Teleinformatics Engineering Department, Federal University of Ceará

Introduction to Gaussian Processes

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Outline

Linear Regression

Curve Fitting

If we have a set of points in the space that comes from observations of an experiment and we want to predict other points, this could be done with **curve fitting** .

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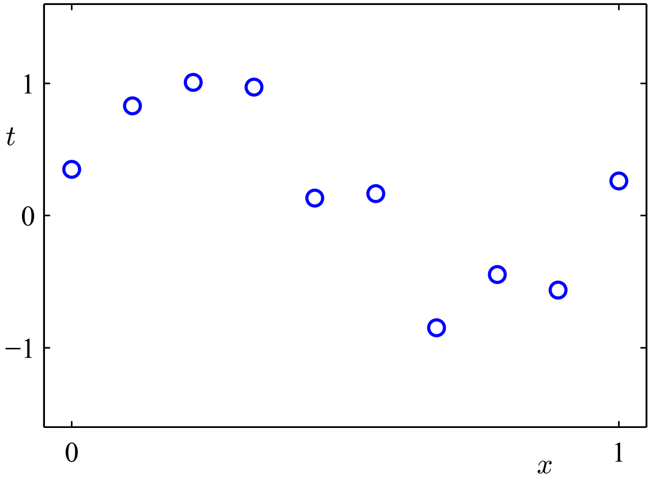
So we could define some strategy to find our model.

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 points below by polynomial curve fitting



Curve Fitting

Be the model chosen

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$$y(x, \mathbf{w}) = w_0 x^0 + w_1 x^1 + w_2 x^2 + \ldots + w_{M-1} x^{M-1} = \sum_{j=1}^{M-1} w_j x^j$$

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For general, we could write this *weighted sum* with any other function. In other words, we can put this in terms of $\phi_n(x) = x^n$, where ϕ could be other *basis function*. For simplicity, we'll carry this notation along.

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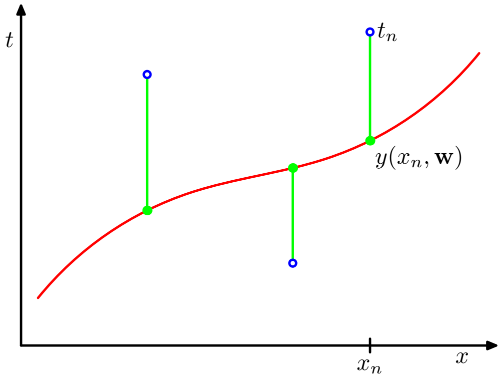
$$y(x, \mathbf{w}) = w_0 \phi_0(x) + w_1 \phi_1(x) + w_2 \phi_2(x) + \ldots + w_{M-1} \phi_{M-1}(x) = \sum_{j=1}^{M-1} w_j \phi_j(x)$$

Curve Fitting

The chosen model will give us some curve that is needed to adjust such that we'll *minimize* his **distance** to the given points, or **targets** (t).



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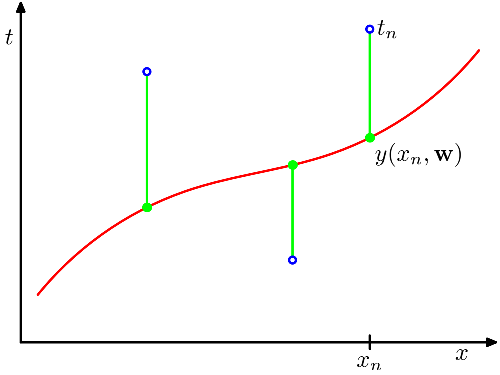

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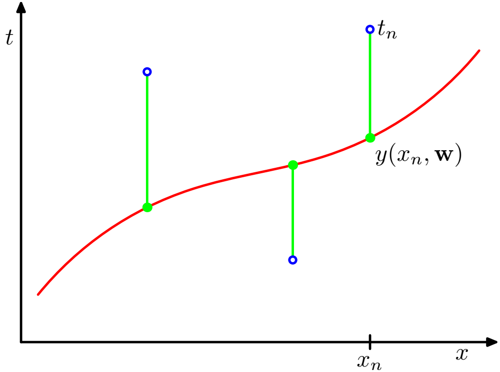
$$E(\mathbf{w}) \triangleq \frac{1}{2} \sum_{n=1}^{N} \{y_n - t_n\}^2$$



