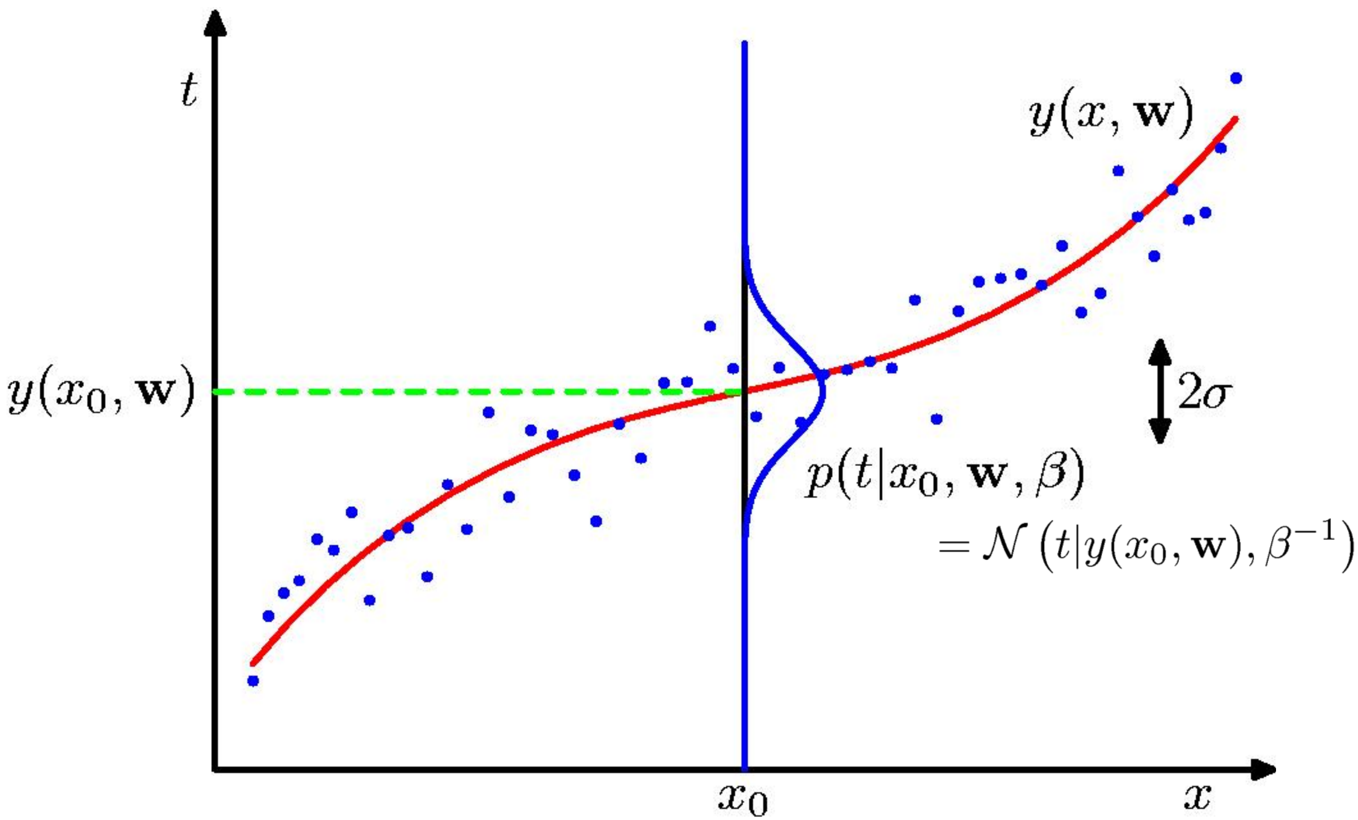
Slides modified from:

PATTERN RECOGNITION AND MACHINE LEARNING

CHRISTOPHER M. BISHOP

Curve Fitting Re-visited



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

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

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

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

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

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

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

$$0 = \sum_{n=1}^{N} t_n \boldsymbol{\phi}(\mathbf{x}_n)^{\mathrm{T}} - \mathbf{w}^{\mathrm{T}} \left(\sum_{n=1}^{N} \boldsymbol{\phi}(\mathbf{x}_n) \boldsymbol{\phi}(\mathbf{x}_n)^{\mathrm{T}} \right)$$

