

Teleinformatics Engineering Department, Federal University of Ceará

Introduction to Gaussian Processes

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Linear Regression

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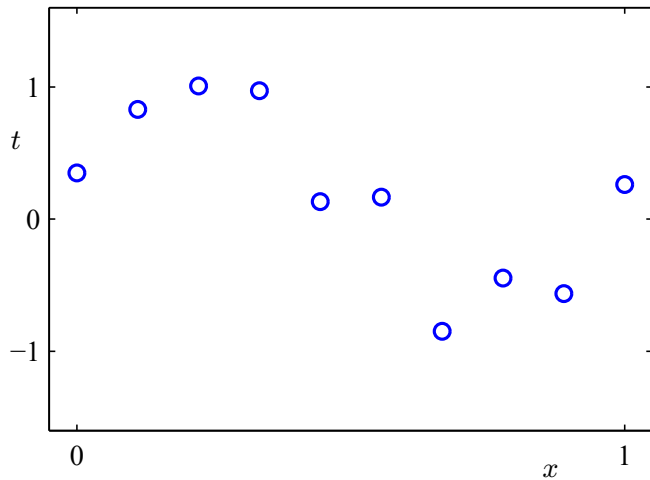
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Strategy

- 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 ϕ could be other *basis function*. For simplicity, we'll carry this notation along.

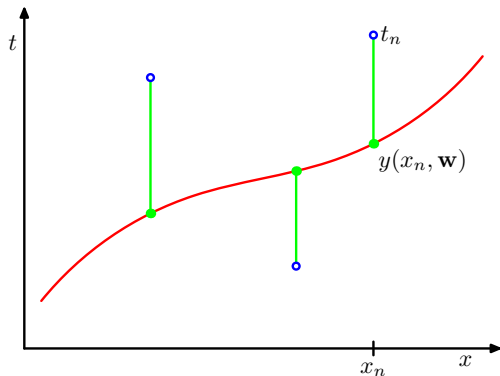
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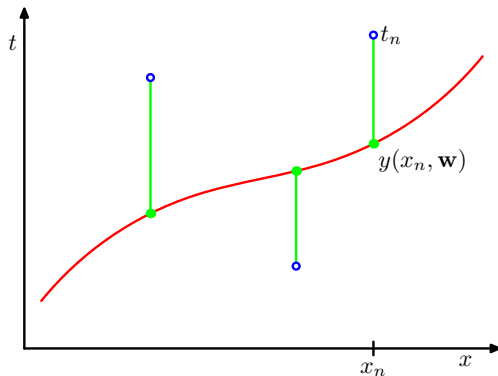
$$y(x, \mathbf{w}) = w_0\phi_0(x) + w_1\phi_1(x) + w_2\phi_2(x) + \dots + w_{M-1}\phi_{M-1}(x) = \sum_{j=1}^{M-1} w_j\phi_j(x)$$

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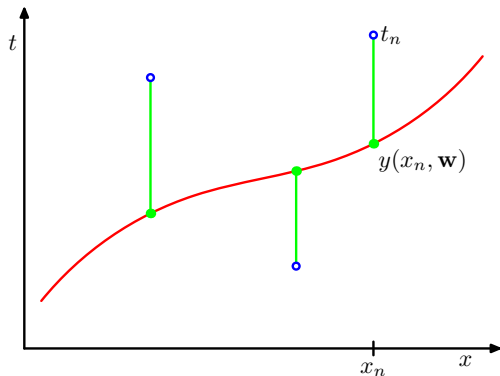
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Here, let's define the sum of these distances as *cost function*, or loss function, and write as