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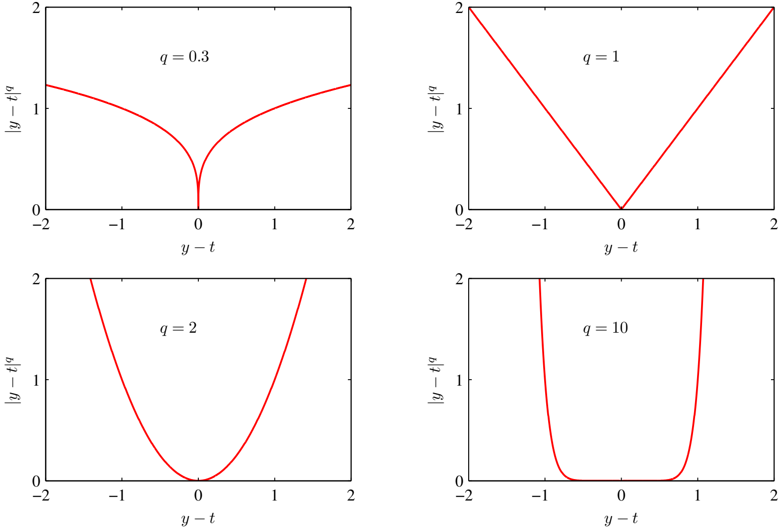


Curve Fitting

Remembering that

$$y_n(x_n, \mathbf{w}) = w_0\phi_0(x_n) + w_1\phi_1(x_n) + w_2\phi_2(x_n) + \ldots + w_{M-1}\phi_{M-1}(x_n)$$

We could put $y_n(x_i, \mathbf{w})$ in the matricial form and get

$$y_n = \begin{bmatrix} \phi_0(x_n) & \phi_1(x_n) & \ldots & \phi_{M-1}(x_n) \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_{M-1} \end{bmatrix}$$

and then

$$\underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{\mathbf{y}} = \underbrace{\begin{bmatrix} \phi_0(x_0) & \phi_1(x_0) & \dots & \phi_{M-1}(x_0) \\ \phi_0(x_1) & \phi_1(x_1) & \dots & \phi_{M-1}(x_1) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(x_{N-1}) & \phi_1(x_{N-1}) & \dots & \phi_{M-1}(x_{N-1}) \end{bmatrix}}_{\Phi} \underbrace{\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_N \end{bmatrix}}_{\mathbf{w}}$$

This represents the system $\mathbf{y} = \Phi\mathbf{w}$. If

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

where $\mathbf{t} = \begin{bmatrix} t_1 & t_2 & \dots & t_n \end{bmatrix}^T$

Then we'll have

$$\begin{aligned} E(\mathbf{w}) =& \frac{1}{2}\left(\mathbf{y}^T\mathbf{y} - \mathbf{t}^T\mathbf{y} - \mathbf{y}^T\mathbf{t} + \mathbf{t}^T\mathbf{t}\right) \\ =& \frac{1}{2}\left((\Phi\mathbf{w})^T(\Phi\mathbf{w}) - \mathbf{t}^T(\Phi\mathbf{w}) - (\Phi\mathbf{w})^T\mathbf{t} + \mathbf{t}^T\mathbf{t}\right) \\ =& \frac{1}{2}\left(\mathbf{w}^T\Phi^T\Phi\mathbf{w} - 2\mathbf{t}^T\Phi\mathbf{w} + \mathbf{t}^T\mathbf{t}\right) \end{aligned}$$

this by the fact that $\alpha = \mathbf{t}^T(\Phi\mathbf{w}) = (\Phi\mathbf{w})^T\mathbf{t}$, being α a scalar.

Curve Fitting

In sequence, we'll try to minimize it in terms of the weights ($\mathbf{w}$) by

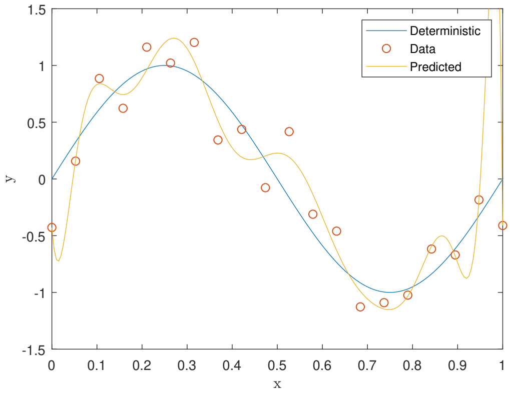
$$
\begin{aligned}
0 =& \frac{\partial E(\mathbf{w})}{\partial \mathbf{w}} \\
0 =& \frac{1}{2}\left(2\mathbf{w}^T\Phi^T\Phi - 2\mathbf{t}^T\Phi + 0\right) \\
\mathbf{w}^T =& \mathbf{t}^T\Phi\left(\Phi^T\Phi\right)^{-1} \\
\mathbf{w} =& \left(\Phi^T\Phi\right)^{-1}\Phi^T\mathbf{t}
\end{aligned}
$$

Here, we've obtained $\mathbf{w}$ for the curve fitting.

```matlab
n = 20;
x = linspace(0,1,n)';
y = @(x) sin(2*pi*x);
e = .2*randn(size(x));
t = y(x) + e;

for M = 1:20
    phi = @(a)(bsxfun(@power,a,0:M-1));
    phix = phi(x);
   W = ((phix'*phix)\phix')*t;
end
```

A visible effect of the *increase of the complexity* of the model, represented here by M, is the *increase of the weights*. We call it **over-fitting**.



