PATTERN RECOGNITION AND MACHINE LEARNING

CHAPTER 3: LINEAR MODELS FOR REGRESSION

Learning Objectives

1、How to achieve linear regression using basis functions?

2、What are the relationships between maximum likelihood and least squares, between maximum a posterior and regularization, and among expected loss, bias, variance, and noise?

3、What are the common regularization methods for regression?

4、How to achieve Bayesian linear regression?

5、What is the kernel for regression?

6、How to choose the model complexity?

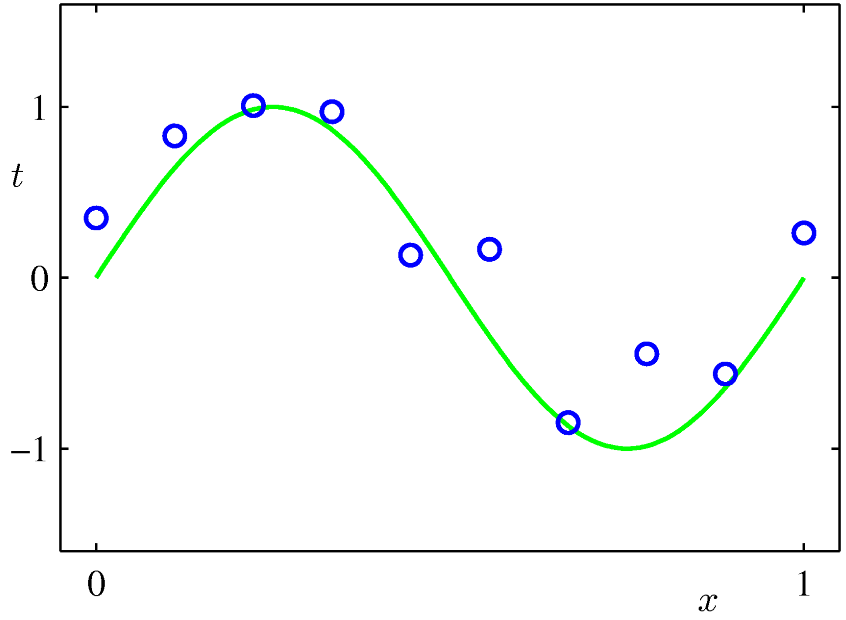
7、What are the evidence approximation and maximization?

Outlines

- Linear Basis Function Models
- Maximum Likelihood and Least Squares
- Bias Variance Decomposition
- Bayesian Linear Regression
- Predictive Distribution
- Bayesian Model Comparison
- Evidence Approximation and Maximization

Linear Basis Function Models (1)

Example: Polynomial Curve Fitting



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

Linear Basis Function Models (2)

- Generally

$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x})$$

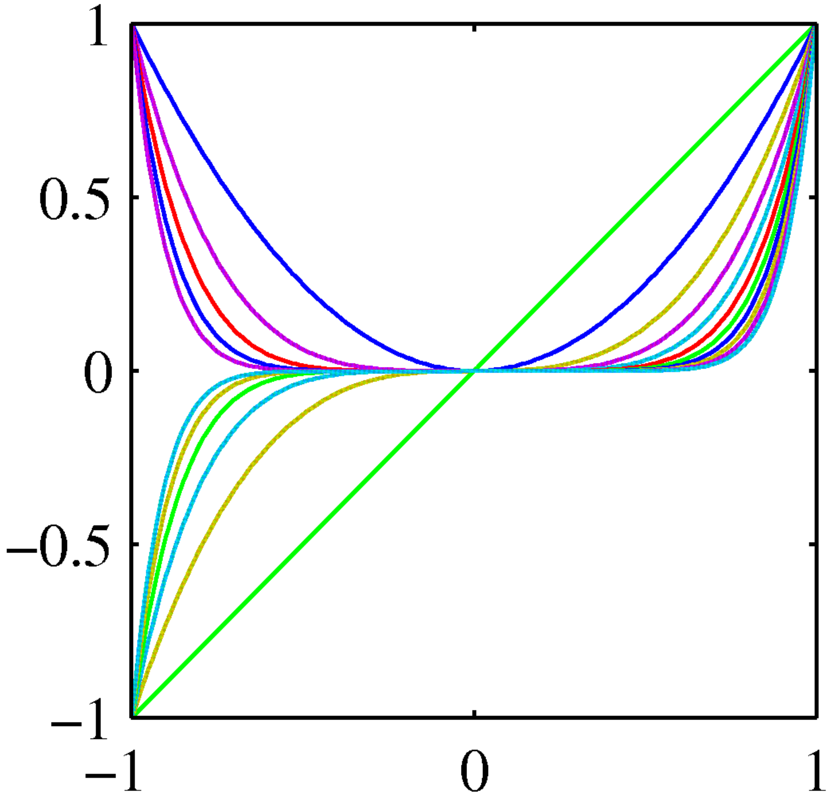
  where $\phi_j(\mathrm{x})$ are known as *basis functions*.
- Typically, $\phi_0(\mathrm{x}) = 1$, so that w_0 acts as a bias.
- In the simplest case, we use linear basis functions : $\phi_d(\mathrm{x}) = x_d$.

Linear Basis Function Models (3)

Polynomial basis functions:

$$\phi_j(x) = x^j.$$

These are global; a small change in x affect all basis functions.

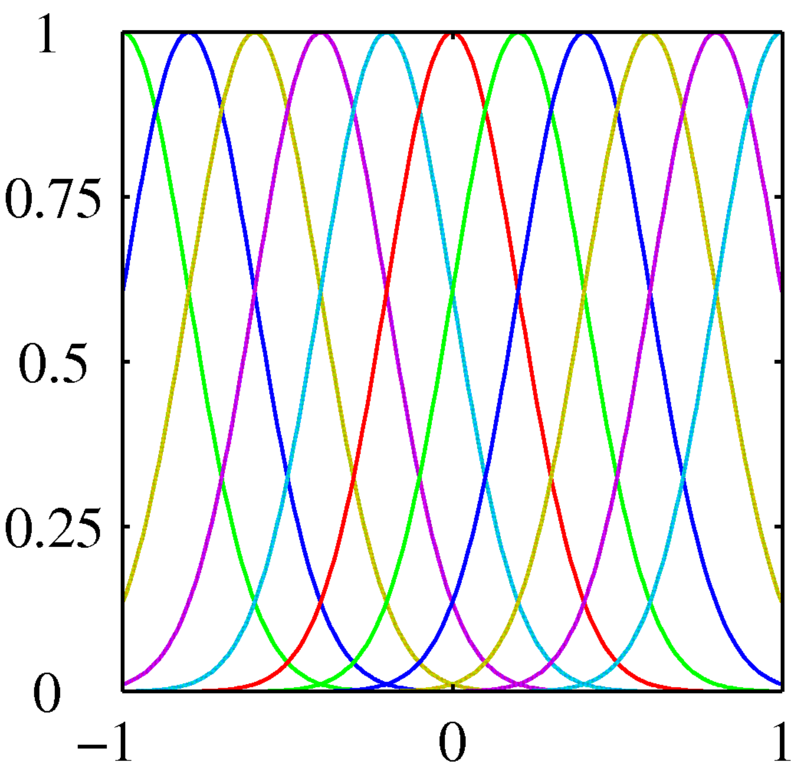


Linear Basis Function Models (4)

Gaussian basis functions:

$$\phi_j(x) = \exp\left\{-\frac{(x-\mu_j)^2}{2s^2}\right\}$$

These are local; a small change in x only affect nearby basis functions. μ_j and s control location and scale (width).



Linear Basis Function Models (5)

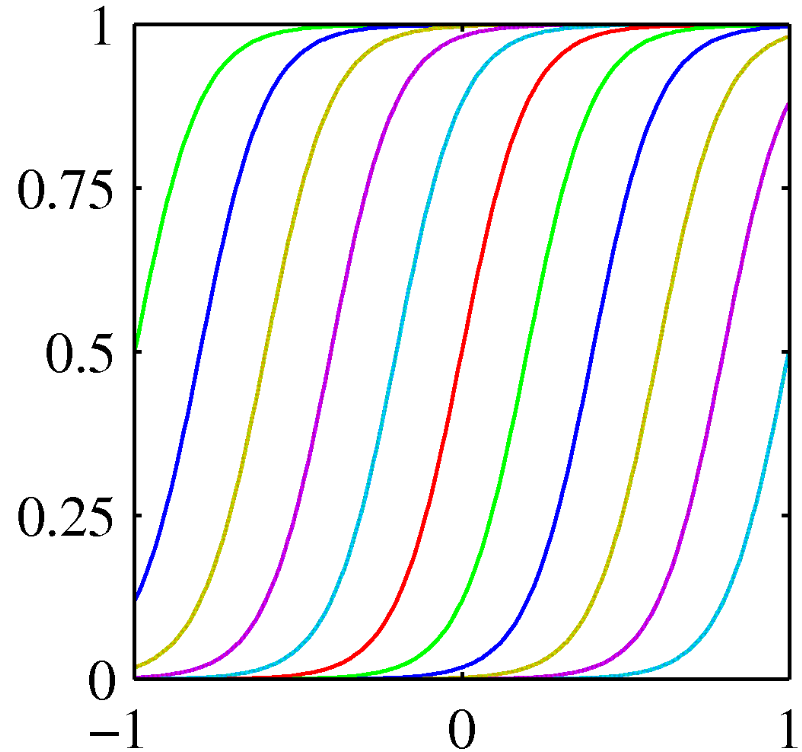
Sigmoidal basis functions:

$$\phi_j(x) = \sigma\left(\frac{x - \mu_j}{s}\right)$$

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)}.$$

Also these are local; a small change in x only affect nearby basis functions. μ_j and s control location and scale (slope).



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Maximum Likelihood and Least Squares (1)

- Assume observations from a deterministic function with added Gaussian noise:

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon \qquad \text{where} \qquad p(\epsilon|\beta) = \mathcal{N}(\epsilon|0, \beta^{-1})$$

  which is the same as saying,

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

- Given observed inputs, $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$, and targets, $\mathbf{t} = [t_1, \dots, t_N]^{\mathrm{T}}$, we obtain the likelihood function

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n|\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}).$$

Maximum Likelihood and Least Squares (2)

Taking the logarithm, we get

$$\begin{aligned}\ln p(\mathbf{t}|\mathbf{w},\beta) &= \sum_{n=1}^{N} \ln \mathcal{N}(t_n|\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n),\beta^{-1}) \\ &= \frac{N}{2}\ln\beta - \frac{N}{2}\ln(2\pi) - \beta E_D(\mathbf{w})\end{aligned}$$

where

$$E_D(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\}^2$$

is the sum-of-squares error.

Maximum Likelihood and Least Squares (3)

Computing the gradient and setting it to zero yields

$$\nabla_{\mathbf{w}} \ln p(\mathbf{t}|\mathbf{w}, \beta) = \beta \sum_{n=1}^{N} \left\{ t_n - \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n) \right\} \boldsymbol{\phi}(\mathbf{x}_n)^{\mathrm{T}} = \mathbf{0}.$$

Solving for $\mathbf{w}$, we get

$$\mathbf{w}_{\mathrm{ML}} = \left(\boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi} \right)^{-1} \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{t}$$

The Moore-Penrose pseudo-inverse, $\boldsymbol{\Phi}^{\dagger}$.

Roger Penrose
2020 Nobel Prize
Laurate in Physics

where

$$\boldsymbol{\Phi} = \begin{pmatrix} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \cdots & \phi_{M-1}(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \phi_1(\mathbf{x}_2) & \cdots & \phi_{M-1}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}_N) & \phi_1(\mathbf{x}_N) & \cdots & \phi_{M-1}(\mathbf{x}_N) \end{pmatrix}.$$

Geometry of Least Squares

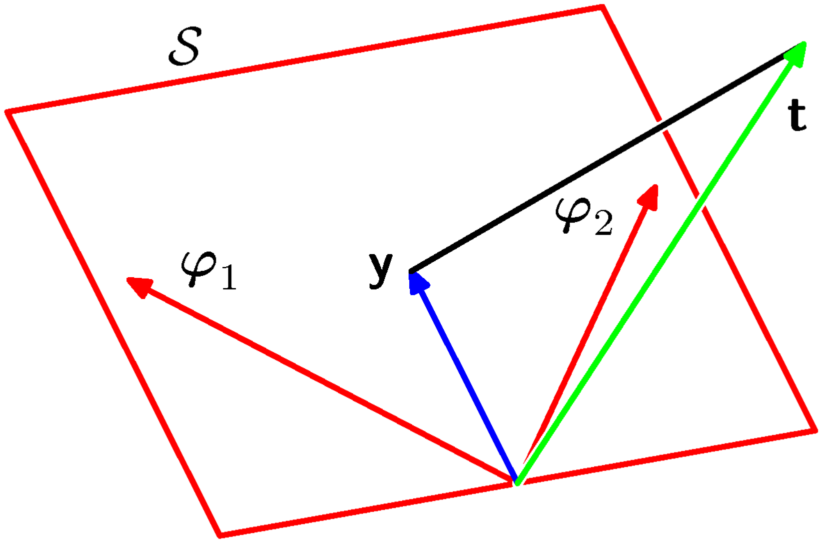
Consider

$$\mathbf{y} = \boldsymbol{\Phi}\mathbf{w}_{\mathrm{ML}} = [\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_M]\,\mathbf{w}_{\mathrm{ML}}.$$

$$\mathbf{y} \in \mathcal{S} \subseteq \mathcal{T} \qquad \mathbf{t} \in \mathcal{T}$$

N-dimensional

M-dimensional



$\mathcal{S}$ is spanned by $\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_M$.

