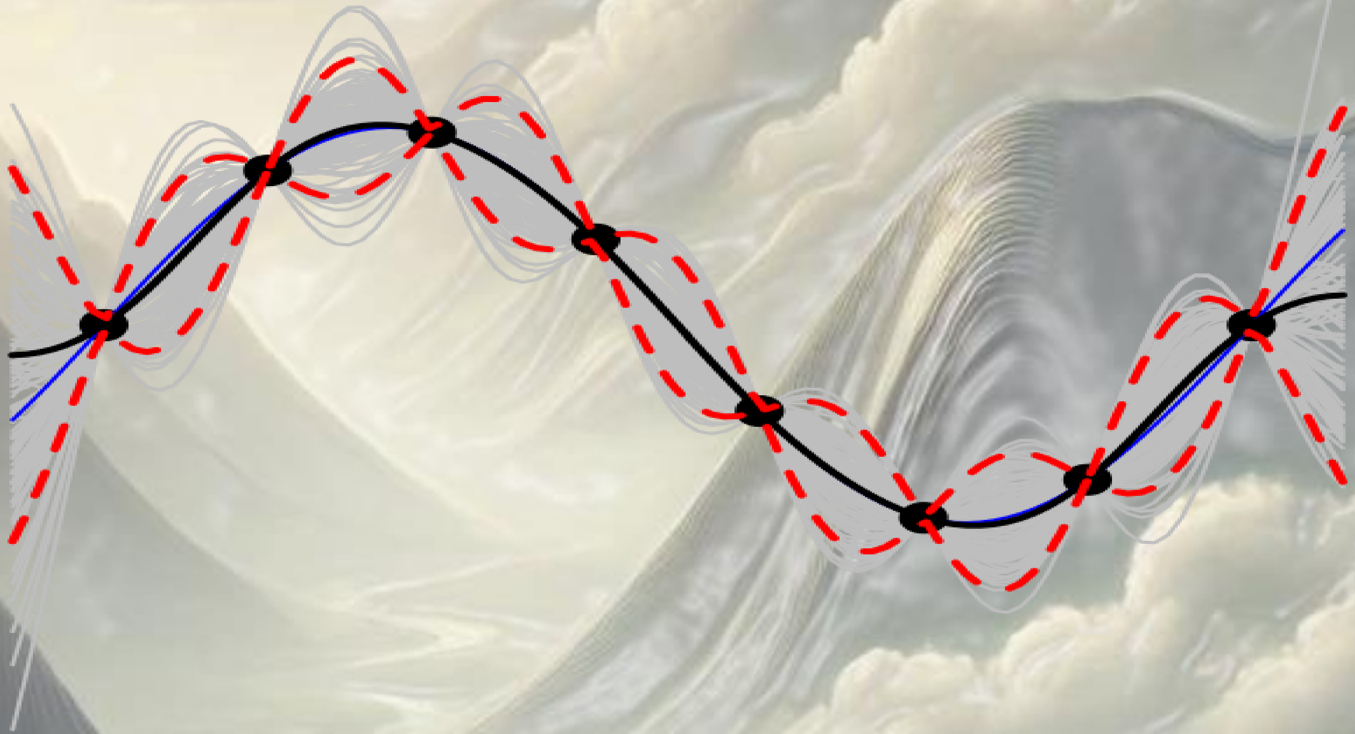
and why they may not be machine learning(?)

Gaussian Processes



Useful references:

Gaussian Processes for Machine Learning by Rasmussen and Williams @ www.GaussianProcess.org/gpml

What are Gaussian Processes?

A ***Gaussian process (GP)*** is a *probability distribution* over possible *functions*; any combination of these functions jointly Gaussian distributed

Key Points:

- GPs can be used as models for both regression and classification
- Since the model is a probability distribution (over a function space that is Gaussian distributed), we can calculate *means* AND *variances*
- The ***mean function*** is calculated from the posterior (recall Baye's) distribution of possible functions → regression predictions
- The ***variances*** provide native uncertainty measures on these predictions, which are typically absent in other ML models (e.g., ANNs)
- The model, as a posterior, can be updated based on new observations

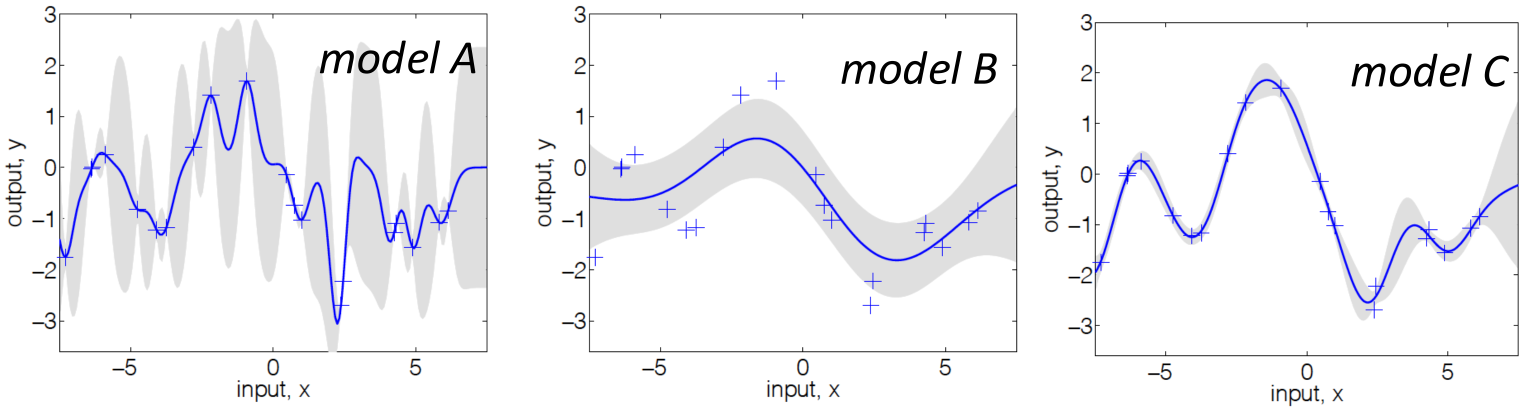
In "math" speak:

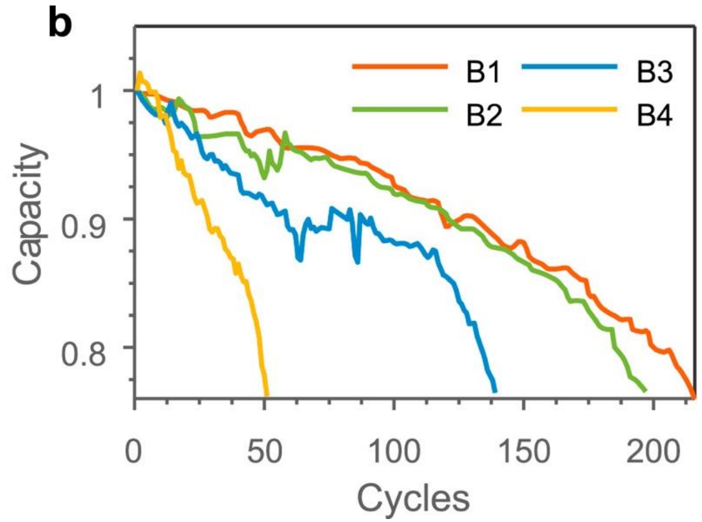
$$\boldsymbol{f}(\boldsymbol{x}) \sim \mathcal{N}(\boldsymbol{\mu}(\boldsymbol{x}), \boldsymbol{K}(\boldsymbol{x}, \boldsymbol{x}'))$$

covariance/Kernel function that dictates model "smoothness"

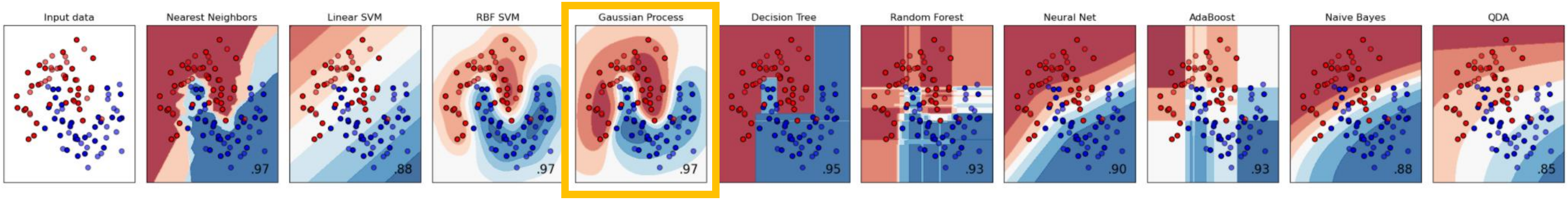
Why should we use them?

- Our observations may be "***noisy***," and it is important to capture that behavior
- They allow you to incorporate ***prior knowledge***
- They provide a reasonable framework to ***regulate model complexity*** and more reliably ***indicate model uncertainty***





