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Introduction to Gaussian Processes

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April 18, 2019

Outline

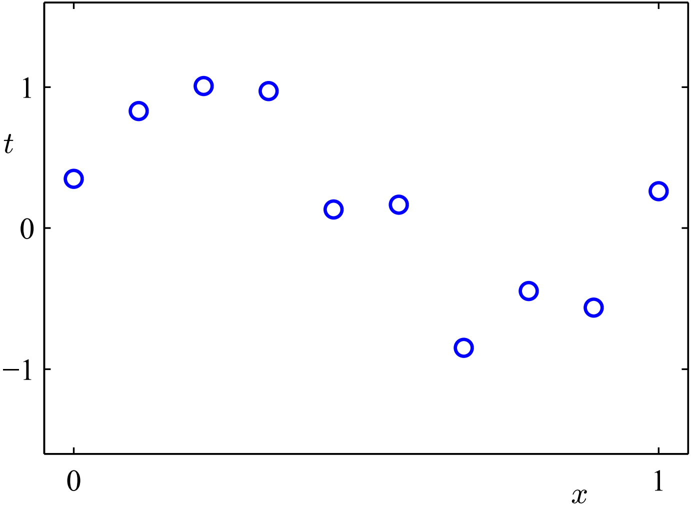
Linear Regression

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

- Let's fit the points below by **polynomial curve fitting**.



- Be the model chosen a **polynomial**, we'll have

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

- In 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**.
- e.g. we could have different ys for different basis functions.

$$\begin{aligned} y(x, \mathbf{w}) &= w_0 \phi_0(x) + w_1 \phi_1(x) + w_2 \phi_2(x) + \ldots + w_{M-1} \phi_{M-1}(x) \\ &= w_0 \exp\left\{-\frac{(x-\mu_0)^2}{2\sigma^2}\right\} + w_1 \exp\left\{-\frac{(x-\mu_1)^2}{2\sigma^2}\right\} + \\ &\ldots + w_{M-1} \exp\left\{-\frac{(x-\mu_{M-1})^2}{2\sigma^2}\right\} \\ &= w_0 \sin(0 \cdot x) + w_1 \cos(1 \cdot x) + \\ &\ldots + w_{M_2} \sin((M-2) \cdot x) + w_{M-1} \cos((M-1) \cdot x) \end{aligned}$$

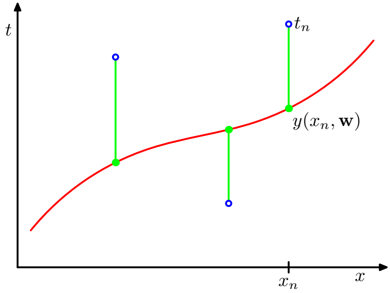
- For simplicity, we'll carry this notation along.

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

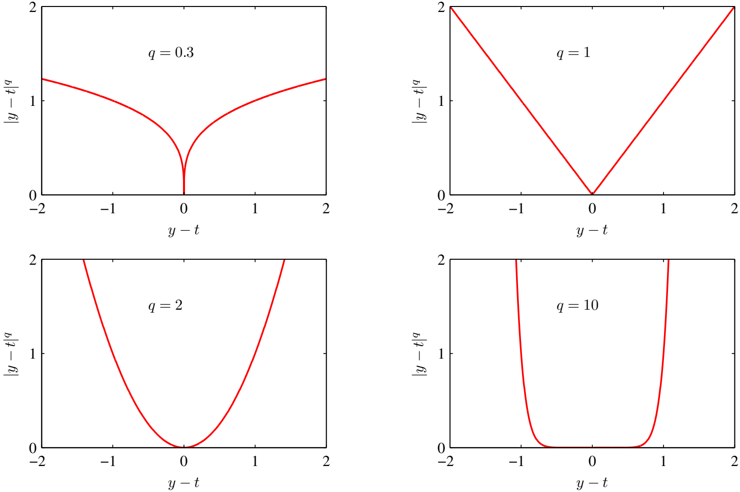
- We'll evaluate ϕ for all x, and then project it in the w vector space, then our model could be formed by **non-linear** functions. But, remaining **linear on parameters**.

