LINEAR REGRESSION

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CSE 4404/5327 Introduction to Machine Learning and Pattern Recognition

Credits

- Some of these slides were sourced and/or modified from:
  - Christopher Bishop, Microsoft UK

Relevant Problems from Murphy

- 7.4, 7.6, 7.7, **7.9**
- Please do 7.9 at least. We will discuss the solution in class.

Linear Regression Topics

- What is linear regression?
- Example: polynomial curve fitting
- Other basis families
- Solving linear regression problems
- Regularized regression
- Multiple linear regression
- Bayesian linear regression

What is Linear Regression?

- In classification, we seek to identify the **categorical** class C_k associate with a given input vector **x**.
- In regression, we seek to identify (or **estimate**) a **continuous** variable *y* associated with a given input vector **x**.
- *y* is called the **dependent variable**.
- **x** is called the **independent variable**.
- If *y* is a vector, we call this multiple regression.
- We will focus on the case where *y* is a scalar.
- Notation:
  - *y* will denote the continuous model of the dependent variable
  - *t* will denote discrete noisy observations of the dependent variable (sometimes called the **target variable**).

Where is the Linear in Linear Regression?

- In regression we assume that y is a function of **x**. The exact nature of this function is governed by an unknown parameter vector **w**:

$$y = y\left(\mathbf{x}, \mathbf{w}\right)$$

- The regression is linear if y is linear in **w**. In other words, we can express y as

$$y = \mathbf{w}^t \phi\left(\mathbf{x}\right)$$

where

$\phi\left(\mathbf{x}\right)$ is some (potentially nonlinear) function of **x**.

Linear Basis Function Models

- 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 Regression Topics

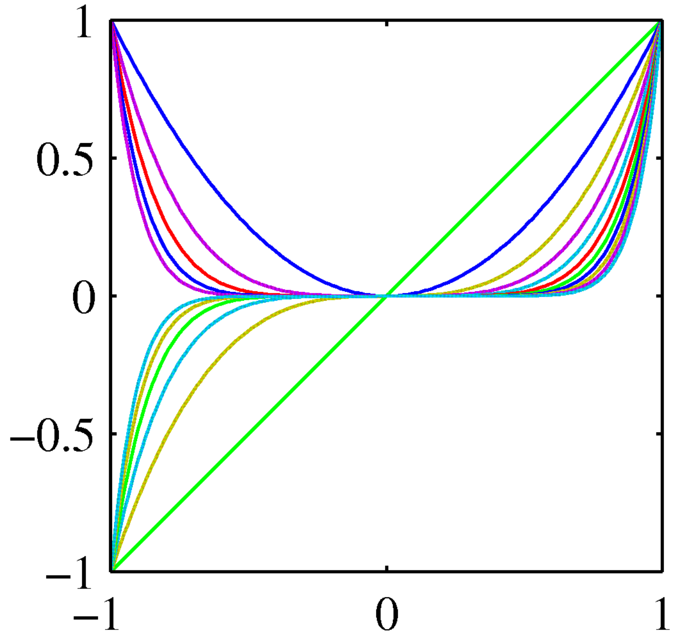
- What is linear regression?
- **Example: polynomial curve fitting**
- Other basis families
- Solving linear regression problems
- Regularized regression
- Multiple linear regression
- Bayesian linear regression

Example: Polynomial Bases

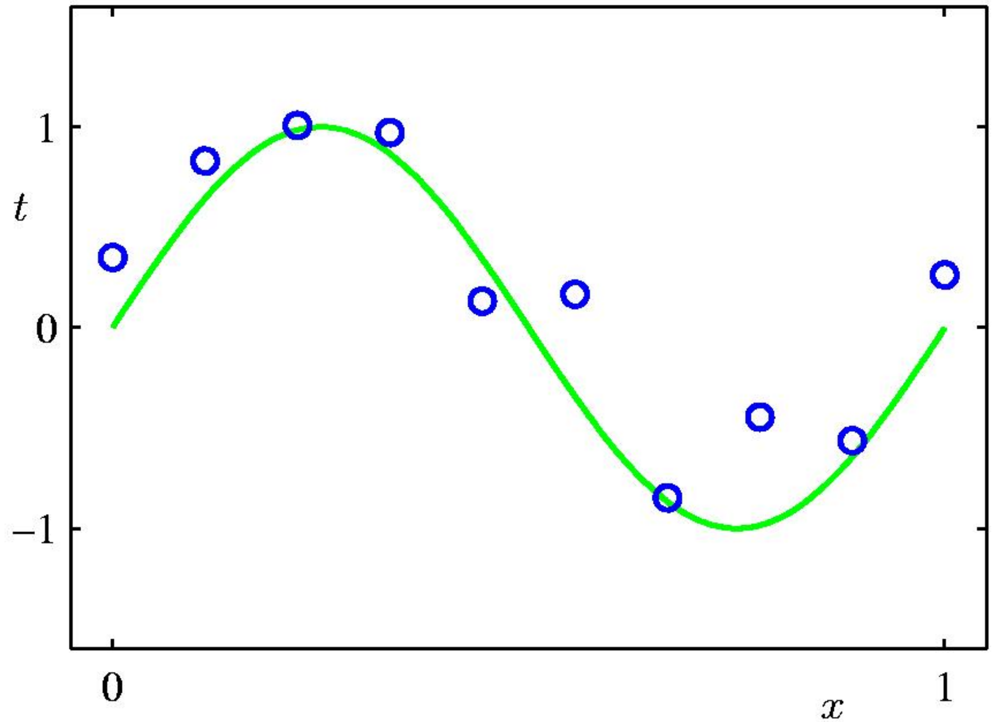
- Polynomial basis functions:

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

- These are global
  - a small change in x affects all basis functions.
  - A small change in a basis function affects y for all x.

