Music and Machine Learning (IFT6080 Winter 08)
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These slides follow closely the (English) course textbook
Pattern Recognition and Machine Learning
by Christopher Bishop

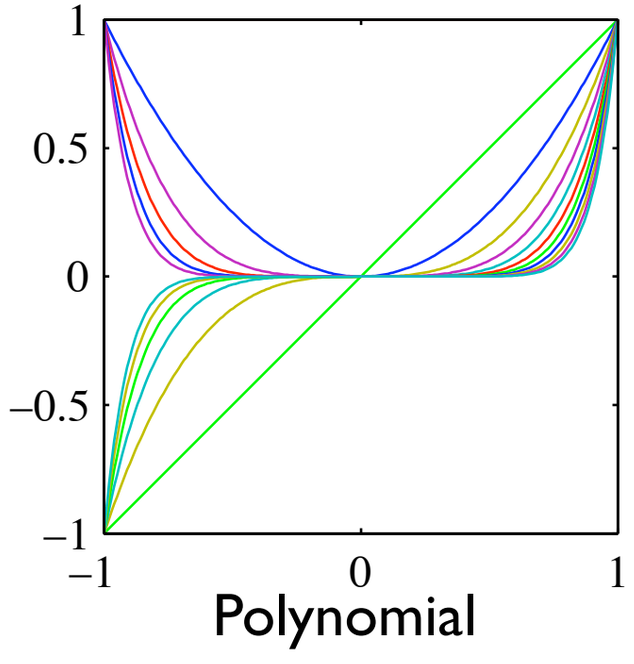
Linear Basis Function Models

- Linear regression extended to consider fixed basis functions:

$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x})$$

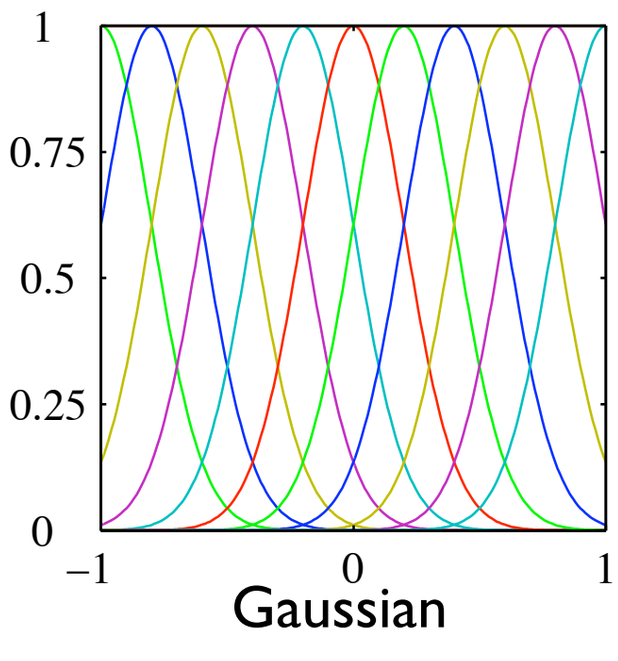
where $\mathbf{w} = (w + 0, ..., w_{M-1})^{\mathrm{T}}$ and $\boldsymbol{\phi} = (\phi_0, ..., \phi_{M-1})^{\mathrm{T}}$

- Possible basis functions include polynomials, Fourier, wavelet, ...



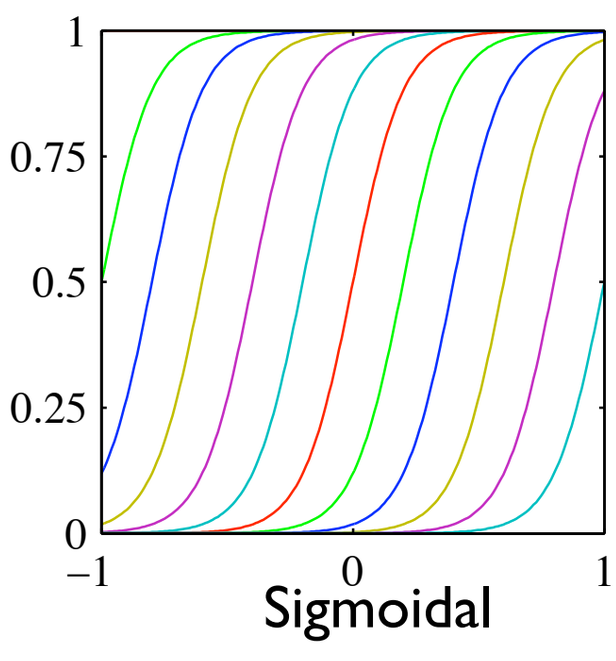
Polynomial

$$\phi_j(x) = x^j$$



Gaussian

$$\phi_j(x) = \exp\left\{\frac{(x - \mu_j)^2}{2s^2}\right\}$$



Sigmoidal

$$\phi_j(x) = \sigma\left(\frac{x = \mu_j}{s}\right)$$

$$\text{where } \sigma(a) = \frac{1}{1 + \exp(-a)}$$

Maximum likelihood and least squares

- Presume target *t* is generated via deterministic function plus gaussian noise ϵ having precision β

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon$$

$$p(t|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1})$$

- With Gaussian conditional distribution conditional mean is:

$$\mathbb{E}[t|\mathbf{x}] = \int tp(t|\mathbf{x})\mathrm{d}t = y(\mathbf{x}, \mathbf{w})$$

- With a set of input points $\mathbf{X} = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$ independently drawn:

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

Maximum likelihood and least squares

- Log likelihood:

$$\begin{aligned}\ln p(\mathbf{t}|\mathbf{w},\beta) &= \sum_{n=1}^{N} \ln \mathcal{N}(t_n|\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n),\beta^{-1}) \\ &= \frac{N}{2}\ln\beta - \frac{N}{2}\ln(2\pi) - \beta E_D(\mathbf{w})\end{aligned}$$

$$\text{where } E_D(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left\{t_n - \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\right\}^2$$

- Gradient:

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

Maximum likelihood and least squares

- Set gradient to 0:

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

- Solve for our weights yields *normal equations* for least squares:

