Machine Learning
ITCS 6156/8156

Linear Regression

Razvan C. Bunescu

Department of Computer Science @ CCI

rbunescu@uncc.edu

Supervised Learning

- **Task** = learn an (unknown) function $t : X \rightarrow T$ that maps input instances $\mathbf{x} \in X$ to output targets $t(\mathbf{x}) \in T$:
  - **Classification**:
    - The output $t(\mathbf{x}) \in T$ is one of a finite set of discrete categories.
  - **Regression**:
    - The output $t(\mathbf{x}) \in T$ is continuous, or has a continuous component.

- Target function $t(\mathbf{x})$ is known (only) through (noisy) set of training examples:

  $(\mathbf{x}_1,t_1), (\mathbf{x}_2,t_2), \ldots (\mathbf{x}_n,t_n)$

Supervised Learning

- **Task** = learn an (unknown) function $t : X \rightarrow T$ that maps input instances $\mathbf{x} \in X$ to output targets $t(\mathbf{x}) \in T$:
  - function t is known (only) through (noisy) set of training examples:
    - Training/Test data: $(\mathbf{x}_1,t_1), (\mathbf{x}_2,t_2), \ldots (\mathbf{x}_n,t_n)$

- **Task** = build a function $h(\mathbf{x})$ such that:
  - h matches t well on the *training data*:
    => h is able to fit data that it has seen.
  - h also matches target t well on *test data*:
    => h is able to generalize to unseen data.

Parametric Approaches to Supervised Learning

- **Task** = build a function $h(\mathbf{x})$ such that:
  - h matches t well on the training data:
    => h is able to fit data that it has seen.
  - h also matches t well on test data:
    => h is able to generalize to unseen data.

- **Task** = choose h from a "nice" *class of functions* that depend on a vector of parameters $\mathbf{w}$:
  - $h(\mathbf{x}) \equiv h_{\mathbf{w}}(\mathbf{x}) \equiv h(\mathbf{w},\mathbf{x})$
  - **what classes of functions are "nice"?**

Linear Regression

1. (Simple) Linear Regression
   – House price prediction

2. Linear Regression with Polynomial Features
   – Polynomial curve fitting
   – Regularization
   – Ridge regression

3. Multiple Linear Regression
   – House price prediction
   – Normal equations

House Price Prediction

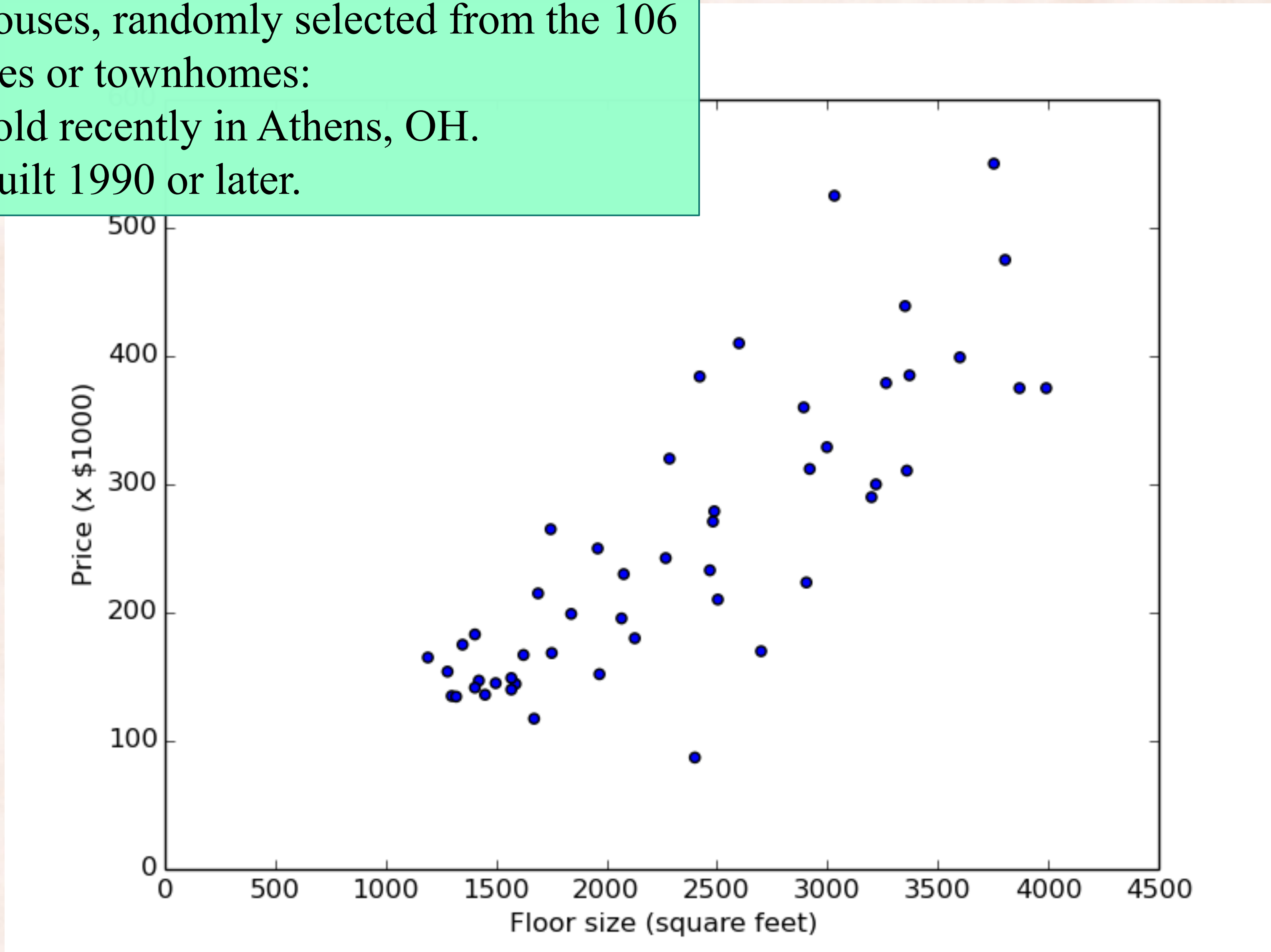
- Given the floor size in square feet, predict the selling price:
  - x is the size, t is the price
  - Need to learn a function h such that $h(x) \approx t(x)$.