$\mathbf{w}_{\mathrm{ML}}$ minimizes the distance between **t** and its orthogonal projection on $\mathcal{S}$, i.e. **y**.

Sequential Learning

- Data items considered one at a time (a.k.a. online learning); use stochastic (sequential) gradient descent:

$$\begin{aligned}\mathbf{w}^{(\tau+1)} &= \mathbf{w}^{(\tau)} - \eta \nabla E_n \\ &= \mathbf{w}^{(\tau)} + \eta (t_n - \mathbf{w}^{(\tau)\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n)) \boldsymbol{\phi}(\mathbf{x}_n).\end{aligned}$$

- This is known as the *least-mean-squares (LMS) algorithm*. Issue: how to choose η?

Regularized Least Squares (1)

- Consider the error function:

$$E_D(\mathbf{w}) + \lambda E_W(\mathbf{w})$$

Data term + Regularization term

- With the sum-of-squares error function and a quadratic regularizer, we get

$$\frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n)\}^2 + \frac{\lambda}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}$$

which is minimized by

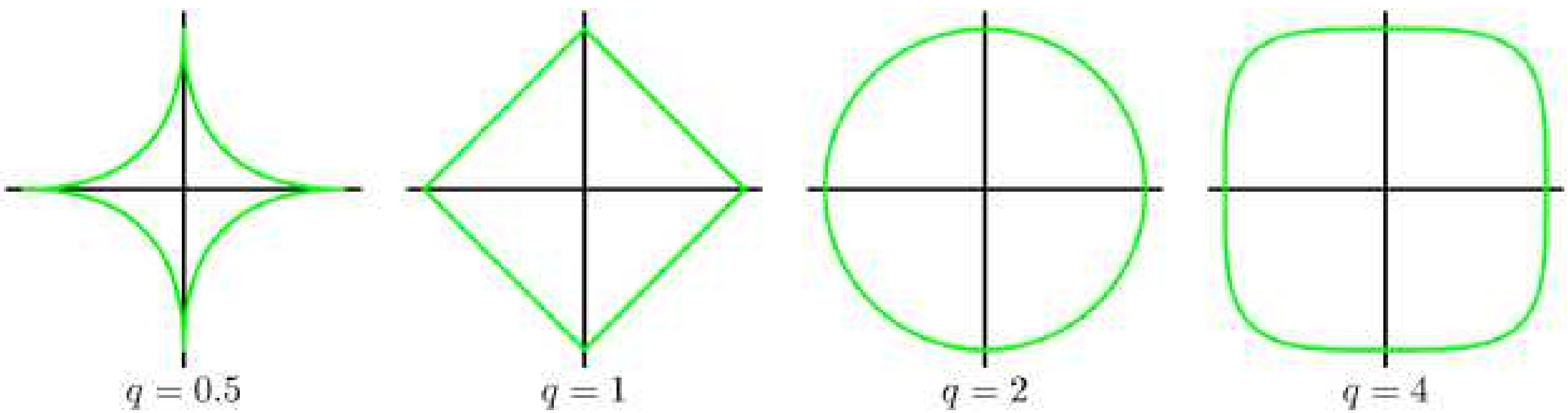
$$\mathbf{w} = \left(\lambda\mathbf{I} + \mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^{\mathrm{T}}\mathbf{t}.$$

λ is called the regularization coefficient.

Regularized Least Squares (2)

With a more general regularizer, we have

$$\frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\}^2 + \frac{\lambda}{2}\sum_{j=1}^{M}|w_j|^q$$

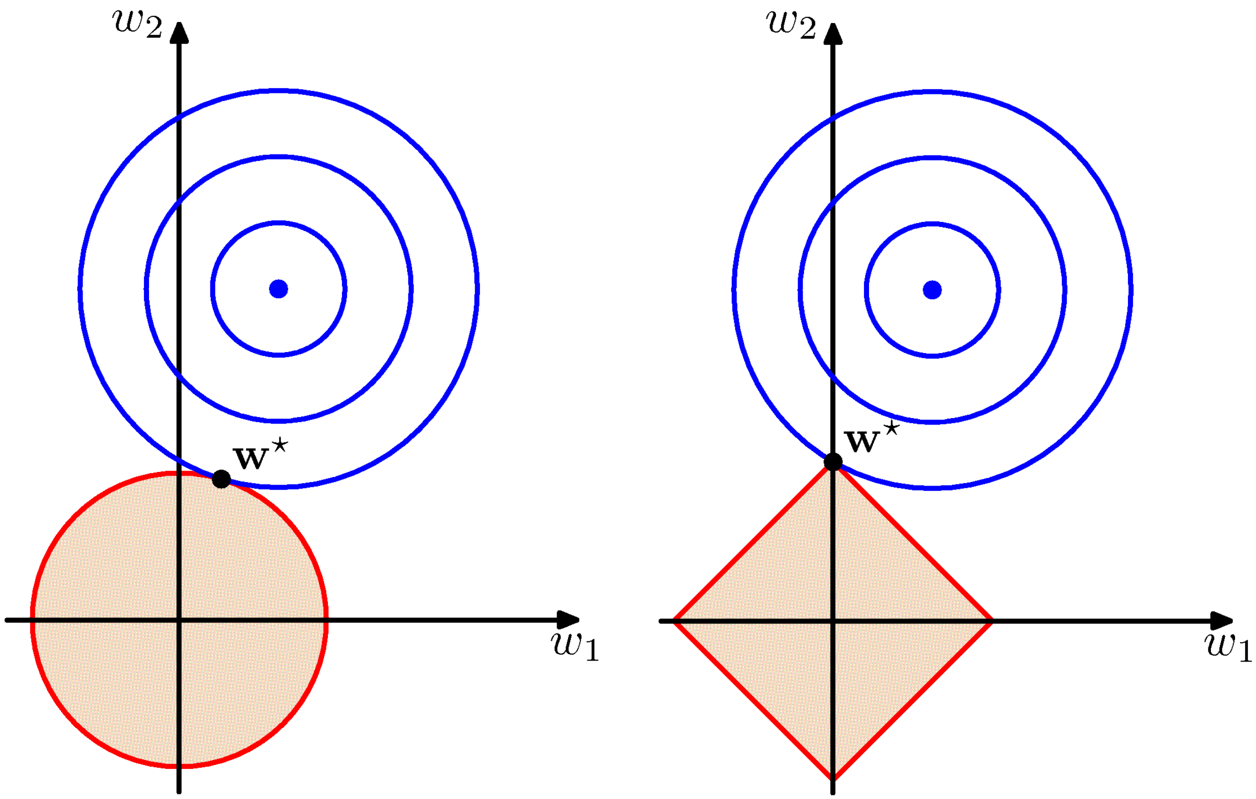


Lasso

Quadratic

Regularized Least Squares (3)

Lasso tends to generate sparser solutions than a quadratic regularizer.



Multiple Outputs (1)

Analogously to the single output case we have:

$$\begin{aligned} p(\mathbf{t}|\mathbf{x}, \mathbf{W}, \beta) &= \mathcal{N}(\mathbf{t}|\mathbf{y}(\mathbf{W}, \mathbf{x}), \beta^{-1}\mathbf{I}) \\ &= \mathcal{N}(\mathbf{t}|\mathbf{W}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}), \beta^{-1}\mathbf{I}). \end{aligned}$$

Given observed inputs, $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, and targets, $\mathbf{T} = [\mathbf{t}_1, \ldots, \mathbf{t}_N]^{\mathrm{T}}$, we obtain the log likelihood function

$$\begin{aligned} \ln p(\mathbf{T}|\mathbf{X}, \mathbf{W}, \beta) &= \sum_{n=1}^{N} \ln \mathcal{N}(\mathbf{t}_n|\mathbf{W}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\mathbf{I}) \\ &= \frac{NK}{2} \ln\left(\frac{\beta}{2\pi}\right) - \frac{\beta}{2}\sum_{n=1}^{N} \left\|\mathbf{t}_n - \mathbf{W}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\right\|^2. \end{aligned}$$

Multiple Outputs (2)

- Maximizing with respect to **W**, we obtain

$$\mathbf{W}_{\mathrm{ML}} = \left(\mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^{\mathrm{T}}\mathbf{T}.$$

- If we consider a single target variable, $\mathbf{t}_{\mathrm{k}}$, we see that

$$\mathbf{w}_k = \left(\mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^{\mathrm{T}}\mathbf{t}_k = \mathbf{\Phi}^{\dagger}\mathbf{t}_k$$

where $\mathbf{t}_k = [t_{1k}, \ldots, t_{Nk}]^{\mathrm{T}}$, which is identical with the single output case.

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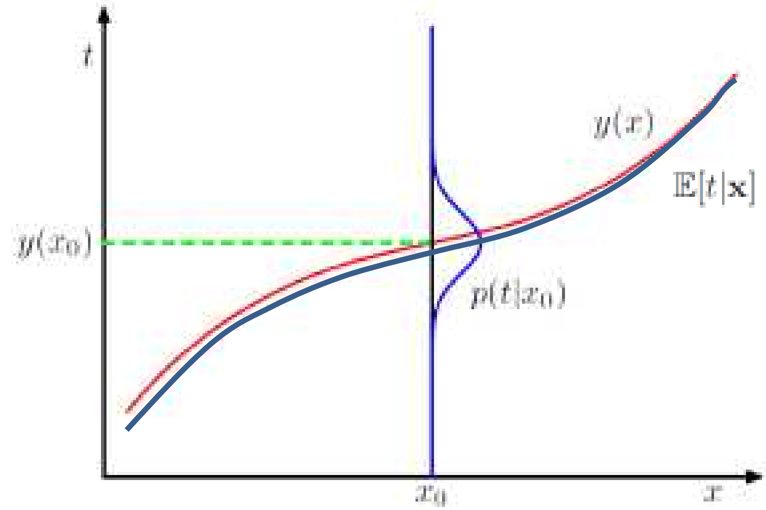
The Expected Squared Loss Function

$$\mathbb{E}[L] = \iint \{\overset{\text{predictor}}{y(\mathbf{x})} - \overset{\text{data}}{t}\}^2 p(\mathbf{x}, t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$



$$\begin{aligned}\{y(\mathbf{x}) - t\}^2 &= \{y(\mathbf{x}) - \overset{\text{ground truth: optimal predictor}}{\mathbb{E}[t|\mathbf{x}]} + \mathbb{E}[t|\mathbf{x}] - t\}^2 \\ &= \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}^2 + \underbrace{2\{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}\{\mathbb{E}[t|\mathbf{x}] - t\}}_{0} + \{\mathbb{E}[t|\mathbf{x}] - t\}^2\end{aligned}$$

$$\mathbb{E}[L] = \int \{\underset{\text{predictor}}{y(\mathbf{x})} - \mathbb{E}[t|\mathbf{x}]\}^2 p(\mathbf{x})\,\mathrm{d}\mathbf{x} + \int \underset{\text{noise}}{\mathrm{var}\,[t|\mathbf{x}]}\, p(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

https://stats.stackexchange.com/questions/228561/loss-functions-for-regression-proof

The Bias-Variance Decomposition (1)

- Recall the *expected squared loss*,

$$\mathbb{E}[L] = \int \{y(\mathbf{x}) - h(\mathbf{x})\}^2 p(\mathbf{x})\,\mathrm{d}\mathbf{x} + \iint \{h(\mathbf{x}) - t\}^2 p(\mathbf{x}, t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

where

$$h(\mathbf{x}) = \mathbb{E}[t|\mathbf{x}] = \int t p(t|\mathbf{x})\,\mathrm{d}t.$$

- The second term of $\mathbb{E}[L]$ corresponds to the noise inherent in the random variable t.

- What about the first term?

