STA 414/2104: Machine Learning

29 January 2018:

Bayesian methods, KNN

Lecture 4, delivered by Mark Ebden With thanks to Russ Salakhutdinov

Outline

- Bayesian methods
 - Bayesian linear regression
 - Bayesian model comparison

K nearest neighbours

Recap

- In our previous classes, we looked at (among other things):
 - 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,
 e.g. Bayesian Linear Regression Models
- Examples of useful perspectives elsewhere:
 - Bishop 2006: sections 3.3 to 3.5
 - Hastie 2013: parts of chapters 6 to 8
 - Murphy 2012: parts of chapter 5, sections 7.6 & 14.7.4

bayes: dataset is fixed, and the parameter are random variables frequentist: dataset is a sample from a random distribution, there are true parameters

Bayesian Approach

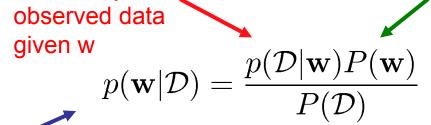
- We formulate our knowledge about the world probabilistically:
 - We define the model that expresses our knowledge qualitatively (e.g. independence assumptions, forms of distributions).
 - Our model will have some unknown parameters.
 - We capture our assumptions, or prior beliefs, about unknown parameters (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.

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:

Probability of

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



Prior probability of weight vector w

Posterior probability of weight vector W given training data D

Marginal likelihood over all possible parameters, which are random (normalizing constant):

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

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

The Rules of Probability

Sum Rule:

$$p(X) = \sum_Y p(X,Y) \quad {}_{\text{marginalizing}}$$

Product Rule:

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

Predictive Distribution

• We can also state Bayes' rule in words:

posterior
$$\propto$$
 likelihood \times prior.

 We can make predictions for a new data point x*, given the training dataset by integrating over the posterior distribution:

$$p(\mathbf{x}^*|\mathcal{D}) = \int p(\mathbf{x}^*|\mathbf{w}, \mathcal{D}) p(\mathbf{w}|\mathcal{D}) d\mathbf{w} = \mathbb{E}_{P(\mathbf{w}|\mathcal{D})} [p(\mathbf{x}^*|\mathbf{w}, \mathcal{D})],$$
posterior distribution,
representing uncertainty with the parameters given data observed

which is sometimes called the predictive distribution.

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

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

Our linear regression techniques

- LLS LR = MLE LR: $\hat{\mathbf{w}} = \mathbf{argmax_w} \ p(D|\mathbf{w})$ likelihood
- $\bullet \quad \mathsf{MAP\ LR:} \qquad \qquad \hat{\mathbf{w}} = \mathbf{argmax_w}\ p(\mathbf{w}|D) \ \ \mathsf{posterior}$
 - L2 regularization combats overfitting
 - 4 regularization does so with sparser solutions model less complex
- Bayesian LR: $p(\mathbf{w}|D)$ no training, throw in all data...
 - Combats overfitting while allowing more data to be used for training
 - Empirical-Bayes LR (future lecture) reduces the assumptions we make about the prior. Note: α (see later) can be tuned per dimension

• 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:

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

where $\phi(\mathbf{x}) = (\phi_0(\mathbf{x}), \phi_1(\mathbf{x}), ..., \phi_{M-1}(\mathbf{x}))^T$ 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 $p(\theta|\mathbf{x})$ are in the same family as the prior probability distribution $p(\theta)$, 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?

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

$$p(\mu|\mathbf{X}) = \mathcal{N}\left(\mu|\mu_{N}, \sigma_{N}^{2}\right) \qquad p(\mu) = \mathcal{N}\left(\mu|\mu_{0}, \sigma_{0}^{2}\right)$$

$$\mu_{N} = \frac{\sigma^{2}}{N\sigma_{0}^{2} + \sigma^{2}}\mu_{0} + \frac{N\sigma_{0}^{2}}{N\sigma_{0}^{2} + \sigma^{2}}\mu_{ML}$$

$$\frac{1}{\sigma_{N}^{2}} = \frac{1}{\sigma_{0}^{2}} + \frac{N}{\sigma^{2}}$$

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

Examples of conjugate priors

• Binomial: β prior

Multinomial: Dirichlet prior

Exponential, Poisson, or γ: γ prior

Normal: Normal prior

Uniform: Pareto prior

NB: This is just a bonus list for reference

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

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

$$\mathbf{S}_N^{-1} = \mathbf{S}_0^{-1} + \beta \mathbf{\Phi}^{\mathrm{T}} \mathbf{\Phi}$$