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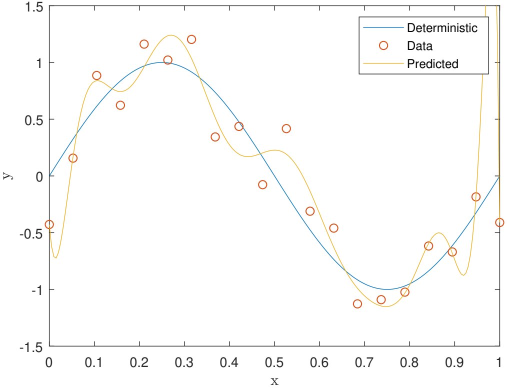

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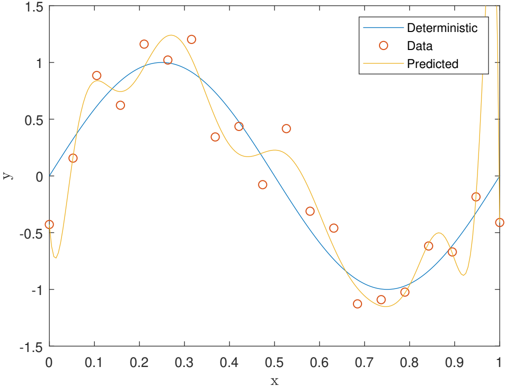
It's reasonable to see that our model start's to differ from the y and starts to interpolate the noise.



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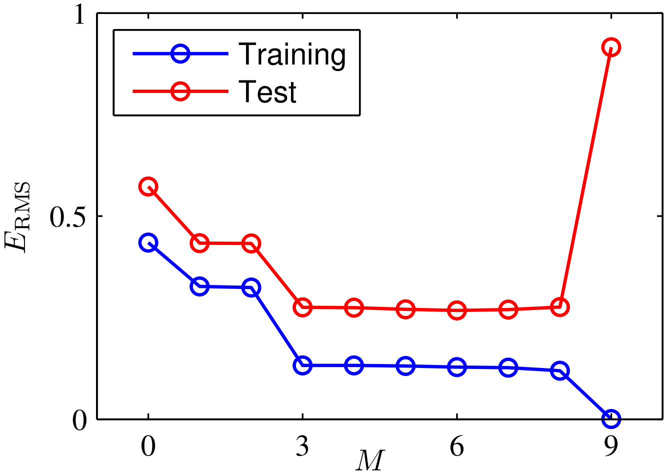

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To control the over-fitting, we try to *regularize* the weights by adding a penalty term (λ) to error function, by this we force the coefficients to not reach high values.

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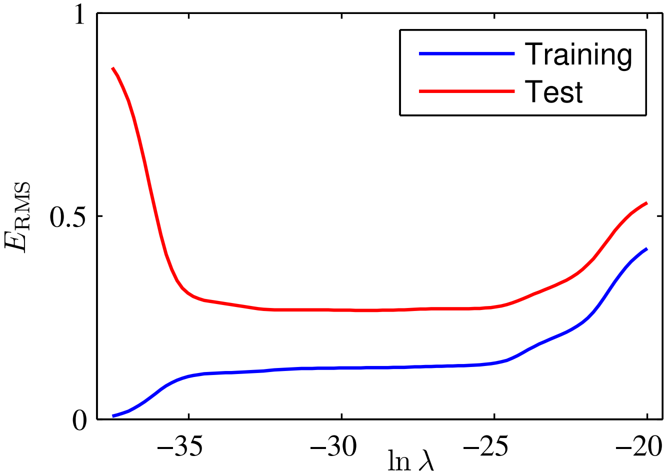
$$
\begin{aligned}
\tilde{E}(\mathbf{w}) =& \frac{1}{2}(\mathbf{y}-\mathbf{t})^T(\mathbf{y}-\mathbf{t}) + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w} \\
=& \frac{1}{2}\left(\mathbf{w}^T\Phi^T\Phi\mathbf{w} - 2\mathbf{t}^T\Phi\mathbf{w} + \mathbf{t}^T\mathbf{t} + \lambda\mathbf{w}^T\mathbf{I}\mathbf{w}\right) \\
\Rightarrow \frac{\partial E(\mathbf{w})}{\partial \mathbf{w}} =& \frac{1}{2}\left(2\mathbf{w}^T\Phi^T\Phi - 2\mathbf{t}^T\Phi + 0 + 2\lambda\mathbf{w}^T\mathbf{I}\right) \\
0 =& \mathbf{w}^T\Phi^T\Phi - \mathbf{t}^T\Phi + \lambda\mathbf{w}^T\mathbf{I} \\
\mathbf{w} =& \left(\Phi^T\Phi + \lambda\mathbf{I}\right)^{-1}\Phi^T\mathbf{t}
\end{aligned}
$$

```
n = 10;
x = linspace(0,1,n)';
y = @(x) sin(2*pi*x);
e = .2*randn(size(x));
t = y(x) + e;
for lambda = 75:-1:1
    M = n;
    plot(Xp,y(Xp),'-');hold on; plot(x,t,'o');
    phi = @(a)(bsxfun(@power,a,0:M-1));
    phix = phi(x);
    W = ((phix'*phix+exp(-lambda)*eye(n))\phix')*t;
end
```

