STA 4273H: Statistical Machine Learning

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Lecture 4

Recap

- In our previous classes, we looked at:

  - Statistical Decision Theory
  - Linear Regression Models
  - Linear Basis Function Models
  - Regularized Linear Regression Models
  - Bias-Variance Decomposition

- We will now look at the Bayesian framework and Bayesian Linear Regression Models.

Bayesian Approach

- We formulate our knowledge about the world probabilistically:
  - We define the model that expresses our knowledge qualitatively (e.g. independence assumptions, forms of distributions).
  - Our model will have some unknown parameters.
  - We capture our assumptions, or prior beliefs, about unknown parameters (e.g. range of plausible values) by specifying the prior distribution over those parameters before seeing the data.
- We observe the data.
- We compute the posterior probability distribution for the parameters, given observed data.
- We use this posterior distribution to:
  - Make predictions by averaging over the posterior distribution
  - Examine/Account for uncertainly in the parameter values.
  - Make decisions by minimizing expected posterior loss.

(See Radford Neal's NIPS tutorial on ``Bayesian Methods for Machine Learning'')

Posterior Distribution

- The posterior distribution for the model parameters can be found by combining the prior with the likelihood for the parameters given the data.

- This is accomplished using Bayes' Rule:

$$P(\text{parameters} \mid \text{data}) = \frac{P(\text{data} \mid \text{parameters})P(\text{parameters})}{P(\text{data})}$$

Probability of observed data given w

Prior probability of weight vector w

$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})P(\mathbf{w})}{P(\mathcal{D})}$$

Posterior probability of weight vector W given training data D

Marginal likelihood (normalizing constant):

$$P(\mathcal{D}) = \int p(\mathcal{D}|\mathbf{w})P(\mathbf{w})\mathrm{d}\mathbf{w}$$

This integral can be high-dimensional and is often difficult to compute.

The Rules of Probability

Sum Rule:

$$p(X) = \sum_Y p(X, Y)$$

Product Rule:

$$p(X, Y) = p(Y|X)p(X)$$

Predictive Distribution

- We can also state Bayes' rule in words:

$$\text{posterior} \propto \text{likelihood} \times \text{prior}.$$

- We can make predictions for a new data point $\mathbf{x}^*$, given the training dataset by integrating over the posterior distribution:

$$p(\mathbf{x}^*|\mathcal{D}) = \int p(\mathbf{x}^*|\mathbf{w},\mathcal{D})p(\mathbf{w}|\mathcal{D})\mathrm{d}\mathbf{w} = \mathbb{E}_{P(\mathbf{w}|\mathcal{D})}\big[p(\mathbf{x}^*|\mathbf{w},\mathcal{D})\big],$$

which is sometimes called predictive distribution.

- Note that computing predictive distribution requires knowledge of the posterior distribution:

$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})P(\mathbf{w})}{P(\mathcal{D})}, \quad \text{where } P(\mathcal{D}) = \int p(\mathcal{D}|\mathbf{w})P(\mathbf{w})\mathrm{d}\mathbf{w}$$

which is usually intractable.

Modeling Challenges

• The first challenge is in specifying suitable model and suitable prior distributions. This can be challenging particularly when dealing with high-dimensional problems we see in machine learning.

- A suitable model should admit all the possibilities that are thought to be at all likely.
- A suitable prior should avoid giving zero or very small probabilities to possible events, but should also avoid spreading out the probability over all possibilities.

• We may need to properly model dependencies between parameters in order to avoid having a prior that is too spread out.

• One strategy is to introduce latent variables into the model and hyperparameters into the prior.

• Both of these represent the ways of modeling dependencies in a tractable way.

Computational Challenges

The other big challenge is computing the posterior distribution. There are several main approaches:

- Analytical integration: If we use "conjugate" priors, the posterior distribution can be computed analytically. Only works for simple models and is usually too much to hope for.

- Gaussian (Laplace) approximation: Approximate the posterior distribution with a Gaussian. Works well when there is a lot of data compared to the model complexity (as posterior is close to Gaussian).

- Monte Carlo integration: Once we have a sample from the posterior distribution, we can do many things. The dominant current approach is Markov Chain Monte Carlo (MCMC) -- simulate a Markov chain that converges to the posterior distribution. It can be applied to a wide variety of problems.

- Variational approximation: A cleverer way to approximate the posterior. It often works much faster compared to MCMC. But often not as general as MCMC.

Bayesian Linear Regression

- Given observed inputs $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\}$, and corresponding target values $\mathbf{t} = [t_1, t_2, ..., t_N]^T$, we can write down the likelihood function:

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

where $\boldsymbol{\phi}(\mathbf{x}) = (\phi_0(\mathbf{x}), \phi_1(\mathbf{x}), ..., \phi_{M-1}(\mathbf{x}))^T$ represent our basis functions.

- The corresponding conjugate prior is given by a Gaussian distribution:

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

- As both the likelihood and the prior terms are Gaussians, the posterior distribution will also be Gaussian.

- If the posterior distributions p(θ|x) are in the same family as the prior probability distribution p(θ), the prior and posterior are then called **conjugate distributions**, and the prior is called a **conjugate prior** for the likelihood.

Bayesian Linear Regression

- Combining the prior together with the likelihood term:

$$p(\mathbf{w}|\mathbf{t}, \mathbf{X}, \mathbf{w}, \beta) \propto \left[\prod_{n=1}^{N} \mathcal{N}(t_n|\mathbf{w}^T\phi(\mathbf{x}_n), \beta^{-1})\right] \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0).$$

- The posterior (with a bit of manipulation) takes the following Gaussian form:

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

where

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

- The posterior mean can be expresses in terms of the least-squares estimator and the prior mean:

$$\mathbf{m}_N = \mathbf{S}_N \left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\mathbf{\Phi}^T\mathbf{\Phi}\mathbf{w}_{ML}\right).$$

$$\boxed{\mathbf{w}_{ML} = (\mathbf{\Phi}^T\mathbf{\Phi})^{-1}\mathbf{\Phi}^T\mathbf{t}.}$$

- As we increase our prior precision (decrease prior variance), we place greater weight on the prior mean relative the data.

Bayesian Linear Regression

• Consider a zero mean isotropic Gaussian prior, which is govern by a single precision parameter α:

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

for which the posterior is Gaussian with:

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

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

• If we consider an infinitely broad prior, $\alpha \rightarrow 0$, the mean $\mathbf{m}_\mathbf{N}$ of the posterior distribution reduces to maximum likelihood value $\mathbf{w}_{\mathbf{ML}}$.

• The log of the posterior distribution is given by the sum of the log-likelihood and the log of the prior:

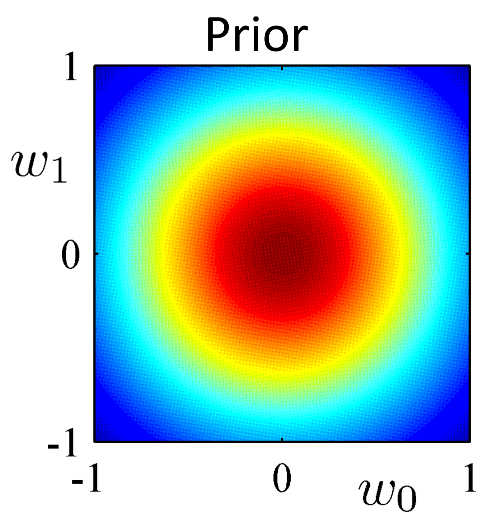
$$\ln p(\mathbf{w}|\mathcal{D}) = -\frac{\beta}{2}\sum_{n=1}^{N}\left(t_n - \mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_n)\right)^2 - \frac{\alpha}{2}\mathbf{w}^T\mathbf{w} + \text{const.}$$

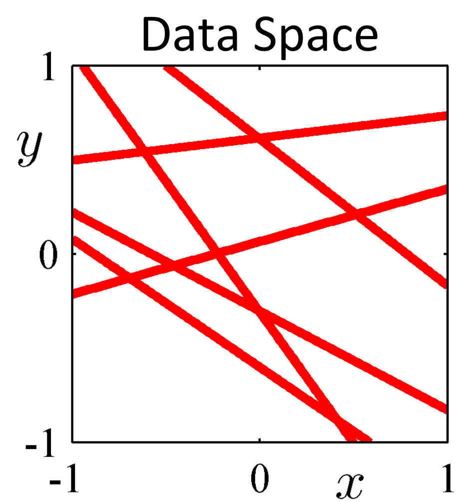
• Maximizing this posterior with respect to **w** is equivalent to minimizing the sum-of-squares error function with a quadratic regulation term $\lambda = \alpha / \beta$.

