ECE521:
Lectures 12 & 13

27 February & 2 March 2017:

PCA continued,
Bayesian methods

With thanks to Russ Salakhutdinov and others

This week

- We will explore the Bayesian framework further, including Bayesian Linear Regression Models

- Examples of additional perspectives:
  - Bishop 2006: section 3.3
  - Murphy 2012: parts of chap. 5, & sec. 7.6

- On Thursday, midterms will be distributed as well

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 uncertainty in the parameter values.
  - Make decisions by minimizing expected posterior loss.

(Bonus: 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:

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

which is sometimes called the predictive distribution.

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

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

which is usually intractable.

Modelling 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 among 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 modelling 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. Chiefly employed for simple models

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- 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).

(We aren't covering the last three here)

- 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.

Our linear regression techniques

- LLS LR = MLE LR: $\hat{\mathbf{w}} = \mathbf{argmax}_{\mathbf{w}}\, p(D|\mathbf{w})$
- MAP LR: $\hat{\mathbf{w}} = \mathbf{argmax}_{\mathbf{w}}\, p(\mathbf{w}|D)$
  - ℓ_2 regularization combats overfitting
  - ℓ_1 regularization does so with sparser solutions
- Bayesian LR: $p(\mathbf{w}|D)$
  - Combats overfitting while allowing more data to be used for training
  - N.B.: something called “Empirical-Bayes LR” (not covered here) reduces the assumptions we make about the prior

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.

Pause: why is the normal distribution's conjugate prior another normal?

$$p(\mu|\mathbf{X}) \propto p(\mathbf{X}|\mu)p(\mu)$$

$$p(\mu|\mathbf{X}) = \mathcal{N}\left(\mu|\mu_N, \sigma_N^2\right)$$

$$p(\mu) = \mathcal{N}\left(\mu|\mu_0, \sigma_0^2\right)$$

$$\mu_N = \frac{\sigma^2}{N\sigma_0^2 + \sigma^2}\mu_0 + \frac{N\sigma_0^2}{N\sigma_0^2 + \sigma^2}\mu_{\mathrm{ML}}$$

$$\frac{1}{\sigma_N^2} = \frac{1}{\sigma_0^2} + \frac{N}{\sigma^2}$$

$$p(\mathbf{X}|\mu) = \prod_{n=1}^{N} p(x_n|\mu) = \frac{1}{(2\pi\sigma^2)^{N/2}} \exp\left\{-\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n - \mu)^2\right\}$$

Examples of conjugate priors

- Binomial: β prior
- Multinomial: Dirichlet prior
- Exponential, Poisson, or γ: γ prior
- Normal: Normal prior
- Uniform: Pareto prior

Back to Bayesian Linear Regression

• Combining the prior together with the likelihood term:

$$p(\mathbf{w}|\mathbf{t},\mathbf{X},\mathbf{w},\beta) \propto \left[\prod_{n=1}^{N}\mathcal{N}(t_n|\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_n),\beta^{-1})\right]\mathcal{N}(\mathbf{w}|\mathbf{m_0},\mathbf{S_0}).$$

• 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

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

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

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

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

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

Bayesian Linear Regression

• Consider a zero-mean, isotropic, Gaussian prior which is governed 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:

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

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

• If we consider an infinitely broad prior, α → 0, the mean $\mathbf{m}_N$ of the posterior distribution reduces to maximum likelihood value $\mathbf{w}_{ML}$. *(Can you see how?)*