- Is this classification or regression?
  - **Regression**, because price is real valued.
    - and there are many possible prices.
  - (Simple) linear regression, because one input value.
  - Would a problem with only two labels $t_1 = 0.5$ and $t_2 = 1.0$ still be regression?

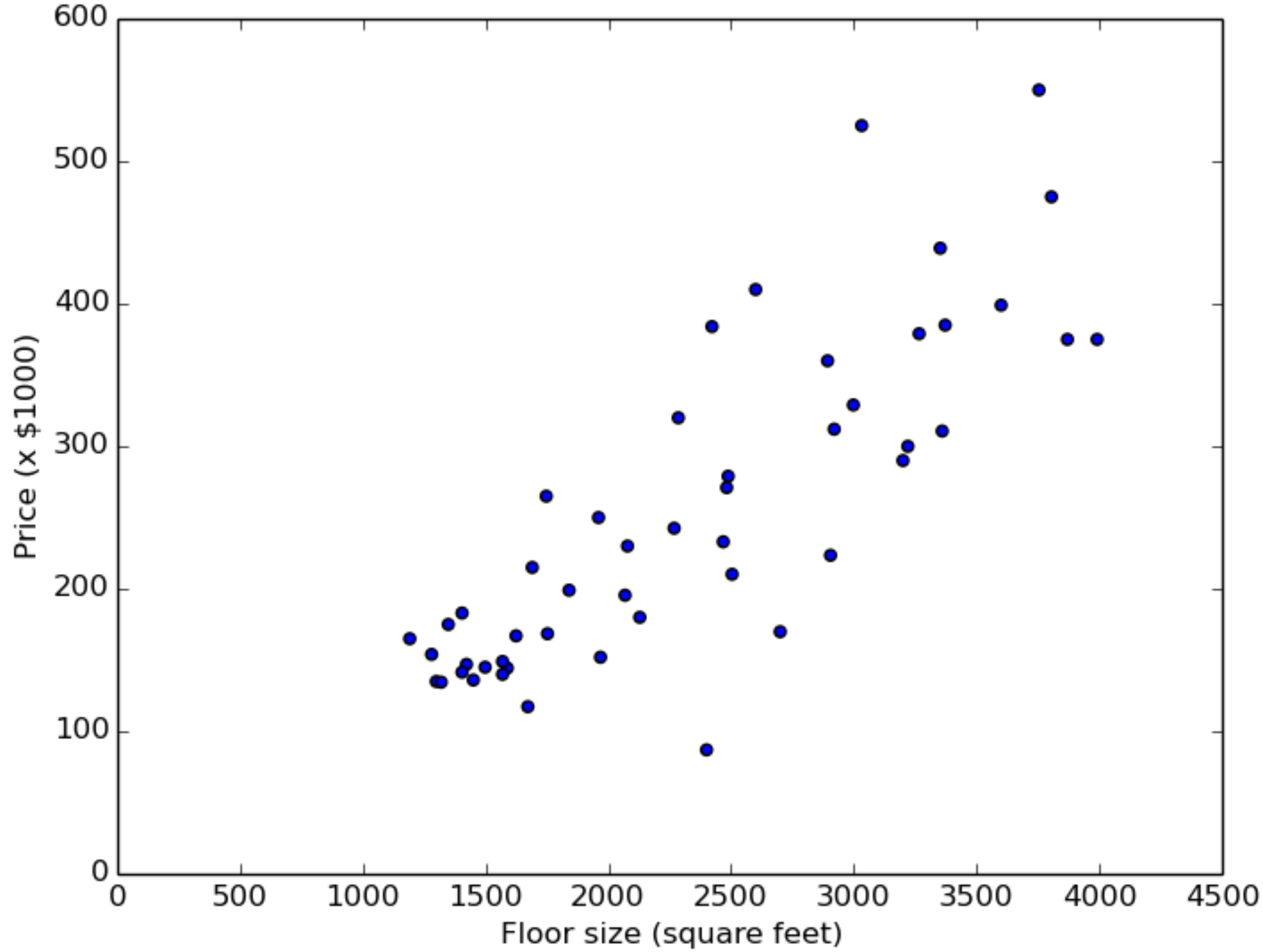
House Prices in Athens

50 houses, randomly selected from the 106 houses or townhomes:

- sold recently in Athens, OH.
- built 1990 or later.



