

Teleinformatics Engineering Department, Federal University of Ceará

# Introduction to Gaussian Processes

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# Linear Regression

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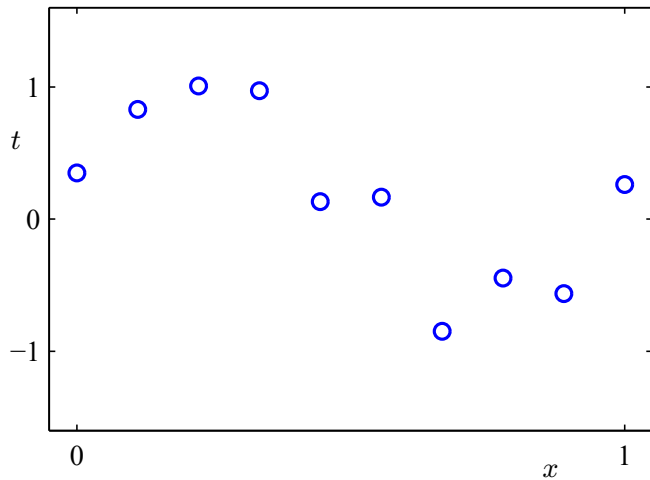
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## Strategy

- 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 points below by polynomial curve fitting



Be the model chosen



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$$y(x, \mathbf{w}) = w_0x^0 + w_1x^1 + w_2x^2 + \dots + w_{M-1}x^{M-1} = \sum_{j=1}^{M-1} w_jx^j$$

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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  $\phi$  could be other *basis function*. For simplicity, we'll carry this notation along.

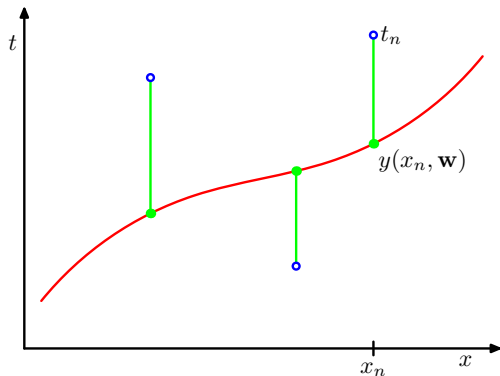
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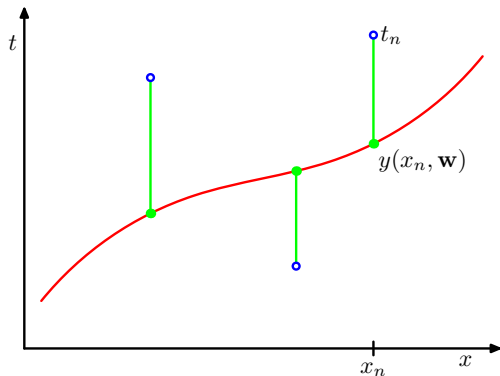
$$y(x, \mathbf{w}) = w_0\phi_0(x) + w_1\phi_1(x) + w_2\phi_2(x) + \dots + w_{M-1}\phi_{M-1}(x) = \sum_{j=1}^{M-1} w_j\phi_j(x)$$

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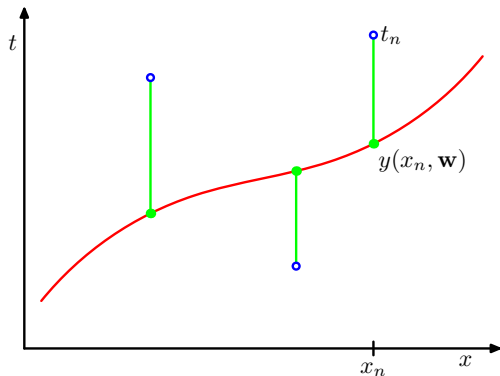
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$$E(\mathbf{w}) \triangleq \frac{1}{2} \sum_{n=1}^N \{y_n - t_n\}^2$$



Insert some *Minkowski* loss.