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

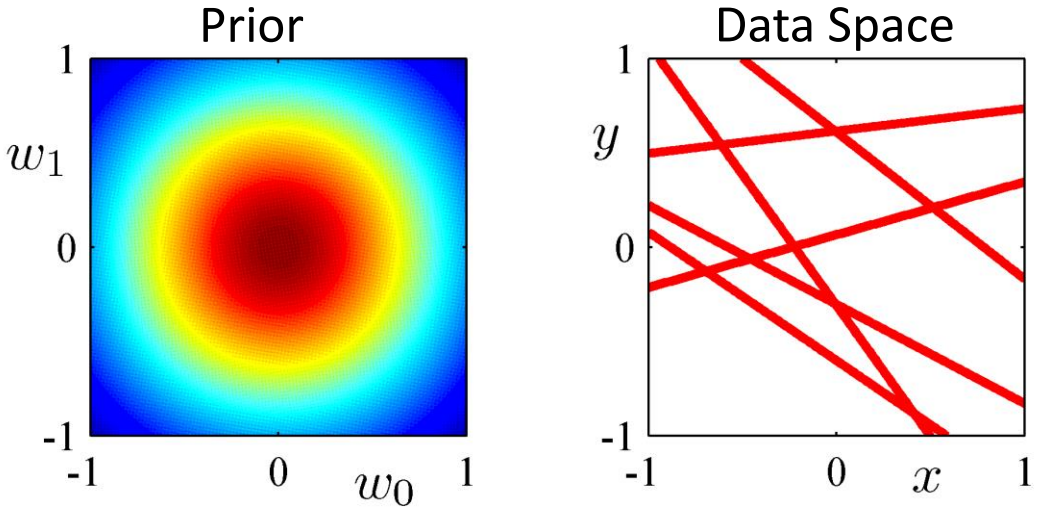
$$\ln p(\mathbf{w}|\mathcal{D}) = -\frac{\beta}{2} \sum_{n=1}^{N} \left(t_n - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n)\right)^2 - \frac{\alpha}{2} \mathbf{w}^T \mathbf{w} + \text{const.}$$

• 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

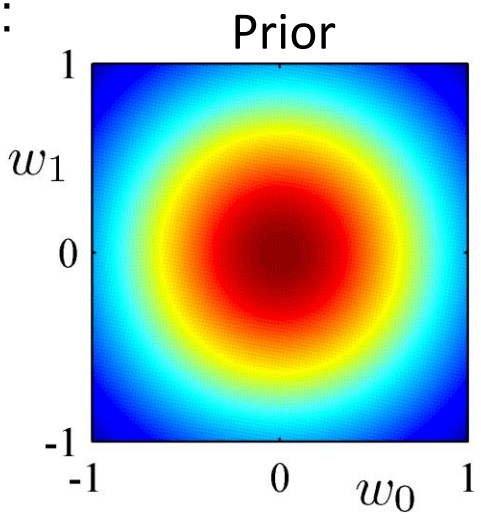
- Consider a linear model of the form: $y(x, \mathbf{w}) = w_0 + w_1 x.$
- The training data is generated from the function $f(x, \mathbf{a}) = a_0 + a_1 x$ with a_0 = -0.3 and a_1 = 0.5 by first choosing x_n uniformly from [-1;1], evaluating $f(x, \mathbf{a})$, and adding a small Gaussian noise.
- Goal: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

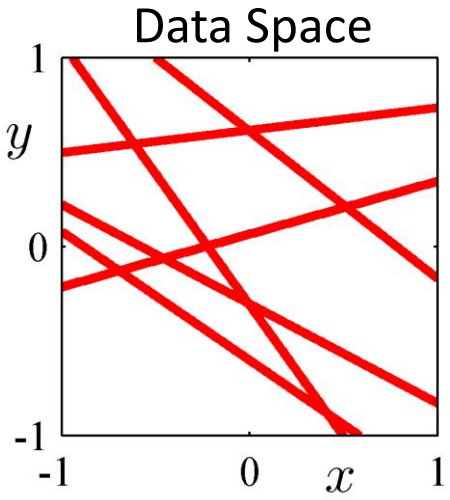
When zero data points have been observed:



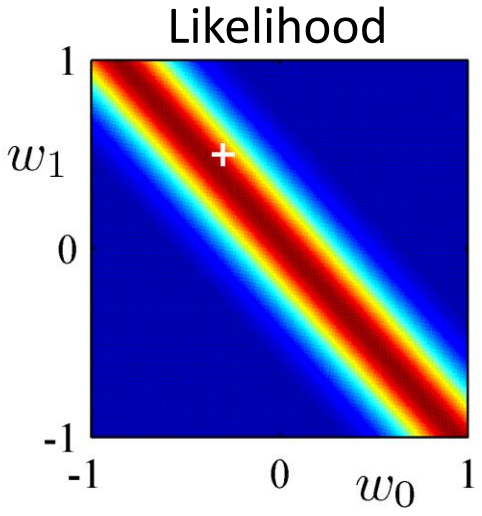
Bayesian Linear Regression

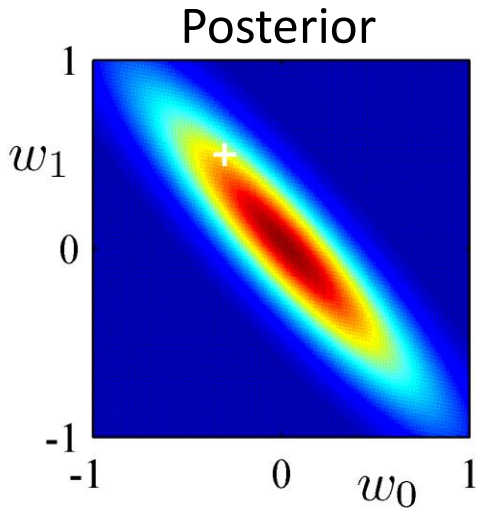
0 data points are observed:

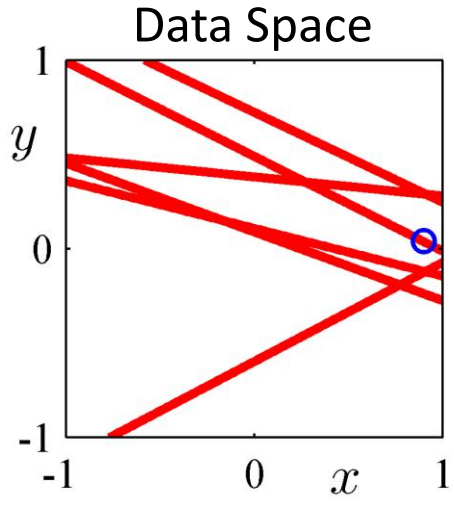




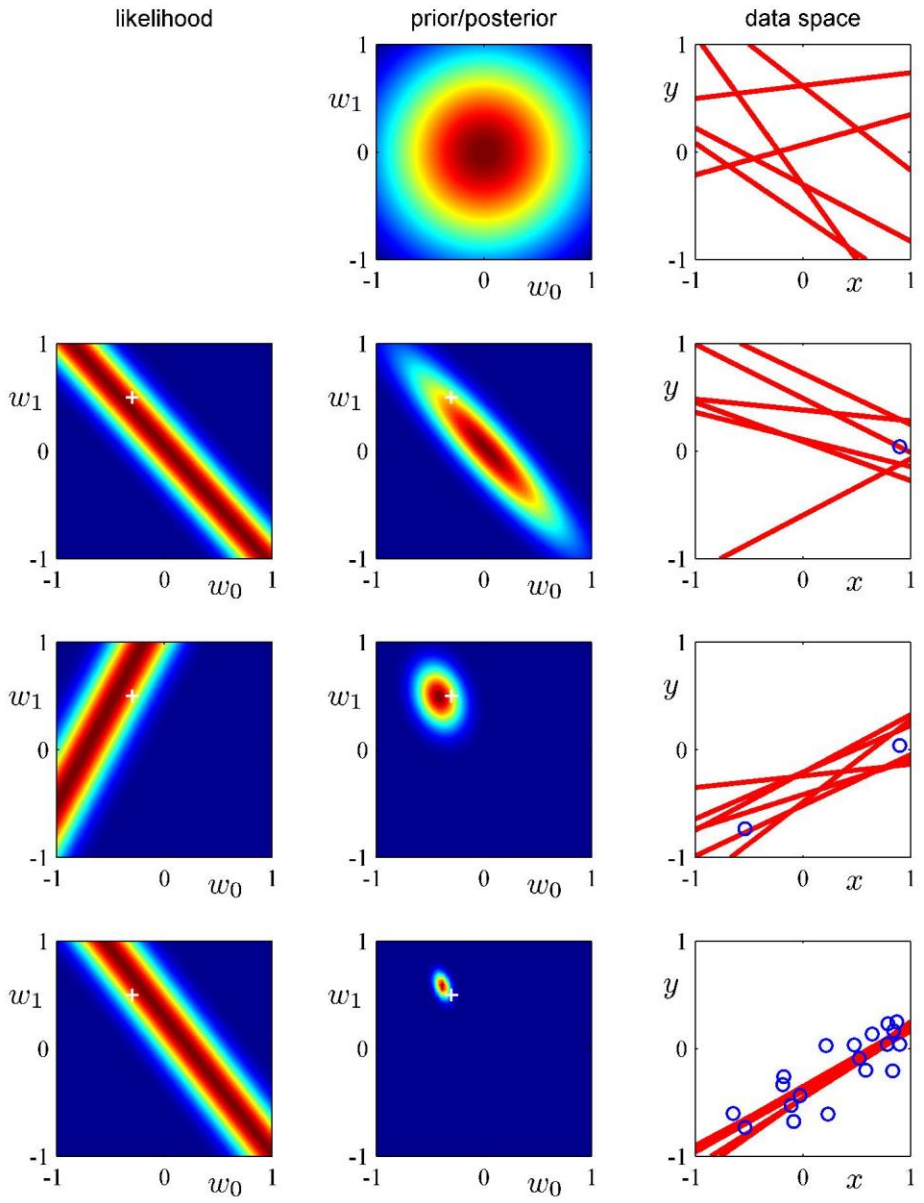
1 data point is observed:







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

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

Noise in the target values

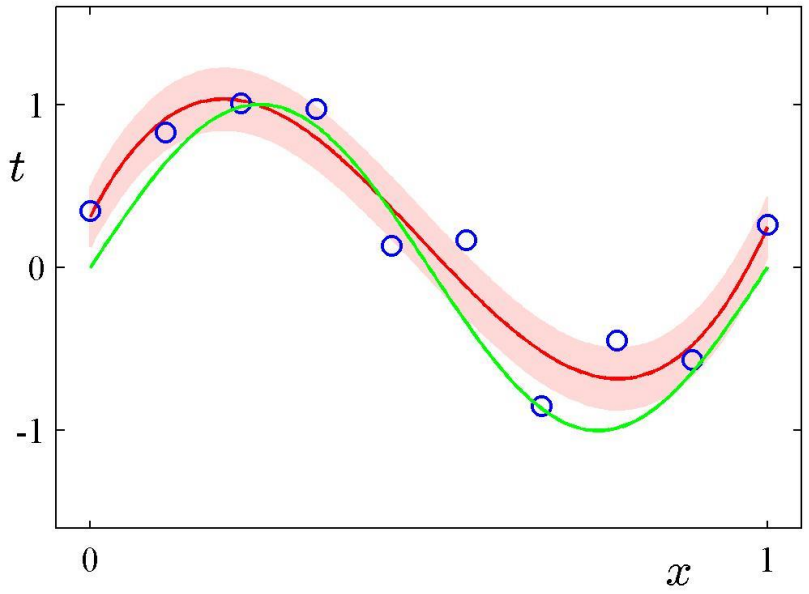
Uncertainty associated with parameter values.