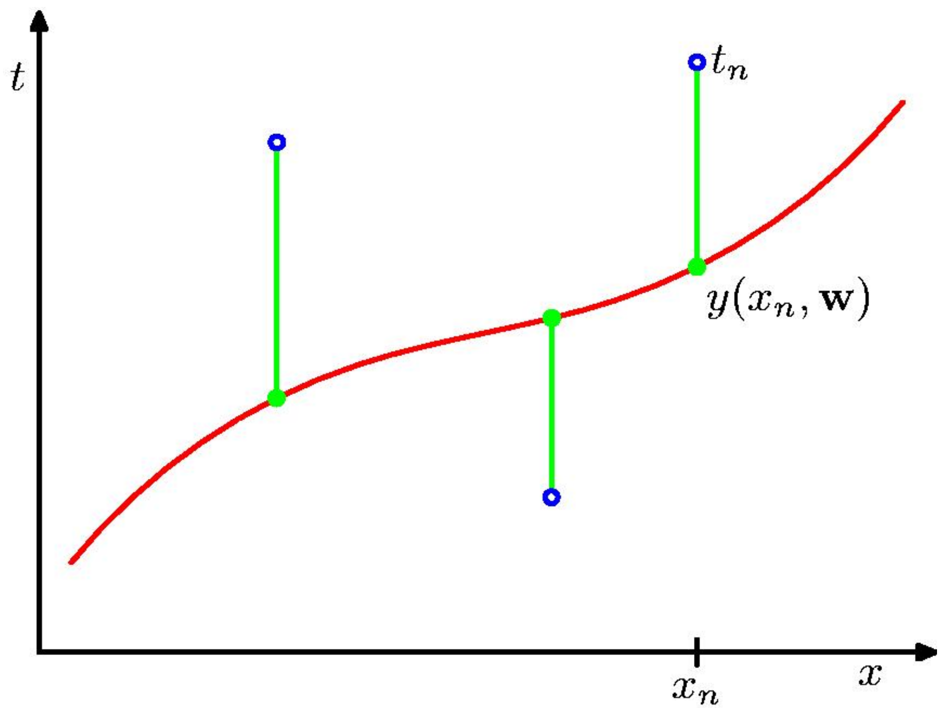


Example: Polynomial Curve Fitting



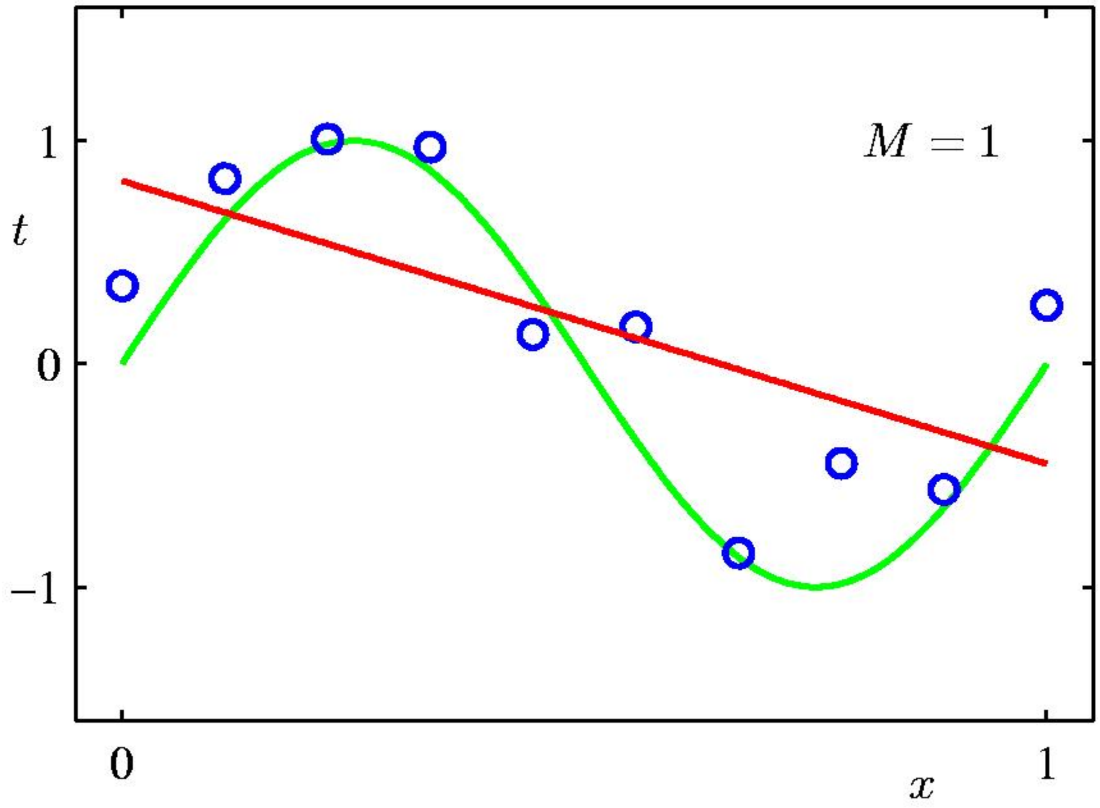
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

Sum-of-Squares Error Function

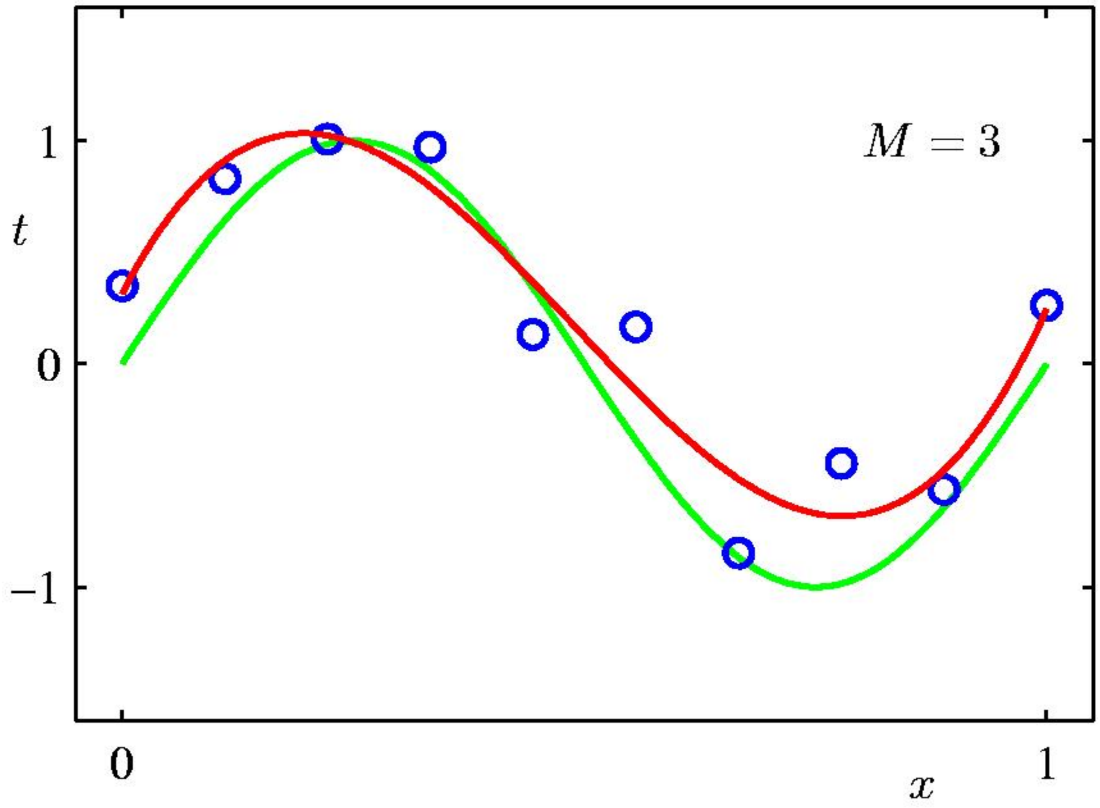


$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2$$

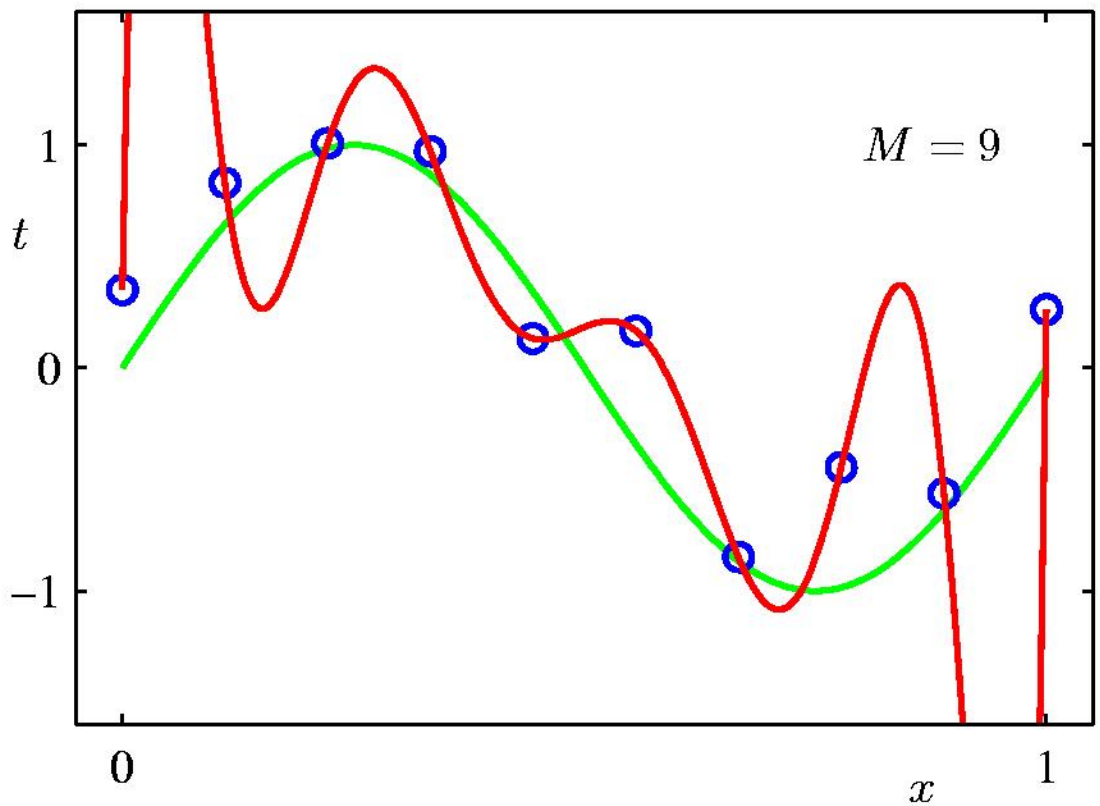
1st Order Polynomial



3rd Order Polynomial



9^{th} Order Polynomial



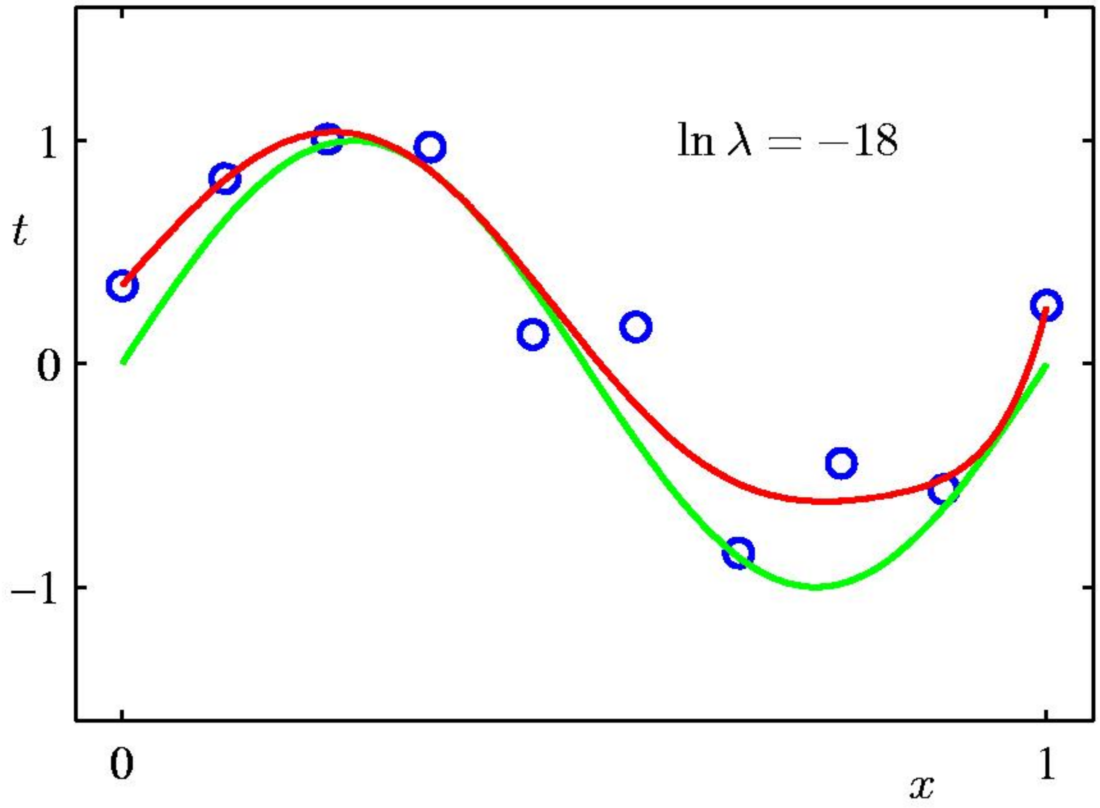
Regularization

- Penalize large coefficient values

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n,\mathbf{w}) - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