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



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

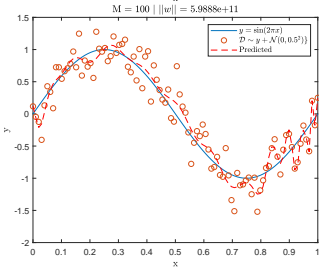
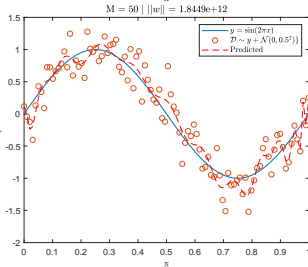
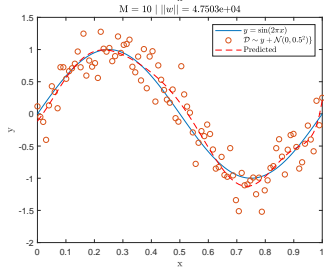
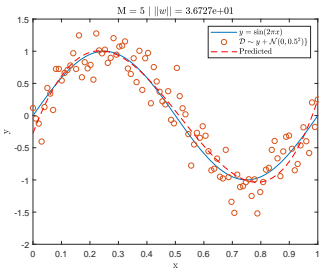
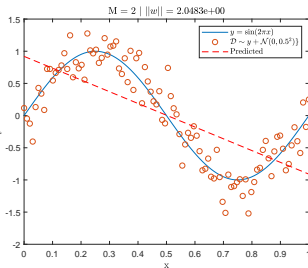
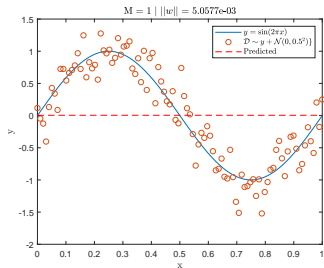
$$\begin{aligned}
 E(\mathbf{w}) &= \frac{1}{2} \left(\mathbf{y}^T \mathbf{y} - \mathbf{t}^T \mathbf{y} - \mathbf{y}^T \mathbf{t} + \mathbf{t}^T \mathbf{t} \right) \\
 &= \frac{1}{2} \left((\Phi \mathbf{w})^T (\Phi \mathbf{w}) - \mathbf{t}^T (\Phi \mathbf{w}) - (\Phi \mathbf{w})^T \mathbf{t} + \mathbf{t}^T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

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

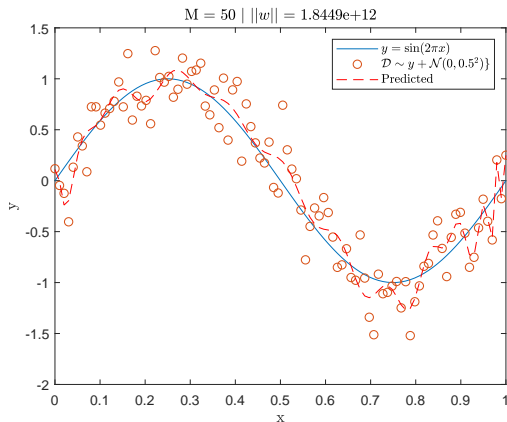
In sequence, we'll try to minimize it in terms of the weights (\mathbf{w}) by

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

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

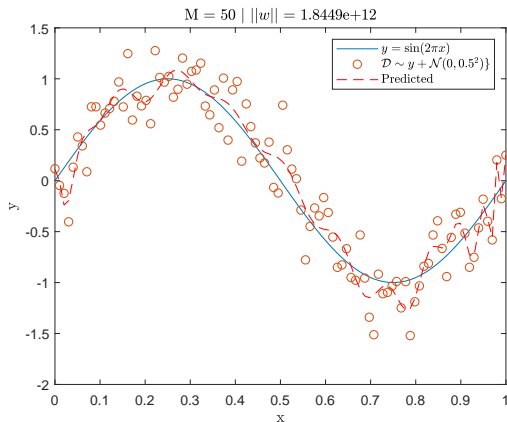


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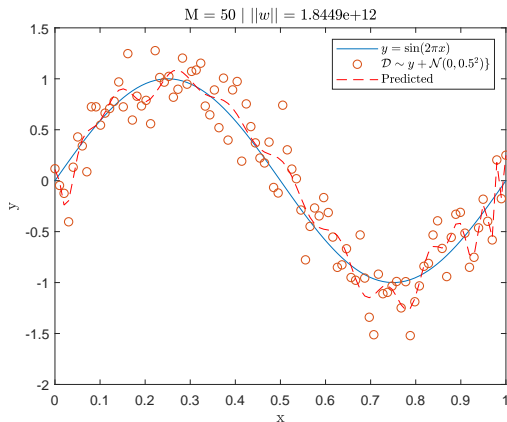
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Last, a basic concept it's that larger weights could imply in massive system inputs, and this sometimes it's wanted to be avoided.