Solving for w, we get

$$\mathbf{w}_{\mathrm{ML}} = \underbrace{\left(\boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi} \right)^{-1} \boldsymbol{\Phi}^{\mathrm{T}}}_{\text{The Moore-Penrose pseudo-inverse, } \boldsymbol{\Phi}^{\dagger}} \mathbf{t}$$

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

where

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

Bayesian Linear Regression (1)

Define a Gaussian prior over w

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

Combining this with the likelihood function

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

and 'completing the square', gives the posterior

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

where

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

Completing the square

$$\frac{1}{2}\mathbf{w}^T C\mathbf{w} + \mathbf{b}^T\mathbf{w} + a$$ C symmetric

Bring into form $$\frac{1}{2}(\mathbf{w}-\mathbf{m})^T S(\mathbf{w}-\mathbf{m}) + u$$

with

$$S = C$$

$$\mathbf{m} = -C^{-1}\mathbf{b}$$

$$u = a - \frac{1}{2}\mathbf{b}^T C^{-1}\mathbf{b}$$

Bayesian Linear Regression (2)

A common choice for the prior is

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

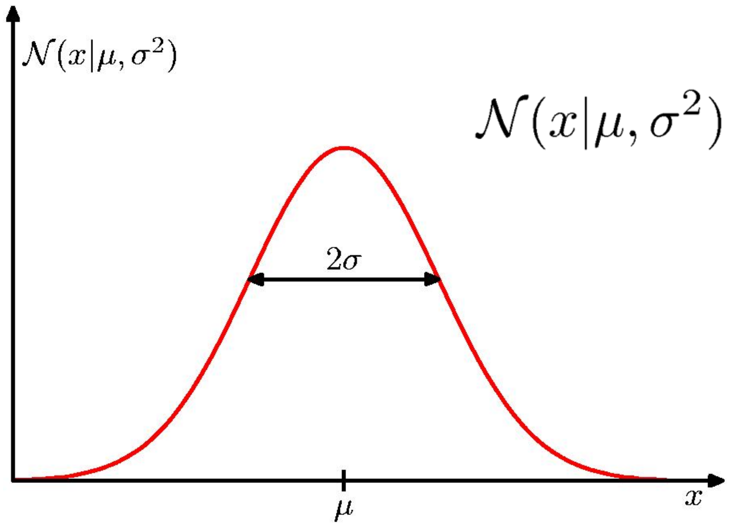
for which

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

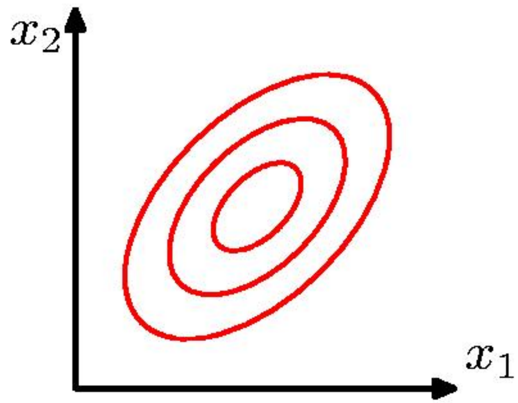
$$\mathbf{m}_N = \beta \mathbf{S}_N \mathbf{\Phi}^{\mathrm{T}} \mathbf{t}$$

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

Reminder: The Gaussian Distribution



$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$



$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

Bayesian Linear Regression (2)

A common choice for the prior is

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

for which

$$\begin{aligned} p(\mathbf{w}|\mathbf{t}) &= \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N) \\ \mathbf{m}_N &= \beta \mathbf{S}_N \mathbf{\Phi}^{\mathrm{T}} \mathbf{t} \\ \mathbf{S}_N^{-1} &= \alpha \mathbf{I} + \beta \mathbf{\Phi}^{\mathrm{T}} \mathbf{\Phi}. \end{aligned}$$