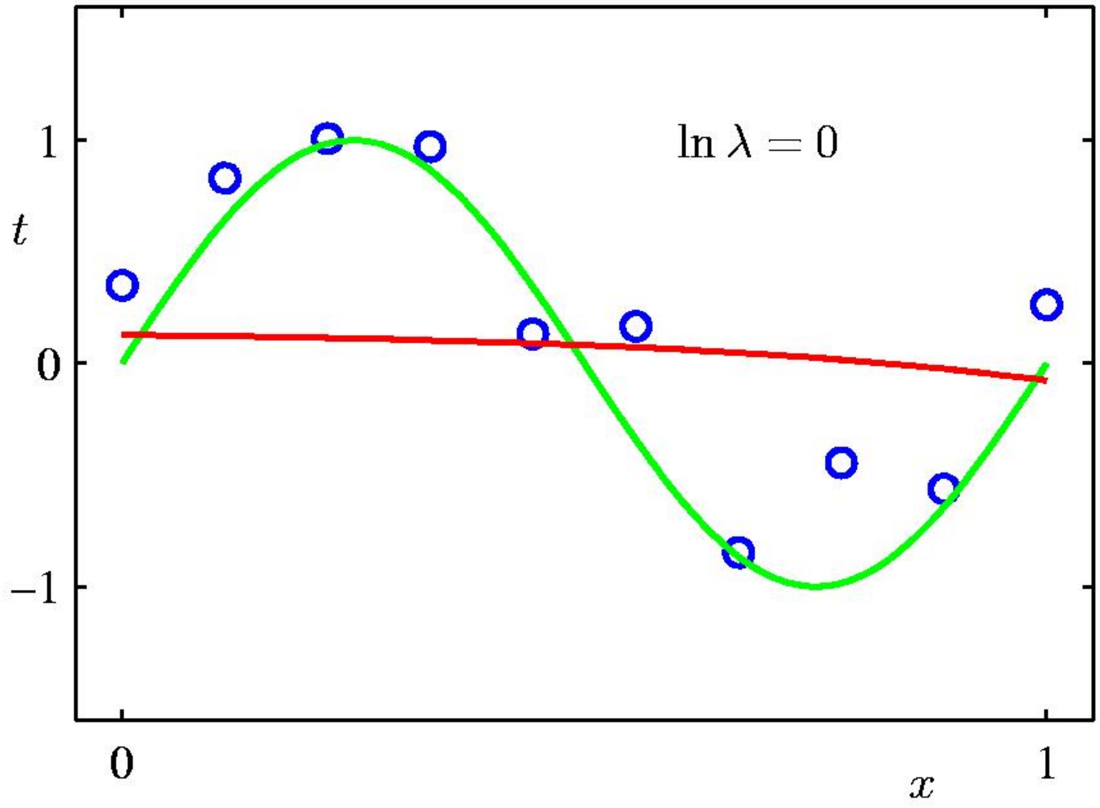
Regularization

9th Order Polynomial



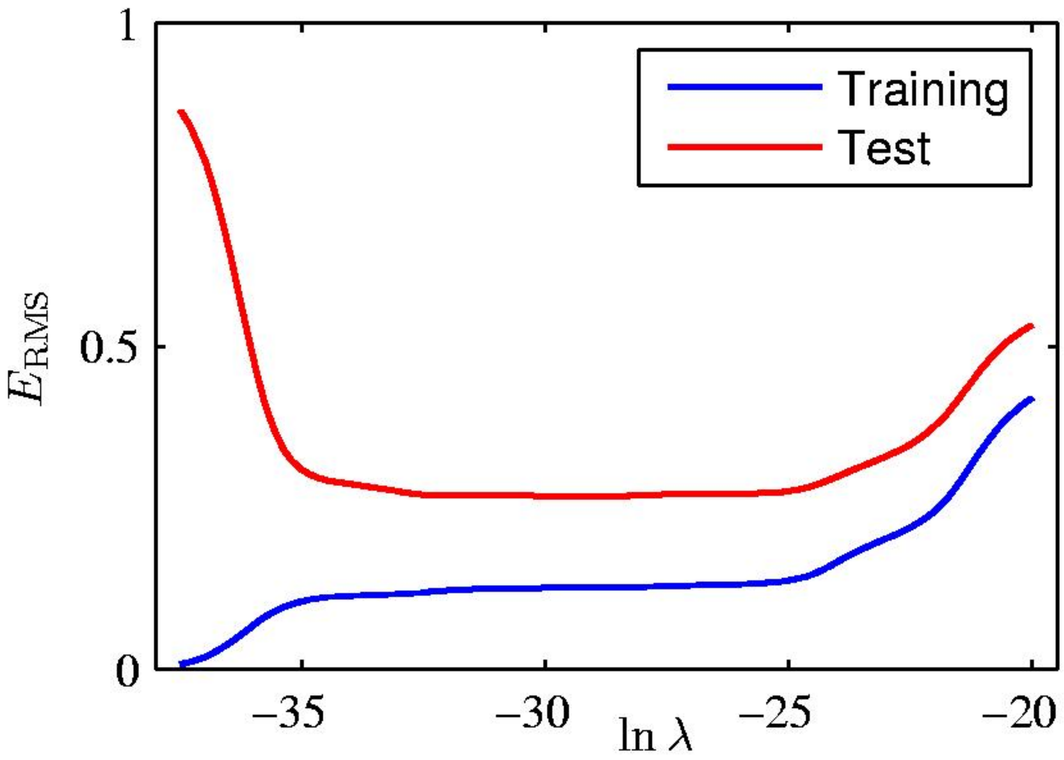
Regularization

9th Order Polynomial



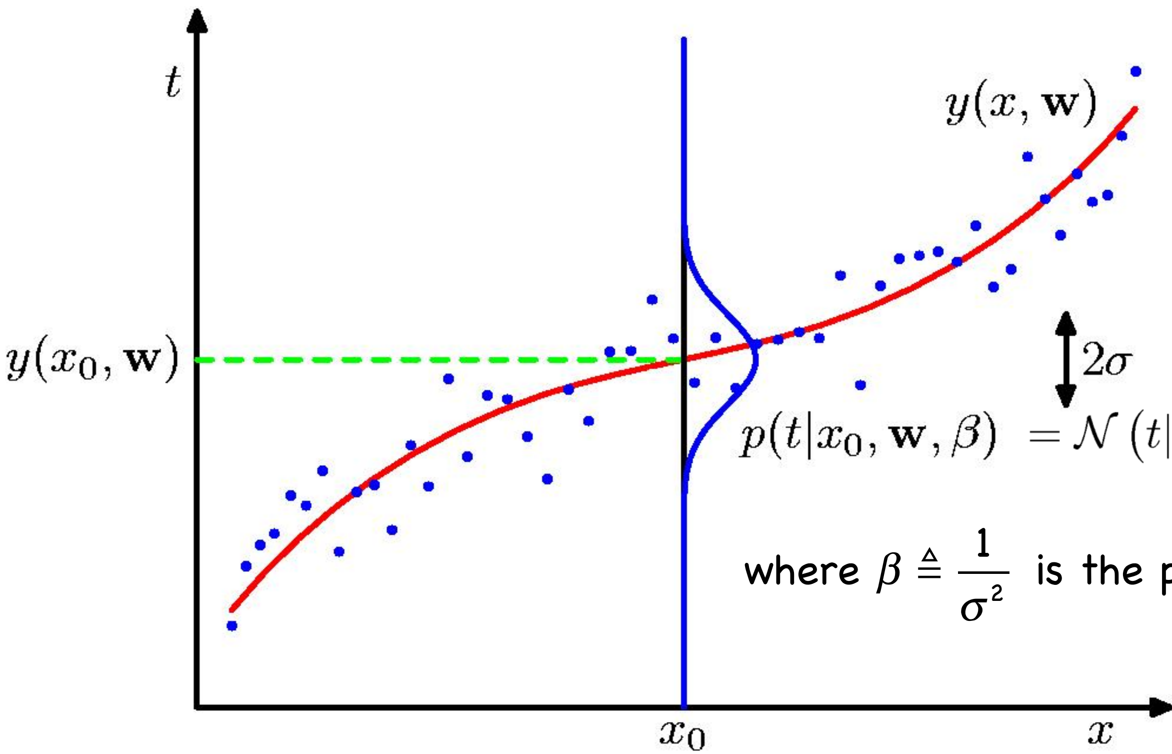
Regularization

9th Order Polynomial



Probabilistic View of Curve Fitting

- Why least squares?
- Model noise (deviation of data from model) as Gaussian i.i.d.



$$p(t|x_0, \mathbf{w}, \beta) = \mathcal{N}\left(t|y(x_0, \mathbf{w}), \beta^{-1}\right)$$

where $\beta \triangleq \dfrac{1}{\sigma^2}$ is the precision of the noise.