House Prices in Athens



Parametric Approaches to Supervised Learning

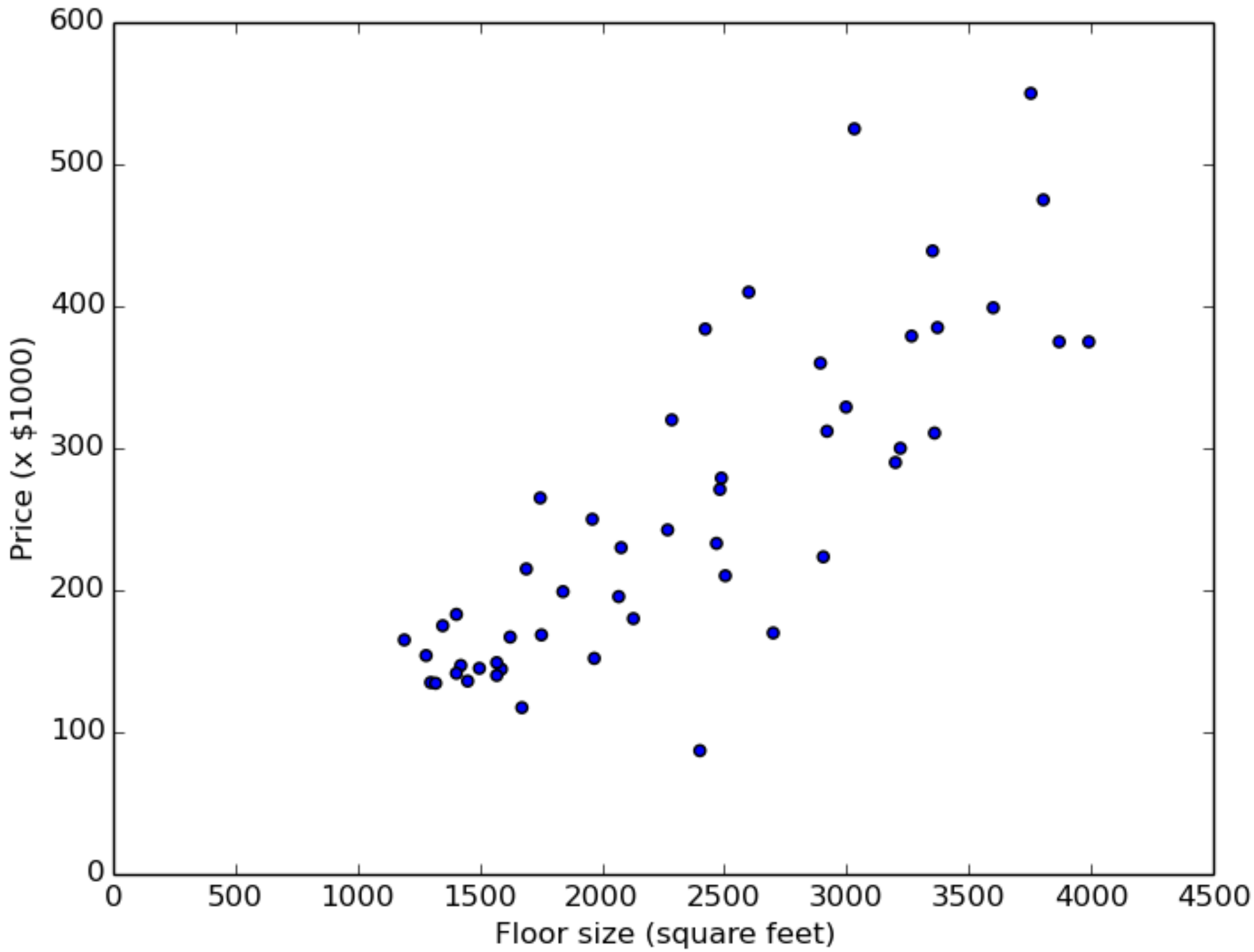
- **Task** = build a function $h(\mathbf{x})$ such that:
  - h matches t well on the training data:

    => h is able to fit data that it has seen.
  - h also matches t well on test data:

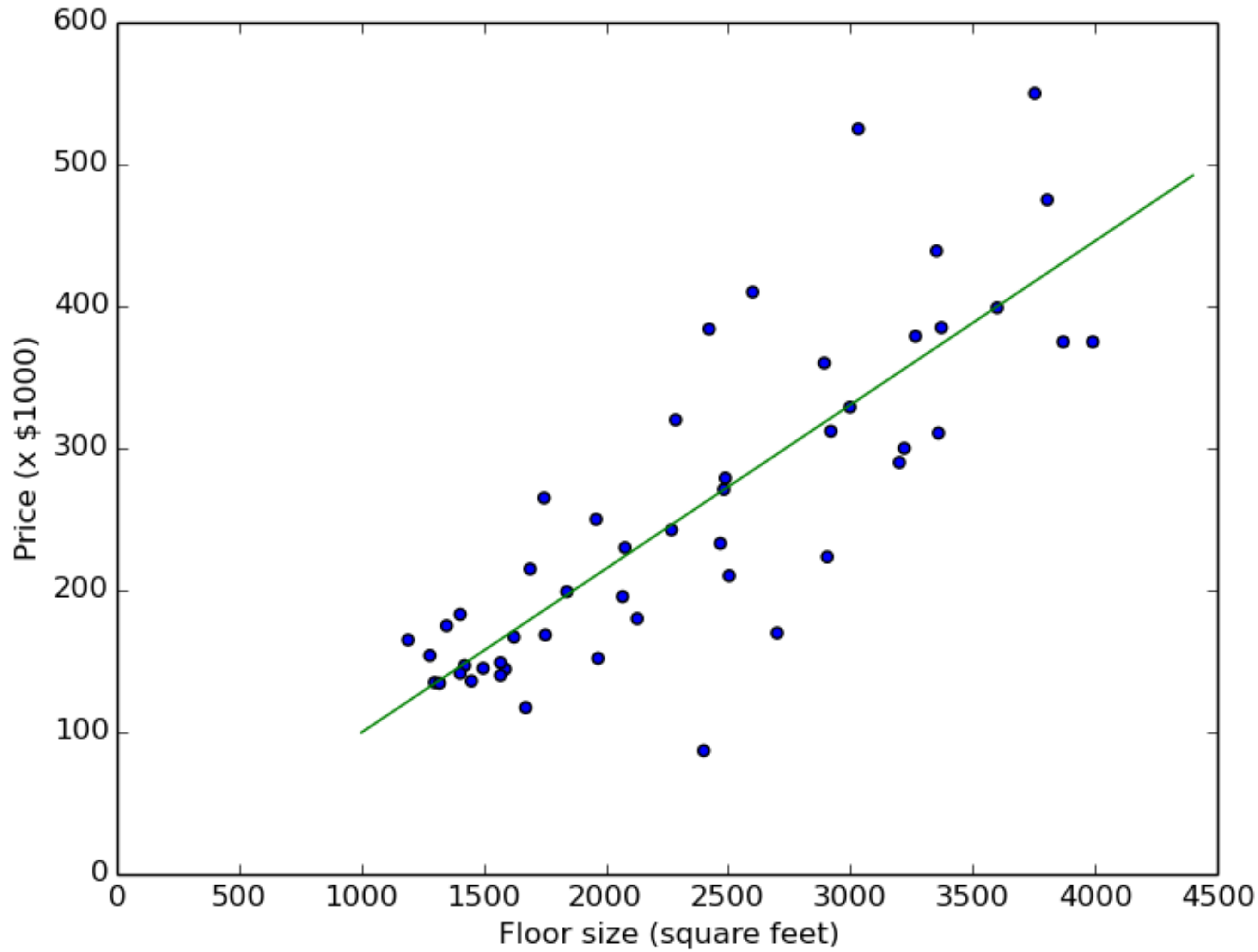
    => h is able to generalize to unseen data.

