Teleinformatics Engineering Department, Federal University of Ceará

Introduction to Gaussian Processes

Filipe P. de Farias, IC
filipepfarias@fisica.ufc.br

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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.

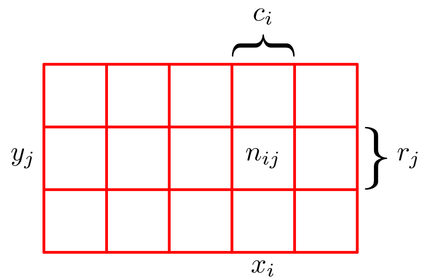
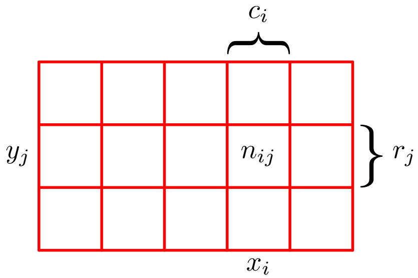


Figure: Considering in the table $X = x_i$ and $Y = y_j$

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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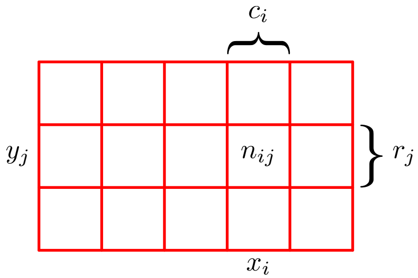

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And so, the probability of choose a cell is defined as $p(X = x_i, Y = y_j) = n_{ij}/N$.

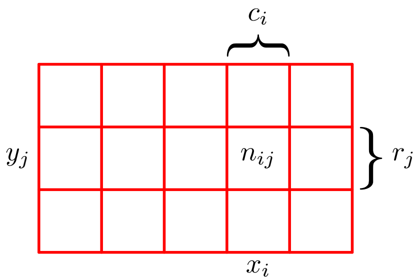

Figure: Considering in the table $X = x_i$ and $Y = y_j$

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

The Rules of Probability

- Sum Rule:

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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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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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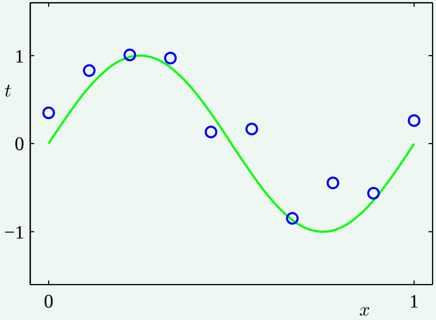
Strategy

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.

Let's fit the example by polynomial curve fitting

Example



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Curve Fitting

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\begin{aligned}
y(x, \mathbf{w}) &= w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M \\
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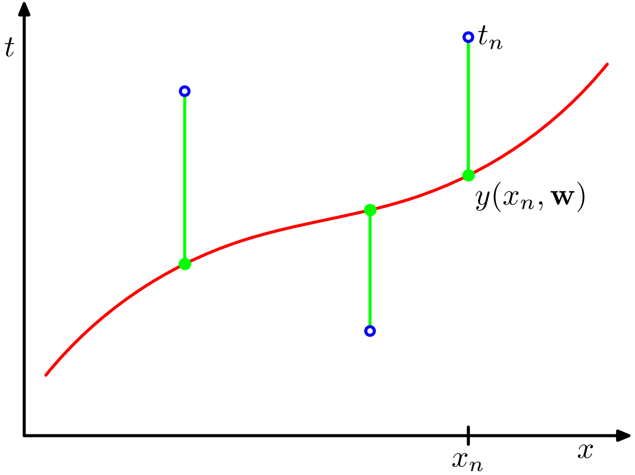
$$E(\mathbf{w}) \triangleq \frac{1}{2} \sum_{n=1}^{N} \{\hat{y}_n - y_n\}^2 \tag{9}$$

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

Curve Fitting



So, we evaluate the error between our model and the target **t**, that is our training data.

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

And try to minimize it by

$$\frac{\partial}{\partial \mathbf{w}} E(\mathbf{w}) = 0$$

$$\sum_{n=1}^{N} \frac{\partial}{\partial \mathbf{w}} y(x, \mathbf{w}) \{y_n(x, \mathbf{w}) - t_n\} = 0 \tag{11}$$

$$\begin{bmatrix} \frac{\partial}{\partial w_1} y(x, \mathbf{w}) \left\{ y(x, \mathbf{w}) - t_n \right\} \\ \frac{\partial}{\partial w_2} y(x, \mathbf{w}) \left\{ y(x, \mathbf{w}) - t_n \right\} \\ \dots \\ \frac{\partial}{\partial w_M} y(x, \mathbf{w}) \left\{ y(x, \mathbf{w}) - t_n \right\} \end{bmatrix} = \tag{12}$$

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

$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})\,\overbrace{p(\mathbf{w})}^{\text{the weights probability}}}{\underbrace{p(\mathcal{D})}_{\text{the data probability}}} \tag{13}$$

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So, if **we have the probability** of the data, we'll could estimate the **future weights**.
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 $y(x, \mathbf{w})$.

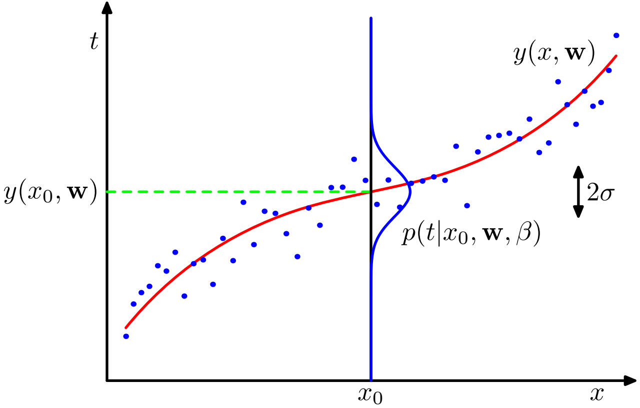

Figure: Schematic of the polynomial function $y(x, \mathbf{w})$ and the gaussian distribution p.

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(15)

(16)

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$$p(t|x, \mathbf{w}, \beta) = \mathcal{N}(t|y(x, \mathbf{w}), \beta^{-1}) \tag{14}$$

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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

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

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$$= \prod_{n=1}^{N} \mathcal{N}(t_n|y(x_n, \mathbf{w}), \beta^{-1}) \tag{16}$$

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

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

$$\ln\left(p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta)\right) = -\frac{\beta}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w} - t_n)\}^2 + \frac{N}{2}\ln(\beta) - \frac{N}{2}\ln(2\pi) \tag{18}$$

Bayesian Curve Fitting

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(19)

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$$\frac{\partial}{\partial \beta} \ln \left(p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta)\right) = 0 \tag{19}$$

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$$\frac{1}{N} \sum_{n=1}^{N} \{y(x_n, \mathbf{w} - t_n)\}^2 = \frac{1}{\beta_{ML}} \tag{21}$$

Where β_{ML} is the maximum likelihood.