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

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

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

i.e. written as a scalar multiple of identity

 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:

$$\mathbf{m}_N = \beta \mathbf{S}_N \mathbf{\Phi}^{\mathrm{T}} \mathbf{t}$$

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

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

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

i.e. regularization coefficient -> 0, equivalent to not using bayesian approach

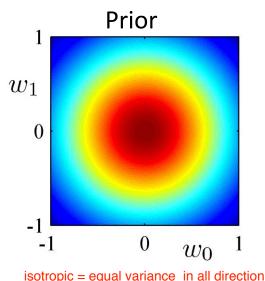
 The log of the posterior distribution is given by the sum of the loglikelihood and the log of the prior:

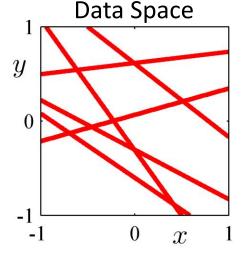
$$\ln p(\mathbf{w}|\mathcal{D}) = -\frac{\beta}{2} \sum_{n=1}^{N} (t_n - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n))^2 - \frac{\alpha}{2} \mathbf{w}^T \mathbf{w} + \text{const.}$$

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

- 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.

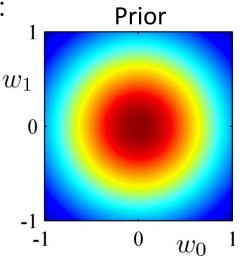
When zero data points have been observed:

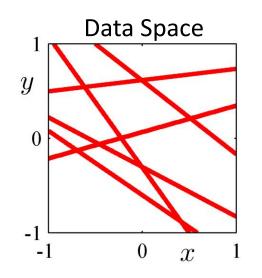




red lines, possible weights in the input space

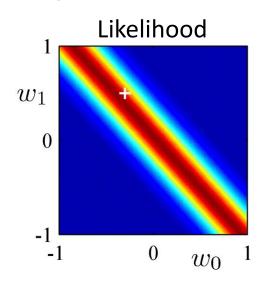
0 data points are observed:

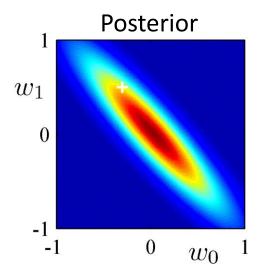


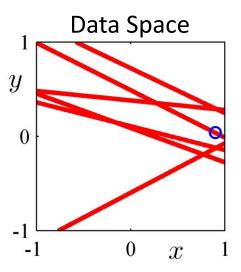


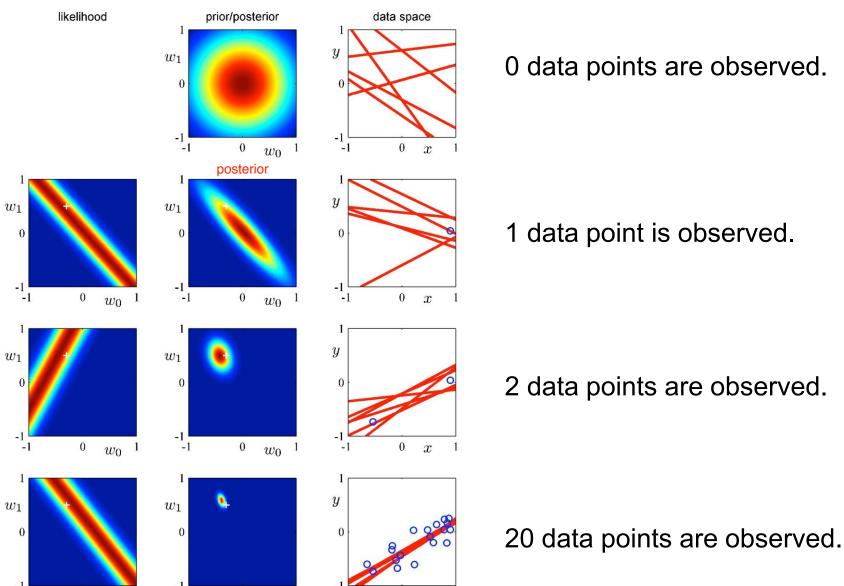
1 data point is observed:

i.e. regions of weights possible to reach the point observed









 w_0^{-1}

Predictive Distribution

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

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

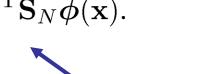
= $\mathcal{N}(t|\mathbf{m}_N^T \boldsymbol{\phi}(\mathbf{x}), \sigma_N^2(\mathbf{x})),$

where

posterior distribution variance

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

Noise in the target values



Uncertainty associated with parameter values.