Bayesian Linear Regression

- Consider a linear model of the form: $y(x, \mathbf{w}) = w_0 + w_1 x.$
- The training data is generated from the function $f(x, \mathbf{a}) = a_0 + a_1 x$ with $a_0 = 0.3; a_1 = 0.5,$ by first choosing x_n uniformly from [-1;1], evaluating $f(x, \mathbf{a}),$ and adding a small Gaussian noise.
- Goal: recover the values of a_0, a_1 from such data.

0 data points are observed:





Bayesian Linear Regression

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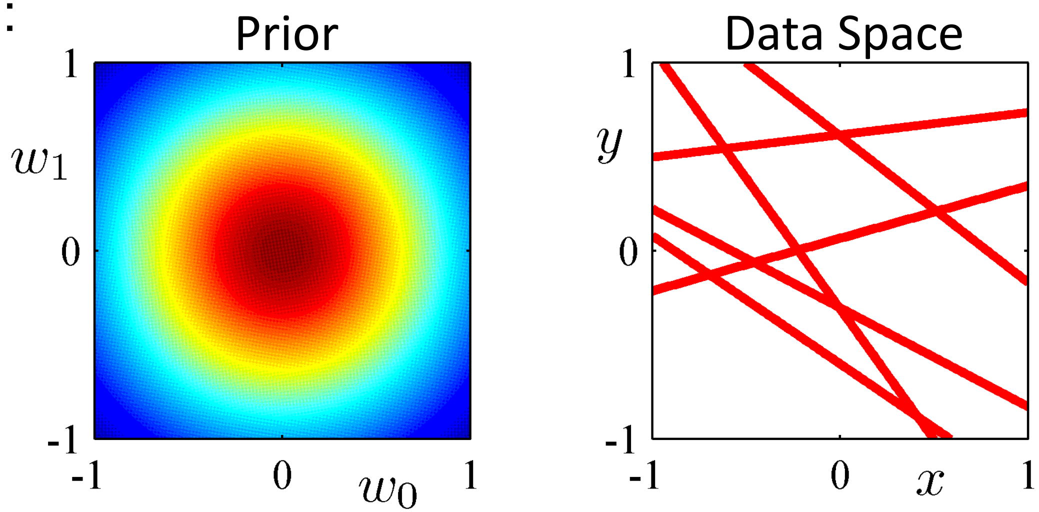
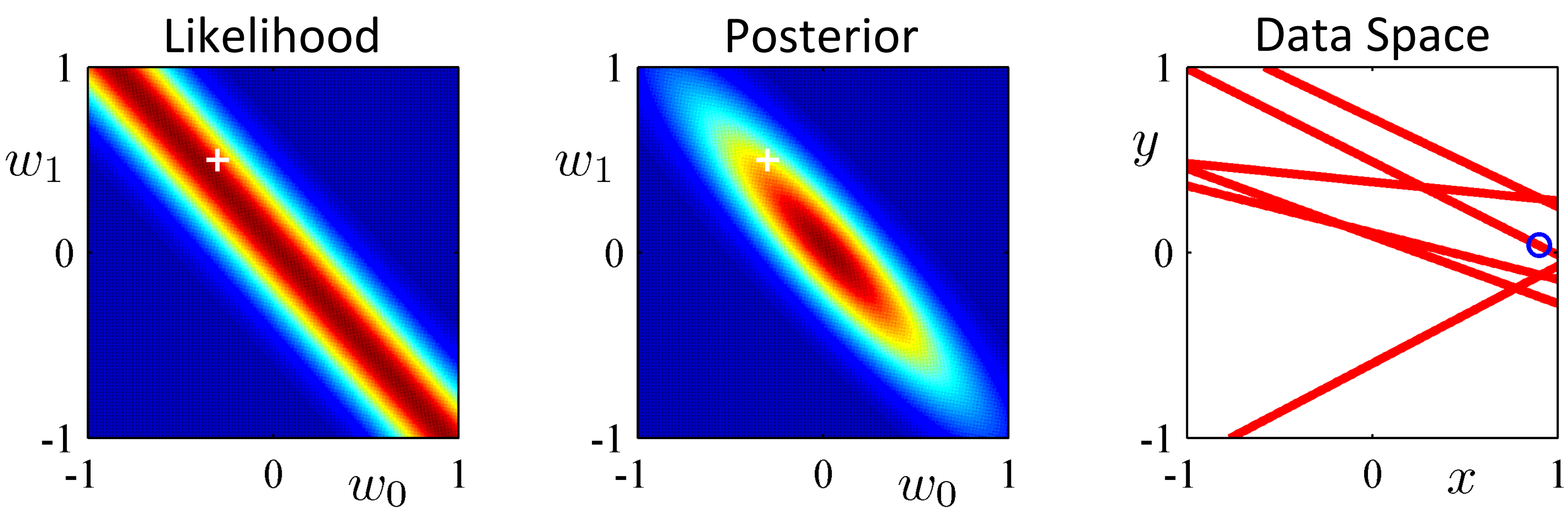
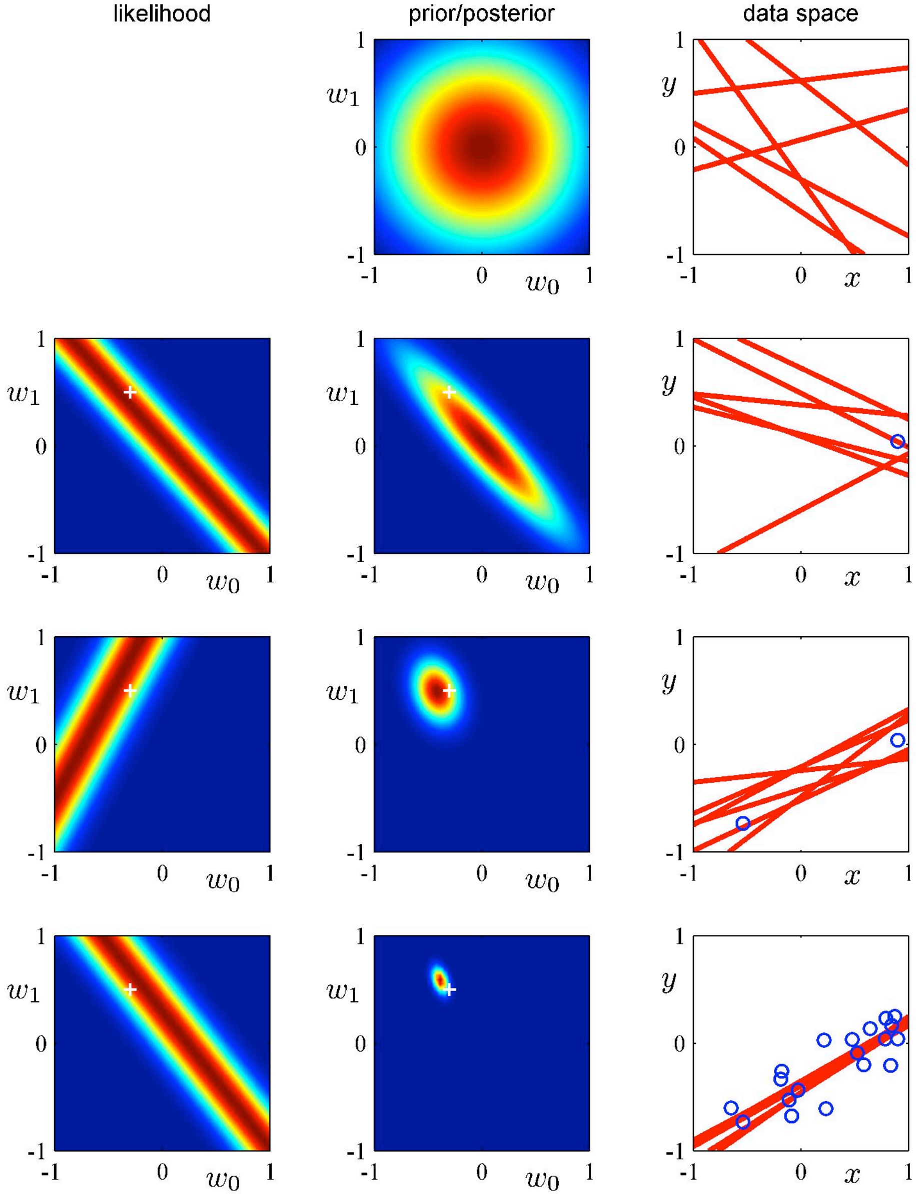


