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Introduction to Gaussian Processes

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Outline

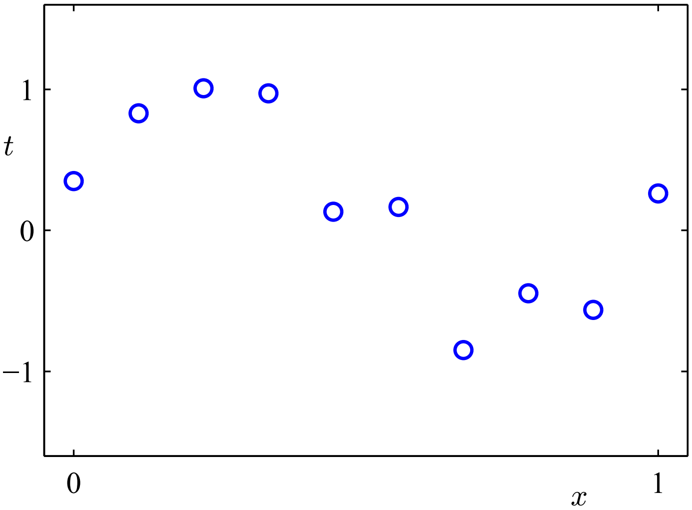
Linear Regression

- 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**

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

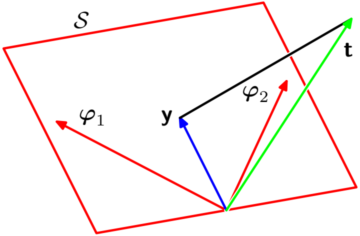
- In general, we could write this **weighted sum** with any other function. In other words, we can put this in terms of $\phi_n(x) = x^n$, where ϕ could be other **basis function**.
- e.g. we could have different $y(x)$ for different basis functions, or **features**.

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

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

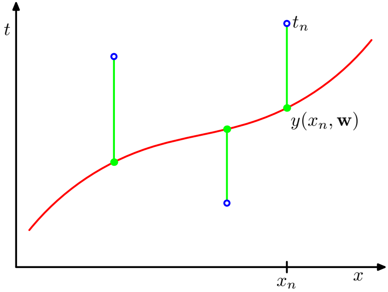
$$
\begin{aligned}
y(x, \mathbf{w}) &= w_0\phi_0(x) + w_1\phi_1(x) + \ldots \\
&\quad + w_{M-1}\phi_{M-1}(x) \\
&= \sum_{j=1}^{M-1} w_j\phi_j(x)
\end{aligned}
$$

- 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**.

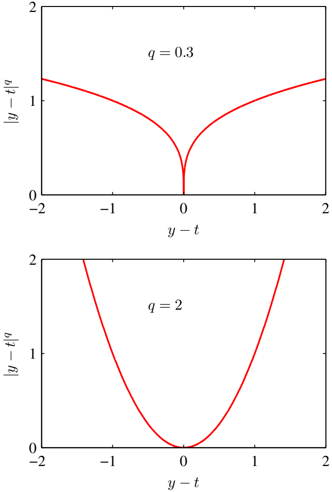


- The chosen model will give us some curve that is needed to adjust such that we'll **minimize its distance** to the **targets** t.
- This approach lead us to use the **least squares** to estimate the weights and minimize the **error** E.

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



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

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

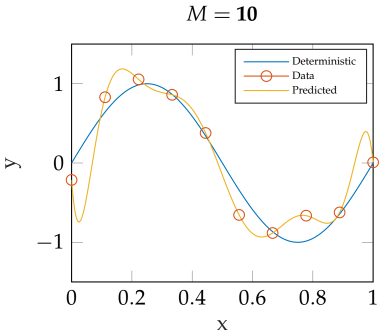
- In sequence, we'll try to minimize it in terms of the weights ($\mathbf{w}$) by

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

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

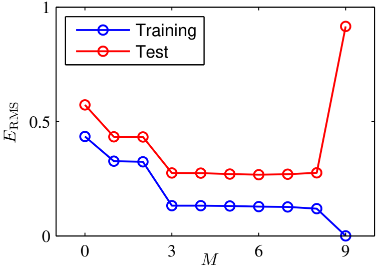
Why the prediction is so distant from the deterministic curve?

- 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**.



