CS60050: Machine Learning

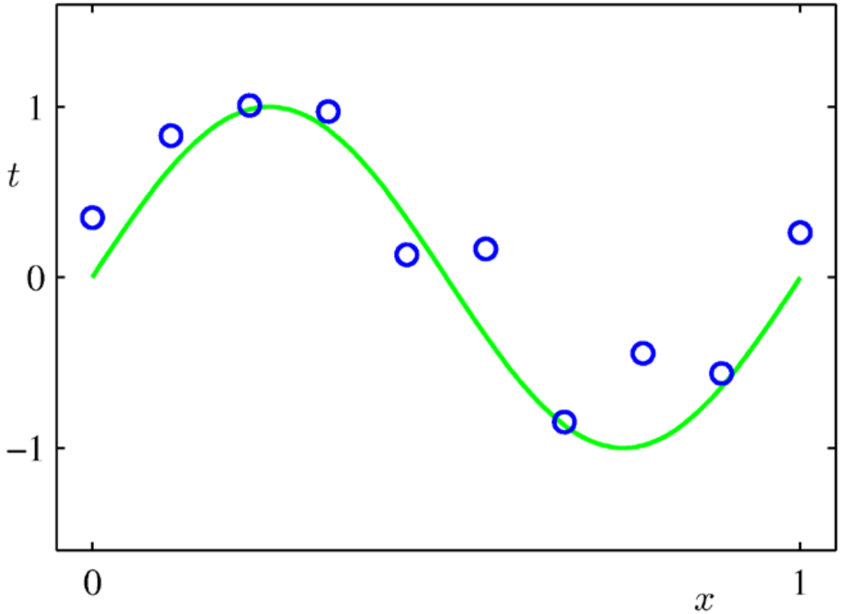
Sourangshu Bhattacharya

Some slides are taken from Christopher Bishop and Geoffrey Hinton's courses

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 $\text{Á}_j(\text{x})$ are known as *basis functions*.

Typically, $\text{Á}_0(\mathrm{x}) = 1$, so that w_0 acts as a bias.

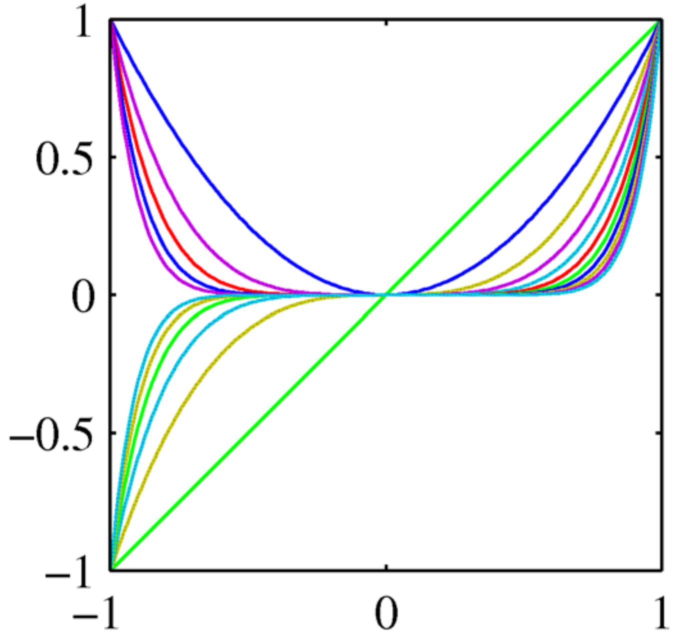
In the simplest case, we use linear basis functions : $\text{Á}_d(\mathrm{x}) = \mathrm{x}_d$.

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.

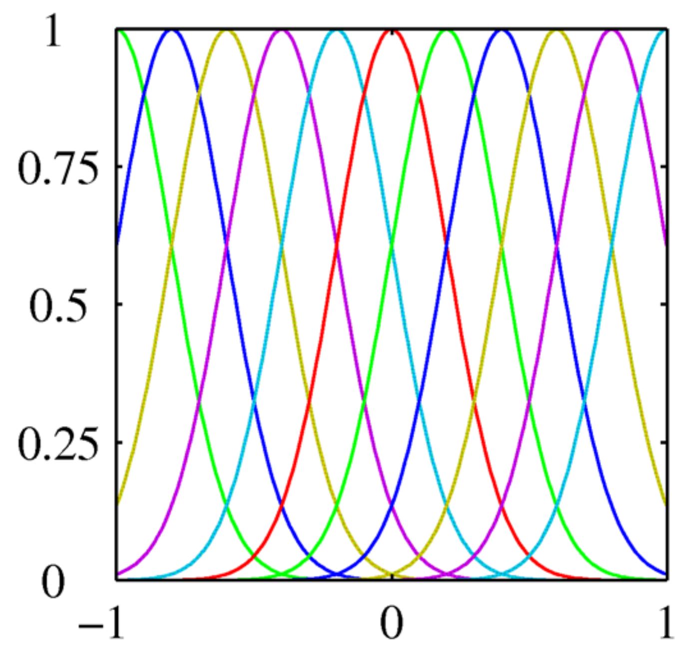


Linear Basis Function Models (4)

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. $^{1}{}_{j}$ and s control location and scale (width).



Linear Basis Function Models (5)

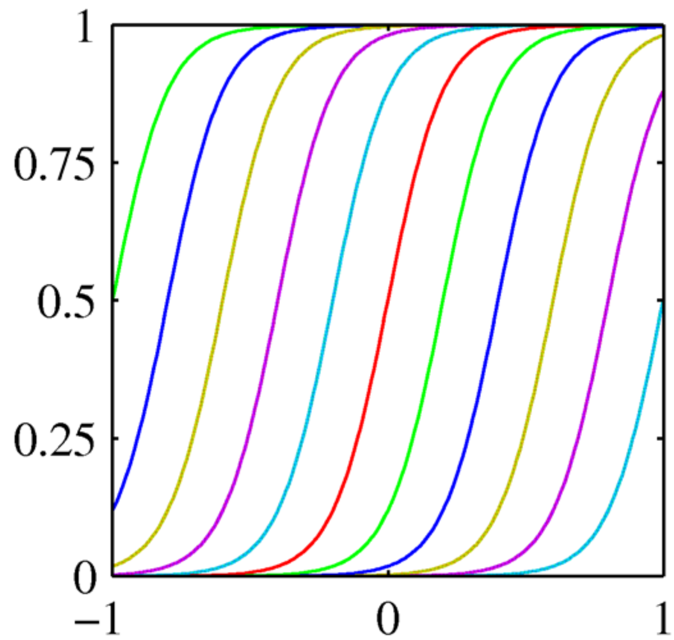
Sigmoidal basis functions:

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

where

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

Also these are local; a small change in x only affect nearby basis functions. $^{1}{}_{j}$ and s control location and scale (slope).

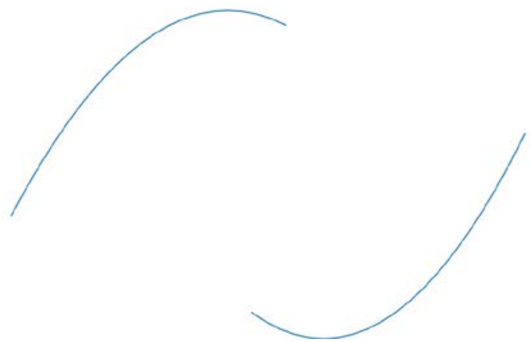


Least Squares Estimation

A a polynomial curve is represented by the parameters w.

$f(x) = x - x^2$

$f(x) = x + x^2$



Error (loss) function for a given parameter:

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

Estimate $w^* = \min_w E(w)$

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

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

Solving for $\mathbf{w}$, we get

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

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

where

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

Geometry of Least Squares

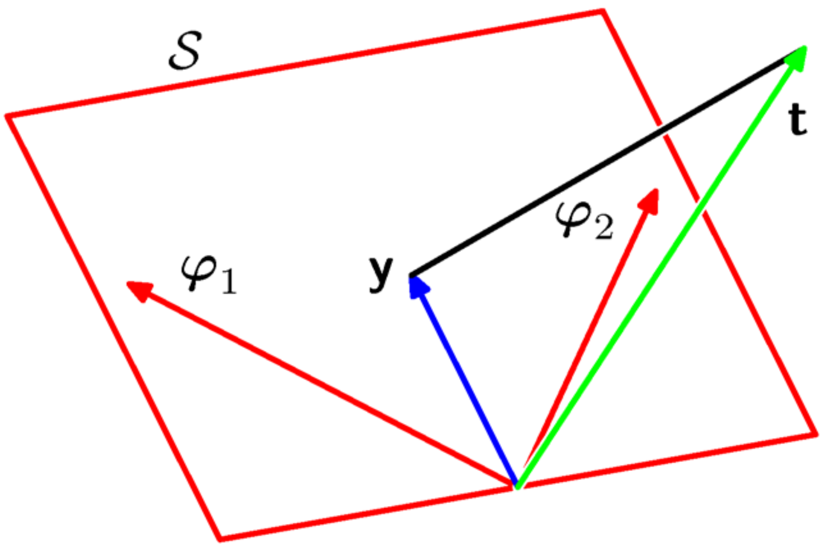
Consider

$$\mathbf{y} = \mathbf{\Phi}\mathbf{w}_{\mathrm{ML}} = [\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_M]\,\mathbf{w}_{\mathrm{ML}}.$$

$$\mathbf{y} \in \mathcal{S} \subseteq \mathcal{T} \qquad \mathbf{t} \in \mathcal{T}$$

N-dimensional

M-dimensional



S is spanned by $\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_M$.

w_{ML} minimizes the distance between t and its orthogonal projection on S, i.e. y.

Normal Equations

$$(\mathbf{A}^T\mathbf{A})\widehat{\beta} = \mathbf{A}^T\mathbf{Y}$$

p xp   p x1   p x1

If $(\mathbf{A}^T\mathbf{A})$ is invertible,

$$\boxed{\widehat{\beta} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{Y} \qquad \widehat{f}_n^L(X) = X\widehat{\beta}}$$

When is $(\mathbf{A}^T\mathbf{A})$ invertible ?
Recall: Full rank matrices are invertible.

What if $(\mathbf{A}^T\mathbf{A})$ is not invertible ?

Gradient Descent

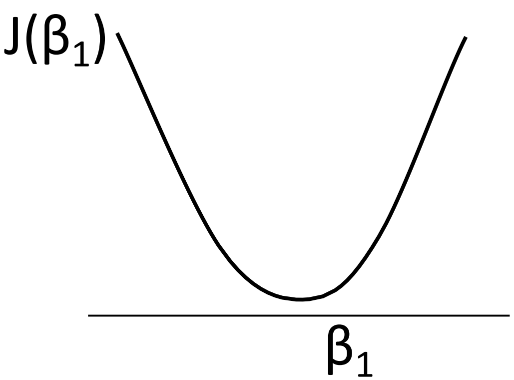
Even when $(\mathbf{A}^T\mathbf{A})$ is invertible, might be computationally expensive if **A** is huge.

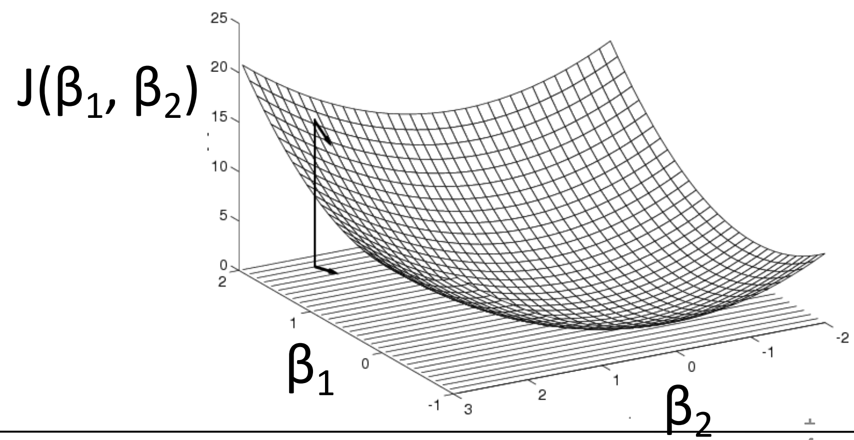
$$\widehat{\beta} = \arg\min_{\beta} \frac{1}{n}(\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y}) = \arg\min_{\beta} J(\beta)$$

Treat as optimization problem

<u>Observation:</u> J(β) is convex in β.

How to find the minimizer?





Gradient Descent

Even when $(\mathbf{A}^T\mathbf{A})$ is invertible, might be computationally expensive if **A** is huge.