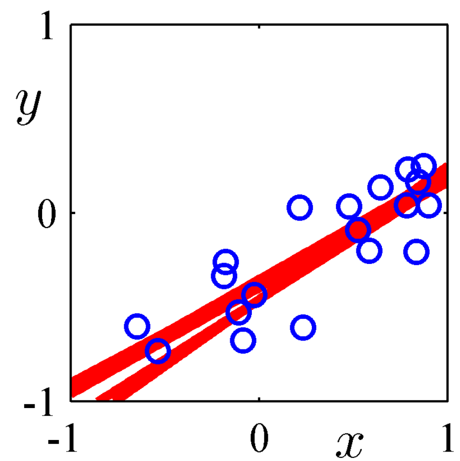
The log of the posterior distribution is given by the sum of the log likelihood and the log of the prior

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

Bayesian Linear Regression (2)

Example: estimate linear model of the form

$$y(x, \mathbf{w}) = w_0 + w_1 x$$



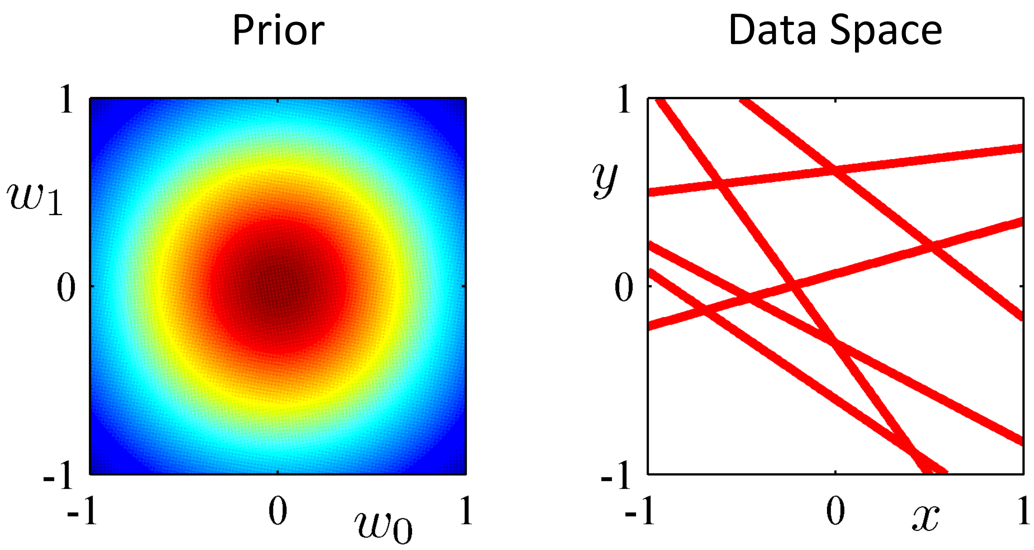
Data: draw x_n from uniform distribution, then plug into

$$f(x, \mathbf{a}) = a_0 + a_1 x$$

then add Gaussian noise to obtain target value t_n

Bayesian Linear Regression (3)