- **Task** = choose h from a "nice" *class of functions* that depend on a vector of parameters $\mathbf{w}$:
  - $h(\mathbf{x}) \equiv h_{\mathbf{w}}(\mathbf{x}) \equiv h(\mathbf{w},\mathbf{x})$
  - **what classes of functions are "nice"?**

House Prices in Athens



House Prices in Athens



Linear Regression

- Use a linear function approximation:
  - $h_{\mathbf{w}}(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} = [w_0, w_1]^{\mathrm{T}}[1, x] = w_1 x + w_0$.
    - w_0 is the intercept (or the bias term).
    - w_1 controls the slope.
  - Learning = optimization:
    - Find $\mathbf{w}$ that obtains the best fit on the training data, i.e. find $\mathbf{w}$ that minimizes the **sum of square errors**:

$$J(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N}\left(h_{\mathbf{w}}(\mathbf{x}_{\mathrm{n}}) - t_n\right)^2$$

$$\widehat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmin}}\, J(\mathbf{w})$$

Univariate Linear Regression

- Learning = finding the “right” parameters $\mathbf{w}^T = [w_0, w_1]$
  - Find $\mathbf{w}$ that minimizes an *error function* $E(\mathbf{w}) = J(\mathbf{w})$ which measures the misfit between $h(\mathbf{x}_n,\mathbf{w})$ and t_n.
  - Expect that $h(\mathbf{x},\mathbf{w})$ performing well on training examples $\mathbf{x}_n \Rightarrow$ $h(\mathbf{x},\mathbf{w})$ will perform well on arbitrary test examples $\mathbf{x} \in X$.

Inductive Learning Hyphotesis

- Sum-of-Squares error function:

$$J(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N} (h_{\mathbf{w}}(\mathbf{x}_{\mathrm{n}}) - t_n)^2$$

Minimizing Sum-of-Squares Error

- Sum-of-Squares error function:

why squared?

$$J(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N} (h_{\mathbf{w}}(\mathbf{x}_{\mathrm{n}}) - t_n)^2$$

- How do we find **w*** that minimizes $E(\mathbf{w})$?

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} J(\mathbf{w})$$

- Least Square solution is found by solving a system of 2 linear equations:

$$\boxed{w_0 N + w_1 \sum_{n=1}^{N} x_n = \sum_{n=1}^{N} t_n}$$

$$\boxed{w_0 \sum_{n=1}^{N} x_n + w_1 \sum_{n=1}^{N} x_n^2 = \sum_{n=1}^{N} t_n\, x_n}$$

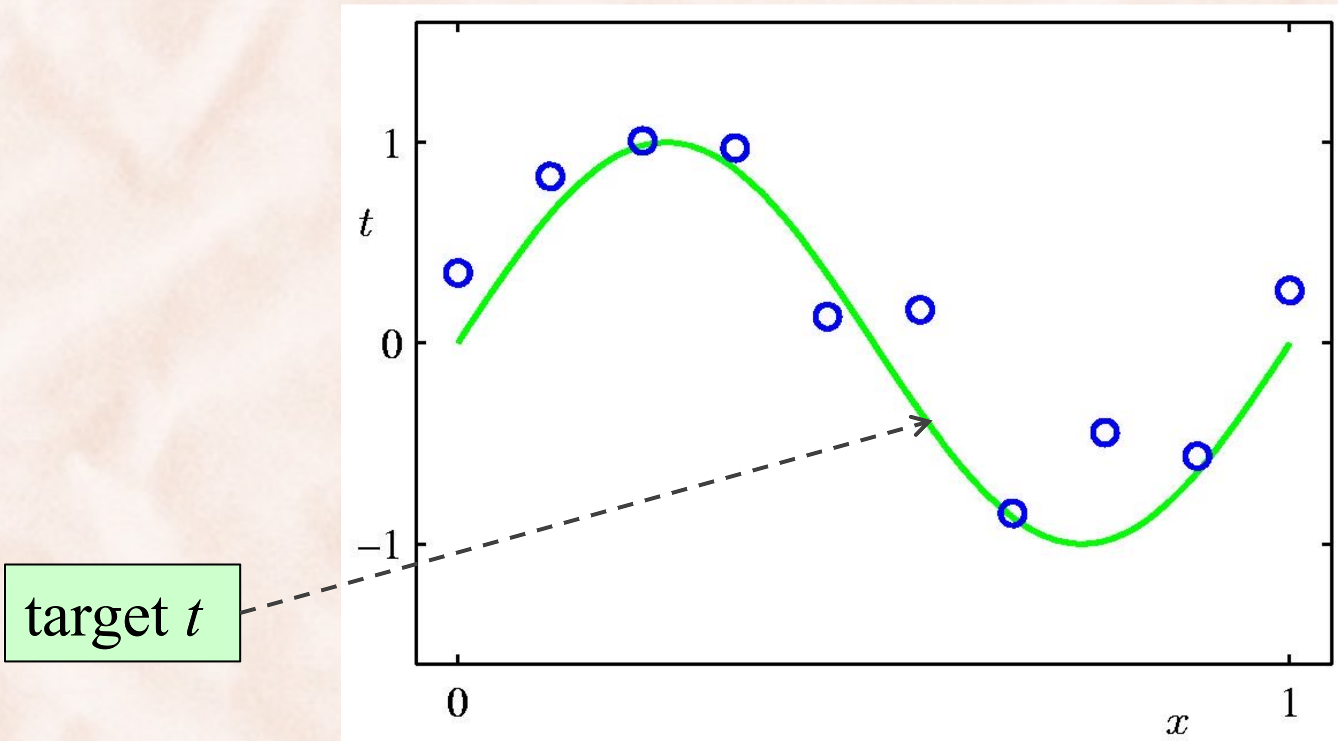
Polynomial Basis Functions

- *Q*: What if the raw feature is insufficient for good performance?
  - Example: non-linear dependency between label and raw feature.