The Bias-Variance Decomposition (2)

- Suppose we were given multiple data sets, each of size N. Any particular data set, $\mathcal{D}$, will give a particular function $y(\mathbf{x};\mathcal{D})$. We then have

$$
\begin{aligned}
&\{y(\mathbf{x};\mathcal{D}) - h(\mathbf{x})\}^2 \\
&\quad = \quad \{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] + \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2 \\
&\quad = \quad \{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2 + \{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2 \\
&\qquad\qquad +2\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}\{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}.
\end{aligned}
$$

The Bias-Variance Decomposition (3)

- Taking the expectation over $\mathbb{D}$ yields

$$
\begin{aligned}
&\mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - h(\mathbf{x})\}^2\right] \\
&\quad = \underbrace{\{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2}_{(\text{bias})^2} + \underbrace{\mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2\right]}_{\text{variance}}.
\end{aligned}
$$

The Bias-Variance Decomposition (4)

- Thus we can write

$$\text{expected loss} = (\text{bias})^2 + \text{variance} + \text{noise}$$

where

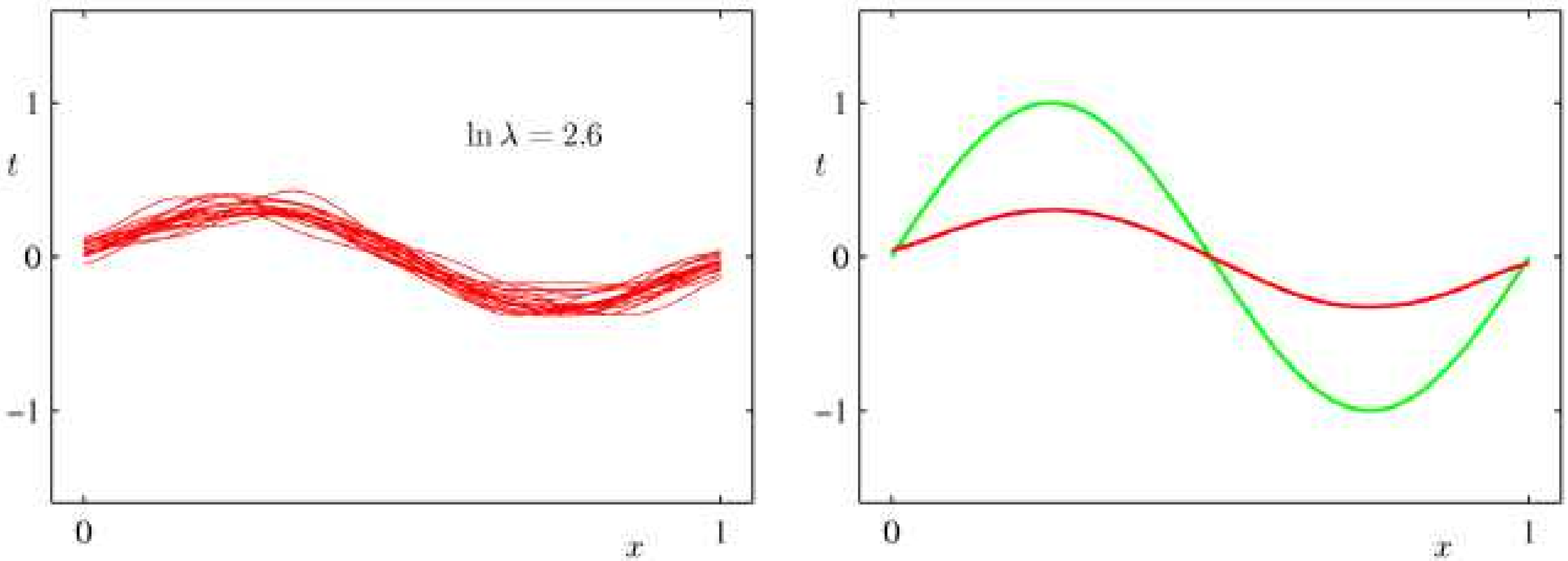
Model:
$$(\text{bias})^2 = \int \{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2 p(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

Model:
$$\text{variance} = \int \mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2\right] p(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

Data:
$$\text{noise} = \iint \{h(\mathbf{x}) - t\}^2 p(\mathbf{x}, t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

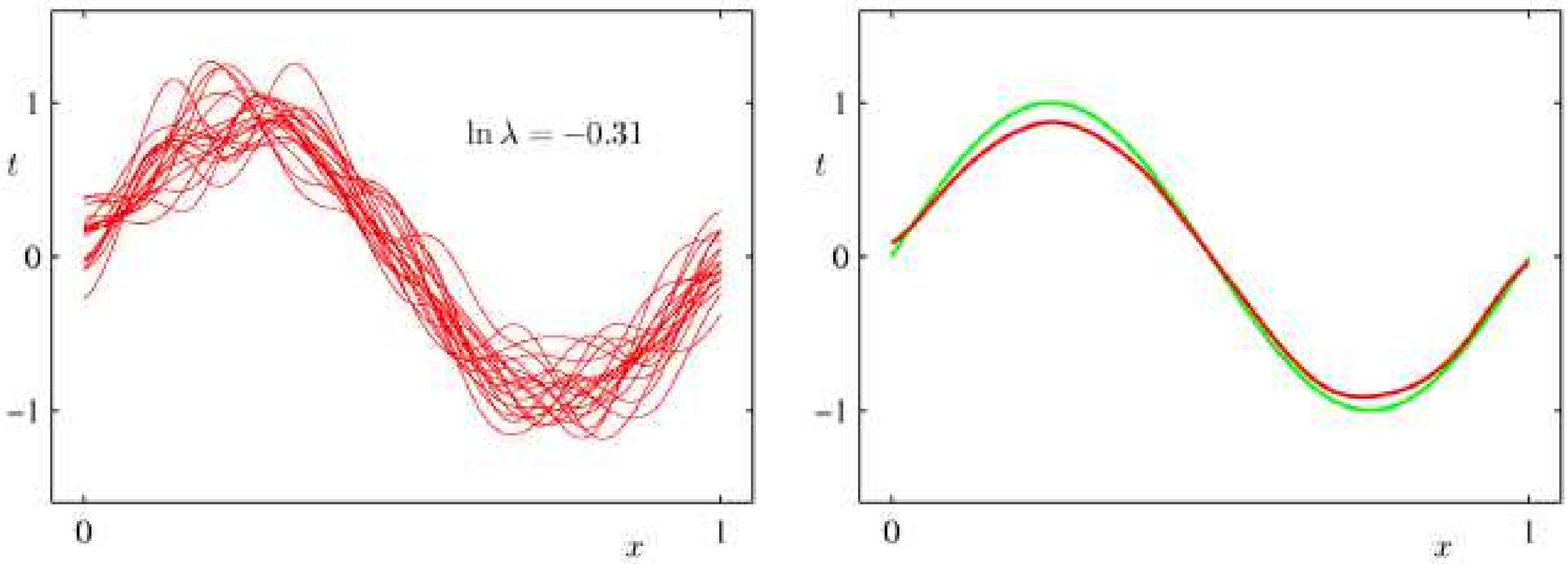
The Bias-Variance Decomposition (5)

- Example: 25 data sets from the sinusoidal, varying the degree of regularization, λ.



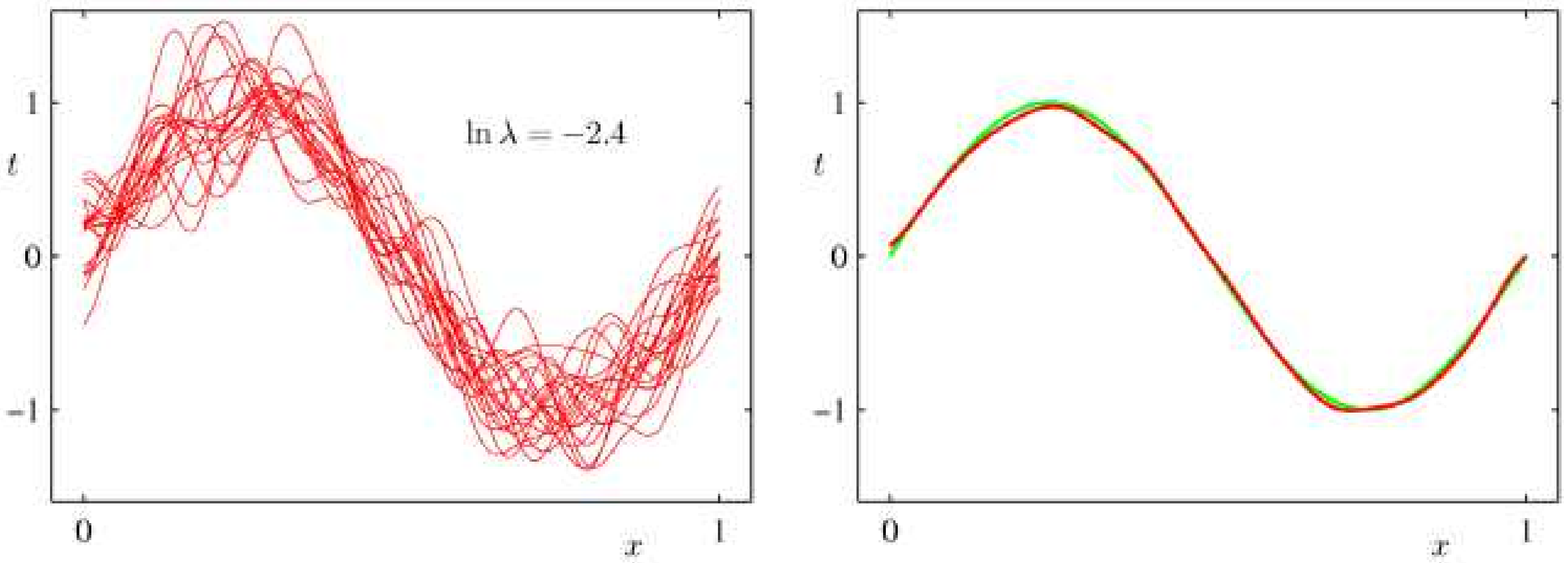
The Bias-Variance Decomposition (6)

- Example: 25 data sets from the sinusoidal, varying the degree of regularization, λ.



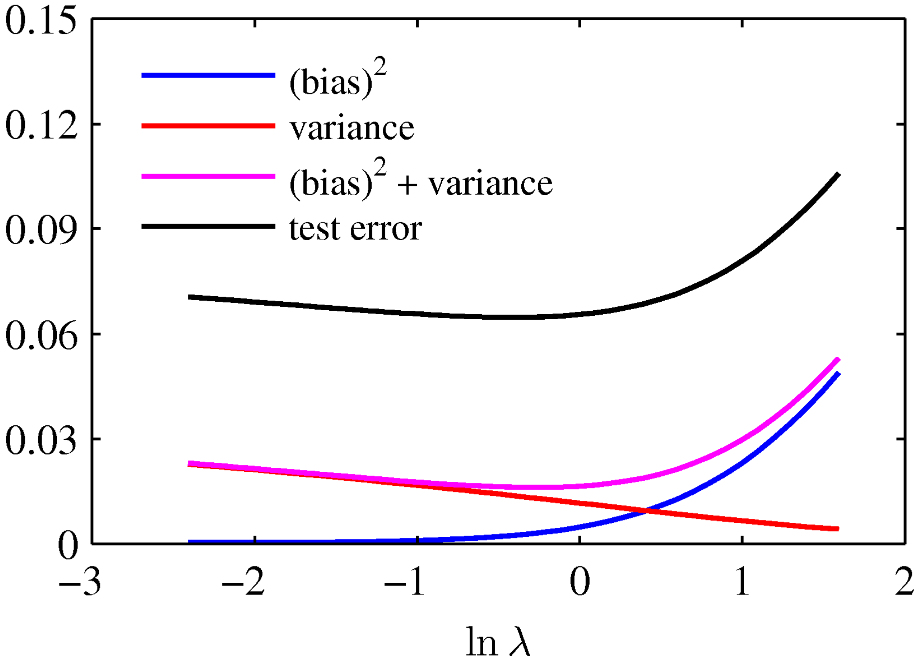
The Bias-Variance Decomposition (7)

- Example: 25 data sets from the sinusoidal, varying the degree of regularization, λ.



The Bias-Variance Trade-off

From these plots, we note that an over-regularized model (large λ) will have a high bias, while an under-regularized model (small λ) will have a high variance.