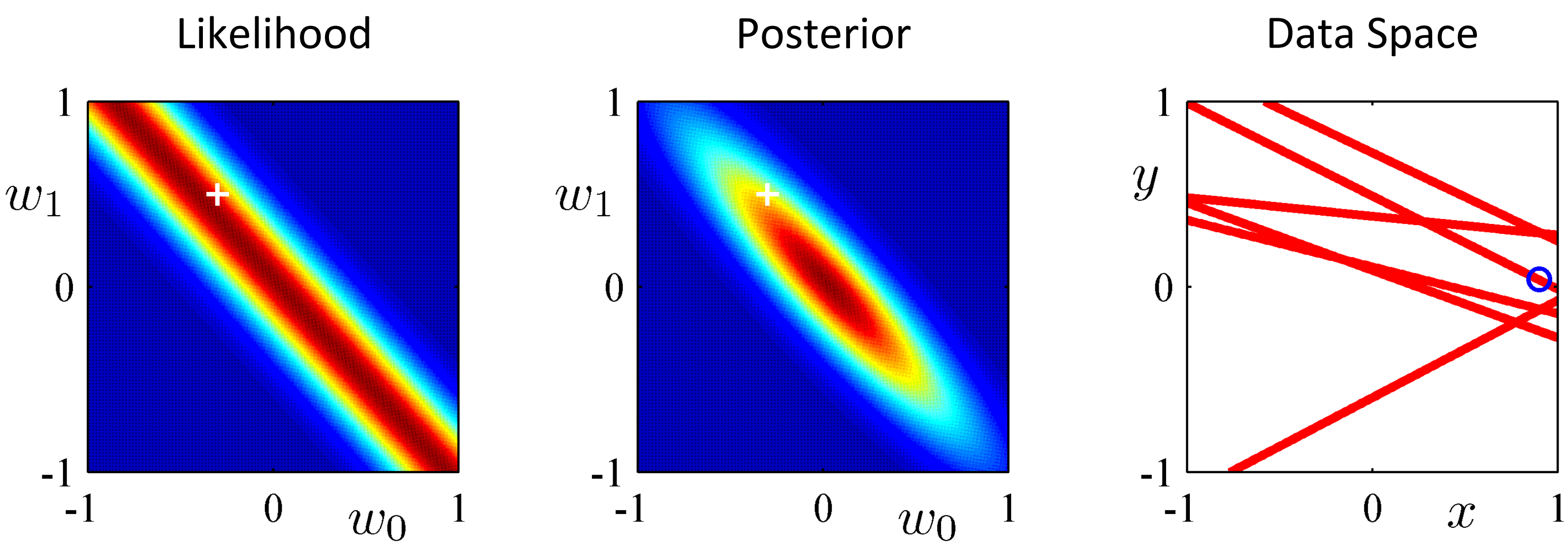
0 data points observed



$$y(x, \mathbf{w}) = w_0 + w_1 x$$

Bayesian Linear Regression (4)

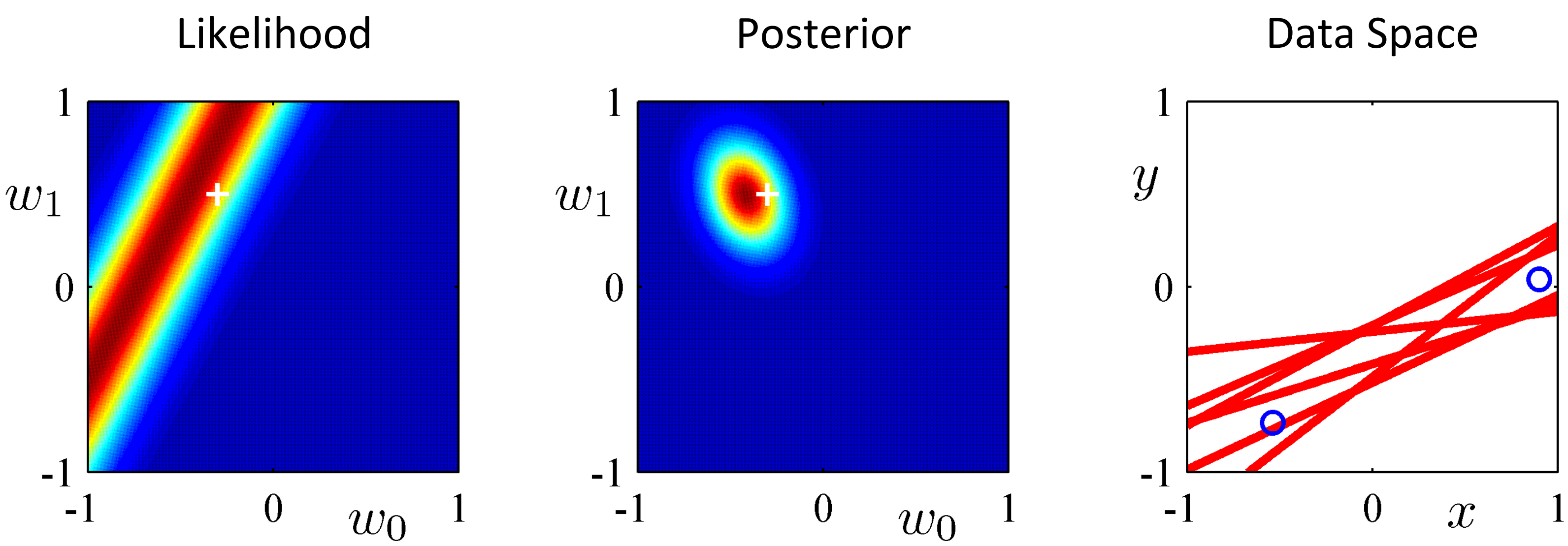
1 data point observed



$$y(x, \mathbf{w}) = w_0 + w_1 x$$

Bayesian Linear Regression (5)