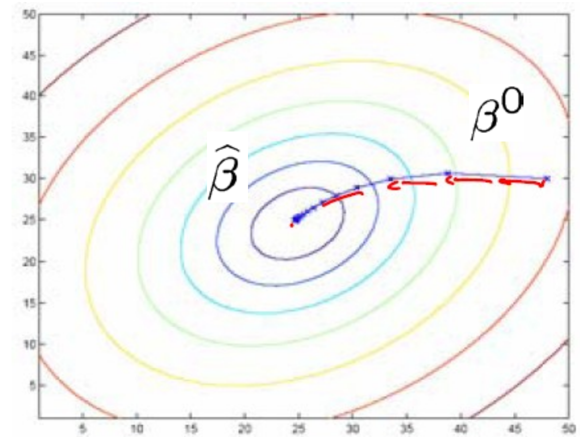
$$\widehat{\beta} = \arg\min_{\beta} \frac{1}{n}(\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y}) = \arg\min_{\beta} J(\beta)$$

Since J(β) is convex, move along negative of gradient

Initialize: β^0

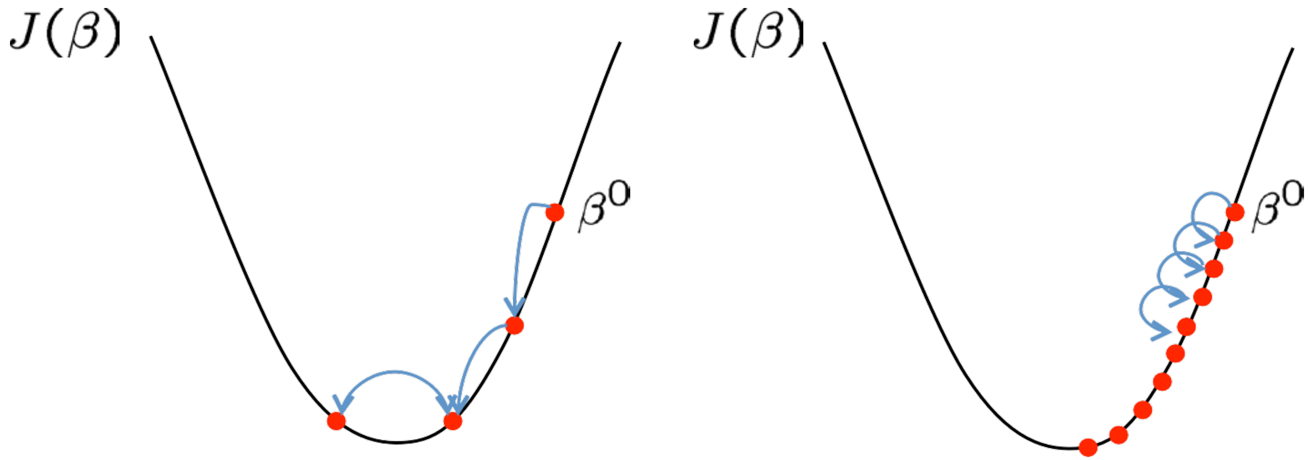
step size

Update:
$$\beta^{t+1} = \beta^t - \frac{\alpha}{2}\frac{\partial J(\beta)}{\partial \beta}\Big|_t = \beta^t - \alpha\, \mathbf{A}^T \underbrace{(\mathbf{A}\beta^t - Y)}_{0 \text{ if } \widehat{\beta} = \beta^t}$$



Stop: when some criterion met e.g. fixed # iterations, or $\frac{\partial J(\beta)}{\partial \beta}\Big|_{\beta^t} < \varepsilon$.

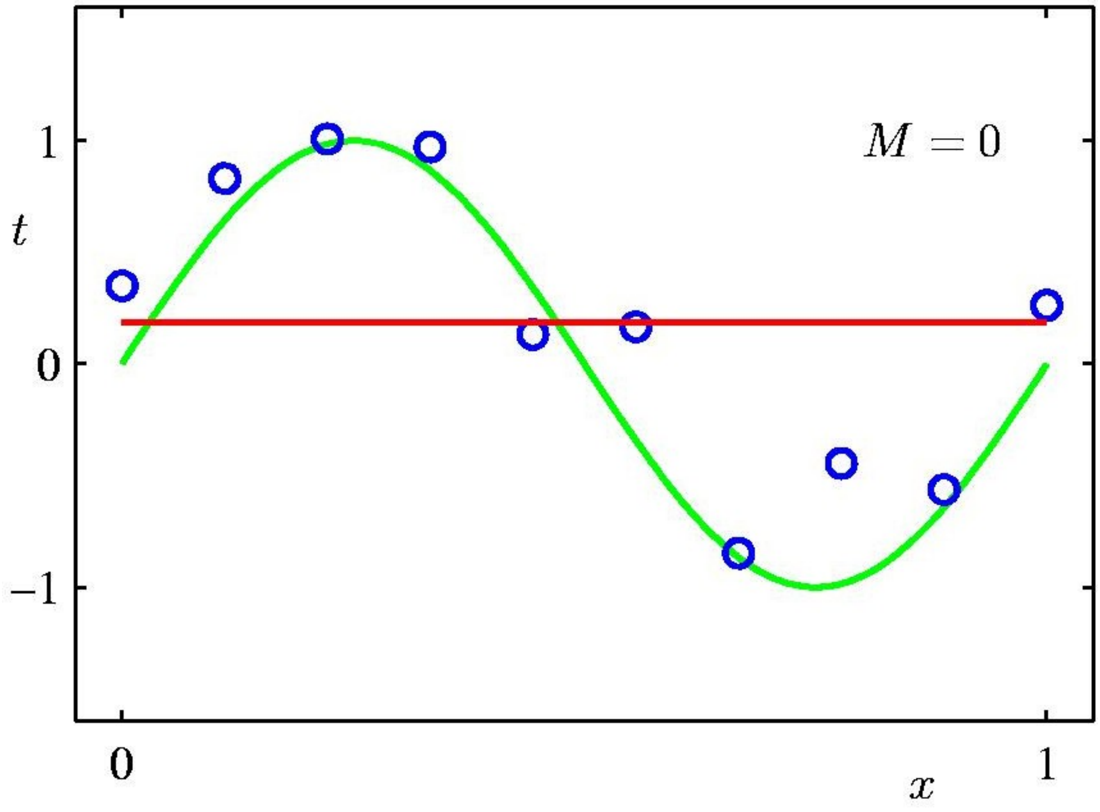
Effect of step-size α



Large α => Fast convergence but larger residual error
Also possible oscillations

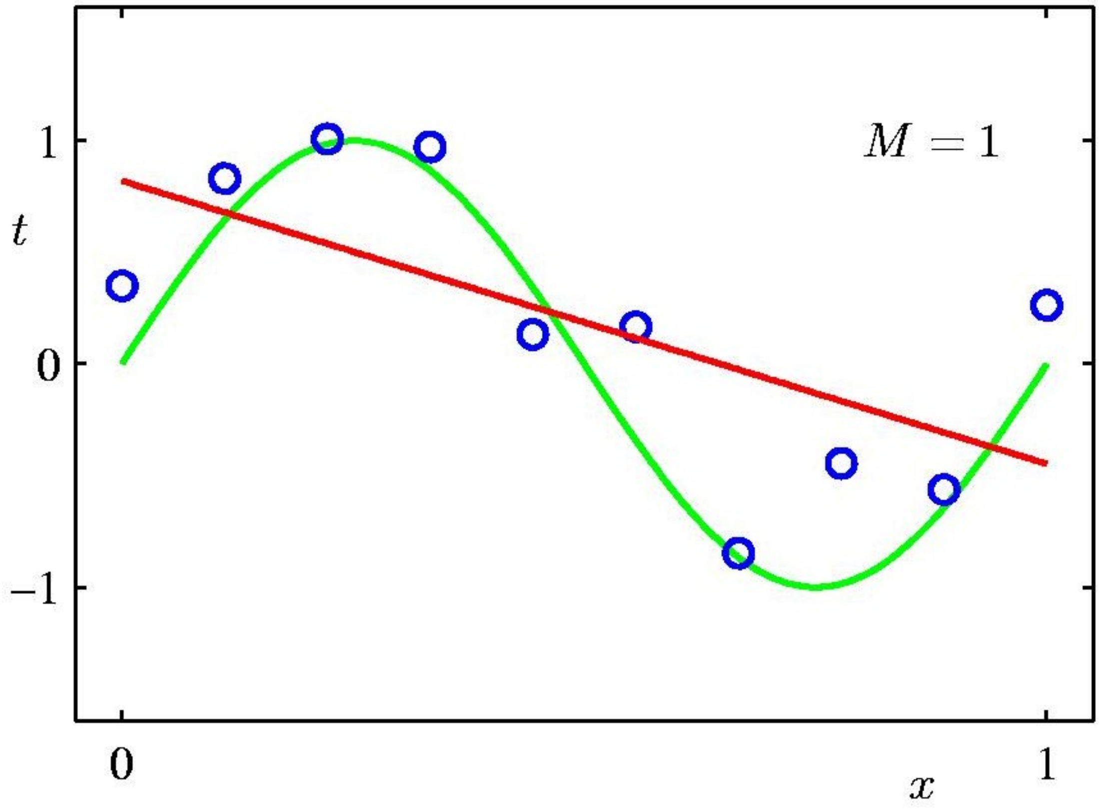
Small α => Slow convergence but small residual error