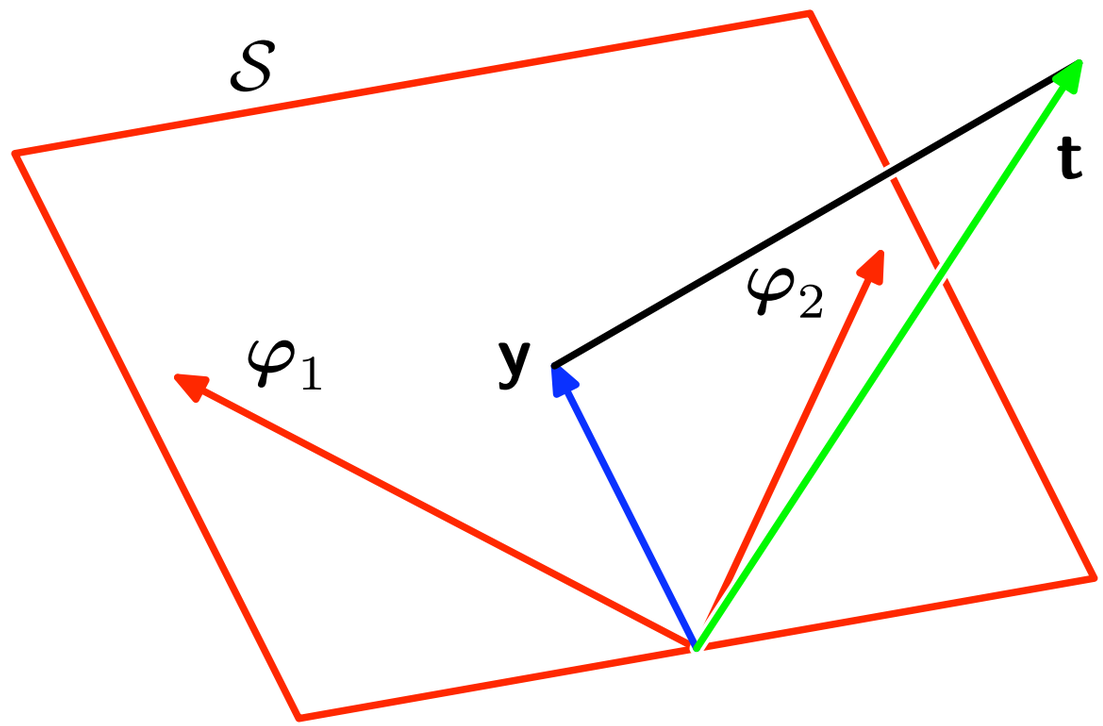
$$\mathbf{w}_{\mathrm{ML}} = \left(\boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi} \right)^{-1} \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{t}$$

- where Φ is the design matrix

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

- and where $\boldsymbol{\Phi}^{\dagger} = \left(\boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi}^{-1} \right) \boldsymbol{\Phi}^{\mathrm{T}}$ is the pseudo-inverse of Φ

Geometry of least squares



- Least-squares regression is obtained by finding the orthogonal projection of the data vector **t** onto the subspace spanned by the basis functions.
- Intuition: Sum of squares error is 1/2 squared Euclidean distance between **y** and **t**. Thus least-squares solution would move **t** as close as possible to **y** in the subspace *S*.

Online learning

- For large datasets may need to learn sequentially on sequences of smaller datasets, summing error

$$E = \sum_n E_n$$

- Sequential gradient descent (also called *stochastic gradient descent*:

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_n$$

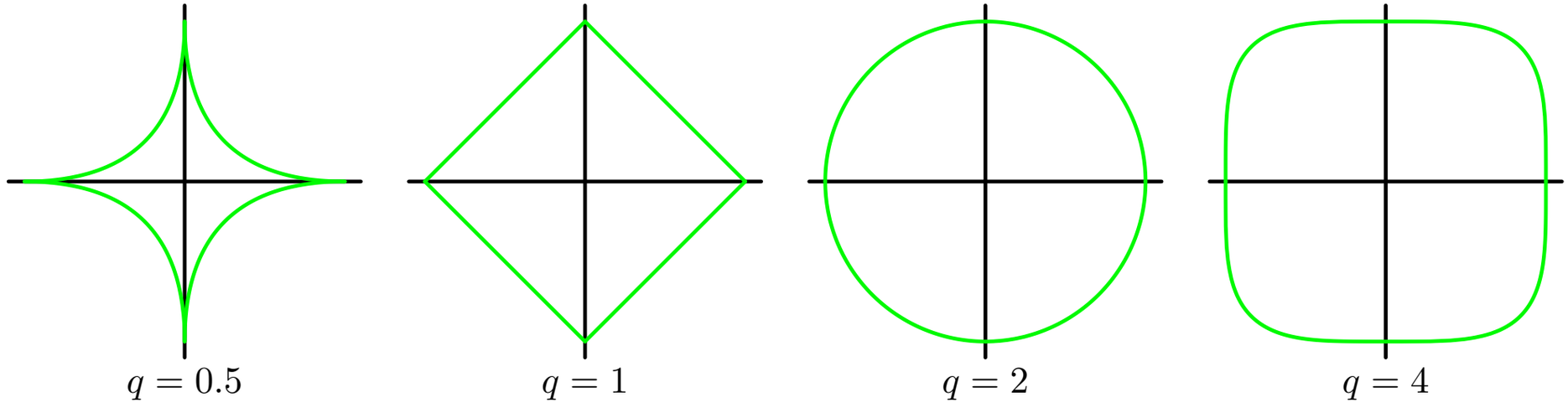
where τ is the iteration number and η is the learning rate

- For sum-of-squares we get Least Mean Squares (LMS):

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} + \eta(t_n - \mathbf{w}^{(\tau)\mathrm{T}}\boldsymbol{\phi}_n)\boldsymbol{\phi}_n$$

- Learning rate must be chosen carefully

Regularized least squares



- Regularize magnitude of weights:

$$\frac{1}{2}\sum_{n=1}^{N}\left\{t_n - \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\right\}^2 + \frac{\lambda}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}$$