Richardson et al. *J. Power Sources* **(2017)**

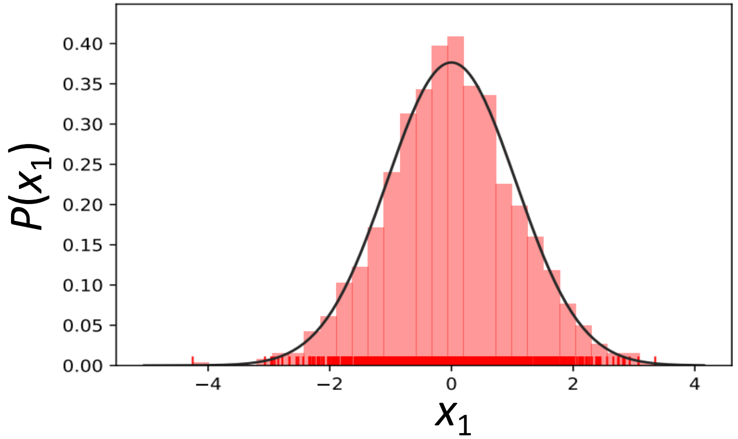


Some basic intuition underlying Gaussian Processes

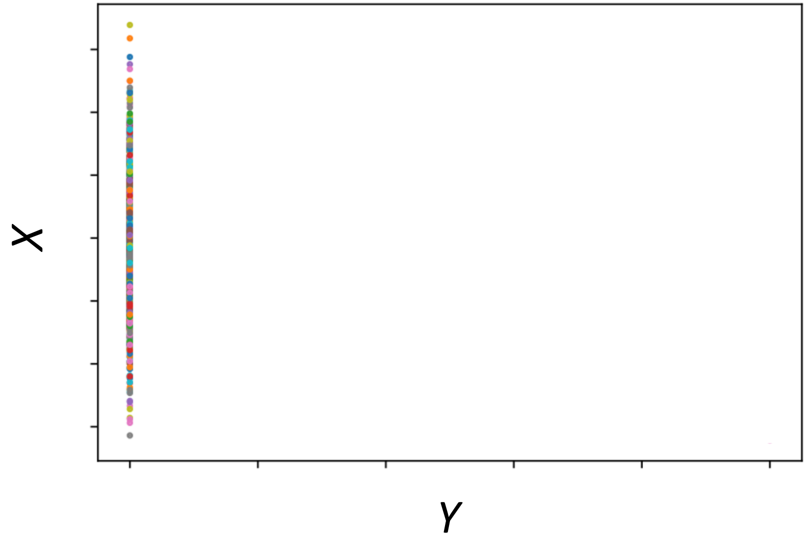
Suppose we have a random variable X_1 with distribution

$$P_{X_1}(x_1) \sim \mathcal{N}(\mu, \sigma^2)$$

We can generate samples from this distribution



and then project them onto a new axis



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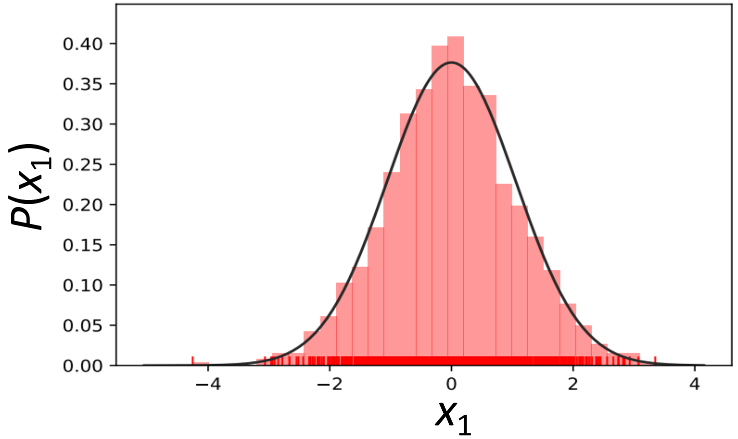

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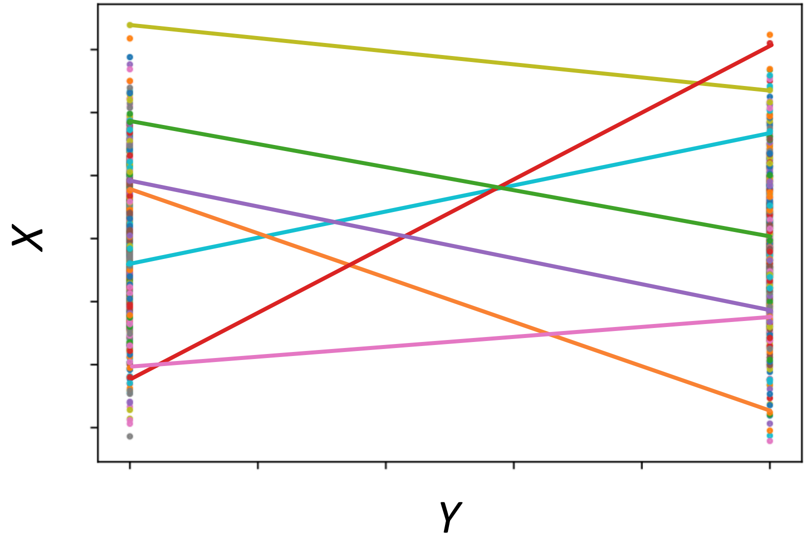

We can do this for another set of samples to obtain two independent Gaussian vectors

Then by connecting random points between the two vectors, we would get a set of linear functions

Some basic intuition underlying Gaussian Processes

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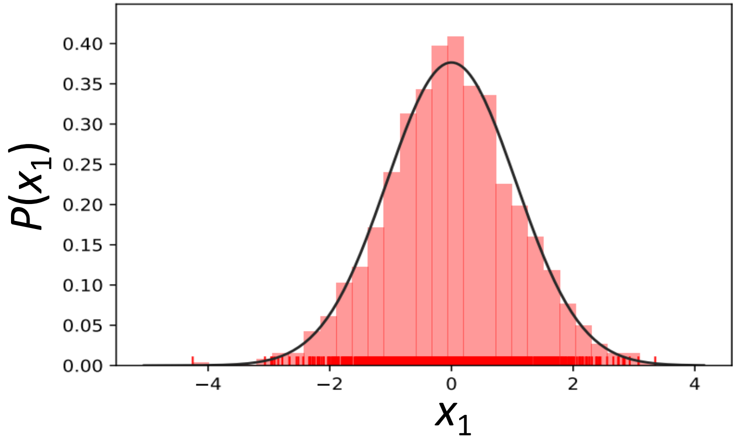

