RMDS - Workshop 4

Gaussian Process Regression

Gaussian Process Regression

What is it?

- A Bayesian nonparametric regression technique
- A method of interpolation where the interpolated values are modeled via a Gaussian process

Gaussian Process Regression (Pros and Cons)

Advantages

- Predictions interpolate our observations
- Predictions come with quantification of uncertainty
- Flexible (Various kernels can be specified) ### Disadvantages
- Not sparse (need entire dataset to produce predictions)
- Lose efficiency in high dimensional spaces

Gaussian Process Regression (History)

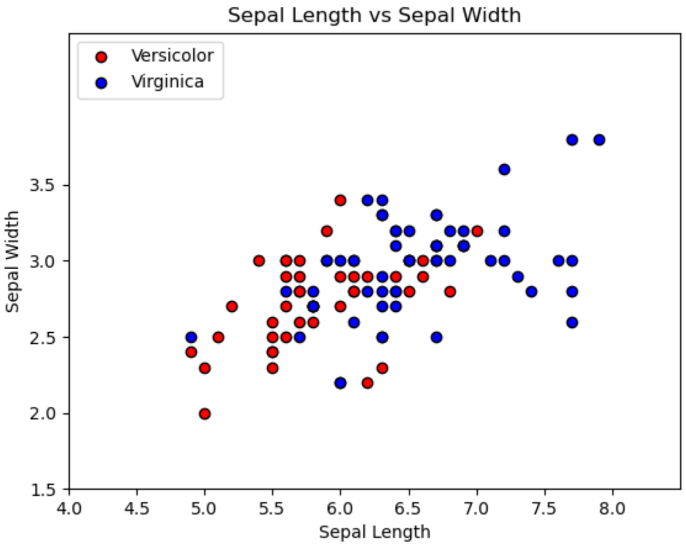
- Herman Wold (1938)
- Andrey Kolmogorov (1941)
- Norbert Wiener (1942)
- Danie Krige (1950s)
- Georges Matheron (1960s)
- Carl Rasmussen & Christopher Williams (1996-present)

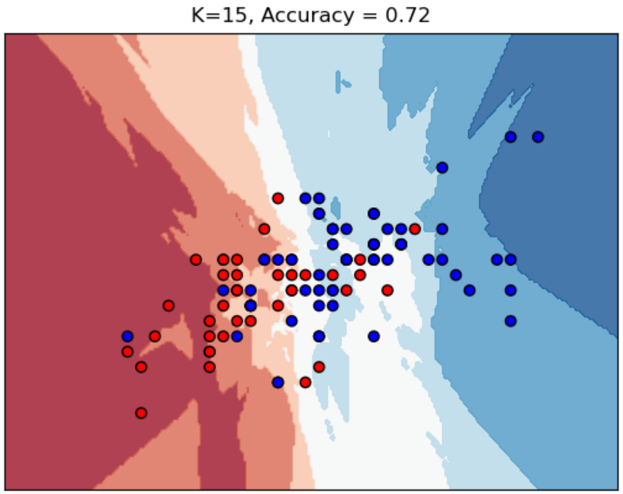
Gaussian Process Regression (A method by many names)