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Bayesian Linear Regression (1)

- Define a conjugate prior over $\mathbf{w}$

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

- Combining this with the likelihood function and using results for marginal and conditional Gaussian distributions, gives the posterior

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$$

where

$$\begin{aligned} \boxed{\mathbf{w}_{\mathrm{MAP}}} \longrightarrow \mathbf{m}_N &= \mathbf{S}_N \left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\boldsymbol{\Phi}^{\mathrm{T}}\mathbf{t}\right) \\ \mathbf{S}_N^{-1} &= \mathbf{S}_0^{-1} + \beta\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}. \end{aligned}$$

Bayesian Linear Regression (2)

$$-\frac{1}{2}(\mathbf{w}-\mathbf{m}_N)^T\ \mathbf{S}_N{}^{-1}(\mathbf{w}-\mathbf{m}_N)\ \propto\ -\frac{1}{2}(\mathbf{t}-\Phi\mathbf{w})^T\beta(\mathbf{t}-\Phi\mathbf{w})$$

$$-\frac{1}{2}(\mathbf{w}-\mathbf{m}_0)^T\ \mathbf{S}_0{}^{-1}(\mathbf{w}-\mathbf{m}_0)$$

Quadratic terms of **w** are equal: (**w**^{T}****w**)

$$\begin{cases} \mathbf{S}_N{}^{-1} = \beta\Phi^T\Phi + \mathbf{S}_0{}^{-1} \\ \mathbf{S}_N{}^{-1}\mathbf{m}_N = \beta\Phi^T\mathbf{t} + \mathbf{S}_0{}^{-1}\mathbf{m}_0 \end{cases}$$

1st order terms of **w** are also equal: (**w**^{T} **)

Bayesian Linear Regression (3)

- A common choice for the prior is

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I})$$

for which

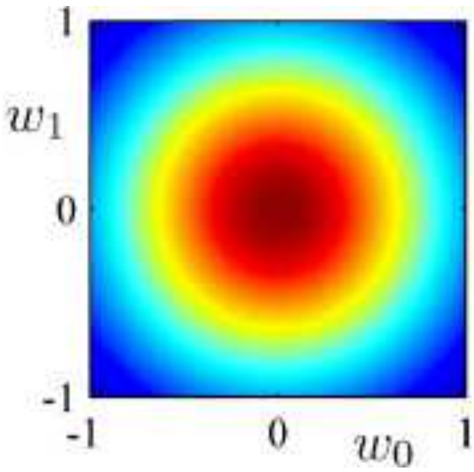
$$\begin{aligned} \boxed{\mathbf{w}_{\mathrm{MAP}}} \longrightarrow \mathbf{m}_N &= \beta \mathbf{S}_N \mathbf{\Phi}^{\mathrm{T}} \mathbf{t} \\ \mathbf{S}_N^{-1} &= \alpha \mathbf{I} + \beta \mathbf{\Phi}^{\mathrm{T}} \mathbf{\Phi}. \end{aligned}$$

- Next we consider an example …

Bayesian Linear Regression (4)

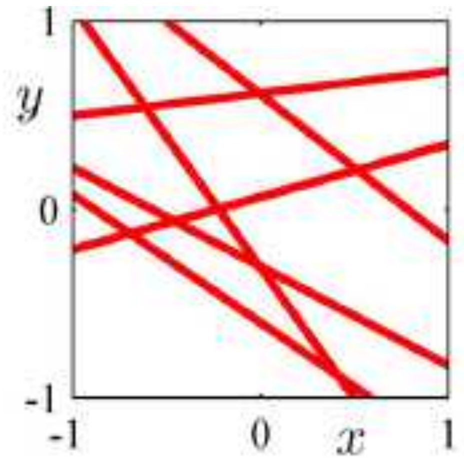
- 0 data points observed

Prior



$p(w_1, w_0)$

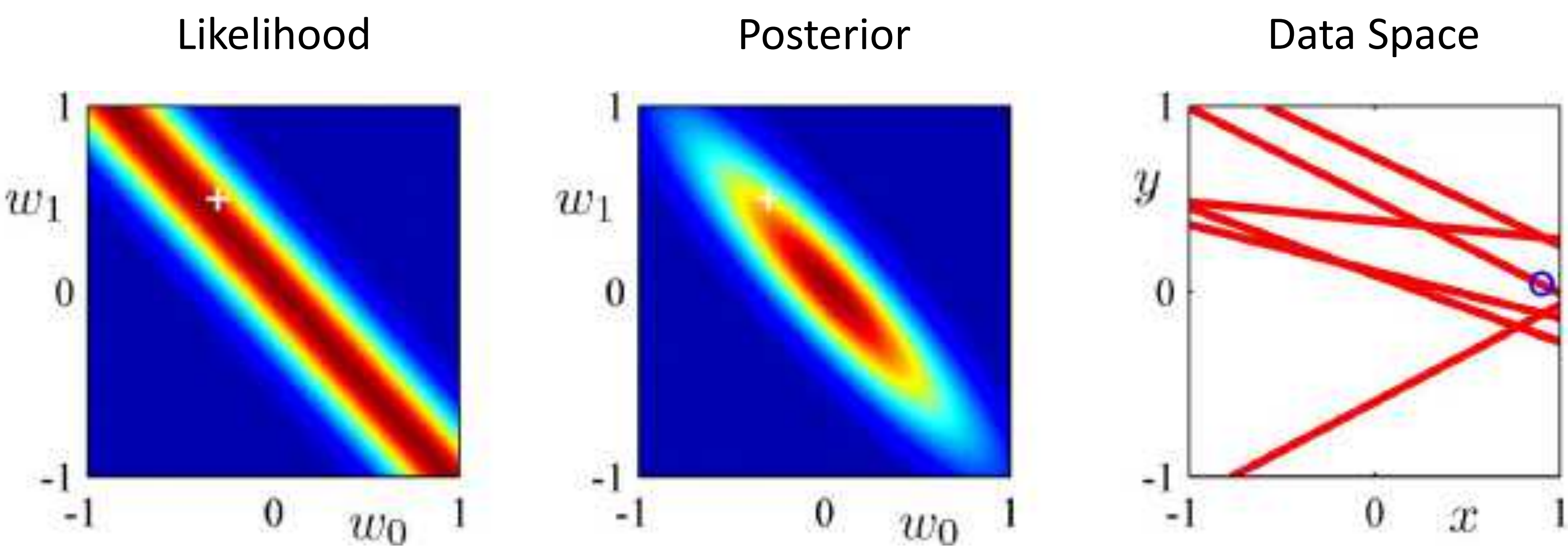
Data Space



$y = w_1 x + w_0$ samples

Bayesian Linear Regression (5)

- 1 data point observed

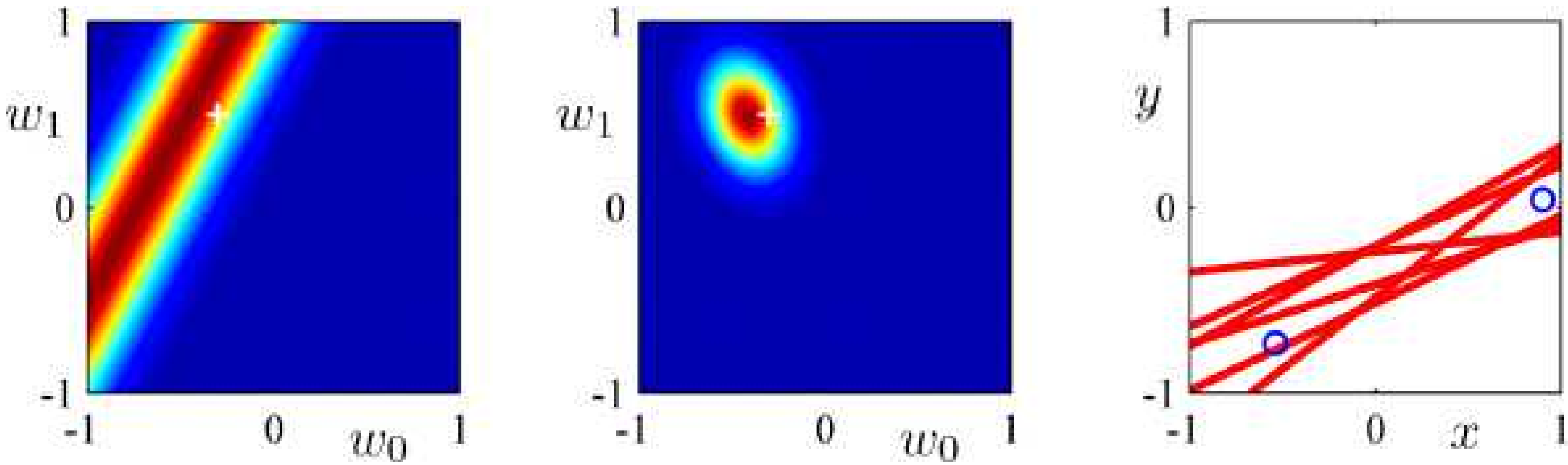


$p(\mathrm{t}|w_1, w_0)$ $p(w_1, w_0|\mathrm{t})$ $y = w_1x + w_0$ samples

Bayesian Linear Regression (6)

- 2 data points observed

Likelihood | Posterior | Data Space

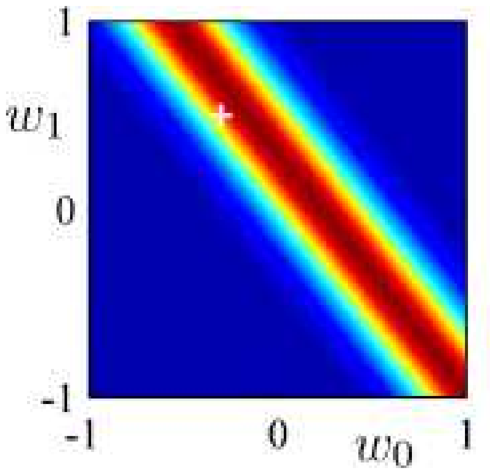


$p(\mathbf{t}|w_1, w_0)$ $\quad$ $p(w_1, w_0|\mathbf{t})$ $\quad$ $y = w_1 x + w_0$ samples

Bayesian Linear Regression (7)

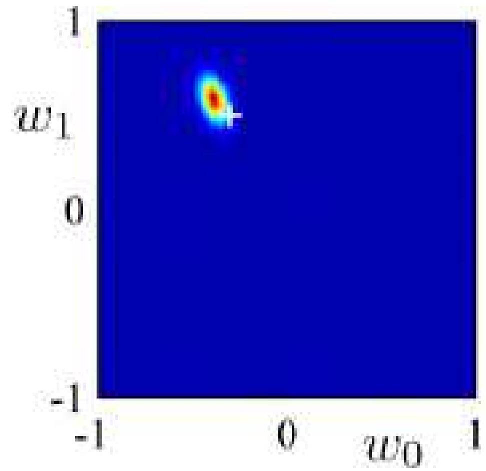
- 20 data points observed

Likelihood



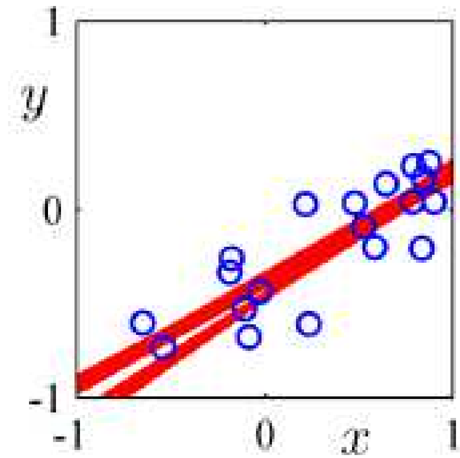
$p(\mathbf{t}|w_1, w_0)$

Posterior



$p(w_1, w_0|\mathbf{t})$

Data Space



$y = w_1 x + w_0$ samples

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Predictive Distribution (1)

- Predict t for new values of $\mathbf{x}$ by integrating over $\mathbf{w}$:

$$p(t|\mathbf{t}, \alpha, \beta) = \int p(t|\mathbf{w}, \beta) p(\mathbf{w}|\mathbf{t}, \alpha, \beta) \, \mathrm{d}\mathbf{w}$$

$$p(t|\mathbf{x}, \mathbf{t}, \alpha, \beta) = \mathcal{N}(t|\mathbf{m}_N^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}), \sigma_N^2(\mathbf{x}))$$

where

$$\sigma_N^2(\mathbf{x}) = \frac{1}{\beta} + \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}} \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x}).$$

Predictive Distribution (2)

- Predict t for new values of $\mathbf{x}$ by expecting over $\mathbf{w}$ and ϵ:

$$t = y(\mathbf{w}, \mathbf{x}) + \epsilon = \mathbf{w}\boldsymbol{\phi}(\mathbf{x}) + \epsilon$$

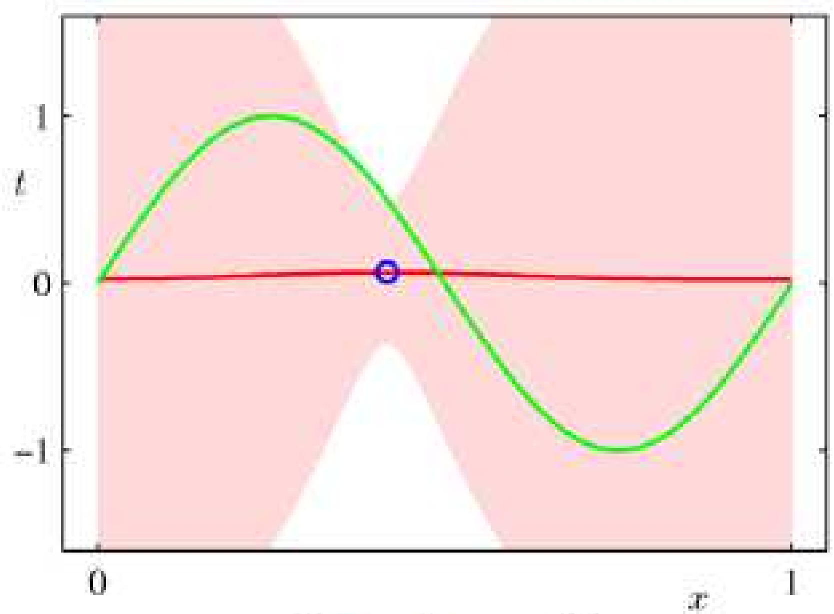
where

$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N) \qquad p(\epsilon|\beta) = \mathcal{N}(\epsilon|0, \beta^{-1})$$