- The chosen model will give us some curve that is needed to adjust such that we'll **minimize its distance** to the **targets** (t).
- Here, let's define the sum of these distances as **cost function**, or error function, and write it as

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



Why choose a quadratic norm distance?



Why choose a quadratic norm distance?

- The first row figures could me used for the derivations, taking care with some **non-continuous derivatives**.
- We'll use the **quadratic norm** because its the minor integer q differentiable, and then the error measures E between the model $y(x, \mathbf{w})$ and the targets t will be euclidean.
- More, increasing the value of q, the smallests than 1 and bigger than 0 errors between the model and the targets that become irrelevant for E.

- Remembering that

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

- We'll evaluate for all x_i values, and then put $y_n(x_i, \mathbf{w})$ in the matrix form and get

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

- And then

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

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

If

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

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.

Defining models

In sequence, we'll try to minimize it in terms of the weights (**w**) by

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

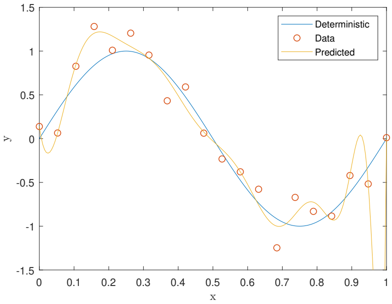
Here, we've obtained **w** for the curve fitting.

```
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
```

Defining models

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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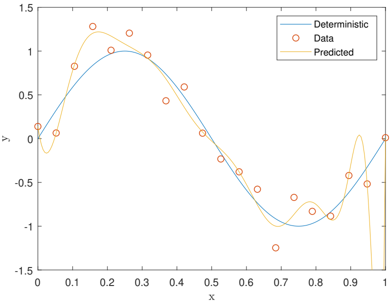

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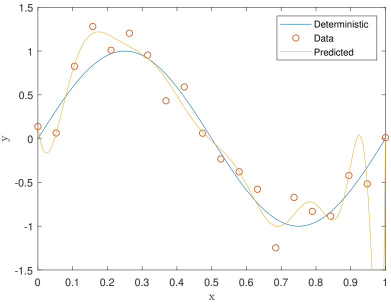
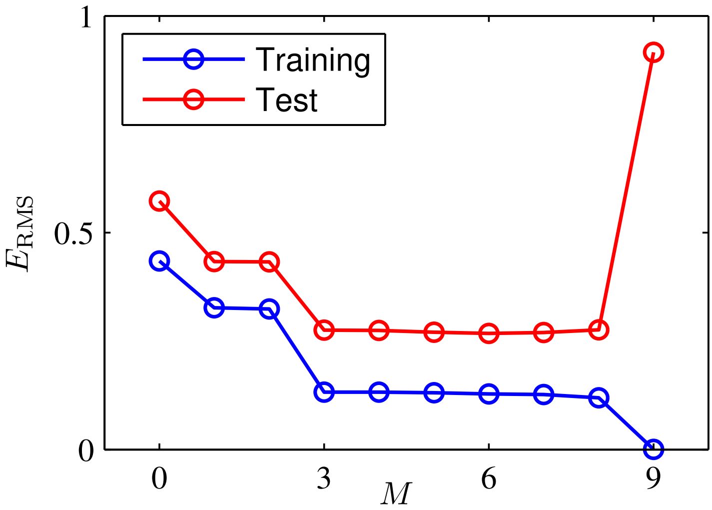
It's reasonable to see that our model start's to differ from the y and starts to interpolate the noise.