- Wiener-Kolmogorov Prediction
- Kriging
- Gaussian Process Regression

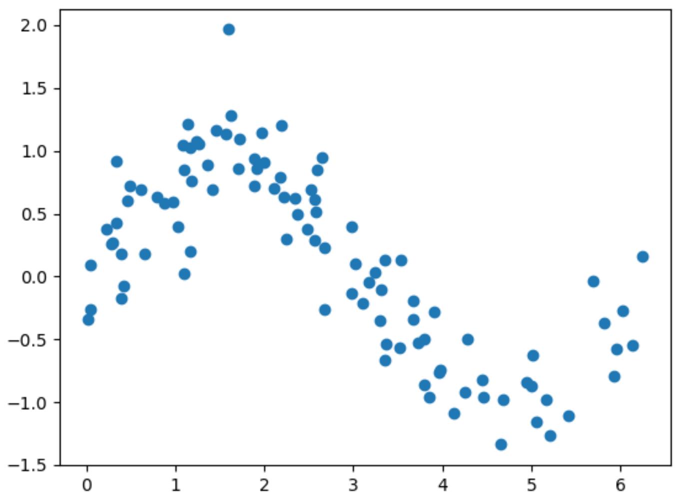
KNN Classification

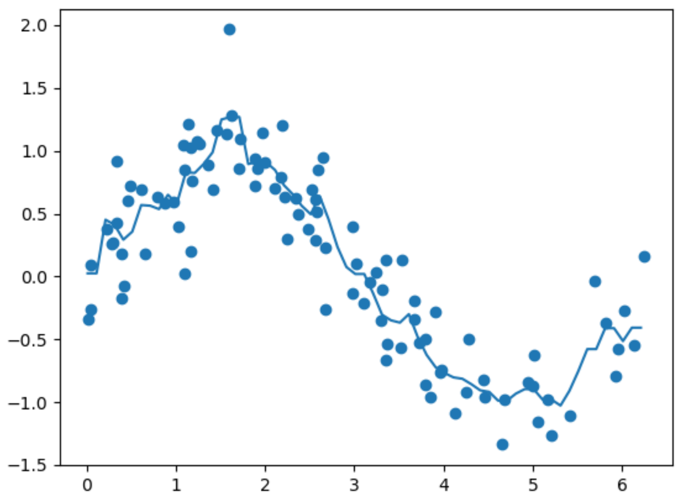
From Workshop 2:



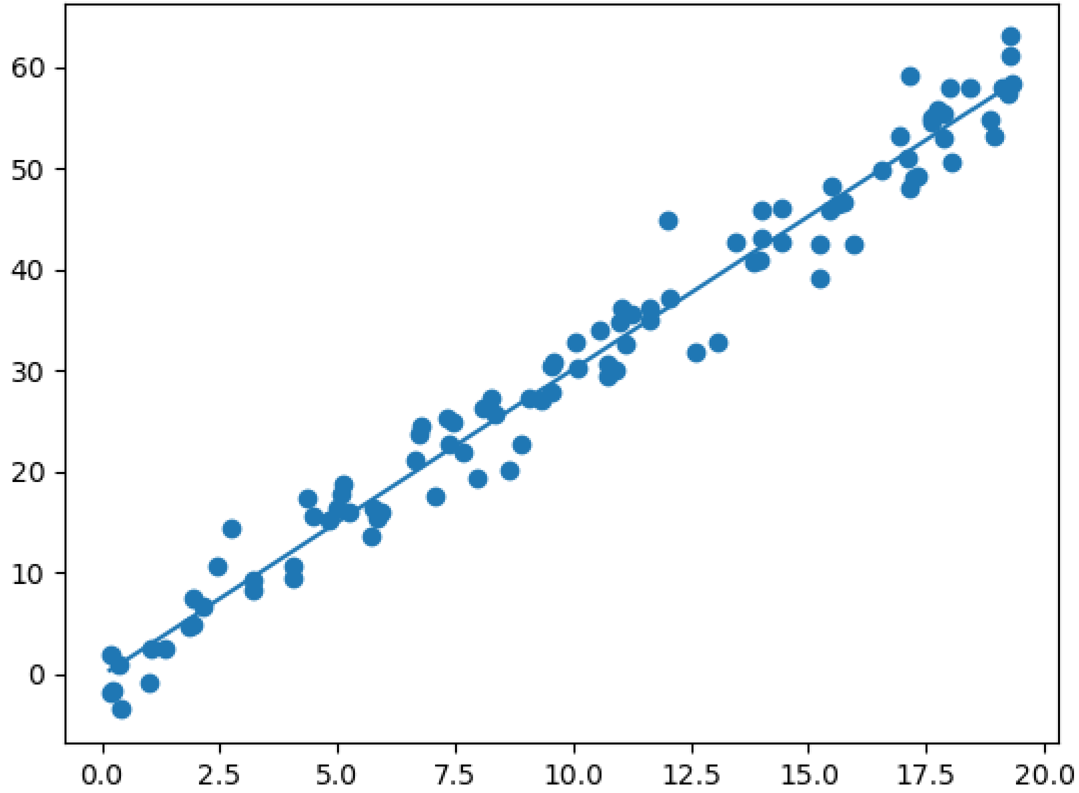


KNN Regression





Ordinary Linear Regression



$$y = \theta^T X + \epsilon \quad \epsilon \sim N(0, \sigma)$$

Solve via maximum likelihood:

$$\hat{\theta}_{MLE} = \arg\max_{\theta} L(\theta) = \arg\max_{\theta} \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} exp\left\{-\frac{(y_i - \theta^T x_i)}{2\sigma^2}\right\}$$

Or equivalently (in this case) via least squares:

$$min_\theta ||\epsilon||_2 = min_\theta \sum_{i=1}^{n} (y - y_i)^2$$

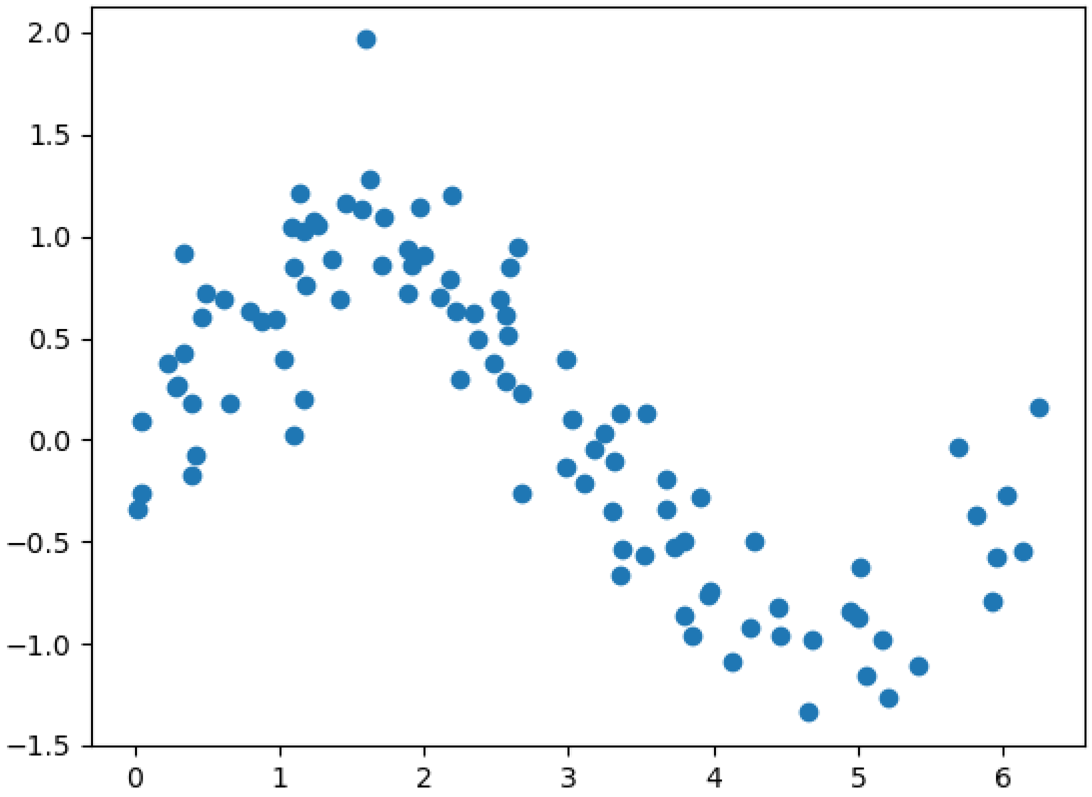
$$\hat{\theta} = (X^T X)^{-1} X^T y$$

A Bayesian Perspective

$$
\begin{aligned}
f(\theta|y) &= \frac{f(y|\theta)f(\theta)}{\int f(y|\theta)f(\theta)d\theta} && (1)\\
&= \text{constant} \times f(\theta)f(y|\theta) && (2)\\
&\propto f(\theta)L(\theta) && (3)
\end{aligned}
$$

$$\hat{\theta}_{MAP} = \arg\max_{\theta} f(\theta|y)$$

But what if our data is not linear?