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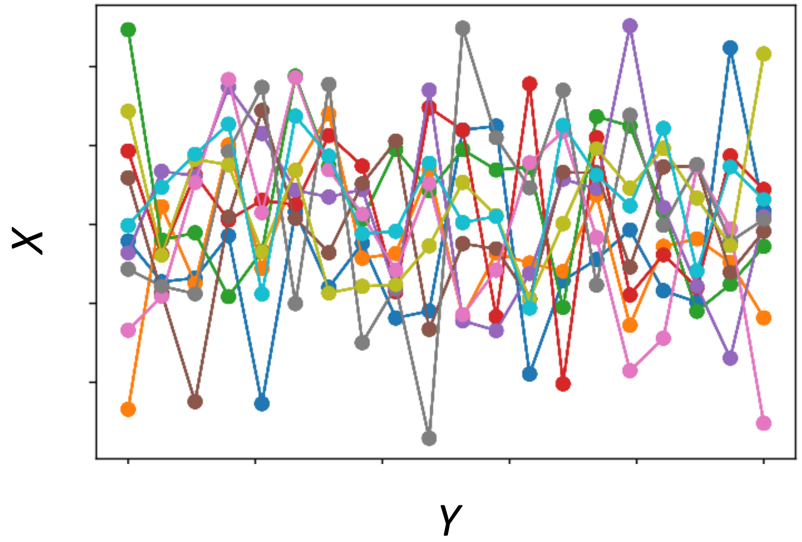

using more and more Gaussian vectors, we could represent more complex functions (showing only ten), but the resulting functions are inherently noisy!

Why?

Some basic intuition underlying Gaussian Processes

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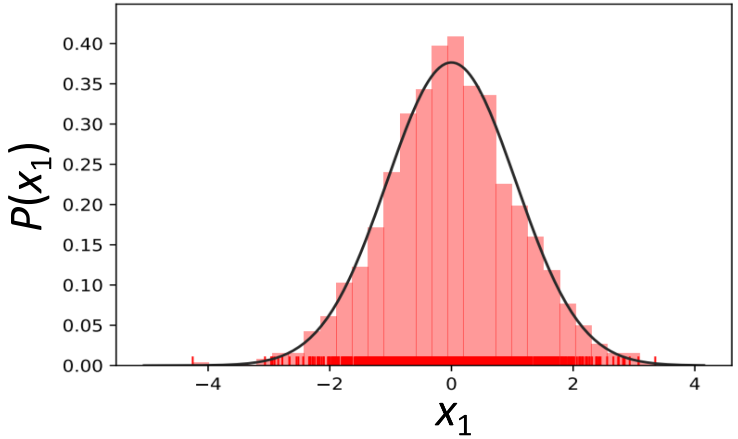

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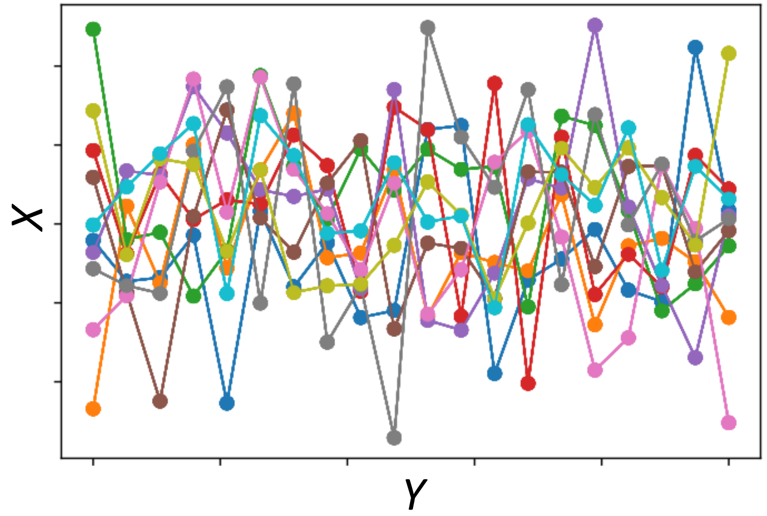
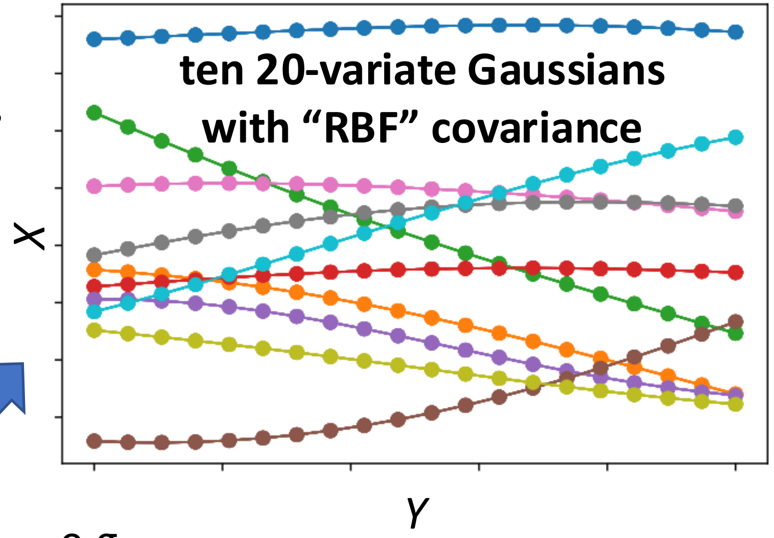


using more and more Gaussian vectors, we could represent more complex functions (showing only ten), but the resulting functions are inherently noisy!