0^{th} Order Polynomial

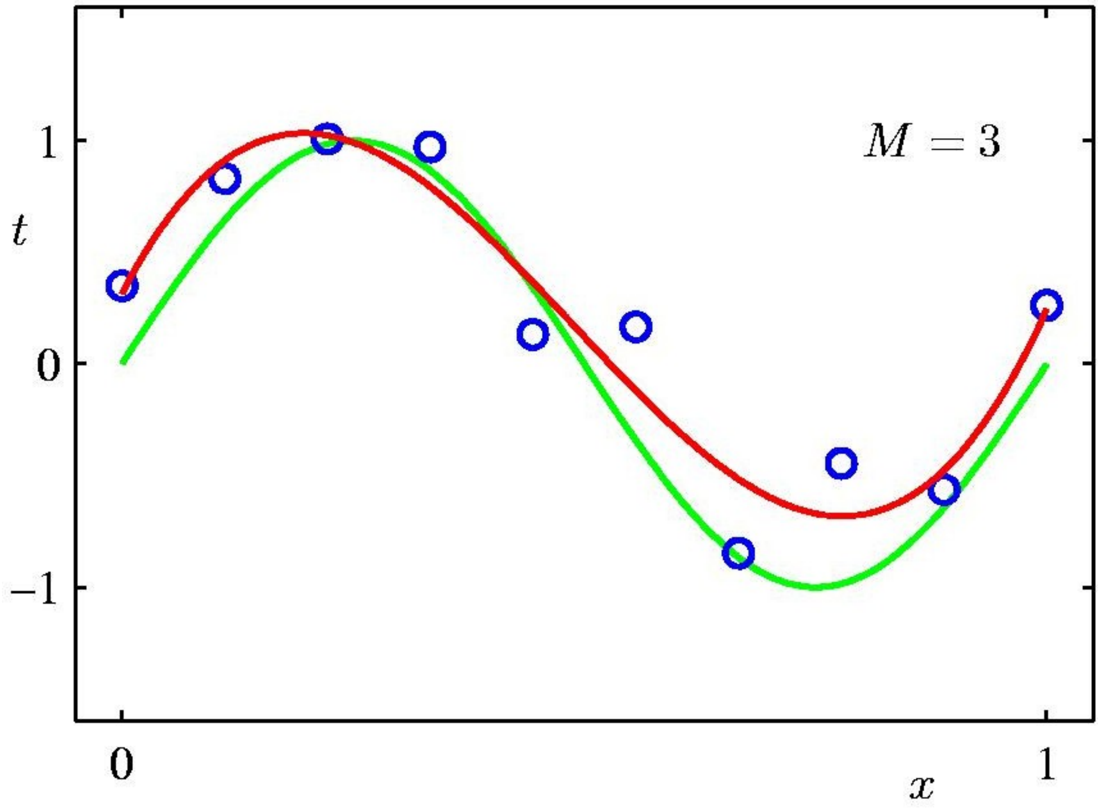


n=10

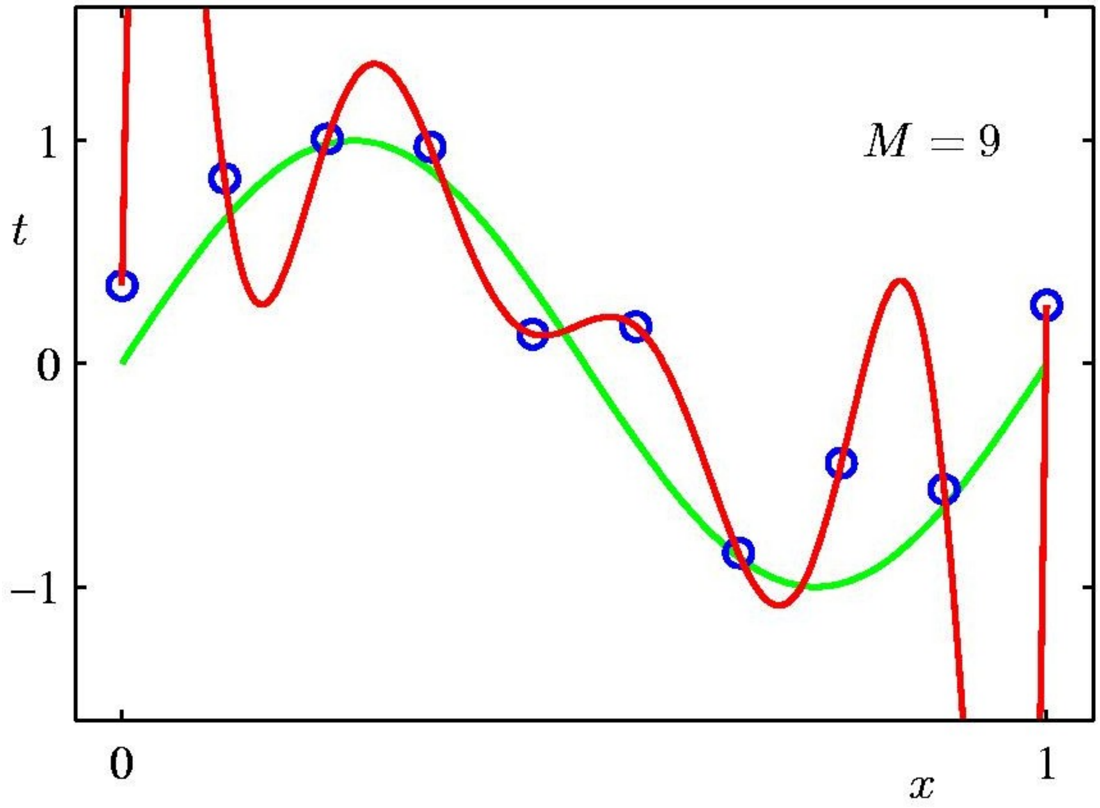
1st Order Polynomial



3^{rd} Order Polynomial



9th Order Polynomial



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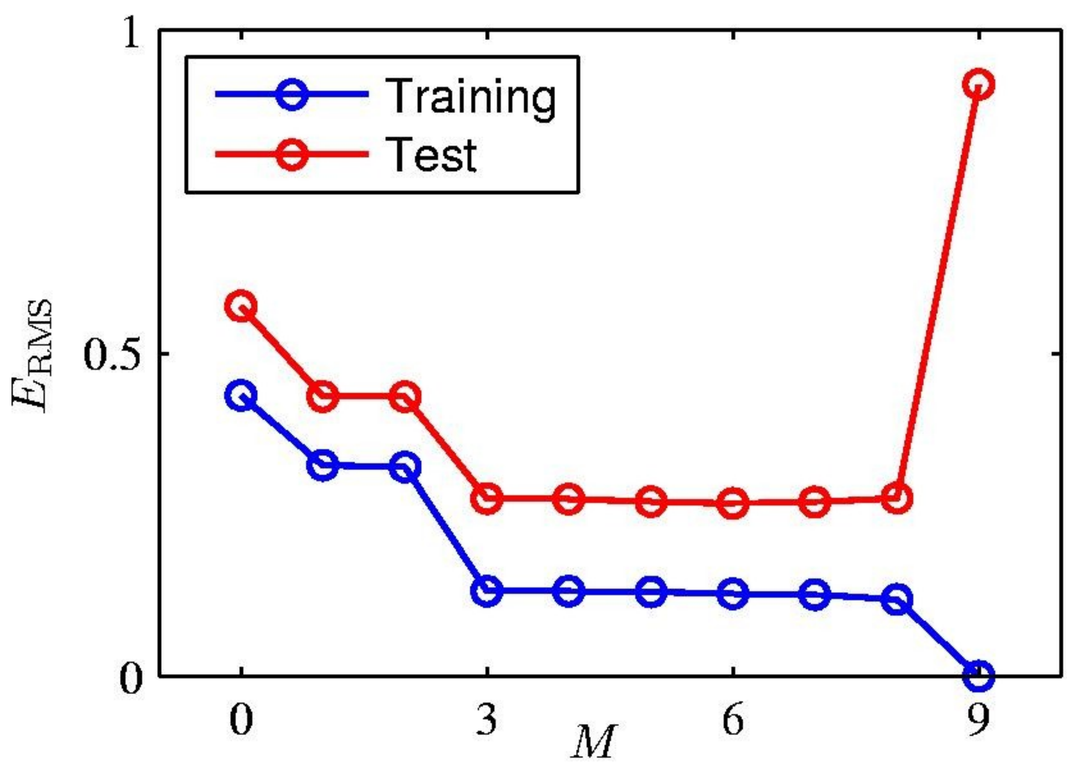
Over-fitting



Root-Mean-Square (RMS) Error

Polynomial Coefficients

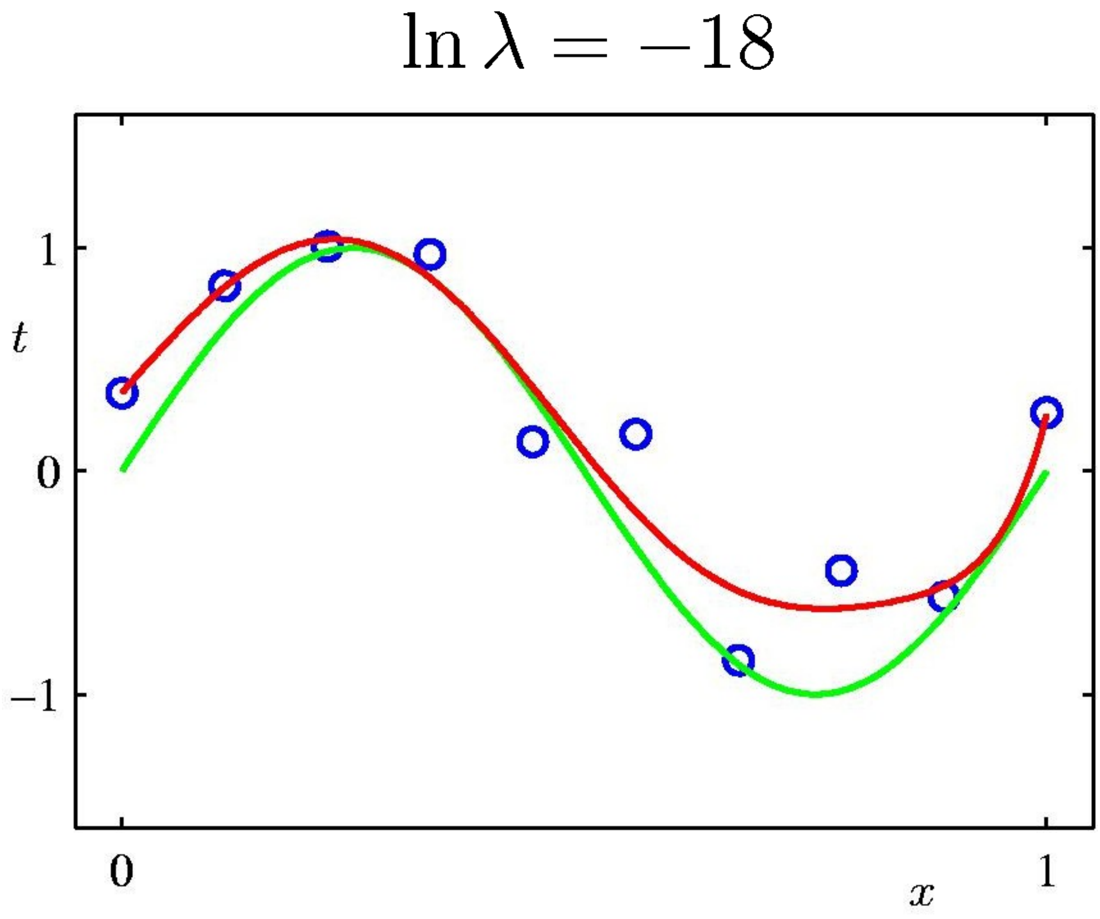
	$M = 0$	$M = 1$	$M = 3$	$M = 9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

Regularization

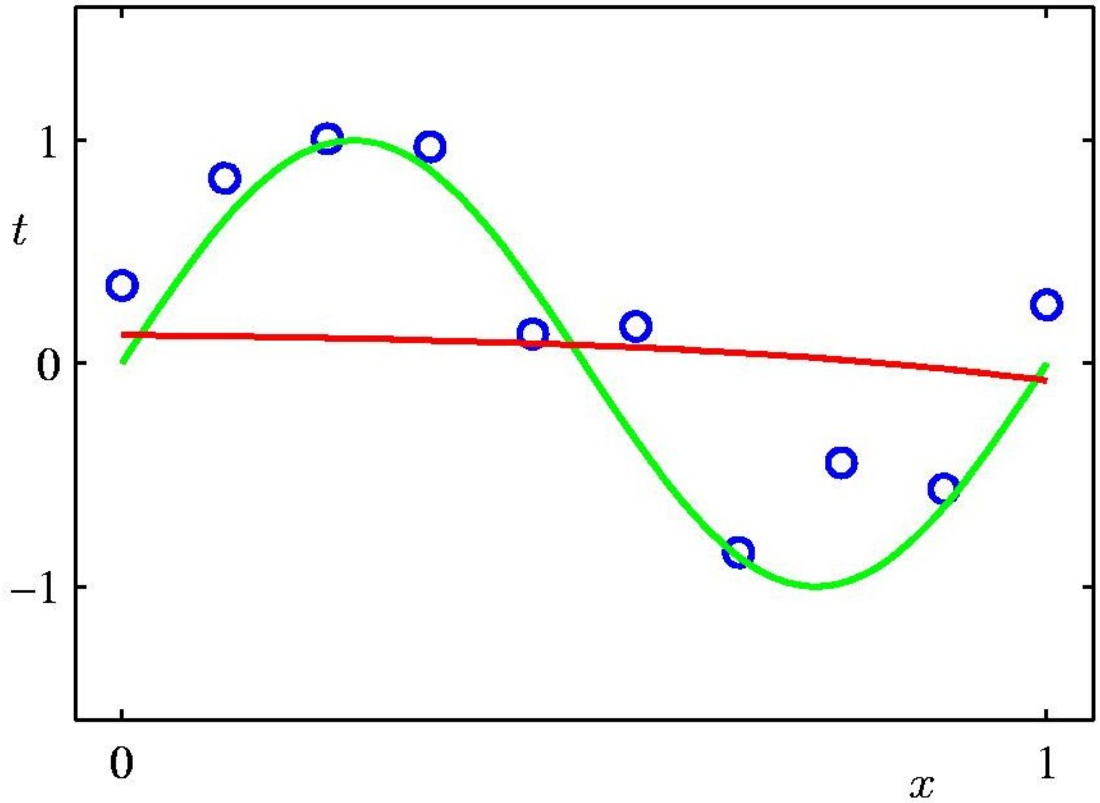
Penalize large coefficient values

$$J_{\mathbf{X},\mathbf{y}}(\mathbf{w}) = \frac{1}{2}\sum_i \left(y^i - \sum_j w_j \phi_j(\mathbf{x}^i) \right)^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

Regularization:



Over Regularization



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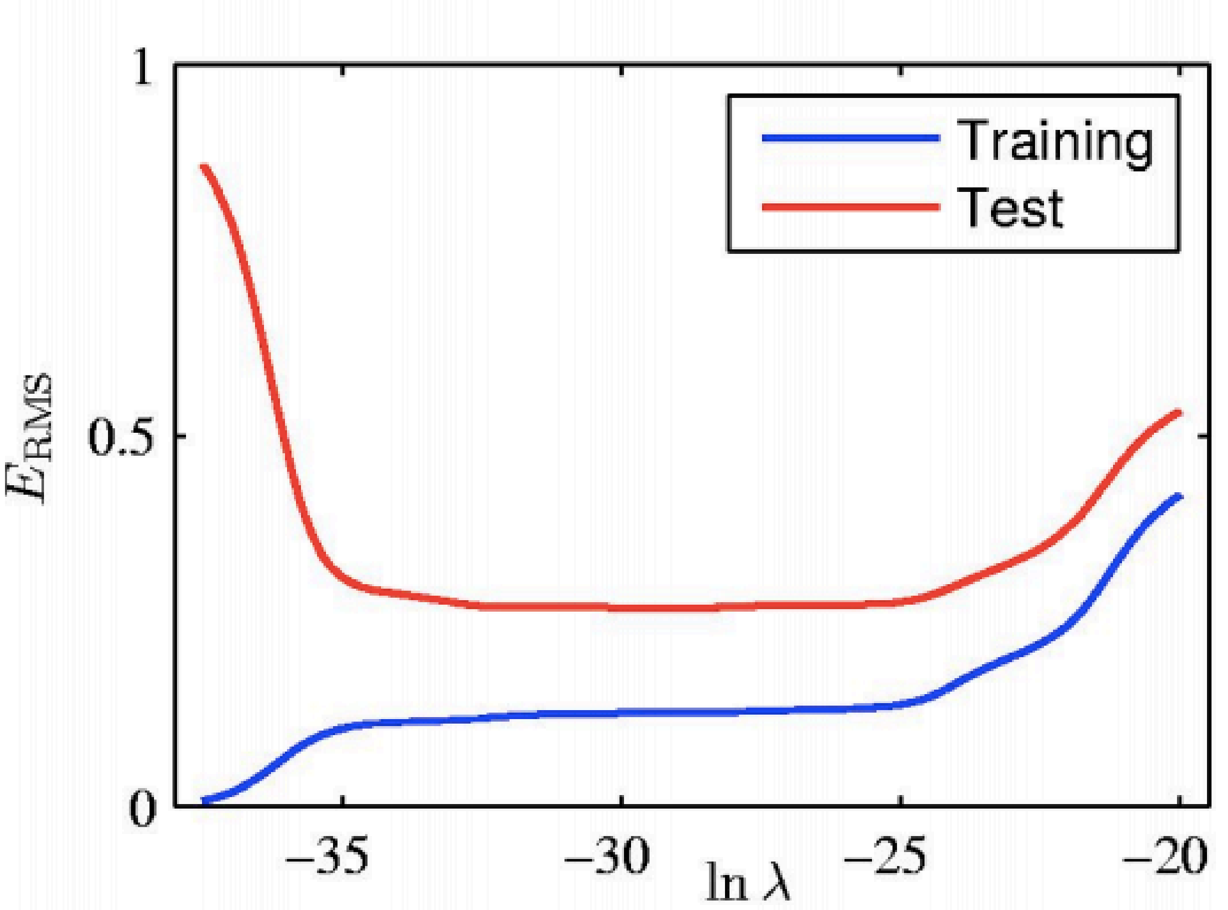
Regularization

9th Order Polynomial



Regularized Least Squares (1)

Consider the error function:

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

Data term + Regularization term

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

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

λ is called the regularization coefficient.