1 data point is observed:



Bayesian Linear Regression



0 data points are observed.

1 data point is observed.

2 data points are observed.

20 data points are observed.

Predictive Distribution

• We can make predictions for a new input vector **x** by integrating over the posterior distribution:

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

where

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

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

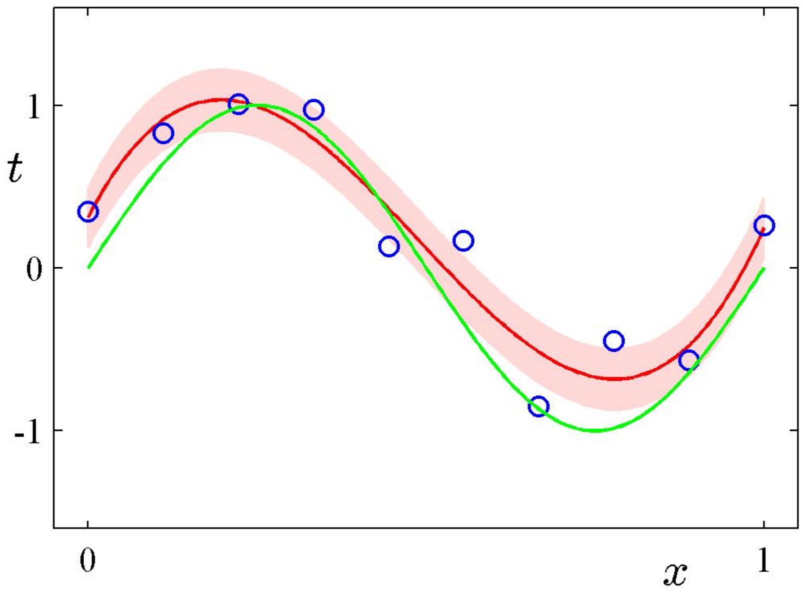
Noise in the target values

Uncertainly associated with parameter values.

• In the limit, as N $\rightarrow \infty$, the second term goes to zero.
• The variance of the predictive distribution arises only from the additive noise governed by parameter β.