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

• 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

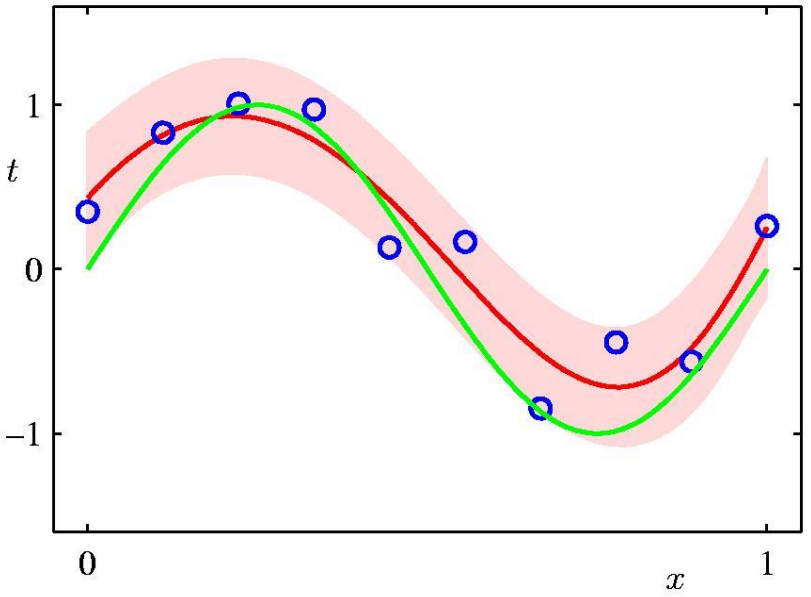
Predictive Distribution: ML vs. Bayes

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



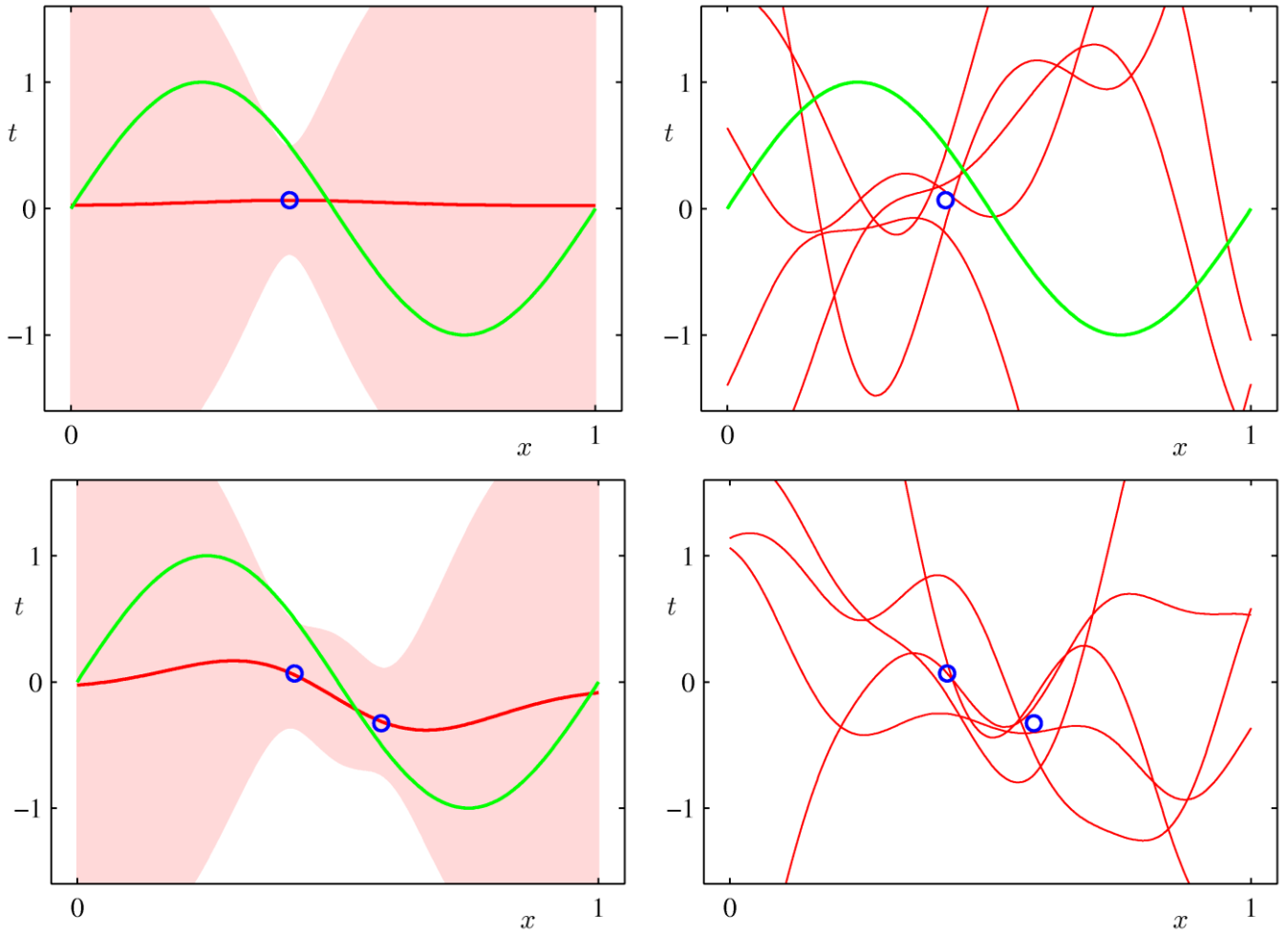
$$p(t|x, \mathbf{t}, \mathbf{X}) = \mathcal{N}\left(t|\mathbf{m}_N^T \boldsymbol{\phi}(x), \sigma_N^2(x)\right)$$

Predictive Distribution

Sinusoidal dataset, nine Gaussian basis functions.