Remembering that

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

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

$$y_n = [\phi_0(x_n) \quad \phi_1(x_n) \quad \dots \quad \phi_{M-1}(x_n)] \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_{M-1} \end{bmatrix}$$



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  $\mathbf{t} = [t_1 \quad t_2 \quad \dots \quad t_n]^T$

Then we'll have

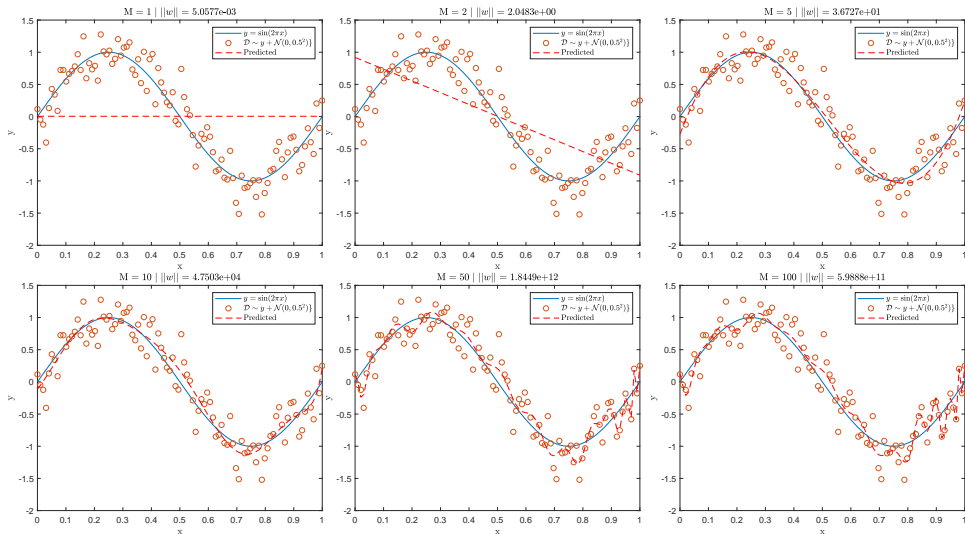
$$\begin{aligned}
 E(\mathbf{w}) &= \frac{1}{2} \left( \mathbf{y}^T \mathbf{y} - \mathbf{t}^T \mathbf{y} - \mathbf{y}^T \mathbf{t} + \mathbf{t}^T \mathbf{t} \right) \\
 &= \frac{1}{2} \left( (\Phi \mathbf{w})^T (\Phi \mathbf{w}) - \mathbf{t}^T (\Phi \mathbf{w}) - (\Phi \mathbf{w})^T \mathbf{t} + \mathbf{t}^T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

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

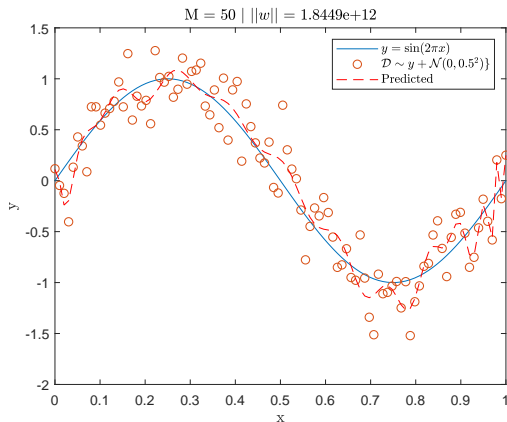
In sequence, we'll try to minimize it in terms of the weights ( $\mathbf{w}$ ) by

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

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

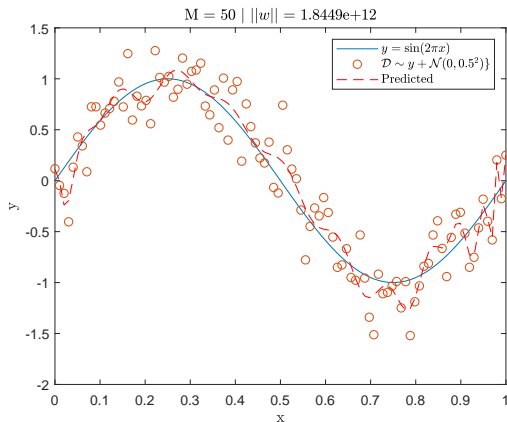


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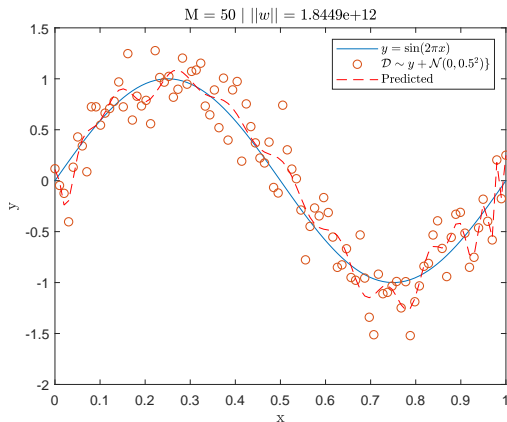
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Last, a basic concept it's that larger weights could imply in massive system inputs, and this sometimes it's wanted to be avoided.



