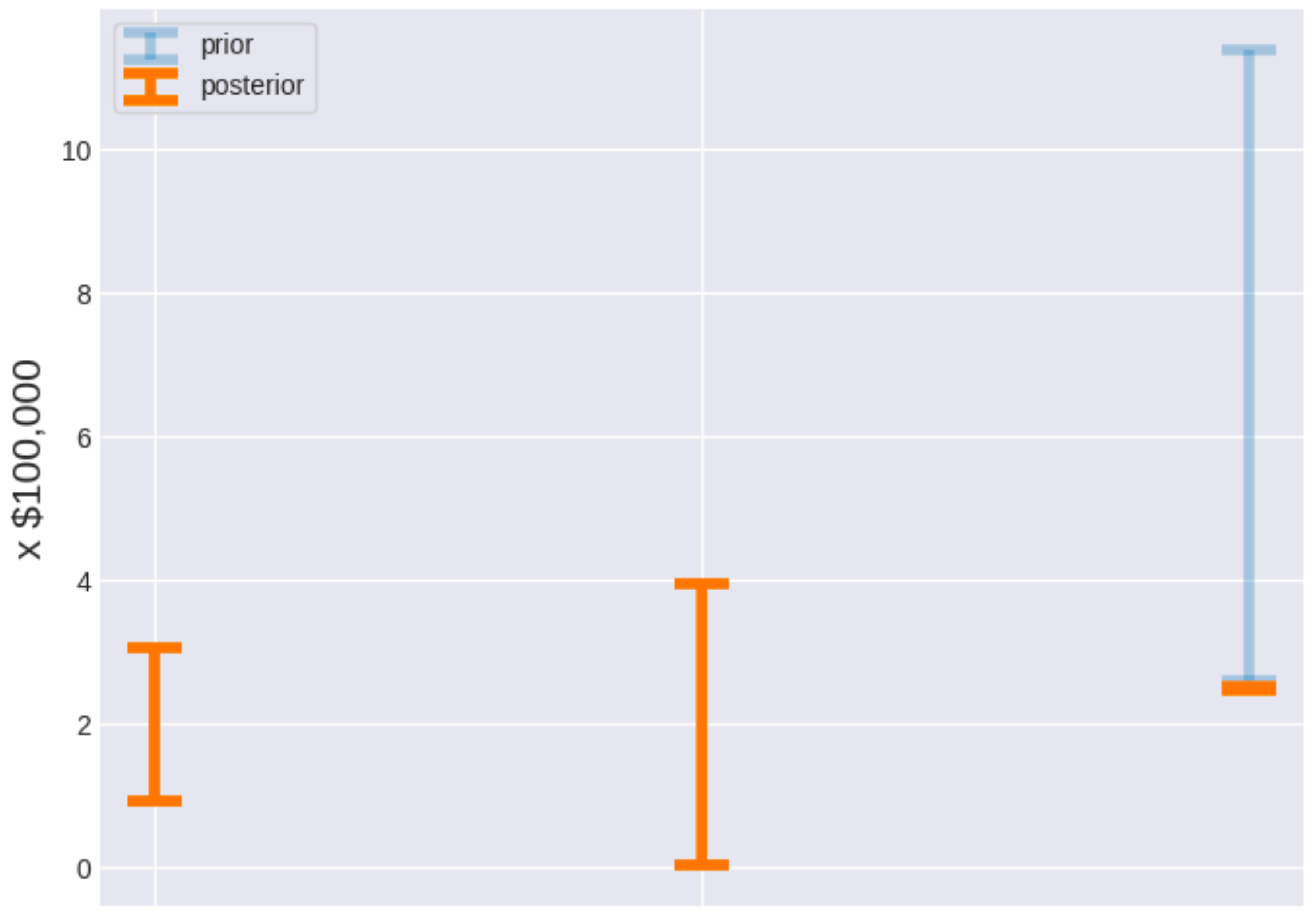

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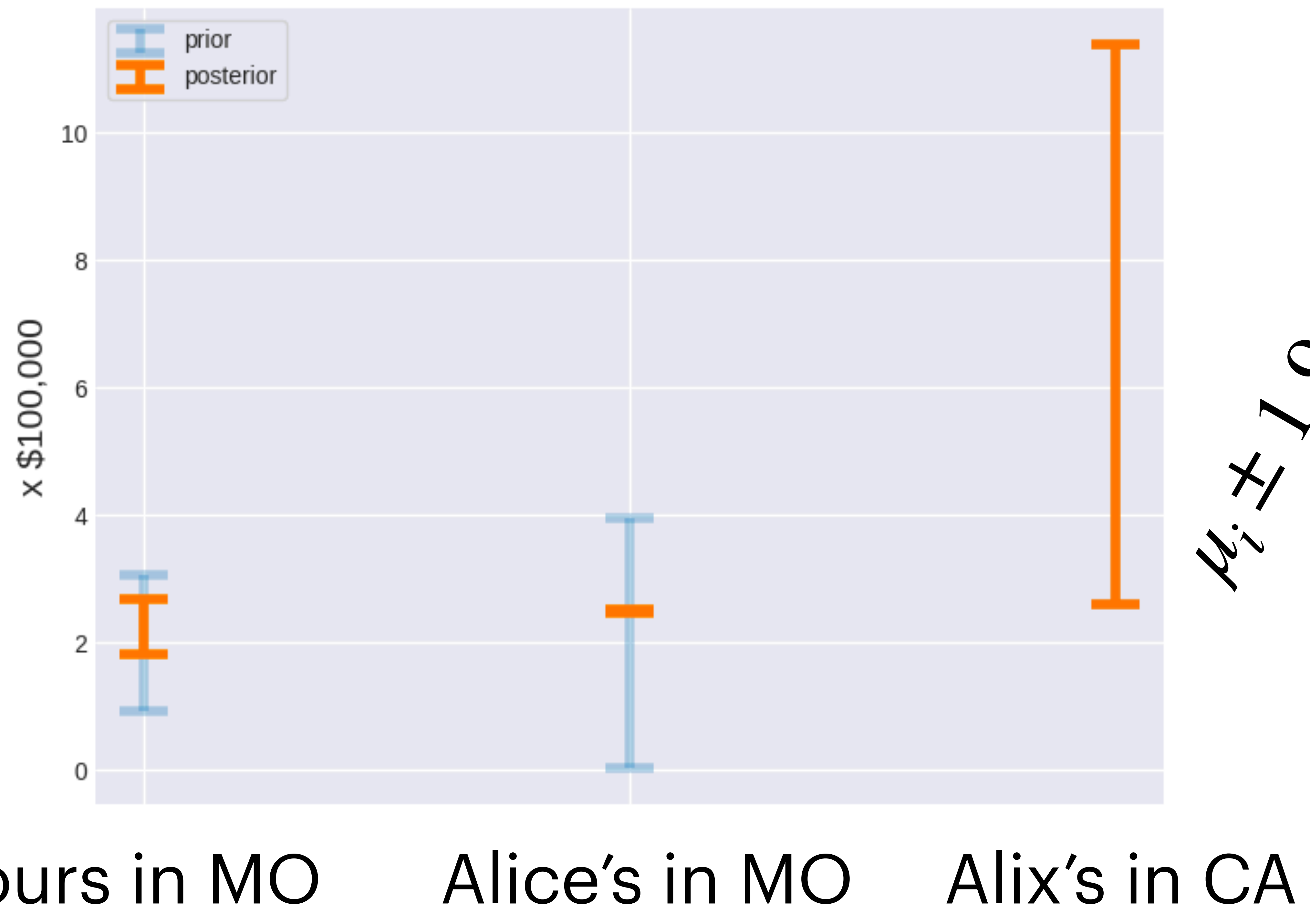

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updating a multivariate Gaussian distribution

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Model unknown house prices as *random variables*

- multivariate Gaussian with appropriate covariances
- once the price of one house is observed, other prices are *updated*

20 houses on a block

- nearby houses have similar prices
- far-away houses have uncorrelated prices

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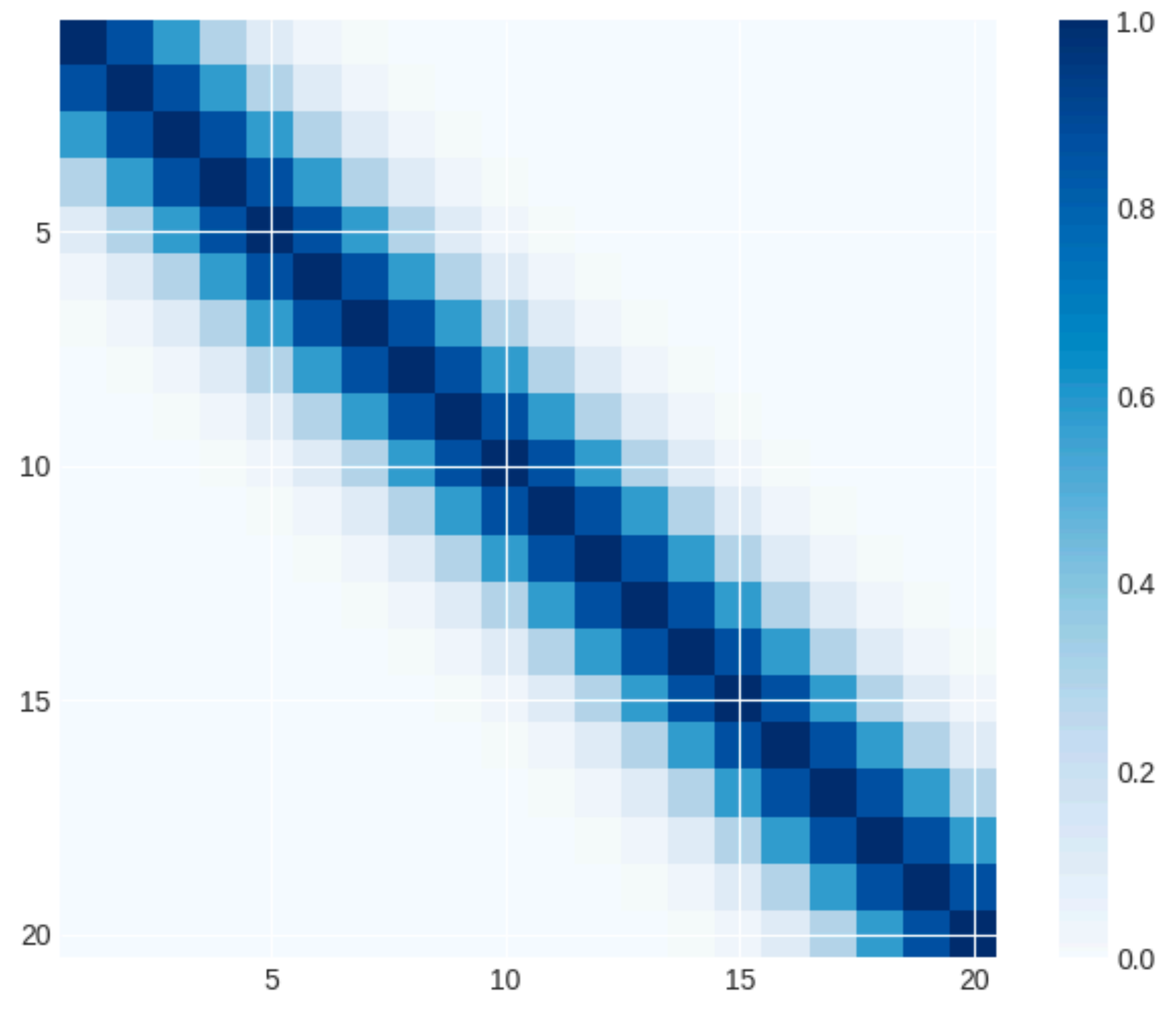