Predictive distribution

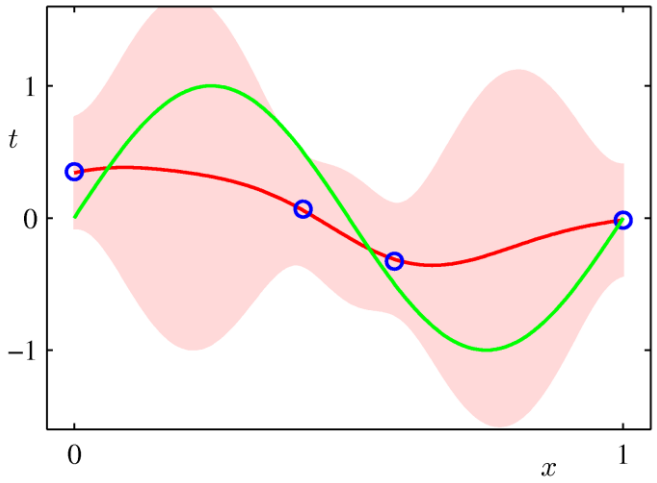
Samples from the posterior



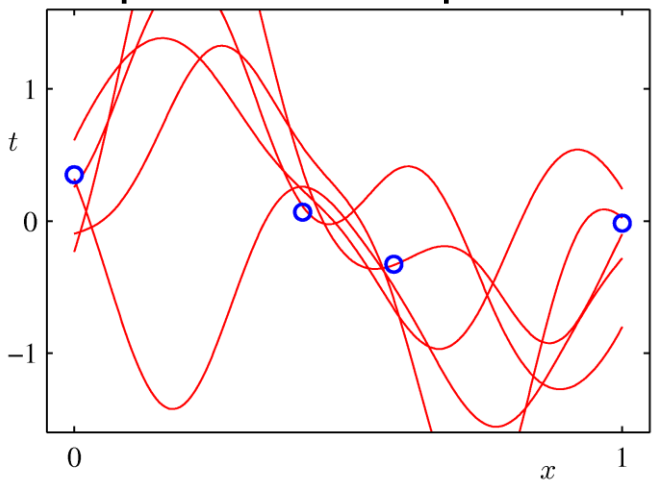
Predictive Distribution

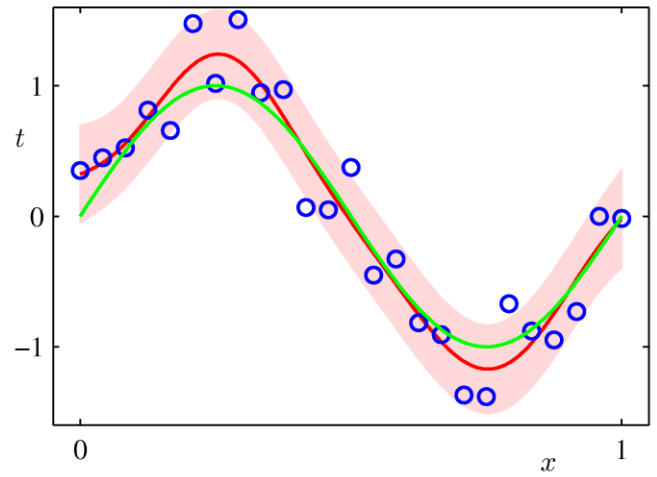
Sinusoidal dataset, nine Gaussian basis functions.