Maximum Likelihood

$$p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}\left(t_n | y(x_n, \mathbf{w}), \beta^{-1}\right)$$

- We determine $\boldsymbol{w}_{ML}$ by minimizing the squared error $E(\boldsymbol{w})$.

$$\ln p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \underbrace{-\frac{\beta}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2}_{\beta E(\mathbf{w})} + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi)$$

- **Thus least-squares regression reflects an assumption that the noise is i.i.d. Gaussian.**

Maximum Likelihood

$$p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}\left(t_n | y(x_n, \mathbf{w}), \beta^{-1}\right)$$

- We determine $\boldsymbol{w}_{ML}$ by minimizing the squared error $E(\boldsymbol{w})$.

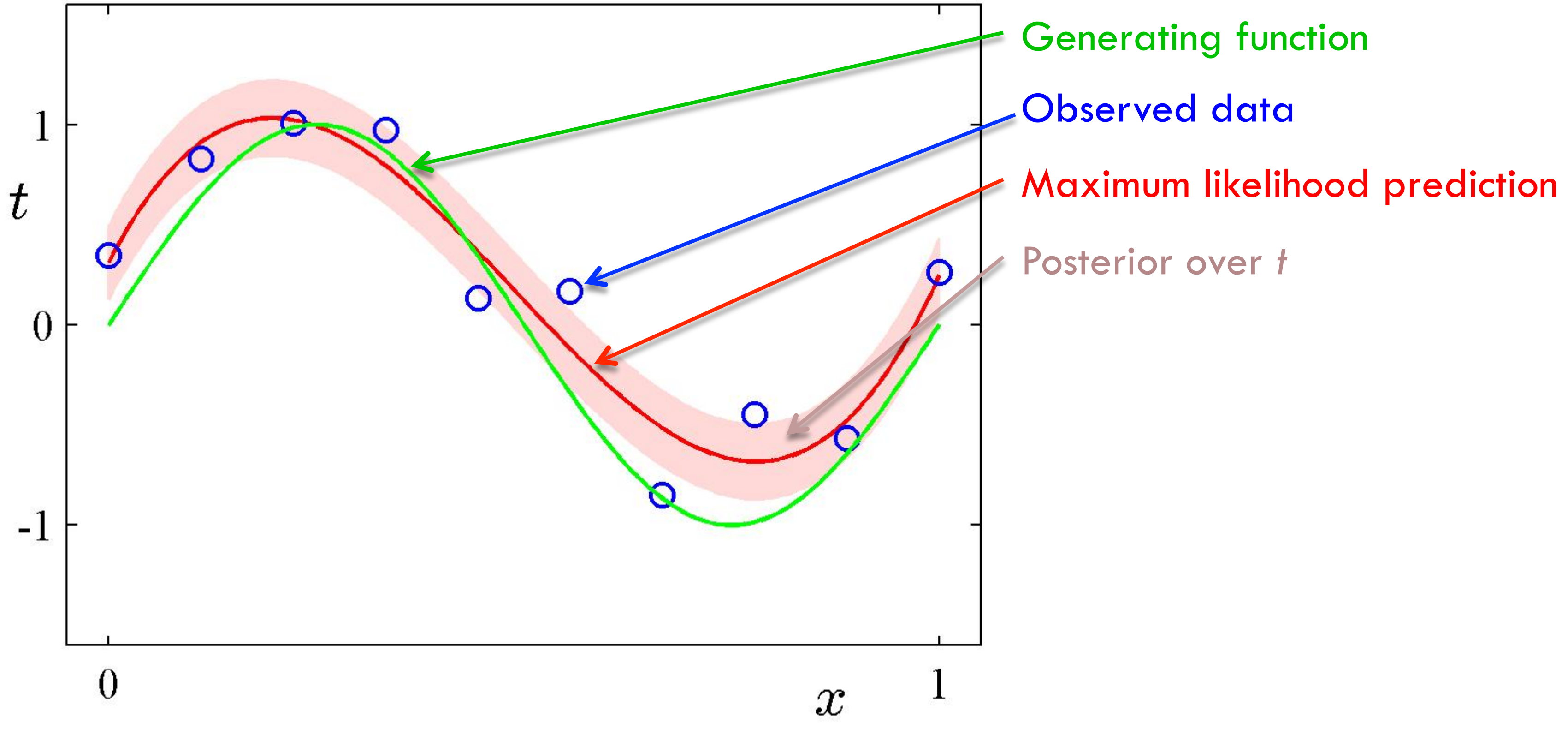
$$\ln p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \underbrace{-\frac{\beta}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2}_{\beta E(\mathbf{w})} + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi)$$

- Now given $\boldsymbol{w}_{ML}$, we can estimate the variance of the noise:

$$\frac{1}{\beta_{\mathrm{ML}}} = \frac{1}{N} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}_{\mathrm{ML}}) - t_n\}^2$$

Predictive Distribution

$$p(t|x, \mathbf{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}}) = \mathcal{N}\left(t|y(x, \mathbf{w}_{\mathrm{ML}}), \beta_{\mathrm{ML}}^{-1}\right)$$



MAP: A Step towards Bayes

- Prior knowledge about probable values of **w** can be incorporated into the regression:

$$p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}) = \left(\frac{\alpha}{2\pi}\right)^{(M+1)/2} \exp\left\{-\frac{\alpha}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}\right\}$$

- Now the posterior over **w** is proportional to the product of the likelihood times the prior:

$$p(\mathbf{w}|\mathbf{x}, \mathbf{t}, \alpha, \beta) \propto p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta)p(\mathbf{w}|\alpha)$$

- The result is to introduce a new quadratic term in **w** into the error function to be minimized:

$$\beta\widetilde{E}(\mathbf{w}) = \frac{\beta}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{\alpha}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}$$

- **Thus regularized (ridge) regression reflects a 0-mean isotropic Gaussian prior on the weights.**

Linear Regression Topics

- What is linear regression?
- Example: polynomial curve fitting
- **Other basis families**
- Solving linear regression problems
- Regularized regression
- Multiple linear regression
- Bayesian linear regression

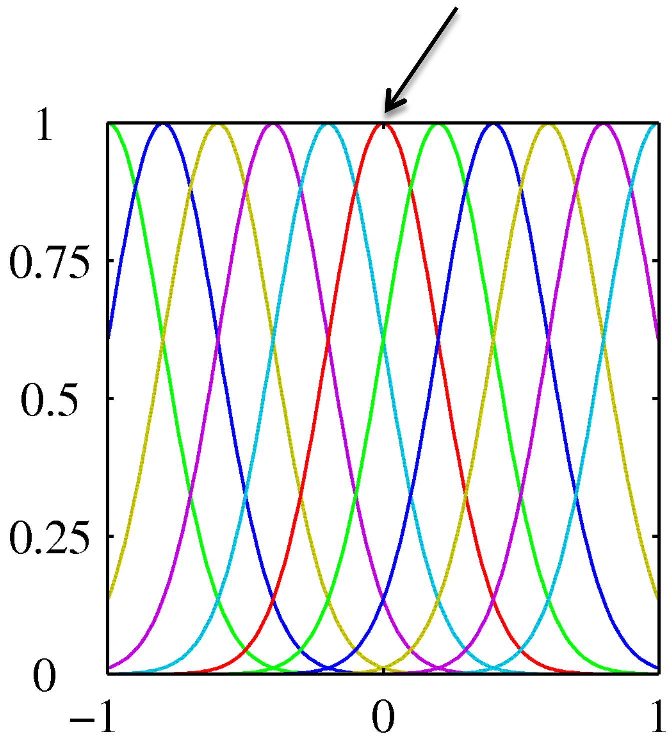
Gaussian Bases

- Gaussian basis functions:

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

- These are local:
  - a small change in x affects only nearby basis functions.
  - a small change in a basis function affects y only for nearby x.
  - μ_j and s control location and scale (width).

Think of these as interpolation functions.



Linear Regression Topics

- What is linear regression?
- Example: polynomial curve fitting
- Other basis families
- **Solving linear regression problems**
- Regularized regression
- Multiple linear regression
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Maximum Likelihood and Linear Least Squares

- 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,

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

- where

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

Maximum Likelihood and Linear Least Squares

- 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 Linear Least Squares

- 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

- Computing the gradient and setting it to zero yields

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

- Solving for **w**, we get

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

- where

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

Linear Regression Topics

- What is linear regression?
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- **Regularized regression**
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- Bayesian linear regression

Regularized Least Squares

- Consider the error function:

$$E_D(\mathbf{w}) + \lambda E_W(\mathbf{w})$$

Data term + Regularization term

λ is called the regularization coefficient.