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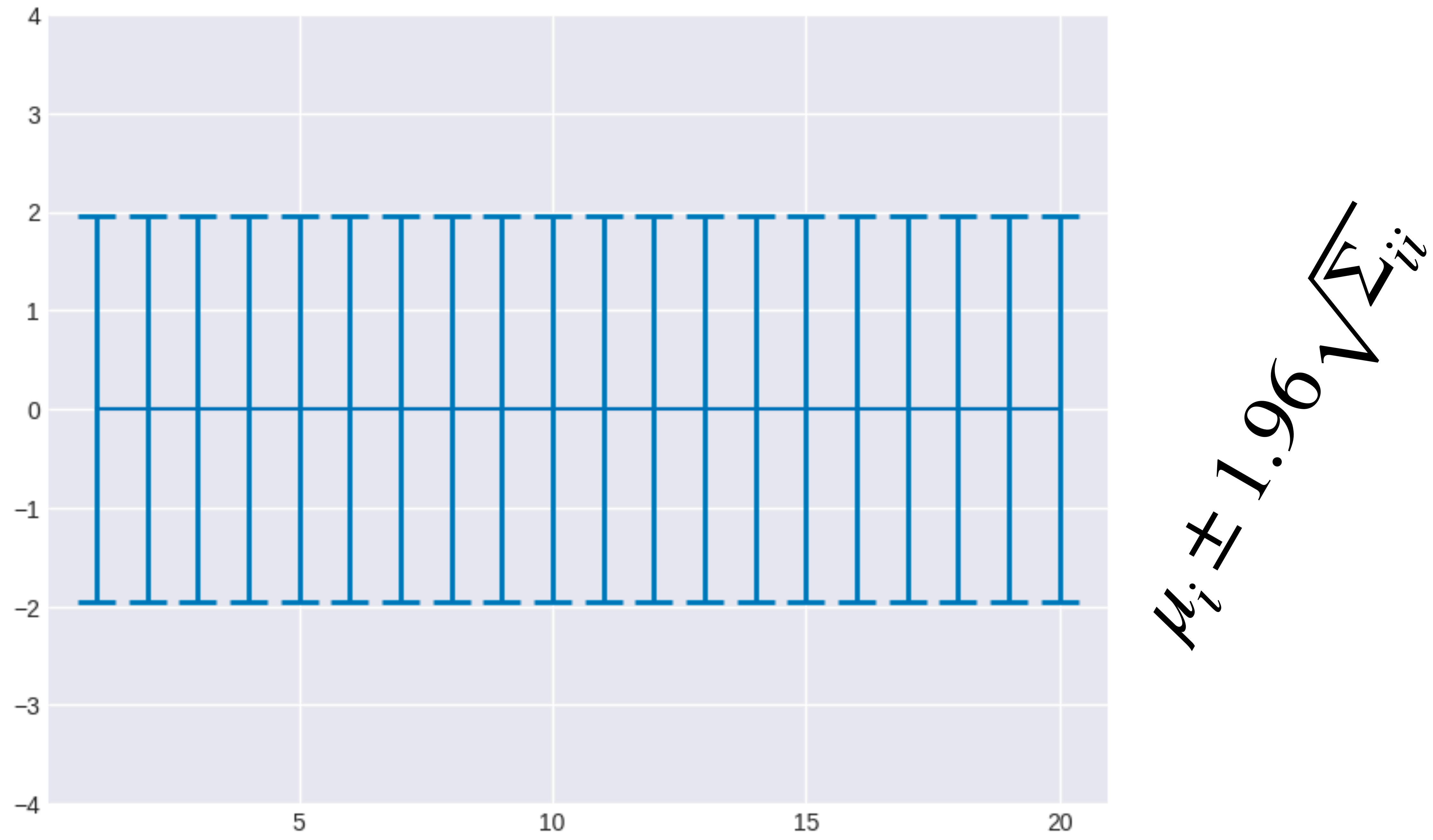

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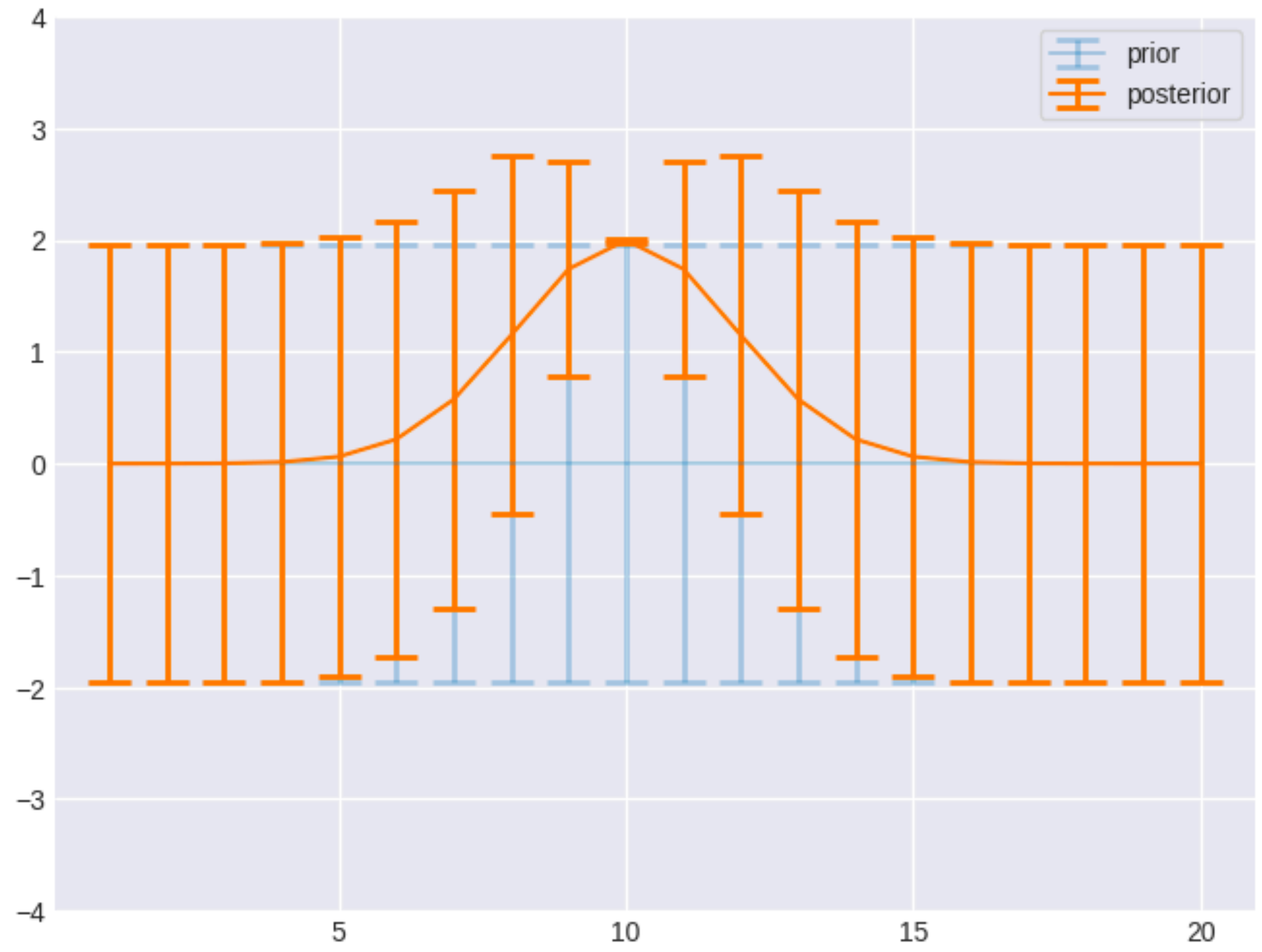
observation $X_{10} = 2$



$\mu_i \pm 1.96\sqrt{\Sigma_{ii}}$

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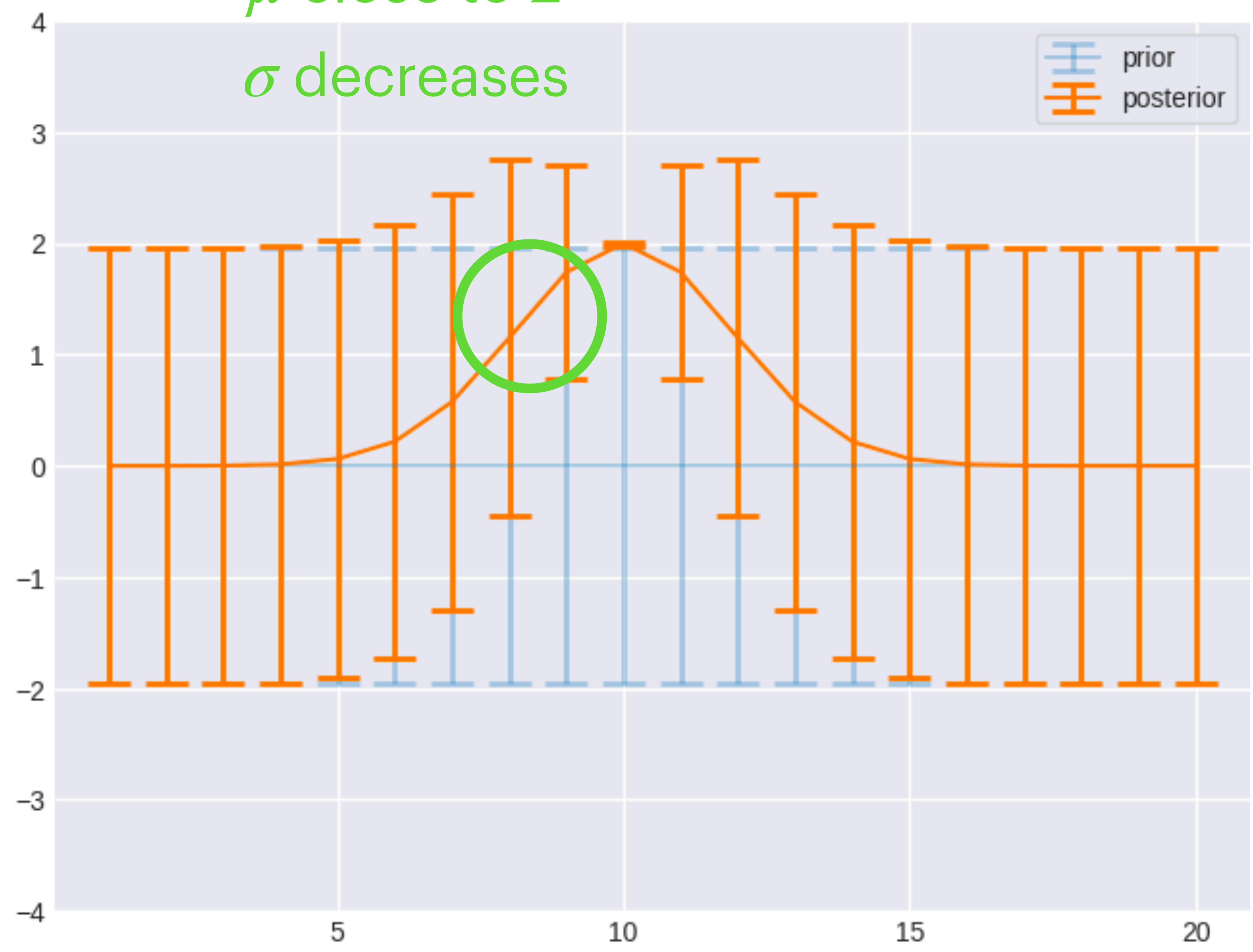

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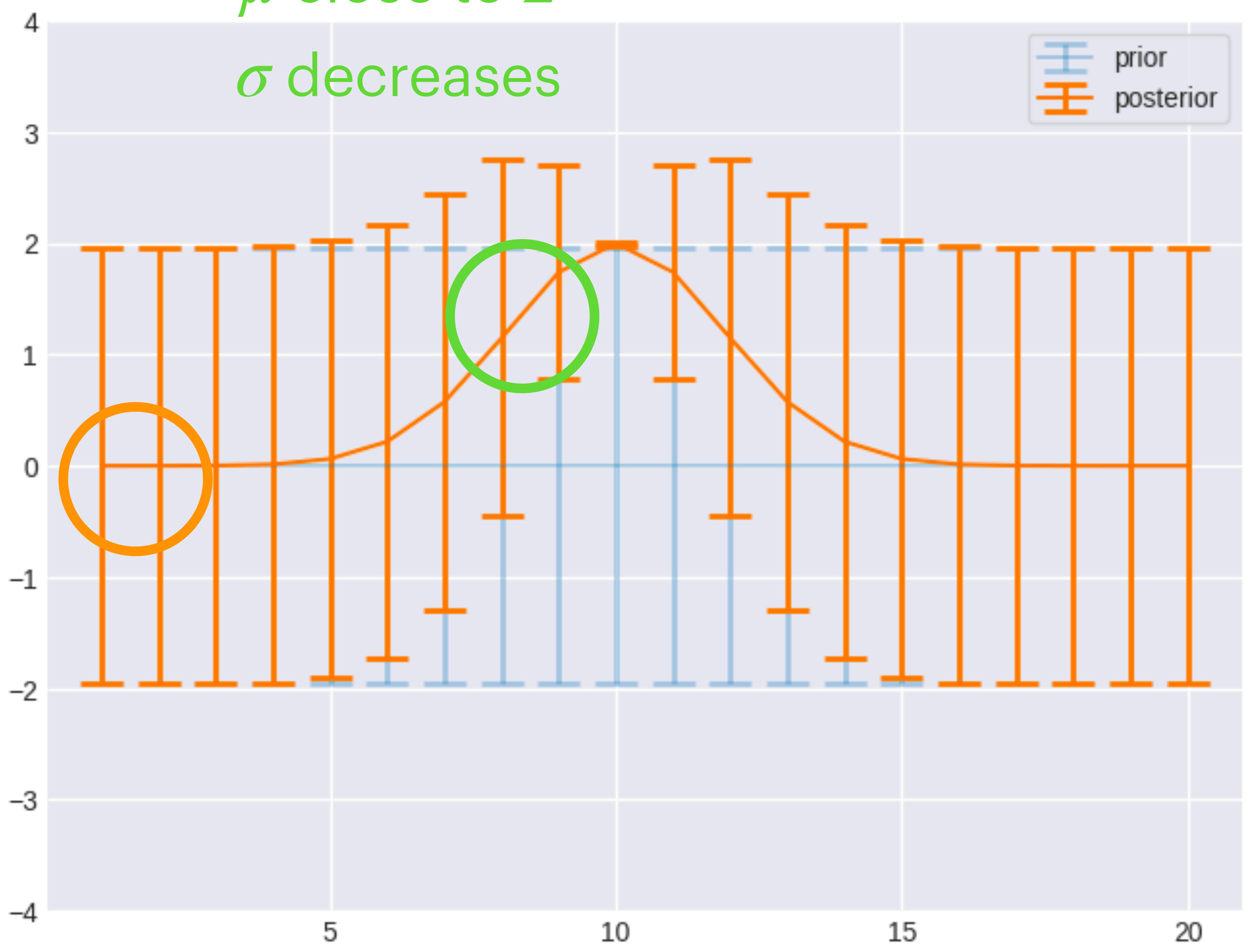
stay the same