$$y = f(x) + \epsilon = \theta\phi(x) + \epsilon$$

The Kernel Trick

$$J(\theta) = \sum_{i=1}^{n} (y_i - \theta^T \phi(x_i))^2$$

Solve for θ yields

$$\begin{aligned}
\hat{\theta} &= \sum_{i=1}^{n} (y_i - \theta^T \phi(x_i)) \phi(x_i) \\
&= \sum_{i=1}^{n} \alpha_i \phi(x_i) \\
&= \phi^T \alpha
\end{aligned}$$

$$
\begin{aligned}
J(\theta) &= \sum_{i=1}^{n} (y_i - \theta^T \phi(x_i))^2 \\
&= (\mathbf{y} - \phi\theta)^T (\mathbf{y} - \phi\theta) \\
&= \mathbf{y}^T \mathbf{y} - \mathbf{y}^T \phi\theta - \theta^T \phi^T \mathbf{y} + \theta^T \phi^T \phi\theta
\end{aligned}
$$

Rewriting in terms of α gives:

$$
\begin{aligned}
J(\alpha) &= \mathbf{y}^T \mathbf{y} - \mathbf{y}^T \phi(\phi^T \alpha) - (\phi^T \alpha)^T \phi^T y + (\phi^T \alpha)^T \phi^T \phi(\phi^T \alpha) \\
&= \mathbf{y}^T \mathbf{y} - \mathbf{y}^T \phi\phi^T \alpha - \alpha^T \phi\phi^T \mathbf{y} + \alpha^T \phi\phi^T \phi\phi^T \alpha \\
&= \mathbf{y}^T \mathbf{y} - \mathbf{y}^T K\alpha - \alpha^T K\mathbf{y} + \alpha^T KK\alpha
\end{aligned}
$$

Reproducing Kernel Hilbert Spaces

Let $x, y \in \mathbb{R}^p$ and consider the space of functionals generated by the span of $\{K(\cdot, y), y \in \mathbb{R}^p\}$

These are functions of the form:

$$f(x) = \sum_m \alpha_m K(x, y_m)$$

Suppose K has an eigen-expansion

$$K(x, y) = \sum_{i=1}^{\infty} \gamma_i \phi_i(x) \phi_i(y)$$

with $\gamma_i \geq 0$ and $\sum_{i=1}^{\infty} \gamma_i < \infty$

Then, elements of $\mathcal{H}_K$ have the form

Examples of Kernels (Polynomial Kernel)

For d-degree polynomials, the polynomial kernel is defined by

$$(x^T y + c)^d$$

A kernel K corresponds to an inner product in some feature space based on some mapping ϕ:

$$k(x, y) =< \phi(x), \phi(y) >$$

For $d = 2$, let's see what this feature map looks like. We have

$$K(x, y) = (\sum_{i=1}^{p} x_i y_i + c)^2 = \sum_{i=1}^{p} x_i^2 y_i^2 + \sum_{i=2}^{p} \sum_{j=1}^{i-1} (\sqrt{2} x_i x_j)(\sqrt{2} y_i y_j) + \sum_{i=1}^{p} 2c\sqrt{x_i y_i} + c^2$$

Examples of Kernels (Squared Exponential AKA RBF AKA Gaussian)

$$K(x, y) = \sigma^2 exp\left(-\frac{(x-y)}{2\ell^2}\right)$$

Here, ℓ controls the wiggliness of functions generated by this kernel.