Curve Fitting



A probabilistic perspective

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

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Sentence

*Having an **uncertainty** in the measured value, we could represent it with a **probability distribuition**.*

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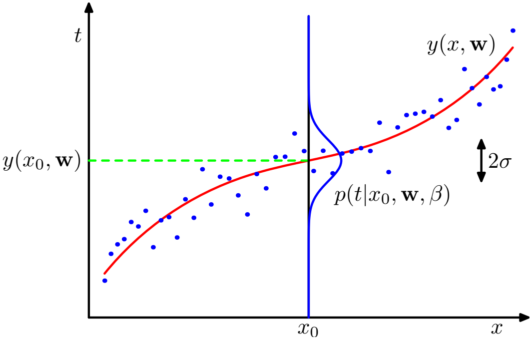
Sentence

Having an ***uncertainty*** *in the measured value, we could represent it with a* ***probability distribuition***.



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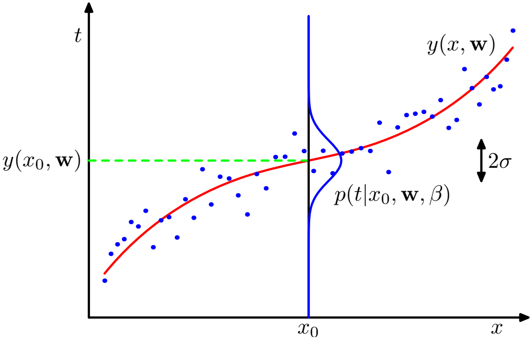
Let's go back to the initial problem of curve fitting. Each observation of the phenomenon is described with a random variable whose *mean* is given by $y(x, \mathbf{w})$, and the *variance* by β.



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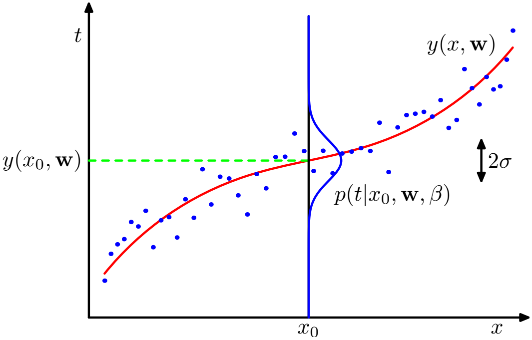
Let's go back to the initial problem of curve fitting. Each observation of the phenomenon is described with a random variable whose *mean* is given by $y(x, \mathbf{w})$, and the *variance* by β.

Then, we want to obtain the probability of the *targets*, given some parameters, in this case $\mathbf{x}$, $\mathbf{w}$ and β.



A probabilistic perspective

So, if we consider that our conditions are such that being the random variables independent and identically distributed, we can say that our *joint probability* is given by

$$p(t|x, \mathbf{w}, \beta) \Rightarrow p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \prod_{n=1}^{N} p\left(t_n|x_n, \mathbf{w}, \beta\right)$$

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Let's assume we have a distribution such that $p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta)$. Our goal is, given the *parameters*, maximize the *probability* of the *targets* given the *parameters*. An approach to do this use the fact that

$$\int_{\infty}^{-\infty} p(x)dx = 1 \text{ and } p(x) \geq 0$$

A probabilistic perspective

Seen this, we're supposing that p could assume values much smaller than one. To avoid computational singularity and for future purposes, we'll take the logarithmic probability. And then

$$\ln\left(p(\mathbf{t}|\mathbf{x},\mathbf{w},\beta)\right)$$

Reminding that

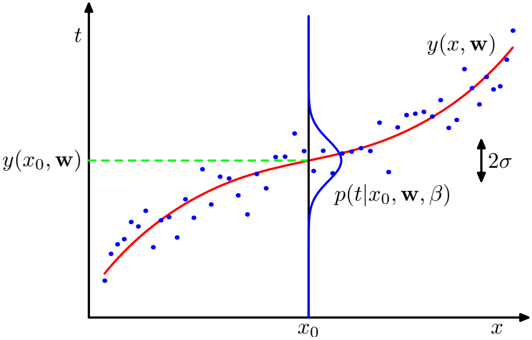
$$p(\mathbf{t}|\mathbf{x},\mathbf{w},\beta) = \prod_{n=1}^{N} p\left(t_n|x_n,\mathbf{w},\beta\right)$$