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Setting infinitely(!) many house prices

updating a Gaussian process

Infinitely many unknown quantities $f(x)$ for all x as random variables

- nearby x_1 and x_2: similar $f(x_1)$ and $f(x_2)$
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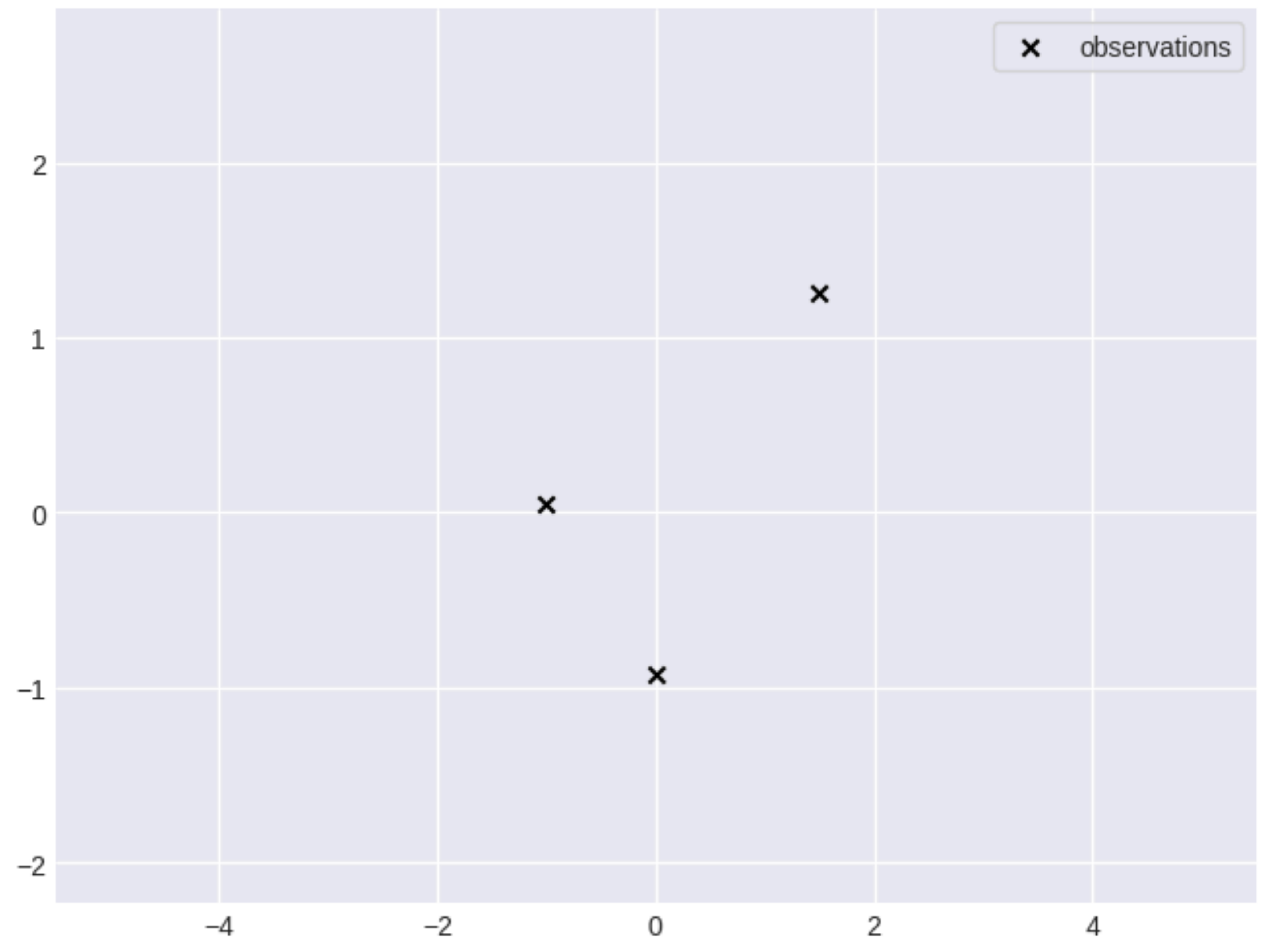

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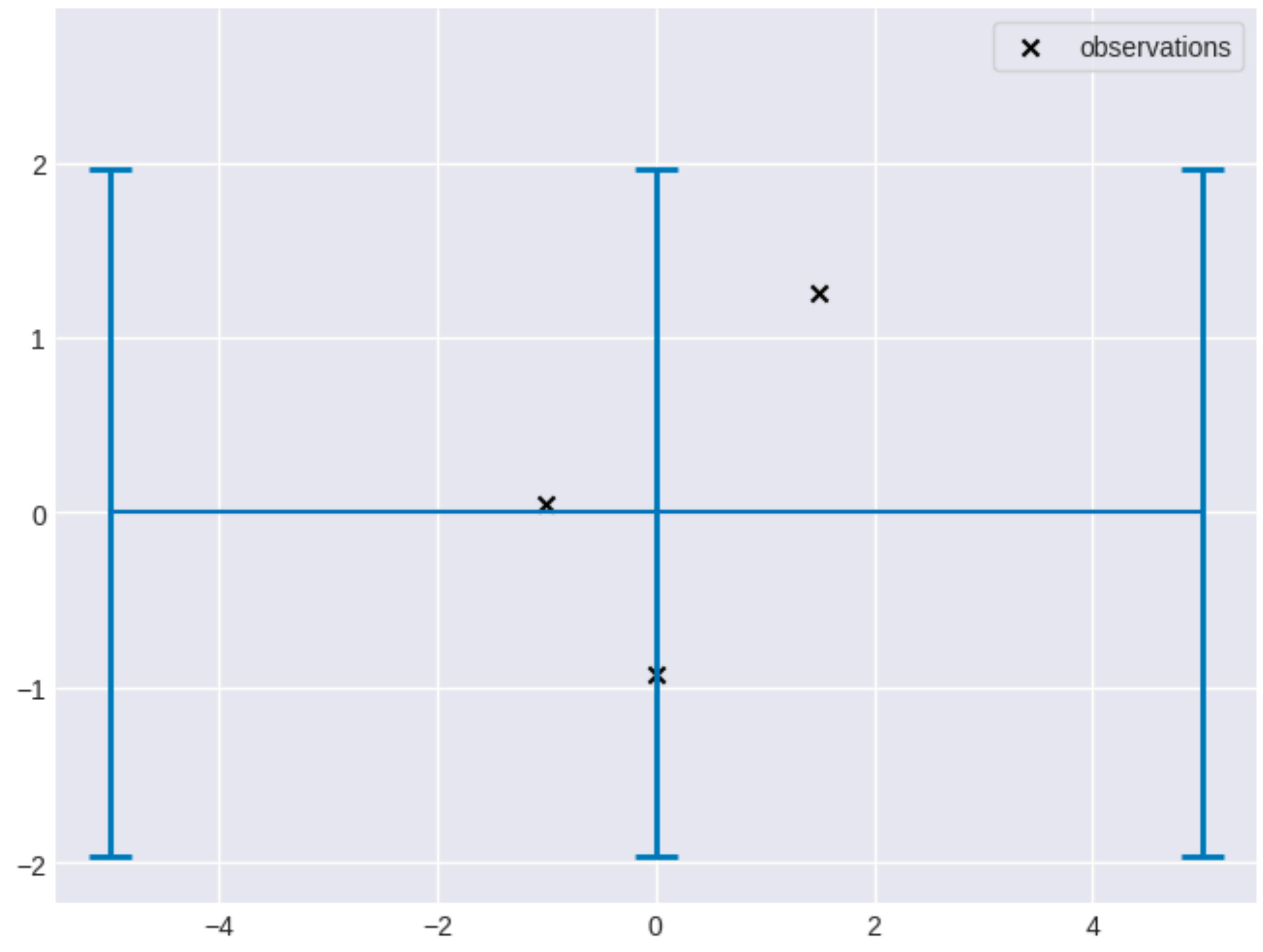

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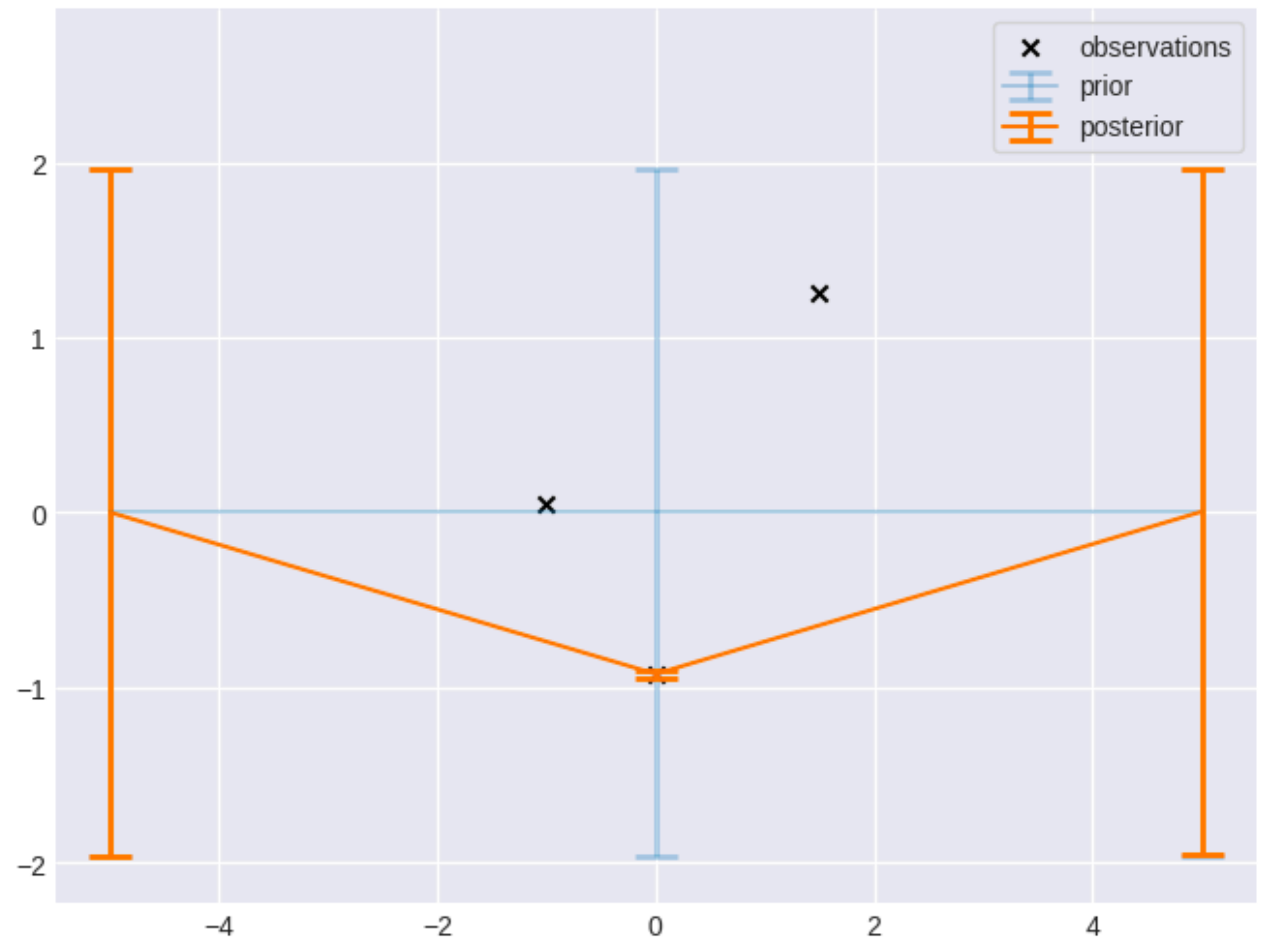