Gaussian Random Fields (Gaussian Processes)

Representation: $\{Z(s)|s \in D \subset \mathbb{R}^d\}$ Suppose a model with additive error:

$$Z(s) = \mu(s) + e(s)$$

The Gaussian process is completely specified by its mean and variance functions:

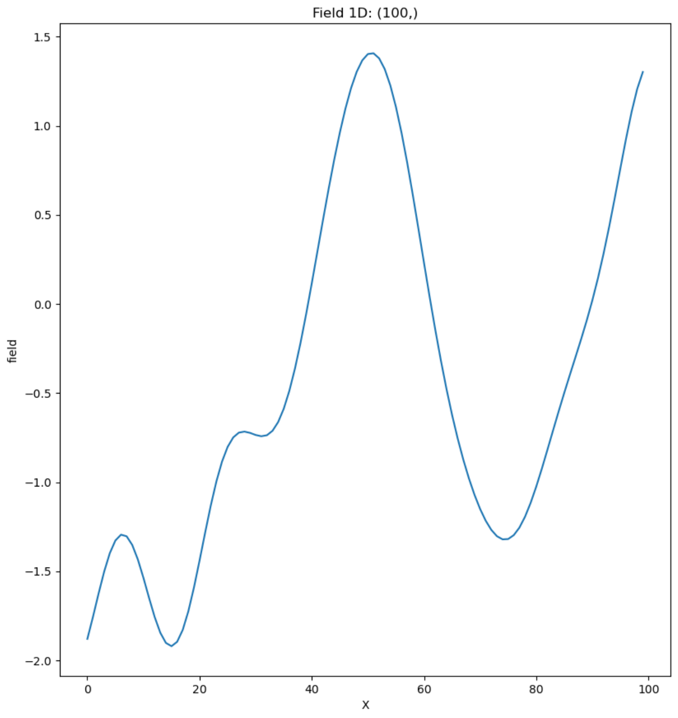
$$\mu(s) = E[Z(s)]$$

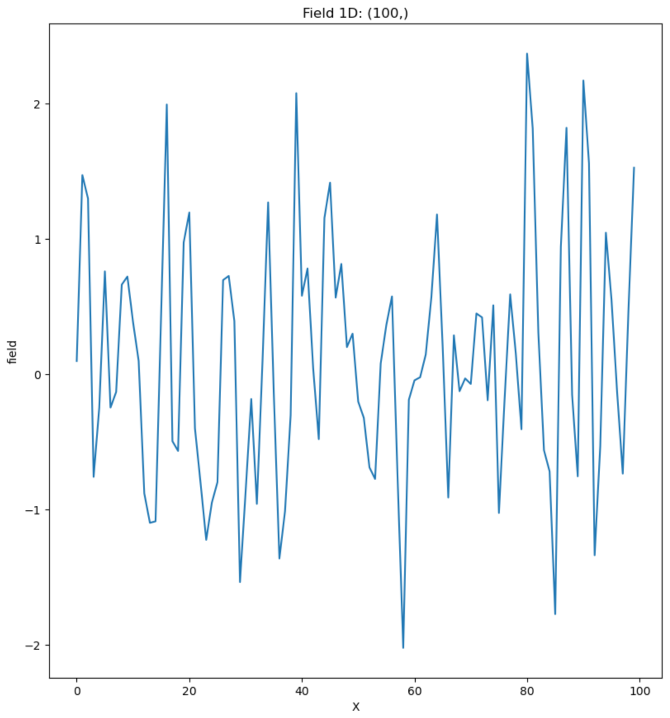
$$K(s, s') = Cov(s, s') = C(h) = Cov[e(s), e(s+h)]$$

This is given by a kernel function. e.g. Gaussian:

$$C(h) = exp\{-h^2/\ell^2\}$$

Samples of Gaussian Random Fields





Gaussian Processes Regression

The data:

$$P(y_1, ..., y_n | x_1, ..., x_n) \sim N(\mathbf{f}, K) \qquad K_{i,j} = K(x_i, x_j)$$