- With the sum-of-squares error function and a quadratic regularizer, we get

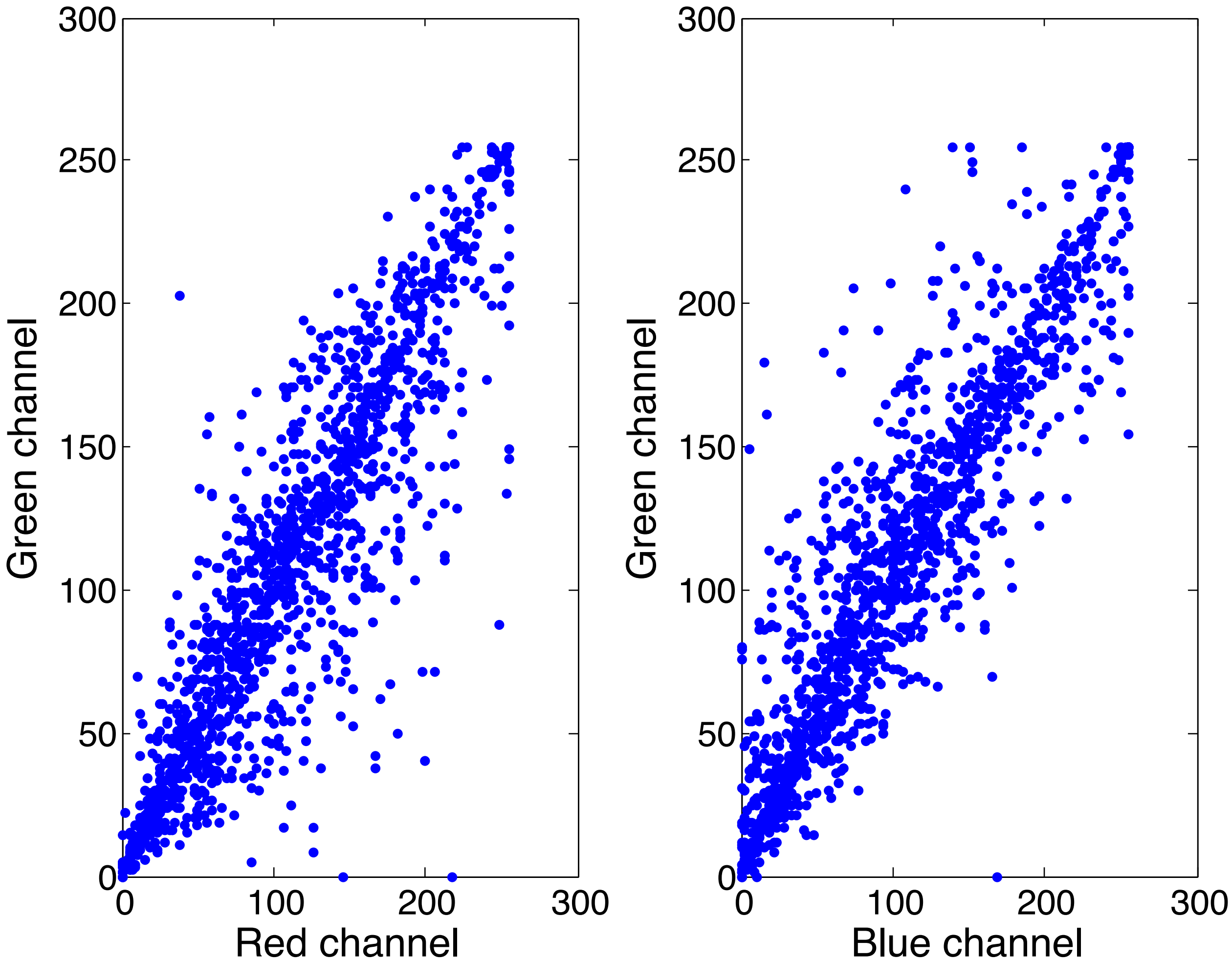
$$\frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n)\}^2 + \frac{\lambda}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}$$

- which is minimized by

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

Thus the name 'ridge regression'

Application: Colour Restoration



Application: Colour Restoration

Original Image

Red and Blue Channels Only

Predicted Image

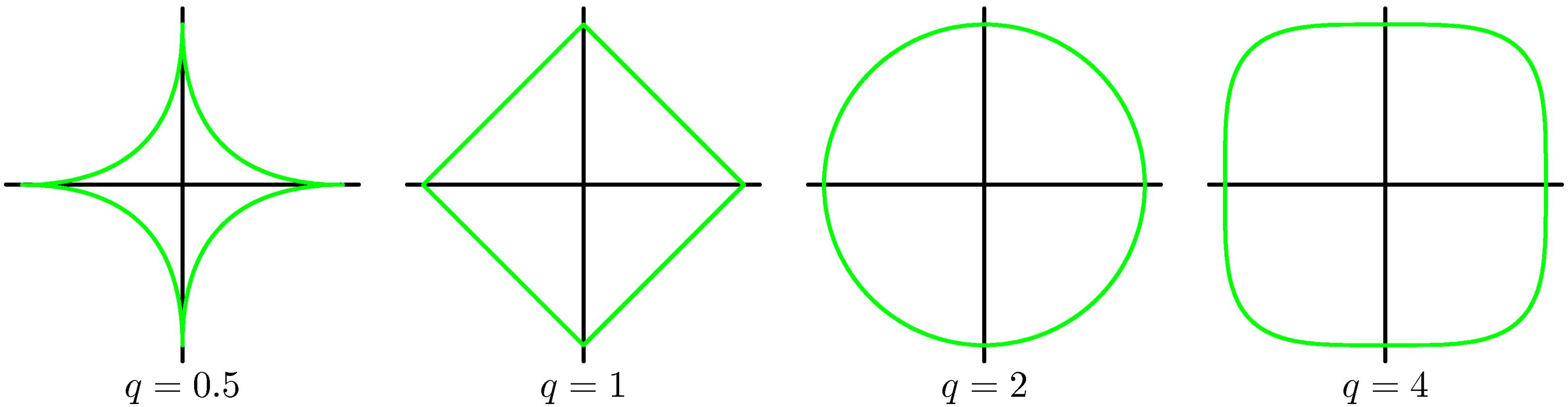
Remove Green

Restore Green

Regularized Least Squares

- A more general regularizer:

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



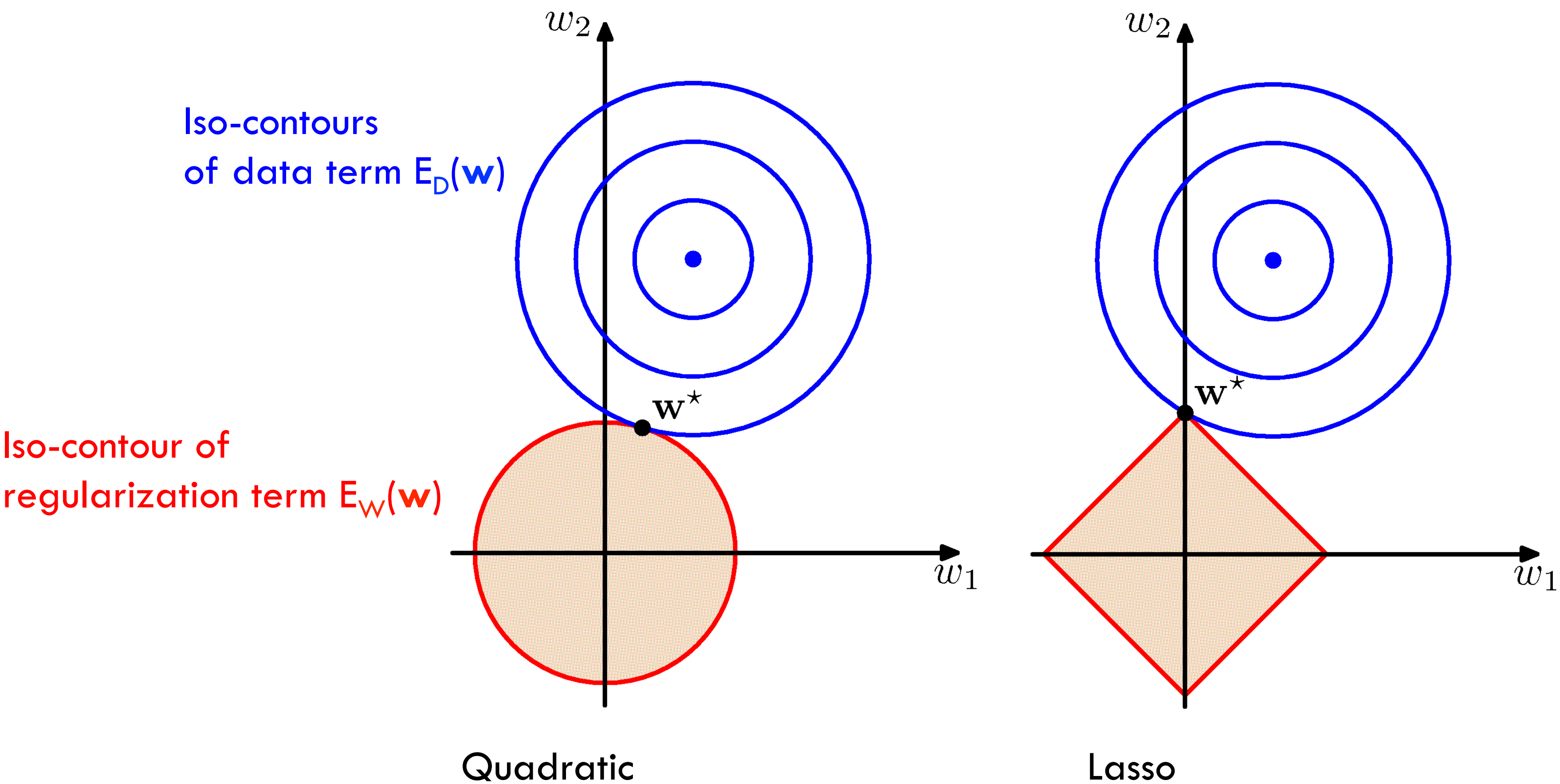
Lasso

Quadratic

(Least absolute shrinkage and selection operator)

Regularized Least Squares

- Lasso generates sparse solutions.