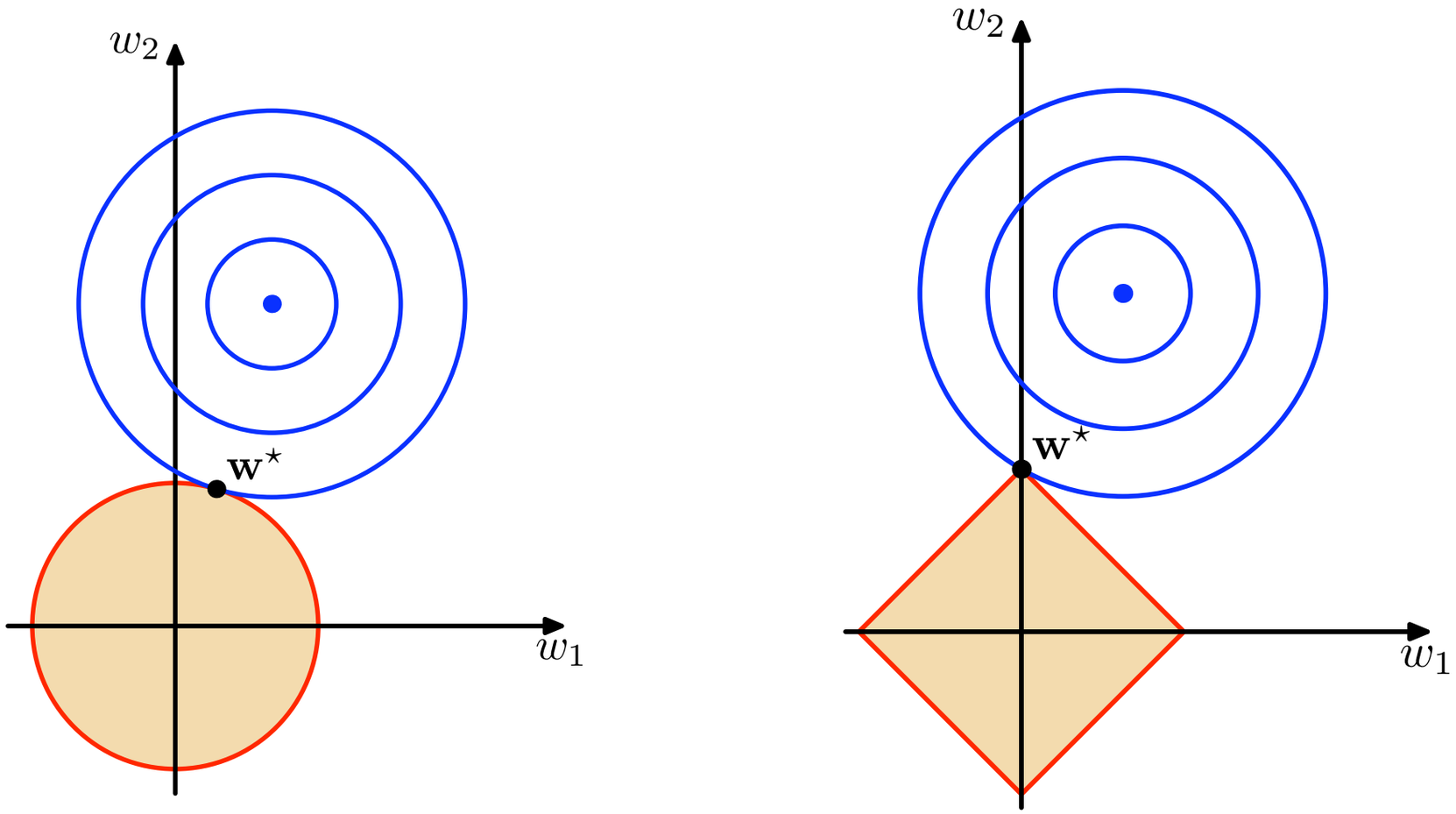
- Gradient with respect to 0 yields extension of least squares:

$$\mathbf{w} = \left(\lambda\mathbf{I} + \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\mathbf{t} \qquad \mathbf{w}_{\mathrm{ML}} = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\mathbf{t}$$

- More general regularizer; when q=1 we have "lasso" regularizer which selects for sparse models:

$$\frac{1}{2}\sum_{n=1}^{N}\left\{t_n - \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\right\}^2 + \frac{\lambda}{2}\sum_{j=1}^{M}|w_j|^q$$

Visualization of regularized least squares



Plot of contours of unregularized error function along with constraint region on the quadratic regularizer (left, q=2) versus lasso regularizer (right, q=1). For lasso, a sparse solution is generated with $w_1=0$

Bias-Variance decomposition

- How to best set the λ parameter for regularization?
- Conditional expectation:

$$h(\mathbf{x}) = \mathbb{E}[t|\mathbf{x}] = \int t p(t|\mathbf{x}) \mathrm{d}t$$

- Expected squared loss written with noise as second term:

$$\mathbb{E}[L] = \int \{y(\mathbf{x}) - h(\mathbf{x})\}^2 p(\mathbf{x})\, \mathrm{d}\mathbf{x} + \int \{h(\mathbf{x}) - t\}^2 p(\mathbf{x}, t)\, \mathrm{d}\mathbf{x}\, \mathrm{d}t$$

- We will minimize the first term. But we cannot hope to ever know the perfect regression function *h*(x)
- In a Bayesian model uncertainty is expressed as posterior over **w**
- In frequentist treatment we make a point-estimate of **w**. Assess confidence by making predictions over subsets of data and taking mean performance.

Bias-Variance decomposition

- Take integrand of first term using some subset of data *D*.
  $\{y(\mathbf{x}, \mathcal{D}) - h(\mathbf{x})\}^2$ which varies with data, thus take its mean

- Add and subtract expected value for the data

$$\{y(\mathbf{x}; \mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x}; \mathcal{D})] + \mathbb{E}_{\mathcal{D}}[y(\mathbf{x}; \mathcal{D})] - h(\mathbf{x})\}^2$$

$$= \{y(\mathbf{x}; \mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x}; \mathcal{D})]\}^2 + \{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x}; \mathcal{D})] - h(\mathbf{x})\}^2$$
$$+2\{y(\mathbf{x}; \mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x}; \mathcal{D})]\}\{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x}; \mathcal{D})] - h(\mathbf{x})\}$$

- Take expectation with respect to *D*; final term vanishes

$$\mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x}; \mathcal{D}) - h(\mathbf{x})\}^2\right]$$
$$= \{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x}; \mathcal{D})] - h(\mathbf{x})\}^2 + \mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x}; \mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x}; \mathcal{D})]\}^2\right]$$

(bias)^2 variance

- First term is bias : extent to which average prediction differs from desired regression function

- Second term is variance: extent to which individual solutions vary around the average. Thus measures sensitivity to data.