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



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

# A probabilistic perspective

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

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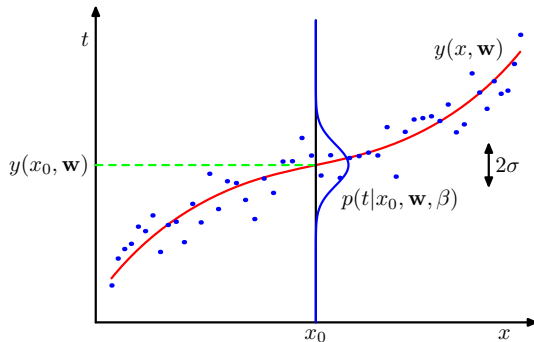
## Sentence

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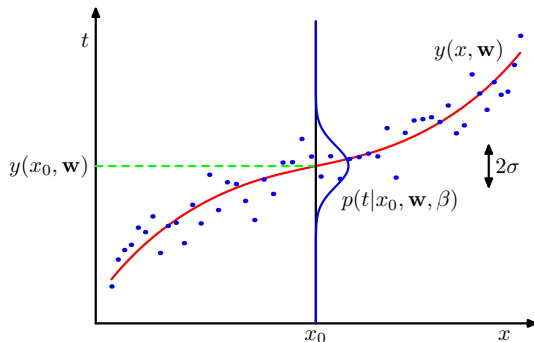
Let's go back to the initial problem of curve fitting. Each observation of the phenomenon is described with a random variable whose *mean* is given by  $y(x, \mathbf{w})$ , and the *variance* by  $\beta$ .

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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

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

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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

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

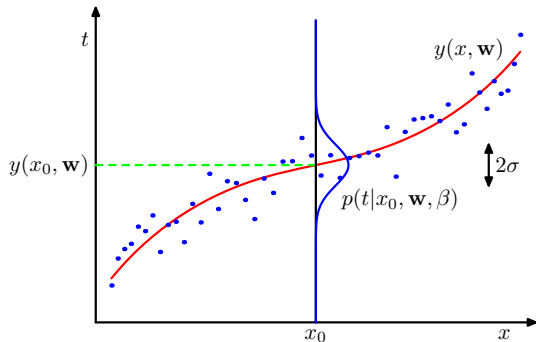
Reminding that

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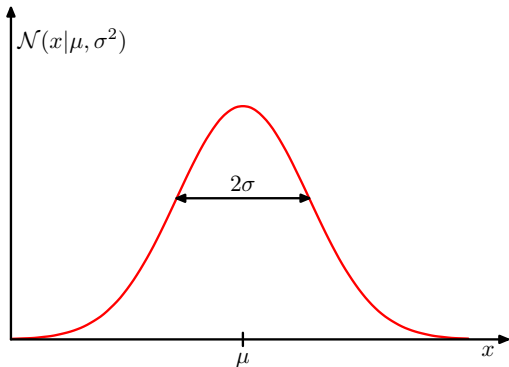
Implies that

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

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 maximizes 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  $\mu$  is the mean and  $\sigma^2$  the variance.

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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

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

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From this, we could obtain the **maximum likelihood**, taking the derivatives of the log probability to zero, according to the terms  $\beta$  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  $\mathbf{w}$ , our expression becomes closer to the *error function* presented previously, added the dependency of  $\beta$

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

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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and by simplicity, consider

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

where  $\alpha$  is the precision of the distribution and  $M + 1$  is the dimension of  $\mathbf{w}$ , for a polynomial of  $M^{th}$  order.



By this, we can find a distribution and its maximum, or most probable value of  $\mathbf{w}$  given the data taking the minimum of the negative logarithm of the inferred expression, that will lead us to a term

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

Note that if we consider  $\lambda = \alpha/\beta$ , this will back to the regularized form of *least squares*.

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 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.

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, let's call this a **Bayesian Linear Regression**.

# Bayesian Linear Regression

Remember the One-dimensional Gaussian distribution

## 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  $\sigma^2$ . 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 identity 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.

## 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:**

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

- **Marginal distribution:**

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



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.

# Bayes' theorem for Gaussian variables

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

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

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So, applying the joint distribution and the its ln after

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

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

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

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

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

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

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

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

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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

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



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By inspection of the linear terms

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

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By inspection of the linear terms

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

And then we we'll have that

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

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

## Marginal and Conditioned Gaussians

From the results above, we'll have

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

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

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

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

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

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

# 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  $\phi(x)$  so that where  $x$  is the input vector and  $\mathbf{w}$  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  $p \times q$

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

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