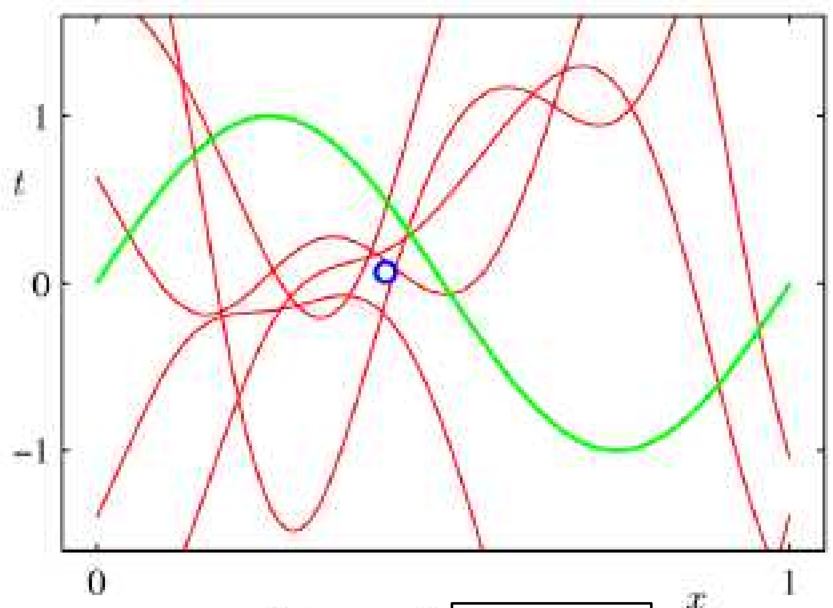
$$\begin{aligned} \mathbf{m}_N &= \beta \mathbf{S}_N \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{t} \\ \mathbf{S}_N^{-1} &= \alpha \mathbf{I} + \beta \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi}. \end{aligned}$$

Predictive Distribution (3)

- Example: Sinusoidal data, 9 Gaussian basis functions, 1 data point



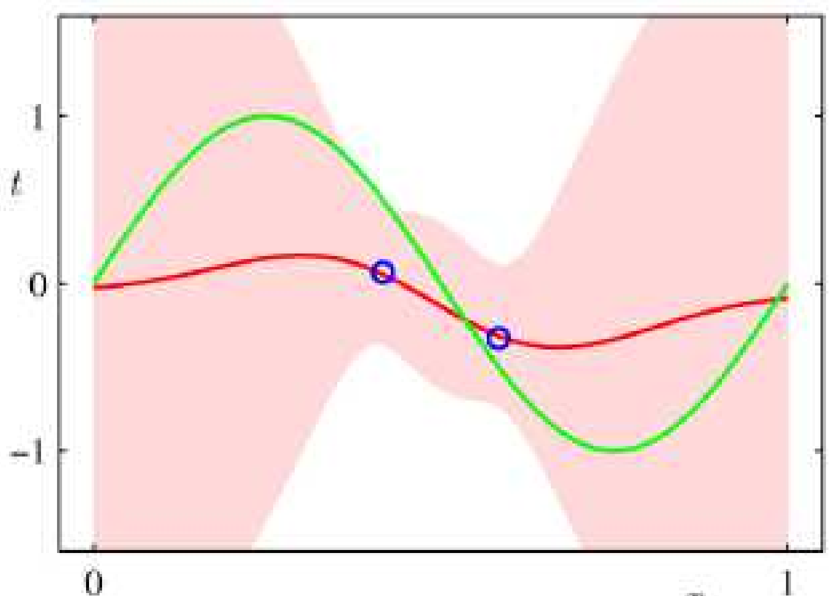
$p(t|\mathbf{x}, \mathbf{t}, \alpha, \beta)$



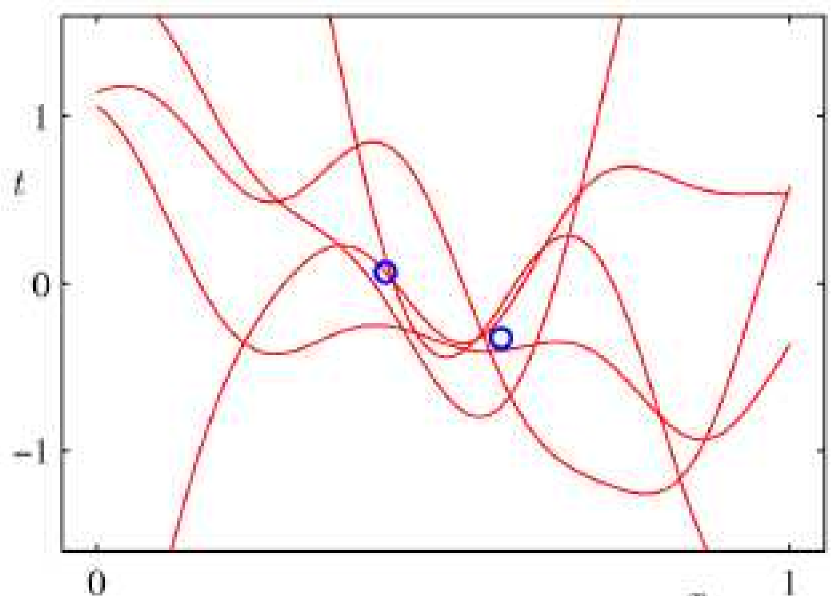
$y(x, \mathbf{w})$ samples

Predictive Distribution (4)

- Example: Sinusoidal data, 9 Gaussian basis functions, 2 data points



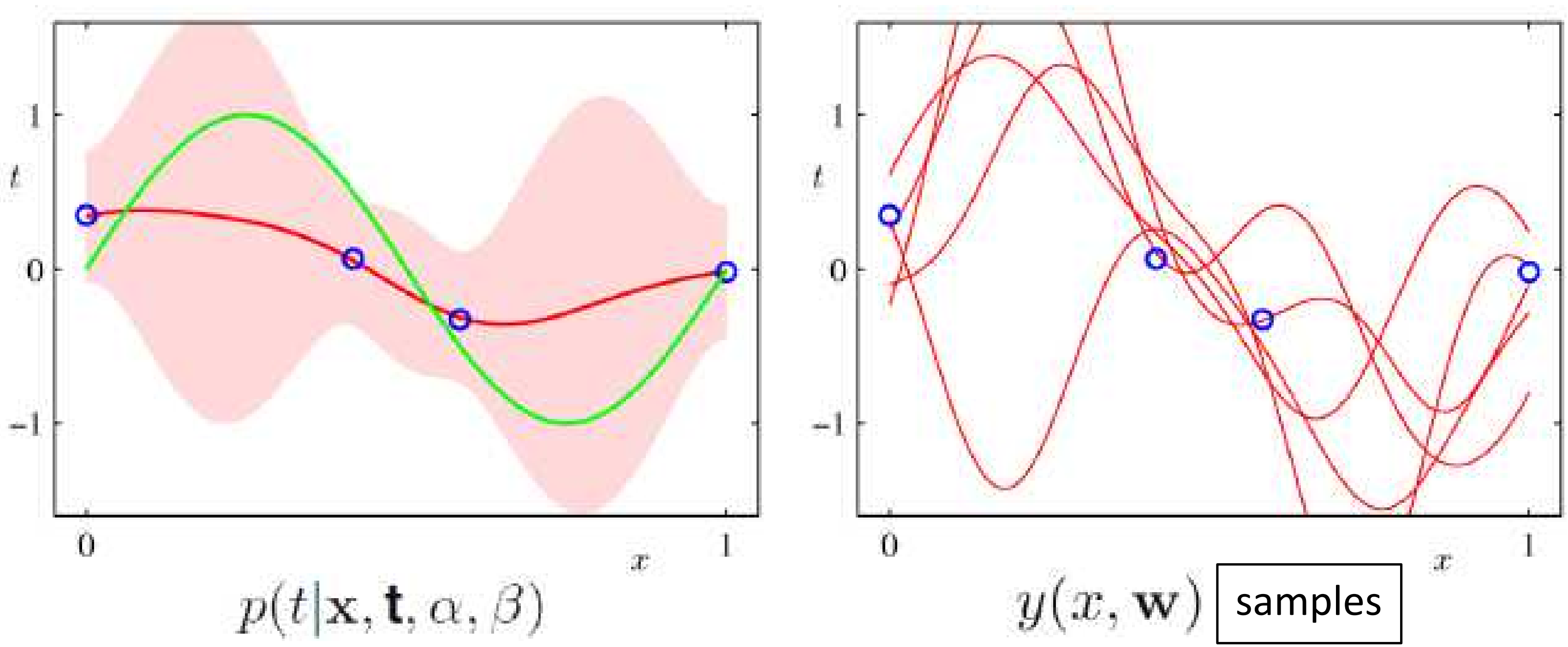
$p(t|\mathbf{x}, \mathbf{t}, \alpha, \beta)$



$y(x, \mathbf{w})$ samples

Predictive Distribution (5)

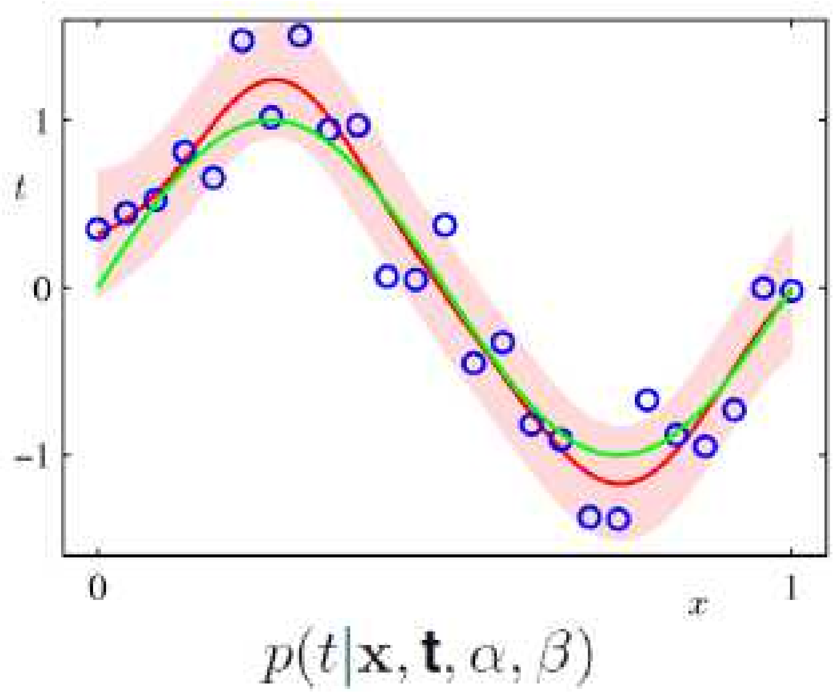
- Example: Sinusoidal data, 9 Gaussian basis functions, 4 data points

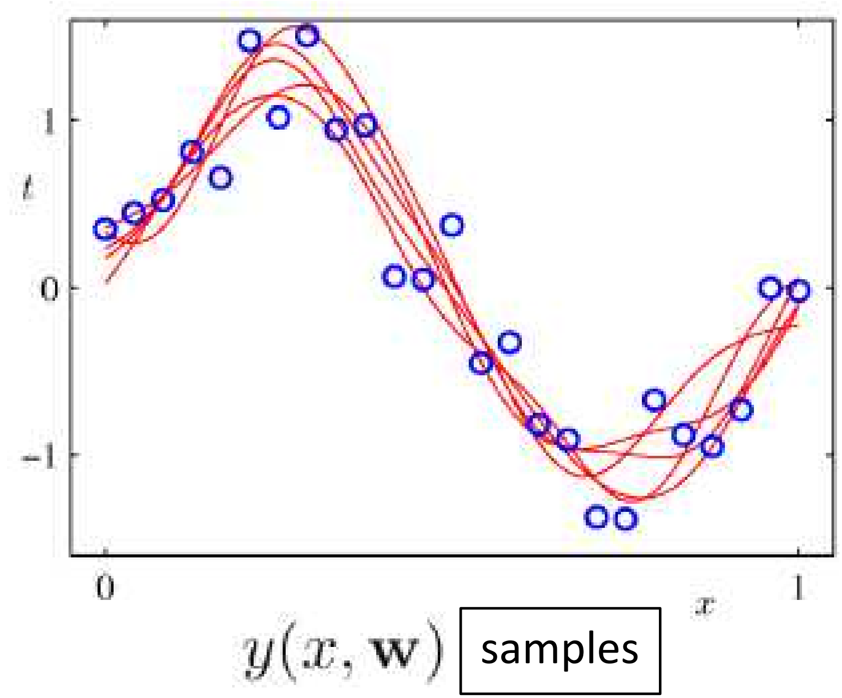


samples

Predictive Distribution (6)

- Example: Sinusoidal data, 9 Gaussian basis functions, 25 data points





Equivalent Kernel (1)