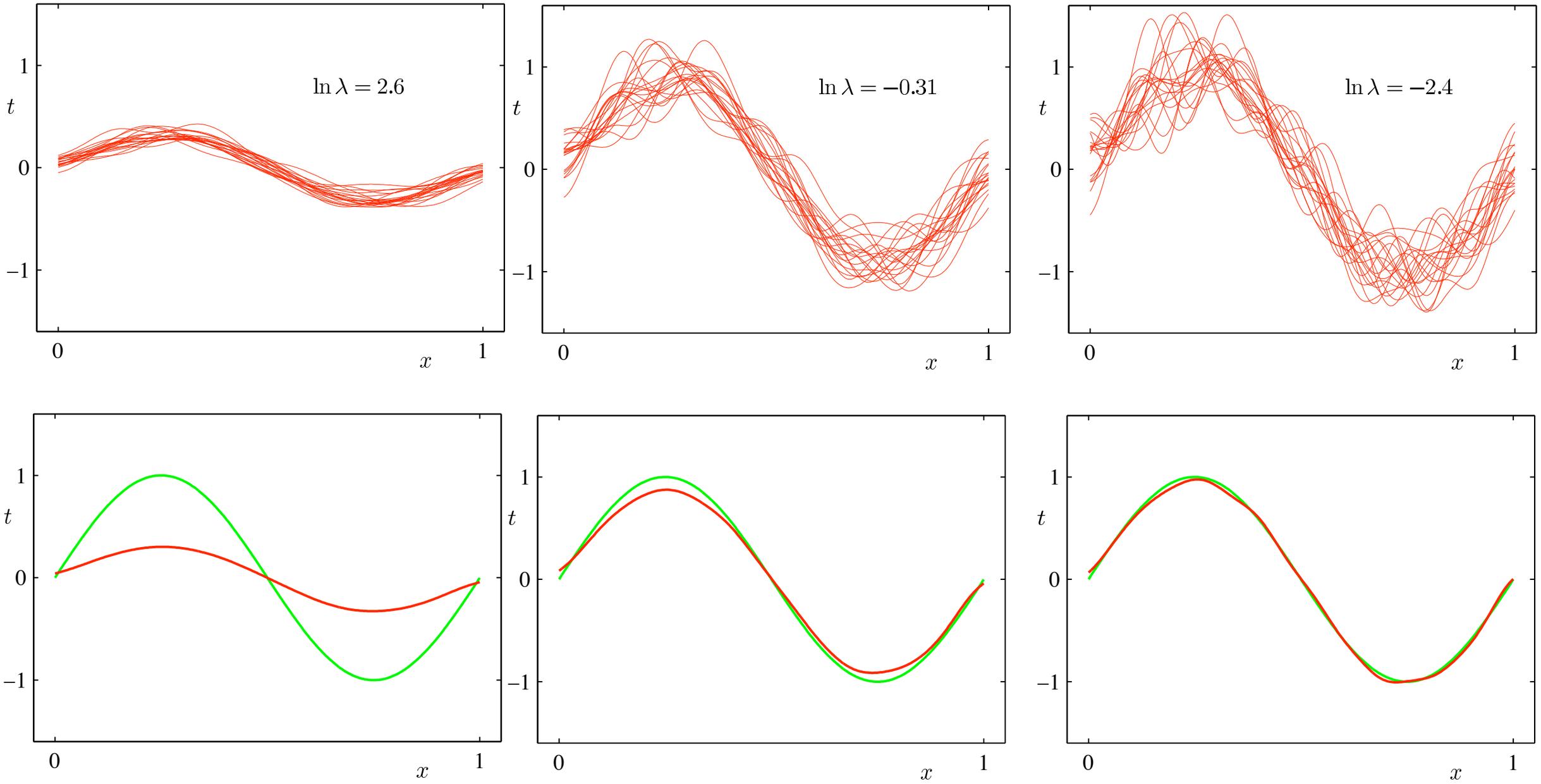
Bias-Variance decomposition

- expected loss = (bias)^2 + variance + noise where:

$$
\begin{aligned}
(\text{bias})^2 &= \int \{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2 p(\mathbf{x})\,\mathrm{d}\mathbf{x} \\
\text{variance} &= \int \mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2\right] p(\mathbf{x})\,\mathrm{d}\mathbf{x} \\
\text{noise} &= \int \{h(\mathbf{x}) - t\}^2 p(\mathbf{x},\mathbf{t})\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{t}
\end{aligned}
$$

- Very flexible models have low bias and high variance
- Relatively rigid models have high bias and low variance
- Optimal model balances the two

Bias variance example



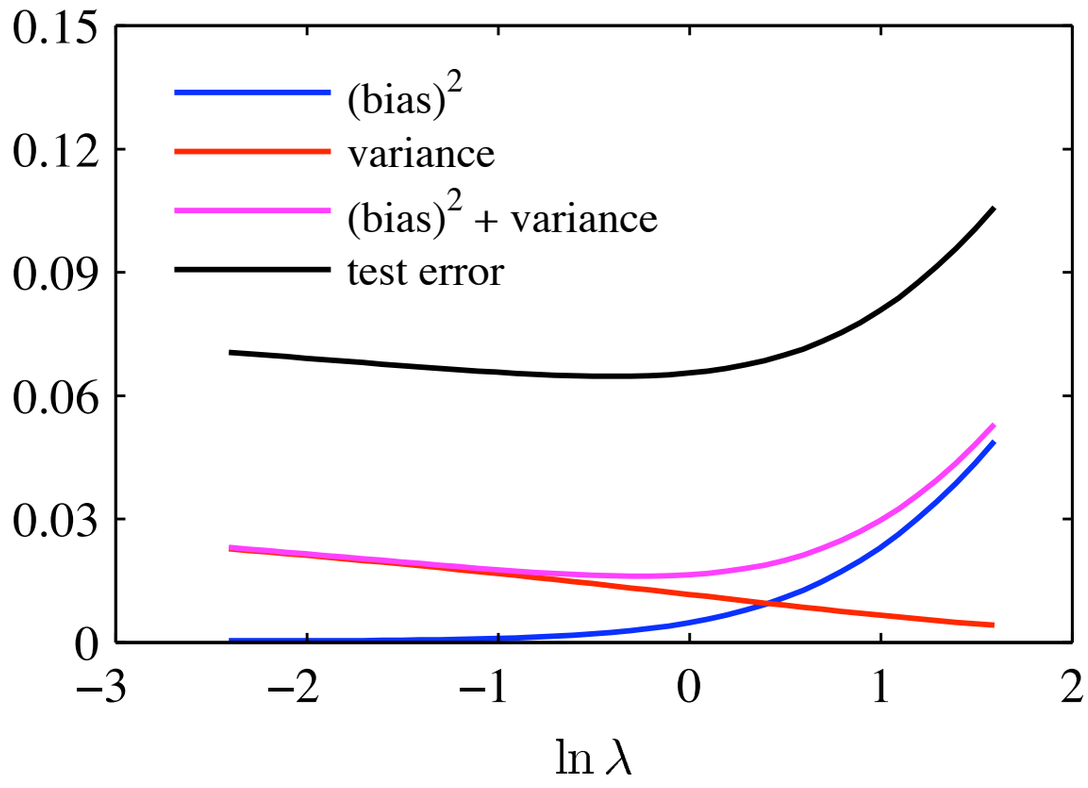
100 datasets each with 25 data points. Fit with 25 Gaussian basis functions.
Regularization parameter λ is varied. Top are individual fits.
Bottom is average fit along with generating sine function in green.

Bias variance example

$$\text{average} = \overline{y}(x) = \frac{1}{L}\sum_{l=1}^{L} y^{(l)}(x)$$

$$(\text{bias})^2 = \frac{1}{N}\sum_{n=1}^{N}\{\overline{y}(x_n) - h(x_n)\}^2$$

$$\text{variance} = \frac{1}{N}\sum_{n=1}^{N}\frac{1}{L}\sum_{l=1}^{L}\left\{y^{(l)}(x_n) - \overline{y}(x_n)\right\}^2$$



Plot of squared bias and variance together with their sum. The minimum is at λ=-0.31 which is close to the value yielding minimum test error

Bayesian Linear Regression

- Bias-variance decomposition requires splitting data. Inefficient.
- Avoids overfitting of maximum likelihood
- Leads to automatic way of determining model complexity
- Now we look quickly at Bayesian approach. Will return to it later in semester.