Prediction:

$$P(y_1, ..., y_n, y_* | x_1, ..., x_n, x_*) \sim N(\mathbf{f}_*, \Sigma)$$

$$P(y_* | y_1, ..., y_n, x_1, ..., x_n, x_*) \sim N(K_*^T K^{-1} y, K_{**} K^{-1} K_*)$$

Where

$$\Sigma = \begin{bmatrix} K & K_* \\ K_*^T & K_{**} \end{bmatrix}$$

GP Regression (An example)

The data:

$$X = \{0.01, 0.02, 0.025, 0.18, 0.19, 0.3, 0.67, .76, .79, 0.88, 0.88, 0.9\}$$

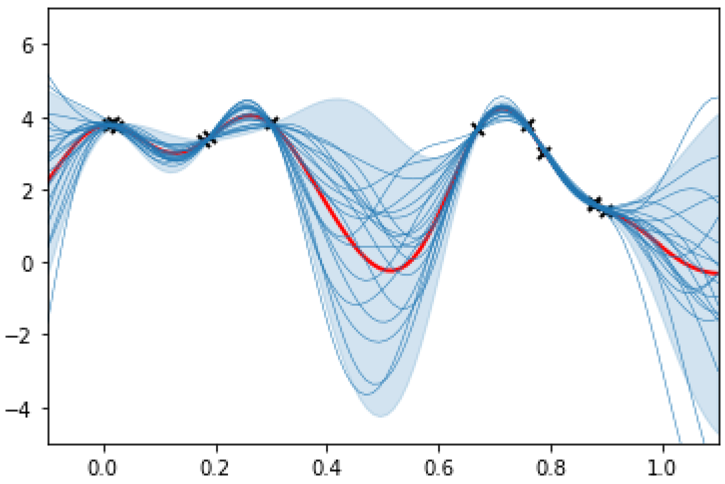
$$Y = \{3.75, 3.80, 3.70, 3.30, 3.45, 3.80, 3.65, 3.75, 3.00, 1.60, 1.55, 1.40\}$$

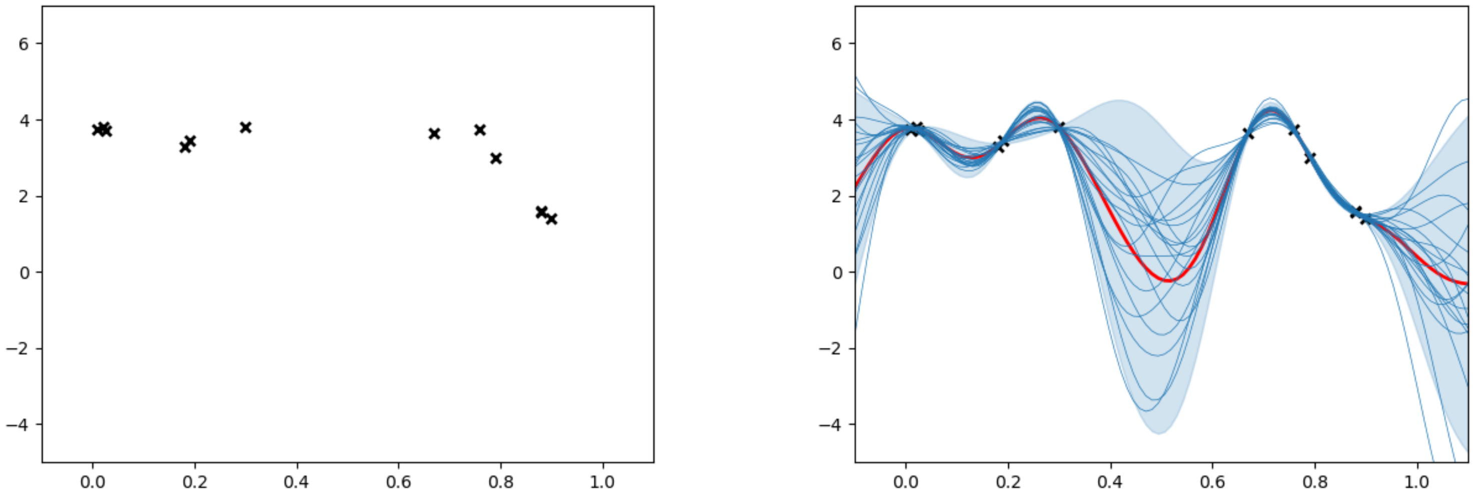
In [22]:

```
import gpflow
import numpy as np
import tensorflow as tf
import matplotlib.pyplot as plt

X = [0.01, 0.02, 0.025, 0.18, 0.19, 0.3, 0.67, .76, .79, 0.88, 0.88, 0.9]
Y = [3.75, 3.80, 3.70, 3.30, 3.45, 3.80, 3.65, 3.75, 3.00, 1.60, 1.55, 1.40]
X = np.array(X).reshape(-1, 1)
Y = np.array(Y).reshape(-1, 1)

k = gpflow.kernels.SquaredExponential()
m = gpflow.models.GPR(data=(X, Y), kernel=k, mean_function=None)
opt = gpflow.optimizers.Scipy()
opt_logs = opt.minimize(m.training_loss, m.trainable_variables, options=dict(maxiter=1000))

## generate test points for prediction
xx = np.linspace(-0.1, 1.1, 100).reshape(100, 1)  # test points must be of shape (N, D)

## predict mean and variance of latent GP at test points
mean, var = m.predict_f(xx)

## generate 20 samples from posterior
tf.random.set_seed(1)  # for reproducibility
samples = m.predict_f_samples(xx, 20)  # shape (10, 100, 1)
```