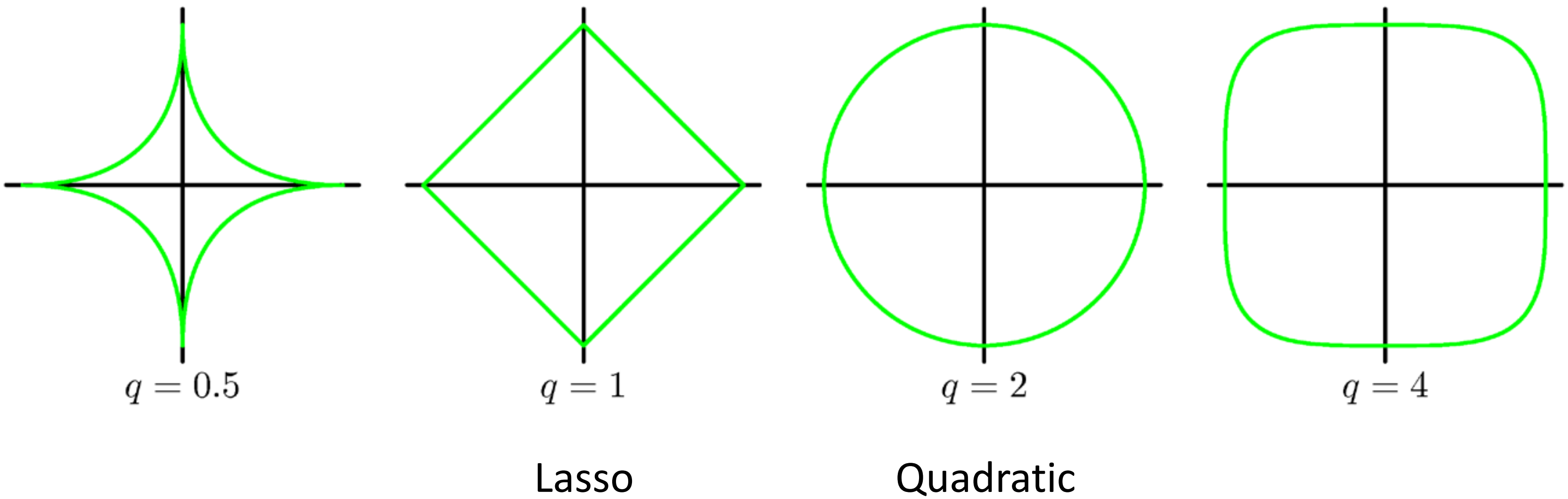
which is minimized by

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

Regularized Least Squares (2)

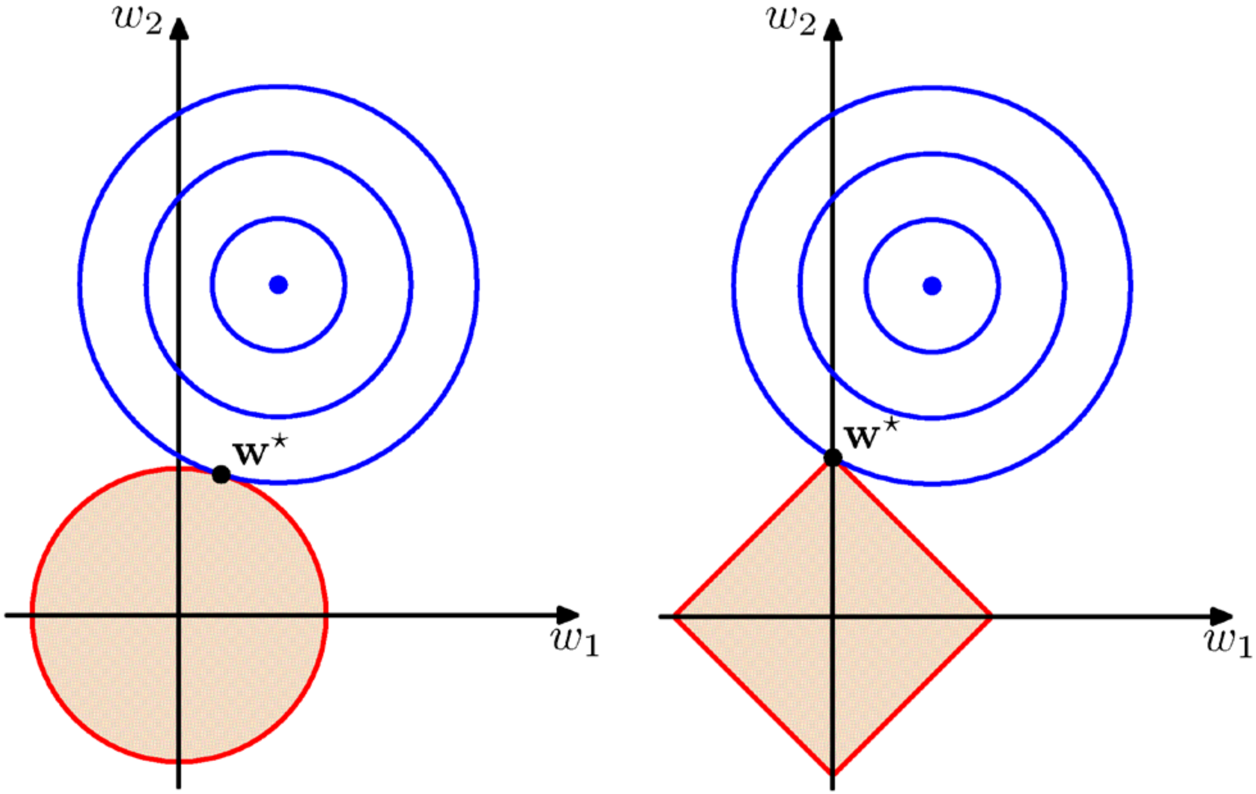
With a more general regularizer, we have

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



Regularized Least Squares (3)

Lasso tends to generate sparser solutions than a quadratic
regularizer.



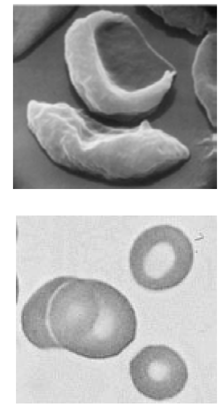
CLASSIFICATION

Discrete and Continuous Labels

Classification

Sports
Science
News

X = Document **Y = Topic**

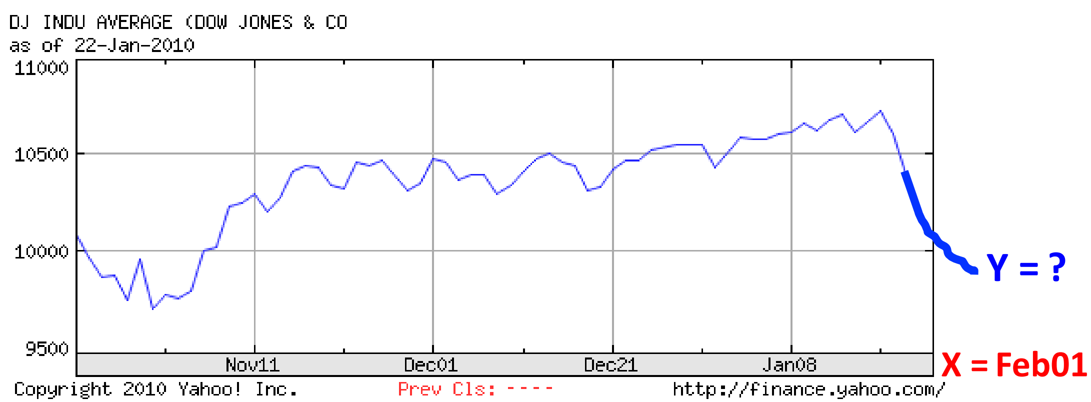


Anemic cell
Healthy cell

X = Cell Image **Y = Diagnosis**

Regression

Stock Market
Prediction



An example application

An emergency room in a hospital measures 17 variables (e.g., blood pressure, age, etc) of newly admitted patients.

A decision is needed: whether to put a new patient in an intensive-care unit.

Due to the high cost of ICU, those patients who may survive less than a month are given higher priority.

Problem: to predict high-risk patients and discriminate them from low-risk patients.

Another application

A credit card company receives thousands of applications for new cards. Each application contains information about an applicant,

- age
- Marital status
- annual salary
- outstanding debts
- credit rating
- etc.

Problem: to decide whether an application should approved, or to classify applications into two categories, approved and not approved.

The data and the goal

Data: A set of data records (also called examples, instances or cases) described by

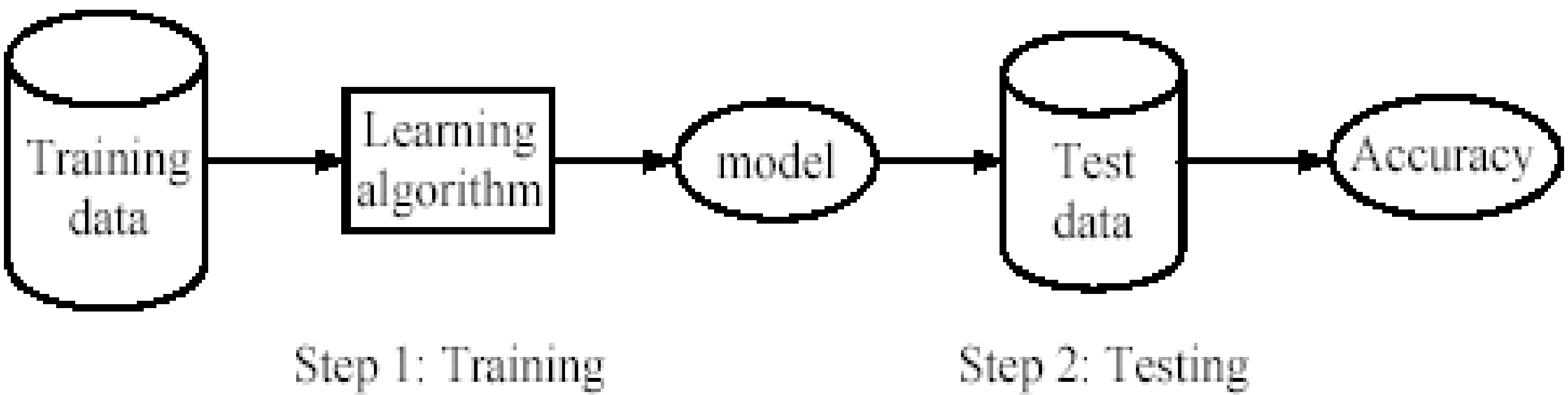
- *k* attributes: $A_1, A_2, \ldots A_k$.
- a class: Each example is labelled with a pre-defined class.

Goal: To learn a classification model from the data that can be used to predict the classes of new (future, or test) cases/instances.

Supervised learning process: two steps

- Learning (training): Learn a model using the training data
- Testing: Test the model using unseen test data to assess the model accuracy

$$Accuracy = \frac{\text{Number of correct classifications}}{\text{Total number of test cases}},$$



Least squares classification

Binary classification.

Each class is described by it's own linear model:

$$y(x) = w^T x + w_0$$

Compactly written as:

$$\mathrm{y}(\boldsymbol{x}) = \boldsymbol{W}^T \boldsymbol{x}$$

W is $[w\ w_0]$.

$$E_D(\boldsymbol{W}) = {}^1\!/_2\,(\boldsymbol{XW} - \boldsymbol{t})^T(\boldsymbol{XW} - \boldsymbol{t})$$

n^{th} row of $\boldsymbol{X}$ is x_n, the n^{th} datapoint.

$\boldsymbol{t}$ is vector of +1, -1.

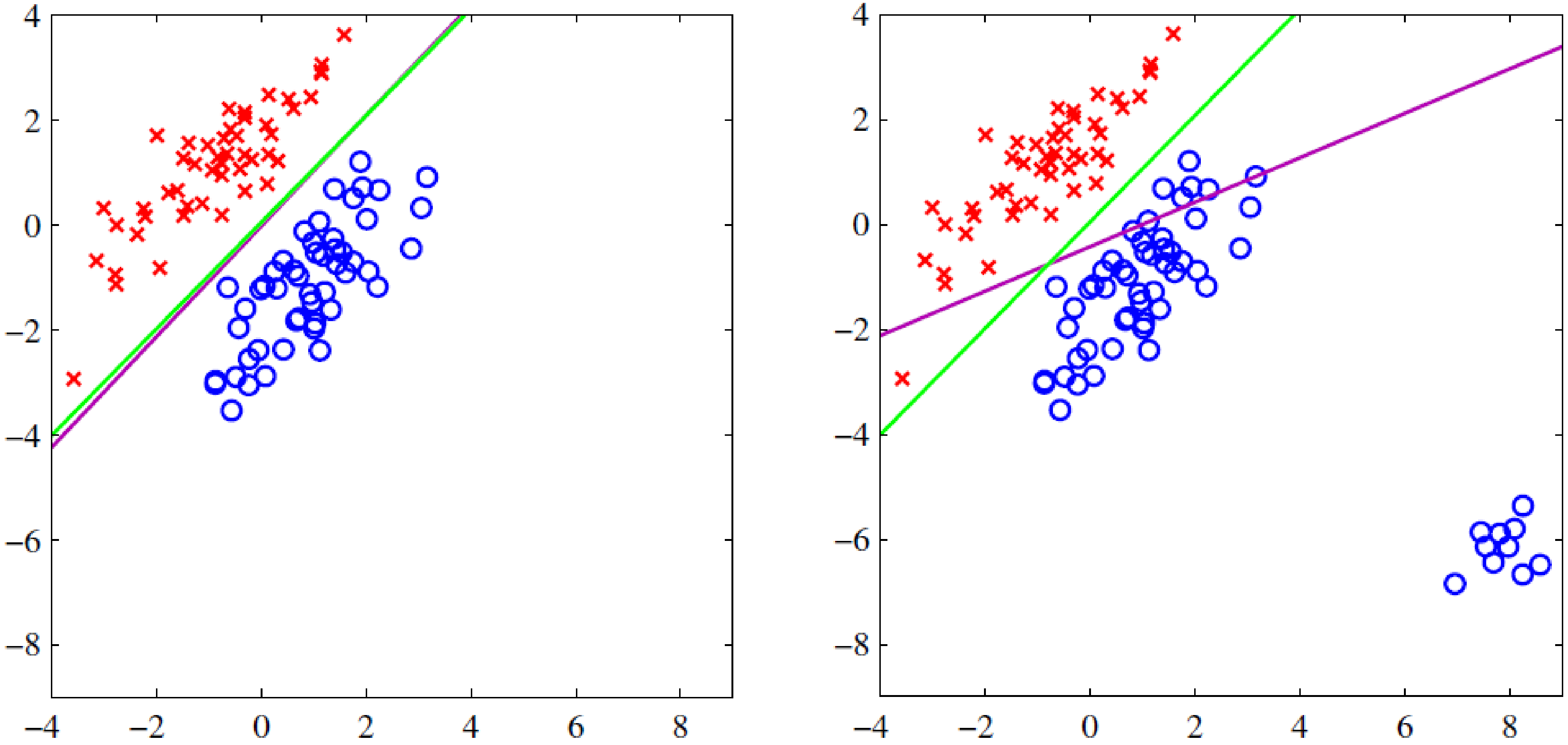
Least squares classification

Least squares $\boldsymbol{W}$ is:

$$\boldsymbol{W} = \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{t}$$

Problem is affected by outliers.