- Define prior over weights using zero-mean Gaussian prior:

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

- Log of posterior is sum of log likelihood and log of prior:

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

with quadratic regularization term $\lambda = \alpha/\beta$ in least squares sense

Sequential Bayesian Learning

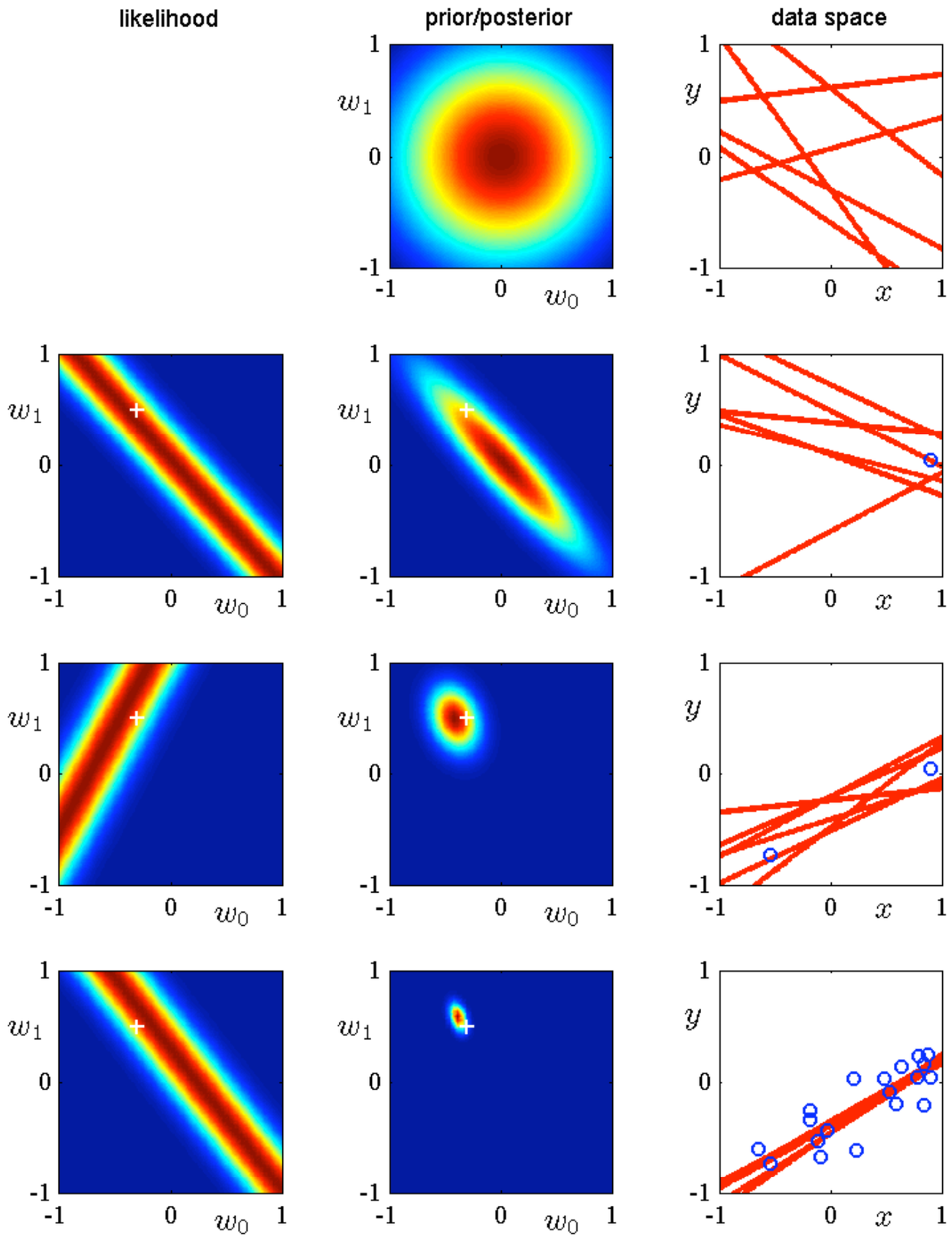
- Consider simple input variable *x*, single target *t* and a linear model of form $y(x, \mathbf{w}) = w_0 + w_1 x$
- Just two weights, can plot prior and posteriors
- Generate synthetic data using $f(x_n, \mathbf{a}) = -0.3 + 0.5 x_n + \epsilon$
- Goal is to recover **a** = {-0.3, 0.5} from data
- Basic algorithm:
  - observe point (*x*,*t*) from dataset
  - calculate likelihood p(*t*|*x*,**w**) based on estimate of noise precision β
  - multiply likelihood by previous prior over **w** to yield new posterior

Sequential Bayesian Learning

Basic algorithm:

- Observe point (*x*,*t*) from dataset
- Calculate likelihood p(*t*|*x*,**w**) based on estimate of noise variance β
- Multiply likelihood by previous prior over **w** to yield new posterior
- Observe another point ...

Samples from posterior are shown on right



Predictive distribution

- We are generally not interested in priors over **w** but rather for predicting new values *t* from x.
- Evaluate predictive distribution

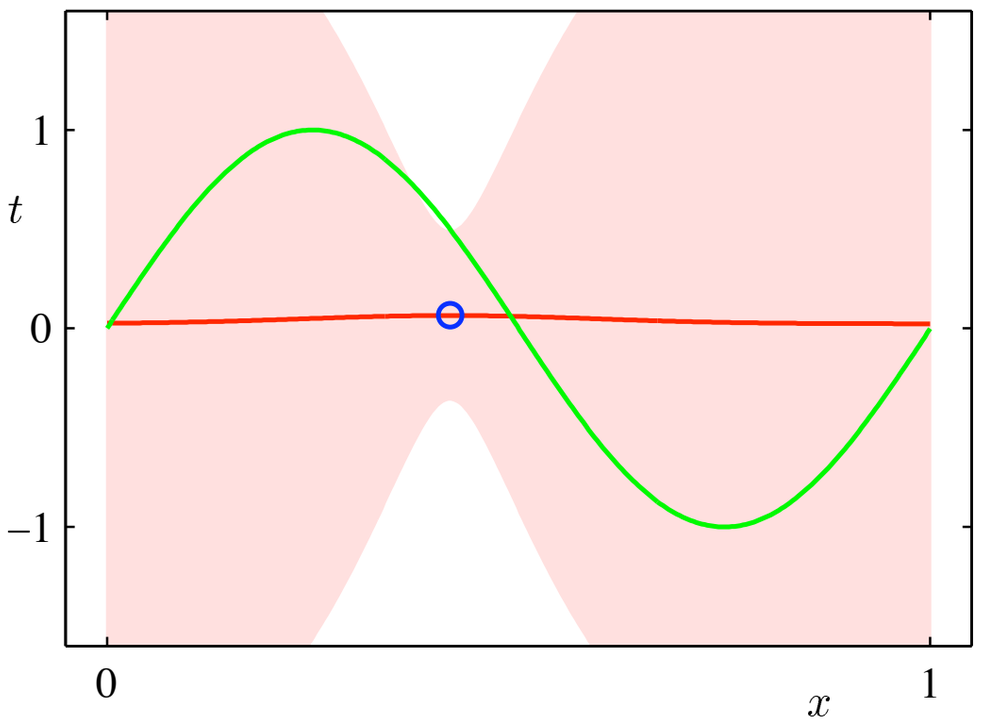
$$p(t|\mathbf{t}, \alpha, \beta) = \int p(t|\mathbf{w}, \beta) p(\mathbf{w}|\mathbf{t}, \alpha, \beta) \, \mathrm{d}\mathbf{w}$$