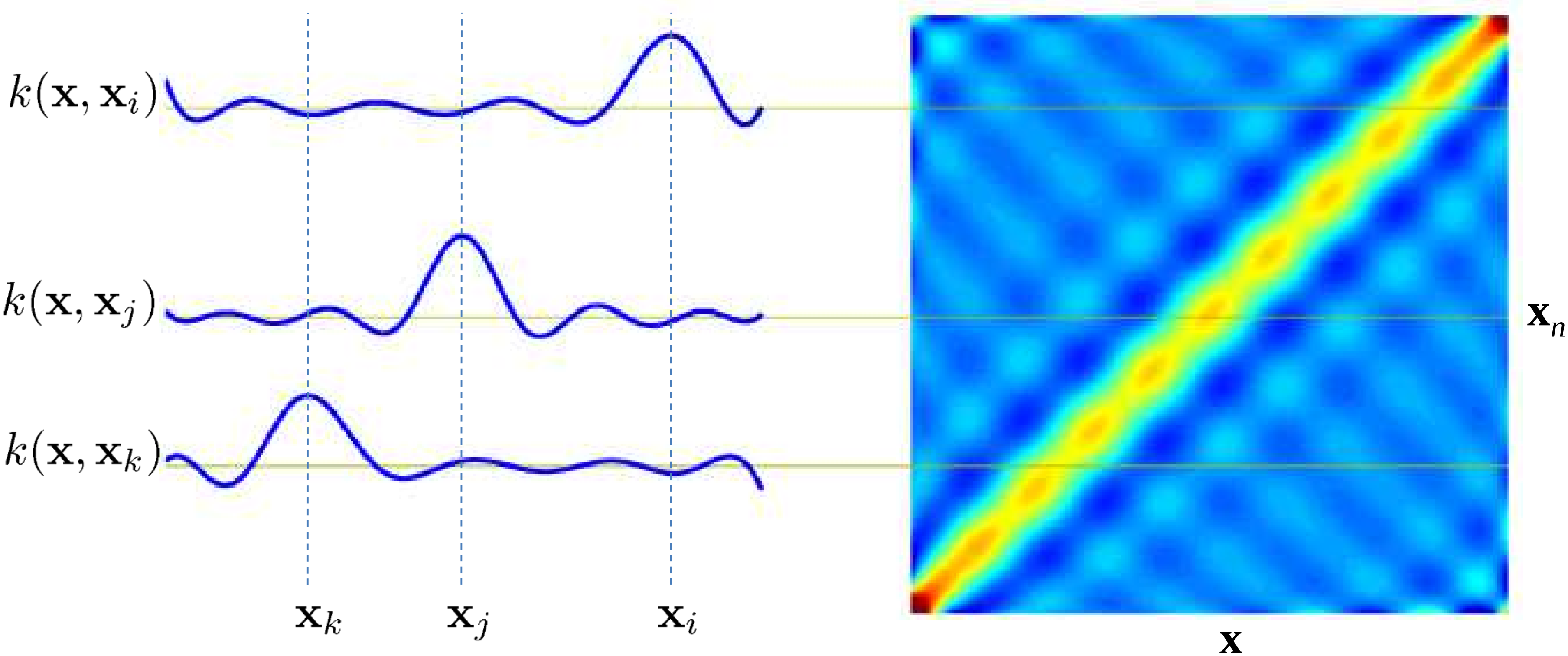
- The predictive mean can be written

$$
\begin{aligned}
y(\mathbf{x}, \mathbf{m}_N) &= \mathbf{m}_N^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}) = \beta \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}} \mathbf{S}_N \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{t} \\
&= \sum_{n=1}^{N} \beta \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}} \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x}_n) t_n \\
&= \sum_{n=1}^{N} k(\mathbf{x}, \mathbf{x}_n) t_n .
\end{aligned}
$$

Equivalent kernel or *smoother matrix*.

- This is a weighted sum of the training data target values, t_n.

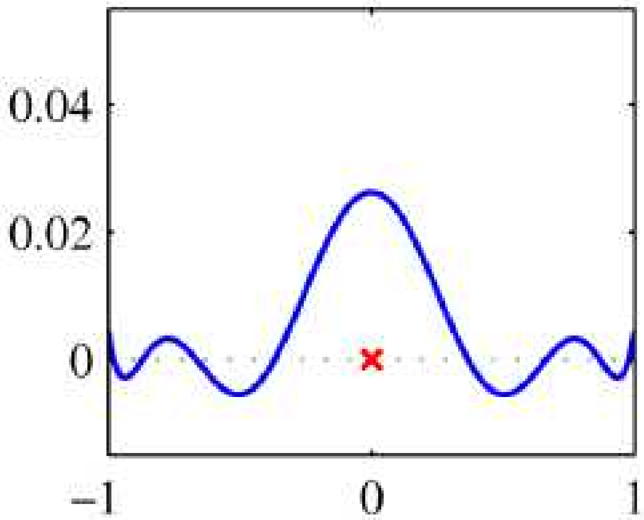
Equivalent Kernel (2)



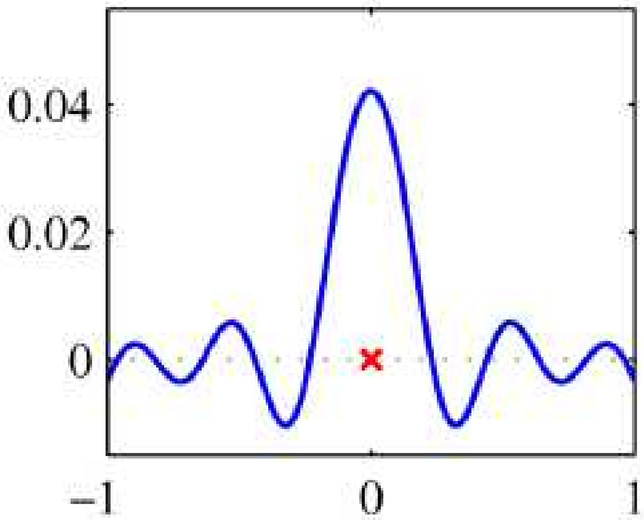
The weight of t_n depends on distance between $\mathbf{x}$ and $\mathbf{x}_n$; nearby $\mathbf{x}_n$ carry more weight.

Equivalent Kernel (3)

Non-local basis functions have local equivalent kernels:



Polynomial



Sigmoidal

Equivalent Kernel (4)

- The kernel as a covariance function: consider

$$\begin{aligned}\mathrm{cov}[y(\mathbf{x}), y(\mathbf{x}')] &= \mathrm{cov}[\boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}}\mathbf{w}, \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}')] \\ &= \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}}\mathbf{S}_N\boldsymbol{\phi}(\mathbf{x}') = \beta^{-1}k(\mathbf{x}, \mathbf{x}').\end{aligned}$$

- We can avoid the use of basis functions and define the kernel function directly, leading to *Gaussian Processes* (Chapter 6).

Equivalent Kernel (5)

$$\sum_{n=1}^{N} k(\mathbf{x}, \mathbf{x}_n) = 1$$

for all values of $\mathbf{x}$; however, the equivalent kernel may be negative for some values of $\mathbf{x}$.

Like all kernel functions, the equivalent kernel can be expressed as an inner product:

$$k(\mathbf{x}, \mathbf{z}) = \boldsymbol{\psi}(\mathbf{x})^{\mathrm{T}} \boldsymbol{\psi}(\mathbf{z})$$

where $\boldsymbol{\psi}(\mathbf{x}) = \beta^{1/2} \mathbf{S}_N^{1/2} \boldsymbol{\phi}(\mathbf{x})$.

Outlines

- Linear Basis Function Models
- Maximum Likelihood and Least Squares
- Bias Variance Decomposition
- Bayesian Linear Regression
- Predictive Distribution
- Bayesian Model Comparison
- Evidence Approximation and Maximization

Bayesian Model Comparison (1)

- How do we choose the 'right' model?
- Assume we want to compare models M_i, $i{=}1, \cdots, L$, using data D; this requires computing

$$p(\mathcal{M}_i|\mathcal{D}) \propto p(\mathcal{M}_i)p(\mathcal{D}|\mathcal{M}_i).$$

Posterior — Prior — *Model evidence* or *marginal likelihood*

- *Bayes Factor*: ratio of evidence for two models

$$\frac{p(\mathcal{D}|\mathcal{M}_i)}{p(\mathcal{D}|\mathcal{M}_j)}$$

Bayesian Model Comparison (2)

- Having comput $p(\mathcal{M}_i|\mathcal{D})$, we can compute the predictive (mixture) distribution

$$p(t|\mathbf{x}, \mathcal{D}) = \sum_{i=1}^{L} p(t|\mathbf{x}, \mathcal{M}_i, \mathcal{D}) p(\mathcal{M}_i|\mathcal{D}).$$

- A simpler approximation, known as *model selection*, is to use the model with the highest evidence.

Bayesian Model Comparison (3)

- For a model with parameters $\mathbf{w}$, we get the model evidence by marginalizing over $\mathbf{w}$

$$p(\mathcal{D}|\mathcal{M}_i) = \int p(\mathcal{D}|\mathbf{w}, \mathcal{M}_i) p(\mathbf{w}|\mathcal{M}_i)\, \mathrm{d}\mathbf{w}.$$

- Note that

$$p(\mathbf{w}|\mathcal{D}, \mathcal{M}_i) = \frac{p(\mathcal{D}|\mathbf{w}, \mathcal{M}_i) p(\mathbf{w}|\mathcal{M}_i)}{p(\mathcal{D}|\mathcal{M}_i)}$$

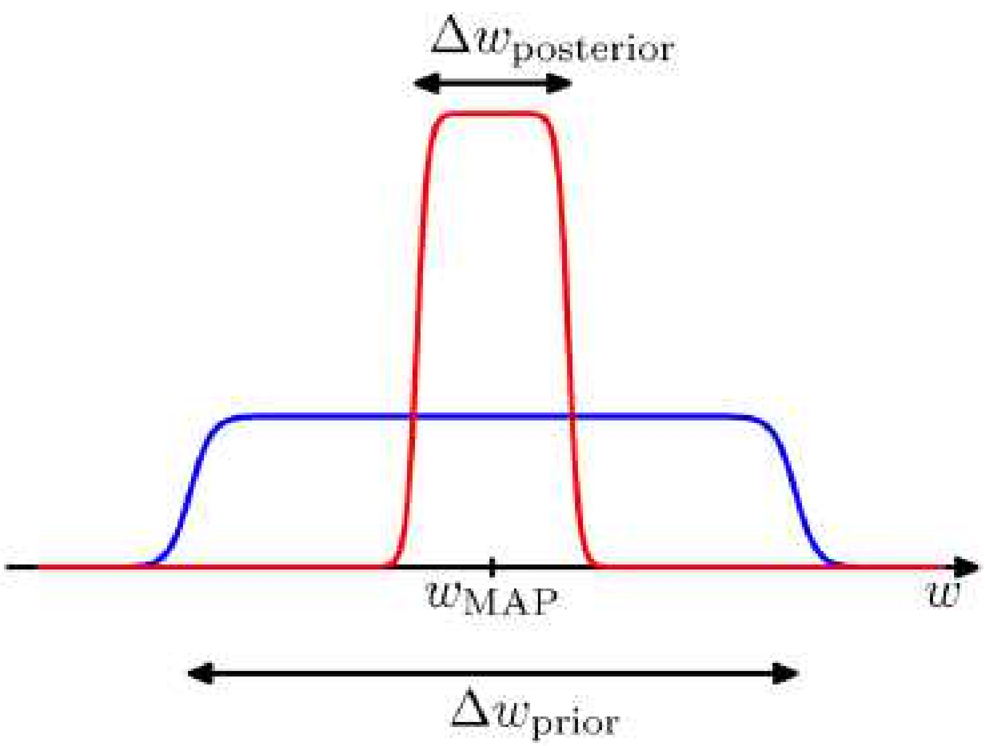
Bayesian Model Comparison (4)

For a given model with a single parameter, w, consider the approximation

$$p(\mathcal{D}) = \int p(\mathcal{D}|w)p(w)\,\mathrm{d}w$$
$$\simeq \quad p(\mathcal{D}|w_{\mathrm{MAP}})\frac{\Delta w_{\mathrm{posterior}}}{\Delta w_{\mathrm{prior}}}$$

where the posterior is assumed to be sharply peaked.

$$p(w) = \frac{1}{\Delta w_{prior}}$$



Bayesian Model Comparison (5)