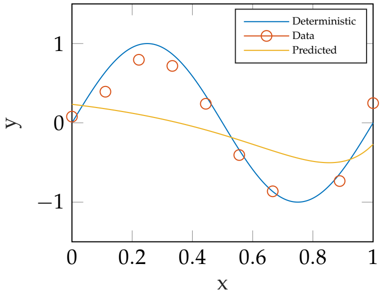
How to control the over-fitting?

- 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.

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

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

$\ln\lambda = \mathbf{0} \mid M = \mathbf{10}$



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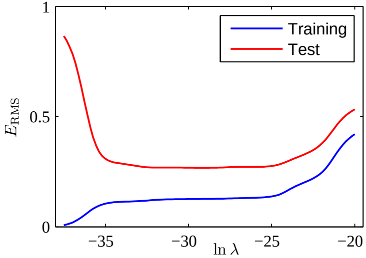
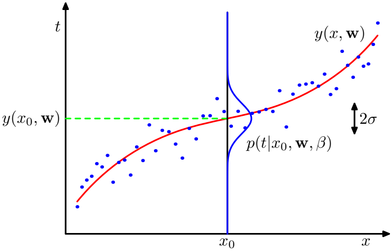


What if we assume not knowing the data exactly?

- Having an **uncertainty** in the measured value, we could represent it with a **probability distribution**.
- 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.
- For this case, we'll consider the distribution being UniOrange**Gaussian**.



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

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

known as **likelihood function**.

- 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

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

- 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, then our assumptions are well grounded.
- With the maximization, we'll obtain the weights $\mathbf{w}$ that **maximize** the log probability of the targets, given the parameters.
- This is called **maximum likelihood**, since we are looking for the **parameters** distribution that are more probable to had been generated the data.
- This is a initial step towards to a **Bayesian** approach.

Bayesian Linear Regression

What if we assume not knowing the data exactly?

- The principle of the Bayesian statistics is express our **degree of belief** in an event.
- This belief could be based on some **prior** knowledge about the event or personal beliefs.
- This differs from frequentist statistics, where the probability is based on the number of trials.
- Suppose a die to be thrown once

Frequentist

There's empiric evidence that similar dice thrown in past produce similar outcomes with the same frequency.

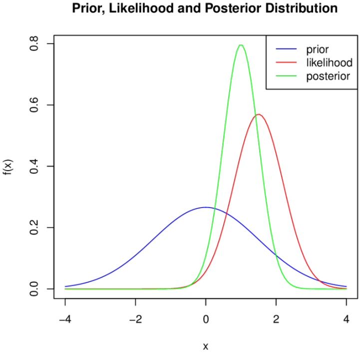


Figure: Aksu 2018

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Bayesian

The last argument is right, but the **belief of the observer** it's important to the statistics.

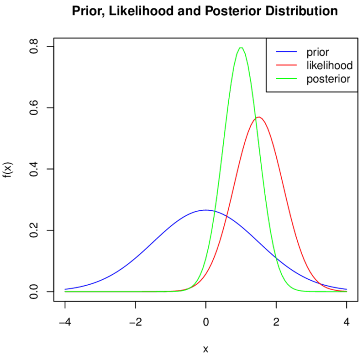


Figure: Aksu 2018

- The main idea of the Bayesian approach is put some **uncertainty** over the parameters and make **inferences**, i.e. obtain some statistics in light over the data.
- This principle is elucidated by the Bayes' Rule

$$\overbrace{p(\mathbf{w}|\mathbf{t})}^{posterior} = \frac{p(\mathbf{t}|\mathbf{w})p(\mathbf{w})}{p(\mathbf{t})} = \frac{\overbrace{p(\mathbf{t}|\mathbf{w})}^{likelihood}\,\overbrace{p(\mathbf{w})}^{prior}}{\underbrace{\int p(\mathbf{t}|\mathbf{w})p(\mathbf{w})d\mathbf{w}}_{marginal\ distribution}}$$

  where we assume some uncertainty over the parameters, i.e. a probability density function $p(\mathbf{w})$.
- We'll use the knowledge about the data with the **likelihood function** and some previous knowledge, or **prior**, that we have about the parameters to obtain the knowledge considering these two, or **posterior**.
- This is called **Bayesian Inference**.