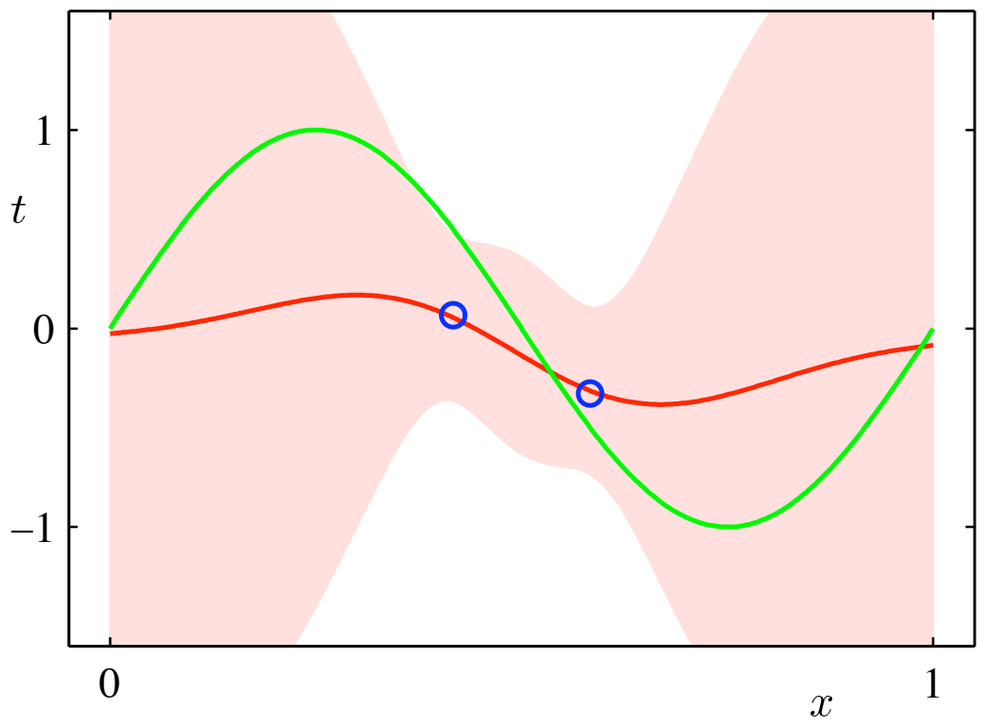
- This is convolution of conditional distribution of target with posterior **w**. For our problem (2 Gaussians) results in:

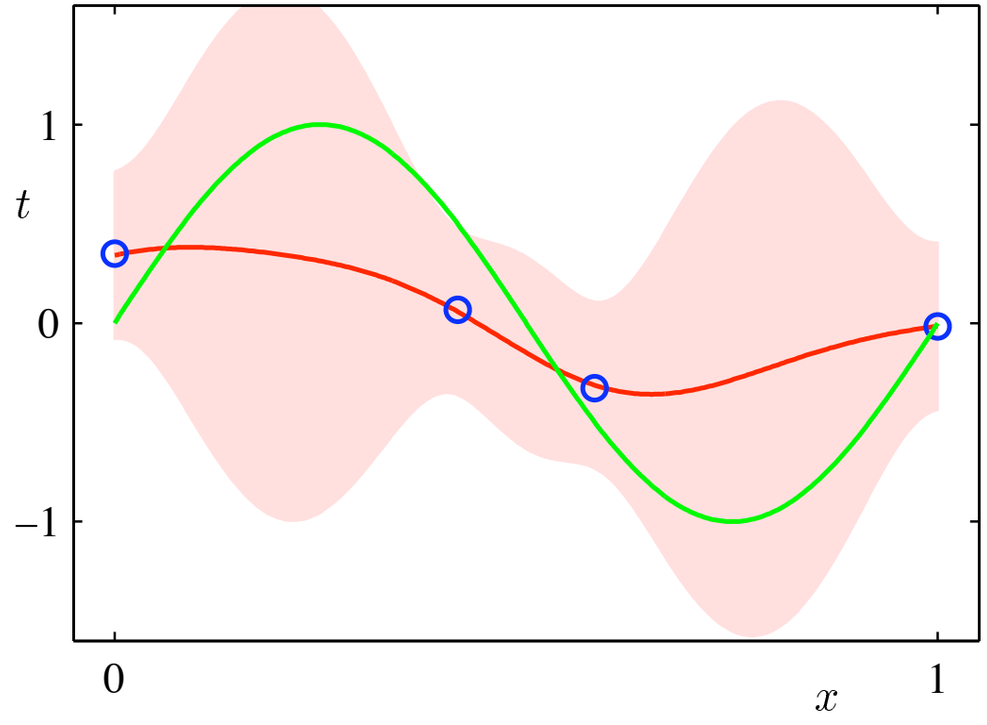
$$p(t|\mathbf{x}, \mathbf{t}, \alpha, \beta) = \mathcal{N}(t|\mathbf{m}_N^T \boldsymbol{\phi}(\mathbf{x}), \sigma_N^2(\mathbf{x}))$$

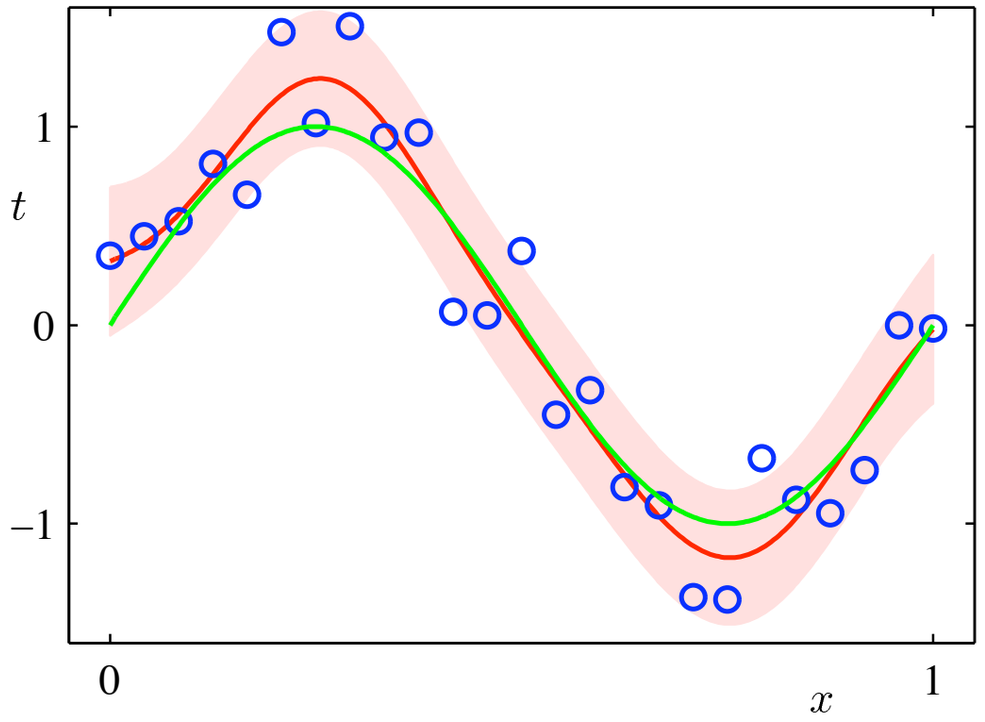
$$\sigma_N^2(\mathbf{x}) = \frac{1}{\beta} + \boldsymbol{\phi}(\mathbf{x})^T \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x})$$