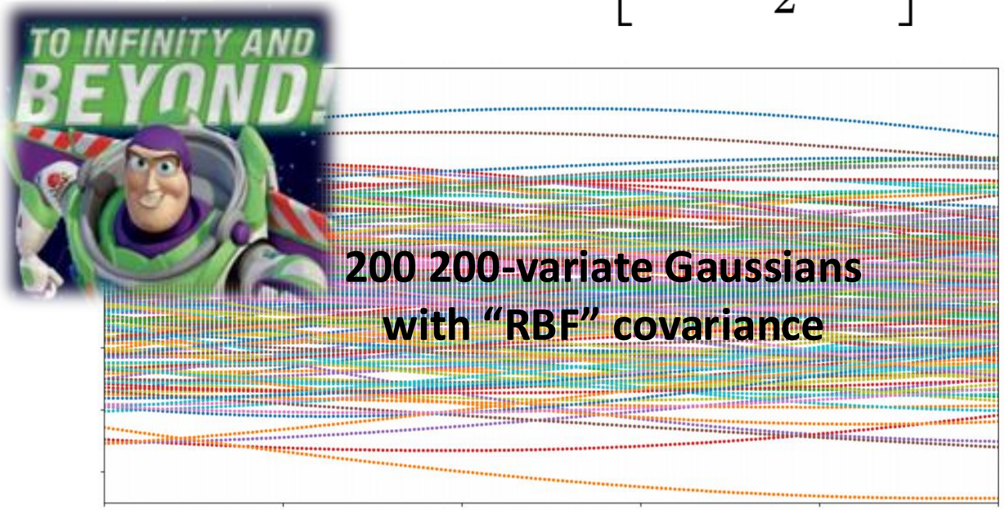
...because the Gaussian vectors are *independent*

using multivariate Gaussians with true covariance enables more smoothly varying functions

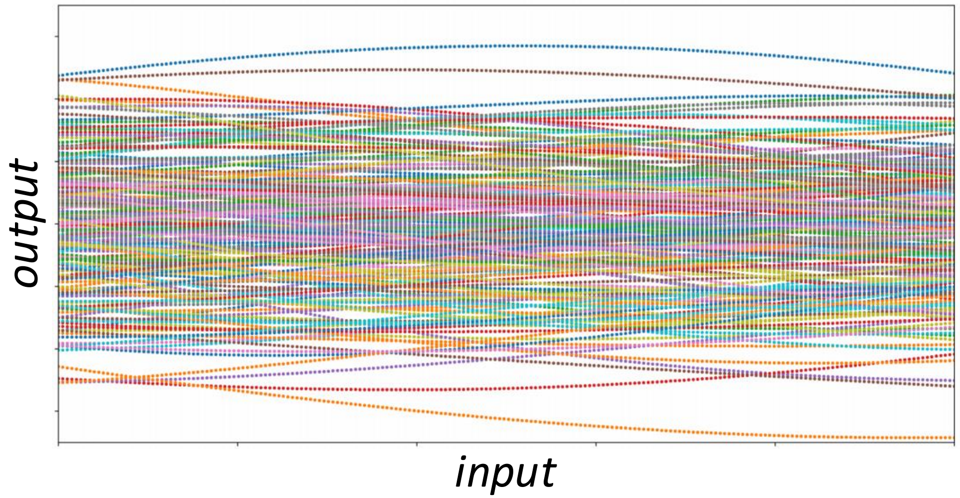


e.g.,

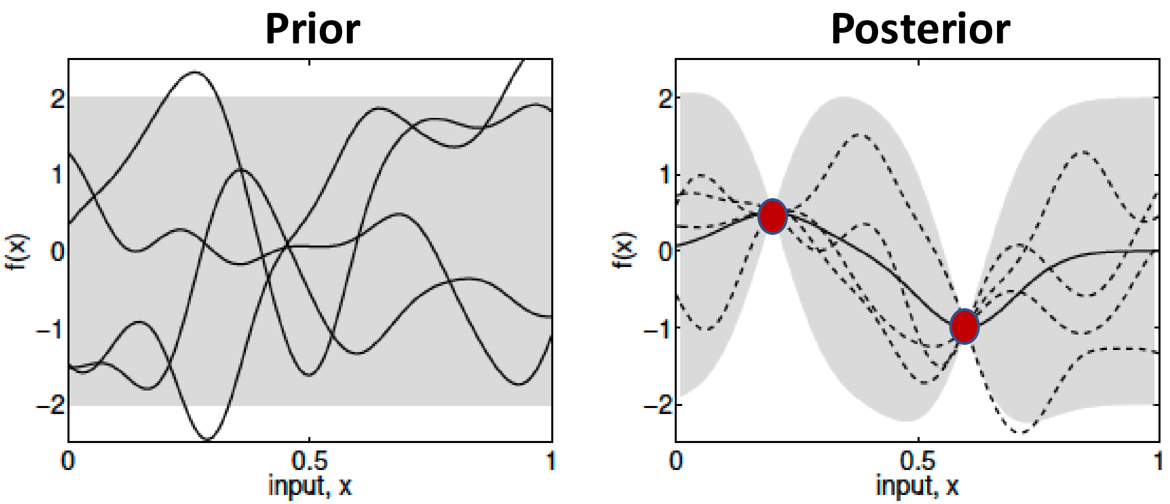
$$K(x_i, x_j) = \exp\left[-\frac{(x_i - x_j)^2}{2}\right]$$



