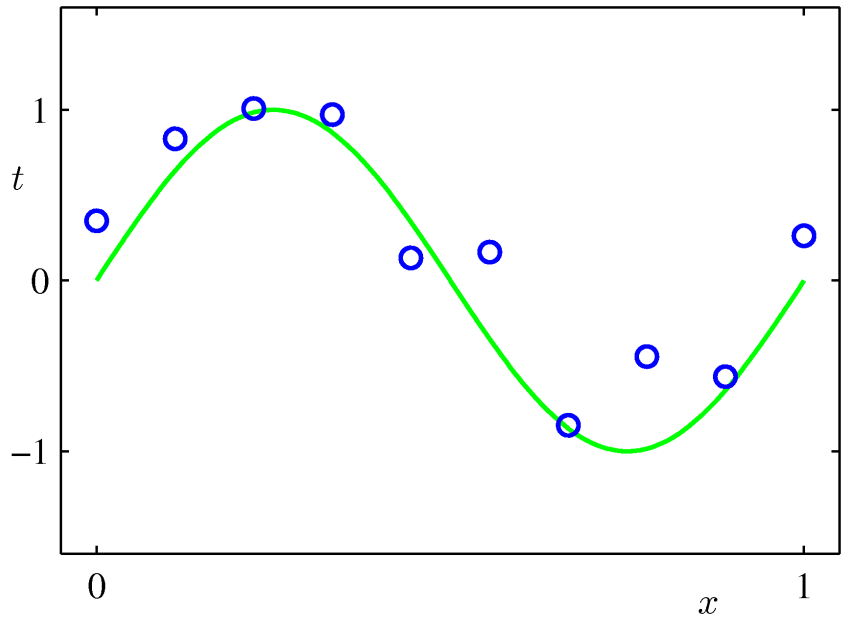
PATTERN RECOGNITION AND MACHINE LEARNING

CHAPTER 3: LINEAR MODELS FOR REGRESSION

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 $\phi_j(\mathbf{x})$ are known as *basis functions*.

Typically, $\phi_0(\mathbf{x}) = 1$, so that w_0 acts as a bias.

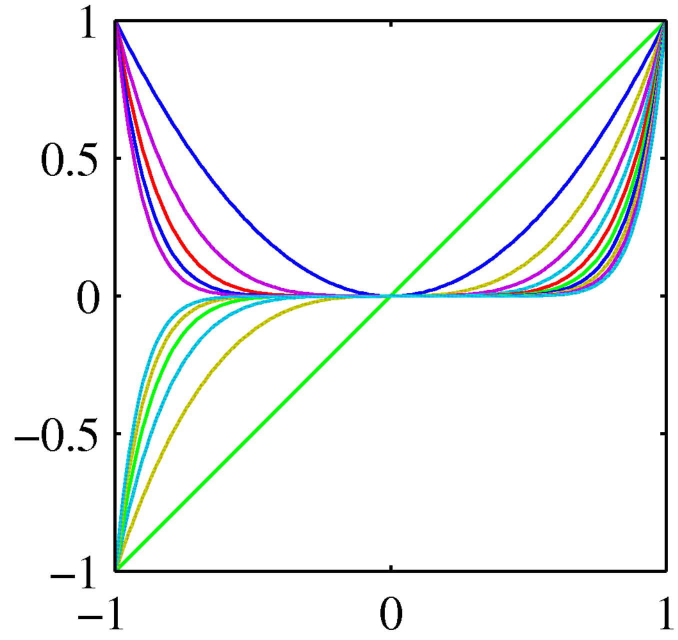
In the simplest case, we use linear basis functions : $\phi_d(\mathbf{x}) = x_d$.

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.