Predictive distribution



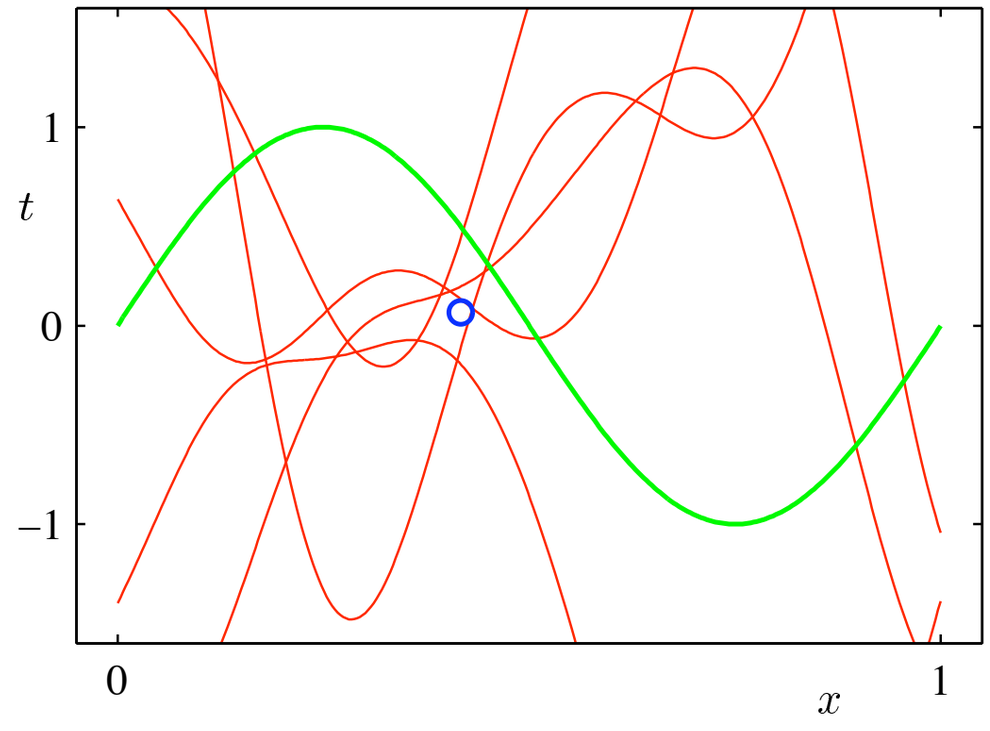


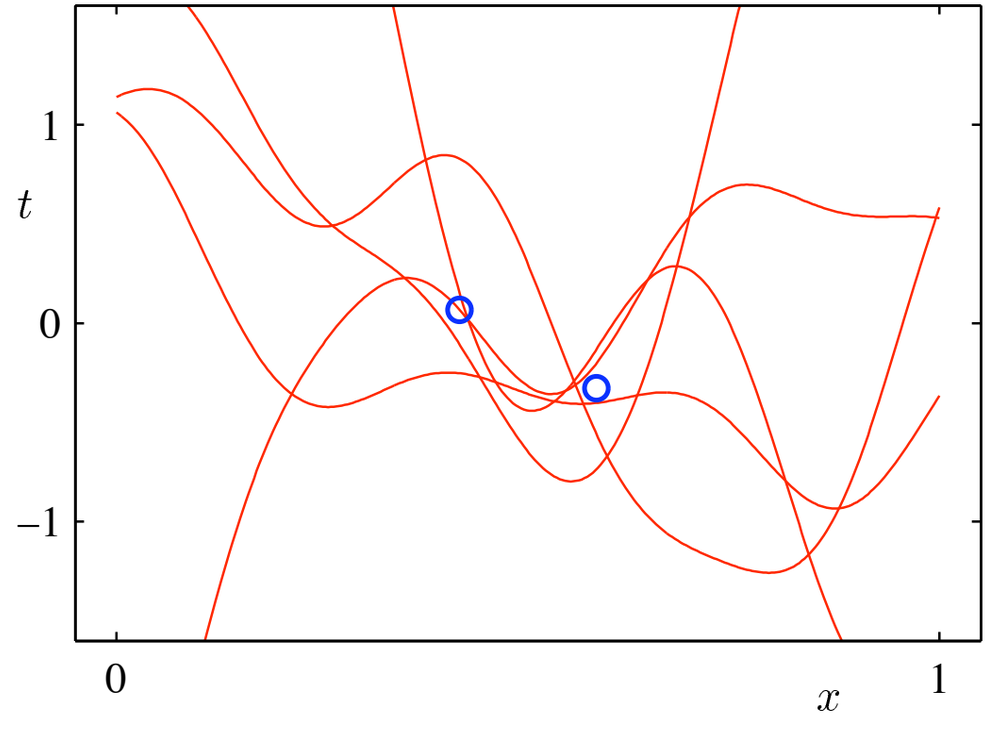


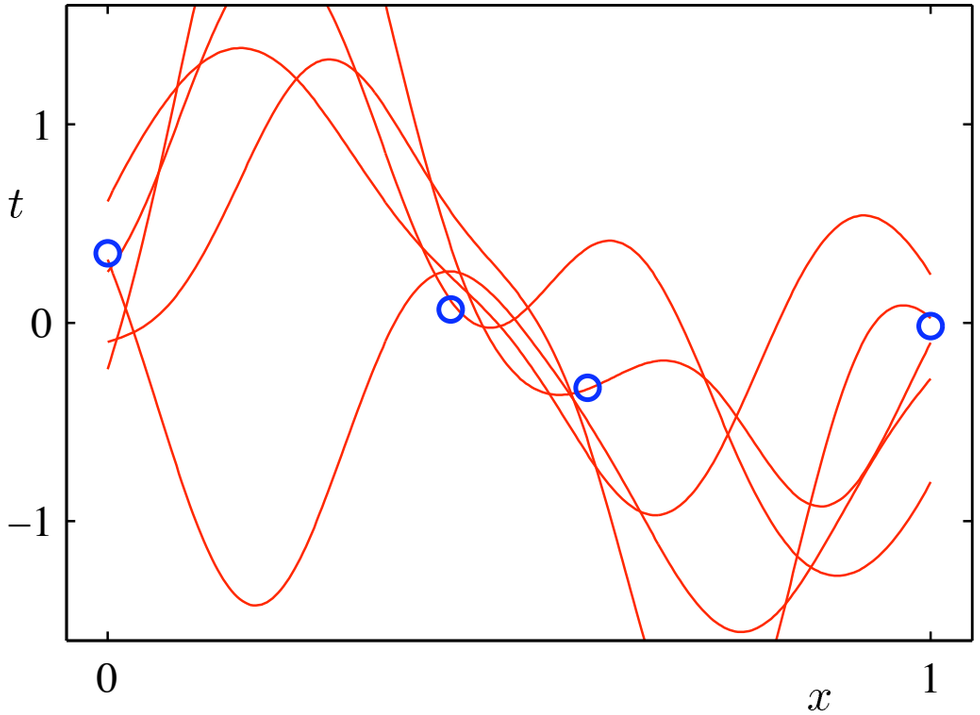


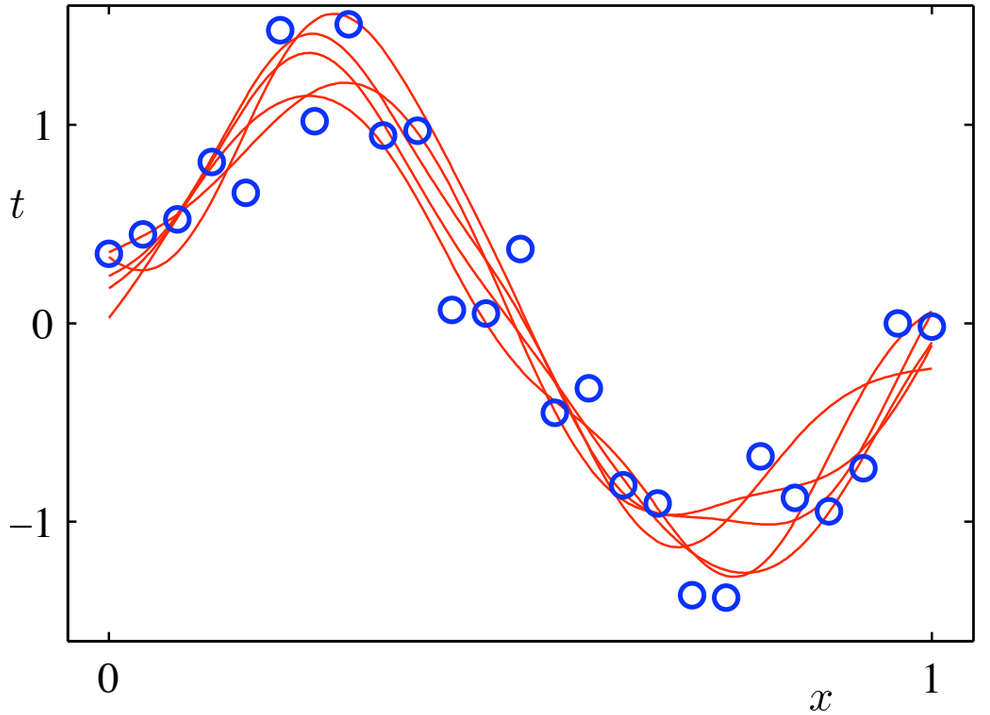
Predictive distributions for 9 Gaussian basis functions fitting f(x)=sin(2Πx)+ϵ in green. Red curve is mean of predictive distributions. Red shaded regions are 1 std dev. away from mean.

Predictive distribution









Plots of the functions y(x,**w**) using samples from the posterior distributions over **w** corresponding to the previous plots.

Equivalent kernel

- Posterior means can be interpreted as kernels; sets stage for kernel methods including Gaussian processes.

- Predictive mean can be written as:

$$y(\mathbf{x}, \mathbf{m}_N) = \mathbf{m}_N^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}) = \beta \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}} \mathbf{S}_N \boldsymbol{\Phi}^{\mathrm{T}} \mathbf{t} = \sum_{n=1}^{N} \beta \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}} \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x}) t_n$$