- Taking logarithms, we obtain

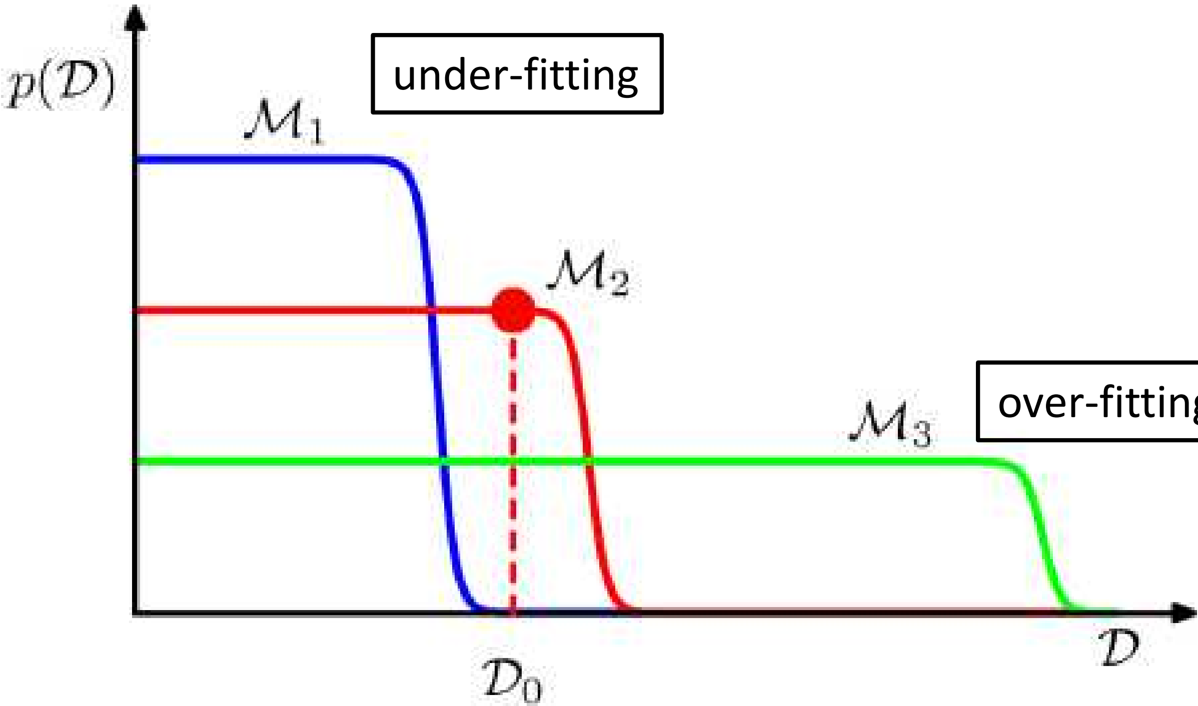
$$\ln p(\mathcal{D}) \simeq \ln p(\mathcal{D}|w_{\mathrm{MAP}}) + \underbrace{\ln\left(\frac{\Delta w_{\mathrm{posterior}}}{\Delta w_{\mathrm{prior}}}\right)}_{\text{Negative}}.$$

- With M parameters, all assumed to have the same ratio $\Delta w_{\mathrm{posterior}}/\Delta w_{\mathrm{prior}}$, we get

$$\ln p(\mathcal{D}) \simeq \ln p(\mathcal{D}|\mathbf{w}_{\mathrm{MAP}}) + \underbrace{M \ln\left(\frac{\Delta w_{\mathrm{posterior}}}{\Delta w_{\mathrm{prior}}}\right)}_{\text{Negative and linear in } M.}.$$

Bayesian Model Comparison (6)

Matching data and model complexity



Outlines

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- Evidence Approximation and Maximization*

The Evidence Approximation (1)*

The fully Bayesian predictive distribution is given by

$$p(t|\mathbf{t}) = \iiint p(t|\mathbf{w}, \beta) p(\mathbf{w}|\mathbf{t}, \alpha, \beta) p(\alpha, \beta|\mathbf{t}) \, \mathrm{d}\mathbf{w} \, \mathrm{d}\alpha \, \mathrm{d}\beta$$

but this integral is intractable. Approximate with

$$p(t|\mathbf{t}) \simeq p\left(t|\mathbf{t}, \widehat{\alpha}, \widehat{\beta}\right) = \int p\left(t|\mathbf{w}, \widehat{\beta}\right) p\left(\mathbf{w}|\mathbf{t}, \widehat{\alpha}, \widehat{\beta}\right) \, \mathrm{d}\mathbf{w}$$

where $\left(\widehat{\alpha}, \widehat{\beta}\right)$ is the mode of $p(\alpha, \beta|\mathbf{t})$, which is assumed to be sharply peaked; a.k.a. *empirical Bayes, type II* or *generalized maximum likelihood,* or *evidence approximation*.

The Evidence Approximation (2)*

From Bayes' theorem we have

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

and if we assume $p(\alpha, \beta)$ to be flat we see that

$$\begin{aligned} p(\alpha, \beta|\mathbf{t}) &\propto p(\mathbf{t}|\alpha, \beta) \\ &= \int p(\mathbf{t}|\mathbf{w}, \beta)p(\mathbf{w}|\alpha)\,\mathrm{d}\mathbf{w}. \end{aligned}$$

General results for Gaussian integrals give

$$p(\mathbf{t} \mid \alpha, \beta) = \left(\frac{\beta}{2\pi}\right)^{\frac{N}{2}} \left(\frac{\alpha}{2\pi}\right)^{\frac{M}{2}} \int \exp\{-E(\boldsymbol{w})\}\,\mathrm{d}\boldsymbol{w}$$

$$\ln p(\mathbf{t}|\alpha, \beta) = \frac{M}{2}\ln\alpha + \frac{N}{2}\ln\beta - E(\mathbf{m}_N) + \frac{1}{2}\ln|\mathbf{S}_N| - \frac{N}{2}\ln(2\pi).$$

The Evidence Approximation (3)*

$$E(\boldsymbol{w}) = E(\boldsymbol{m}_N) + \frac{1}{2}(\boldsymbol{w} - \boldsymbol{m}_N)^T \boldsymbol{A}(\boldsymbol{w} - \boldsymbol{m}_N)$$

Precision: $\boldsymbol{A} = \alpha \boldsymbol{I} + \beta \boldsymbol{\Phi}^T \boldsymbol{\Phi} \quad \boldsymbol{A} = \boldsymbol{S}_N^{-1}$

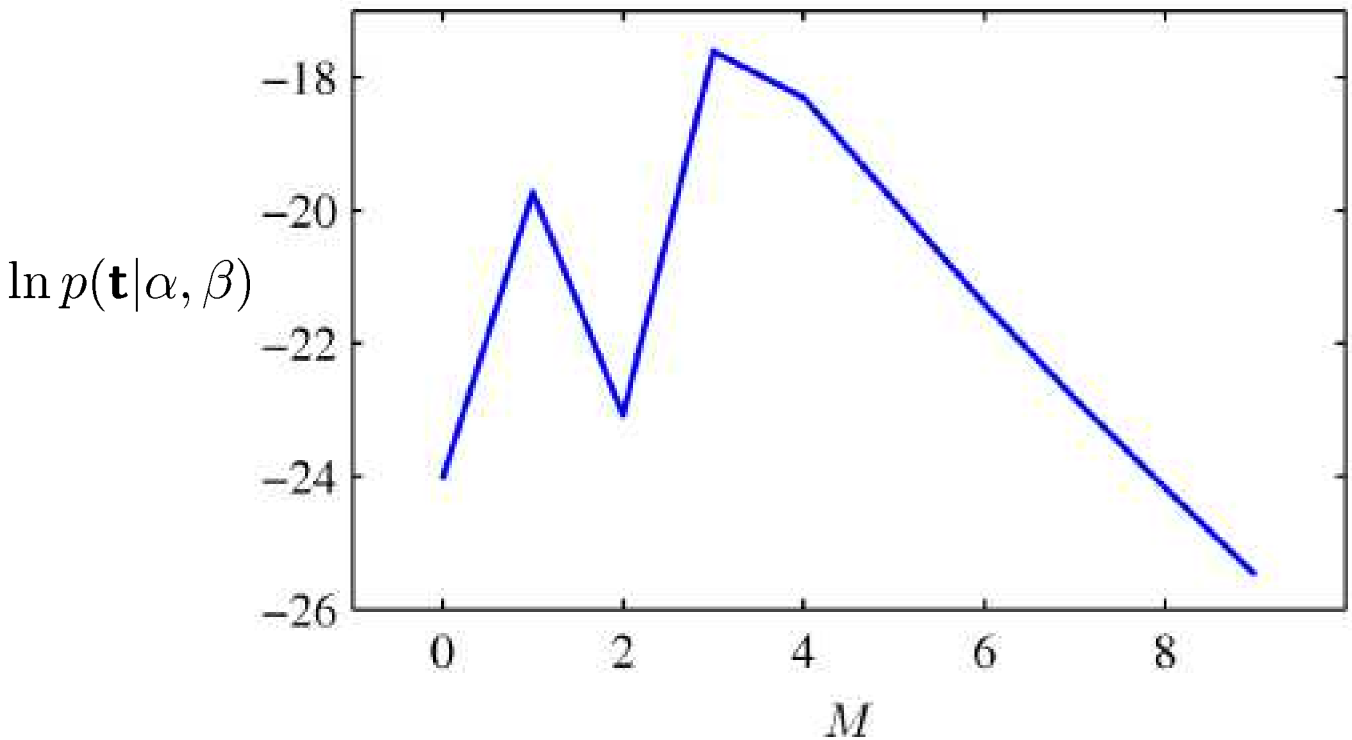
$$\mathbf{m}_N = \beta \mathbf{S}_N \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{t}$$
$$\mathbf{S}_N^{-1} = \alpha \mathbf{I} + \beta \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi}.$$

$$E(\boldsymbol{m}_N) = \frac{\beta}{2}\|\mathbf{t} - \boldsymbol{\Phi}\boldsymbol{m}_N\|^2 + \frac{\beta}{2}\boldsymbol{m}_N^T \boldsymbol{m}_N$$

$$\int \exp\{-E(\boldsymbol{w})\}\,\mathrm{d}\,\boldsymbol{w}$$
$$= \exp\{-E(\boldsymbol{m}_N)\} \int \exp\left\{-\frac{1}{2}(\boldsymbol{w} - \boldsymbol{m}_N)^T \boldsymbol{A}(\boldsymbol{w} - \boldsymbol{m}_N)\right\} \mathrm{d}\boldsymbol{w}$$
$$= \exp\{-E(\boldsymbol{m}_N)\}(2\pi)^{\frac{M}{2}} |\boldsymbol{A}|^{-\frac{1}{2}}$$

The Evidence Approximation (4)*

- Example: sinusoidal data, M^{th} degree polynomial, $\alpha = 5 \times 10^{-3}$



Maximizing the Evidence Function (1)*

- To maximise $\ln p(\mathbf{t}|\alpha, \beta)$ w.r.t. α and β, we define the eigenvector equation

$$\boxed{\text{Precision:}} \quad \left(\beta \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi}\right) \mathbf{u}_i = \lambda_i \mathbf{u}_i.$$

- Thus

$$\boxed{\text{Precision:}} \quad \mathbf{A} = \mathbf{S}_N^{-1} = \alpha \mathbf{I} + \beta \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi}$$

has eigenvalues $\lambda_i + \alpha$.

Maximizing the Evidence Function (2)*

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\ln|\boldsymbol{A}| = \frac{\mathrm{d}}{\mathrm{d}\alpha}\ln\prod_i(\lambda_i+\alpha) = \frac{\mathrm{d}}{\mathrm{d}\alpha}\sum_i\ln(\lambda_i+\alpha) = \sum_i\frac{1}{\lambda_i+\alpha}$$

$$\frac{\partial p(\mathbf{t}|\alpha,\beta)}{\partial\alpha} = \; 0 = \frac{M}{2\alpha} - \frac{1}{2}\boldsymbol{m}_N^T\boldsymbol{m}_N - \frac{1}{2}\sum_i\frac{1}{\lambda_i+\alpha}$$

$$\frac{\mathrm{d}}{\mathrm{d}\beta}\ln|\boldsymbol{A}| = \frac{\mathrm{d}}{\mathrm{d}\beta}\sum_i\ln(\lambda_i+\alpha) = \frac{1}{\beta}\sum_i\frac{\lambda_i}{\lambda_i+\alpha} = \frac{\gamma}{\beta}$$

$$\frac{\partial p(\mathbf{t}|\alpha,\beta)}{\partial\beta} = \; 0 = \frac{N}{2\beta} - \frac{1}{2}\sum_{n=1}^{N}\{t_n - \boldsymbol{m}_N^T\boldsymbol{\phi}(\boldsymbol{x}_n)\}^2 - \frac{\gamma}{2\beta}$$

