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Introduction to Gaussian Processes

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Outline

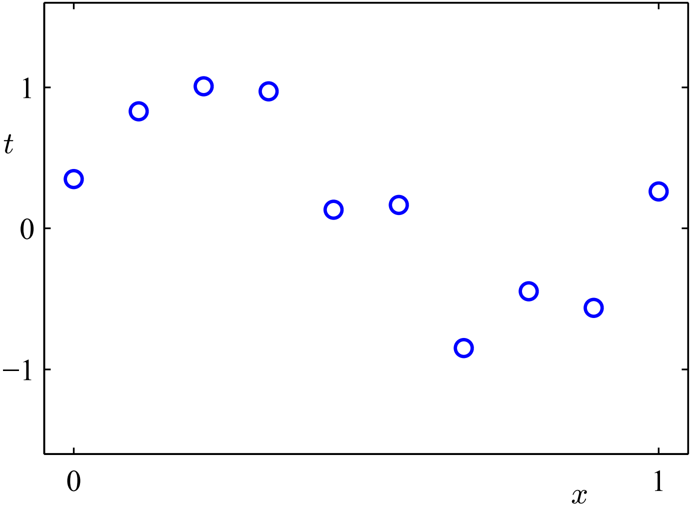
Linear Regression

- 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 take the points below generated from the function $y(x) = \sin(2\pi x)$ with addition of Gaussian noise with zero mean and 0.2 of standard deviation.



- We can express the curve with a polynomial, being the **model**

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

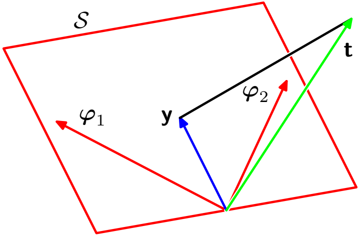
- In general, we could write this **weighted sum** with any other function. In other words, we can put this in terms of $\phi_n(x) = x^n$, where ϕ could be other **basis function**.
- e.g. we could have different $y(x)$ for different basis functions, or **features**.

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

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

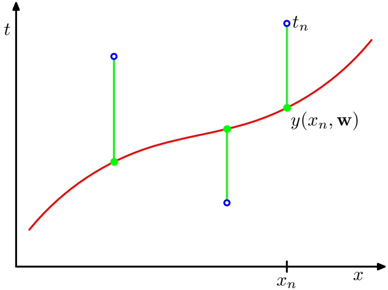
$$
\begin{aligned}
y(x, \mathbf{w}) &= w_0\phi_0(x) + w_1\phi_1(x) + \dots \\
&\quad + w_{M-1}\phi_{M-1}(x) \\
&= \sum_{j=1}^{M-1} w_j\phi_j(x)
\end{aligned}
$$

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

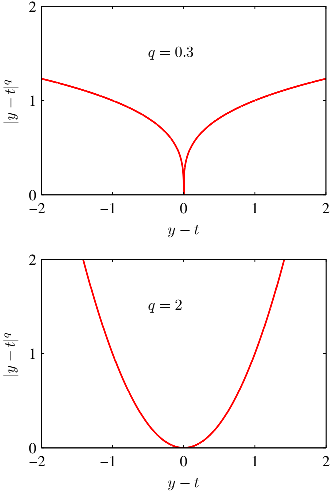


- The chosen model will give us some curve that is needed to adjust such that we'll **minimize its distance** to the **targets** t.
- This approach lead us to use the **least squares** to estimate the weights and minimize the **error** E.

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



Why choose a quadratic norm distance?



Why choose a quadratic norm distance?[1]

- The first row figures could be 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.

[1] See Appendix ?

- 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

$$\underbrace{\begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_{N-1} \end{bmatrix}}_{\mathbf{y}} = \underbrace{\begin{bmatrix} \phi_0(x_0) & \phi_1(x_0) & \ldots & \phi_{M-1}(x_0) \\ \phi_0(x_1) & \phi_1(x_1) & \ldots & \phi_{M-1}(x_1) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(x_{N-1}) & \phi_1(x_{N-1}) & \ldots & \phi_{M-1}(x_{N-1}) \end{bmatrix}}_{\Phi} \underbrace{\begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_{N-1} \end{bmatrix}}_{\mathbf{w}}$$

  where Φ is the **design matrix**.
- This represents the system $\mathbf{y} = \Phi\mathbf{w}$.