Some basic intuition underlying Gaussian Processes



- If the dimensionality of the ***multivariate Gaussians*** (MVG) becomes infinite → a continuous function
- With an infinite number of such functions, we could make predictions at any point
- Functions as MVGs is our initial assumption (***prior***)
- The functions shown provide expected outputs as a function of inputs *without having observed any data*



- As data is collected, we can downselect from infinite functions to only the functions that describe the data/observations → ***posterior*** (kind of like wavefunctions in quantum mechanics, if that helps)
- As we add more data, the current posterior can be used as the prior to obtain a new posterior

Theoretical Development of GPs for Regression

A ***Gaussian process (GP)*** is a *probability distribution* over possible *functions*; any combination of these functions jointly Gaussian distributed

$$f(\boldsymbol{x}) \sim \mathcal{GP}(\mu(\boldsymbol{x}), k(\boldsymbol{x}, \boldsymbol{x}'))$$

this is a stochastic function, i.e., a collection of random variables

$$\mu(\boldsymbol{x}) = \mathbb{E}\left[f(\boldsymbol{x})\right]$$

its distribution is characterized by its mean and covariance function

$$k(\boldsymbol{x}, \boldsymbol{x}') = \mathrm{Cov}\left[f(\boldsymbol{x}), f(\boldsymbol{x}')\right] = \mathbb{E}\left[(f(\boldsymbol{x}) - \mu(\boldsymbol{x}))(f(\boldsymbol{x}') - \mu(\boldsymbol{x}'))\right]$$

A simple example $f(\boldsymbol{x}) = \phi(\boldsymbol{x})^T \boldsymbol{w}$

weighting coefficients BUT $\boldsymbol{w} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_p)$

some vector field, e.g., $\phi(\boldsymbol{x})^T = (\sum_i x_i, \sum_i x_i^2, \ldots, \sum_i x_i^m)$

for such a process, it is easy to show that $\mu(\boldsymbol{x}) = 0;\; k(\boldsymbol{x}, \boldsymbol{x}') = \phi(\boldsymbol{x})^T \boldsymbol{\Sigma}_p \phi(\boldsymbol{x}')$

that is just to say that f(x) and f(x’) are indeed jointly Gaussian with the above mean and covariance → any number of input points will be jointly Gaussian

Theoretical Development of GPs for Regression

Let's suppose we have a dataset now $\mathcal{D} := \{(\boldsymbol{x}_i, f_i = f(\boldsymbol{x}_i)) \text{ for } i = 1, \ldots, n\}$

$\boldsymbol{f}, \boldsymbol{x}$ **training** $\boldsymbol{f}_*, \boldsymbol{x}_*$ **test**

These two sets should be jointly distributed according to our Gaussian prior as

$$\begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{f}_* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} k(\boldsymbol{x}, \boldsymbol{x}) & k(\boldsymbol{x}, \boldsymbol{x}_*) \\ k(\boldsymbol{x}_*, \boldsymbol{x}) & k(\boldsymbol{x}_*, \boldsymbol{x}_*) \end{bmatrix}\right)$$

prior distribution

Now, to get the posterior distribution, we must restrict our prior distribution to only the set of functions that "agree" with our observations/training data (i.e., we should make our prior distribution conditional on our observations)

Theoretical Development of GPs for Regression

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prior distribution

from math review

$$p(\boldsymbol{x}, \boldsymbol{y}) = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_x \\ \boldsymbol{\mu}_y \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{xx} & \boldsymbol{\Sigma}_{xy} \\ \boldsymbol{\Sigma}_{yx} & \boldsymbol{\Sigma}_{yy} \end{bmatrix}\right)$$

$$p(\boldsymbol{x} \mid \boldsymbol{y}) = \mathcal{N}(\boldsymbol{\mu}_{x \mid y}, \boldsymbol{\Sigma}_{x \mid y})$$

$$\boldsymbol{\mu}_{x \mid y} = \boldsymbol{\mu}_x + \boldsymbol{\Sigma}_{xy} \boldsymbol{\Sigma}_{yy}^{-1} (\boldsymbol{y} - \boldsymbol{\mu}_y)$$

$$\boldsymbol{\Sigma}_{x \mid y} = \boldsymbol{\Sigma}_{xx} - \boldsymbol{\Sigma}_{xy} \boldsymbol{\Sigma}_{yy}^{-1} \boldsymbol{\Sigma}_{yx}$$

$$\boldsymbol{f}_* \mid \boldsymbol{f}, \boldsymbol{x}, \boldsymbol{x}_* \sim \mathcal{N}\big(k(\boldsymbol{x}_*, \boldsymbol{x}) k(\boldsymbol{x}, \boldsymbol{x})^{-1} \boldsymbol{f}, \; k(\boldsymbol{x}_*, \boldsymbol{x}_*) - k(\boldsymbol{x}_*, \boldsymbol{x}) k(\boldsymbol{x}, \boldsymbol{x})^{-1} k(\boldsymbol{x}, \boldsymbol{x}_*)\big)$$

easy to just sample function values from the posterior by computing the mean and covariance in the above!