Maximizing the Evidence Function (3)*

- We can now differentiate $\ln p(\mathbf{t}|\alpha,\beta)$ w.r.t. α and β, and set the results to zero, to get

$$\alpha = \frac{\gamma}{\mathbf{m}_N^{\mathrm{T}}\mathbf{m}_N}$$

$$\boxed{\frac{1}{\beta_{\mathrm{MAP}}}:} \quad \frac{1}{\beta} = \frac{1}{N-\gamma}\sum_{n=1}^{N}\left\{t_n - \mathbf{m}_N^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\right\}^2$$

where

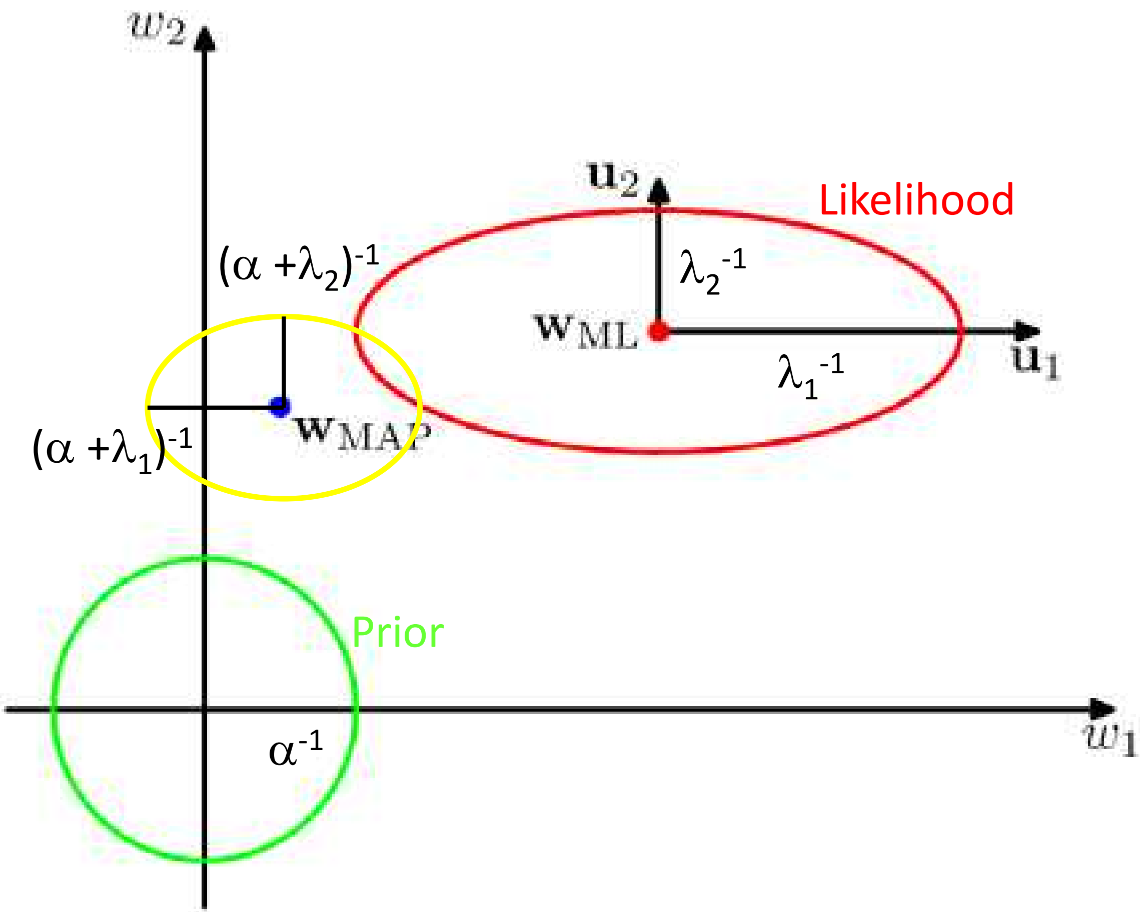
$$\gamma = \sum_i \frac{\lambda_i}{\alpha+\lambda_i}.$$

γ depends on both α and β.

recall

$$\boxed{\frac{1}{\beta_{\mathrm{ML}}} = \frac{1}{N}\sum_{n=1}^{N}\{t_n - \mathbf{w}_{\mathrm{ML}}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\}^2}$$

Effective Number of Parameters (1)*



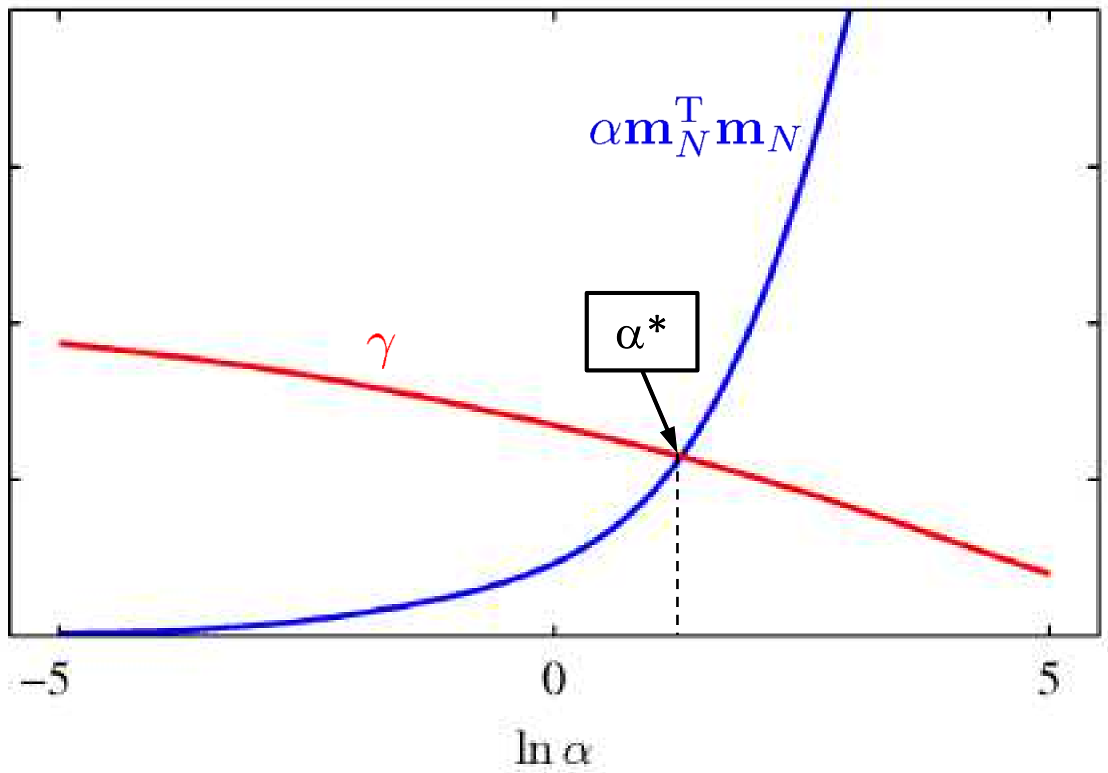
$\lambda_1 \ll \alpha$
w_1 is not well determined by the likelihood when more disturbed from β

$\lambda_2 \gg \alpha$
w_2 is well determined by the likelihood when less disturbed from β

γ is the number of well determined parameters

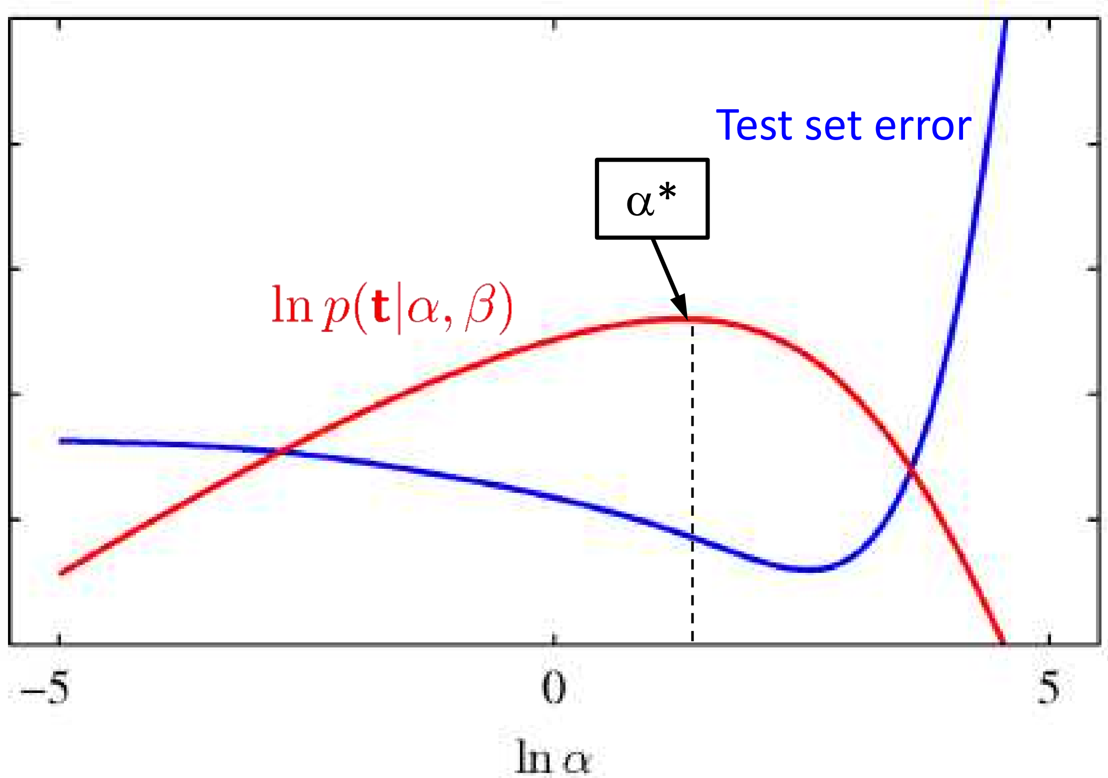
Effective Number of Parameters (2)*

- Example: sinusoidal data, 9 Gaussian basis functions, $\beta = 11.1$ (true value β*).



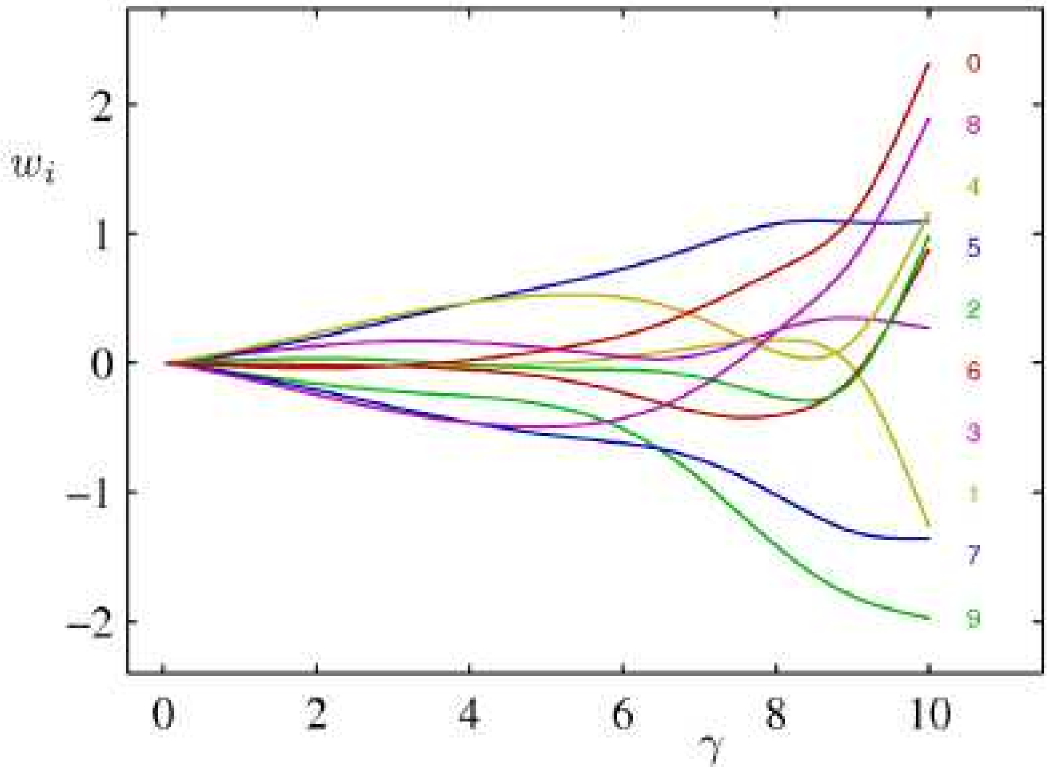
Effective Number of Parameters (3)*

- Example: sinusoidal data, 9 Gaussian basis functions, $\beta = 11.1$ (true value β*).



Effective Number of Parameters (4)*

- Example: sinusoidal data, 9 Gaussian basis functions, $\beta = 11.1$ (true value β*).



$\infty > \alpha \geq 0$

$0 \leq \gamma \leq 10$

Effective Number of Parameters (5)*

- In the limit $N \gg M$, $\gamma = M$ and we can consider using the easy-to-compute approximation

$$\alpha = \frac{M}{\mathbf{m}_N^{\mathrm{T}}\mathbf{m}_N}$$

$$\frac{1}{\beta} = \frac{1}{N}\sum_{n=1}^{N}\left\{t_n - \mathbf{m}_N^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\right\}^2.$$

$$\boxed{\frac{1}{\beta_{\mathrm{ML}}} = \frac{1}{N}\sum_{n=1}^{N}\{t_n - \mathbf{w}_{\mathrm{ML}}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\}^2}$$

Limitations of Fixed Basis Functions

- M basis function along each dimension of a D-dimensional input space requires M^D basis functions: the curse of dimensionality.
- In later chapters, we shall see how we can get away with fewer basis functions, by choosing these using the training data.