1
0.5
0
E_{RMS}
0
3
6
9
M
Training
Test

Defining models

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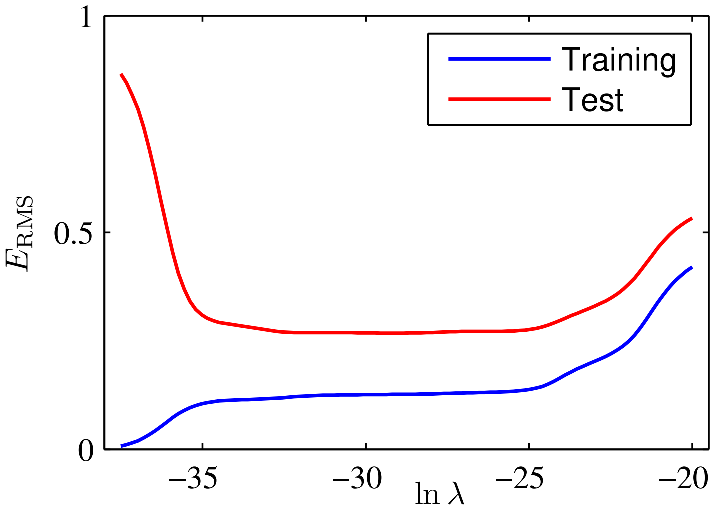
$$
\begin{aligned}
\tilde{E}(\mathbf{w}) =& \frac{1}{2}(\mathbf{y}-\mathbf{t})^T(\mathbf{y}-\mathbf{t}) + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w} \\
=& \frac{1}{2}\left(\mathbf{w}^T\Phi^T\Phi\mathbf{w} - 2\mathbf{t}^T\Phi\mathbf{w} + \mathbf{t}^T\mathbf{t} + \lambda\mathbf{w}^T\mathbf{I}\mathbf{w}\right)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

```
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
```


1
0.5
0
E_{RMS}
−35
−30
−25
−20
$\ln \lambda$
Training
Test

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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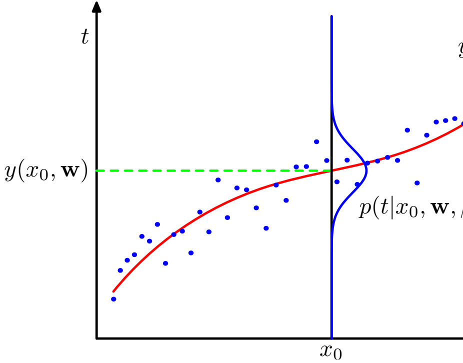
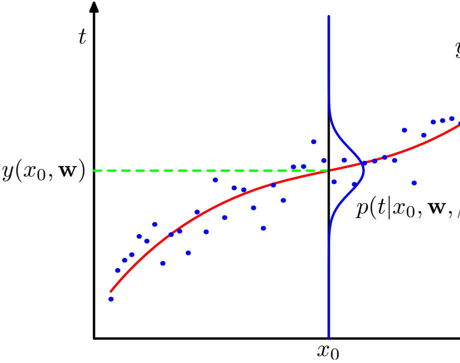


A probabilistic perspective

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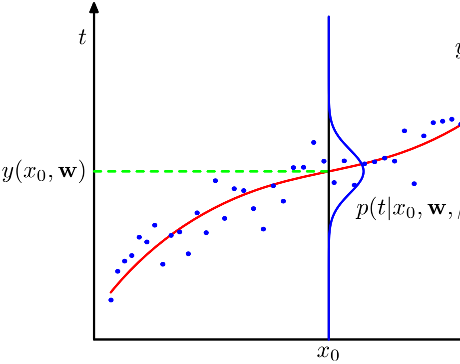
Then, we want to obtain the probability of the *targets*, given some parameters, in this case $\mathbf{x}$, $\mathbf{w}$ and β.



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

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

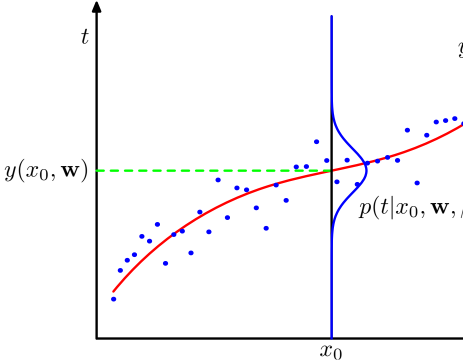
Reminding that

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

Implies that

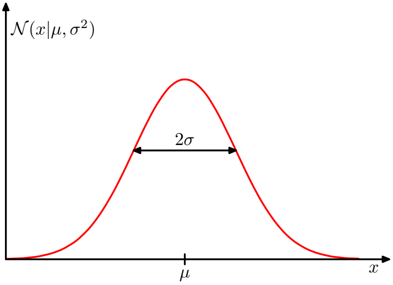
$$\ln\left(p(\mathbf{t}|\mathbf{x},\mathbf{w},\beta)\right) = \sum_{n=1}^{N} \ln\left(p\left(t_n|x_n,\mathbf{w},\beta\right)\right)$$

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.