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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

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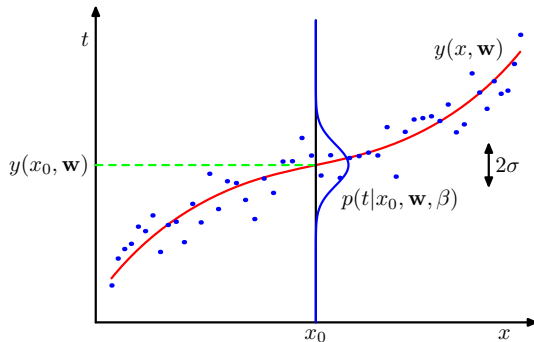
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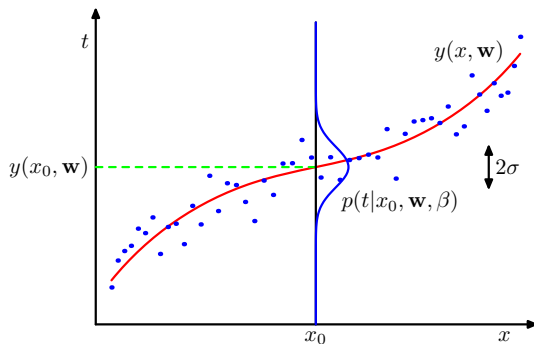
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Then, we want to obtain the probability of the *targets*, given some parameters, in this case \mathbf{x} , \mathbf{w} and β .



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

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

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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

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

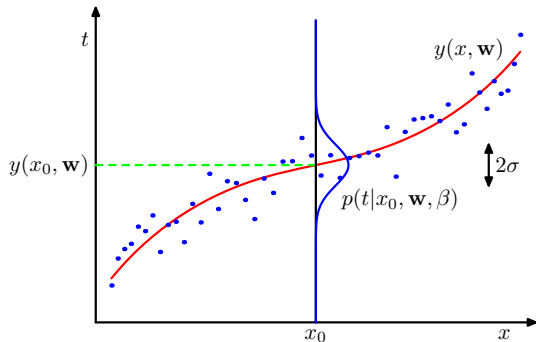
Reminding that

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

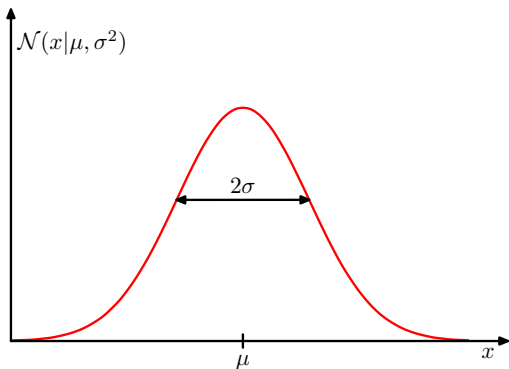
Implies that

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

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

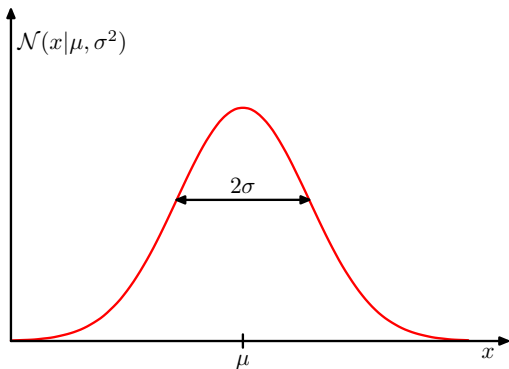


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First we'll consider a geometrical approach by the quadratic distance $(x - \mu)^2$ normalized by the variance σ^2 . This comprehension will help us with the D-dimensional case.



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

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

We could observe that taking the derivative with respect to \mathbf{w} , our expression becomes closer to the *error function* presented previously, added some 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**. But there's a difference between the equations by the term β .

So, here our objective is to find the parameters to minimize the error and maximize the log probability. But it's reasonable to think that we'll face the same **over-fitting** problem presented before. Added to the fact that we don't apply yet a fully *bayesian* treatment of regression, let's introduce some machinery

Bayesian Linear Regression

Remember the One-dimensional Gaussian distribution

One-dimensional Gaussian distribution

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

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

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

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

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

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 partitionated 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

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

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

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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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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 $p \times q$

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

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

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