Least squares classification



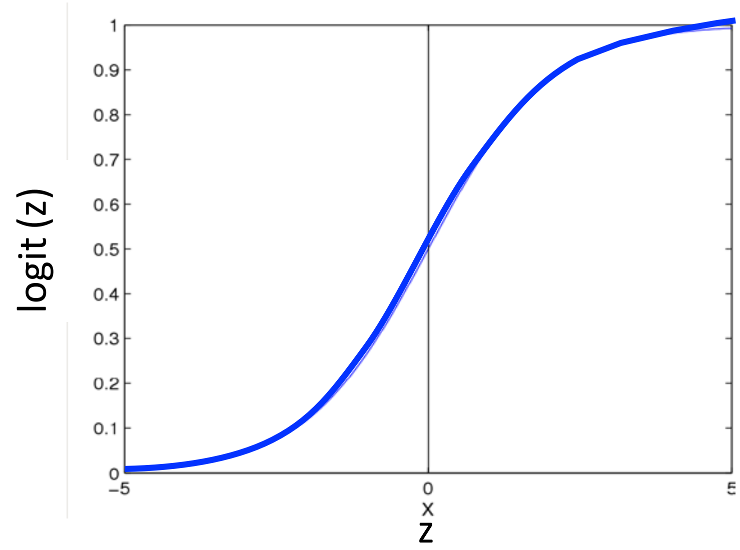
From Linear to Logistic Regression

Assumes the following functional form for P(Y|X):

$$P(Y=1|X) = \frac{1}{1+\exp(w_0 + \sum_i w_i X_i)}$$

Logistic function applied to a linear function of the data

Logistic function (or Sigmoid): $\frac{1}{1+exp(-z)}$



Features can be discrete or continuous!

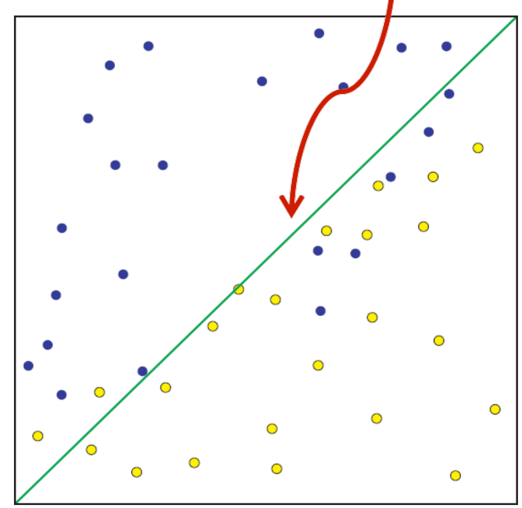
Logistic Regression is a Linear Classifier!

Assumes the following functional form for P(Y|X):

$$P(Y=1|X) = \frac{1}{1+\exp(w_0 + \sum_i w_i X_i)}$$

$$w_0 + \sum_i w_i X_i = 0$$

Decision boundary:



$$P(Y=0|X) \underset{1}{\overset{0}{\gtrless}} P(Y=1|X)$$

$$w_0 + \sum_i w_i X_i \underset{1}{\overset{0}{\gtrless}} 0$$

(Linear Decision Boundary)

Logistic Regression is a Linear Classifier!

Assumes the following functional form for P(Y|X):

$$P(Y=1|X) = \frac{1}{1+\exp(w_0 + \sum_i w_i X_i)}$$

$$\Rightarrow P(Y=0|X) = \frac{\exp(w_0 + \sum_i w_i X_i)}{1+\exp(w_0 + \sum_i w_i X_i)}$$

$$\Rightarrow \frac{P(Y=0|X)}{P(Y=1|X)} = \exp(w_0 + \sum_i w_i X_i) \quad \overset{0}{\underset{1}{\gtrless}} 1$$

$$\Rightarrow \boxed{w_0 + \sum_i w_i X_i \quad \overset{0}{\underset{1}{\gtrless}} 0}$$

Logistic Regression

Label t $\in \{+1, -1\}$modeled as:

$$P(t = 1|x, w) = \sigma(w^T x)$$

$$P(y|x, w) = \sigma(yw^T x), y \in \{+1, -1\}$$

Given a set of parameters w, the probability or likelihood of a datapoint *(x,t):*

$$P(t|x, w) = \sigma(tw^T x)$$

Logistic Regression

Given a training dataset $\{(x_1, t_1), \ldots, (x_N, t_N)\}$, log likelihood of a model w is given by:

$$L(w) = \sum_n \ln(P(t_n | x_n, w))$$

Using principle of maximum likelihood, the best w is given by:

$$w^* = \arg\max_w L(w)$$

Logistic Regression

Final Problem:

$$\max_{w} \sum_{i=1}^{n} -\log(1 + \exp(-t_n w^T x_n))$$

Or, $\min\limits_{w} \sum_{i=1}^{n} \log(1 + \exp(-t_n w^T x_n))$

Error function:

$$E(w) = \sum_{i=1}^{n} \log(1 + \exp(-t_n w^T x_n))$$

$E(w)$ is convex.

Logistic Regression

Final Problem:

$$\max_{w} \sum_{i=1}^{n} -\log(1 + \exp(-t_n w^T x_n))$$

Regularized Version:

$$max \sum_{i=1}^{n} -\log(1 + \exp(-t_n w^T x_n)) - \lambda w^T w$$

Or, $\min_{w} \sum_{i=1}^{n} \log(1 + \exp(-t_n w^T x_n)) + \lambda \left|\left|w\right|\right|^2$

Properties of Error function

Derivatives:

$$\nabla E(w) = \sum_{i=1}^{n} -\big(1 - \sigma(t_i w^T x_i)\big)(t_i x_i)$$

$$\nabla^2 E(w) = \sum_{i=1}^{n} \sigma(t_i w^T x_i)\big(1 - \sigma(t_i w^T x_i)\big) x_i x_i^T$$

Gradient Descent

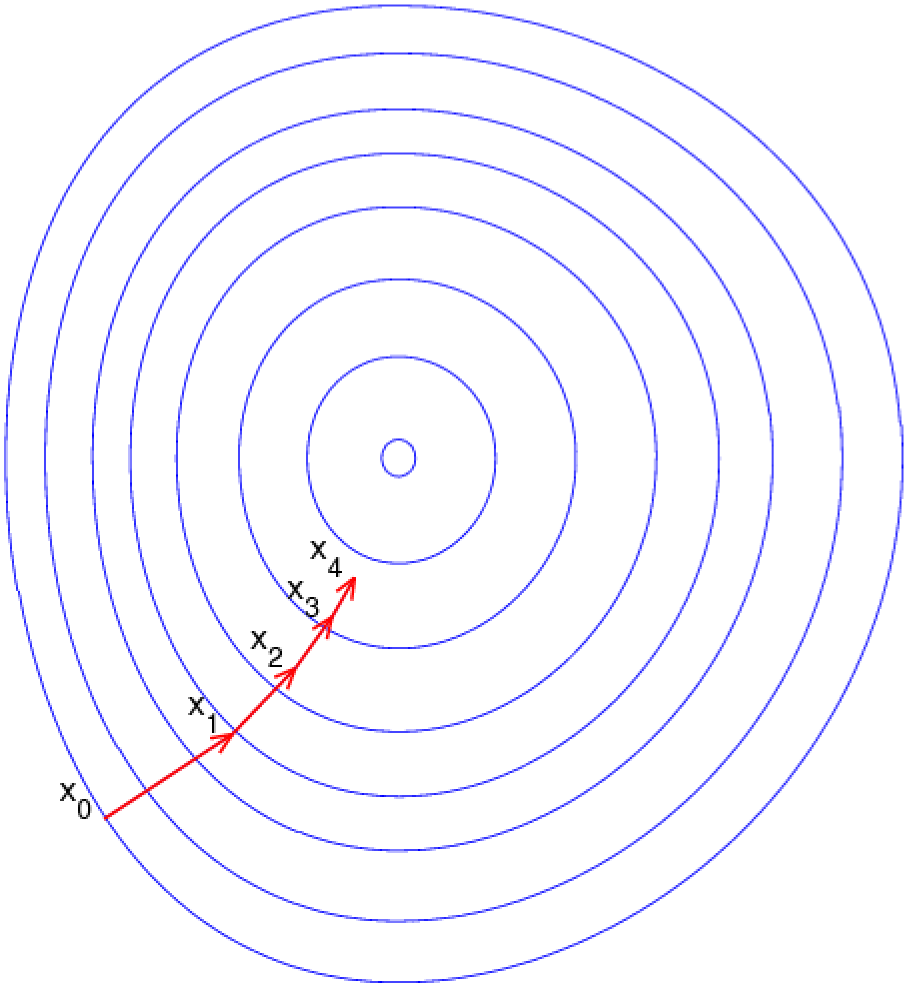
Problem: min f(x)

f(x): differentiable

g(x): gradient of f(x)

Negative gradient is steepest descent direction.

At each step move in the gradient directic so that there is "sufficient decrease



Gradient Descent

input : Function f, Gradient ∇f
output: Optimal solution w^*

Initialize $w_0 \leftarrow 0$, $k \leftarrow 0$
while $|\nabla f_k| > \epsilon$ **do**
  Compute $\alpha_k \leftarrow \text{linesearch}(f, -\nabla f_k, w_k)$
  Set $w_{k+1} \leftarrow w_k - \alpha_k \nabla f_k$
  Evaluate ∇f_{k+1}
  $k \leftarrow k + 1$
end
$w^* \leftarrow w_k$

Logistic Regression for more than 2 classes

- Logistic regression in more general case, where
  Y $\{y_1,\ldots,y_K\}$

  for $k<K$

$$P(Y=y_k|X)=\frac{\exp(w_{k0}+\sum_{i=1}^{d}w_{ki}X_i)}{1+\sum_{j=1}^{K-1}\exp(w_{j0}+\sum_{i=1}^{d}w_{ji}X_i)}$$

  for $k=K$ (normalization, so no weights for this class)

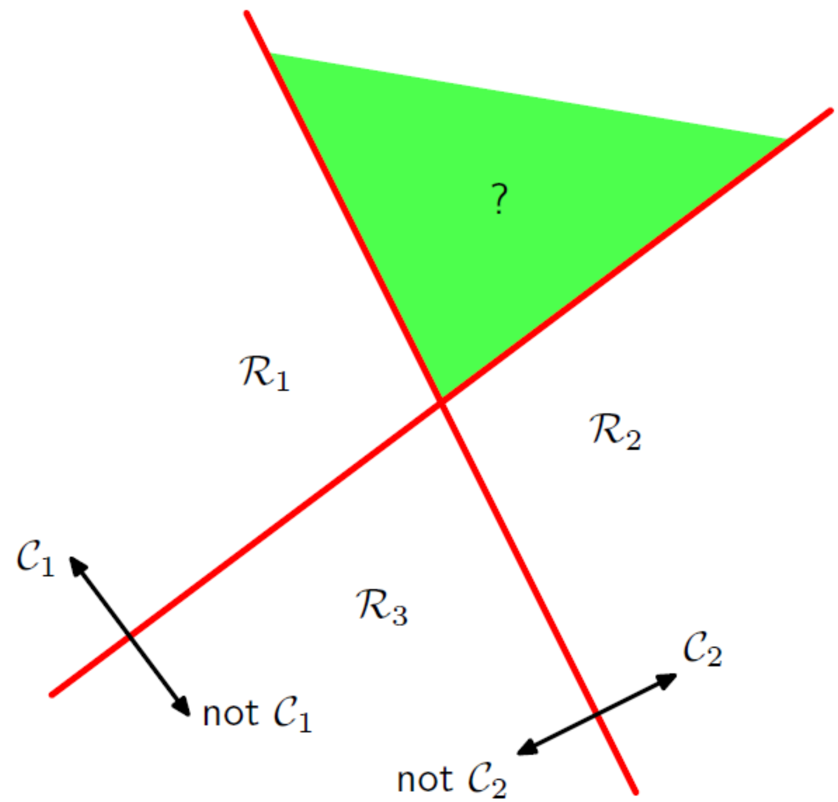
$$P(Y=y_K|X)=\frac{1}{1+\sum_{j=1}^{K-1}\exp(w_{j0}+\sum_{i=1}^{d}w_{ji}X_i)}$$

Multiple classes

One-vs-all: $K - 1$ hyperplanes each separating $C_1, \ldots, C_{K-1}$ classes from rest.

Otherwise C_K

Low number of classifiers.

