Teleinformatics Engineering Department, Federal University of Ceará

Introduction to Gaussian Processes

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Outline

Linear Regression

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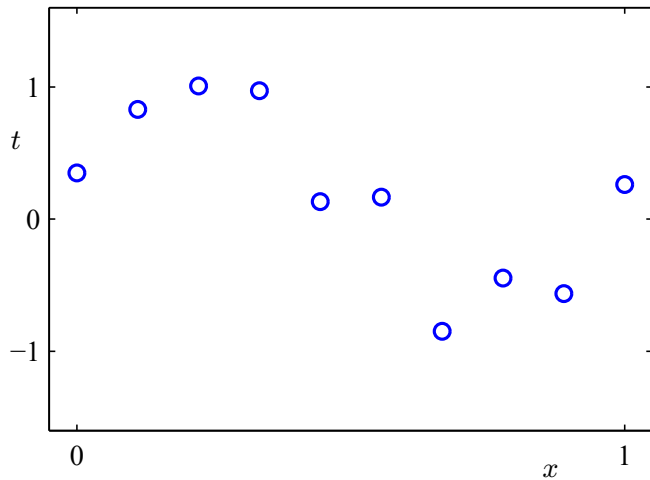
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$$y(x, \mathbf{w}) = w_0 x^0 + w_1 x^1 + w_2 x^2 + ... + w_{M-1} x^{M-1} = \sum_{j=1}^{M-1} w_j x^j$$

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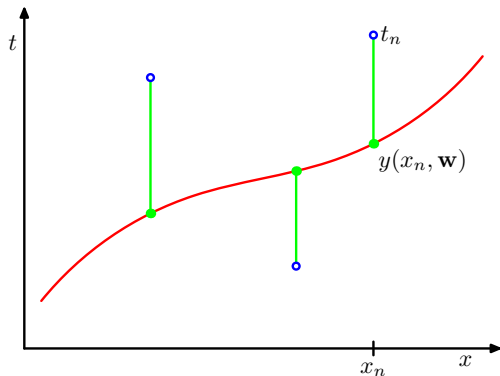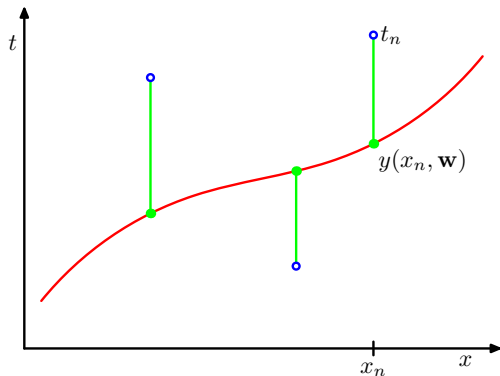
$$y(x, \mathbf{w}) = w_0 \phi_0(x) + w_1 \phi_1(x) + w_2 \phi_2(x) + ... + w_{M-1} \phi_{M-1}(x) = \sum_{j=1}^{M-1} w_j \phi_j(x)$$

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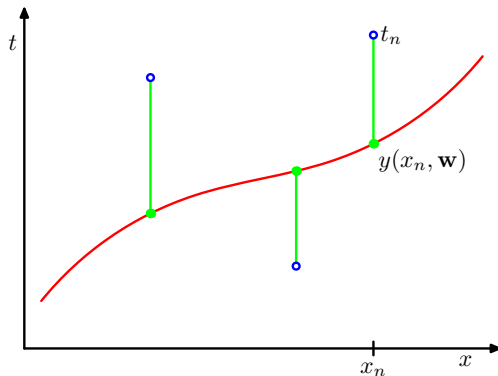
Here, let's define the sum of these distances as *cost function*, or loss function, and write as

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

Remembering that

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

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

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

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.