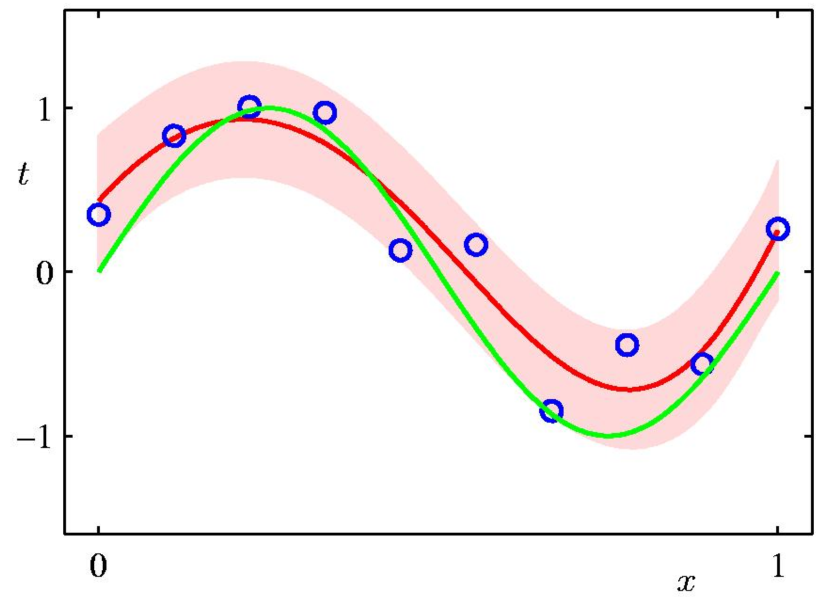
Predictive Distribution: Bayes vs. ML

Predictive distribution based on maximum likelihood estimates



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

Bayesian predictive distribution

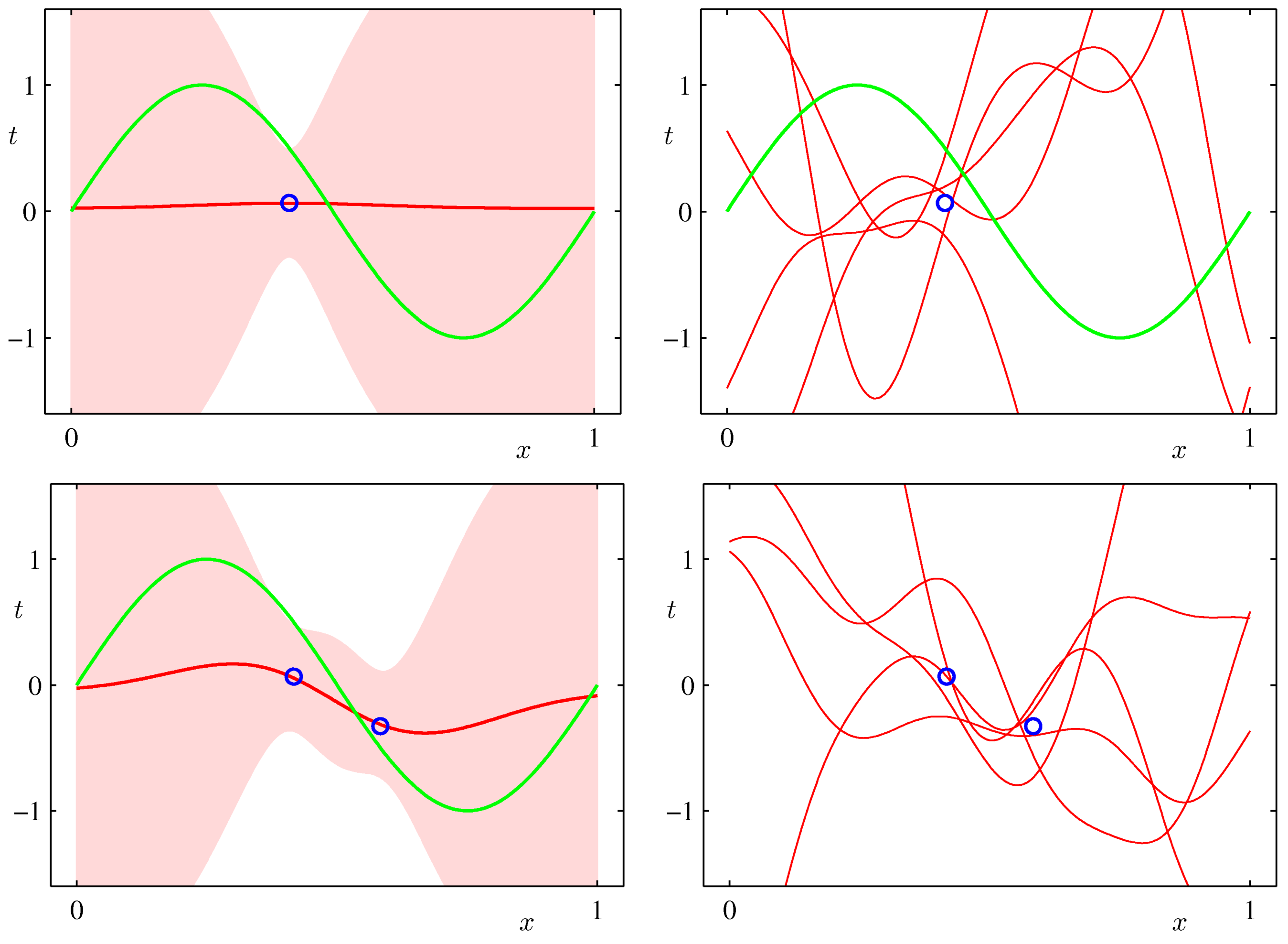


$$p(t|x, \mathbf{t}, \mathbf{X}) = \mathcal{N}\left(t|\mathbf{m}_N^T \boldsymbol{\phi}(x), \sigma_N^2(x)\right)$$

Predictive Distribution

Sinusoidal dataset, 9 Gaussian basis functions.

Predictive distribution   Samples from the posterior



Predictive Distribution

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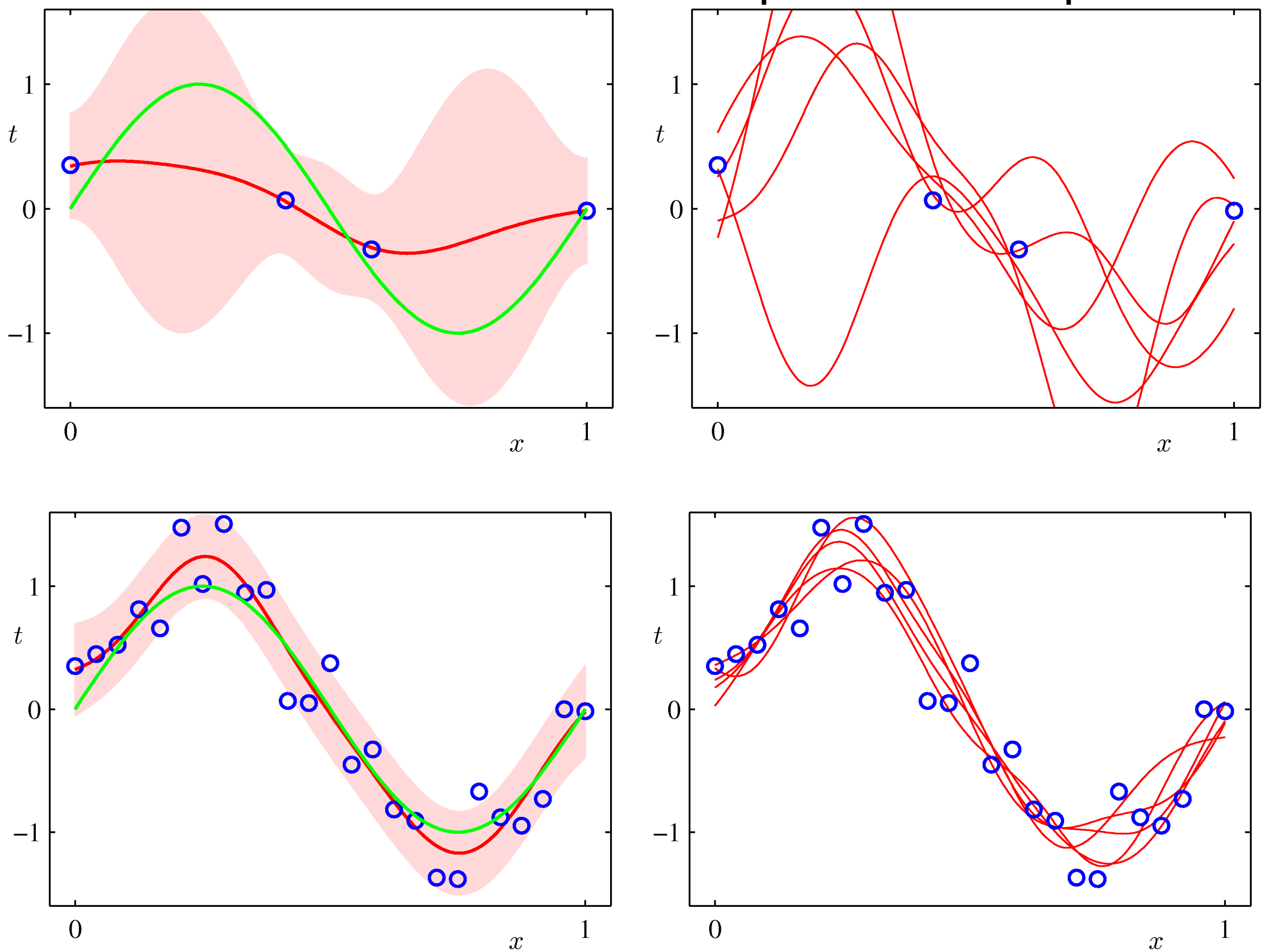
Predictive distribution Samples from the posterior



Gamma-Gaussian Conjugate Prior

- So far we have assumed that the noise parameter β is known.
- If both **w** and β are treated as unknown, then we can introduce a conjugate prior distribution that will be given by the Gaussian-Gamma distribution:

$$p(\mathbf{w}, \beta) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \beta^{-1}\mathbf{S}_0)\mathrm{Gam}(\beta|a_0, b_0),$$

where the Gamma distribution is given by:

$$\mathrm{Gam}(\beta|a, b) = \frac{1}{\Gamma(a)} b^a \beta^{a-1} \exp(-b\beta), \qquad \Gamma(a) = \int_0^\infty u^{a-1} e^{-u} \mathrm{d}u.$$

- The posterior distribution takes the same functional form as the prior:

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \beta^{-1}\mathbf{S}_N)\mathrm{Gam}(\beta|a_N, b_N).$$

Equivalent Kernel

- The predictive mean can be written as:

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

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

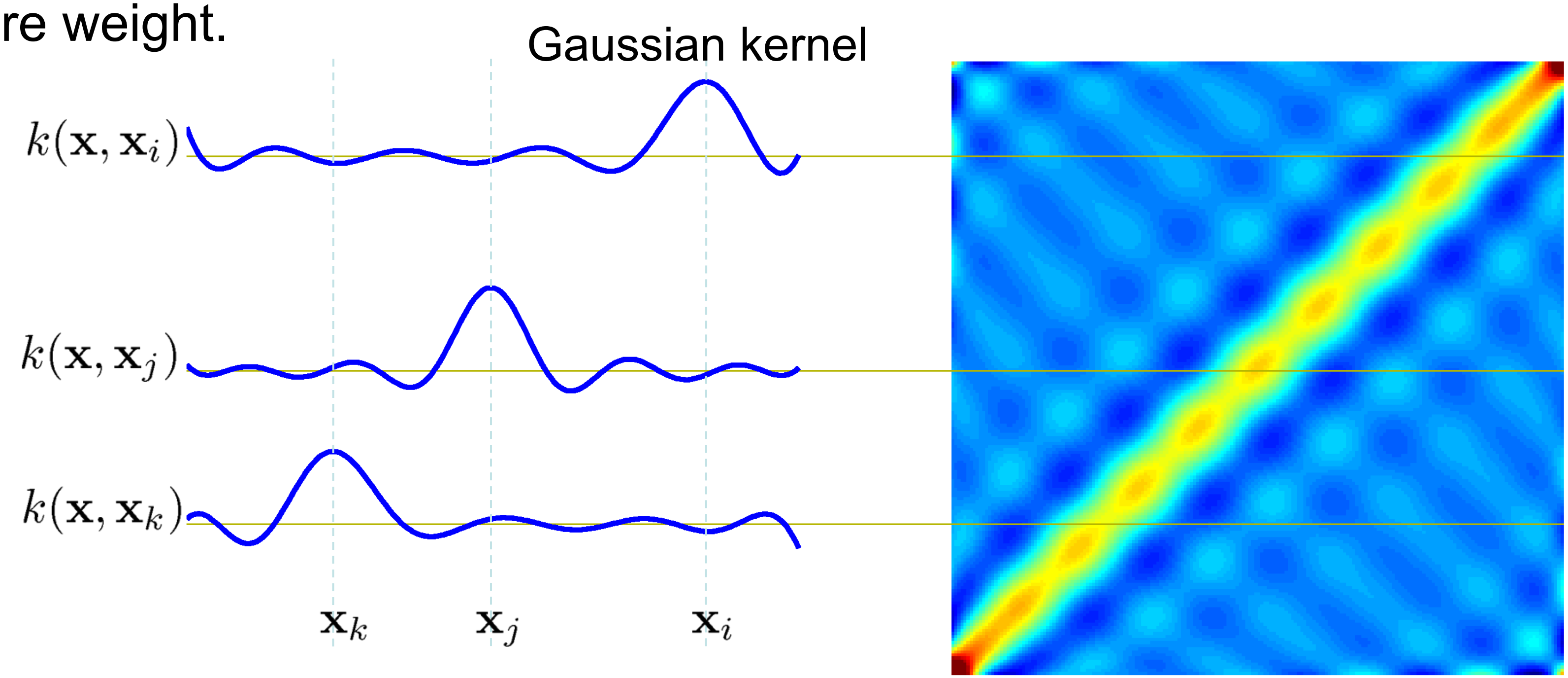
Equivalent kernel or smoother matrix.

- The mean of the predictive distribution at a time **x** can be written as a linear combination of the training set target values.

- Such regression functions are called linear smoothers.

Equivalent Kernel

• The weight of t_n depends on distance between x and x_n; nearby x_n carry more weight.



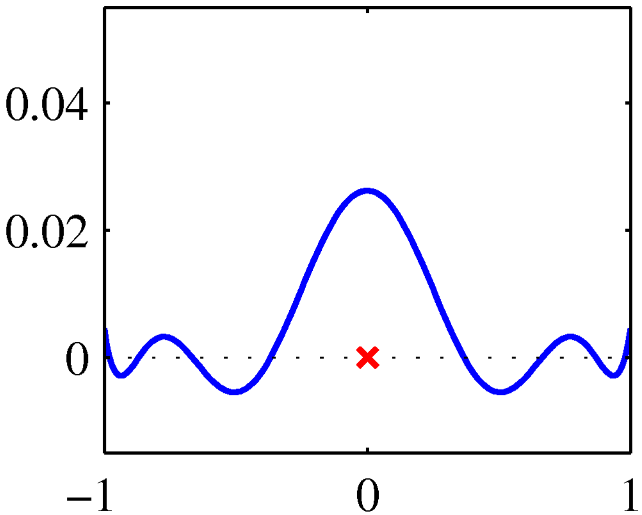
- The kernel as a covariance function:

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

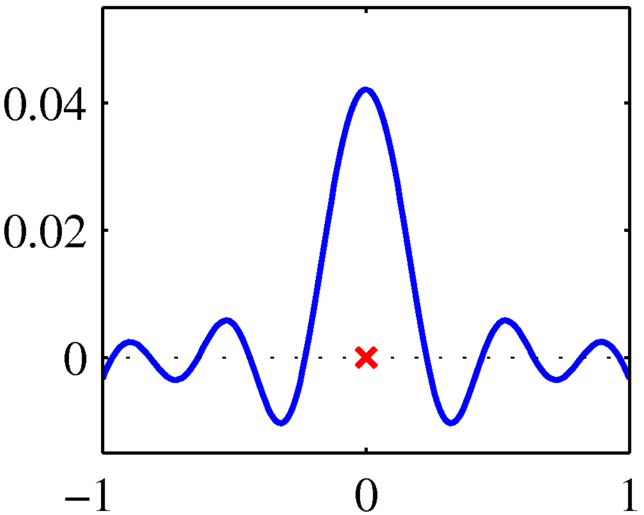
• We can avoid the use of basis functions and define the kernel function directly, leading to *Gaussian Processes.*

Other Kernels

- Examples of kernels k(x,x') for x=0, plotted as a function corresponding to x'.



Polynomial



Sigmoidal

- Note that these are localized functions of x'.

Bayesian Model Comparison

- The Bayesian view of model comparison involves the use of probabilities to represent uncertainty in the choice of the model.
- We would like to compare a set of L models $\{\mathcal{M}_i\}$, where $i = 1, 2, ..., L,$ using a training set D.
- We specify the prior distribution over the different models $p(\mathcal{M}_i)$.
- Given a training set D, we evaluate the posterior:

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

Posterior Prior *Model evidence* or *marginal likelihood*

- For simplicity, we will assume that all model are a-priori equal.
- The model evidence expresses the preference shown by the data for different models.
- The ratio of two model evidences for two models is known as Bayes factor:

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

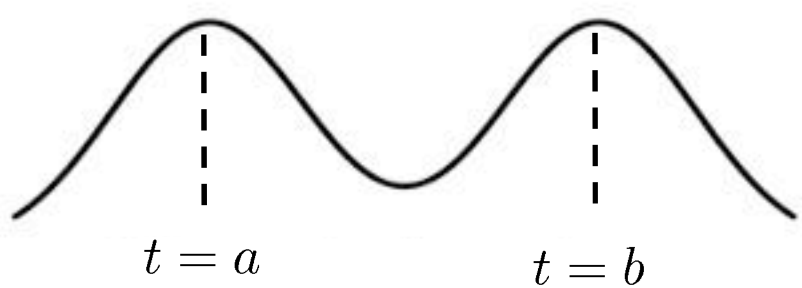
Bayesian Model Comparison

• Once we compute the posterior $p(M_i|\mathcal{D})$, we can compute the predictive (mixture) distribution:

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

• The overall predictive distribution is obtained by averaging the predictive distributions of individual models, weighted by the posterior probabilities.