Implies that

$$\ln\left(p(\mathbf{t}|\mathbf{x},\mathbf{w},\beta)\right) = \sum_{n=1}^{N} \ln\left(p\left(t_n|x_n,\mathbf{w},\beta\right)\right)$$

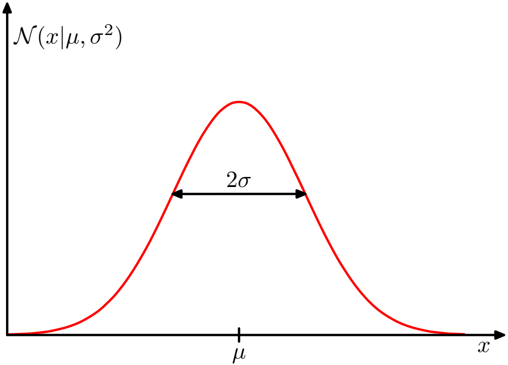
A probabilistic perspective

To proceed, we need to know what distribution p is. Let's choose the **Gaussian distribution**.



A probabilistic perspective

The **Gaussian distribution** comes from many different contexts, as the one that maximize the entropy among of all ones with fixed variance and from the sum of multiple random variables with finite variance.



A probabilistic perspective

One-dimensional Gaussian distribution

$$\mathcal{N}(x|\mu, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\} > 0$$

where μ is the mean and σ^2 the variance.

A probabilistic perspective

Now, back to the discussion of the maximization of

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

A probabilistic perspective

And then, from the *joint probability* of the Gaussians distributions

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

From this, we could obtain the **maximum likelihood**, or the *best estimation for the parameters*, taking the derivatives of the log probability to zero, according to the terms β and $\mathbf{w}$, our model parameters.

A probabilistic perspective

We could observe that taking the derivative with respect to **w**, our expression becomes closer to the *error function* presented previously, added the dependency of β

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

Then some behaviors could be expected, as the **over-fitting**.

A probabilistic perspective

We'll obtain the best β by

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

remembering that $\mathbf{w}_{ML}$ is already known from the regular linear regression.

A probabilistic perspective

At this point, we have a probabilistic model and we may want to predict values for x. Then, we need a *predictive distribution*.

Let's say we have the probabilities of some idea we desire to update it in the light of some new evidence. This could be done with **Bayes' Rule**, to convert a *prior* probability in a *posterior* probability and put some uncertainty in the parameters too.

A probabilistic perspective

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$$\underbrace{p\left(\mathbf{w}|\mathbf{x},\mathbf{t},\alpha,\beta\right)}_{\text{posterior}} \propto \underbrace{p\left(\mathbf{t}|\mathbf{w},\mathbf{x},\beta\right)}_{\text{likelihood}}\underbrace{p\left(\mathbf{w}|\alpha\right)}_{\text{prior}}$$

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and for simplicity, consider the follow prior for $\mathbf{w}$

$$p\left(\mathbf{w}|\alpha\right) = \mathcal{N}\left(\mathbf{w}|\mathbf{0},\alpha^{-1}\mathbf{I}\right) = \left(\frac{\alpha}{2\pi}\right)^{(M+1)/2}\exp\left\{-\frac{\alpha}{2}\mathbf{w}^T\mathbf{w}\right\}$$

where α the precision of the distribution and $M+1$ is the dimension of $\mathbf{w}$, for a polynomial of M^{th} order. Variables such α are called *hyperparameters* and control the distribuition of model parameters.

A probabilistic perspective

By this, we can find a distribution and its maximum, or most probable value of **w** given the data taking the minimum of the negative logarithm of the infered expression, that will lead us to a term

$$\sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{\alpha}{2}\mathbf{w}^T\mathbf{w} + \text{const.}$$

Note that if we consider $\lambda = \alpha/\beta$, this will back to the regularized form of *least squares*. This technique is called *maximum posterior* (MAP).

A probabilistic perspective

So, observe that even making some probabilistic assumptions, we don't have yet a fully bayesian model, given that finding the *maximum likelihood*, we're finding only the parameters given one model such that maximize our targets probabilities. Furthermore, even with some probabilistic assumptions, our model still have a **over-fitting** problem, given that we obtained the same expressions for the simple regression, adding some constants.

The next step is put some **uncertainty in predictive model**, and makes adjustments in the light of our new evidences. By that we could obtain a "more Bayesian" model, in other words, a **Bayesian Linear Regression**.

Bayesian Linear Regression

Bayesian Linear Regression

Seeking a Bayesian approach, the next steps consists to apply the **sum** and **product** rules of probability to evaluate the predictive distribution. By now we assume that the hyperparameters are fixed, but they could assume a distribution too.

