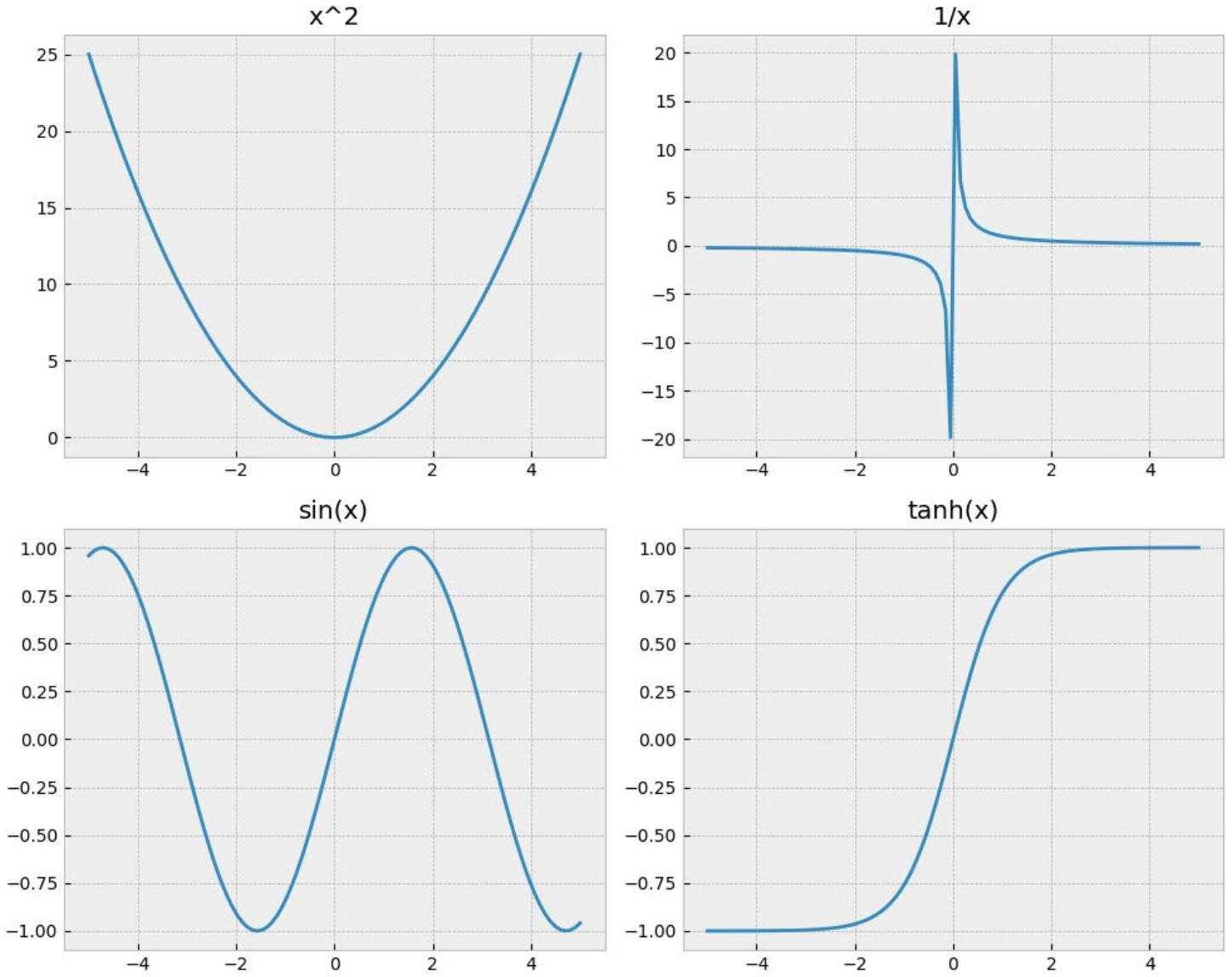
THE UNIVERSITY of TENNESSEE KNOXVILLE

Lecture 22: Gaussian Processes and Bayesian Optimization

Instructor: Sergei V. Kalinin