- *A*: Engineer / Learn higher-level features, as functions of the raw feature.

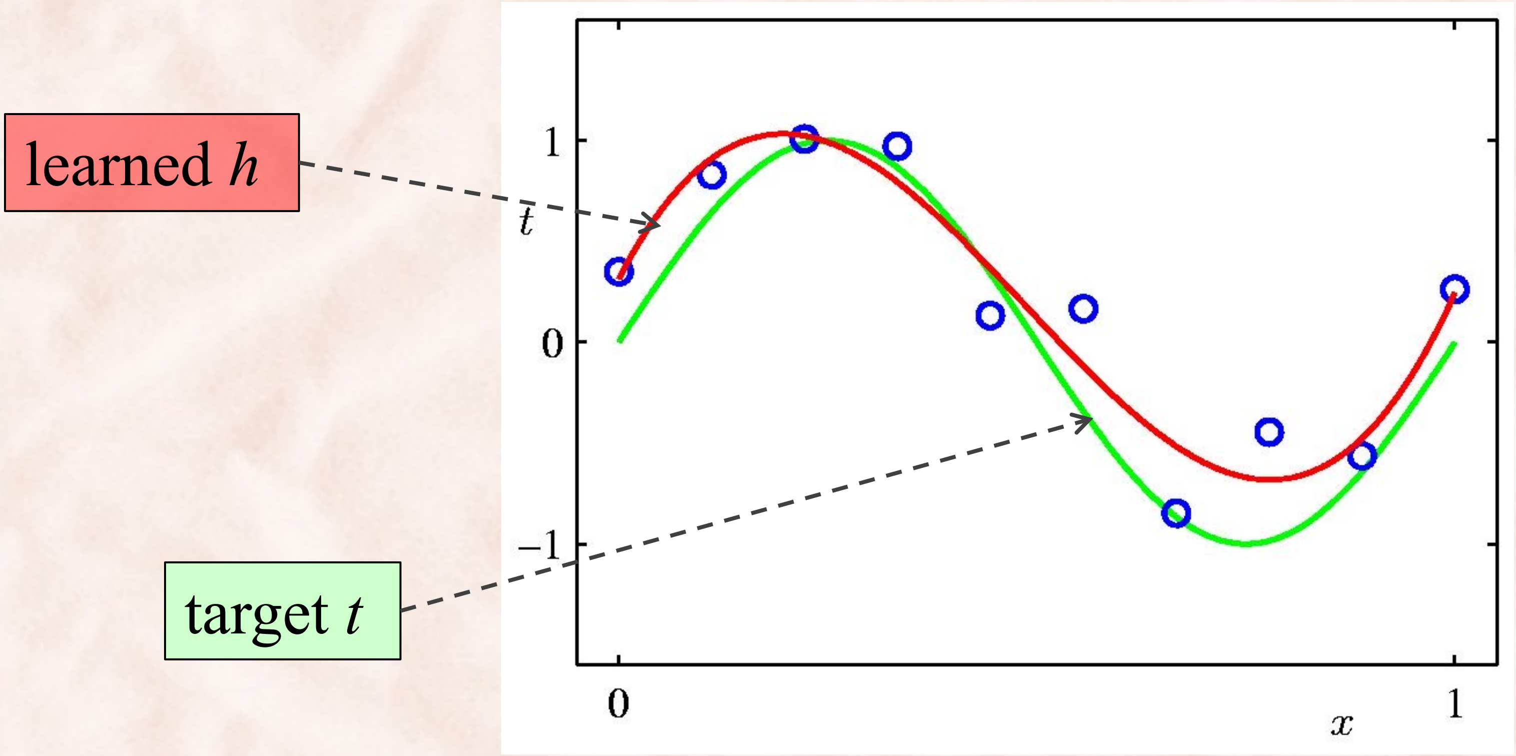
- **Polynomial curve fitting**:
  - Add new features, as polynomials of the original feature.