- We can introduce the **maximum *a posteriori*** (MAP) as the direct estimator for the Bayes' Rule.
- The approach is similar to what was done by maximizing the likelihood function, but now maximizing the posterior distribuition of the parameters given the data.
- We consider the **marginal distribution** $p(\mathbf{t})$ being a constant in the parameters

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

- Here, we'll consider out prior knowledge about the parameters being

$$\mathbf{w} \sim \mathcal{N}\left(\mathbf{0}, \alpha^{-1}\mathbf{I}\right)$$

- We obtain by the derivative w.r.t. $\mathbf{w}$ of the negative log that

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

what is similar to the regularized linear regression considering $\lambda = \alpha/\beta$.

Aren't we ignoring possible solutions?

- The main idea in the Bayesian approach is that our knowledge is in the **statistics** and not in a singular value.
- With MAP we just consider the **most probable** value of a full distribution of possible values.
- In the next we'll obtain the statistics of the distributions involved in Bayes' Rule, including the posterior.
- But before, we need some tools...

Partitioned Gaussians

Be $\mathbf{x}$ a n-dimensional vector with a Gaussian distribution $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$, then the partitioned will be

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

Preserved the symmetry $\boldsymbol{\Sigma}^\top = \boldsymbol{\Sigma}$, we say the covariance matrix is positive definite. And be the multivariate Gaussian

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

We define too, just for convenience of work, the precision matrix $\boldsymbol{\Lambda}$ by

$$\boldsymbol{\Lambda} = \begin{pmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{pmatrix} \equiv \boldsymbol{\Sigma}^{-1}$$

assuming all matrices have inverses.

Closure under linear transformations and marginalization

Being $\mathbf{x}_b$ conditioned on $\mathbf{x}_a$ and Gaussian distributed as

$$p\left(\mathbf{x}_a\right) = \mathcal{N}\left(\mathbf{x}_a | \boldsymbol{\mu}_a, \boldsymbol{\Sigma}_a\right), \quad p\left(\mathbf{x}_b | \mathbf{x}_a\right) = \mathcal{N}\left(\mathbf{x}_b | \mathbf{M}\mathbf{x}_a + \mathbf{d}, \boldsymbol{\Sigma}_{b|a}\right)$$

$\mathbf{M}$ a constant matrix and $\mathbf{d}$ a constant vector, both with the appropriate dimensions. Then conditional distribution $p(\mathbf{x}_a | \mathbf{x}_b)$ is given by

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

with

$$\boldsymbol{\mu}_{a|b} = \boldsymbol{\Sigma}_{a|b}\left(\mathbf{M}^\top \boldsymbol{\Sigma}_{b|a}^{-1}\left(\mathbf{x}_b - \mathbf{d}\right) + \boldsymbol{\Sigma}_a^{-1}\boldsymbol{\mu}_a\right), \quad \boldsymbol{\Sigma}_{a|b} = \left(\boldsymbol{\Sigma}_a^{-1} + \mathbf{M}^\top \boldsymbol{\Sigma}_{b|a}^{-1}\mathbf{M}\right)^{-1}.$$

The marginal density of $\mathbf{x}_b$ is given by

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

with

$$\boldsymbol{\mu}_b = \mathbf{M}\boldsymbol{\mu}_a + \mathbf{d}, \quad \boldsymbol{\Sigma}_b = \boldsymbol{\Sigma}_{b|a} + \mathbf{M}\boldsymbol{\Sigma}_a\mathbf{M}^\top.$$

Substituting...

Being $\mathbf{M}$ the design matrix Φ and $\mathbf{d}$ a zero vector, we have the posterior distribution

$$p(\mathbf{w}|\mathbf{t}, \alpha, \beta) = \mathcal{N}\left(\mathbf{w}|\boldsymbol{\mu}_{\mathbf{w}|\mathbf{t}}, \boldsymbol{\Sigma}_{\mathbf{w}|\mathbf{t}}\right)$$

being

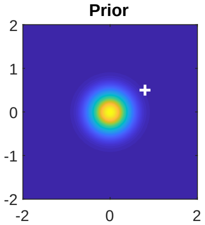
$$\boldsymbol{\mu}_{\mathbf{w}|\mathbf{t}} = \boldsymbol{\Sigma}_{\mathbf{w}|\mathbf{t}}\left(\beta\Phi^{\top}\mathbf{t} + \boldsymbol{\Sigma}_{\mathbf{w}}^{-1}\boldsymbol{\mu}_{\mathbf{w}}\right), \quad \boldsymbol{\Sigma}_{\mathbf{w}|\mathbf{t}} = \left(\boldsymbol{\Sigma}_{\mathbf{w}}^{-1} + \beta\Phi^{\top}\Phi\right)^{-1}.$$