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

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

Here, we've obtained $\mathbf{w}$ for the curve fitting.
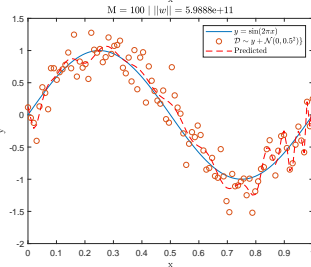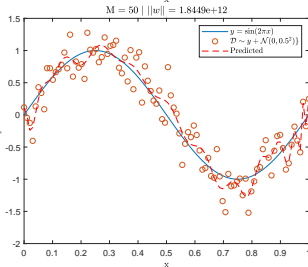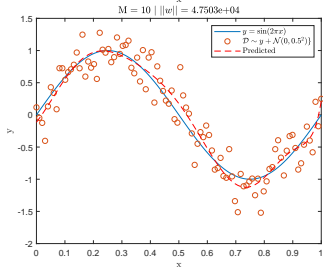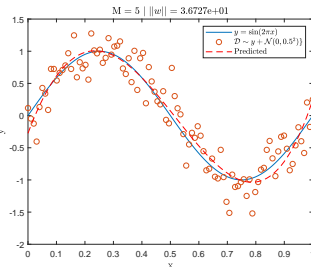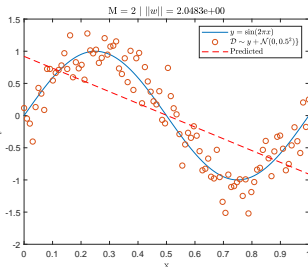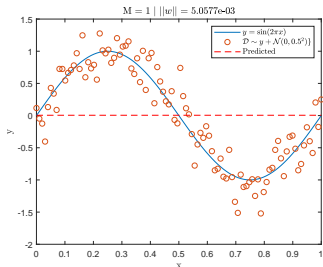
A visible effect of the *increase of the complexity* of the model, represented here by *M*, is the *increase of the weights*. We call it **over-fitting**.

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This phenomenon illustrate a method of ever search for the *best estimation for the parameters*.

M = 50 | $||w|| = 1.8449e+12$
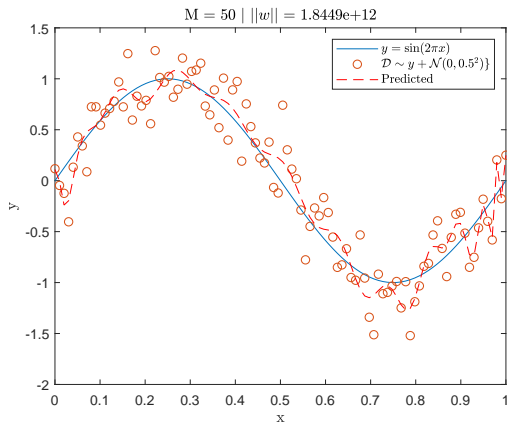
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This phenomenon illustrate a method of ever search for the *best estimation for the parameters*.

It's reasonable to see that our model start's to differ from the y and starts to interpolate the noise.
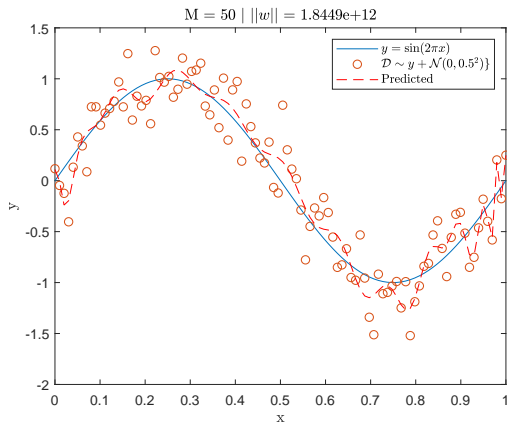
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Legend:
- $y = \sin(2\pi x)$
- $\mathcal{D} \sim y + \mathcal{N}(0, 0.5^2)\}$
- Predicted

