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Introduction to Gaussian Processes

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Preamble

The Gaussian Processes are the widely used stochastic processes for modeling dependent data observed over time, space or even time and space. Here, we'll iniciate our study with a **Probability and Random Process Theory Review** taking some points to base our journey, going through **Linear Regression** and finally the GP.

Outline

Probability and Random Process Theory Review

Basic Concepts of Probability Theory

A key concept in the field of pattern recognition is that of **uncertainty**, that arises from both through noise on measurements, as well as through the finite size of data sets. To find this uncertainty we'll talk about a little of the **Probability Theory**. Let's begin from a simple example.

Basic Concepts of Probability Theory

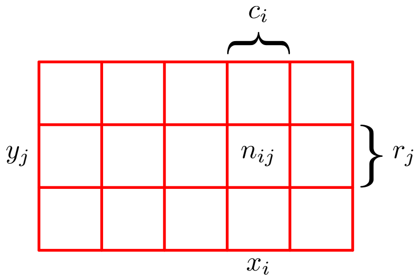
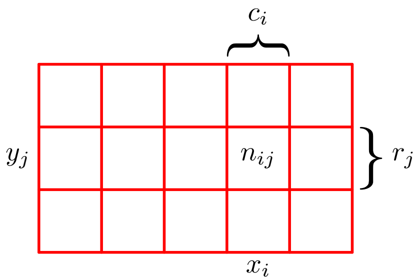


Figure: Considering in the table $X = x_i$ and $Y = y_j$

Let's choose a cell in the 6. We define the probability of choose a cell in a given column is $p(X = x_i) = c_i/N$, being N the total number of cells and $c_i = \sum_j n_{ij}$.



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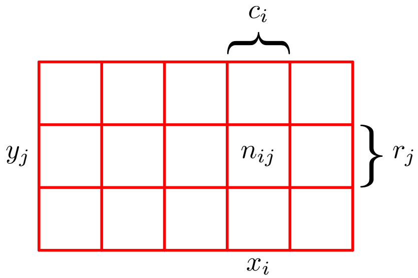
We could say that the probability of choose a cell in a given a row is defined as $p(Y = y_j | X = x_i) = n_{ij}/c_i$.



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And so, the probability of choose a cell is defined as $p(X = x_i, Y = y_j) = n_{ij}/N$.

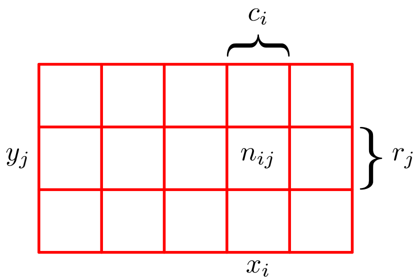

Figure: Considering in the table $X = x_i$ and $Y = y_j$

Here, we could see some properties that we call **The Rules of Probability**

The Rules of Probability

- Sum Rule:

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- Product Rule:

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$$p(Y = y_j, X = x_i) = n_{ij}/N = n_{ij}/c_i \cdot c_i/N \Rightarrow p(X, Y) = p(Y|X)p(X) \tag{2}$$

And by the **Product Rule** we prove that

Bayes' Theorem

$$p(X, Y) = p(Y|X)p(X) = p(X|Y)p(Y) \Rightarrow p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)} \tag{3}$$

So, from **The Rules of Probability**, we could show that too

Total Probability Theorem

$$p(X) = \sum_{Y} p(Y|X)p(X) \tag{4}$$

An important propriety of probability is the **Independence of events**. So, let's say that two events occurs without that one has occurred, so by the **Bayes' Theorem** we make

$$p(X|Y) = p(X) \text{ and } p(Y|X) = p(Y) \Rightarrow p(X,Y) = p(X)p(Y) \tag{5}$$

Random Variables

Simplifying, the **Random Variables** will treat the probability defined before in the *continuous domain*. So we define a random variable X as a function that assigns a real number, $X(\zeta)$, to each outcome ζ, so $X(\zeta) = x$.

