

### (3.) Mathematics

Given  $(x, P(x))$  to find  $f(x)$  that passes thro  $\phi$  all the point.

Normally we find a function w parameters which fits our data well and then define the function with the parameters.

We have data  $D$  we find  $\hat{w} \rightarrow$  param then we predict  $y = w^T x$ .  
In GP instead we try to find the ~~function directly~~ <sup>prediction directly without limiting to one function</sup> which fits with the data.

so we find

$$P(y|x, D) = \int_w P(y|x, w) P(w|D) dw$$

We assume that our data is continuous and follows Gaussian distribution.

So we  $P(y|x, w) \rightarrow$  gaussian and  $P(w) \rightarrow$  gaussian,  $P(D|w) \rightarrow$  gaussian

$$P(w|D) = \frac{P(D|w) P(w)}{Z}$$

and hence  $P(w|D)$  will be gaussian.

Hence  $P(y|x, D)$  will be gaussian.

Now we know  $P(y|x, D)$  is gaussian so we assume our data with both test and training data to be gaussian.

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$$P([y_1, y_2, \dots, y_n] | [x_1, x_2, \dots, x_n]) \sim N(\mu, \Sigma)$$

Now we can normalise the data so make the mean 0

$$P\left(\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \middle| \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, x^*\right) \sim N(0, \Sigma)$$

where  $\Sigma$  is the covariance matrix the test in linear case to find covariance matrix we have to do Cholesky decomposition of the covariance matrix's Cholesky decomposition decomposes the matrix into  $U^T D U$  which is kind of taking square root.

~~$$X \rightarrow V^T V^T$$~~ 
$$X \rightarrow V^T V$$

$X$  can be decomposed into  $V^T V$ .

Now  $X$  needs to be positive semi-definite to do Cholesky decomposition because

Now  $X \rightarrow V^T V$

~~$$Y^T X Y \rightarrow Y^T V^T V Y$$~~

$$Y^T X Y \rightarrow (V Y)^T V Y$$

$$Y^T X Y \rightarrow \|V Y\|^2$$

$$Y^T X Y \geq 0$$

Hence  $X$  is positive semi-definite.

The covariance matrix can be is a kernel because it is positive semi-definite. So

We can define the covariance matrix by a kernel function. We can use RBF kernel function as it is infinite dimensional kernel.

RBF kernel =  $k(x, z) = e^{-\frac{\|x-z\|^2}{2\sigma^2}}$   $\sigma$  is a free parameter.

So far we have

$$P\left(\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \middle| \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}\right) = \mathcal{N}(0, \Sigma) \text{ where } \Sigma = K =$$

$$K_{ij} = k(x_i, x_j)$$

We now need to know  $[y_1, y_2, \dots, y_n]$  given in our data and we need to find  $y^*$  at our testing point.

$$P(y^* | y_1, y_2, \dots, y_n, x_1, \dots, x_n, x^*)$$

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By conditioning

$$p(y^* | y_1, y_2, \dots, y_n, x_1, x_2, \dots, x_n, x^*) = N(\mu_{y^* | (y_1, \dots, y_n, x_1, \dots, x_n, x^*)}, \Sigma_{y^* | (y_1, \dots, y_n, x_1, \dots, x_n, x^*)})$$

By conditioning identity.

$$\mu_{y^* | (y_1, \dots, y_n, x_1, \dots, x_n, x^*)} = K_*^T K^{-1} y$$

where  $K_*$  is the kernel covariance matrix b/w  $x^*$  and  $x$  Training points and Testing point.

$K$  is the covariance matrix/kernel matrix of Training data.

$y$  is our Training data.

and

$$\Sigma_{y^* | (y_1, \dots, y_n, x_1, \dots, x_n, x^*)} = \cancel{K_*^T K^{-1} K_*} K_* - K_*^T K^{-1} K_*$$

where  $K_{**}$  is the covariance matrix of Testing point.

This completes the GP model.

We can define how well our model extrapolates by the variance of the extrapolated points, if the variance is very large then we say that it is poorly extrapolated.  
Yes we need to optimize it, we can optimize by choosing the right parameter of the kernel RBF kernel.