

Gaussian Process Regression

Let us first consider a function as given $f(x)$ for any x . In this case, for an example I am considering a toy dataset as given in the question.

So, let $f(x) = x+2$ at $x=1, x=2, x=3$

If I consider the extrapolation at $x'=4$. I am not considering any noise in this case.

So, we can consider $y = f(x) = [3, 4, 5]$

From the text, I understood that,

For prediction, let us apply a kernel.

For GPR, kernel is defined as

$$k(x, x') = \sigma_f^2 e^{-\frac{(x-x')^2}{2l^2}}$$

$$\text{and } K = \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & k(x_1, x_3) \\ k(x_2, x_1) & k(x_2, x_2) & k(x_2, x_3) \\ k(x_3, x_1) & k(x_3, x_2) & k(x_3, x_3) \end{bmatrix}$$

$$K_* = [k(x', x), k(x', x_2), k(x', x_3)]$$

$$K_{**} = k(x', x')$$

So, let the predicted function be $F(x)$.

So, we define

the best fit of y as \bar{y}_* (which is mean of y) is defined as

$$\bar{y}_* = K_* K^{-1} \bar{y} \quad \text{and } \text{var}(\bar{y}_*) = K_{**} - K_* K^{-1} K^T$$

Here, I have two hyperparameters.
they are σ_f^2 & l .

σ_f^2 is most significant for getting the "spread".
here σ_f^2 corresponds to the maximum allowed covariance

In this case, since the gaussian noise is not present
I will consider σ_f^2 to be small, say 0.1.

l is the length (or distance) between the known
point and the ~~pre~~ x' value to be used for
prediction. Since, the distance is $x - x'$ is
not so small compared to the spread of x , I
will consider it to be relatively equal to the size
of the spread of x . say $l = 10$.

In case we have some more spread in y values
along with some noise, we may use the
formule ~~from the~~ for the kernel as

$$k(x, x') = \sigma_f^2 \exp \left[\frac{-(x - x')^2}{2l^2} \right] + \sigma_n^2 \delta(x, x')$$

Where $\delta =$ Kronecker δ fn.

The implementation is in the colab notebook
as well as the second part ~~to~~ (and the bonus
part) are present in it as well as this text (previous
& this page).