Solving Regularized Systems

- Quadratic regularization has the advantage that the solution is closed form.
- Non-quadratic regularizers generally do not have closed form solutions
- Lasso can be framed as minimizing a quadratic error with linear constraints, and thus represents a convex optimization problem that can be solved by quadratic programming or other convex optimization methods.
- We will discuss quadratic programming when we cover SVMs

Linear Regression Topics

- What is linear regression?
- Example: polynomial curve fitting
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- Regularized regression
- **Multiple linear regression**
- Bayesian linear regression

Multiple Outputs

- Analogous to the single output case we have:

$$\begin{aligned} p(\mathbf{t}|\mathbf{x}, \mathbf{W}, \beta) &= \mathcal{N}(\mathbf{t}|\mathbf{y}(\mathbf{W}, \mathbf{x}), \beta^{-1}\mathbf{I}) \\ &= \mathcal{N}(\mathbf{t}|\mathbf{W}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}), \beta^{-1}\mathbf{I}). \end{aligned}$$

- Given observed inputs $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, and targets $\mathbf{T} = [\mathbf{t}_1, \ldots, \mathbf{t}_N]^{\mathrm{T}}$

  we obtain the log likelihood function

$$\begin{aligned} \ln p(\mathbf{T}|\mathbf{X}, \mathbf{W}, \beta) &= \sum_{n=1}^{N} \ln \mathcal{N}(\mathbf{t}_n|\mathbf{W}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\mathbf{I}) \\ &= \frac{NK}{2} \ln\left(\frac{\beta}{2\pi}\right) - \frac{\beta}{2}\sum_{n=1}^{N}\left\|\mathbf{t}_n - \mathbf{W}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\right\|^2. \end{aligned}$$

Multiple Outputs

- Maximizing with respect to W, we obtain

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

- If we consider a single target variable, t_k, we see that

$$\mathbf{w}_k = \left(\mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^{\mathrm{T}}\mathbf{t}_k = \mathbf{\Phi}^{\dagger}\mathbf{t}_k$$

- where $\mathbf{t}_k = [t_{1k}, \ldots, t_{Nk}]^{\mathrm{T}}$, which is identical with the single output case.

Some Useful MATLAB Functions

- polyfit
  - Least-squares fit of a polynomial of specified order to given data
- regress
  - More general function that computes linear weights for least-squares fit

Linear Regression Topics

- What is linear regression?
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- Multiple linear regression
- **Bayesian linear regression**

Bayesian Linear Regression

Rev. Thomas Bayes, 1702 - 1761

Bayesian Linear Regression

- In least-squares, we determine the weights **w** that minimize the least squared error between the model and the training data.
- This can result in overlearning!
- Overlearning can be reduced by adding a regularizing term to the error function being minimized.
- Under specific conditions this is equivalent to a Bayesian approach, where we specify a prior distribution over the weight vector.

Bayesian Linear Regression

- Define a conjugate prior over **w**:

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

- Combining this with the likelihood function and matching terms, we obtain

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

- where

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

Bayesian Linear Regression

- A common choice for the prior is

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

- for which

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

- Thus $\boldsymbol{m}_N$ represents the ridge regression solution with

$$\lambda = \alpha / \beta$$

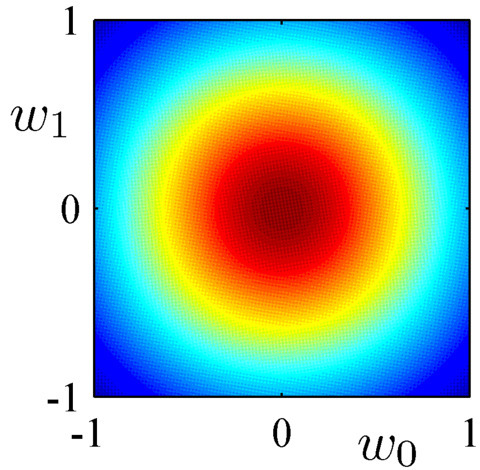
- Next we consider an example …

Bayesian Linear Regression

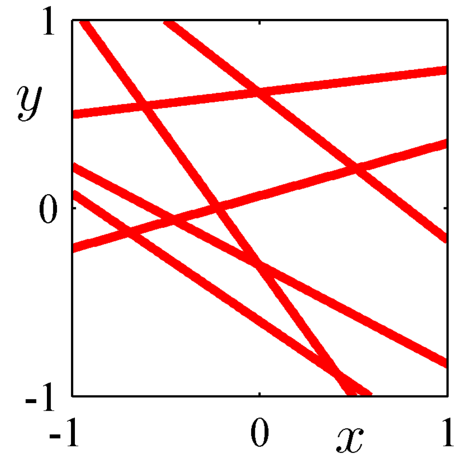
Example: fitting a straight line

0 data points observed

Prior

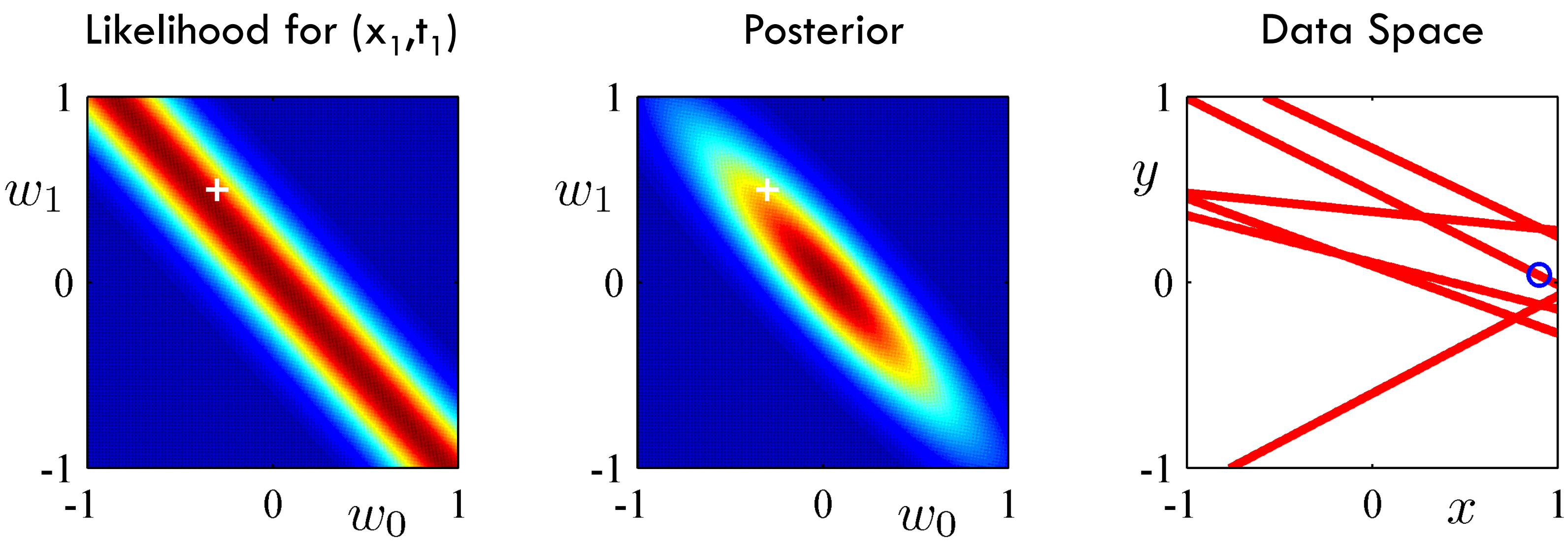


Data Space



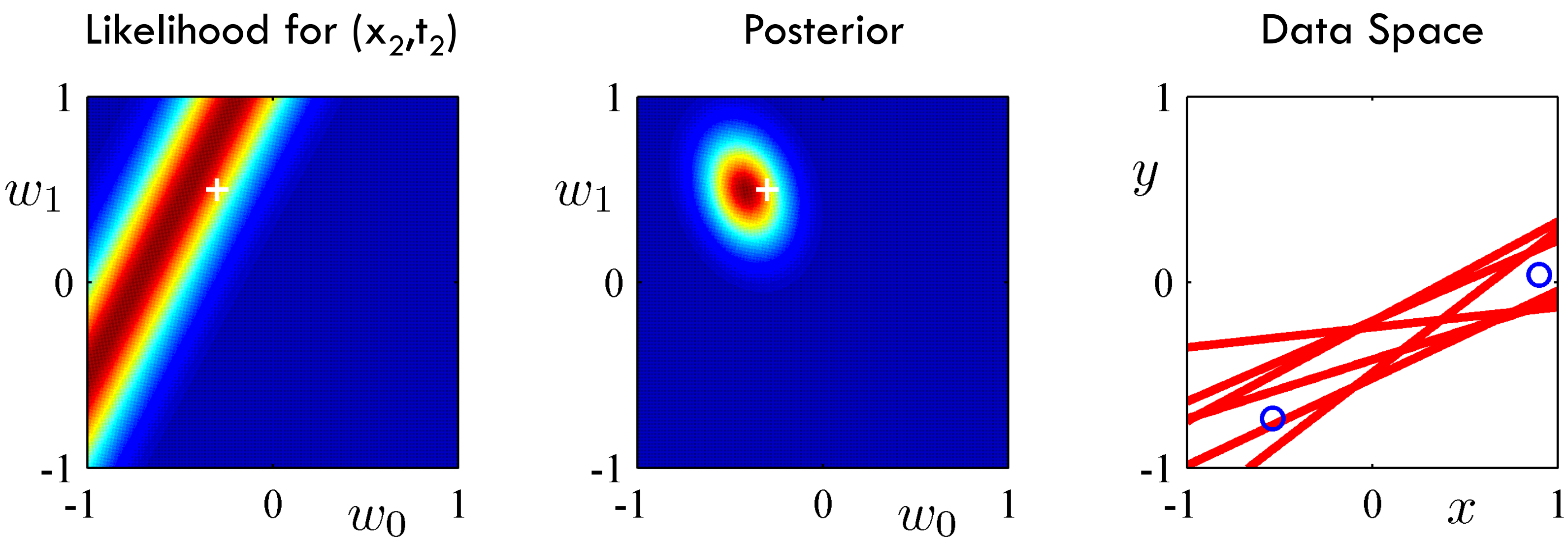
Bayesian Linear Regression

1 data point observed



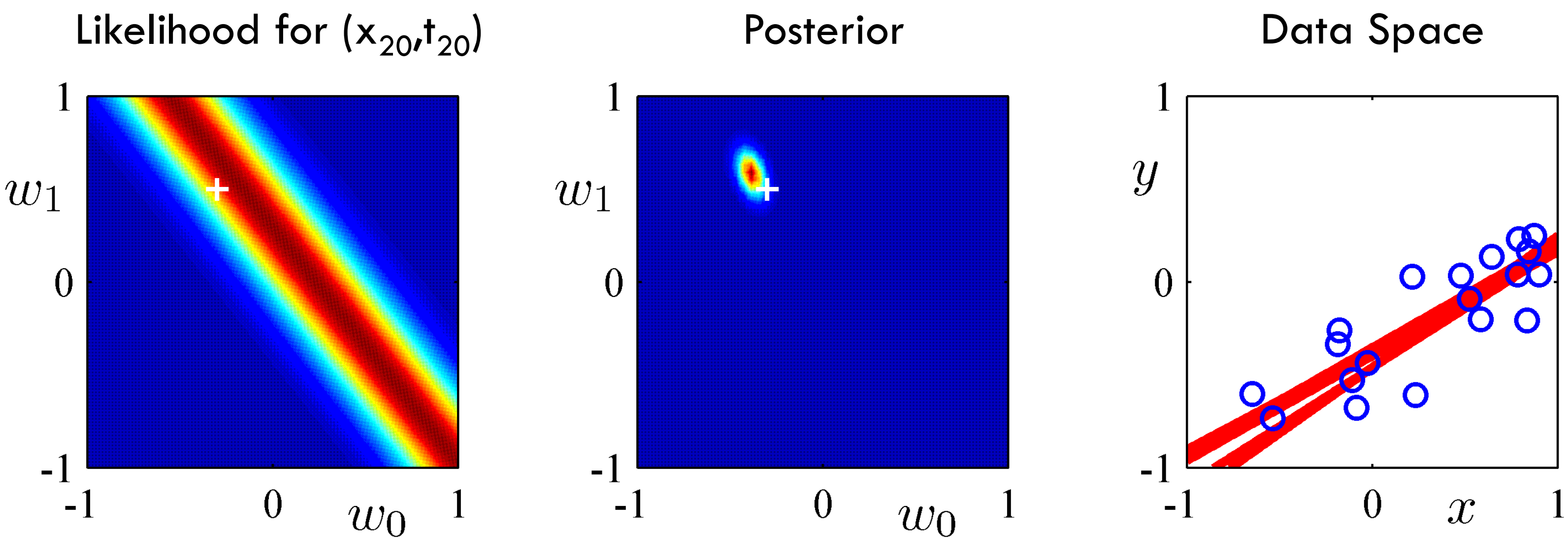
Bayesian Linear Regression

2 data points observed



Bayesian Linear Regression

20 data points observed



Bayesian Prediction

- In least-squares, or regularized least-squares, we determine specific weights w that allow us to predict a specific value y(**x**,**w**) for every observed input **x**.
- However, our estimate of the weight vector **w** will never be perfect! This will introduce error into our prediction.
- In Bayesian prediction, we model the posterior distribution over our predictions, taking into account our uncertainty in model parameters.

Predictive Distribution

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

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

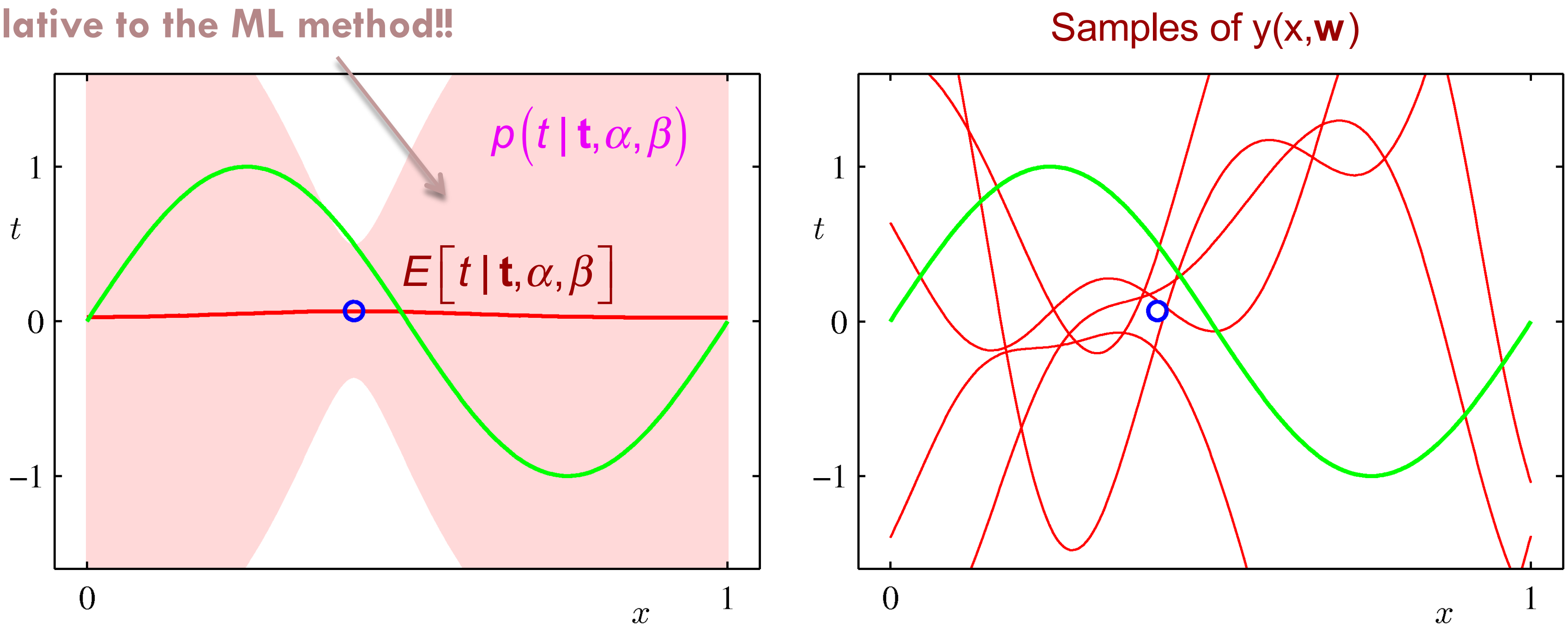
- where

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

Predictive Distribution

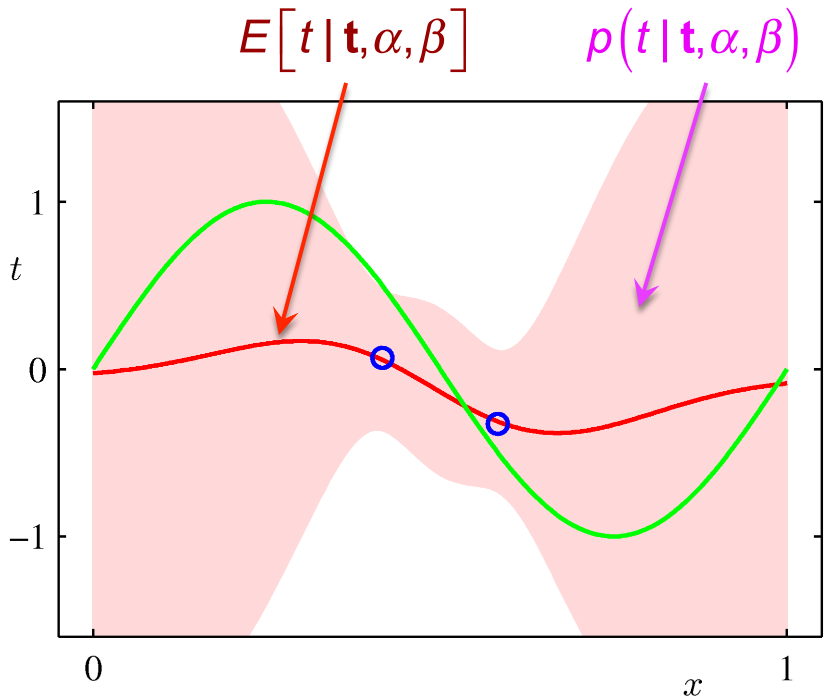
- Example: Sinusoidal data, 9 Gaussian basis functions, 1 data point