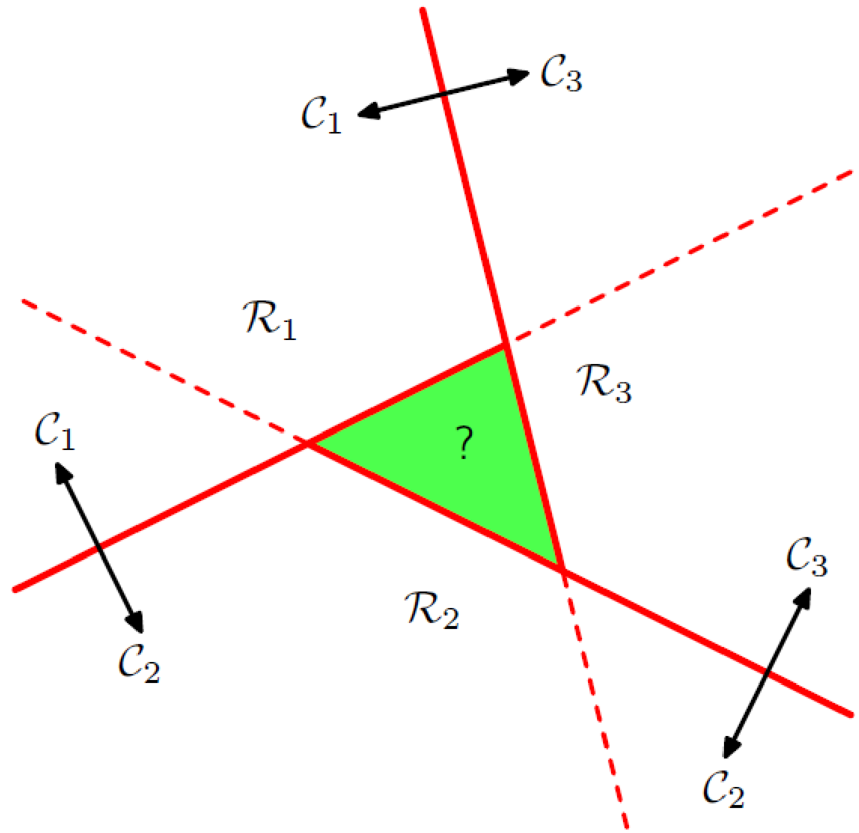


Multiple classes

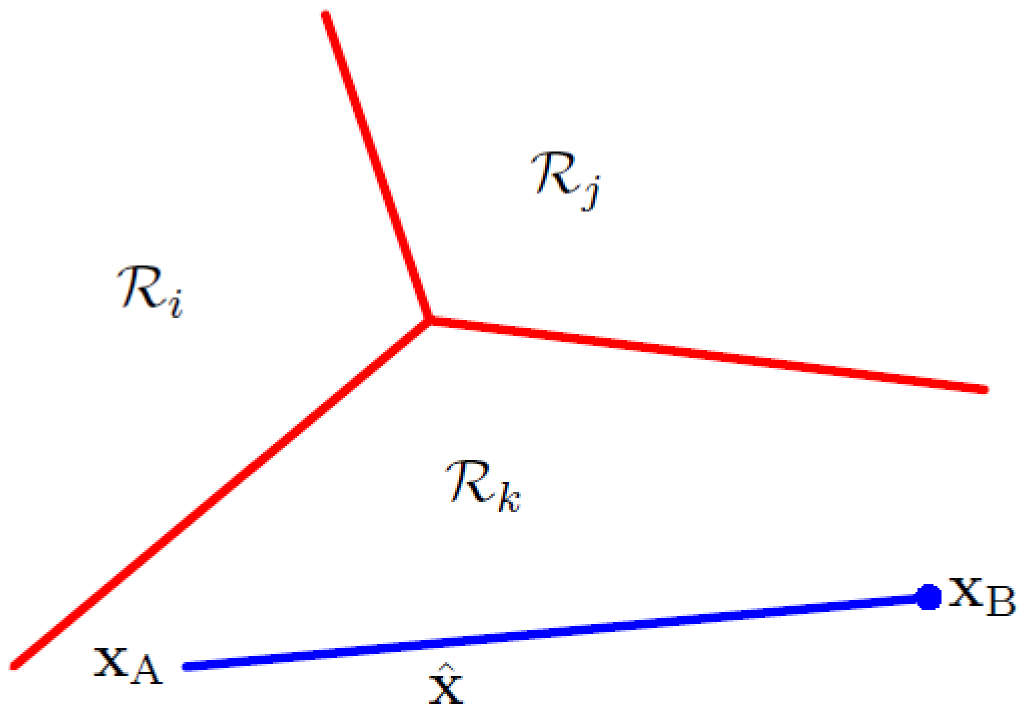
One-vs-one: Every pair $C_i - C_j$ get a boundary.

Final by majority vote.

High number of classifiers.



Multiple Classes



Multiple classes

K-linear discriminant functions:

$$y_k(x) = w_k^T \boldsymbol{x} + w_{k0}$$

Assign x to C_k if $y_k(x) \geq y_j(x)$ for all $j \neq k$

Decision boundary:

$$\left(w_k - w_j\right)^T \boldsymbol{x} + \left(w_{k0} - w_{j0}\right) = 0$$

Decision region is singly connected:

$$x = \lambda x_A + (1 - \lambda) x_B$$

If x_A and x_B have same label, so does x.

MORE REGRESSION

The Bias-Variance Decomposition (1)

Recall the *expected squared loss,*

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

where

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

The second term of $\mathbb{E}[L]$ corresponds to the noise inherent in the random variable t.

What about the first term?

The Bias-Variance Decomposition (2)

Suppose we were given multiple data sets, each of size N. Any particular data set, D, will give a particular function y(x;D). We then have

$$
\begin{aligned}
&\{y(\mathbf{x};\mathcal{D}) - h(\mathbf{x})\}^2 \\
&\quad = \{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] + \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2 \\
&\quad = \{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2 + \{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2 \\
&\qquad +2\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}\{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}.
\end{aligned}
$$

The Bias-Variance Decomposition (3)

Taking the expectation over D yields

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

The Bias-Variance Decomposition (4)

Thus we can write

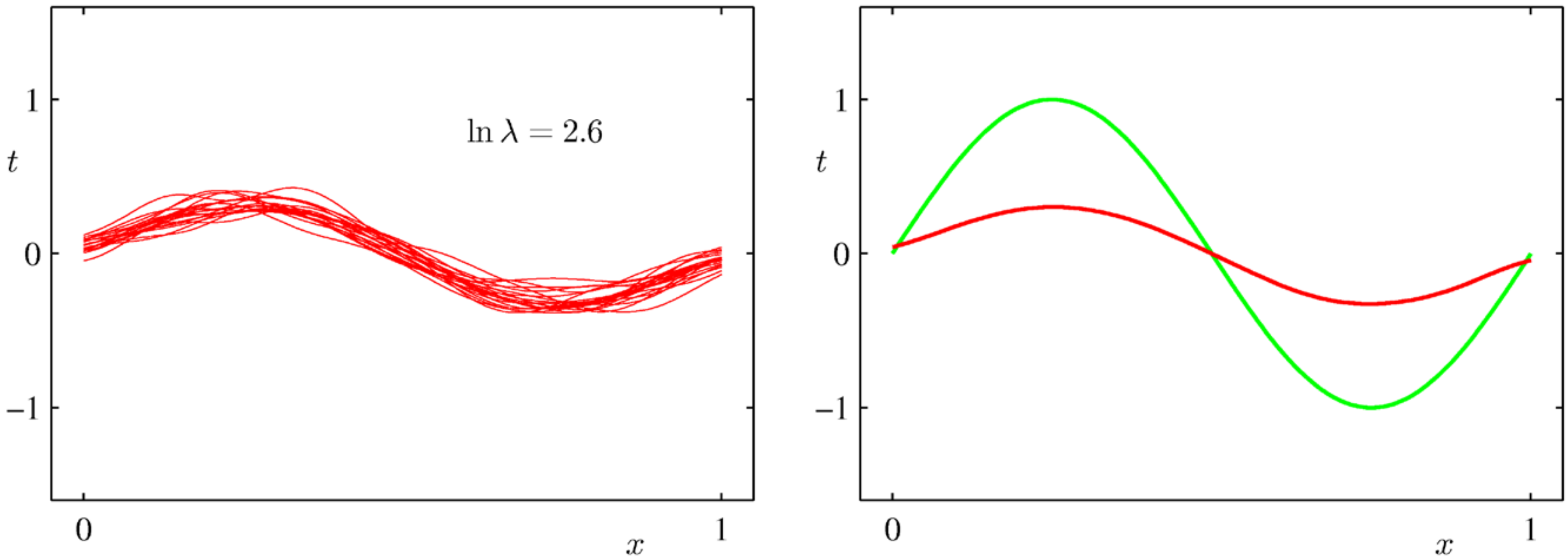
$$\text{expected loss} = (\text{bias})^2 + \text{variance} + \text{noise}$$

where

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

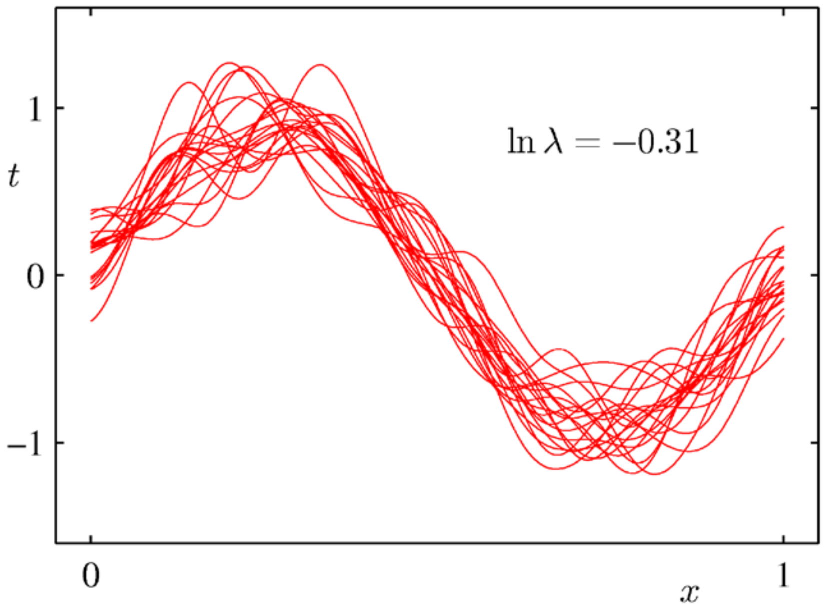
The Bias-Variance Decomposition (5)

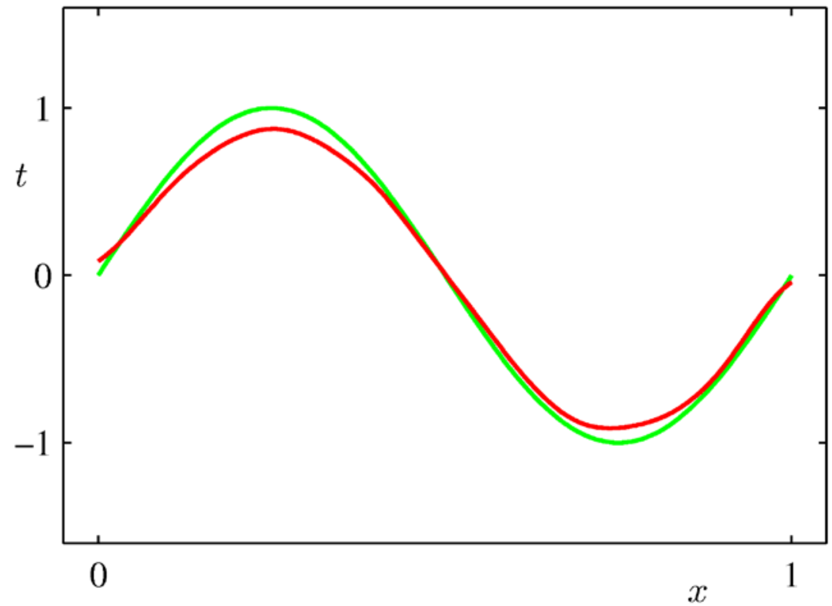
Example: 25 data sets from the sinusoidal, varying the degree of regularization, ¸ .



The Bias-Variance Decomposition (6)

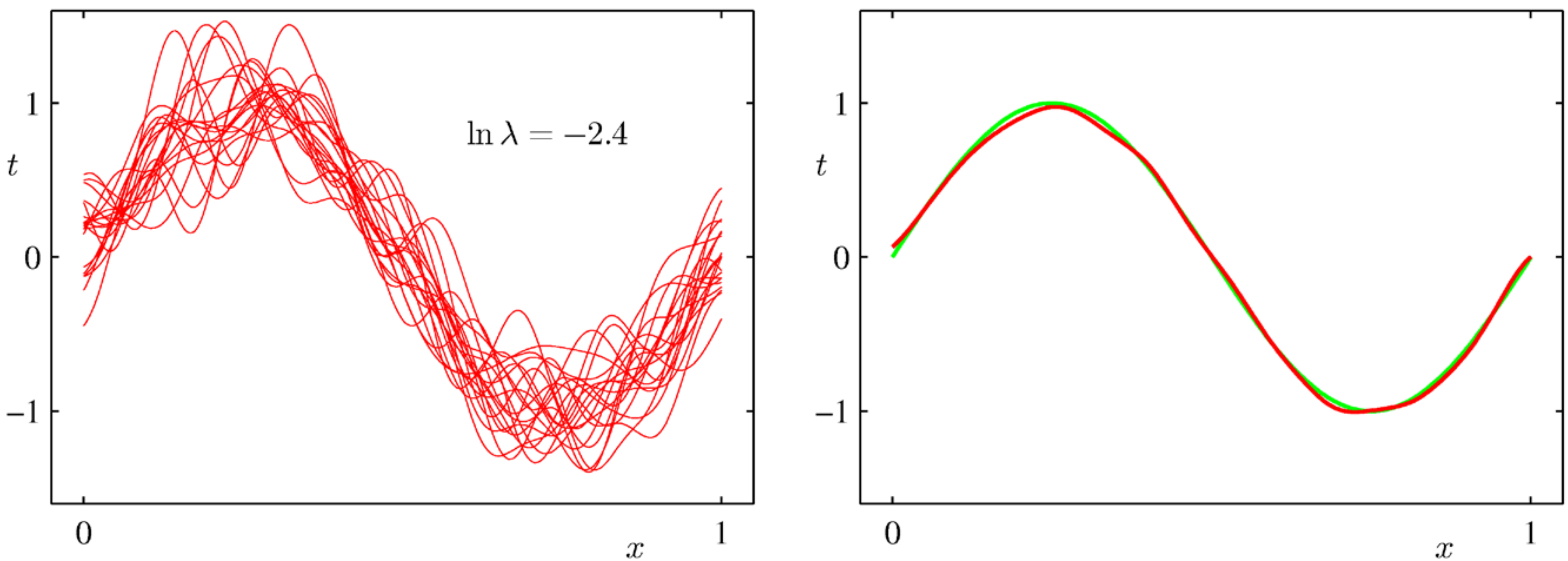
Example: 25 data sets from the sinusoidal, varying the degree of regularization, ¸ .