• For example, if we have two models, and one predicts a narrow distribution around t=a while the other predicts a narrow distribution around t=b, then the overall predictions will be bimodal:



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

Bayesian Model Comparison

- Remember, the posterior is given by

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

For a model governed by a set of parameters **w**, the model evidence can be computed as follows:

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

- Observe that the evidence is the normalizing term that appears in the denominator in Bayes' rule:

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

- The model evidence is also often called marginal likelihood.

Bayesian Model Comparison

- We next get some insight into the model evidence by making simple approximations.

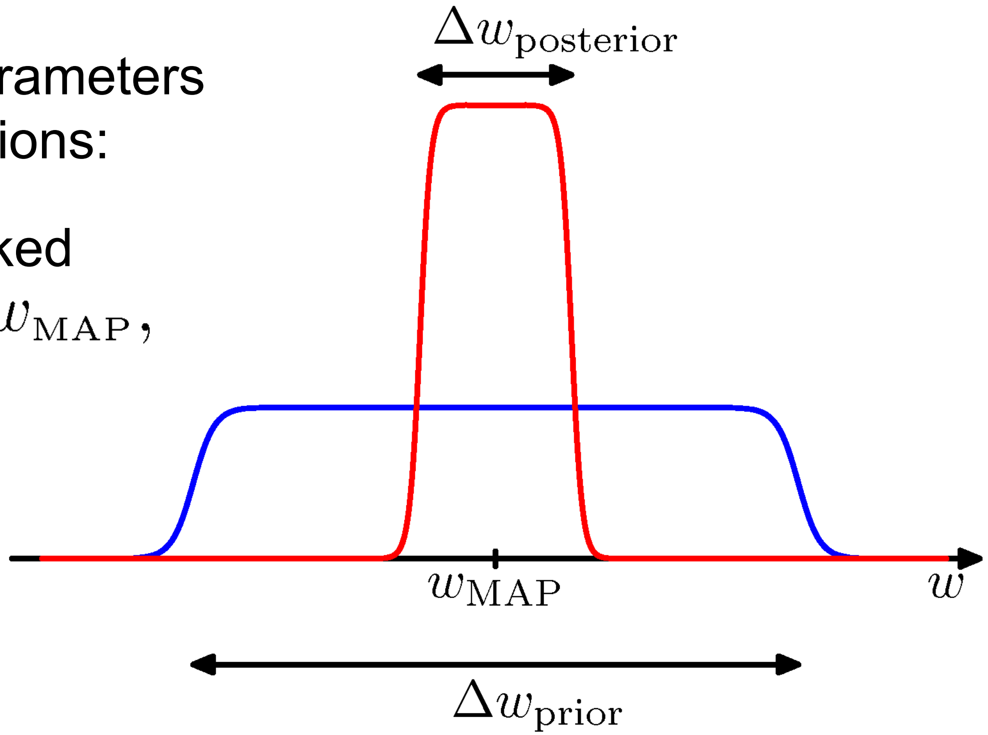
- For a give model with a single parameters parameter, w, consider approximations:

  - Assume that the posterior is picked around the most probable value w_{MAP}, with width $\Delta w_{\mathrm{posterior}}$

  - Assume that the prior is flat with width $\Delta w_{\mathrm{prior}}$

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

$$\simeq \quad p(\mathcal{D}|w_{\mathrm{MAP}})\frac{\Delta w_{\mathrm{posterior}}}{\Delta w_{\mathrm{prior}}}$$



Bayesian Model Comparison

- Taking the logarithms, we obtain:

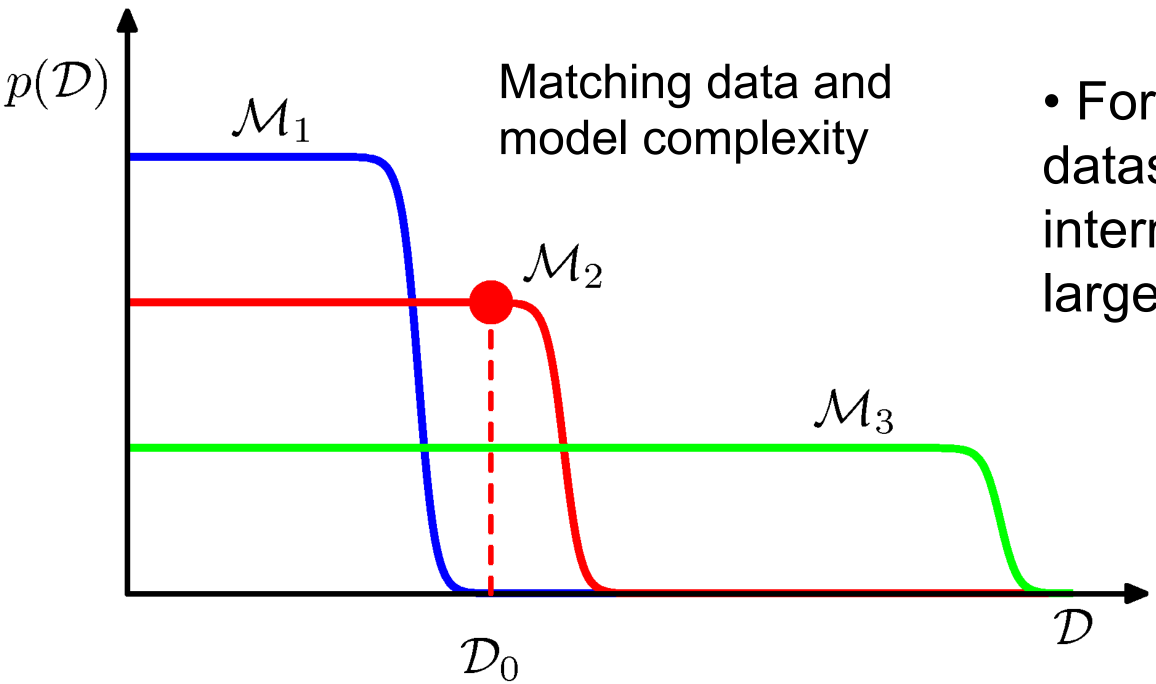
$$\ln p(\mathcal{D}) \simeq \ln p(\mathcal{D}|w_{\mathrm{MAP}}) + \underbrace{\ln \left(\frac{\Delta w_{\mathrm{posterior}}}{\Delta w_{\mathrm{prior}}} \right)}_{\text{Negative}}.$$

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

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

- As we increase the complexity of the model (increase the number of adaptive parameters M), the first term will increase, whereas the second term will decrease due to the dependence on M.
- The optimal model complexity: trade-off between these two competing terms.

Bayesian Model Comparison



- For the particular observed dataset $\mathcal{D}_0$, the model $\mathcal{M}_2$ with intermediate complexity has the largest evidence.

- The simple model cannot fit the data well, whereas the more complex model spreads its predictive probability and so assigns relatively small probability to any one of them.

- The marginal likelihood is very sensitive to the prior used!

- Computing the marginal likelihood makes sense only if you are certain about the choice of the prior.

Evidence Approximation

• In the fully Bayesian approach, we would also specify a prior distribution over the hyperparameters $p(\alpha, \beta)$.

• The fully Bayesian predictive distribution is then given by marginalizing over model parameters as well as hyperparameters:

Likelihood

posterior over weights

posterior over hyperparameters

$$p(t^*|\mathbf{x}^*, \mathcal{D}) = \iiint p(t^*|\mathbf{x}^*, \mathbf{w}, \beta)p(\mathbf{w}|\mathcal{D}, \alpha, \beta)p(\alpha, \beta|\mathcal{D})\mathrm{d}\mathbf{w}\,\mathrm{d}\alpha\,\mathrm{d}\beta.$$

target and input on test case

precision of output noise

precision of the prior

training data: inputs and targets

• However, this integral is intractable (even when everything is Gaussian). Need to approximate.