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

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

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we can state a Gaussian distribution for each target and then

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

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

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

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.

Mathematically, by Bayes' Rule, we could infer

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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 **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 **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

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

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

Remember the One-dimensional Gaussian distribution

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

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

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

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

And then

D-dimensional Gaussian distribution

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

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:

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

- Marginal distribution:

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

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 $p\left(\mathbf{y}\right)$ and the conditional distribution $p\left(\mathbf{x}|\mathbf{y}\right)$, given

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

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

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

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

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

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

Bayes' rule for Gaussian variables

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

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

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

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

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

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

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

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

By inspection of the linear terms

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

Bayes' rule for Gaussian variables

And then we we'll have that

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

Bayes' rule for Gaussian variables

And then we we'll have that

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

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

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 $\mathbf{S}_0$.

Marginal and Conditioned Gaussians

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

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

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

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

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

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

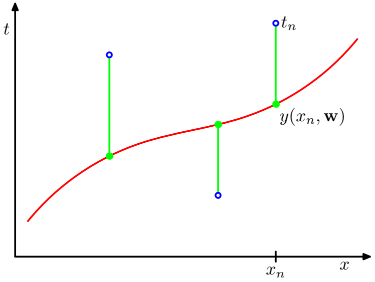
And then $p(\mathbf{w}|\mathbf{t}) = \mathcal{N}\left(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N\right)$ where

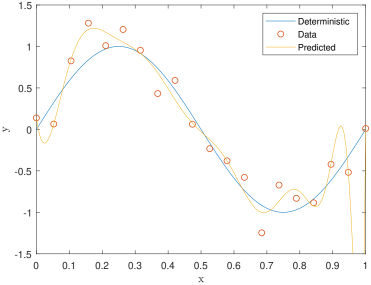
$$\begin{aligned} \mathbf{m}_N &= \mathbf{S}_N \left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\mathbf{\Phi}^\top \mathbf{t}\right) \\ \mathbf{S}_N^{-1} &= \mathbf{S}_0^{-1} + \beta\mathbf{\Phi}^\top \mathbf{\Phi} \end{aligned}$$

Gaussian Processes

What was done until here?

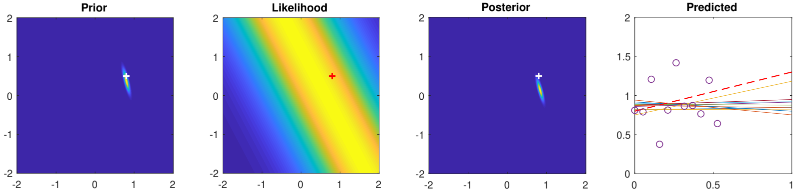
- We assumed that our targets t were **i.i.d.** and given by $t = y(\mathbf{x}) + \varepsilon$, where $\varepsilon \sim \mathcal{N}(0, \beta)$.
- Our model is given by $\mathbf{y}(\mathbf{x}) = \Phi^\top \mathbf{w}$, where Φ is the **design matrix**, and this caracterize our model as **linear in parameters**.
- The **design matrix** was defined as $\phi_{i,j} = \phi_i(\mathbf{x}_j)$.
- The **parameters** were given by $\mathbf{w} = \left(\Phi^\top \Phi\right)^{-1} \Phi^\top \mathbf{t}$.
- These **parameters** calculated at the minimum of the cost function are called **maximum likelihood**.





What was done until here?

- We put an **uncertainty** over the targets t and the parameters $\mathbf{w}$.
- We assumed that targets being **distributed** as $p(t|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1})$.
- By **Bayes' Rule** we obtained that $p\left(\mathbf{w}|\mathbf{x}, \mathbf{t}, \alpha, \beta\right) \propto p\left(\mathbf{t}|\mathbf{w}, \mathbf{x}, \beta\right) p\left(\mathbf{w}|\alpha\right)$
- This allowed to make an **inference** to obtain a **prediction** of the parameters in the **weight-space**.