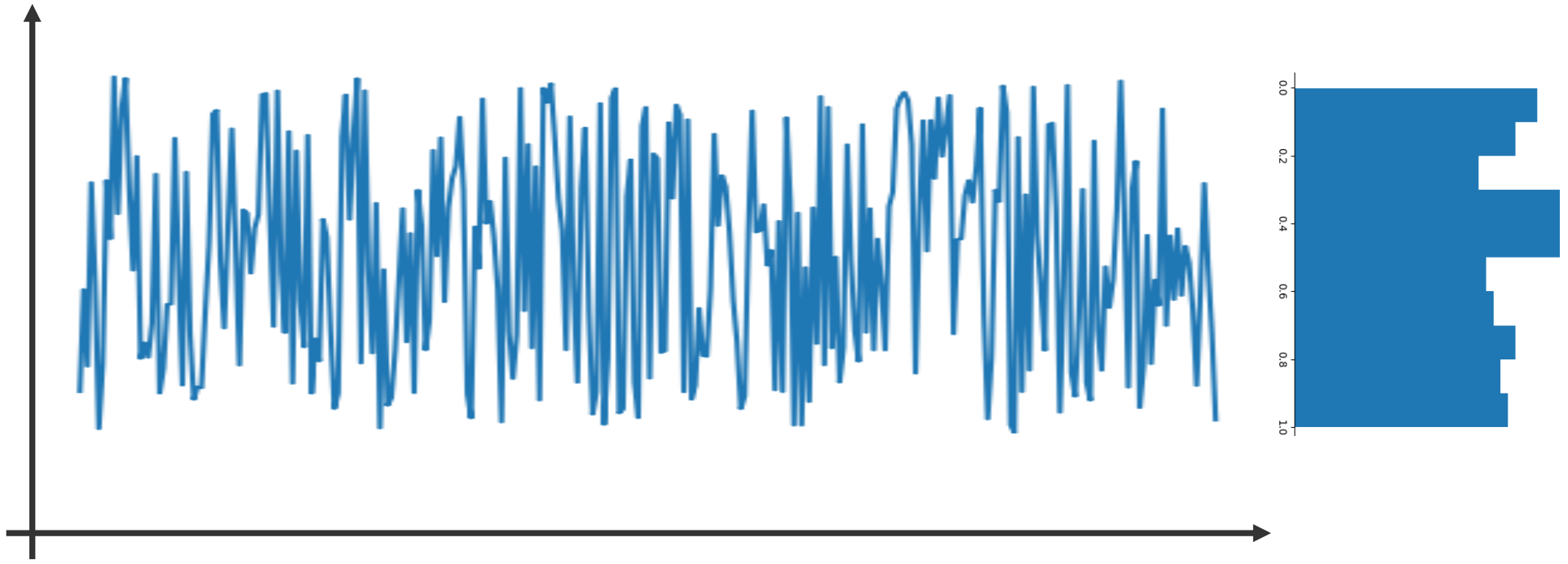
Functions are nice!



"*Well! I've often seen a cat without a grin,*' thought Alice *'but a grin without a cat! It's the most curious thing i ever saw in my life!*"