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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}
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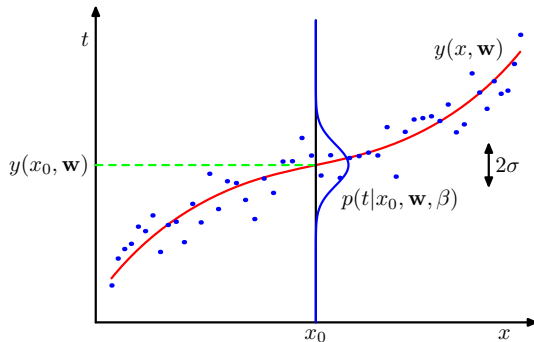
Let's go back to the initial problem of curve fitting. Each observation of the phenomenon is described with a random variable whose *mean* is given by $y(x, \mathbf{w})$, and the *variance* by β.
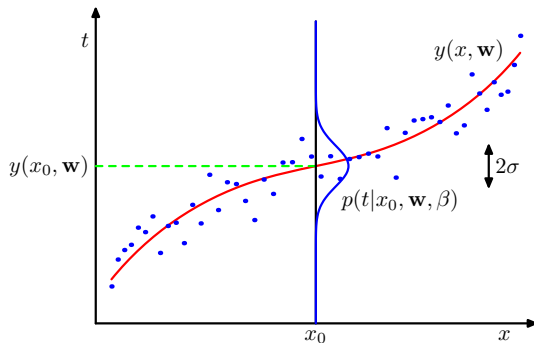
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Then, we want to obtain the probability of the *targets*, given some parameters, in this case $\mathbf{x}$, $\mathbf{w}$ and β.
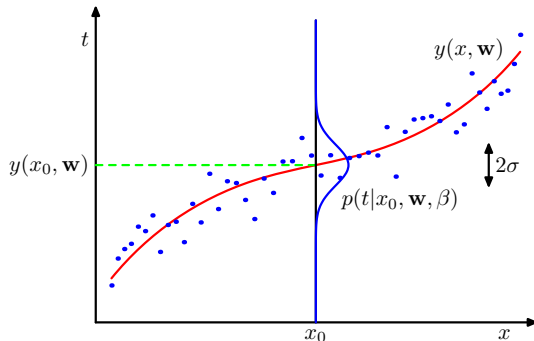
So, if we consider that our conditions are such that being the random variables independent and identically distributed, we can say that our *joint probability* is given by

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

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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

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

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

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

To proceed, we need to know what distribution p is. Let's choose the **Gaussian distribution**.
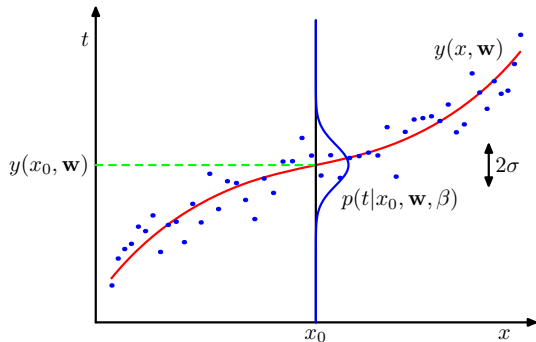
The **Gaussian distribution** comes from many different contexts, as the one that maximize the entropy among of all ones with fixed variance and from the sum of multiple random variables with finite variance.
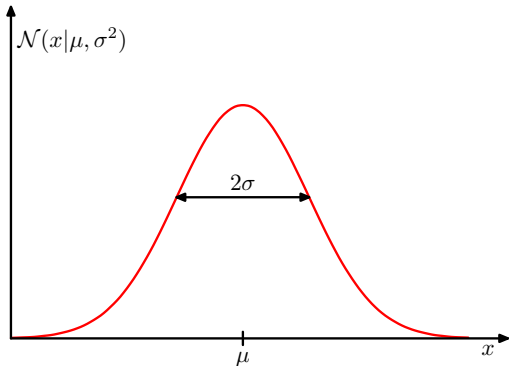
One-dimensional Gaussian distribution

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

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

Now, back to the discussion of the maximization of

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

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

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

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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. We'll obtain

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

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

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**.

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' Theorem**, to convert a *prior* probability in a *posterior* probability.