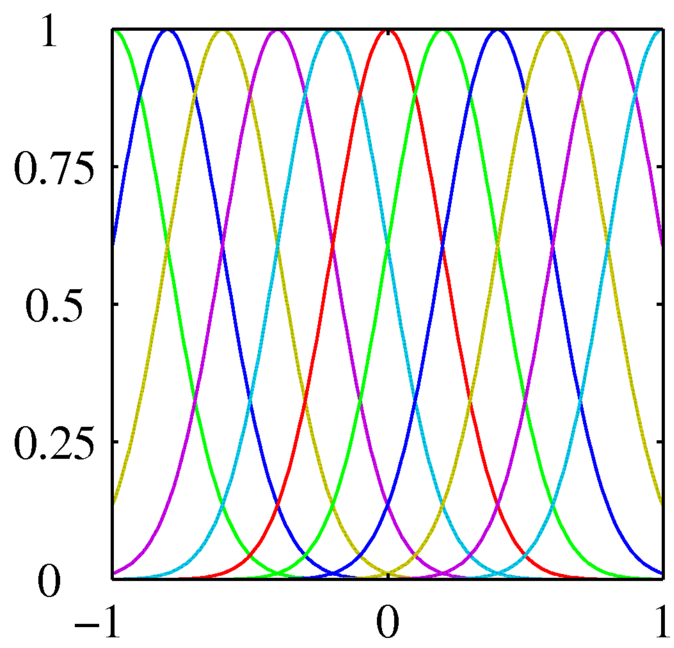


Linear Basis Function Models (4)

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).



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

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

Bayesian Model Comparison (1)

How do we choose the 'right' model?

Assume we want to compare models $\mathcal{M}_i,\ i=1,\ \ldots,L$, using data $\mathcal{D}$; 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 computed $p(\mathcal{M}_i|\mathcal{D})$, 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

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

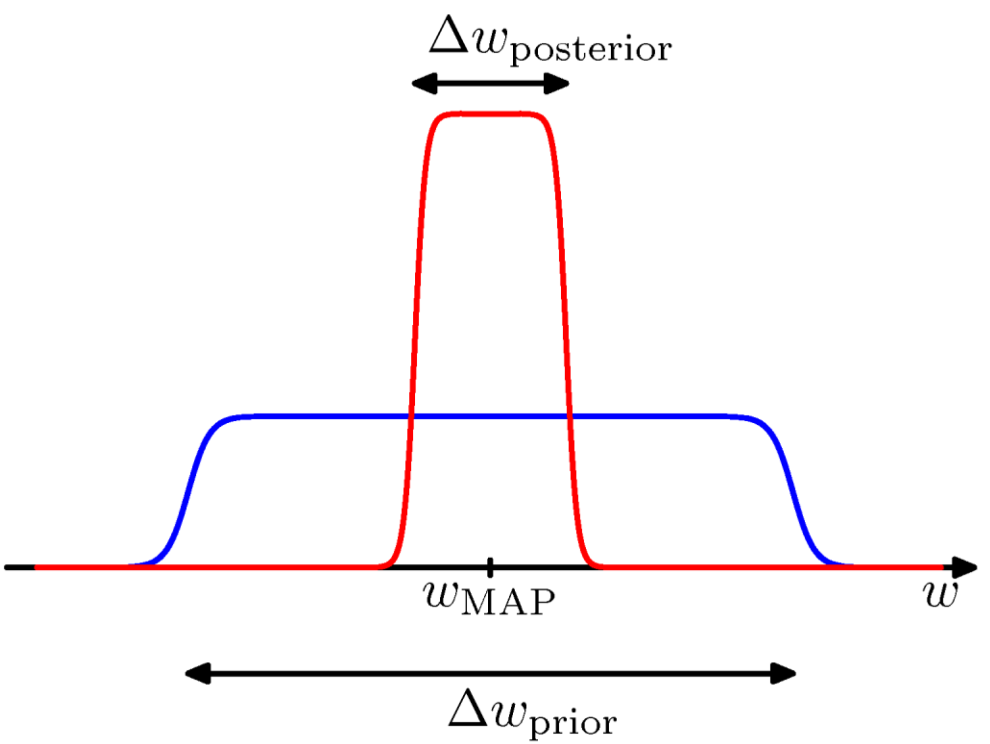
Bayesian Model Comparison (4)

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.



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