Regression: Curve Fitting



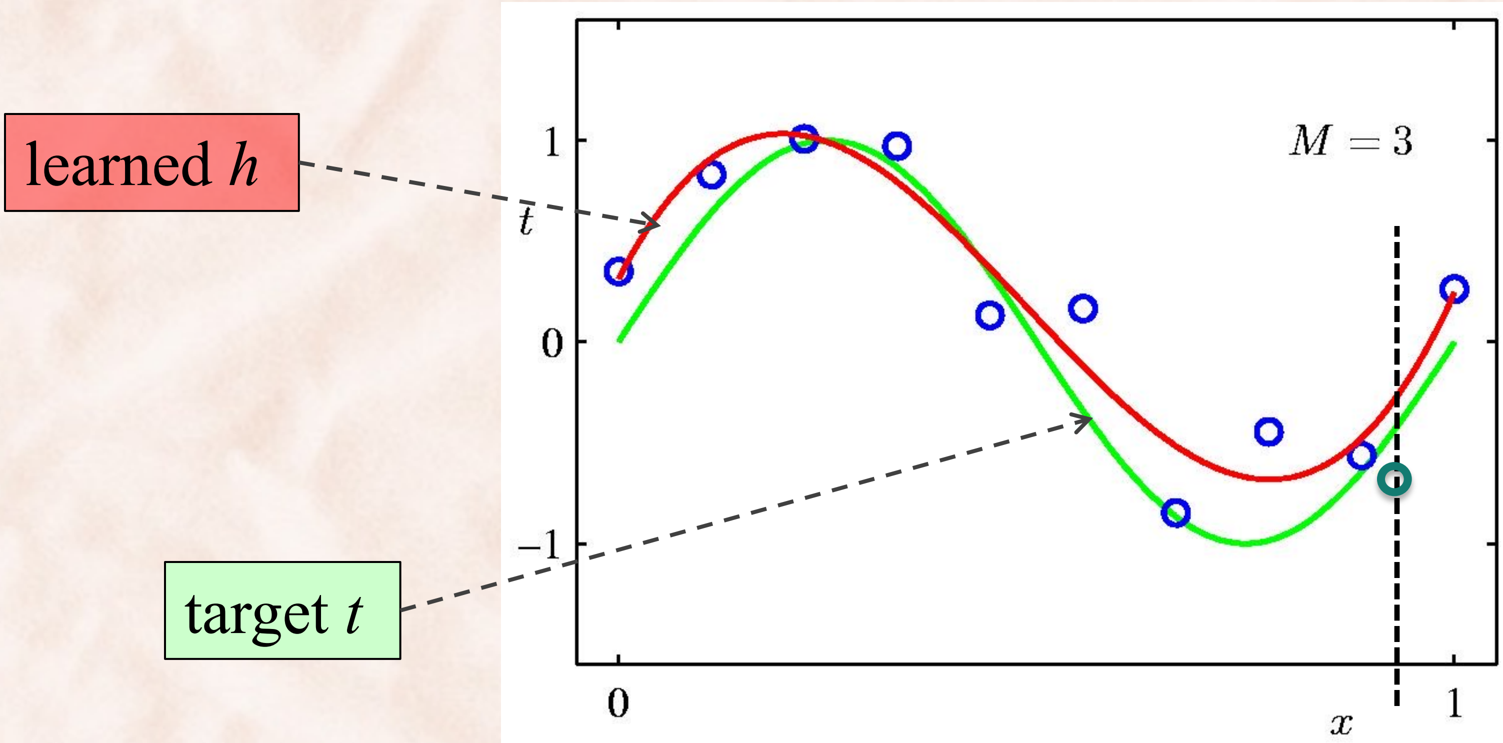
- **Training**: Build a function $h(x)$, based on (noisy) training examples (x_1,t_1), (x_2,t_2), … (x_N,t_N)

Regression: Curve Fitting



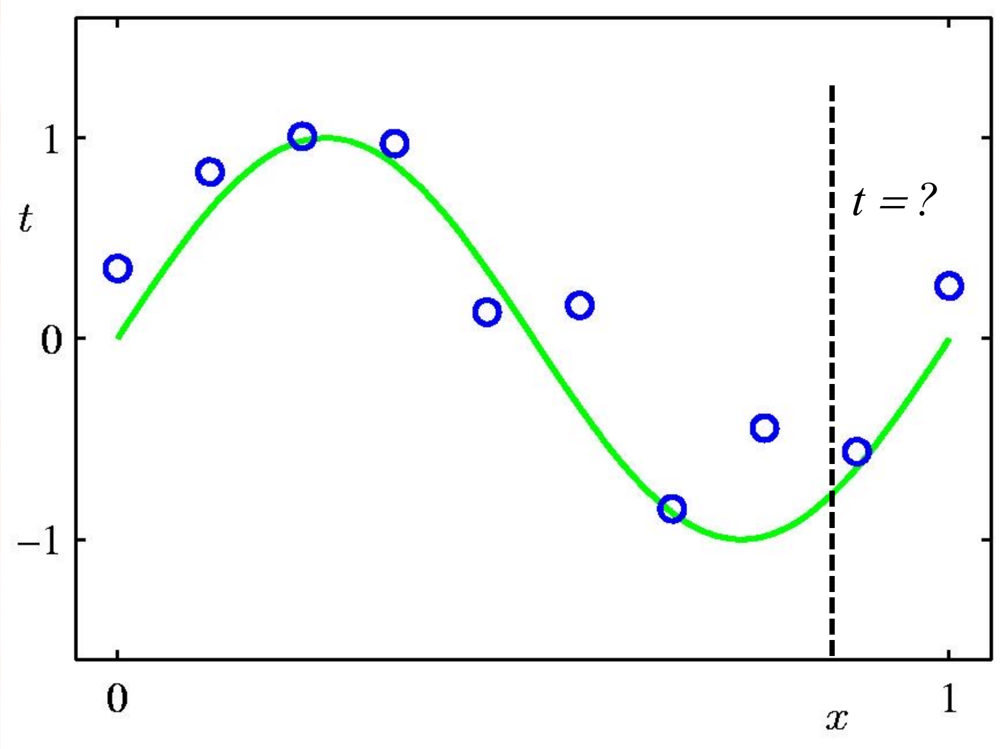
- **Training**: Build a function $h(x)$, based on (noisy) training examples (x_1,t_1), (x_2,t_2), … (x_N,t_N)

Regression: Curve Fitting



- **Testing**: for arbitrary (unseen) instance $x \in X$, compute target output $h(x)$; want it to be close to $t(x)$.