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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 Mth order. Variables such α are called *hyperparameters* and control the distribuition of model parameters.

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).

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

Seeking a Bayesian approach, the next steps consists to apply the **sum** and **product** rules of probability to evaluate the predictive distribution $p(t|x, \mathbf{x}, \mathbf{t})$. By now we assume that the hyperparameters are fixed, but they could assume a distribution too.

We saw that the posterior distribution for $\mathbf{w}$ could be given by

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

To reach the equality

$$p\left(\mathbf{w}|\mathbf{x}, \mathbf{t}\right) = \frac{p\left(\mathbf{t}|\mathbf{w}, \mathbf{x}\right) p\left(\mathbf{w}\right)}{p(\mathbf{w}, \mathbf{x})}$$

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 $\mathbf{S}_0$.

Remember the One-dimensional Gaussian distribution

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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.

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×D-dimensional variance matrix and $|\boldsymbol{\Sigma}|$ its determinant.

Partitioned Gaussians

Given a joint Gaussian distribution $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with $\boldsymbol{\Lambda} \equiv \boldsymbol{\Sigma}^{-1}$ and

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix}, \boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{pmatrix}, \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{pmatrix}, \boldsymbol{\Lambda} = \begin{pmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{pmatrix}.$$

Will give us

- Conditional distribution:

$$p\left(\mathbf{x}_a|\mathbf{x}_b\right) = \mathcal{N}\left(\mathbf{x}_a|\boldsymbol{\mu}_{a|b}, \boldsymbol{\Lambda}_{aa}^{-1}\right), \; \boldsymbol{\mu}_{a|b} = \boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ab}\left(\mathbf{x}_b - \boldsymbol{\mu}_b\right)$$

- Marginal distribution:

$$p\left(\mathbf{x}_a\right) = \mathcal{N}\left(\mathbf{x}_a|\boldsymbol{\mu}_a, \boldsymbol{\Sigma}_{aa}\right)$$

We stated before that the Bayes' theorem could be used to **adjust** our model parameters as we obtain evidences. Let's partitionate our distribution $\mathbf{z}$ as

$$\mathbf{z} = \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}$$

The strategy here is to make predictions for $\mathbf{y}$. We do this evaluating the probabilities for the whole distribution $\mathbf{z}$. And the key idea is, being $\mathbf{y}$ part of $\mathbf{z}$, we can evaluate its probabilities from $\mathbf{x}$, assuming that the partionated distributions remains Gaussian.

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

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

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$$p(\mathbf{x}) = \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}\right)$$

$$p(\mathbf{y}|\mathbf{x}) = \mathcal{N}\left(\mathbf{y}|\mathbf{A}\mathbf{x} + \mathbf{b}, \mathbf{L}^{-1}\right)$$

So, applying the joint distribution and the its ln after

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

$$\ln p(\mathbf{z}) = \ln p(\mathbf{y}|\mathbf{x}) + \ln p(\mathbf{x})$$

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

$$-\frac{1}{2}(\mathbf{y} - \mathbf{A}\mathbf{x} - \mathbf{b})^T \mathbf{L} (\mathbf{y} - \mathbf{A}\mathbf{x} - \mathbf{b}) + \text{const}$$

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

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

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So, applying the joint distribution and the its ln after

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

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

$$\ln p\left(\mathbf{z}\right) = -\frac{1}{2}\mathbf{x}^T\left(\mathbf{\Lambda} + \mathbf{A}^T\mathbf{L}\mathbf{A}\right)\mathbf{x} - \frac{1}{2}\mathbf{y}^T\mathbf{L}\mathbf{y} + \frac{1}{2}\mathbf{y}^T\mathbf{L}\mathbf{A}\mathbf{x} + \frac{1}{2}\mathbf{x}^T\mathbf{A}^T\mathbf{L}\mathbf{y}$$

$$= -\frac{1}{2}\begin{pmatrix}\mathbf{x}\\\mathbf{y}\end{pmatrix}^T\begin{pmatrix}\mathbf{\Lambda} + \mathbf{A}^T\mathbf{L}\mathbf{A} & -\mathbf{A}^T\mathbf{L}\\-\mathbf{L}\mathbf{A} & \mathbf{L}\end{pmatrix}\begin{pmatrix}\mathbf{x}\\\mathbf{y}\end{pmatrix} = -\frac{1}{2}\mathbf{z}^T\mathbf{R}\mathbf{z}$$