— Lewis Carroll, **Alice in Wonderland**

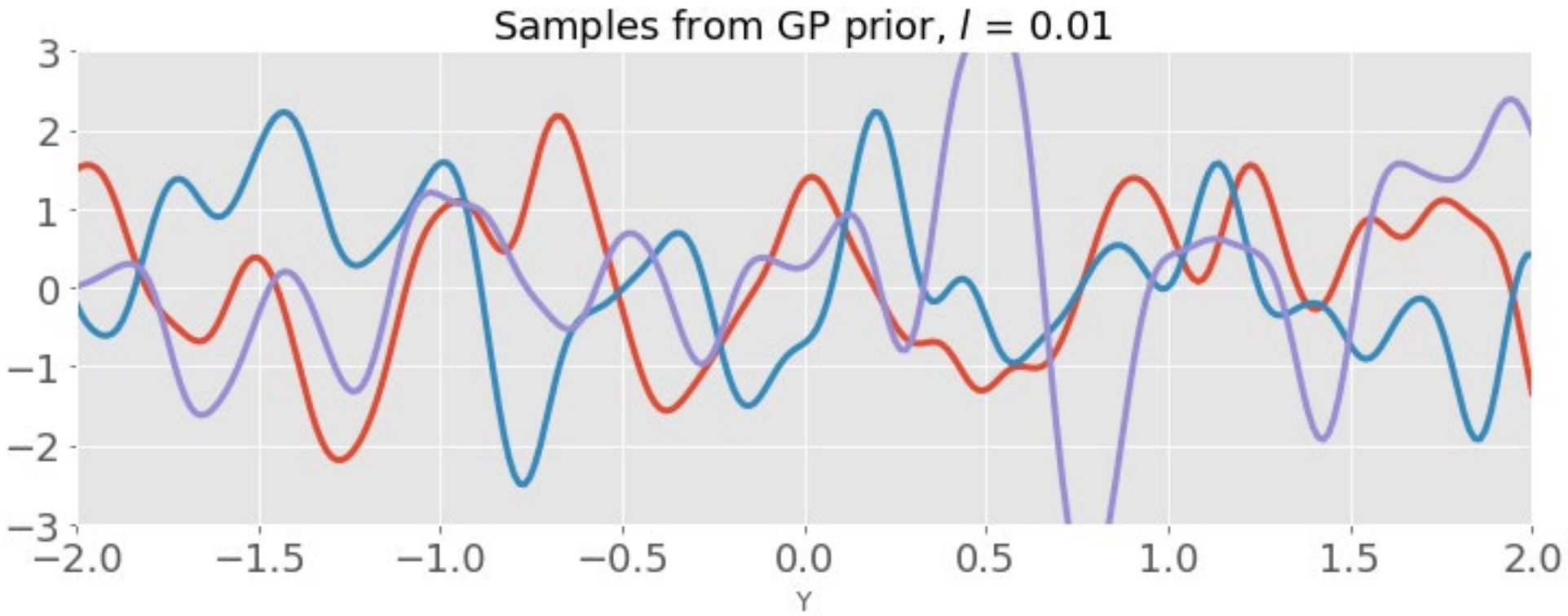
What do we know if we do not know anything?



Gaussian Process Regression

- Covariance matrix determines what type of functions we will allow.

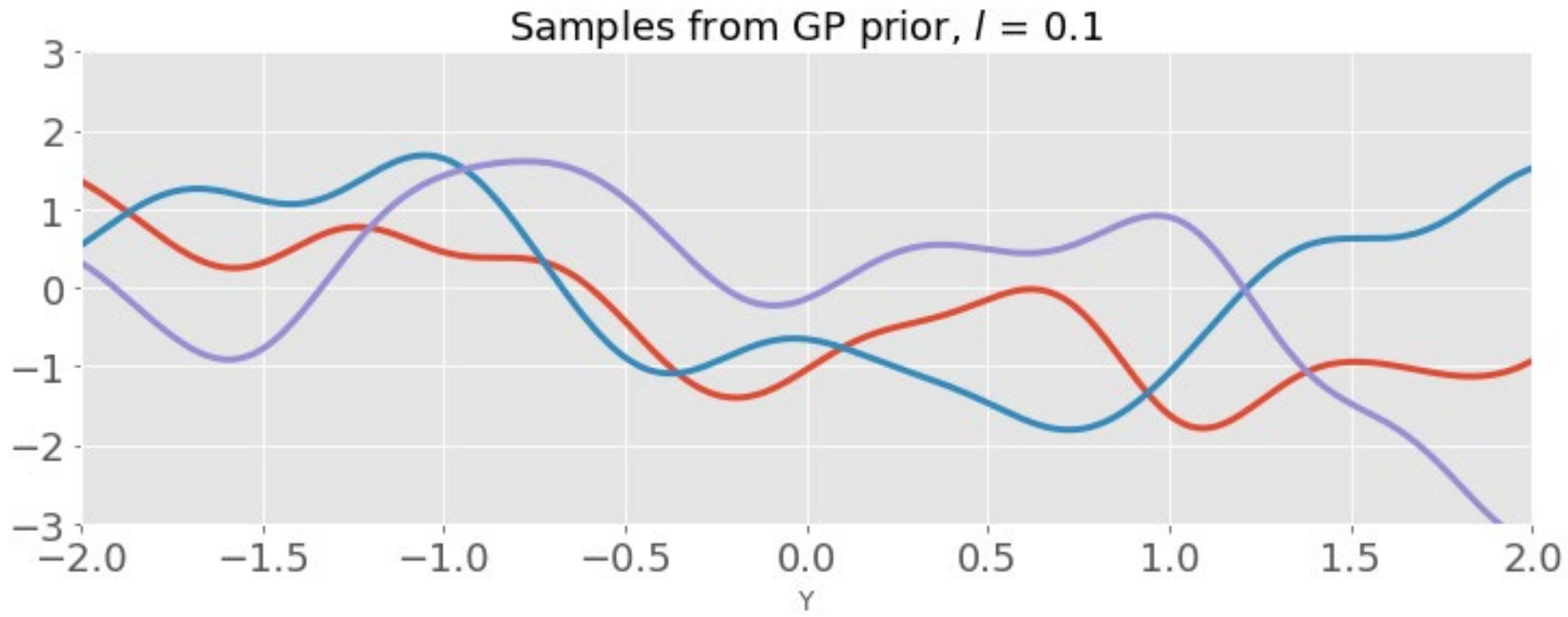
$$\mathrm{k}(\mathrm{x}, \mathrm{x}') = \exp\left(-\frac{1}{2l}(x - x')^2\right)$$