From Bayesian inference

- We have

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

- We'll change from **weight-space**

$$p(\mathbf{t}_*|\mathbf{x}_*, \mathbf{x}, \mathbf{t}) = \int p(\mathbf{t}_*|\mathbf{x}_*, \mathbf{w})p(\mathbf{w}|\mathbf{x}, \mathbf{t})\mathrm{d}\mathbf{w}$$

- To **feature-space**

$$\begin{aligned} p\left(f_*|\mathbf{x}_*, \Phi, \mathbf{t}\right) &= \int p\left(f_*|\mathbf{x}_*, \mathbf{w}\right) p(\mathbf{w}|\Phi, \mathbf{t})d\mathbf{w} = \int \mathbf{x}_*^\top \mathbf{w}\, p(\mathbf{w}|\Phi, \mathbf{t})d\mathbf{w} \\ &= \mathcal{N}\left(\beta\boldsymbol{\phi}(\mathbf{x}_*)^\top \mathbf{S}_N \Phi \mathbf{t}, \boldsymbol{\phi}(\mathbf{x}_*)^\top \mathbf{S}_N^{-1} \boldsymbol{\phi}(\mathbf{x}_*)\right) \end{aligned}$$

where $f_* \triangleq f\left(\mathbf{x}_*\right)$ at $\mathbf{x}_*$ and $\Phi = \Phi(\mathbf{x})$

Alternative formulation

$$f_*|\mathbf{x}_*, \Phi, \mathbf{t} \sim \mathcal{N}\left(\boldsymbol{\phi}_*^\top \mathbf{S}_0 \Phi \left(K + \beta^{-2} I\right)^{-1} \mathbf{t}, \boldsymbol{\phi}_*^\top \mathbf{S}_0 \boldsymbol{\phi}_* - \boldsymbol{\phi}_*^\top \mathbf{S}_0 \Phi \left(K + \beta^{-2} I\right)^{-1} \Phi^\top \mathbf{S}_0 \boldsymbol{\phi}_*\right)$$

where $K = \Phi^\top \mathbf{S}_0 \Phi$

What is kernel?

$$f_*|\mathbf{x}_*, \Phi, \mathbf{t} \sim \mathcal{N}\left(\boldsymbol{\phi}_*^\top \mathbf{S}_0 \Phi \left(K + \beta^{-2} I\right)^{-1} \mathbf{t}, \boldsymbol{\phi}_*^\top \mathbf{S}_0 \boldsymbol{\phi}_* - \boldsymbol{\phi}_*^\top \mathbf{S}_0 \Phi \left(K + \beta^{-2} I\right)^{-1} \Phi^\top \mathbf{S}_0 \boldsymbol{\phi}_*\right)$$

- We could observe the appearance of terms like $\Phi^\top \mathbf{S}_0 \Phi$, $\boldsymbol{\phi}_*^\top \mathbf{S}_0 \Phi$, or $\boldsymbol{\phi}_*^\top \mathbf{S}_0 \boldsymbol{\phi}_*$.
- The common term between these operations is $k(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^\top \mathbf{S}_0 \boldsymbol{\phi}(\mathbf{x}')$
- Then we define $k(\cdot, \cdot)$ as **kernel function**
- This technique is particularly valuable in situations where it is more convenient to compute the kernel than the design matrix vectors themselves.

- Previously we make the inference in the **feature-space** and then we find the function distribution.
- Now we'll make the inference directly on **function-space**.
- Let's define

Definition

*A **Gaussian process** is a collection of random variables which any finite number of them have a joint Gaussian distribution.*

Mean and covariance function

- As the Gaussian distribution, the $\mathcal{GP}$ is characterized by its **mean function** $m(\mathbf{x})$ and its **covariance function** $k(\mathbf{x}, \mathbf{x}')$ of a real process $f(\mathbf{x})$.
- For a Gaussian processes

$$f(\mathbf{x}) \sim \mathcal{GP}\left(m(\mathbf{x}), k\left(\mathbf{x}, \mathbf{x}'\right)\right)$$

- We have

$$\begin{aligned} m(\mathbf{x}) &= \mathbb{E}[f(\mathbf{x})] \\ k\left(\mathbf{x}, \mathbf{x}'\right) &= \mathbb{E}\left[(f(\mathbf{x}) - m(\mathbf{x}))\left(f\left(\mathbf{x}'\right) - m\left(\mathbf{x}'\right)\right)\right] \end{aligned}$$

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