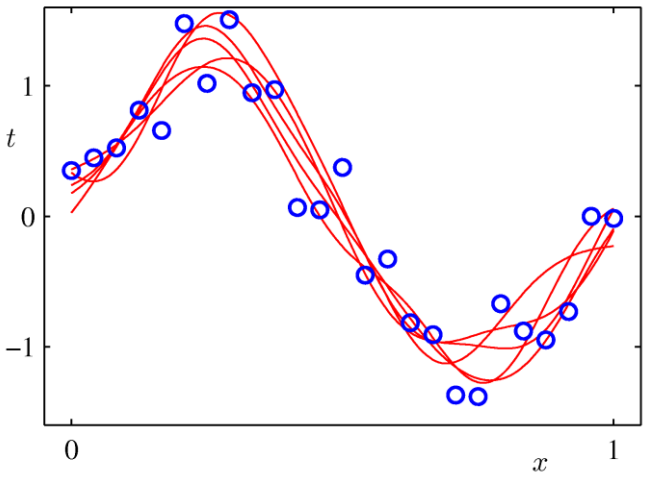
Predictive distribution



Samples from the posterior







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 $\mathcal{D}$.
- We specify the prior distribution over the different models $p(\mathcal{M}_i)$.
- Given a training set $\mathcal{D}$, 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 models are a-priori equally likely
- 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 a Bayes factor:

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

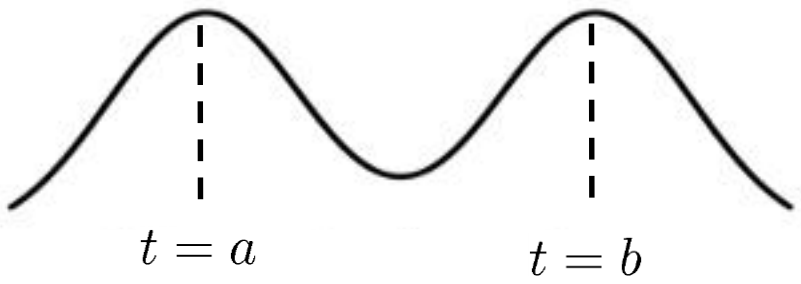
Bayesian Model Comparison

• 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.

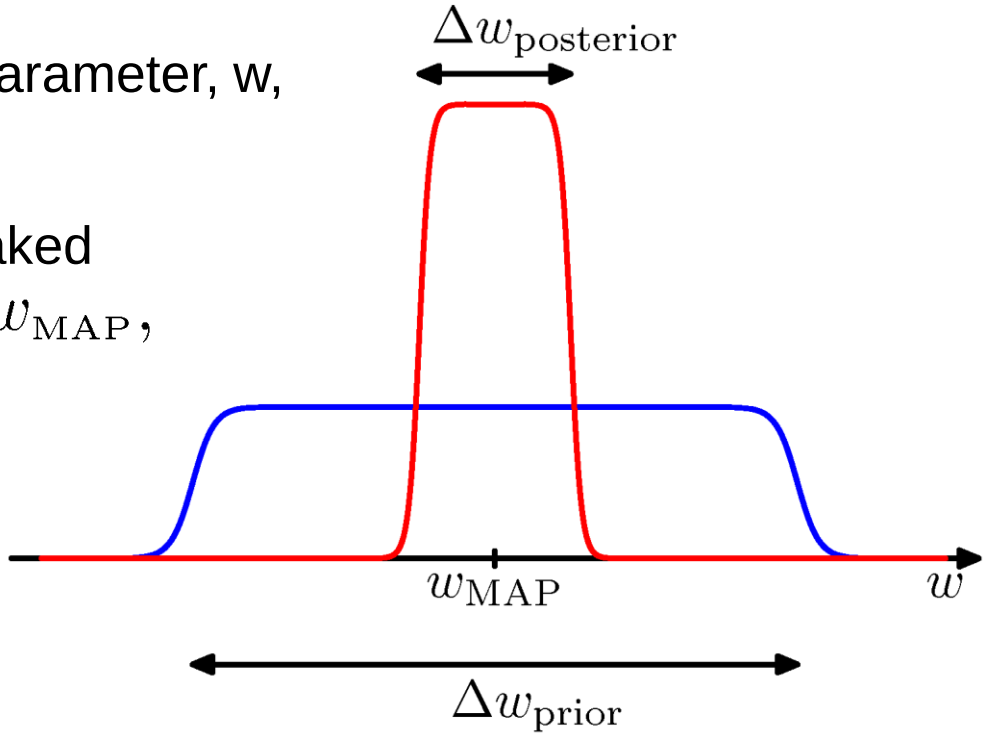
Bayesian Model Comparison

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

• For a given model with a single parameter, w, consider approximations:

- Assume that the posterior is peaked 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:

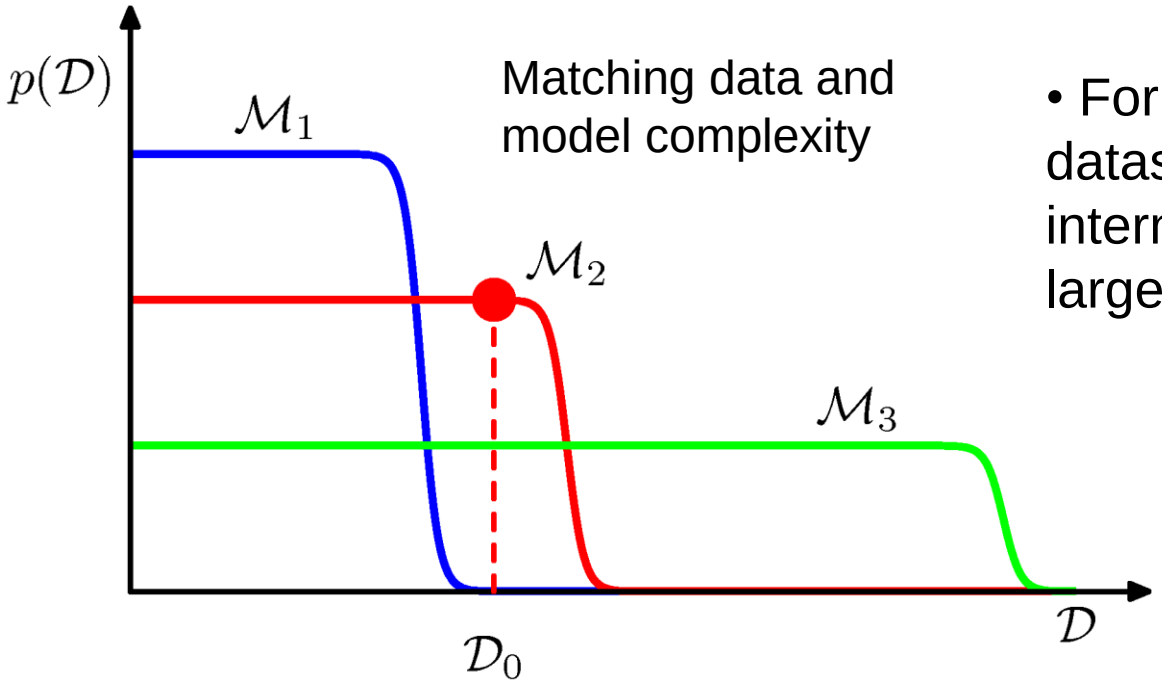
$$\ln p(\mathcal{D}) \simeq \ln p(\mathcal{D}|w_{\mathrm{MAP}}) + \underbrace{\ln\left(\frac{\Delta w_{\mathrm{posterior}}}{\Delta w_{\mathrm{prior}}}\right)}_{\text{Negative}}.$$

- 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



Matching data and model complexity

• 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.

Hint for the question on slide 11

The exponent in the right-hand side is:

$$-\frac{1}{2\sigma_0^2}(\mu-\mu_0)^2-\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n-\mu)^2$$

$$=-\frac{\mu^2}{2}\left(\frac{1}{\sigma_0^2}+\frac{N}{\sigma^2}\right)+\mu\left(\frac{\mu_0}{\sigma_0^2}+\frac{1}{\sigma^2}\sum_{n=1}^{N}x_n\right)+\text{const.}$$

Compare this, term by term, to a single Gaussian's exponent:

$$-\frac{1}{2}\left(\frac{\mu-\mu_N}{\sigma_N}\right)^2=-\frac{\mu^2}{2}\left(\frac{1}{\sigma_N}\right)^2+\mu\left(\frac{\mu_N}{{\sigma_N}^2}\right)\quad+\text{const.}$$

And you arrive at the terms on the left-hand side of slide 12.