Gaussian Process Regression

- Covariance matrix determines what type of functions we will allow.

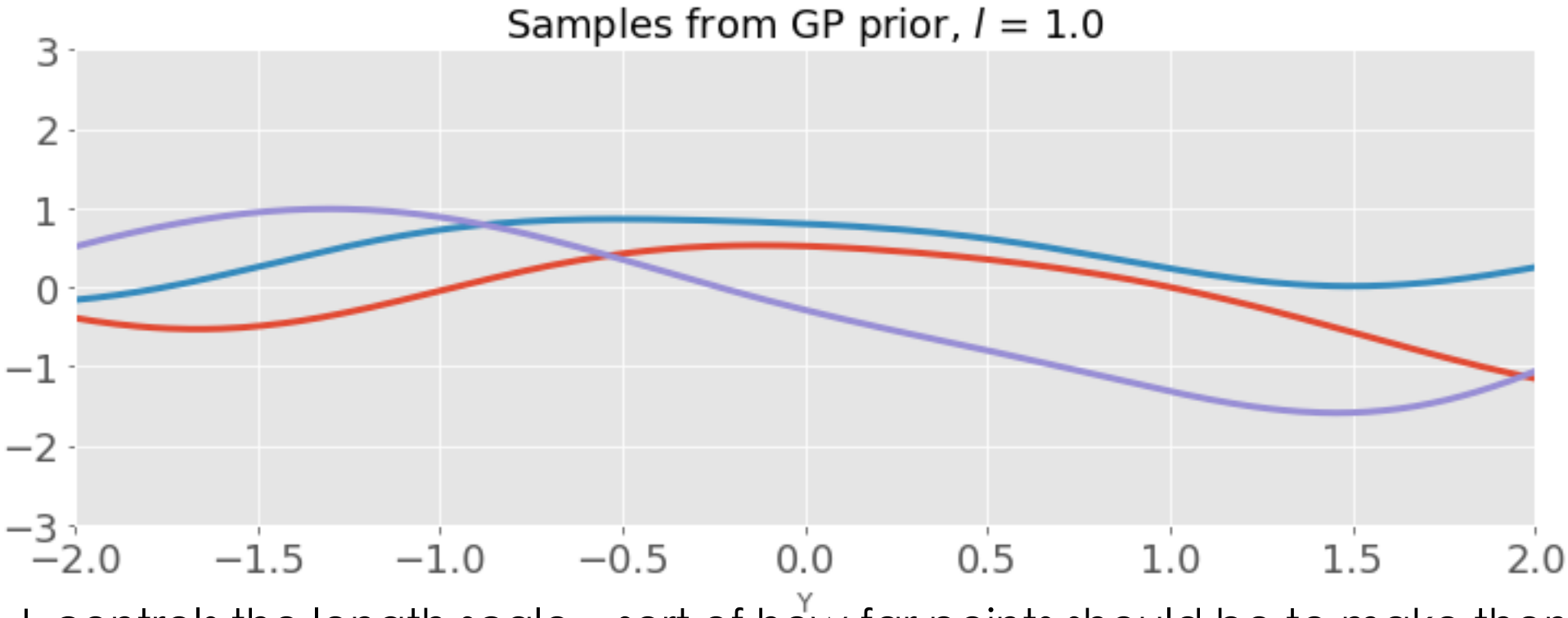
$$\mathrm{k}(\mathrm{x}, \mathrm{x}') = \exp\left(-\frac{1}{2l}(x - x')^2\right)$$