In [23]:

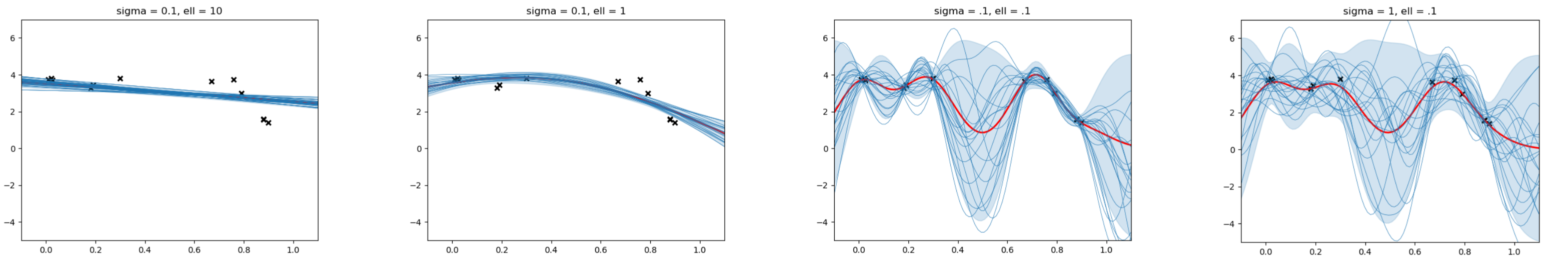
```
plt.figure()
plt.xlim(-.1, 1.1)
plt.ylim(-5, 7)
plt.plot(X, Y, "kx", mew=2)
plt.plot(xx, mean, "red", lw=2)
plt.fill_between(
    xx[:, 0],
    mean[:, 0] - 1.96 * np.sqrt(var[:, 0]),
    mean[:, 0] + 1.96 * np.sqrt(var[:, 0]),
    color="C0",
    alpha=0.2,
)

plt.plot(xx, samples[:, :, 0].numpy().T, "C0", linewidth=0.5)
_ = plt.xlim(-0.1, 1.1)
```





6
4
2
0
−2
−4
0.0
0.2
0.4
0.6
0.8
1.0
6
4
2
0
−2
−4
0.0
0.2
0.4
0.6
0.8
1.0

What if we chose a different value for σ and ℓ?



Questions?