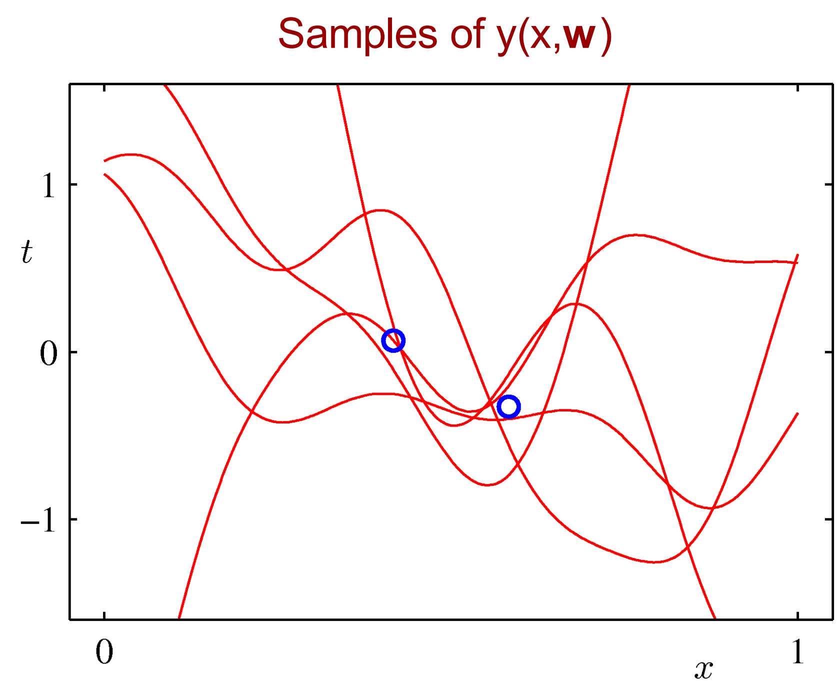
Notice how much bigger our uncertainty is relative to the ML method!!



Predictive Distribution

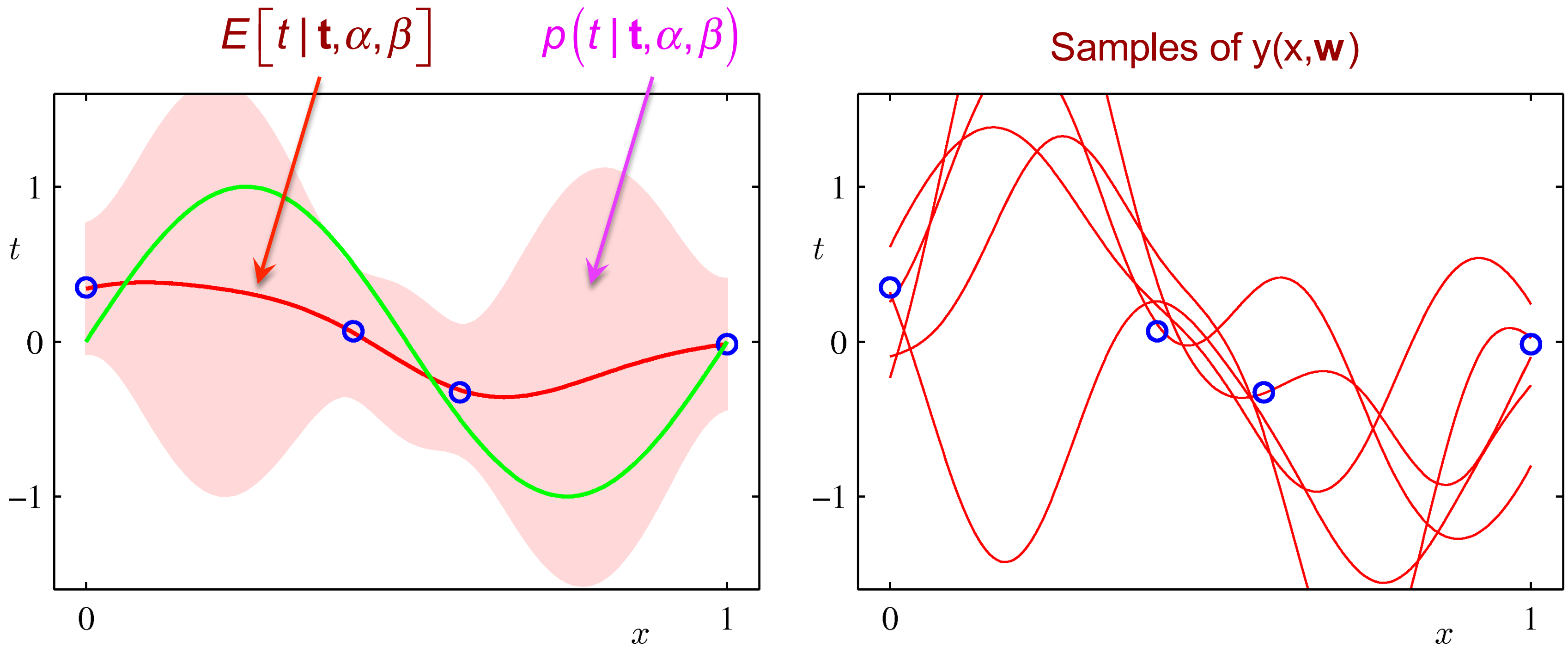
- Example: Sinusoidal data, 9 Gaussian basis functions, 2 data points





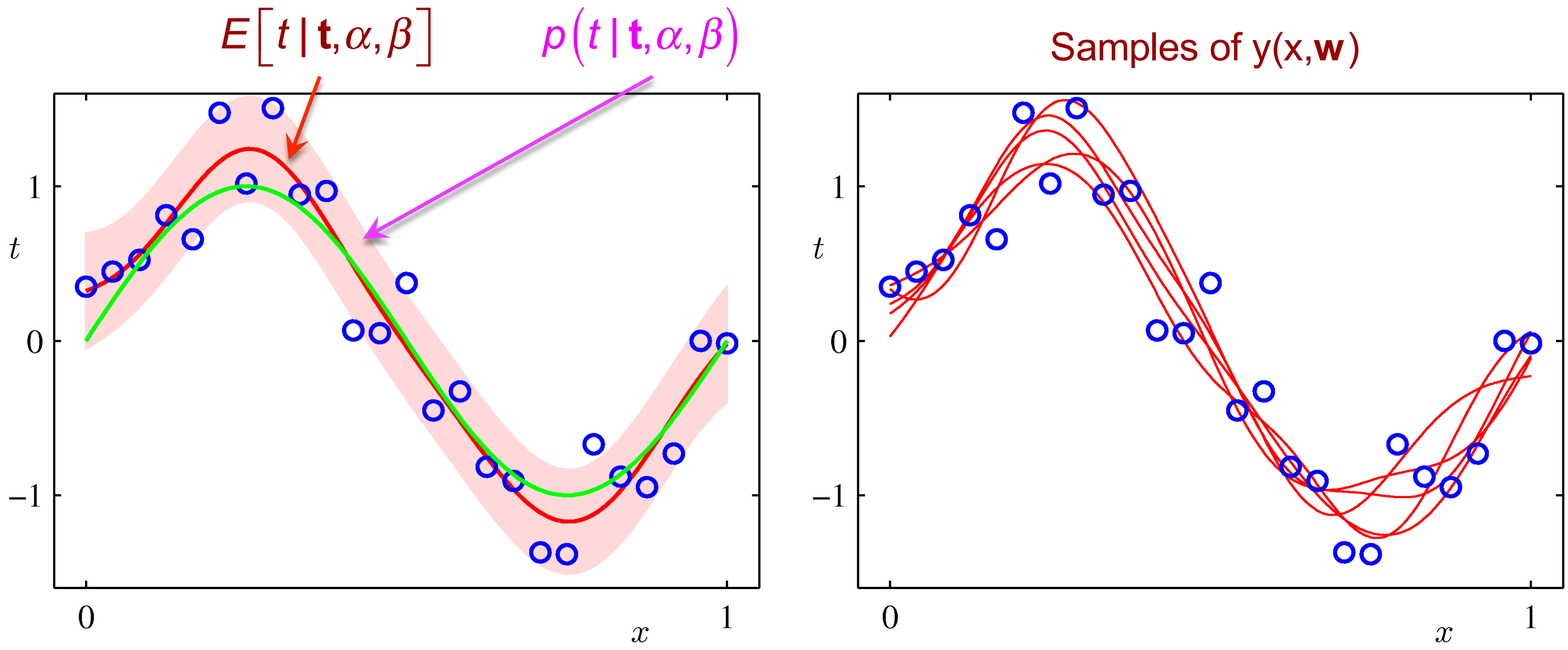
Predictive Distribution

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



Predictive Distribution

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



Linear Regression Topics

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- Example: polynomial curve fitting
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