Regression: Polynomial Curve Fitting



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

parameters *features*

Polynomial Curve Fitting

- Parametric model:

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

- Polynomial curve fitting is (Multiple) Linear Regression:

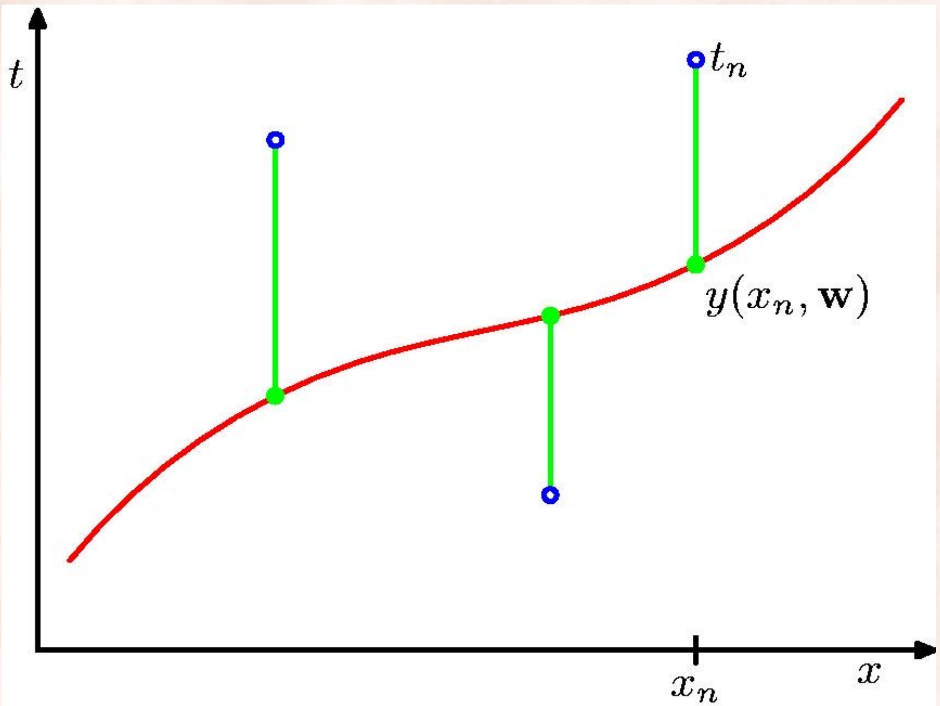
$\mathbf{x} = [1, x, x^2, ..., x^M]^T$

$h(x) = h(\mathbf{x},\mathbf{w}) = h_{\mathbf{w}}(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$

- **Learning** = minimize the Sum-of-Squares error function:

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} J(\mathbf{w}) \qquad J(\mathbf{w}) = \frac{1}{2N} \sum_{n=1}^{N} (h_{\mathbf{w}}(\mathbf{x}_n) - t_n)^2$$

Sum-of-Squares Error Function



$$J(\mathbf{w}) = \frac{1}{2N} \sum_{n=1}^{N} (h_{\mathbf{w}}(\mathbf{x}_n) - t_n)^2$$

- How to find **w*** that minimizes $E(\mathbf{w})$, i.e. $\mathbf{w}^* = \arg\min_{\mathbf{w}} E(\mathbf{w})$
- Solve $\nabla J(\mathbf{w}) = 0$.

Polynomial Curve Fitting

- *Least Square* solution is found by solving a set of M + 1 linear equations:

$$A\mathbf{w} = T$$

$$\sum_{j=0}^{M} A_{ij} w_j = T_i \text{ , where } A_{ij} = \sum_{n=1}^{N} x_n^{i+j} \text{, and } T_i = \sum_{n=1}^{N} t_n x_n^i$$

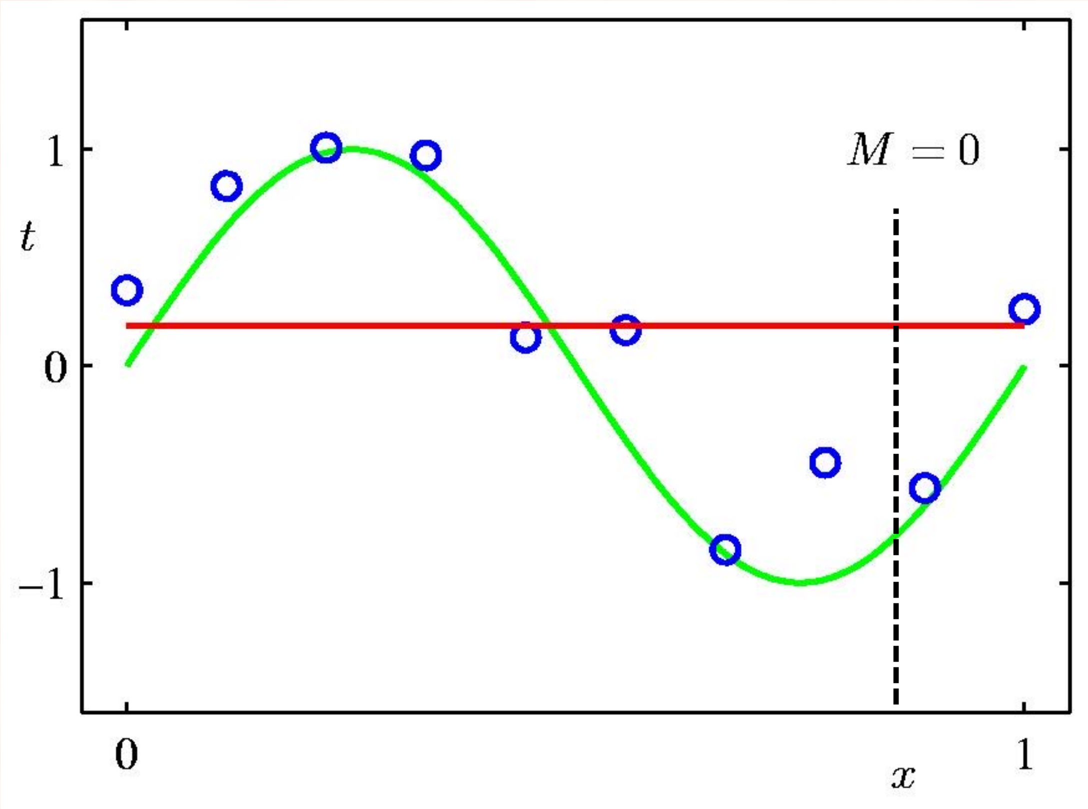
- Prove it.