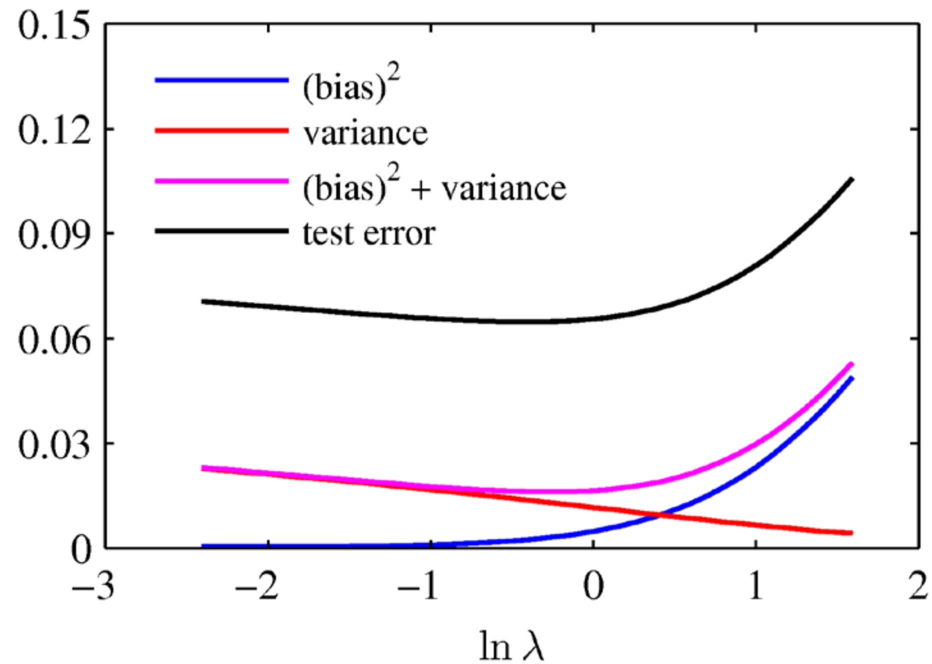
The Bias-Variance Decomposition (7)

Example: 25 data sets from the sinusoidal, varying the degree of regularization, ¸ .



The Bias-Variance Trade-off

From these plots, we note that an over-regularized model (large ¸) will have a high bias, while an under-regularized model (small ¸) will have a high variance.



Bayesian Linear Regression (1)

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 using results for marginal and conditional Gaussian distributions, gives the posterior

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

where

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

Bayesian Linear Regression (2)

A common choice for the prior is

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

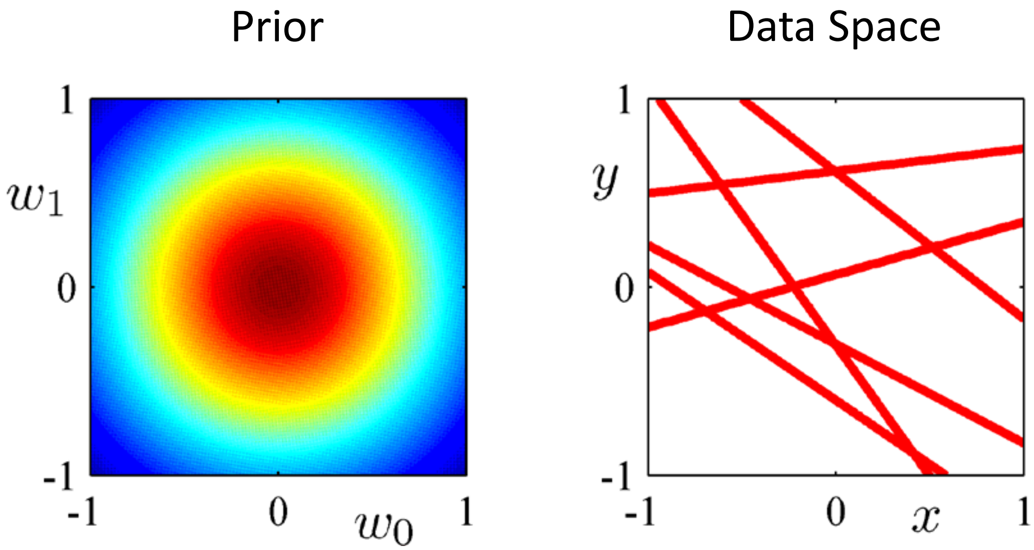
for which

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

Next we consider an example …

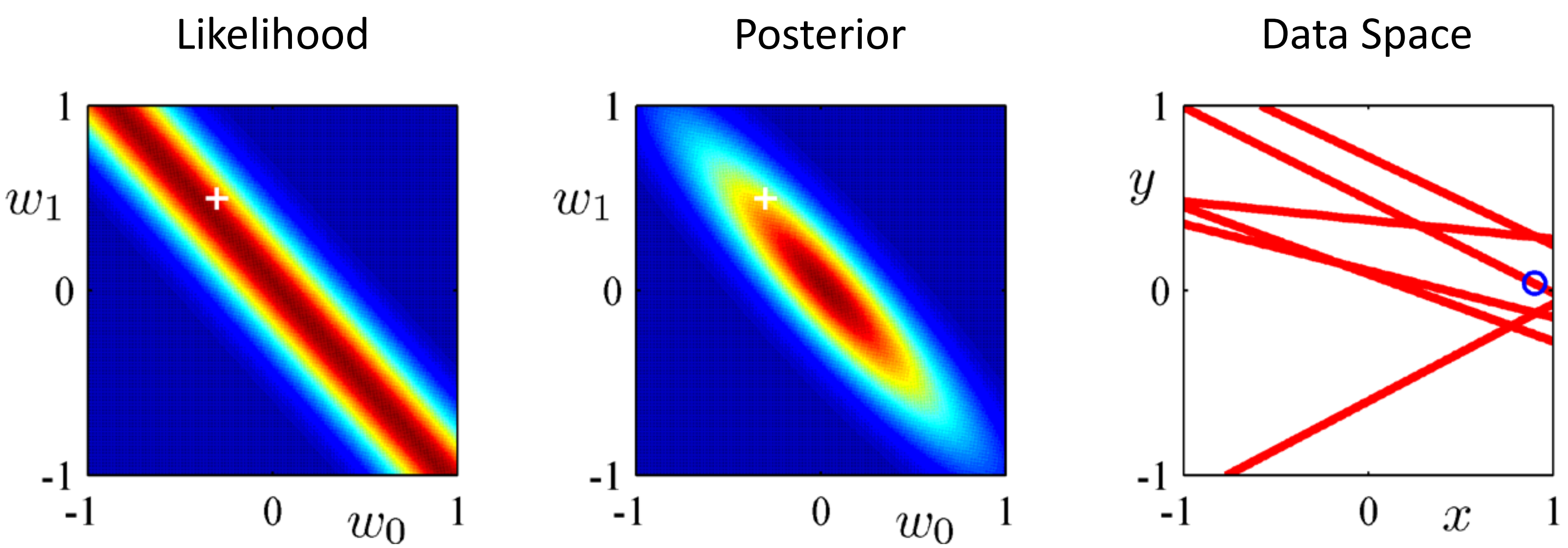
Bayesian Linear Regression (3)

0 data points observed



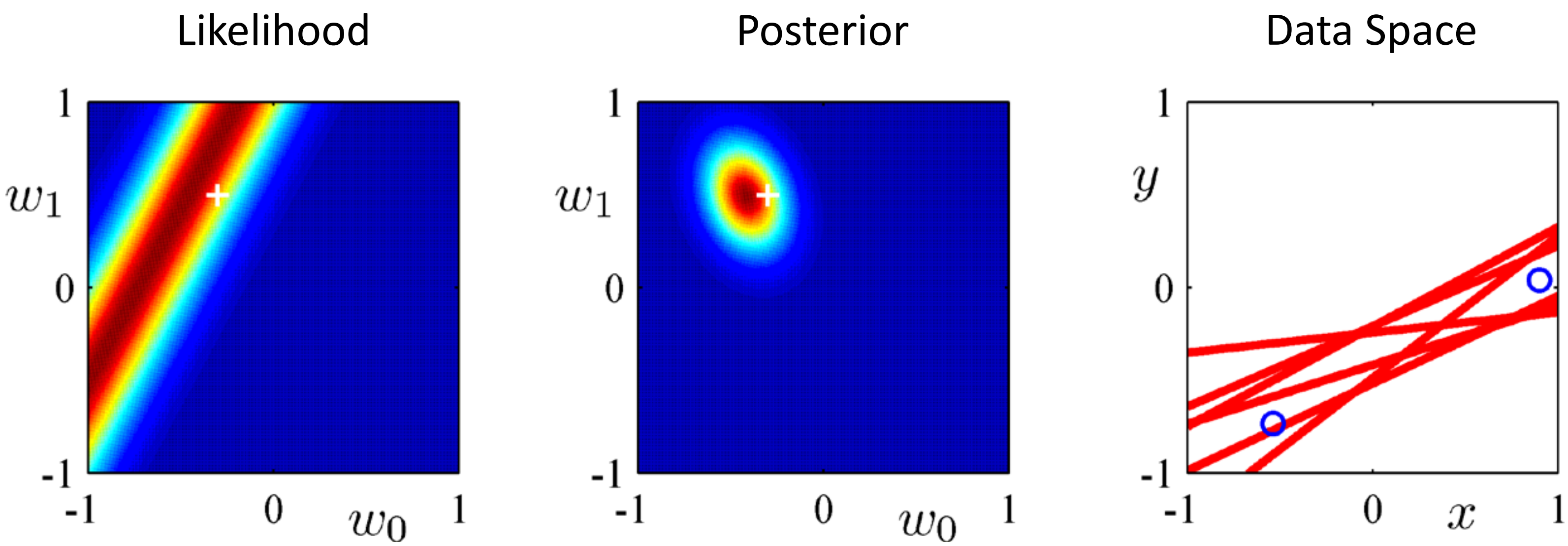
Bayesian Linear Regression (4)

1 data point observed



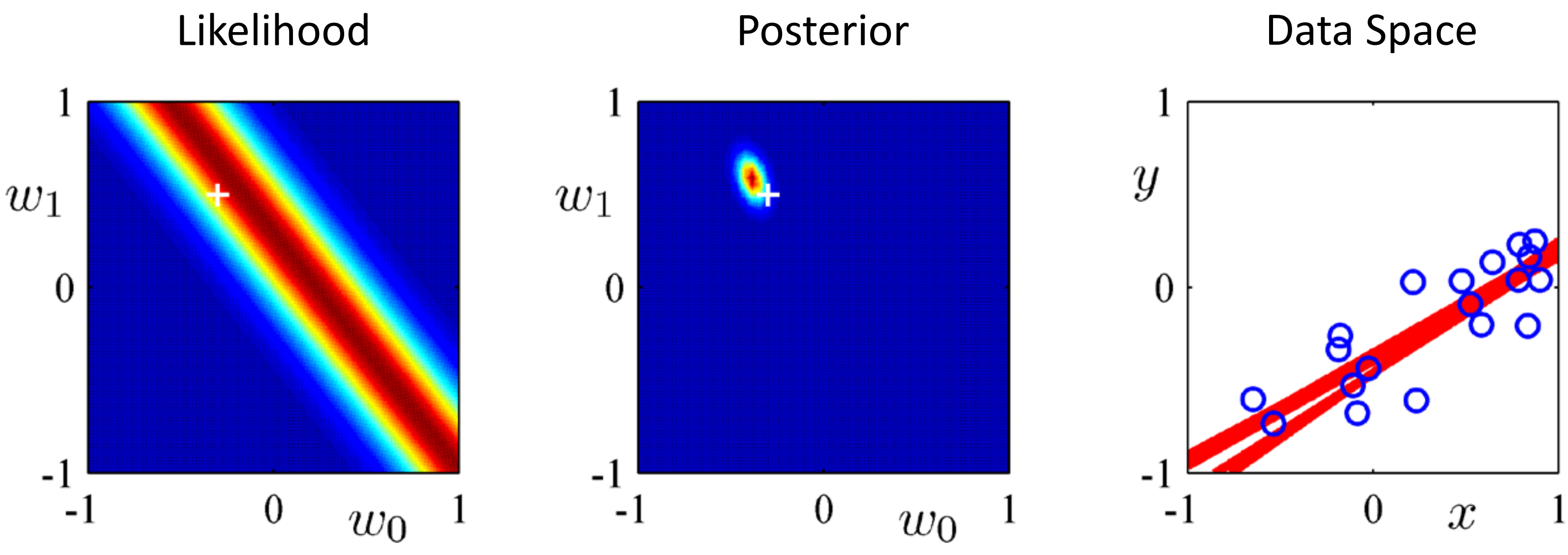
Bayesian Linear Regression (5)