Gaussian Process Regression

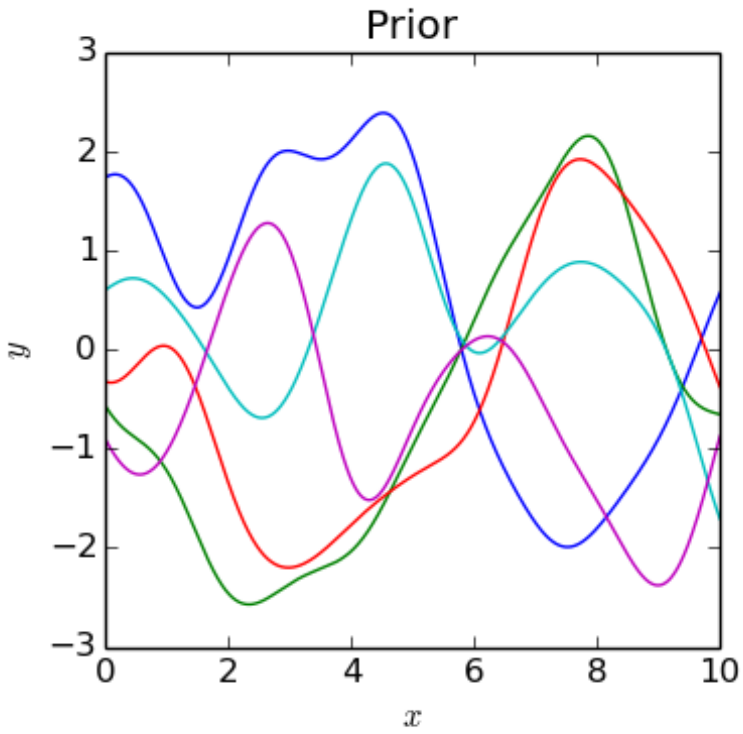
- Covariance matrix (kernel) determines what type of functions we will allow.

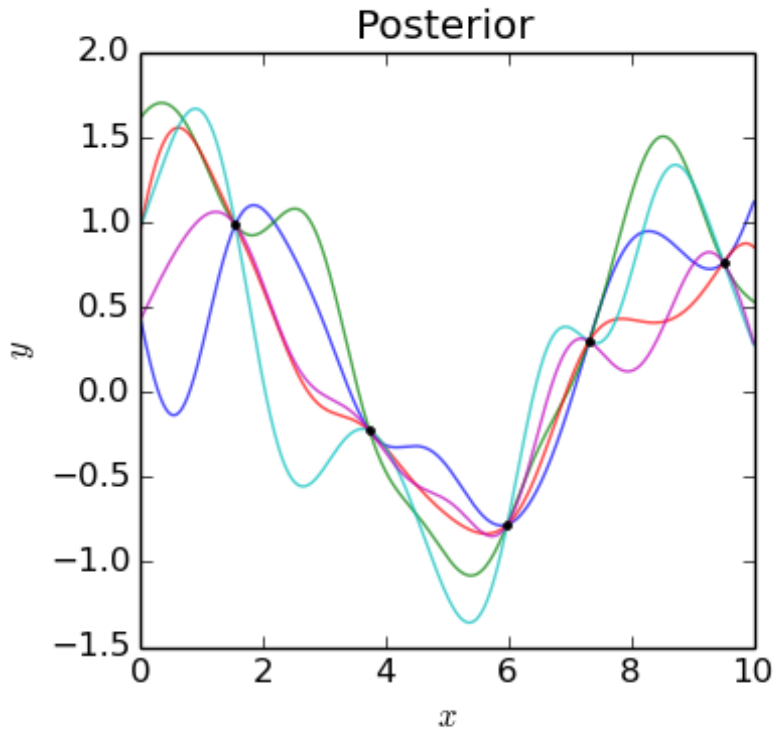
$$\mathrm{k}(\mathrm{x}, \mathrm{x}') = \exp\left(-\frac{1}{2l}(x - x')^2\right)$$