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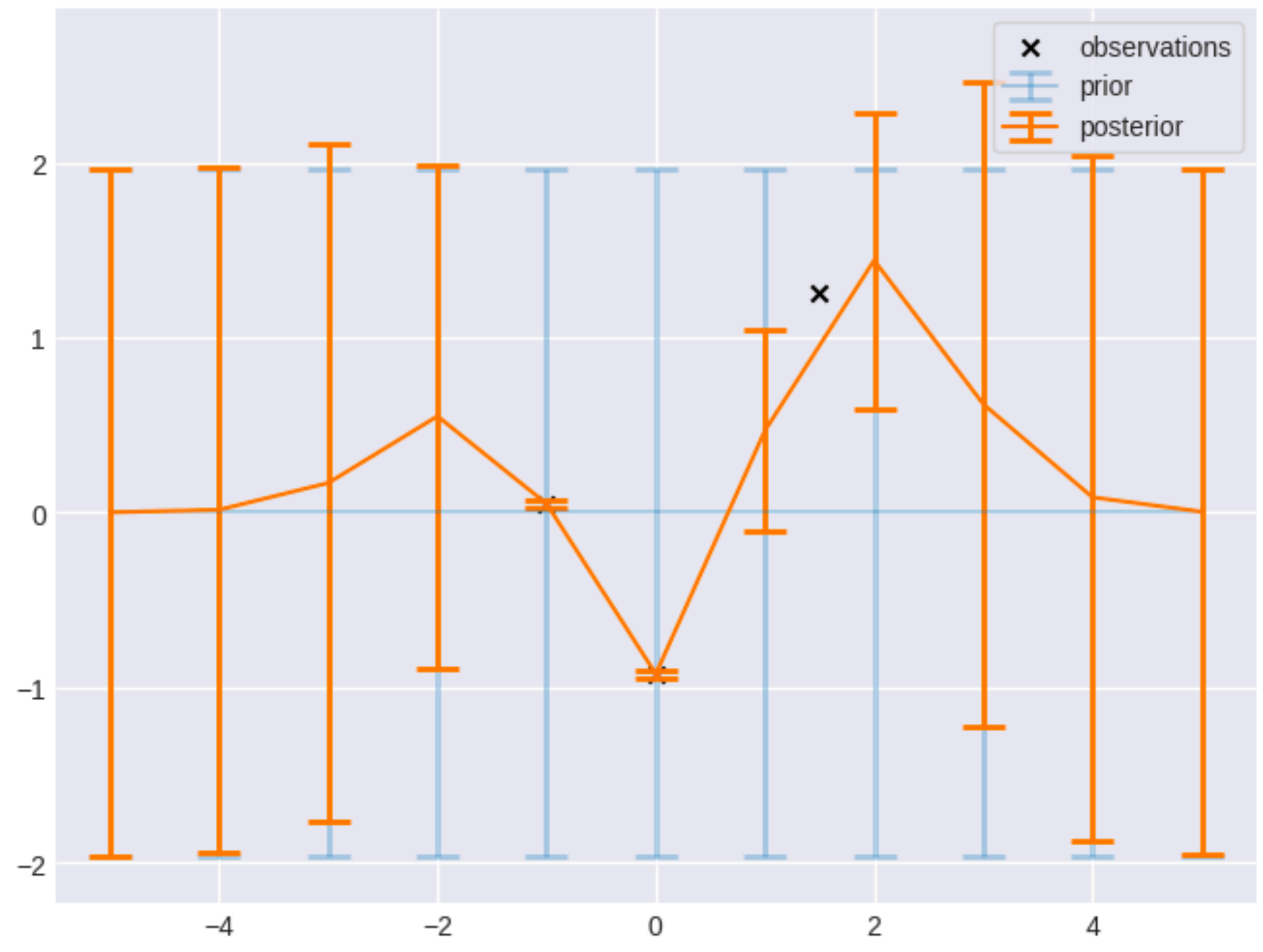

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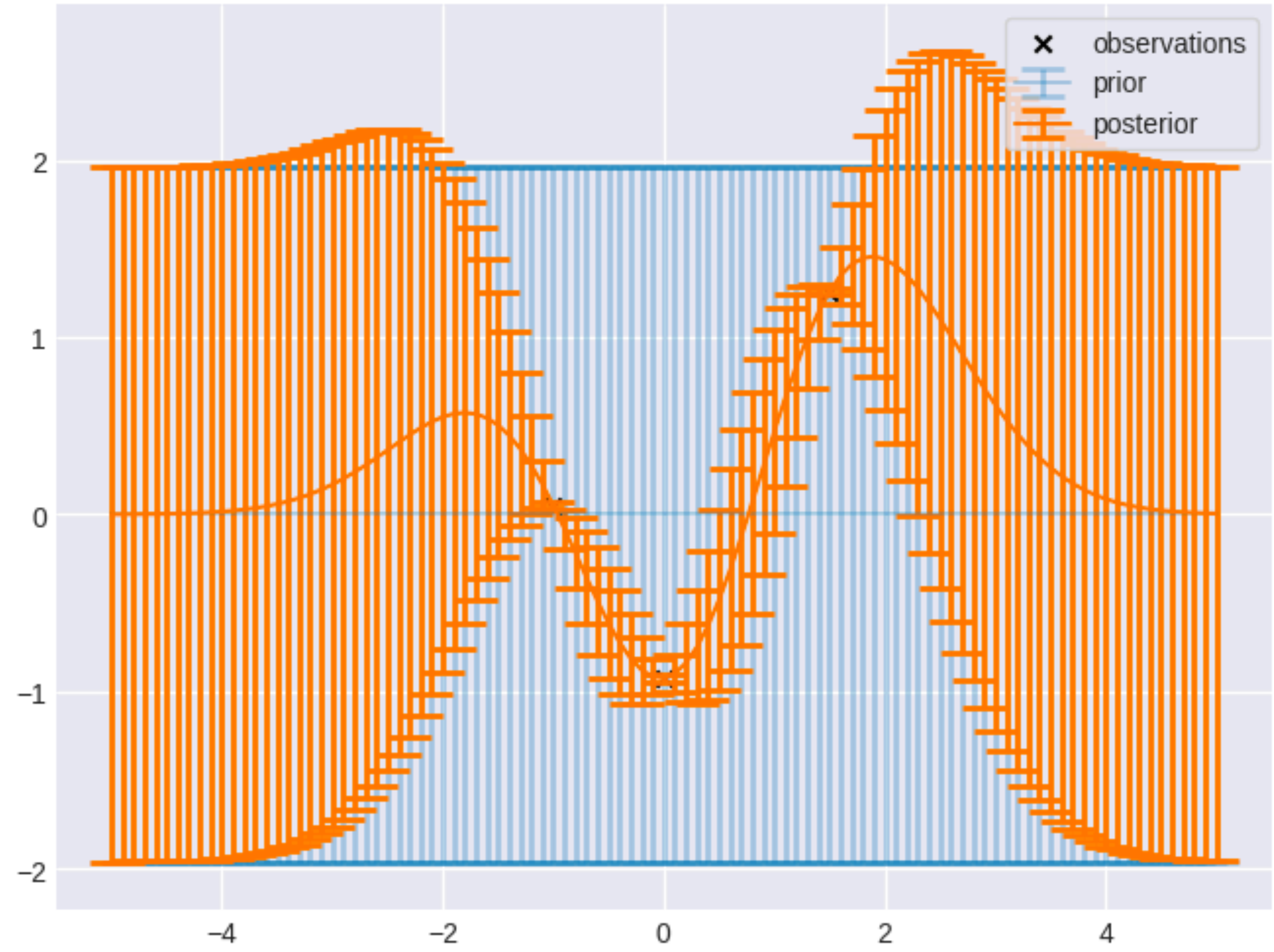

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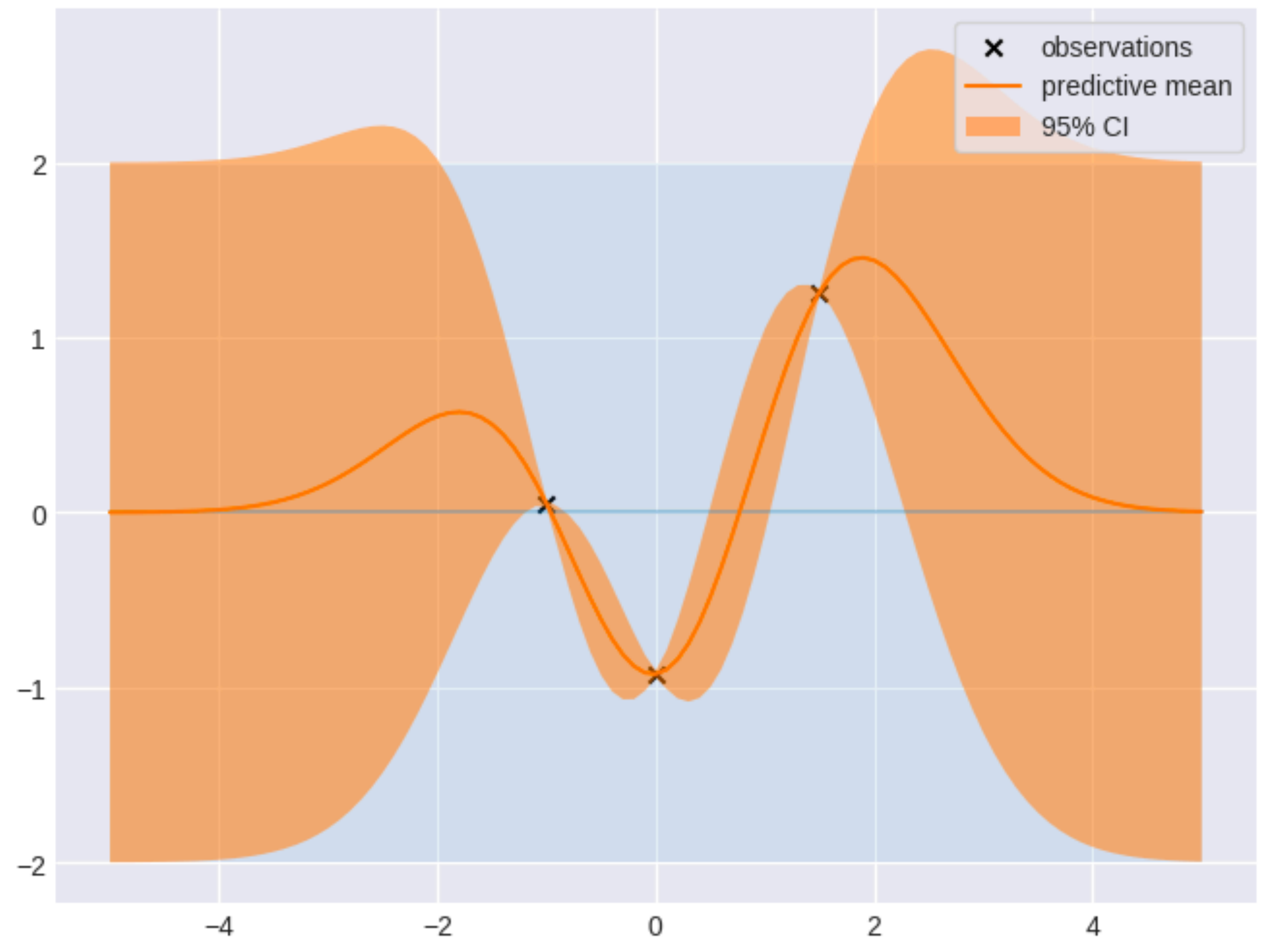

Implementing Gaussian processes in Python

using state-of-the-art software

GPyTorch for Gaussian process modeling

modular implementation of Gaussian processes

Need to declare two components:

- **Mean function** models the *expected trend*
- **Kernel** models *smoothness*

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```
class GPModel(ExactGP):
    def __init__(self, train_x, train_y, likelihood):
        super().__init__(train_x, train_y, likelihood)
        self.mean_module = ConstantMean()
        self.covar_module = RBFKernel()

    def forward(self, x):
        mean_x = self.mean_module(x)
        covar_x = self.covar_module(x)
        return MultivariateNormal(mean_x, covar_x)
```

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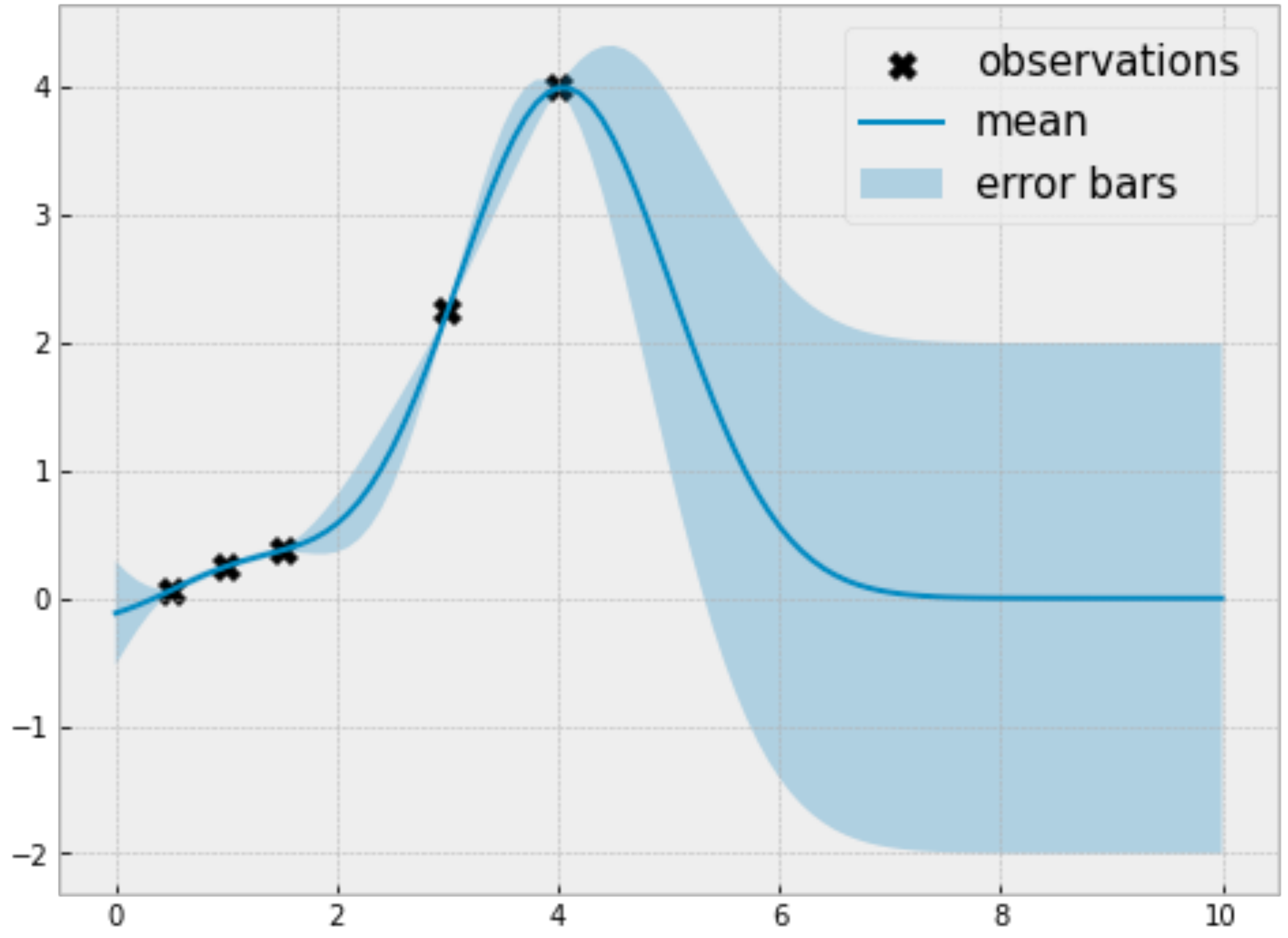

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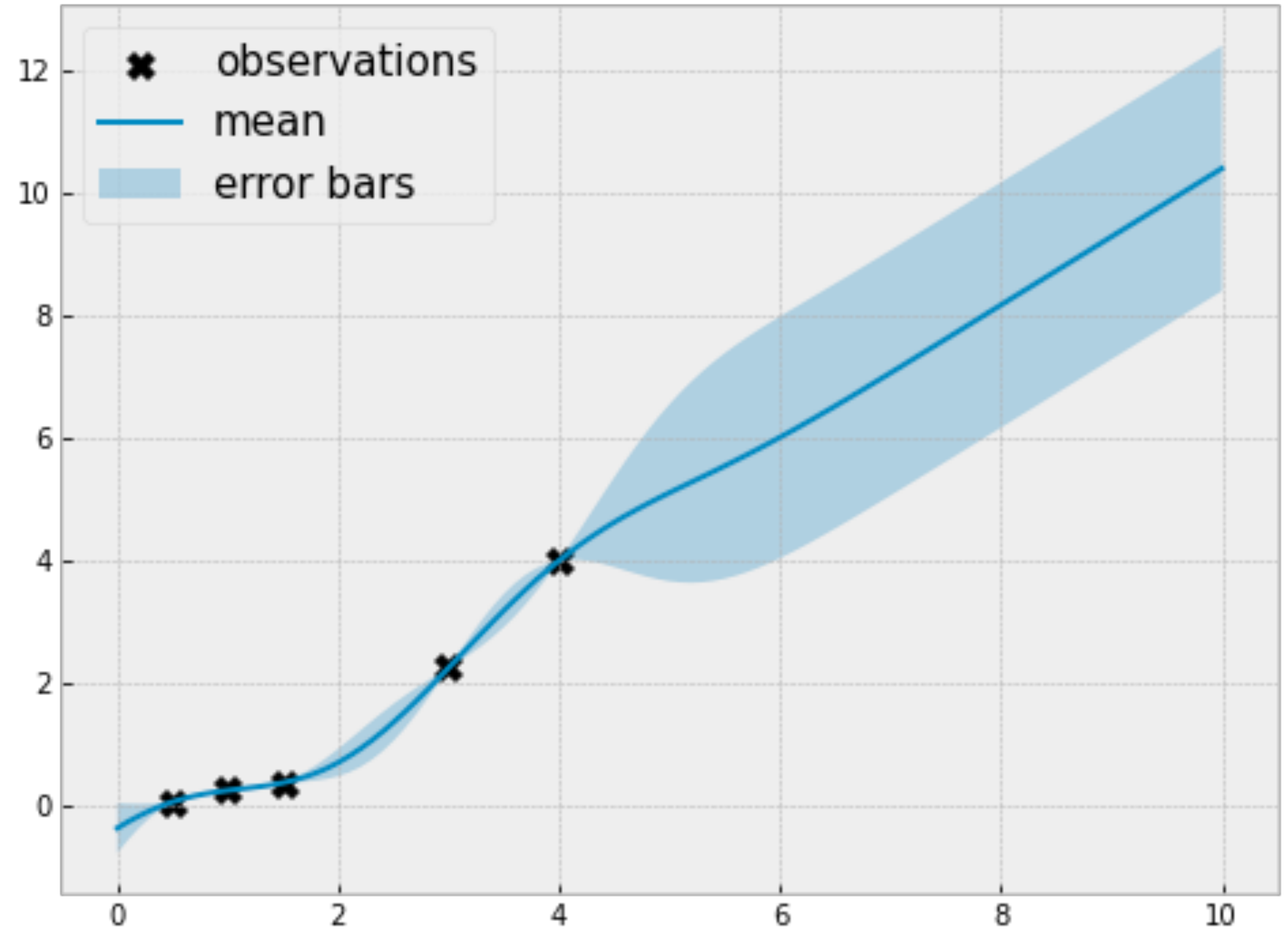
```
class GPModel(ExactGP):
    def __init__(self, train_x, train_y, likelihood):
        super().__init__(train_x, train_y, likelihood)