We saw that the posterior distribution for **w** could be given by

$$\underbrace{p\left(\mathbf{w}|\mathbf{x},\mathbf{t}\right)}_{\text{posterior}} \propto \underbrace{p\left(\mathbf{t}|\mathbf{w},\mathbf{x}\right)}_{\text{likelihood}}\underbrace{p\left(\mathbf{w}\right)}_{\text{prior}}$$

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First we'll consider a geometrical approach by the quadratic distance $(x-\mu)^2$ normalized by the variance σ^2. This comprehension will help us with the D-dimensional case.

The D-dimensional Gaussian Distribution

To more than one dimensions, we'll consider the points (x) distance for the mean of the distribution, as we done in the one dimensional case, by adding a term to prioritize some dimension distribution in particular. Then

$$\Delta^2 = (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})$$

called *Mahalanobis distance*. And it's becomes the *Euclidean distance*, when $\boldsymbol{\Sigma}$ is the indentity matrix. This means that the all the distances are equally normalized. The matrix $\boldsymbol{\Sigma}$ is the covariance matrix of the distributions, by definition.

And then

D-dimensional Gaussian distribution

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{ -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right\}$$

where $\boldsymbol{\mu}$ is the D-dimensional mean vector, $\boldsymbol{\Sigma}$ the D$\times$D-dimensional variance matrix and $|\boldsymbol{\Sigma}|$ its determinant.

Bayes' rule for Gaussian variables

To proceed we'd like to prove that the Gaussians are **closed under linear transformations**. This will allow us to transform the Gaussians under the likelihood distribution given a prior. For example, given a distribution

$$p(\mathbf{z}) = p(\mathbf{x}, \mathbf{y})$$

Bayes’ rule for Gaussian variables

In other words, we’re trying to find the parginal distribution $p(\mathbf{y})$ and the conditional distribution $p(\mathbf{x}|\mathbf{y})$, given

$$
\begin{aligned}
p(\mathbf{x}) =& \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}\right) \\
p(\mathbf{y}|\mathbf{x}) =& \mathcal{N}\left(\mathbf{y}|\mathbf{A}\mathbf{x} + \mathbf{b}, \mathbf{L}^{-1}\right)
\end{aligned}
$$

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\end{aligned}$$

So, applying the joint distribution and the its $\ln$ after

$$\begin{aligned}
p\left(\mathbf{z}\right) &= p\left(\mathbf{x}, \mathbf{y}\right) = p\left(\mathbf{y}|\mathbf{x}\right) p\left(\mathbf{x}\right) \\
\ln p\left(\mathbf{z}\right) &= \ln p\left(\mathbf{y}|\mathbf{x}\right) + \ln p\left(\mathbf{x}\right) \\
&= -\frac{1}{2}\left(\mathbf{x} - \boldsymbol{\mu}\right)^{T} \boldsymbol{\Lambda}\left(\mathbf{x} - \boldsymbol{\mu}\right) \\
&\quad -\frac{1}{2}\left(\mathbf{y} - \mathbf{A}\mathbf{x} - \mathbf{b}\right)^{T} \mathbf{L}\left(\mathbf{y} - \mathbf{A}\mathbf{x} - \mathbf{b}\right) + \text{const}
\end{aligned}$$

The "const" is the term independent of **x** and **y**. Then, expanding the quadratic form

$$\begin{aligned}\ln p(\mathbf{z}) &= -\frac{1}{2}\mathbf{x}^T\left(\boldsymbol{\Lambda}+\mathbf{A}^T\mathbf{L}\mathbf{A}\right)\mathbf{x}-\frac{1}{2}\mathbf{y}^T\mathbf{L}\mathbf{y}+\frac{1}{2}\mathbf{y}^T\mathbf{L}\mathbf{A}\mathbf{x}+\frac{1}{2}\mathbf{x}^T\mathbf{A}^T\mathbf{L}\mathbf{y}\\ &= -\frac{1}{2}\begin{pmatrix}\mathbf{x}\\ \mathbf{y}\end{pmatrix}^T\begin{pmatrix}\boldsymbol{\Lambda}+\mathbf{A}^T\mathbf{L}\mathbf{A} & -\mathbf{A}^T\mathbf{L}\\ -\mathbf{L}\mathbf{A} & \mathbf{L}\end{pmatrix}\begin{pmatrix}\mathbf{x}\\ \mathbf{y}\end{pmatrix}=-\frac{1}{2}\mathbf{z}^T\mathbf{R}\mathbf{z}\end{aligned}$$