The Gaussian distribution

The **Gaussian distribution** is defined as

$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\} \tag{6}$$

where μ is the mean and σ^2 the standard deviation.

Independence of two random variables

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X and Y are independent random variables if *any* event A_1 defined in terms of X is independent of *any* event A_2 defined in terms of Y

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that means in other words that *if X and Y are independent discrete random variables, then the **joint probability mass function (pmf)** is equal to the product of the marginal pmf's.*

Linear Regression

Curve Fitting

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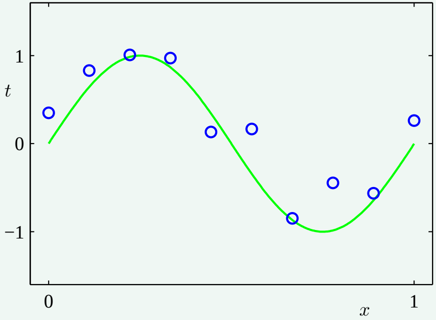
Strategy

1. Purpose a model, e.g. functions like exponential, polynomial and others.
2. Train our model with the training data set, finding the unknown parameters.

Curve Fitting

Let's fit the example by polynomial curve fitting

Example



Curve Fitting

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$$
\begin{aligned}
y_i(x_i, \mathbf{w}) &= w_0 x_i^0 + w_1 x_i + w_2 x_i^2 + \ldots + w_M x_i^M \\
&= \sum_{j=0}^{M} w_j x_i^j
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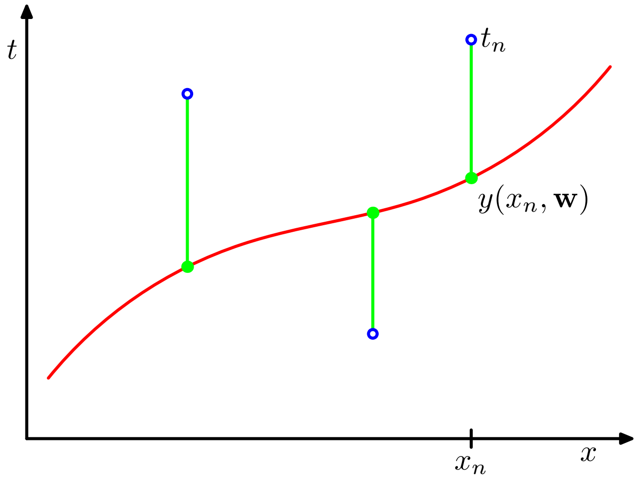
So we'll try to minimize the mean squared error between the model and the training data set. So, if the MSE is defined as

$$
E(\mathbf{w}) \triangleq \frac{1}{2} \sum_{n=1}^{N} \{\hat{y}_n - y_n\}^2 \tag{9}
$$

where $\hat{y}$ is our predict.

Curve Fitting



So, we evaluate the error between our model and the target $\mathbf{t}$, that is our training data.

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y_n(x_i, \mathbf{w}) - t_n\}^2 \tag{10}$$

We could make this evaluation in the matrix form. So

$$E(\mathbf{w}) = \frac{1}{2}(\mathbf{y} - \mathbf{t})^T(\mathbf{y} - \mathbf{t}) \tag{11}$$

where $\mathbf{y} = \mathbf{xw}$. This represents the system

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} = \begin{bmatrix} x_1^1 & x_1^2 & \dots & x_1^M \\ x_2^1 & x_2^2 & \dots & x_2^M \\ \vdots & \vdots & \ddots & \vdots \\ x_N^1 & x_N^2 & \dots & x_N^M \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_N \end{bmatrix} \tag{12}$$

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y_n(x_i, \mathbf{w}) - t_n\}^2 \tag{13}$$

And try to minimize it by

$$\begin{aligned} 0 &= \frac{\partial}{\partial \mathbf{w}} E(\mathbf{w}) \\ 0 &= \sum_{n=1}^{N} \frac{\partial}{\partial \mathbf{w}} y_n(x_n, \mathbf{w}) \{y_n(x_n, \mathbf{w}) - t_n\} \end{aligned} \tag{14}$$