$$\mathbf{m}_N = \beta \mathbf{S}_N \mathbf{\Phi}^{\mathrm{T}} \mathbf{t}$$

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

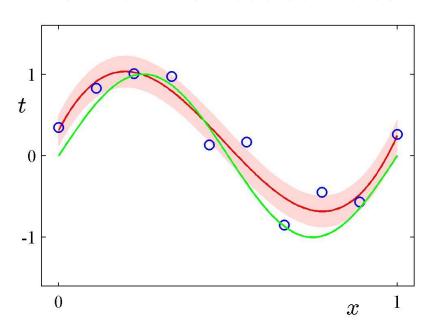
i.e. uncertainty in estimating the parameter given a particular datase

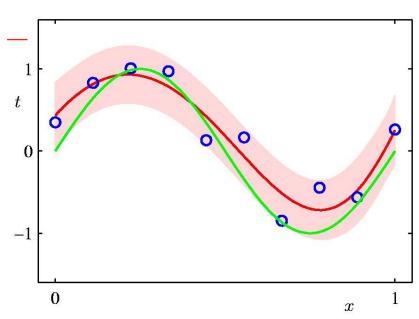
- As $N \rightarrow \infty$:
 - The second term goes to zero
- idea is with enough training sample, we are really confident about distribution of parameter estimated
- The variance of the predictive distribution arises only from the additive noise governed by parameter β

Predictive Distribution: ML vs. Bayes

Predictive distribution based on maximum likelihood estimates

Bayesian predictive distribution





$$p(t|x, \mathbf{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}}) = \mathcal{N}\left(t|y(x, \mathbf{w}_{\mathrm{ML}}), \beta_{\mathrm{ML}}^{-1}\right) \quad p(t|x, \mathbf{t}, \mathbf{X}) = \mathcal{N}\left(t|\mathbf{m}_{N}^{T} \boldsymbol{\phi}(x), \sigma_{N}^{2}(x)\right)$$

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

distribution is based a point LS estimation

distribution take into account uncertainty in estimating w

Predictive Distribution

w are samples from posterior

 \boldsymbol{x}

Sinusoidal dataset, nine Gaussian basis functions.

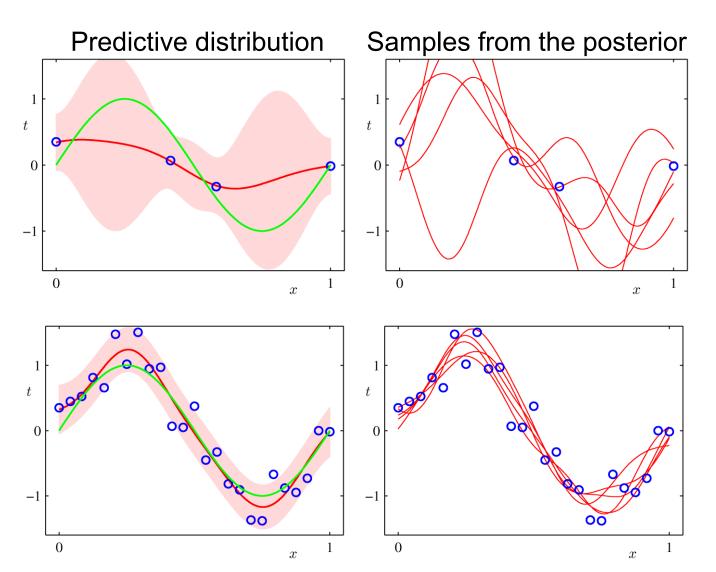
0

plot the regression function y(x,w)Predictive distribution Samples from the posterior t0 0 -1

0

Predictive Distribution

Sinusoidal dataset, nine Gaussian basis functions.



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:

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

where the Gamma distribution is given by:

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

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

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

- 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

can be viewed as a likelihood function over the space of models, in which parameters have been marginalized out

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

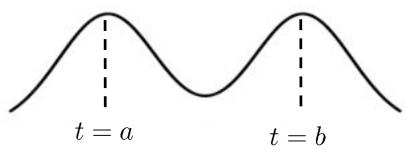
• Once we compute the posterior $p(M_i|\mathcal{D})$, we can compute the predictive (mixture) distribution:

$$p(t|\mathbf{x}, \mathcal{D}) = \sum_{i=1}^{L} p(t|\mathbf{x}, \mathcal{M}_i, \mathcal{D}) p(\mathcal{M}_i|\mathcal{D}).$$
predictive distribution posterior probability of the mode

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

compare to mle, we can get multimodal models by keeping track of multiple models

• 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.

i.e. instead of averaging, pick the model with largest posterior probability

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:

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

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

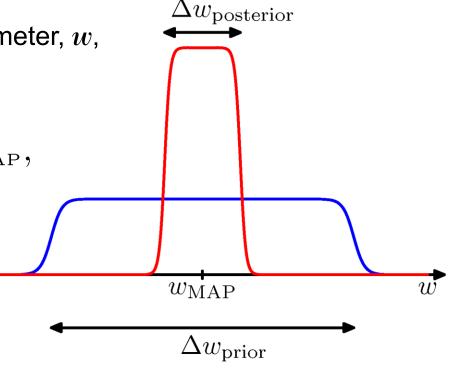
$$p(\mathbf{w}|\mathcal{D}, \mathcal{M}_i) = \frac{p(\mathcal{D}|\mathbf{w}, \mathcal{M}_i)p(\mathbf{w}|\mathcal{M}_i)}{p(\mathcal{D}|\mathcal{M}_i)}$$

The model evidence is also often called marginal likelihood.

- We next get some insight into the model evidence by making simple approximations.
- ullet For a given model with a single parameter, w, consider approximations:
 - Assume that the posterior is peaked around the most probable value $w_{\rm MAP},$ with width $\Delta w_{\rm posterior}$
 - Assume that the prior is flat with width $\Delta w_{\rm prior}$ so p(w) = 1 / delta(w) prior

$$p(\mathcal{D}) = \int p(\mathcal{D}|w)p(w) dw$$

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



Taking the logarithms, we obtain:

 $\ln p(\mathcal{D}) \simeq \ln p(\mathcal{D}|w_{\text{MAP}}) + \ln \left($

fit to data given by most probable parameter values

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

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

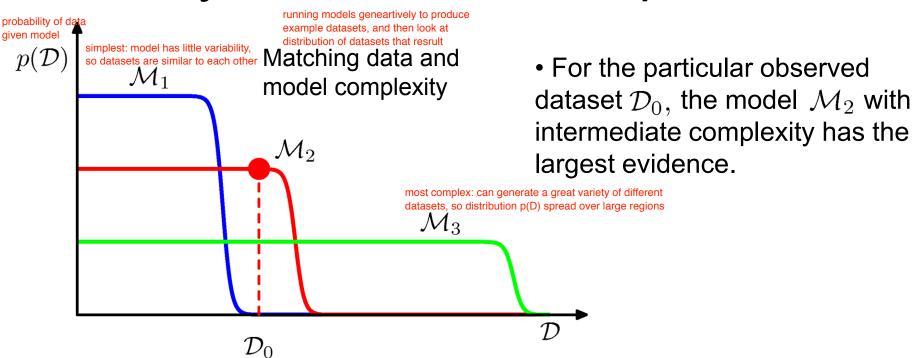
Negative and linear in *M*.

size of penalty increases linearly with number

penalizes the model according to its complexity

Negative

- 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. decrease because a more complex model can be a better fit to data
- The optimal model complexity: trade-off between these two competing terms.



- 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.

A limitation of all these LBFMs

1. basis functions are fixed before training data is observed,

a. curse of dimensionality, number of basis needs to grow rapidly, exponential, with dimension D of input space With M basis functions along each dimension of a D-dimensional input space, you require MD basis functions: the curse of dimensionality. determine if they are really there is not trivial

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.

using localized basis function such that they scatter in input space only in regions containing data

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

nerual nets exploit this property by choosing directions in input space to which basis functions respond

the good with assumption of linearity

- closed form to LS problem
- 2. tractable Bayesian treatment
- 3. model arbitrary nonlinearities in mapping input to targets

Our linear regression techniques

assumptions

iid data

- LLS LR = MLE LR: $\hat{\mathbf{w}} = \operatorname{\mathbf{argmax}}_{\mathbf{w}} p(D|\mathbf{w})$
- MAP LR: $\hat{\mathbf{w}} = \mathbf{argmax_w} \ p(\mathbf{w}|D)$
 - L_2 regularization combats overfitting
 - \mathcal{L}_1 regularization does so with sparser solutions
- Bayesian LR: $p(\mathbf{w}|D)$ the prior needs to be set reasonably
 - Combats overfitting while allowing more data to be used for training
 - Empirical-Bayes LR (future lecture) reduces the assumptions we make about the prior. Note: α can be tuned per dimension

What assumptions are we making in each case?

Hint for the question on slide 12

The exponent in the right-hand side is:

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

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

idea is to match the coefficients to 2nd order and 1st order of mu

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

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

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

Outline

- Bayesian methods
 - Bayesian linear regression
 - Bayesian model comparison
 - Evidence approximation

K nearest neighbours