        self.mean_module = LinearMean(1)
        self.covar_module = RBFKernel()
```



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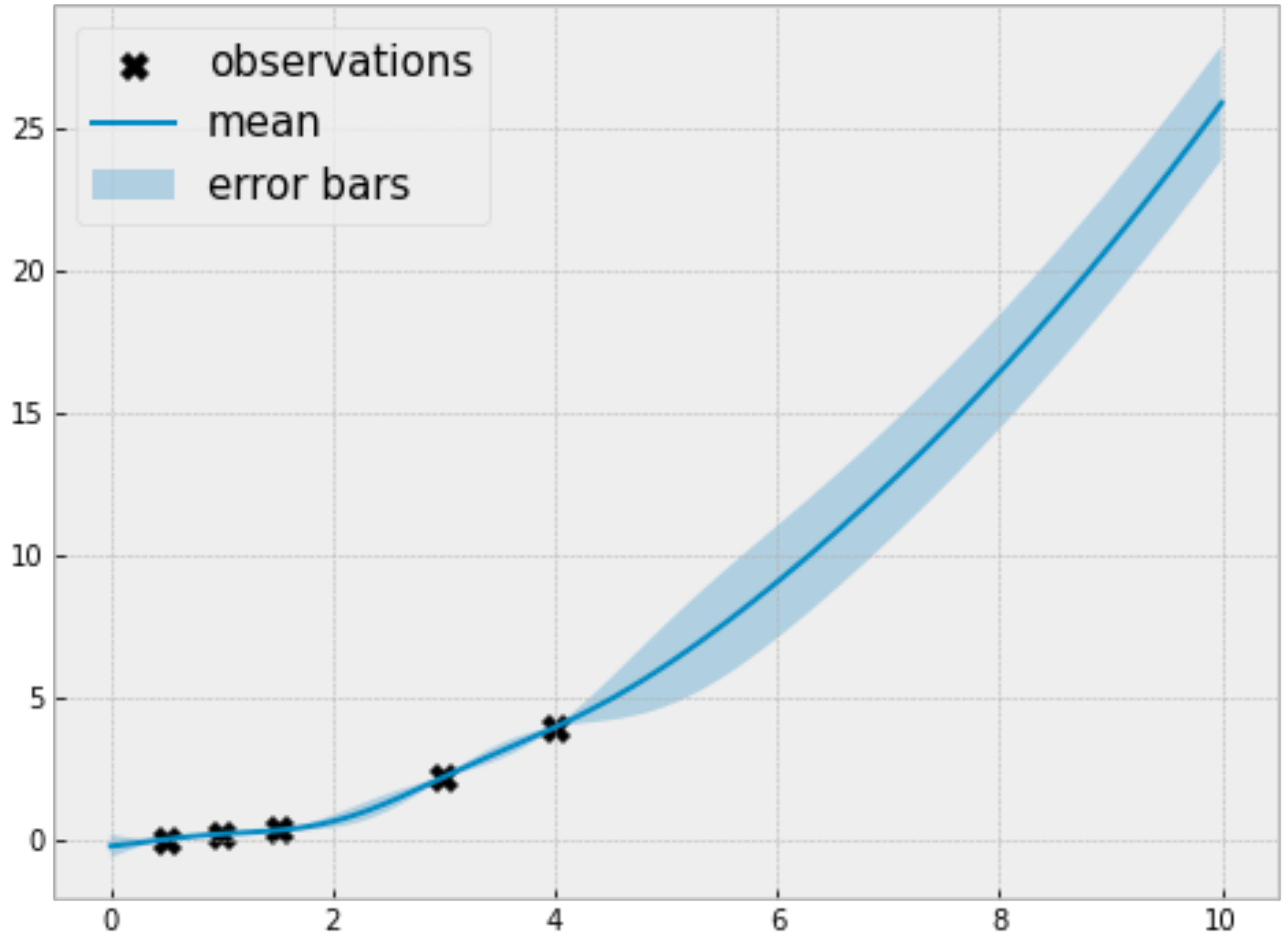
```
class QuadraticMean(Mean):
    def forward(self, x):
        res = (
            x.pow(2).matmul(self.second)
            + x.matmul(self.first)
            + self.bias
        )
        return res
```



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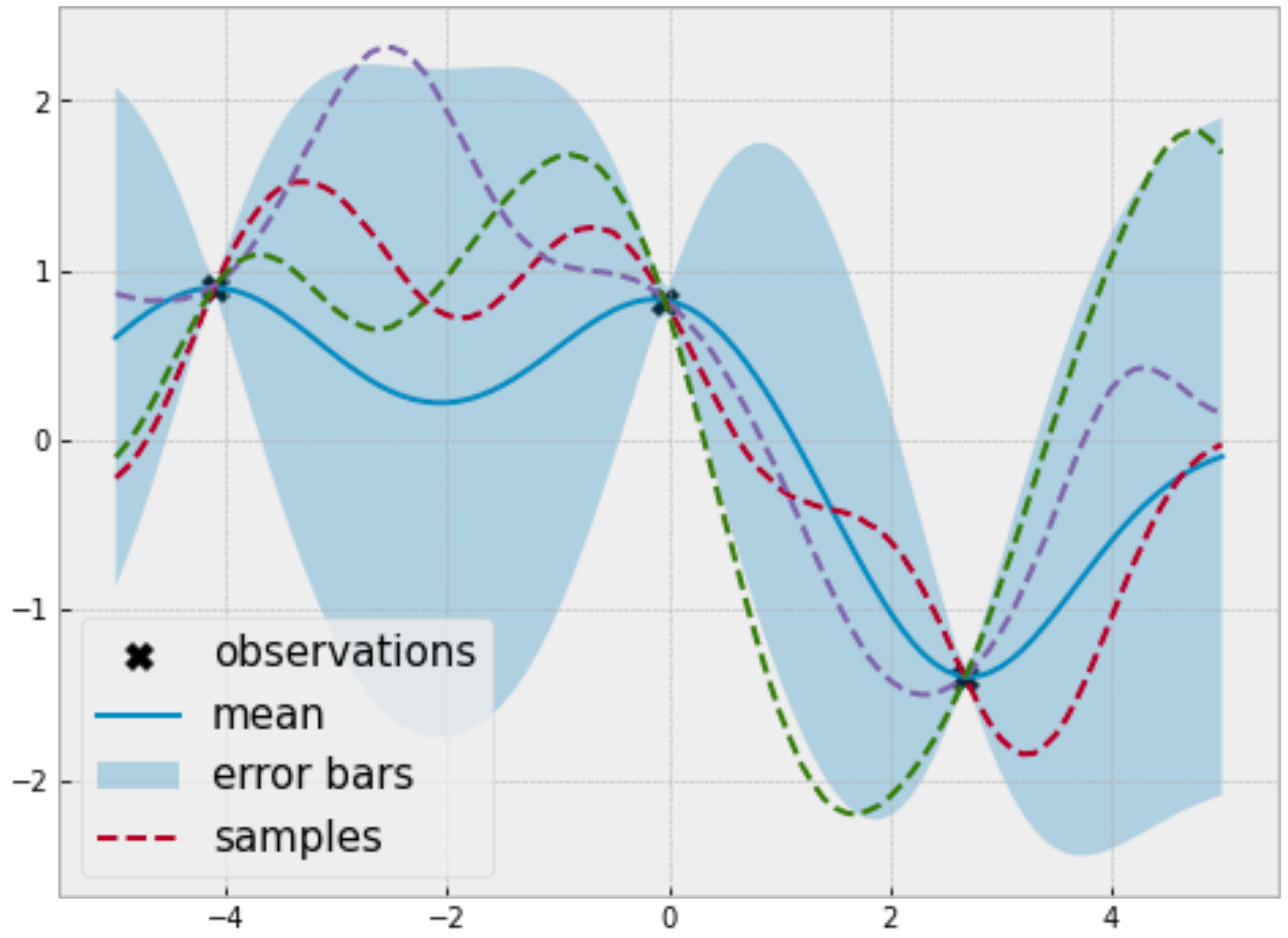

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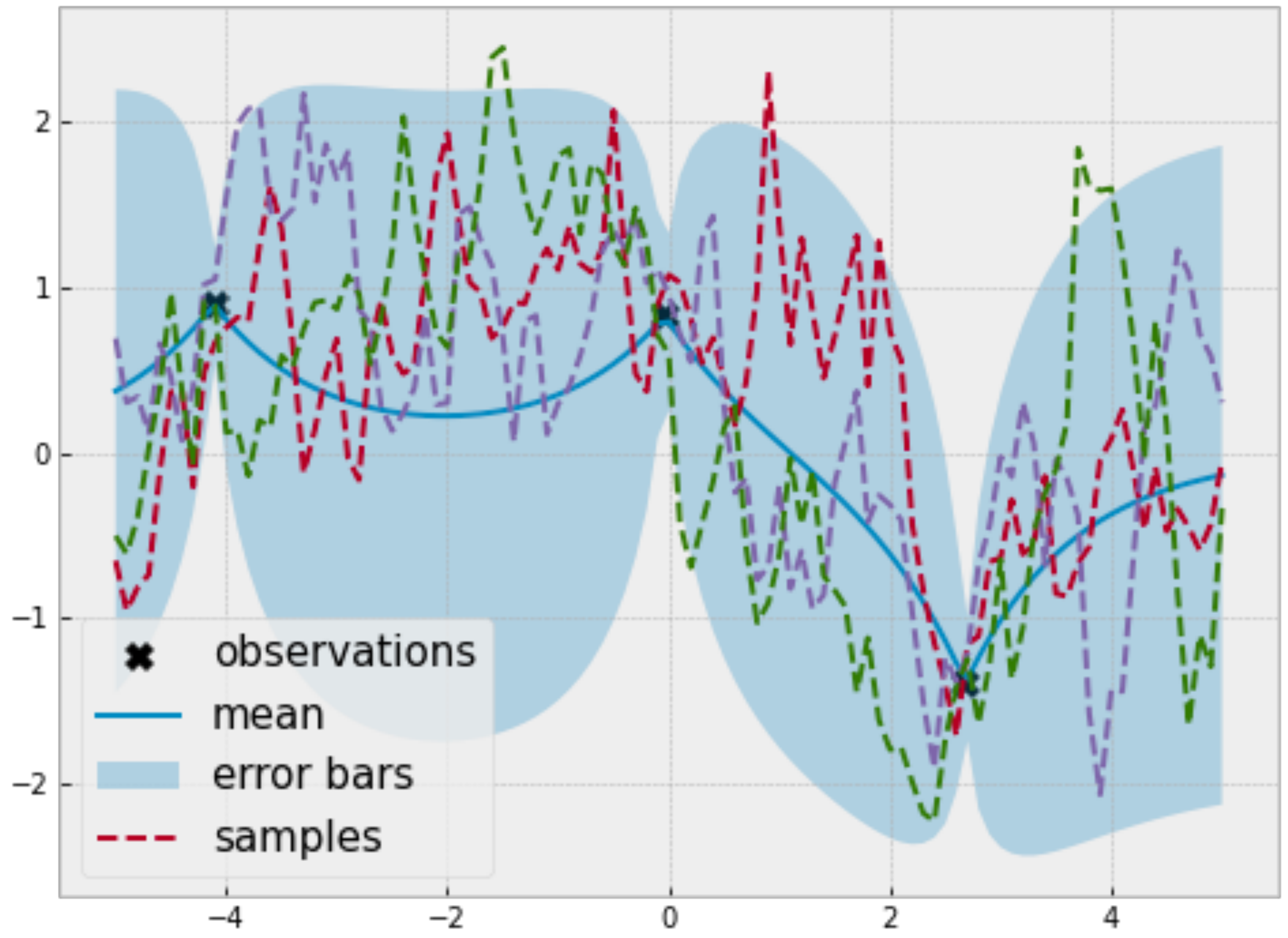
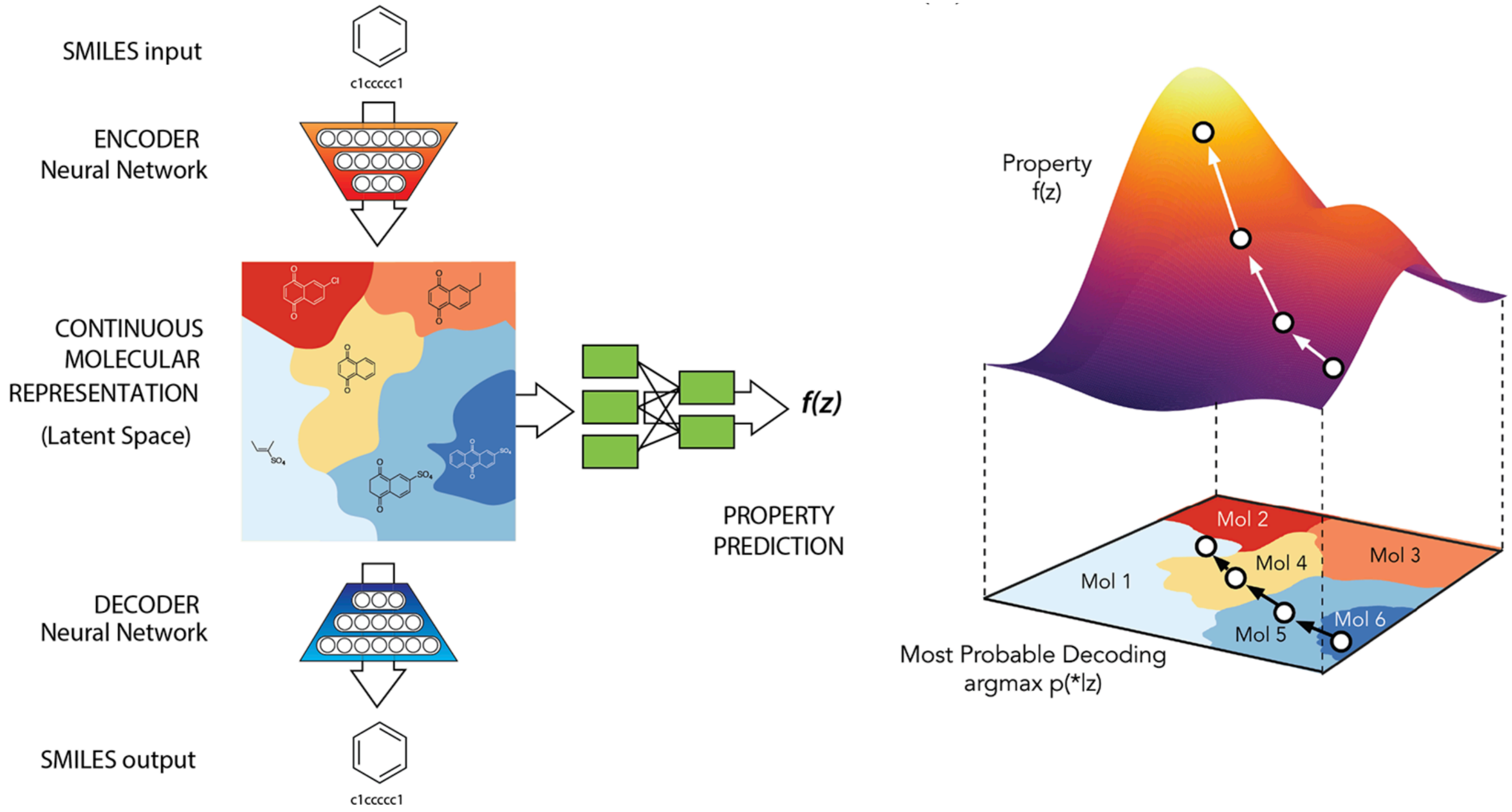
class GPModel(ExactGP):
    def __init__(self, train_x, train_y, likelihood):
        super().__init__(train_x, train_y, likelihood)
        self.mean_module = ConstantMean()
        self.covar_module = MaternKernel(nu=0.5)
```