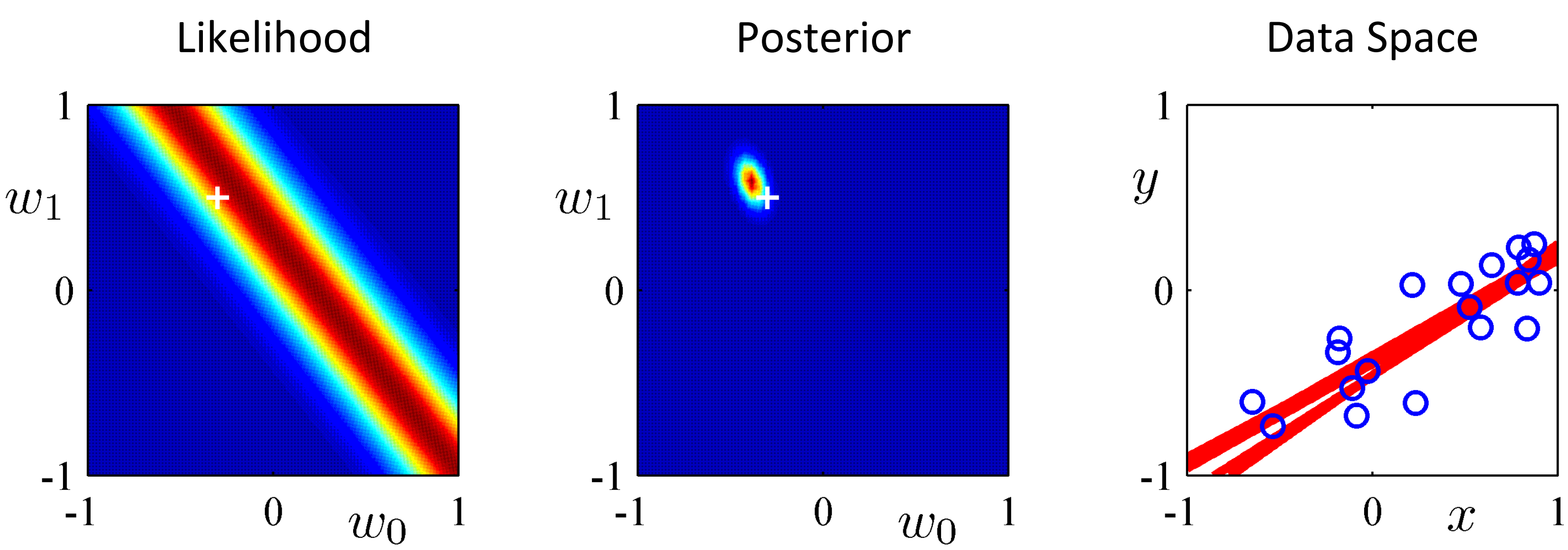
2 data points observed



$$y(x, \mathbf{w}) = w_0 + w_1 x$$

Bayesian Linear Regression (6)

20 data points observed



$$y(x, \mathbf{w}) = w_0 + w_1 x$$

Predictive Distribution (1)

Predict t for new values of x by integrating over w:

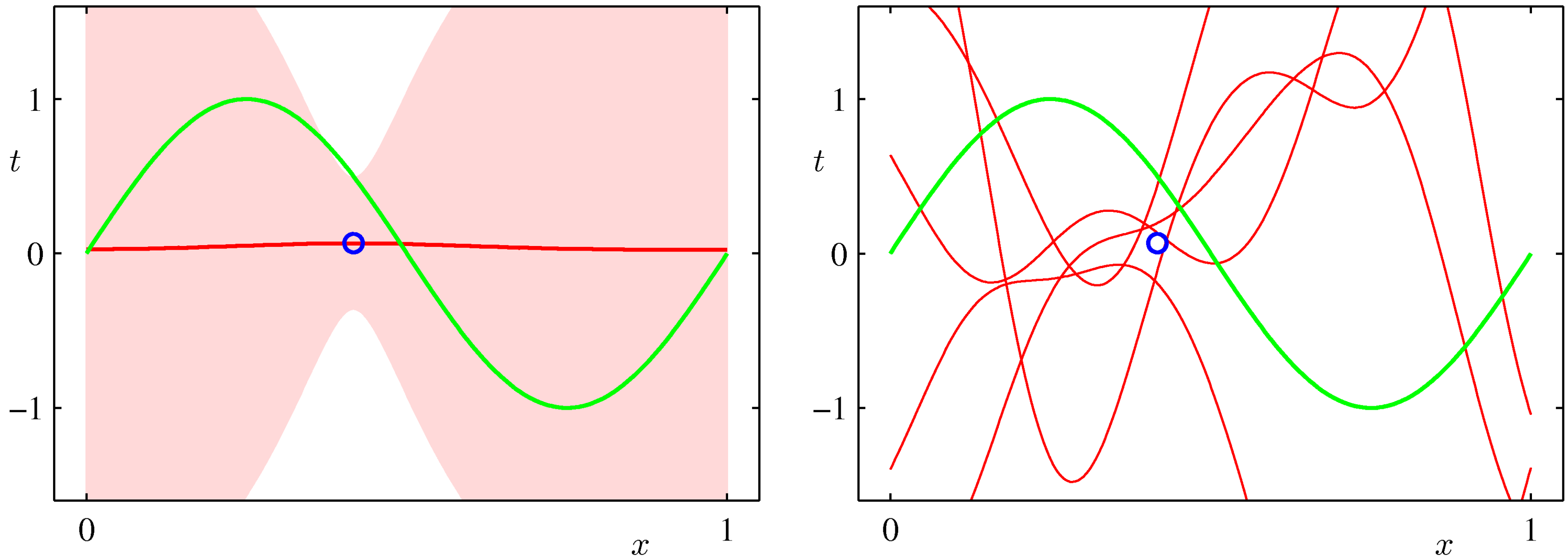
$$\begin{aligned} p(t|\mathbf{t}, \alpha, \beta) &= \int p(t|\mathbf{w}, \beta) p(\mathbf{w}|\mathbf{t}, \alpha, \beta) \, \mathrm{d}\mathbf{w} \\ &= \mathcal{N}(t|\mathbf{m}_N^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}), \sigma_N^2(\mathbf{x})) \end{aligned}$$

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)

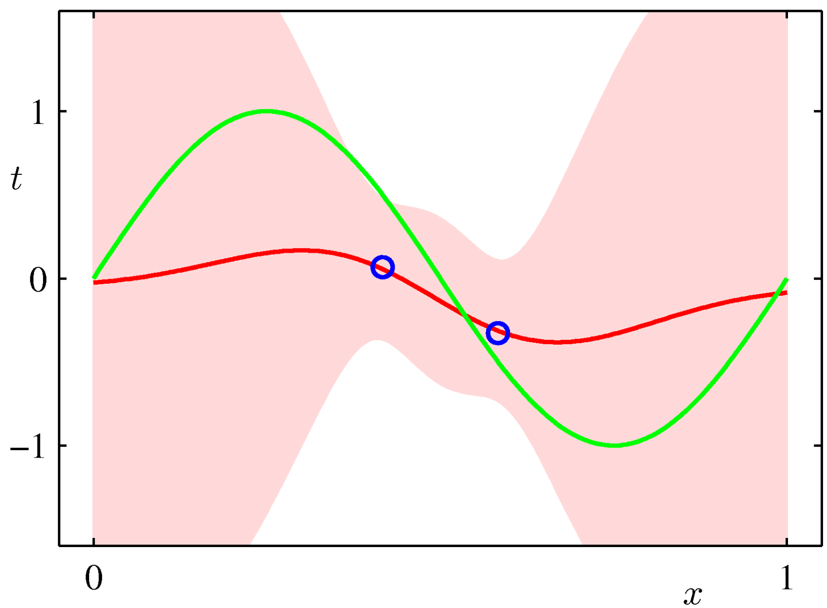
Example: Sinusoidal data, 9 Gaussian basis functions, 1 data point