Bayes' rule for Gaussian variables

The "const" is the term independent of $\mathbf{x}$ and $\mathbf{y}$. Then, expanding the quadratic form

$$\begin{aligned}
\ln p(\mathbf{z}) &= -\frac{1}{2}\mathbf{x}^T\left(\boldsymbol{\Lambda} + \mathbf{A}^T\mathbf{L}\mathbf{A}\right)\mathbf{x} - \frac{1}{2}\mathbf{y}^T\mathbf{L}\mathbf{y} + \frac{1}{2}\mathbf{y}^T\mathbf{L}\mathbf{A}\mathbf{x} + \frac{1}{2}\mathbf{x}^T\mathbf{A}^T\mathbf{L}\mathbf{y} \\
&= -\frac{1}{2}\begin{pmatrix}\mathbf{x}\\ \mathbf{y}\end{pmatrix}^T \begin{pmatrix}\boldsymbol{\Lambda} + \mathbf{A}^T\mathbf{L}\mathbf{A} & -\mathbf{A}^T\mathbf{L} \\ -\mathbf{L}\mathbf{A} & \mathbf{L}\end{pmatrix}\begin{pmatrix}\mathbf{x}\\ \mathbf{y}\end{pmatrix} = -\frac{1}{2}\mathbf{z}^T\mathbf{R}\mathbf{z}
\end{aligned}$$

We'll apply the partitioned matrices inversion to obtain $\mathbf{R}^{-1}$

$$\mathbf{R}^{-1} = \begin{pmatrix}\boldsymbol{\Lambda}^{-1} & \boldsymbol{\Lambda}^{-1}\mathbf{A}^T \\ \mathbf{A}\boldsymbol{\Lambda}^{-1} & \mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^T\end{pmatrix}$$

Bayes' rule for Gaussian variables

The expanded form of $\ln p(\mathbf{z})$ give us the mean too by the linear terms, then

$$\mathbf{x}^T \boldsymbol{\Lambda}\boldsymbol{\mu} - \mathbf{x}^T \mathbf{A}^T \mathbf{L}\mathbf{b} + \mathbf{y}^T \mathbf{L}\mathbf{b} = \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}^T \begin{pmatrix} \boldsymbol{\Lambda}\boldsymbol{\mu} - \mathbf{A}^T \mathbf{L}\mathbf{b} \\ \mathbf{L}\mathbf{b} \end{pmatrix}$$

Bayes' rule for Gaussian variables

The expanded form of $\ln p\left(\mathbf{z}\right)$ give us the mean too by the linear terms, then

$$\mathbf{x}^T\boldsymbol{\Lambda}\boldsymbol{\mu} - \mathbf{x}^T\mathbf{A}^T\mathbf{L}\mathbf{b} + \mathbf{y}^T\mathbf{L}\mathbf{b} = \begin{pmatrix}\mathbf{x}\\ \mathbf{y}\end{pmatrix}^T \begin{pmatrix}\boldsymbol{\Lambda}\boldsymbol{\mu} - \mathbf{A}^T\mathbf{L}\mathbf{b}\\ \mathbf{L}\mathbf{b}\end{pmatrix}$$

By inspection of the linear terms

$$\mathbb{E}[\mathbf{z}] = \mathbf{R}^{-1}\begin{pmatrix}\boldsymbol{\Lambda}\boldsymbol{\mu} - \mathbf{A}^T\mathbf{L}\mathbf{b}\\ \mathbf{L}\mathbf{b}\end{pmatrix}$$

Bayes' rule for Gaussian variables

The expanded form of $\ln p(\mathbf{z})$ give us the mean too by the linear terms, then

$$\mathbf{x}^T\boldsymbol{\Lambda}\boldsymbol{\mu} - \mathbf{x}^T\mathbf{A}^T\mathbf{L}\mathbf{b} + \mathbf{y}^T\mathbf{L}\mathbf{b} = \begin{pmatrix}\mathbf{x}\\ \mathbf{y}\end{pmatrix}^T \begin{pmatrix}\boldsymbol{\Lambda}\boldsymbol{\mu} - \mathbf{A}^T\mathbf{L}\mathbf{b}\\ \mathbf{L}\mathbf{b}\end{pmatrix}$$

Bayes' rule for Gaussian variables

The expanded form of $\ln p(\mathbf{z})$ give us the mean too by the linear terms, then

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By inspection of the linear terms

$$\mathbb{E}[\mathbf{z}] = \mathbf{R}^{-1}\begin{pmatrix}\boldsymbol{\Lambda}\boldsymbol{\mu} - \mathbf{A}^T\mathbf{L}\mathbf{b}\\ \mathbf{L}\mathbf{b}\end{pmatrix} = \begin{pmatrix}\boldsymbol{\mu}\\ \mathbf{A}\boldsymbol{\mu} + \mathbf{b}\end{pmatrix}$$

Bayes' rule for Gaussian variables

And then we we'll have that

$$\mathbb{E}[\mathbf{y}] = \mathbf{A}\boldsymbol{\mu} + \mathbf{b}$$
$$\mathrm{cov}[\mathbf{y}] = \mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^T$$