- If $E(\mathbf{w}) = \frac{1}{2}\left(\mathbf{y}-\mathbf{t}\right)^\top\left(\mathbf{y}-\mathbf{t}\right)$ where $\mathbf{t} = \begin{bmatrix} t_1 & t_2 & \dots & t_n \end{bmatrix}^\top$
- Then we'll have

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

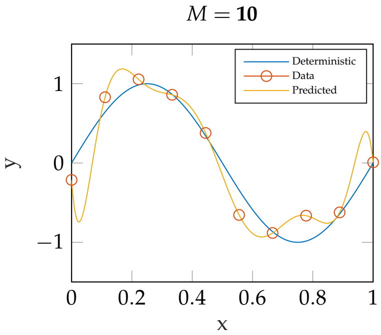
- In sequence, we'll try to minimize it in terms of the weights ($\mathbf{w}$) by

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

- Here, we've obtained the weights $\mathbf{w}^*$ with the **best fit** of the curve.
- We could say that the model **learned** the parameters.

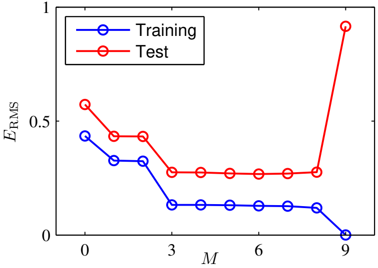
Why the prediction is so distant from the deterministic curve?

- A visible effect of the **increase of the complexity** of the model, is the increase of the **number of features** M.
- It's easy to see that our model start's to differ from the y and starts to interpolate the noise. We call this of **over-fitting**.
- This phenomenon illustrate a method of always search for the **best estimation of the parameters**.



Could be over-fitting a problem?

- We could **train** our model, it means evaluate $\mathbf{w}^*$, for only a part of our dataset.
- If the model be a good one, the error must be small when its **testing**, i.e. the error must be small when we evaluate all dataset with the $\mathbf{w}^*$ of the trained part.
- But this in general does not occur and the **error increases**.

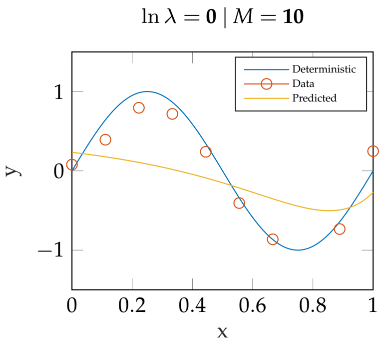


How to control the over-fitting?

- With the increase of the model complexity, the value of $\mathbf{w}^*$ increases too.
- A solution could be add a **penalty term** as the norm of the weights increases.
- 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.

$$\tilde{E}(\mathbf{w}) = \frac{1}{2}(\mathbf{y}-\mathbf{t})^\top(\mathbf{y}-\mathbf{t}) + \frac{\lambda}{2}\mathbf{w}^\top\mathbf{w}$$

$$\Rightarrow \mathbf{w}^*_{\text{reg}} = \left(\Phi^\top\Phi + \lambda\mathbf{I}\right)^{-1}\Phi^\top\mathbf{t}$$



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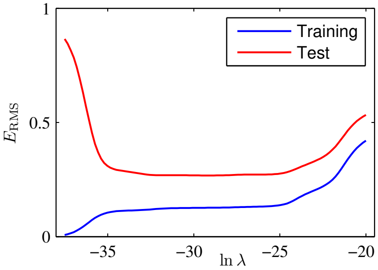
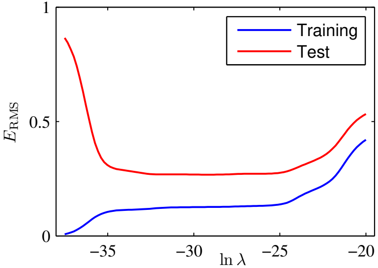
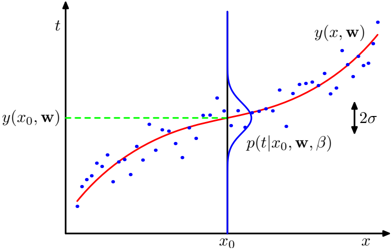


A more sophisticated approach?