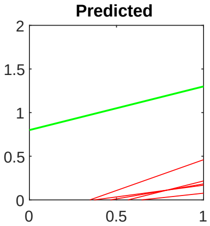
Assuming the prior

$$\mathbf{w} \sim \mathcal{N}\left(\mathbf{0}, \alpha^{-1}\mathbf{I}\right)$$

we have

$$\boldsymbol{\mu}_{\mathbf{w}|\mathbf{t}} = \beta\boldsymbol{\Sigma}_{\mathbf{w}|\mathbf{t}}\Phi^{\top}\mathbf{t}, \quad \boldsymbol{\Sigma}_{\mathbf{w}|\mathbf{t}} = \left(\alpha^{-1}\mathbf{I} + \beta\Phi^{\top}\Phi\right)^{-1}.$$


Prior
2
1
0
-1
-2
-2
0
2


Predicted
2
1.5
1
0.5
0
0
0.5
1

From Bayesian inference

- In the most of the cases, we are more interested in making predictions of $\mathbf{t}$ than in the parameters $\mathbf{w}$ in the space of the parameters, or **weight-space**, for the new values of $\mathbf{x}$. We'll define from the Bayes' Rule a **predictive distribution**

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

- And turn to the **feature-space**

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

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

Alternative formulation

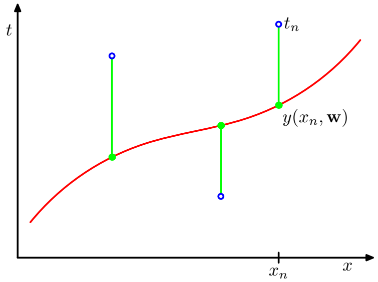
$$f_* | \mathbf{x}_*, \Phi, \mathbf{t} \sim \mathcal{N}\left(\boldsymbol{\phi}_*^\top \mathbf{S}_0 \Phi \left(K + \beta^{-2} I\right)^{-1} \mathbf{t}, \boldsymbol{\phi}_*^\top \mathbf{S}_0 \boldsymbol{\phi}_* - \boldsymbol{\phi}_*^\top \mathbf{S}_0 \Phi \left(K + \beta^{-2} I\right)^{-1} \Phi^\top \mathbf{S}_0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

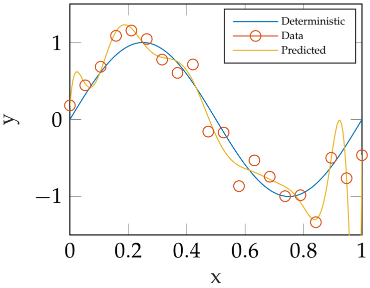
where $K = \Phi^\top \mathbf{S}_0 \Phi$

Gaussian Processes

What was done until here?

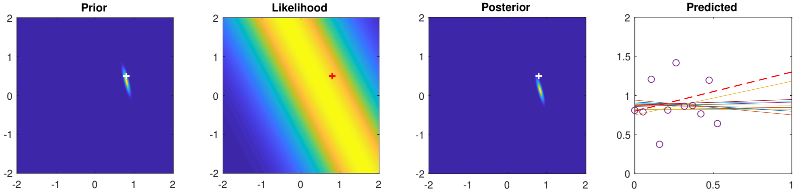
- We assumed that our targets t were **i.i.d.** and given by $t = y(\mathbf{x}) + \varepsilon$, where $\varepsilon \sim \mathcal{N}(0, \beta)$.
- Our model is given by $\mathbf{y}(\mathbf{x}) = \Phi^\top \mathbf{w}$, where Φ is the **design matrix**, and this caracterize our model as **linear in parameters**.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



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 $k(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^\top \mathbf{S}_0 \boldsymbol{\phi}\left(\mathbf{x}'\right)$
- 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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