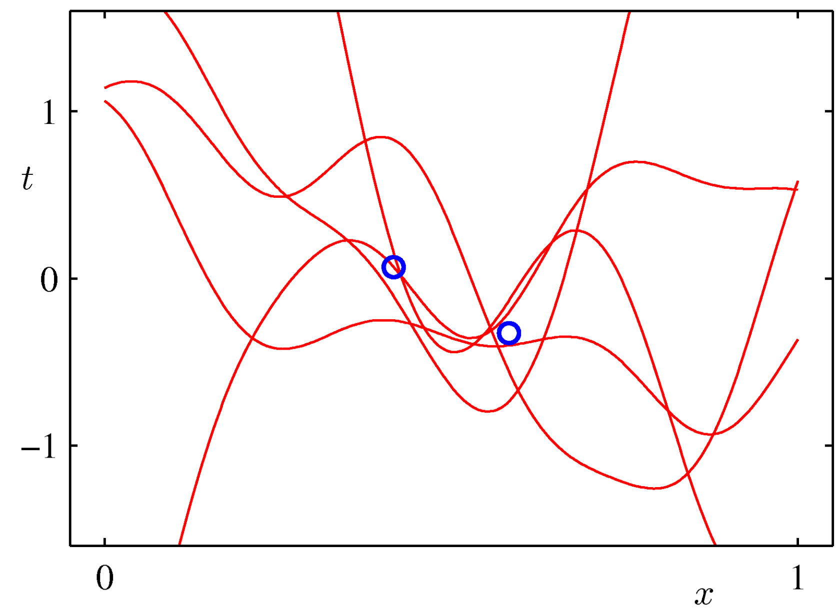
$\mathcal{N}(t|\mathbf{m}_N^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}), \sigma_N^2(\mathbf{x}))$ $y(x, \mathbf{w})$

Predictive Distribution (3)

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



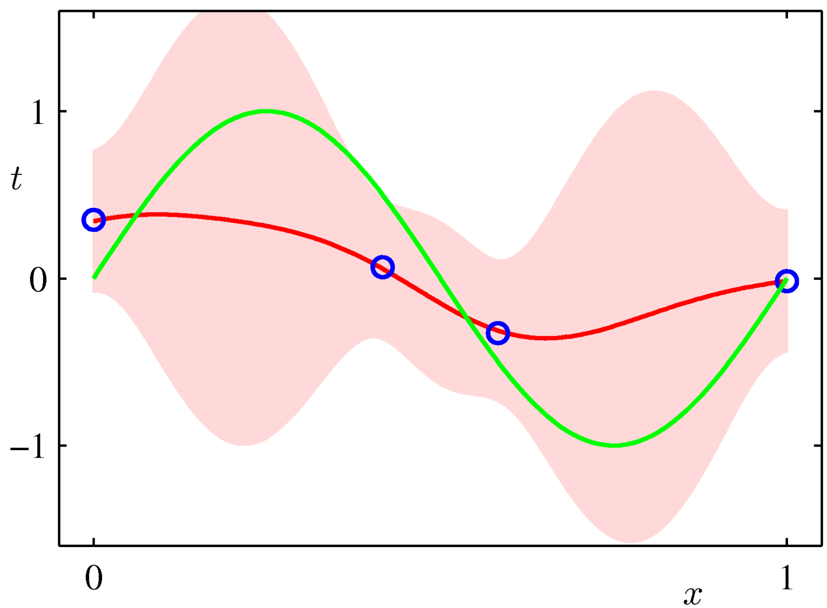
$$\mathcal{N}(t|\mathbf{m}_N^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}), \sigma_N^2(\mathbf{x}))$$