Theoretical Development of GPs for Regression

Let's suppose we have a dataset now $\mathcal{D} := \{(\boldsymbol{x}_i, f_i = f(\boldsymbol{x}_i)) \text{ for } i = 1, \dots, n\}$

$$\boldsymbol{f}, \boldsymbol{x} \qquad\qquad \boldsymbol{f}_*, \boldsymbol{x}_*$$

training ***test***

In the prior example, our observations were treated as Noise-free; otherwise…

$$y = f(\boldsymbol{x}) + \varepsilon \qquad \varepsilon \sim \mathcal{N}(0, \sigma_n^2) \qquad \operatorname{cov}(\boldsymbol{y}, \boldsymbol{y}) = k(\boldsymbol{x}, \boldsymbol{x}) + \sigma_n^2 \boldsymbol{I}$$

This would slightly modify our joint distribution as

$$\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{f}_* \end{bmatrix} \sim \mathcal{N}\left(\boldsymbol{0}, \begin{bmatrix} k(\boldsymbol{x}, \boldsymbol{x}) + \sigma_n^2 \boldsymbol{I} & k(\boldsymbol{x}, \boldsymbol{x}_*) \\ k(\boldsymbol{x}_*, \boldsymbol{x}) & k(\boldsymbol{x}_*, \boldsymbol{x}_*) \end{bmatrix}\right)$$

Then, the posterior is obtained by again conditioning on our observations

these are governing equations

$$\boldsymbol{f}_* | \boldsymbol{y}, \boldsymbol{x}, \boldsymbol{x}_* \sim \mathcal{N}(\bar{\boldsymbol{f}}_*, \operatorname{cov}(\boldsymbol{f}_*, \boldsymbol{f}_*))$$

$$\bar{\boldsymbol{f}}_* := \mathbb{E}\left[\boldsymbol{f}_* | \boldsymbol{y}, \boldsymbol{x}, \boldsymbol{x}_*\right] = k(\boldsymbol{x}_*, \boldsymbol{x}) \left[k(\boldsymbol{x}, \boldsymbol{x}) + \sigma_n^2 \boldsymbol{I}\right]^{-1} \boldsymbol{y}$$

$$\mathbb{V}\left[\boldsymbol{f}_*\right] = \operatorname{cov}(\boldsymbol{f}_*, \boldsymbol{f}_*) = k(\boldsymbol{x}_*, \boldsymbol{x}_*) - k(\boldsymbol{x}_*, \boldsymbol{x}) \left[k(\boldsymbol{x}, \boldsymbol{x}) + \sigma_n^2 \boldsymbol{I}\right]^{-1} k(\boldsymbol{x}, \boldsymbol{x}_*)$$

Log Marginal Likelihood

"marginal likelihood" or "evidence"

$$p(\boldsymbol{y}|\boldsymbol{x}) = \int p(\boldsymbol{y}|\boldsymbol{f},\boldsymbol{x})p(\boldsymbol{f}|\boldsymbol{x})d\boldsymbol{f}$$

→ *how likely would we observe the data that we have given the data originates from **f**(**x**)*

Assuming a Gaussian process, we can show that

$$\log p(\boldsymbol{y}|\boldsymbol{x}) = -\frac{1}{2}\boldsymbol{y}^T(\boldsymbol{K}+\sigma_n^2\boldsymbol{I})^{-1}\boldsymbol{y} - \frac{1}{2}\log|\boldsymbol{K}+\sigma_n^2\boldsymbol{I}| - \frac{n}{2}\log 2\pi$$

"log marginal likelihood""

- All the terms necessary to evaluate this are also used to obtain the mean function
- Useful metric for evaluating different models
- Hyperparameter optimization based on minimizing log likelihood

Basic Algorithm Outline

1. Define data/models: $\boldsymbol{x}, \boldsymbol{y}, k, \sigma_n^2, \boldsymbol{x}_*$

2. Perform Cholesky decomposition $\boldsymbol{L} := \text{cholesky}(k(\boldsymbol{x}, \boldsymbol{x}) + \sigma_n^2 \boldsymbol{I})$

3. Compute predictive mean function $\boldsymbol{\alpha} := \boldsymbol{L}^T \backslash (\boldsymbol{L} \backslash \boldsymbol{y})$

$$\bar{f}_* := k(\boldsymbol{x}, \boldsymbol{x}_*)^T \boldsymbol{\alpha}$$

4. Compute predictive variance

$$\boldsymbol{v} := \boldsymbol{L} \backslash k(\boldsymbol{x}, \boldsymbol{x}_*)$$

$$\mathbb{V}[f_*] = k(\boldsymbol{x}_*, \boldsymbol{x}_*) - \boldsymbol{v}^T \boldsymbol{v}$$

5. Compute log marginal likelihood

$$\log p(\boldsymbol{y}|\boldsymbol{x}) = -\frac{1}{2} \boldsymbol{y}^T \boldsymbol{\alpha} - \sum_i \log L_{ii} - \frac{n}{2} \log 2\pi$$

6. Return mean, variance, log marginal likelihood

Basic Algorithm Outline

1. Define data/models: $\boldsymbol{x}, \boldsymbol{y}, k, \sigma_n^2, \boldsymbol{x}_*$

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Go to Jupyter Notebook

5. Compute log marginal likelihood

$$\log p(\boldsymbol{y}|\boldsymbol{x}) = -\frac{1}{2}\boldsymbol{y}^T\boldsymbol{\alpha} - \sum_i \log L_{ii} - \frac{n}{2}\log 2\pi$$

6. Return mean, variance, log marginal likelihood

Gaussian Distribution

Gaussian distribution is the most well-studied distribution in science, engineering, and ML

