A probabilistic approach to ML

Bayesian approach: find y that maximizes $\mathbb{P}(Y = y | \text{data}, X = x)$

This problem of Bayesian inference is hard to solve without additional hypothesis.

A probabilistic approach to ML

Gaussian Processes

- Compute the most probable function that passes through the data points, given a priori information about how related two data points are (through a covariance kernel);
- Also provide a measure of prediction uncertainty in each point;
- Are computed offline and require an $N \times N$ matrix inversion for N data points in the training set (computationnally costly);
- Careful engineering of covariance kernels can help incorporate priori knowledge into Gaussian Processes;
- Are suitable both for regression and classification.

A probabilistic approach to ML

Note that Gaussian Processes are widely used in preliminary design phases, especially as surrogate models that replace physics computations.