Advanced Gaussian process models

taking Gaussian processes to the next level

- Combining neural networks and Gaussian processes



Gomez-Bombarelli *et al. Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules*. ACS Central Science, 2018.

Advanced Gaussian process models

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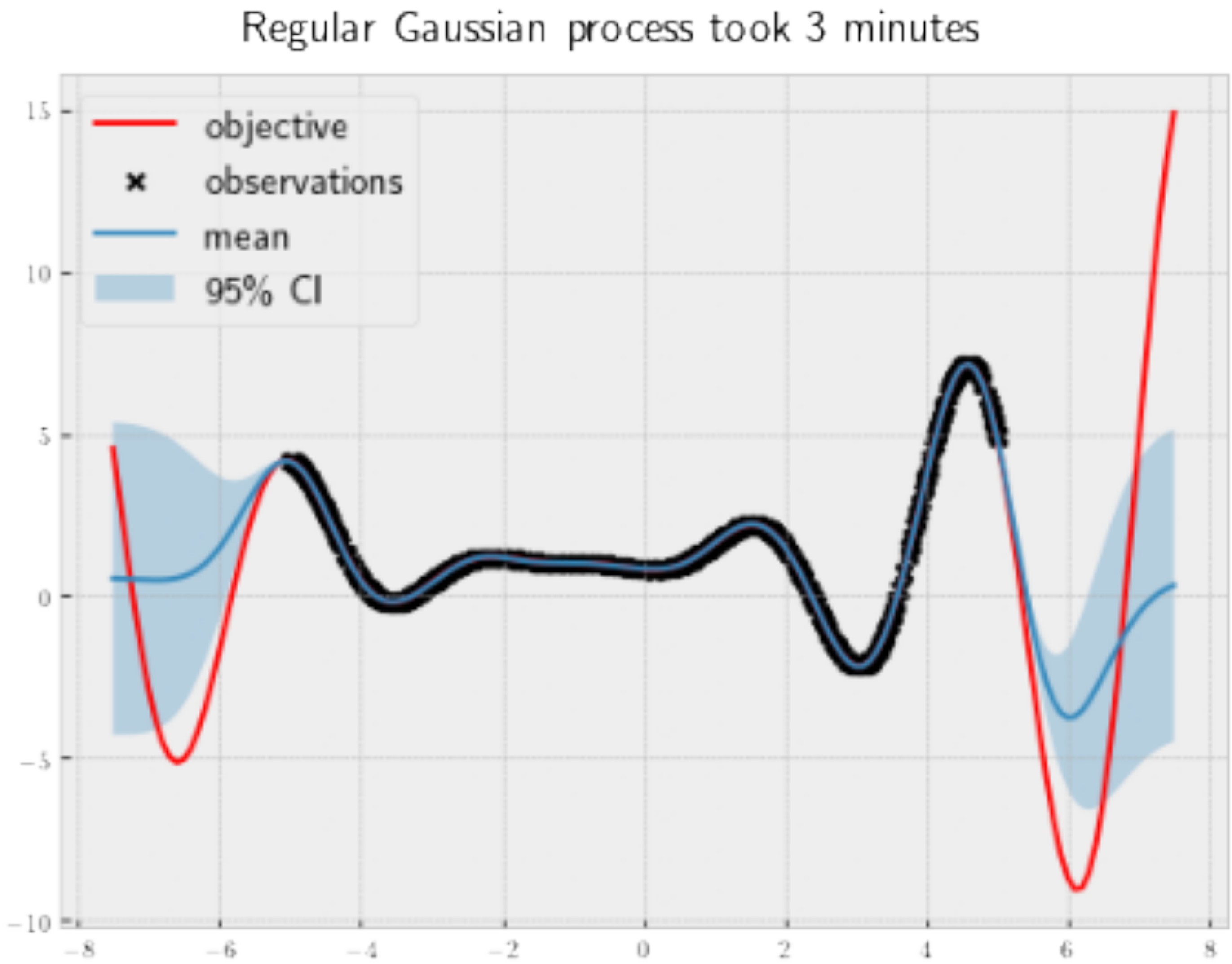
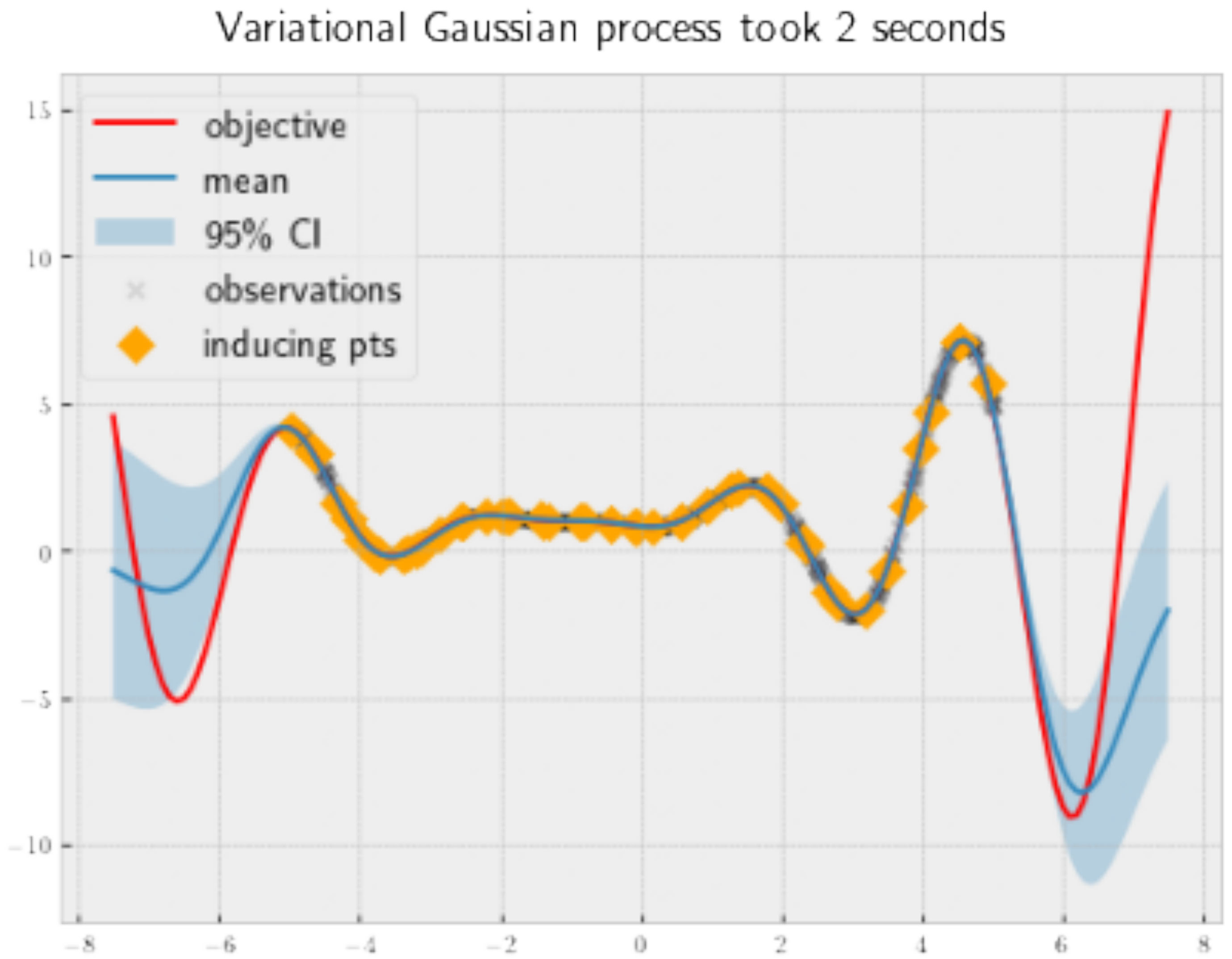
- Combining neural networks and Gaussian processes
- Scaling Gaussian processes to large data sets using representative data

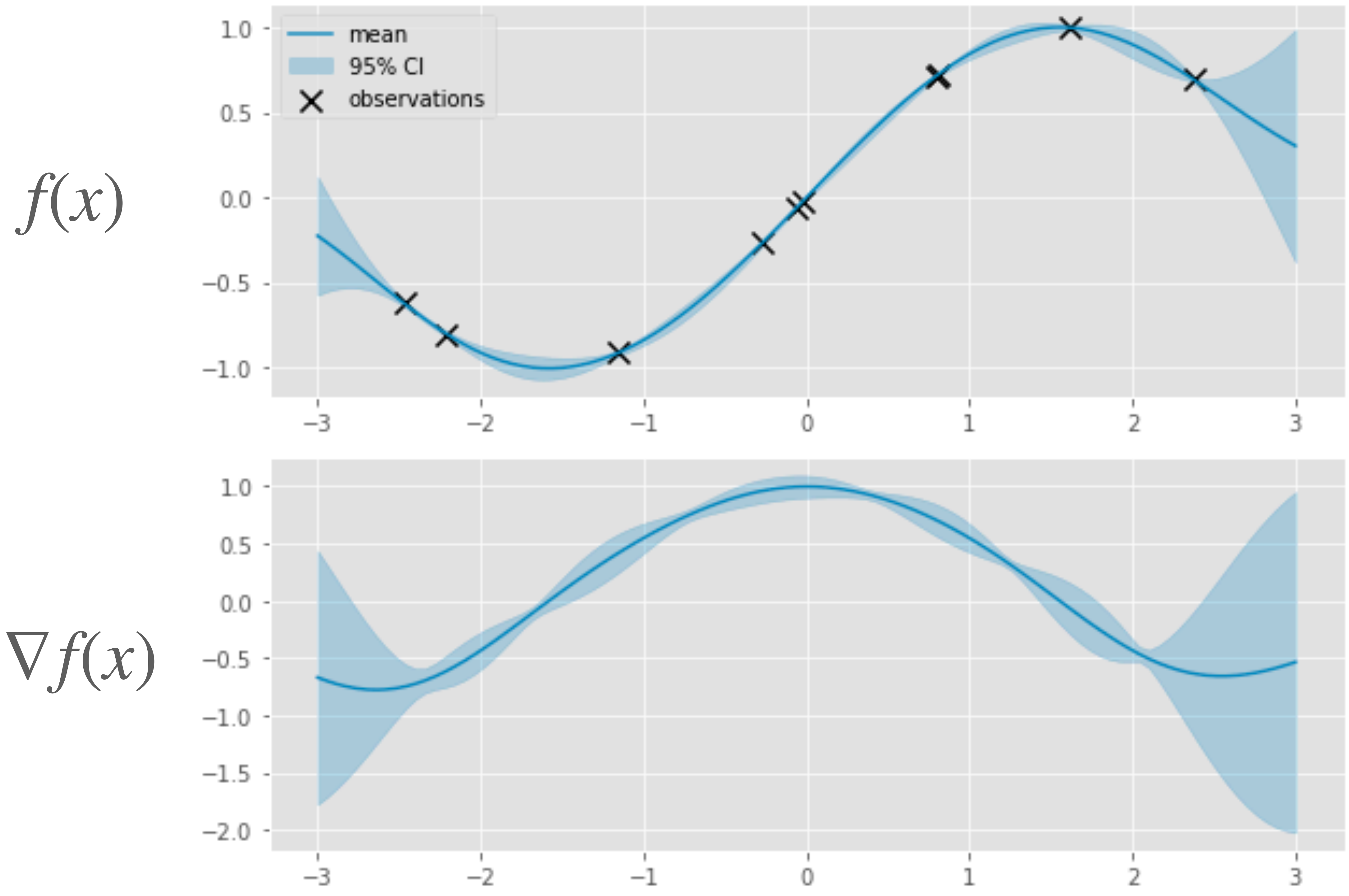




Advanced Gaussian process models

taking Gaussian processes to the next level

- Combining neural networks and Gaussian processes
- Scaling Gaussian processes to large data sets using representative data
- Learn from and/or predicting derivatives – derivative follows a GP



Bayesian optimization

blackbox optimization with Gaussian processes

- Last year's PyData Global talk
- https://www.manning.com/books/bayesian-optimization-in-action
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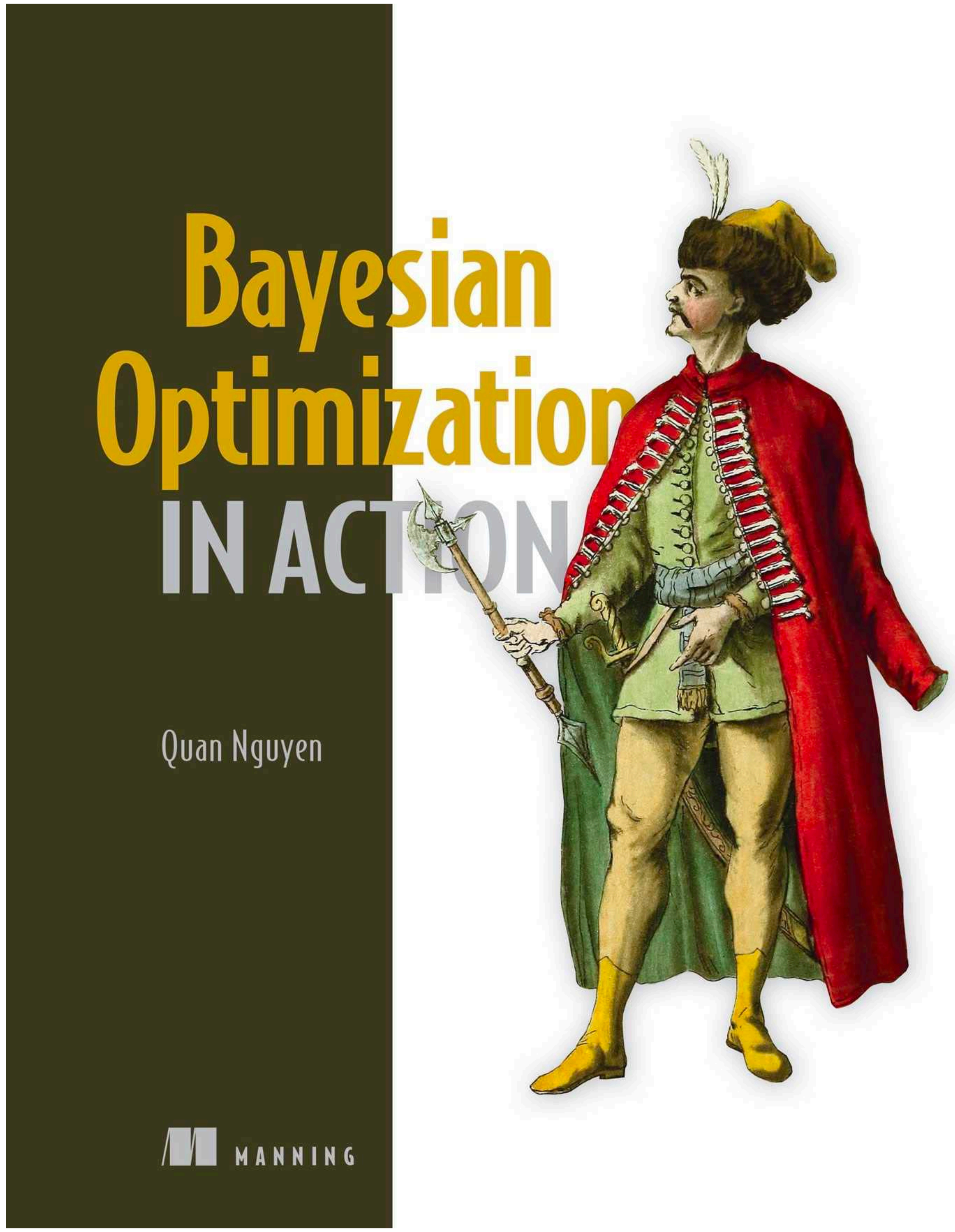
- Discount code: **ctwpydata45**