Curve Fitting

$$\begin{bmatrix} \frac{\partial}{\partial w_1} y_(x, \mathbf{w}) \left\{ y(x, \mathbf{w}) - t_n \right\} \\ \frac{\partial}{\partial w_2} y(x, \mathbf{w}) \left\{ y(x, \mathbf{w}) - t_n \right\} \\ \dots \\ \frac{\partial}{\partial w_M} y(x, \mathbf{w}) \left\{ y(x, \mathbf{w}) - t_n \right\} \end{bmatrix} = \tag{15}$$

Bayesian Curve Fitting

So, we'll start to look the regression with a statistical approach. To encourage you, let's take the sentence.

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If we could update the ***regression weights*** *as we acquire some new values of the experiment?*

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Bayes Theorem

$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})\,\overbrace{p(\mathbf{w})}^{\text{the weights probability}}}{\underbrace{p(\mathcal{D})}_{\text{the data probability}}} \tag{16}$$

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But, how?

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A good ideia is to express our target values $\mathbf{t}$ in terms of **gaussians distributions** with the mean equals to $y(x, \mathbf{w})$.

Bayesian Curve Fitting

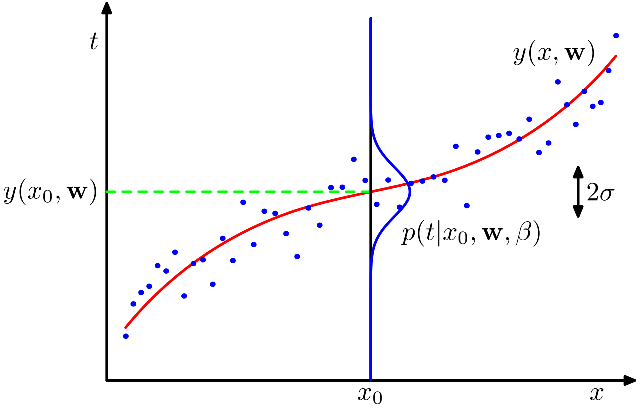

Figure: Schematic of the polynomial function $y(x, \mathbf{w})$ and the gaussian distribution p.

By the 25, we assume the relation

(18)

(19)

Bayesian Curve Fitting

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$$p(t|x, \mathbf{w}, \beta) = \mathcal{N}(t|y(x, \mathbf{w}), \beta^{-1}) \tag{17}$$

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and then, assume that the training data $\{\mathbf{x}, \mathbf{t}\}$ is indenpendent and identically distributed (i.i.d.) and put on **product form**, i.e. the joint probability is

$$p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(t_0|y(x_1, \mathbf{w}), \beta^{-1}) \cap \mathcal{N}(t_n|y(x_0, \mathbf{w}), \beta^{-1}) \ldots \cap \mathcal{N}(t_n|y(x_0, \mathbf{w}), \beta^{-1}) \tag{18}$$

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$$= \prod_{n=1}^{N} \mathcal{N}(t_n|y(x_n, \mathbf{w}), \beta^{-1}) \tag{19}$$

regarding that $\beta^{-1} = \sigma^2$.

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Applying the **Gaussian distribution** (see 6) will result

$$\ln\left(p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta)\right) = -\frac{\beta}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w} - t_n)\}^2 + \frac{N}{2}\ln(\beta) - \frac{N}{2}\ln(2\pi) \tag{21}$$

And taking the derivatives with respect to β to minimize the error

(22)

(24)

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$$\frac{\partial}{\partial \beta} \ln \left(p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta)\right) = 0 \tag{22}$$

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$$\frac{1}{N}\sum_{n=1}^{N}\{y(x_n, \mathbf{w} - t_n)\}^2 = \frac{1}{\beta_{ML}} \tag{24}$$

Where β_{ML} is the maximum likelihood.