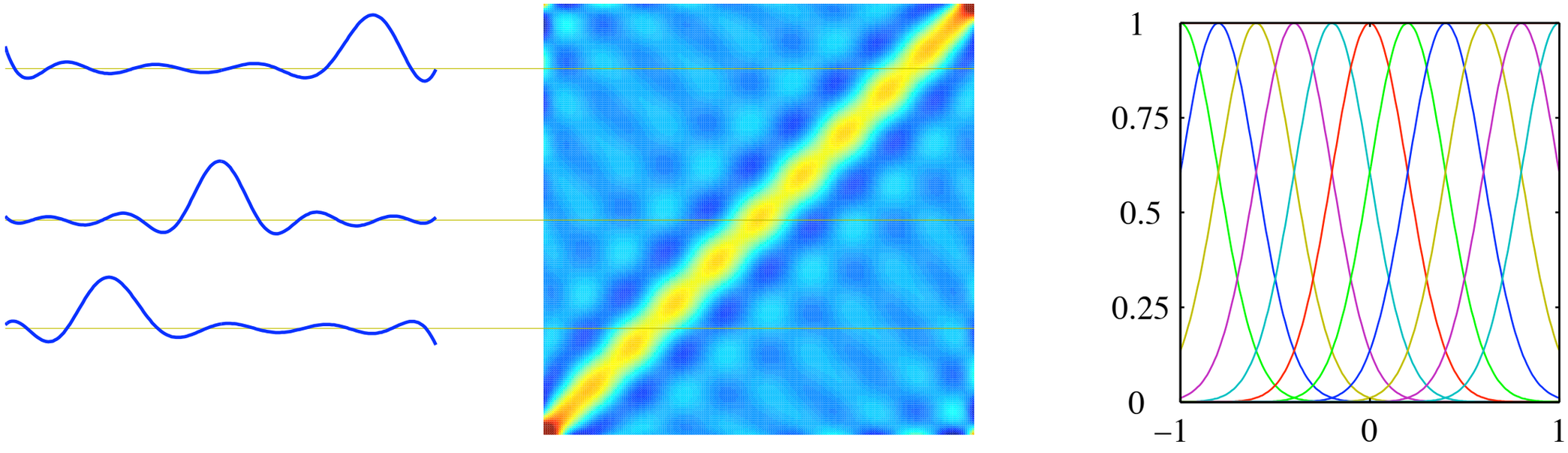
- We can also rewrite this as a kernel function:

$$y(\mathbf{x}, \mathbf{m}_N) = \sum_{n=1}^{N} k(\mathbf{x}, rbx_n) t_n$$

where the function $k(\mathbf{x}, \mathbf{x}') = \beta \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}} \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x}')$ is known as the *smoother matrix* or *equivalent kernel*

- Regression functions which predict using linear combinations of target values are known as *linear smoothers*

Equivalent kernel



Equivalent kernel (left, middle) for Gaussian basis function (right)

- Above $k(x,x')$ is plotted as a function of x. Note that it is localized around x.
- Mean of predictive distribution at x given by $y(x,\mathbf{m}_N)$ is obtained using a weighted combination where points close to x are given higher weight.
- Idea of using a localized kernel in place of a set of basis functions leads to *Gaussian processes* (to be covered later).