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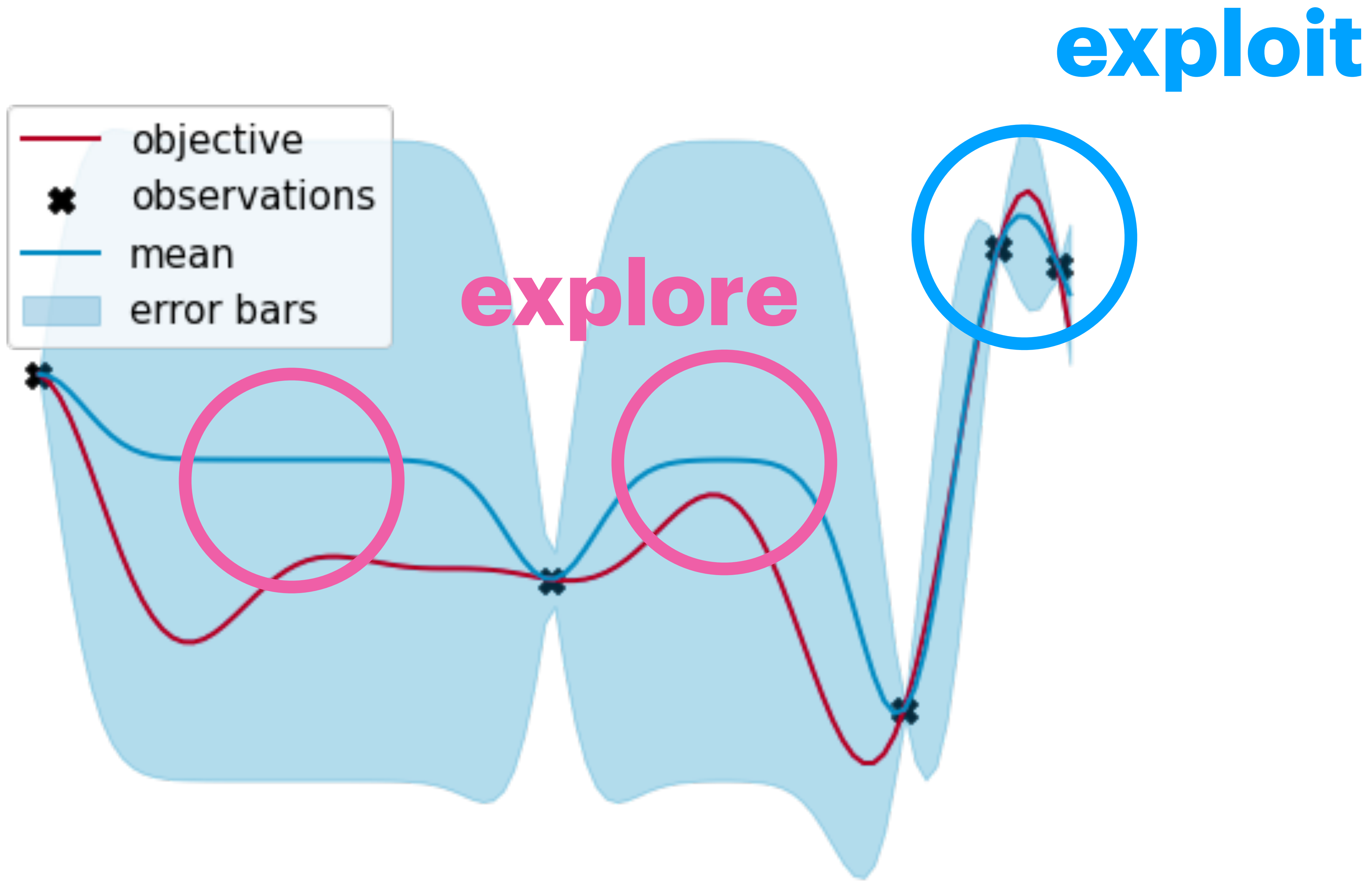

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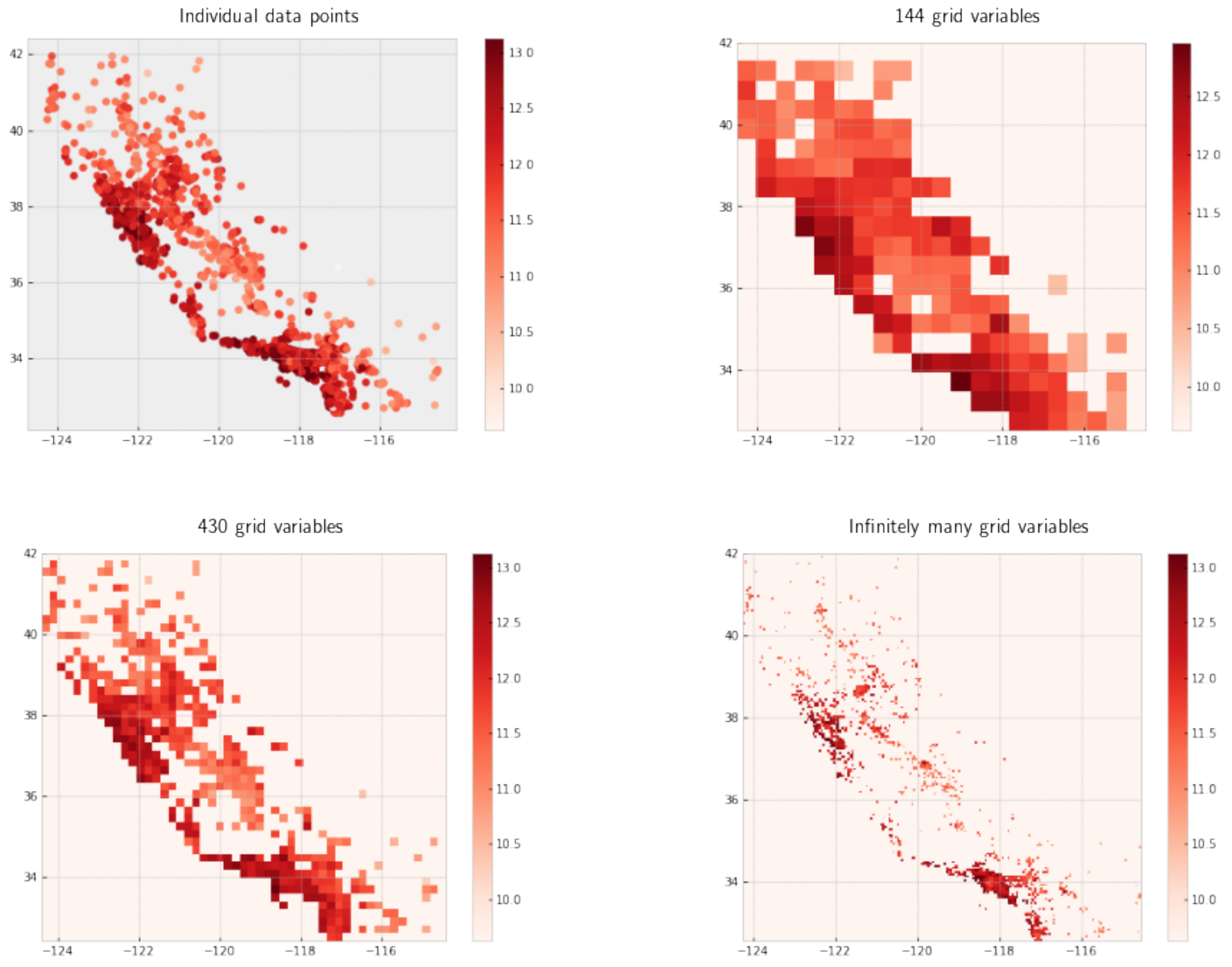

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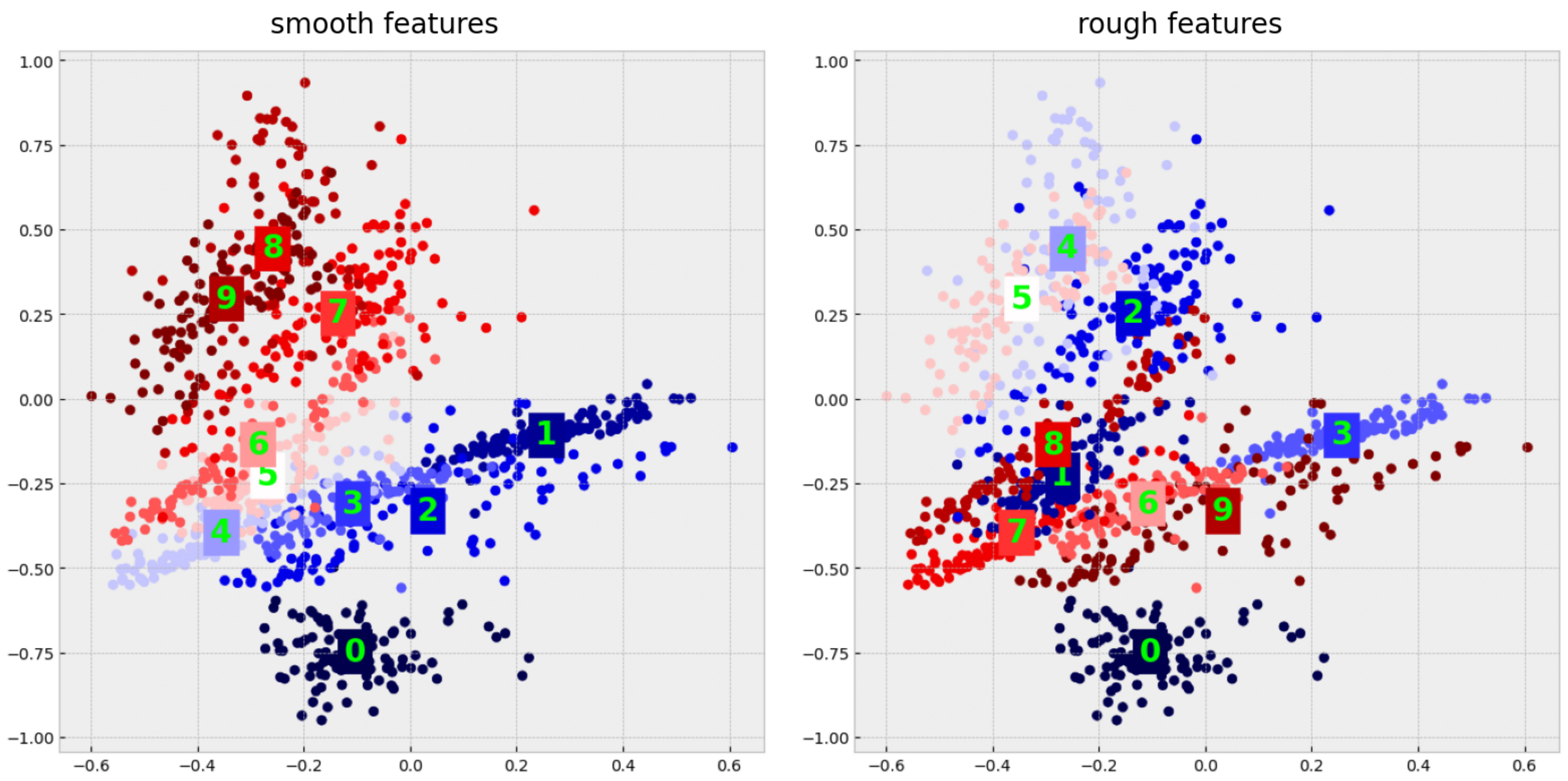

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