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

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

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

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

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

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

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By inspection of the linear terms

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

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

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

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By inspection of the linear terms

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

And then we we'll have that

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

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

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

Marginal and Conditioned Gaussians

From the results above, we'll have

- For $\mathbf{y}$ given $\mathbf{x}$:

$$p\left(\mathbf{y}|\mathbf{x}\right) = \mathcal{N}\left(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}\right)$$

$$p\left(\mathbf{x}\right) = \mathcal{N}\left(\mathbf{y}|\mathbf{A}\mathbf{x} + \mathbf{b}, \mathbf{L}^{-1}\right)$$

- For $\mathbf{x}$ given $\mathbf{y}$:

$$p\left(\mathbf{x}|\mathbf{y}\right) = \mathcal{N}\left(\mathbf{y}|, \boldsymbol{\Sigma}\left\{\mathbf{A}^T\mathbf{L}(\mathbf{y} - \mathbf{b} + \boldsymbol{\Sigma}\boldsymbol{\mu})\right\}, \boldsymbol{\Sigma}\right)$$

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

We'll make the same optimization we made for the mono-variate case. So the logarithmic likelihood results

Maximum likelihood for the Gaussian

$$\ln p\left(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\Sigma}\right) = -\frac{ND}{2}\ln(2\pi) - \frac{N}{2}\ln|\boldsymbol{\Sigma}| - \frac{1}{2}\sum_{n=1}^{N}\left(\mathbf{x}_n - \boldsymbol{\mu}\right)^T \Sigma^{-1}\left(\mathbf{x}_n - \boldsymbol{\mu}\right)$$

Gaussian Processes

In order to motivate the Gaussian process viewpoint, let us return to the linear regression example and re-derive the predictive distribution by working in terms of distributions over functions $y(x, \mathbf{w})$. This will provide a specific example of a Gaussian process. Consider a model defined in terms of a linear combination of M fixed basis functions given by the elements of the vector (x) so that where x is the input vector and w is the M-dimensional weight vector.

Appendix

Definition (Matrix Multiplication)

Given $\mathbf{A}$ being $m \times n$ and $\mathbf{B}$ being $p \times q$

$$\mathbf{AB} = \left[\sum_{s=1}^{n} a_{is} b_{sj} \right], \text{ with } n = p$$

$$\mathbf{BA} = \left[\sum_{k=1}^{r} b_{ik} a_{kj} \right], \text{ with } m = q$$

Definition (Matrix Multiplication)

Given $\mathbf{A}$ being $m \times n$ and $\mathbf{B}$ being $p \times q$

$$[\mathbf{AB}]^T = \left[\sum_{s=1}^{m} a_{is} b_{sj} \right]^T = \left[\sum_{s=1}^{n} b_{is} a_{sj} \right] = \mathbf{B}^T \mathbf{A}^T, \text{ with } n = p$$

Proposition

Given $\mathbf{y}$ being $m \times 1$, $\mathbf{x}$ being $n \times 1$, $\mathbf{A}$ being $m \times n$ independent of $\mathbf{x}$ and

$$\mathbf{y} = \mathbf{A}\mathbf{x}$$

Then

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \mathbf{A}$$

Definition (Matrix Derivative)

Given $\mathbf{A}$ being $m \times n$ and $\mathbf{B}$ being $p \times q$

$$\mathbf{AB} = \left[\sum_{s=1}^{n} a_{is} b_{sj} \right]$$

$$\mathbf{BA} = \left[\sum_{k=1}^{r} b_{ik} a_{kj} \right]$$

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