• Note: the fully Bayesian approach is to integrate over the posterior distribution for $\{\alpha, \beta, \mathbf{w}\}$. This can be done by MCMC, which we will consider later. For now, we will use evidence approximation: much faster.

Evidence Approximation

• The fully Bayesian predictive distribution is given by:

$$p(t^*|\mathbf{x}^*, \mathcal{D}) = \iiint p(t^*|\mathbf{x}^*, \mathbf{w}, \beta) p(\mathbf{w}|\mathcal{D}, \alpha, \beta) p(\alpha, \beta|\mathcal{D}) \mathrm{d}\mathbf{w}\, \mathrm{d}\alpha\, \mathrm{d}\beta.$$

• If we assume that the posterior over hyperparameters α and β is sharply picked, we can approximate:

$$p(t^*|\mathbf{x}^*, \mathcal{D}) \approx p(t^*|\mathbf{x}^* \mathcal{D}, \hat{\alpha}, \hat{\beta}) = \int p(t^*|\mathbf{x}^*, \mathcal{D}, \hat{\beta}) p(\mathbf{w}|\mathcal{D}, \hat{\alpha}, \hat{\beta}) \mathrm{d}\mathbf{w}.$$

where $\left(\widehat{\alpha}, \widehat{\beta}\right)$ is the mode of the posterior $p(\alpha, \beta|\mathcal{D})$.

• So we integrate out parameters but maximize over hyperparameters.

• This is known as empirical Bayes, Type II Maximum Likelihood, Evidence Approximation.

Evidence Approximation

• From Bayes' rule we obtain:

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

• If we assume that the prior over hyperparameters $p(\alpha, \beta)$ is flat, we get:

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

• The values $\left(\widehat{\alpha}, \widehat{\beta}\right)$ are obtained by maximizing the marginal likelihood $p(\mathbf{t}|\mathbf{X}, \alpha, \beta)$.

• This will allow us to determine the values of these hyperparameters from the training data.

• Recall that the ratio α/β is analogous to the regularization parameter.

Evidence Approximation

- The marginal likelihood is obtained by integrating out parameters:

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

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

- We can write the evidence function in the form:

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

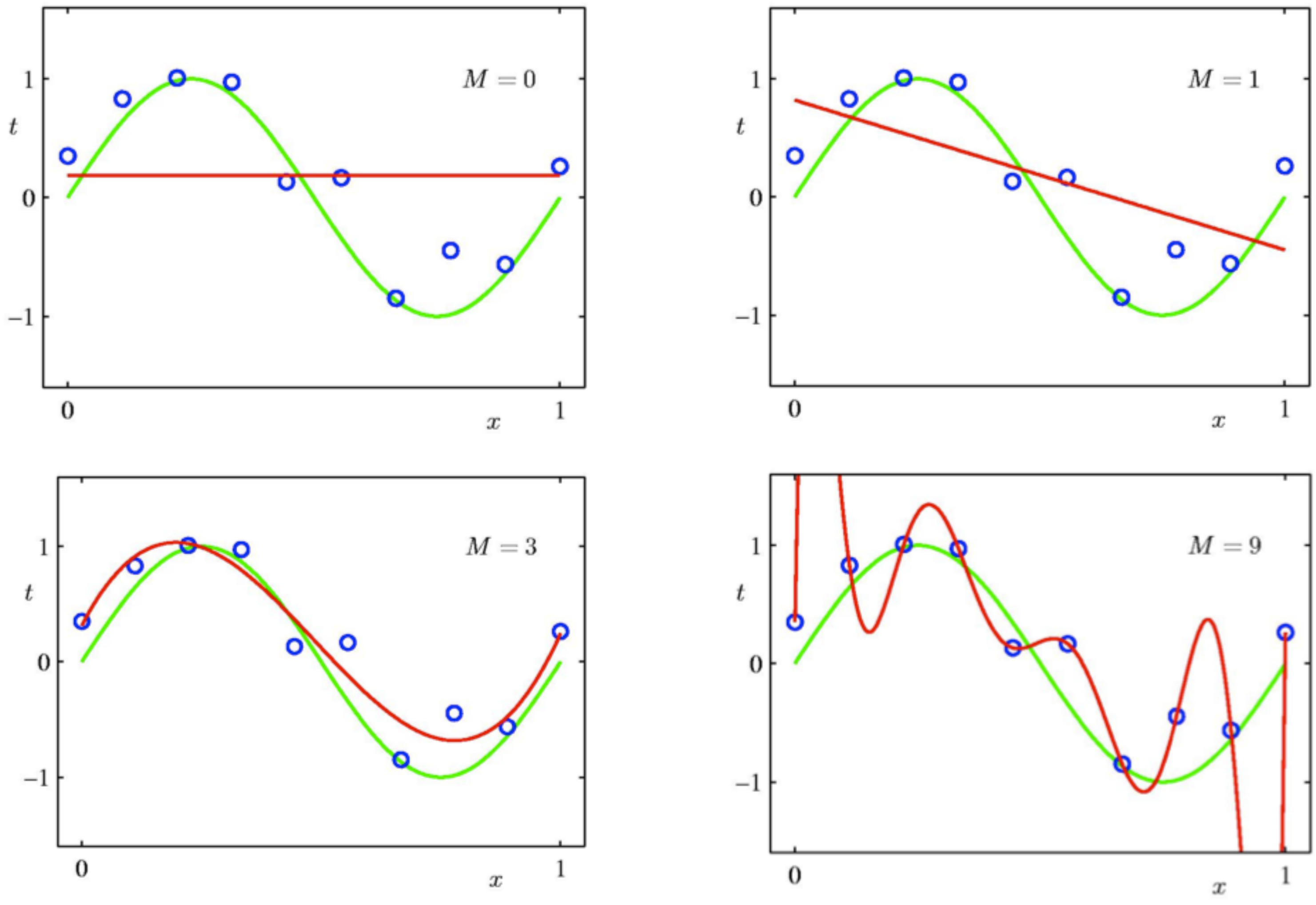
where

$$E(\mathbf{w}) = \beta E_{\mathcal{D}}(\mathbf{w}) + \alpha E_W(\mathbf{w}) = \frac{\beta}{2}||\mathbf{t}-\mathbf{\Phi}\mathbf{w}||^2 + \frac{\alpha}{2}\mathbf{w}^T\mathbf{w}.$$

- Using standard results for the Gaussian distribution, we obtain:

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

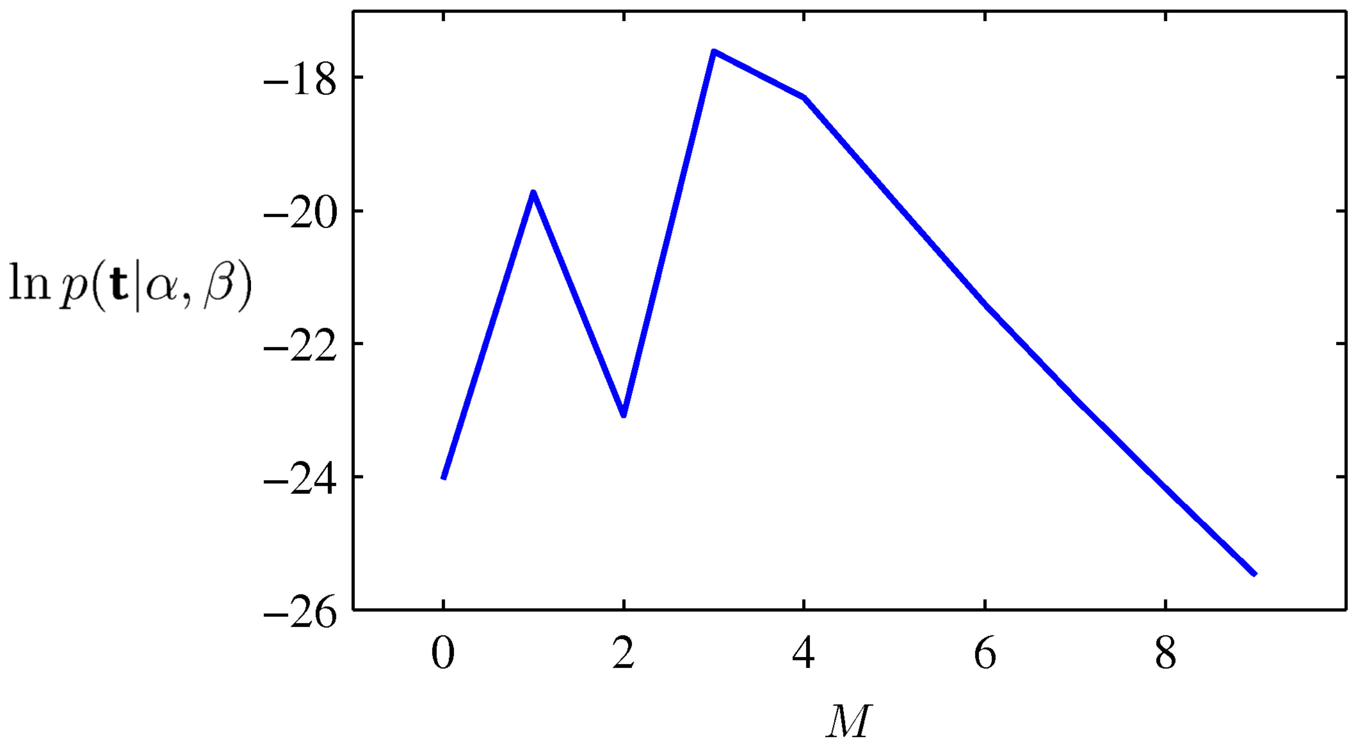
Some Fits to the Data



For M=9, we have fitted the training data perfectly.

Evidence Approximation

Using sinusoidal data, M^{th} degree polynomial.



The evidence favours the model with M=3.

Maximizing the Evidence

- Remember:

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

- To maximize the evidence $p(\mathbf{t}|\mathbf{X}, \alpha, \beta)$ with respect to α and β, define the following eigenvector equation:

$$\left(\beta\mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi}\right)\mathbf{u}_i = \lambda_i\mathbf{u}_i.$$

Precision matrix of the Gaussian posterior distribution

- Therefore the matrix:

$$\mathbf{A} = \mathbf{S}_N^{-1} = \alpha\mathbf{I} + \beta\mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi}$$

has eigenvalues $\alpha + \lambda_i$.

- The derivative:

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

Maximizing the Evidence

- Remember:

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

where

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

- Differentiating $\ln p(\mathbf{t}|\alpha, \beta)$, the stationary points with respect to α satisfy:

$$\frac{M}{2\alpha} - \frac{1}{2}\mathbf{m}_N^T\mathbf{m}_N - \frac{1}{2}\sum_i \frac{1}{\alpha + \lambda_i} = 0.$$

$$\alpha\mathbf{m}_N^T\mathbf{m}_N = M - \alpha\sum_i \frac{1}{\alpha + \lambda_i} = \gamma,$$

where the quantity γ, effective number of parameters, can be defined as:

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

Maximizing the Evidence

- The stationary points with respect to α satisfy:

$$\alpha \mathbf{m}_N^T \mathbf{m}_N = M - \alpha \sum_i \frac{1}{\alpha + \lambda_i} = \gamma,$$

where the quantity γ, effective number of parameters, is defined as:

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

Note that the eigenvalues need to be computed only once.

- Iterate until convergence:

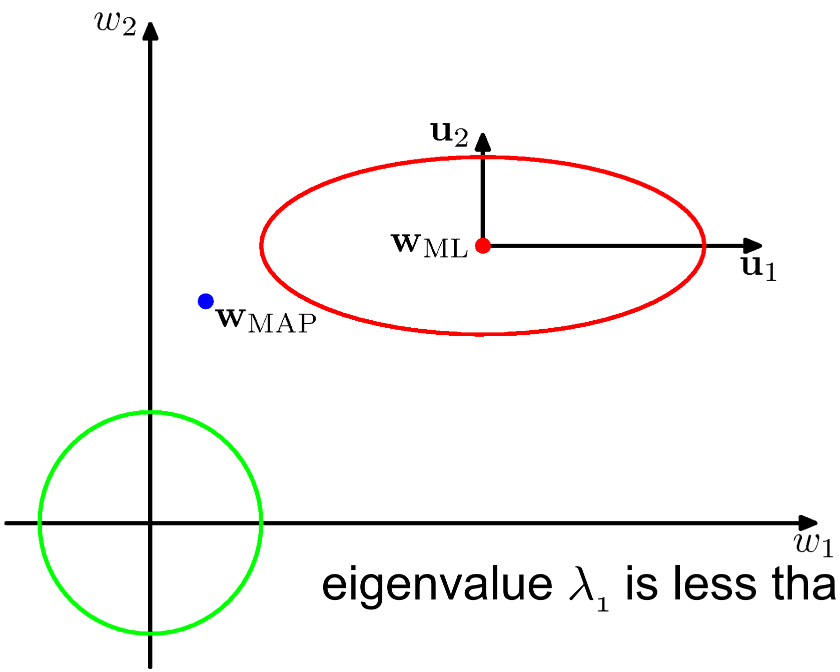
$$\alpha = \frac{\gamma}{\mathbf{m}_N^T \mathbf{m}}; \quad \gamma = \sum_i \frac{\lambda_i}{\lambda_i + \alpha}; \quad \begin{aligned} \mathbf{m}_N &= \beta \mathbf{S}_N \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{t} \\ \mathbf{S}_N^{-1} &= \alpha \mathbf{I} + \beta \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi}.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

- Similarly:

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

Effective Number of Parameters

- Consider the contours of the likelihood function and the prior.



eigenvalue λ_1 is less than λ_2.

- The eigenvalue λ_i measures the curvature of the log-likelihood function.
- The quantity γ will lie $0 \leq \gamma \leq M$.
- For $\lambda_i \gg \alpha$, the corresponding parameter $\mathbf{w_i}$ will be close to its maximum likelihood. The ratio:

$$\frac{\lambda_i}{\lambda_i + \alpha}$$ will be close to one.

- Such parameters are called well determined, as their values are highly constrained by the data.
- For $\lambda_i \ll \alpha$, the corresponding parameters will be close to zero (pulled by the prior), as will the ratio $\lambda_i/(\lambda_i + \alpha)$.
- We see that γ measures the effective total number of well determined parameters.

Quick Approximation

- In the limit $N \gg M$, γ = M, and we consider to use the easy to compute approximations:

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

Limitations

• M basis function along each dimension of a D-dimensional input space requires M^D basis functions: the curse of dimensionality.

• Fortunately, we can get away with fewer basis functions, by choosing these using the training data (e.g. adaptive basis functions), which we will see later.

• Second, the data vectors typically lie close to a nonlinear low-dimensional manifold, whose intrinsic dimensionality is smaller than that of the input space.