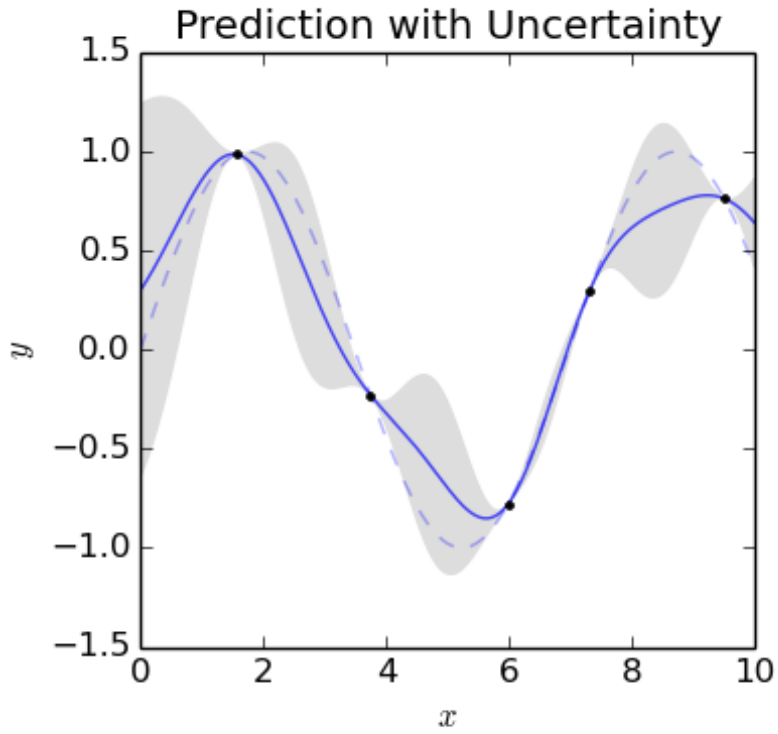


L controls the length scale – sort of how far points should be to make them independent of each other.

Gaussian Process Regression







Prior: What can the function be before the measurement
Data: Measurement
Posterior: What can the function be after measurement

Policy: How do we balance exploration and exploitation (acquisition function)

GP Vocabulary

- Gaussian Process
- Kernel and kernel parameters
- Kernel Priors
- Noise Priors
- Posteriors

Kernels in Molecular Spaces

Graph Kernels: Since chemical molecules can be represented as graphs with atoms as nodes and bonds as edges, graph kernels are a natural choice. Graph kernels measure the similarity between graphs and can be used in GPs to model molecular properties. Examples include the Random Walk Kernel, Weisfeiler-Lehman (WL) Kernel, and Graphlet Kernel.

Molecular Fingerprint Kernels: Molecular fingerprints are binary vectors representing the presence or absence of certain substructures within a molecule. Kernels can be defined on these fingerprints, such as the Tanimoto Kernel (also known as the Jaccard Index), which measures the similarity between two fingerprint vectors. This approach is particularly popular in cheminformatics for its interpretability and efficiency.

Spectral Kernels: Spectral methods can be used to define kernels on the spectrum (eigenvalues) of the Laplacian matrix of molecular graphs. These kernels can capture the topological and spectral properties of molecules, offering a powerful way to model molecular similarities.

Kernels in Molecular Spaces

Gaussian Molecular Kernels: This type of kernel measures the similarity between molecules based on Gaussian-shaped functions centered on atoms. The overlap between these Gaussian functions for different molecules can be used to compute a kernel value, incorporating both structural and spatial information.

Physicochemical Property Kernels: Kernels can be designed based on the physicochemical properties of molecules, such as hydrophobicity, charge distribution, or molecular weight. By defining a similarity measure based on the distance between these property vectors of different molecules, one can construct a kernel that reflects the similarities in physical and chemical properties.

Deep Learning-Based Kernels: With the rise of deep learning, kernels can also be derived from the embeddings or latent spaces generated by neural networks trained on molecular data. For instance, a neural network can be trained to generate molecular embeddings, and a kernel can be defined as the dot product or cosine similarity between these embeddings.

Colab