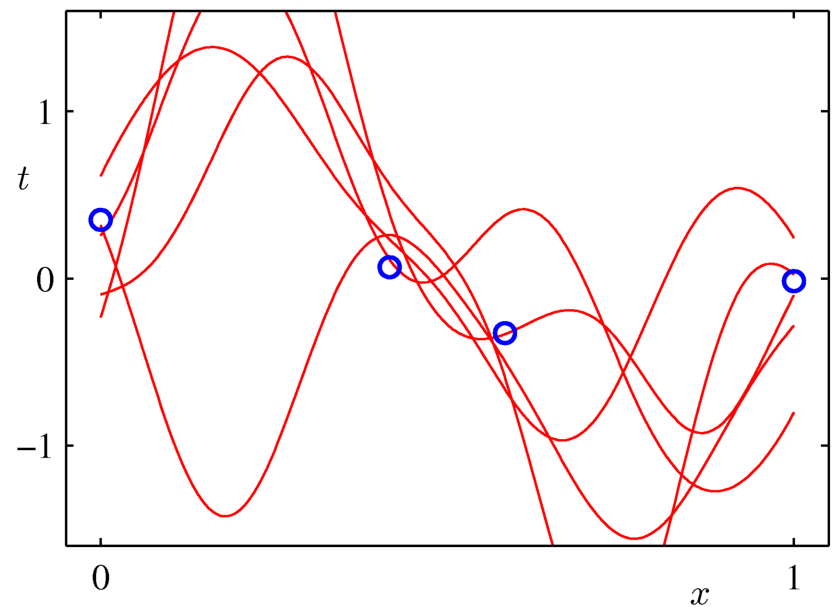
$$y(x, \mathbf{w})$$

Predictive Distribution (4)

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



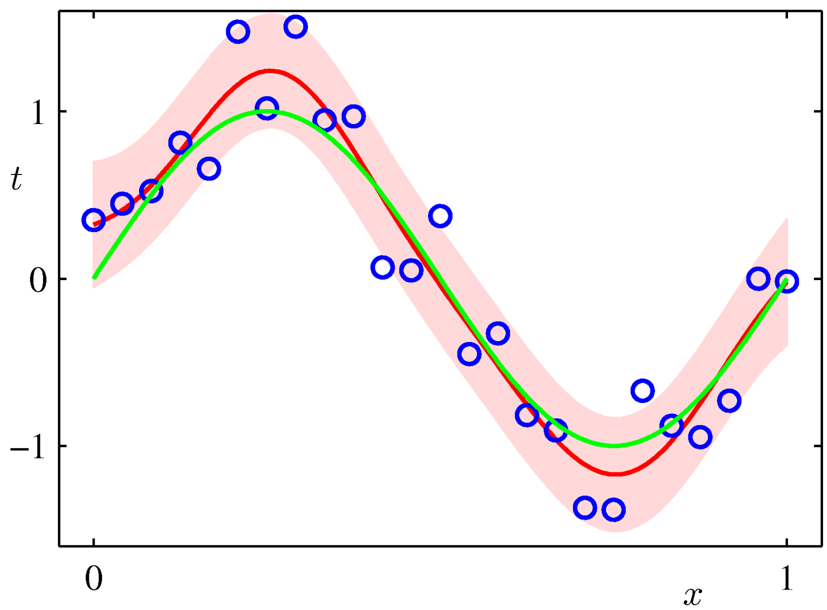
$$\mathcal{N}(t|\mathbf{m}_N^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}),\sigma_N^2(\mathbf{x}))$$



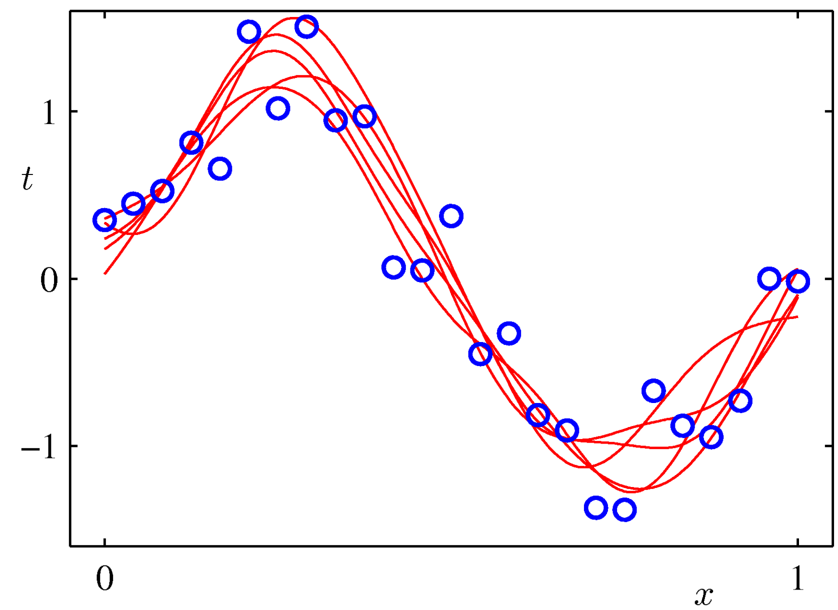
$$y(x,\mathbf{w})$$

Predictive Distribution (5)

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



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



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