Bayes' rule for Gaussian variables

And then we we'll have that

$$\mathbb{E}[\mathbf{y}] = \mathbf{A}\boldsymbol{\mu} + \mathbf{b}$$
$$\operatorname{cov}[\mathbf{y}] = \mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^T$$

$$\mathbb{E}[\mathbf{x}|\mathbf{y}] = \left(\boldsymbol{\Lambda} + \mathbf{A}^T\mathbf{L}\mathbf{A}\right)^{-1}\left\{\mathbf{A}^T\mathbf{L}(\mathbf{y}-\mathbf{b}) + \boldsymbol{\Lambda}\boldsymbol{\mu}\right\}$$
$$\operatorname{cov}[\mathbf{x}|\mathbf{y}] = \left(\boldsymbol{\Lambda} + \mathbf{A}^T\mathbf{L}\mathbf{A}\right)^{-1}$$

Bayesian Linear Regression

In the next step, we'll assume a **prior distribution over parameters**, $p(\mathbf{w})$, and define it as a Gaussian distribution, then

$$p(\mathbf{w}) = \mathcal{N}\left(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0\right)$$

with mean $\mathbf{m}_0$ and variance $\mathbf{S}_0$.

Bayes' rule for Gaussian variables

Marginal and Conditioned Gaussians

- For y given x:

$$
\begin{aligned}
p\left(\mathbf{x}\right) =& \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}\right) \\
p\left(\mathbf{y}|\mathbf{x}\right) =& \mathcal{N}\left(\mathbf{y}|\mathbf{A}\mathbf{x} + \mathbf{b}, \mathbf{L}^{-1}\right)
\end{aligned}
$$

- For x given y:

$$
\begin{aligned}
p\left(\mathbf{x}|\mathbf{y}\right) &= \mathcal{N}\left(\mathbf{y}|, \boldsymbol{\Sigma}\left\{\mathbf{A}^T\mathbf{L}(\mathbf{y} - \mathbf{b} + \boldsymbol{\Sigma}\boldsymbol{\mu})\right\}, \boldsymbol{\Sigma}\right) \\
p\left(\mathbf{y}\right) &= \mathcal{N}\left(\mathbf{y}|\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^T\right), \text{where } \boldsymbol{\Sigma} = \left(\boldsymbol{\Lambda} + \mathbf{A}^T\mathbf{L}\mathbf{A}\right)^{-1}
\end{aligned}
$$

Bayes' rule for Gaussian variables

By the derivations, we make the assumptions of given $p(\mathbf{w})$ and for $p(\mathbf{t}|\mathbf{w})$ such that

$$\begin{aligned} p(\mathbf{t}|\mathbf{w}) &= \mathcal{N}\left(\mathbf{t}|y(\mathbf{x},\mathbf{w}),\beta^{-1}\right) \\ &= \mathcal{N}\left(\mathbf{t}|\boldsymbol{\Phi}^T\mathbf{w},\beta^{-1}\right) \end{aligned}$$

And then $p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$ where

$$\begin{aligned} \mathbf{m}_N &= \mathbf{S}_N\left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\boldsymbol{\Phi}^T\mathbf{t}\right) \\ \mathbf{S}_N^{-1} &= \mathbf{S}_0^{-1} + \beta\boldsymbol{\Phi}^T\boldsymbol{\Phi} \end{aligned}$$

Gaussian Processes

Bibliography I

C.M. Bishop (2016). *Pattern Recognition and Machine Learning*. Information Science and Statistics. Springer New York. ISBN: 9781493938438. URL: https://books.google.com.br/books?id=kOXDtAEACAAJ.

J.L. Crassidis and J.L. Junkins (2011). *Optimal Estimation of Dynamic Systems*. Chapman & Hall/CRC Applied Mathematics & Nonlinear Science. CRC Press. ISBN: 9781439839867. URL: https://books.google.com.br/books?id=CmjRBQAAQBAJ.

P.J. Dhrymes (2013). *Mathematics for Econometrics*. SpringerLink : Bücher. Springer New York. ISBN: 9781461481454. URL: https://books.google.com.br/books?id=HIK8BAAAQBAJ.

J. L. Doob (Sept. 1944). "The Elementary Gaussian Processes". In: *Ann. Math. Statist.* 15.3, pp. 229–282. DOI: 10.1214/aoms/1177731234. URL: https://doi.org/10.1214/aoms/1177731234.

Bibliography II

F.A. Graybill (2001). *Matrices with Applications in Statistics*. Duxbury Classic Series. Brooks/Cole. ISBN: 9780534401313. URL: https://books.google.com.br/books?id=BV3CAAAACAAJ.

T.B. Schön (2011). *Manipulating the Multivariate Gaussian Density*. URL: http://user.it.uu.se/~thosc112/pubpdf/schonl2011.pdf.