- We could **train and test** and evaluate the error for several values of λ.
- Even yet, it's too wasteful partitionate and optimize data to find good model parameters or even a **flexible** one.
- We need a more sophisticated approach.



- Having an **uncertainty** in the measured value, we could represent it with a **probability distribuition**.
- Now, each **target** could be expressed as a **random variable**.
- Its **mean** is given by $y(x, \mathbf{w})$, and the **variance** by $1/\sigma^2 = \beta$.
- β is known as **precision parameter** too.



- Being the random variables independent and identically distributed, we can say that our **joint probability** is given by

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

- Our goal is, given the **parameters** $\mathbf{w}$, maximize the **probability** of the **targets**.
- Before, consider a property of the probability distribuitions

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

- Then, to avoid computational singularity and obtain a monotonically increasing function, we apply

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

- From the **joint probability** of the Gaussians distributions we have

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

- If we make

$$
\frac{\partial}{\partial \mathbf{w}} \ln\left(p(\mathbf{t}|\mathbf{x},\mathbf{w},\beta)\right) = 0
$$

  we'll obtain the **cost function** obtained before in the linear regression.
- In other words, we'll obtain the weights $\mathbf{w}$ that **maximize** the log probability of the targets.
- Next we'll take a step towards to a **Bayesian** approach.

Bayesian Linear Regression

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 $\mathbf{w}$

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

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

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

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

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**.

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 $\mathbf{w}$ could be given by

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

The D-dimensional Gaussian Distribution

Remember the One-dimensional Gaussian distribution

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.

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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

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

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

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

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

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

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

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

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

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

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

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

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

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By inspection of the linear terms

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

Bayes' rule for Gaussian variables

And then we we'll have that

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

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

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

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

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

Bayes' rule for Gaussian variables

Marginal and Conditioned Gaussians

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

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

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

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

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

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

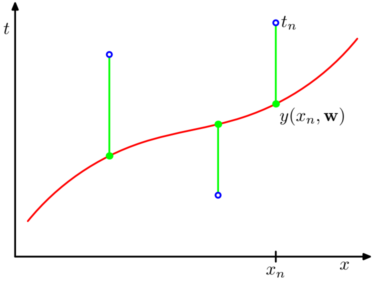
And then $p(\mathbf{w}|\mathbf{t}) = \mathcal{N}\left(\mathbf{w}|\mathbf{m}_N,\mathbf{S}_N\right)$ where

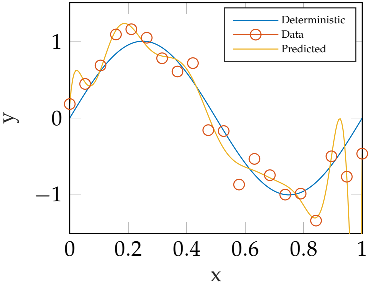
$$\begin{aligned} \mathbf{m}_N &= \mathbf{S}_N\left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\boldsymbol{\Phi}^\top\mathbf{t}\right) \\ \mathbf{S}_N^{-1} &= \mathbf{S}_0^{-1} + \beta\boldsymbol{\Phi}^\top\boldsymbol{\Phi} \end{aligned}$$

Gaussian Processes

What was done until here?

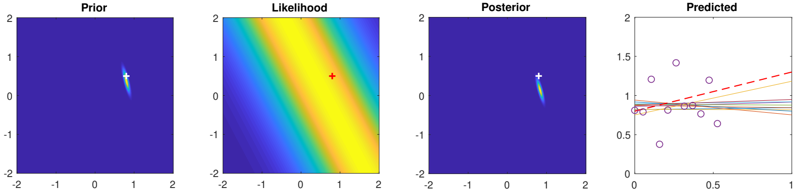
- We assumed that our targets t were **i.i.d.** and given by $t = y(\mathbf{x}) + \varepsilon$, where $\varepsilon \sim \mathcal{N}(0, \beta)$.
- Our model is given by $\mathbf{y}(\mathbf{x}) = \Phi^\top \mathbf{w}$, where Φ is the **design matrix**, and this caracterize our model as **linear in parameters**.
- 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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