2 data points observed



Bayesian Linear Regression (6)

20 data points observed



Predictive Distribution (1)

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

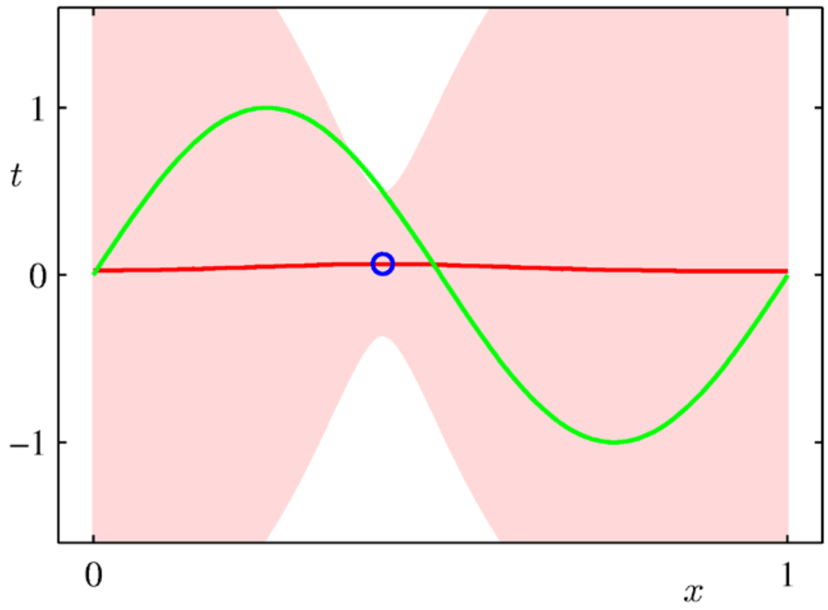
$$
\begin{aligned}
p(t|\mathbf{t}, \alpha, \beta) &= \int p(t|\mathbf{w}, \beta) p(\mathbf{w}|\mathbf{t}, \alpha, \beta) \, \mathrm{d}\mathbf{w} \\
&= \mathcal{N}(t|\mathbf{m}_N^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}), \sigma_N^2(\mathbf{x}))
\end{aligned}
$$

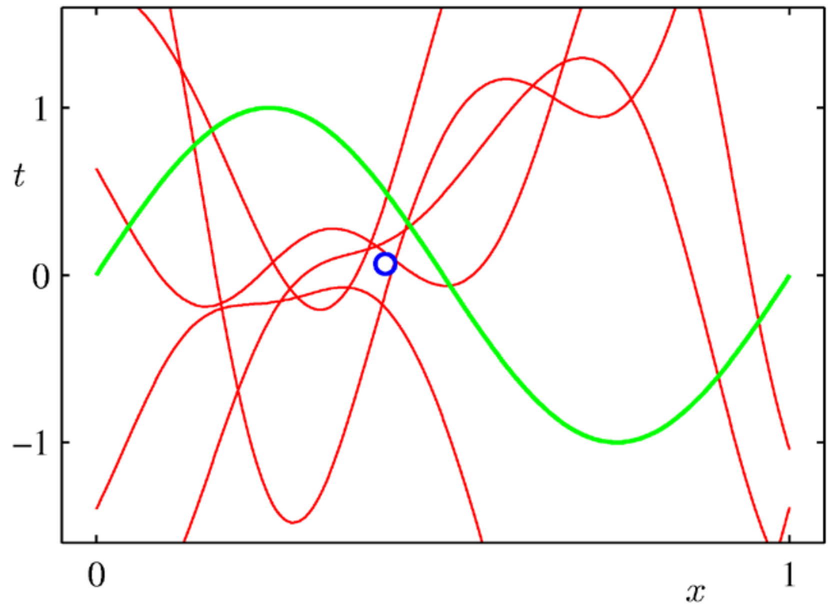
where

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

Predictive Distribution (2)

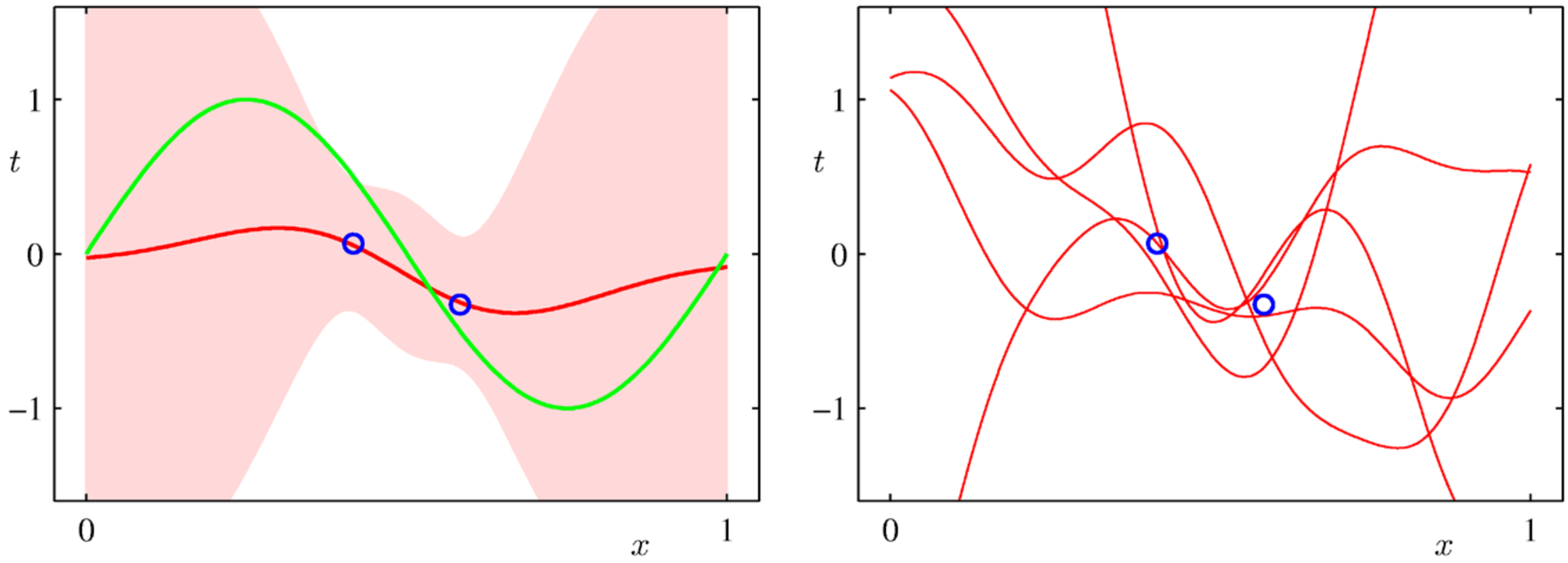
Example: Sinusoidal data, 9 Gaussian basis functions, 1 data point





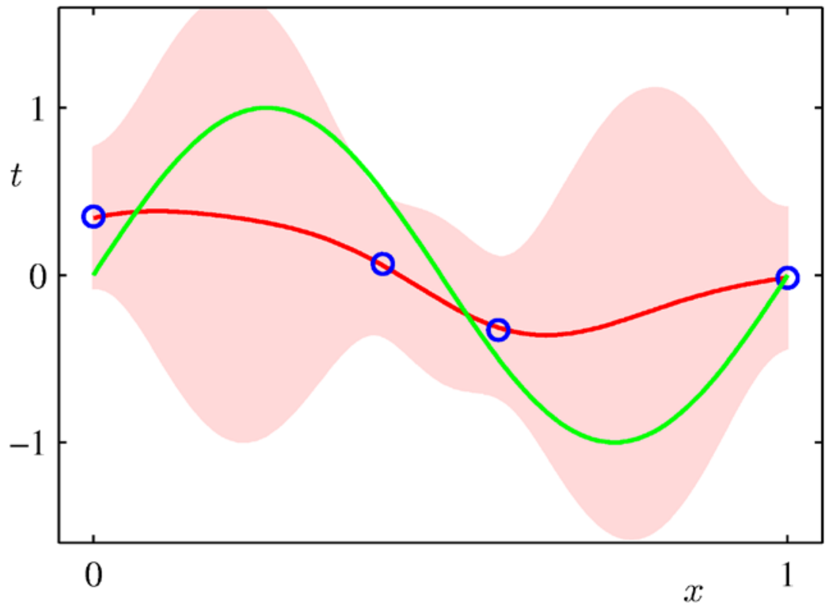
Predictive Distribution (3)

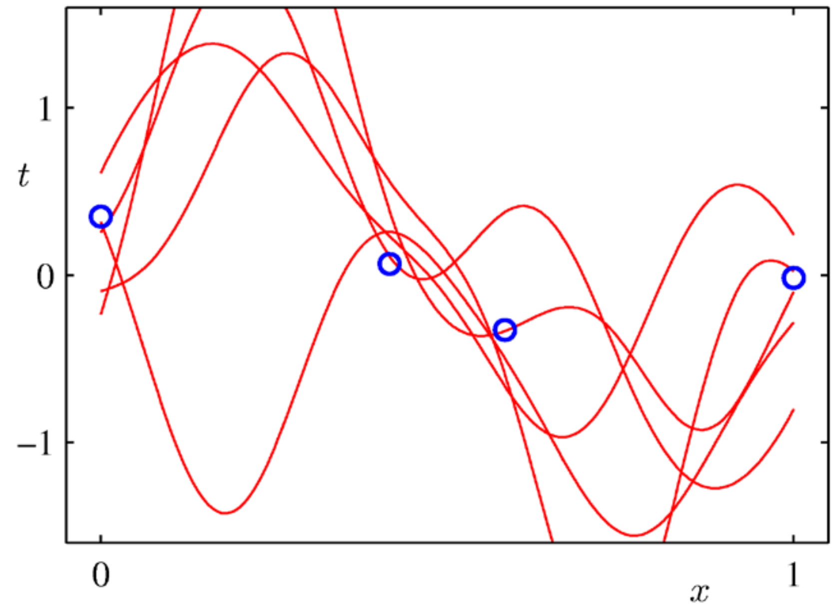
Example: Sinusoidal data, 9 Gaussian basis functions, 2 data points



Predictive Distribution (4)

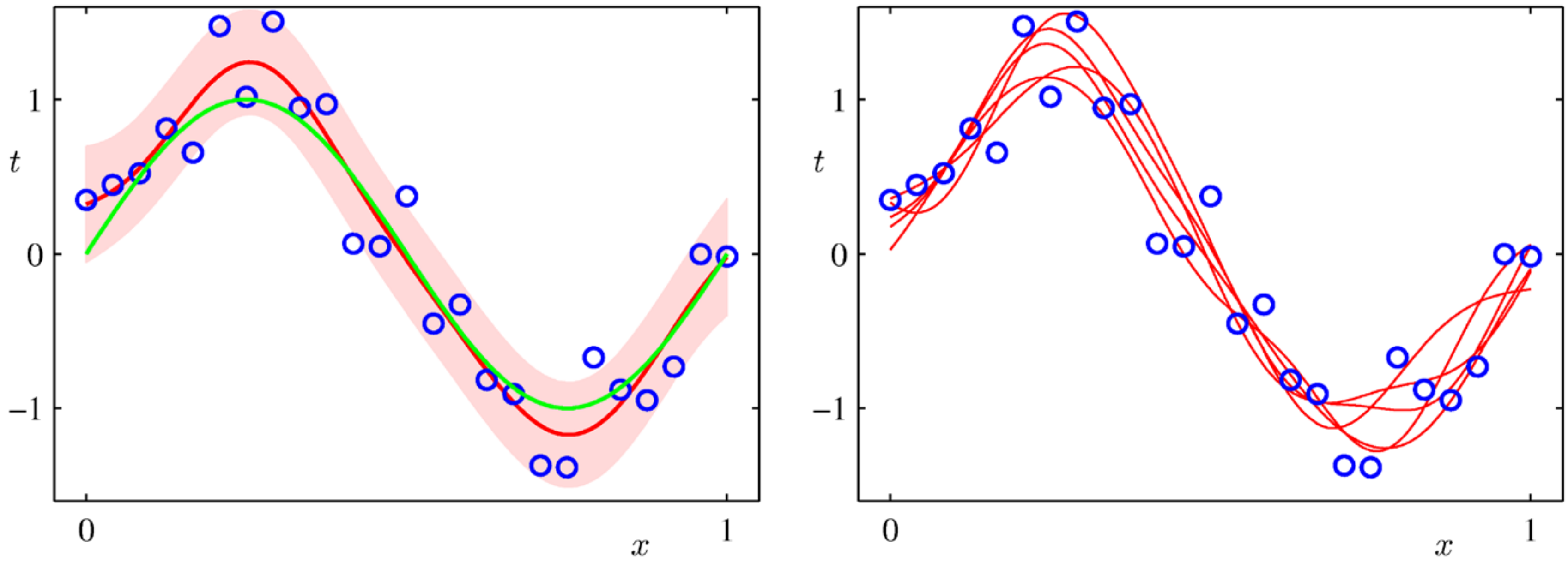
Example: Sinusoidal data, 9 Gaussian basis functions, 4 data points





Predictive Distribution (5)

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



Multiple Outputs (1)

Analogously 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 (2)

Maximizing with respect to W , we obtain

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

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

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

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