- *ubiquity (often stemming from* ***central limit theorem****)*
- *computationally convenient*

<u>univariate</u>

$$p(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

<u>multivariate</u>

$$p(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{m/2}} |\boldsymbol{\Sigma}|^{-1/2} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T \boldsymbol{\sigma}^{-1} (\boldsymbol{x}-\boldsymbol{\mu})\right)$$

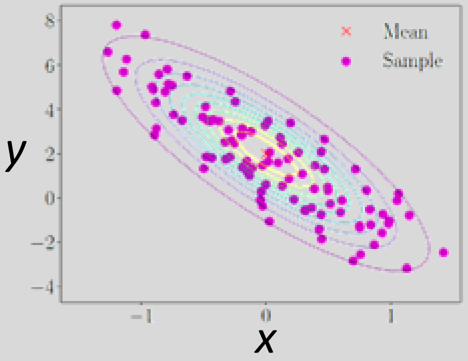
$$p(\boldsymbol{x}) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$$ for short

standard normal distribution → ***0*** mean and $\boldsymbol{I}_n$ as the covariance matrix

<u>**Basic tenant of Gaussian distributions**</u>**:** *doing things with Gaussians results in Gaussians*

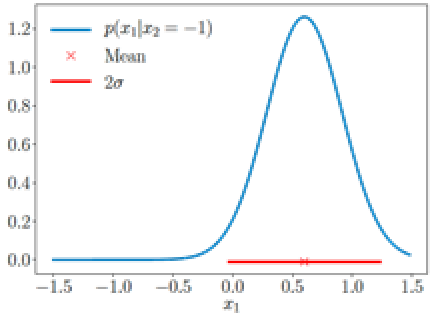
Gaussian Distribution

Consider the joint distribution over *X* and *Y*:



$$p(\boldsymbol{x}, \boldsymbol{y}) = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_x \\ \boldsymbol{\mu}_y \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{xx} & \boldsymbol{\Sigma}_{xy} \\ \boldsymbol{\Sigma}_{yx} & \boldsymbol{\Sigma}_{yy} \end{bmatrix} \right)$$

- *Conditionals of Gaussians are Gaussians*



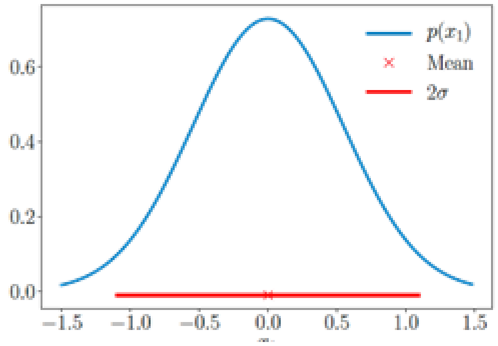
$$p(\boldsymbol{x} \,|\, \boldsymbol{y}) = \mathcal{N}\left(\boldsymbol{\mu}_{x\,|\,y}, \, \boldsymbol{\Sigma}_{x\,|\,y}\right)$$

$$\boldsymbol{\mu}_{x\,|\,y} = \boldsymbol{\mu}_x + \boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yy}^{-1}(\boldsymbol{y} - \boldsymbol{\mu}_y)$$

$$\boldsymbol{\Sigma}_{x\,|\,y} = \boldsymbol{\Sigma}_{xx} - \boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yy}^{-1}\boldsymbol{\Sigma}_{yx}$$

- *Marginals over Gaussians are Gaussians*

$$p(\boldsymbol{x}) = \int p(\boldsymbol{x}, \boldsymbol{y})\mathrm{d}\boldsymbol{y} = \mathcal{N}\left(\boldsymbol{x} \,|\, \boldsymbol{\mu}_x, \, \boldsymbol{\Sigma}_{xx}\right)$$



- *The product of Gaussians is Gaussian*

$$\mathcal{N}(\boldsymbol{x}|\boldsymbol{a}, \boldsymbol{A})\mathcal{N}(\boldsymbol{x}|\boldsymbol{b}, \boldsymbol{B}) \rightarrow c\mathcal{N}(\boldsymbol{x}|\boldsymbol{c}, \boldsymbol{C})$$

$$\boldsymbol{C} = (\boldsymbol{A}^{-1} + \boldsymbol{B}^{-1})^{-1}$$

$$\boldsymbol{c} = \boldsymbol{C}(\boldsymbol{A}^{-1}\boldsymbol{a} + \boldsymbol{B}^{-1}\boldsymbol{b}) \quad c = \mathcal{N}(\boldsymbol{a}|\boldsymbol{b}, \boldsymbol{A} + \boldsymbol{B})$$

- *The sum over independent Gaussian variables is… Gaussian*

$$p(\boldsymbol{x}, \boldsymbol{y}) = p(\boldsymbol{x})p(\boldsymbol{y})$$

$$p(\boldsymbol{x} + \boldsymbol{y}) = \mathcal{N}(\boldsymbol{\mu}_x + \boldsymbol{\mu}_y, \boldsymbol{\Sigma}_x + \boldsymbol{\Sigma}_y)$$

- *Any linear transformation of Gaussians is Gaussian* $p(a\boldsymbol{x} + b\boldsymbol{y}) = \mathcal{N}\left(a\boldsymbol{\mu}_x + b\boldsymbol{\mu}_y, \, a^2\boldsymbol{\Sigma}_x + b^2\boldsymbol{\Sigma}_y\right)$