Polynomial Curve Fitting

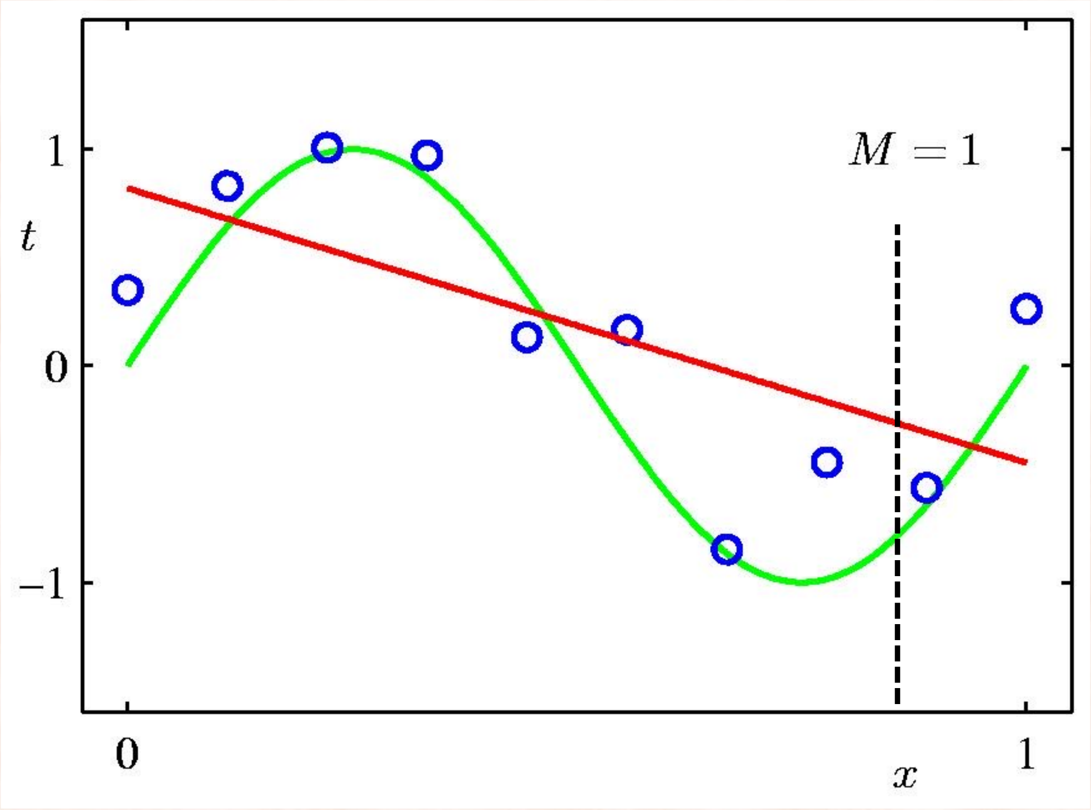
- Generalization = how well the parameterized $h(x,\mathbf{w})$ performs on arbitrary (unseen) test instances $x \in X$.

- Generalization performance depends on the value of M.

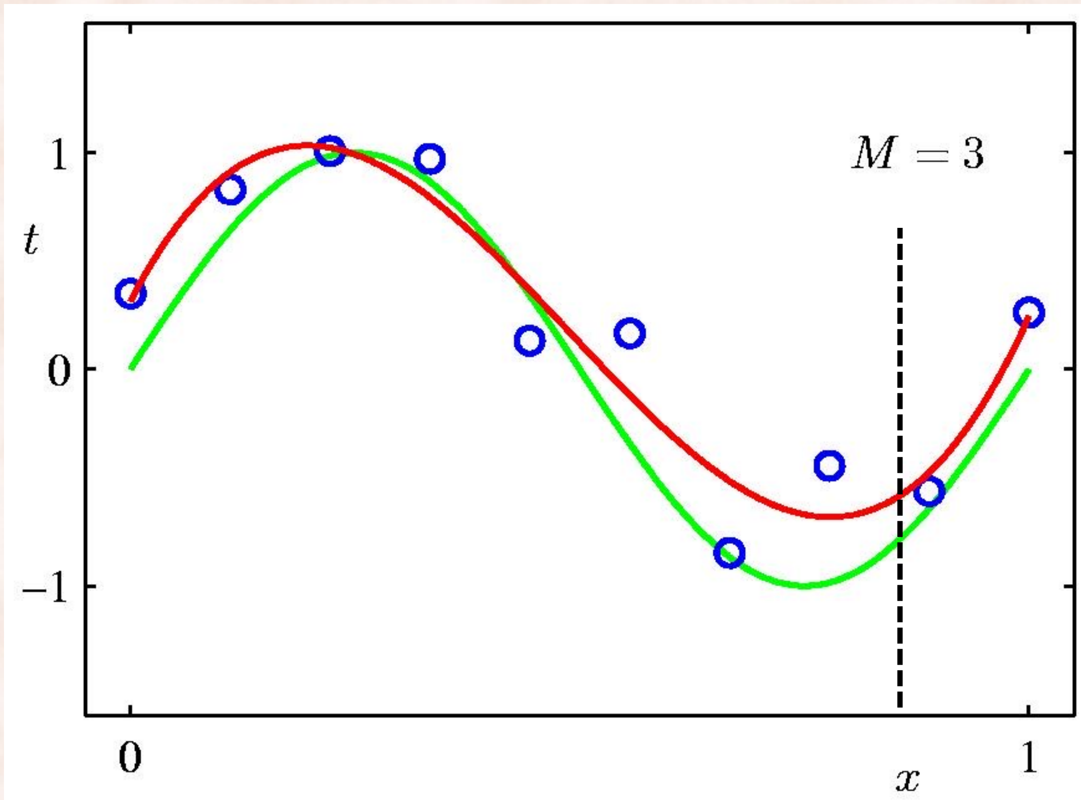
0^{th} Order Polynomial



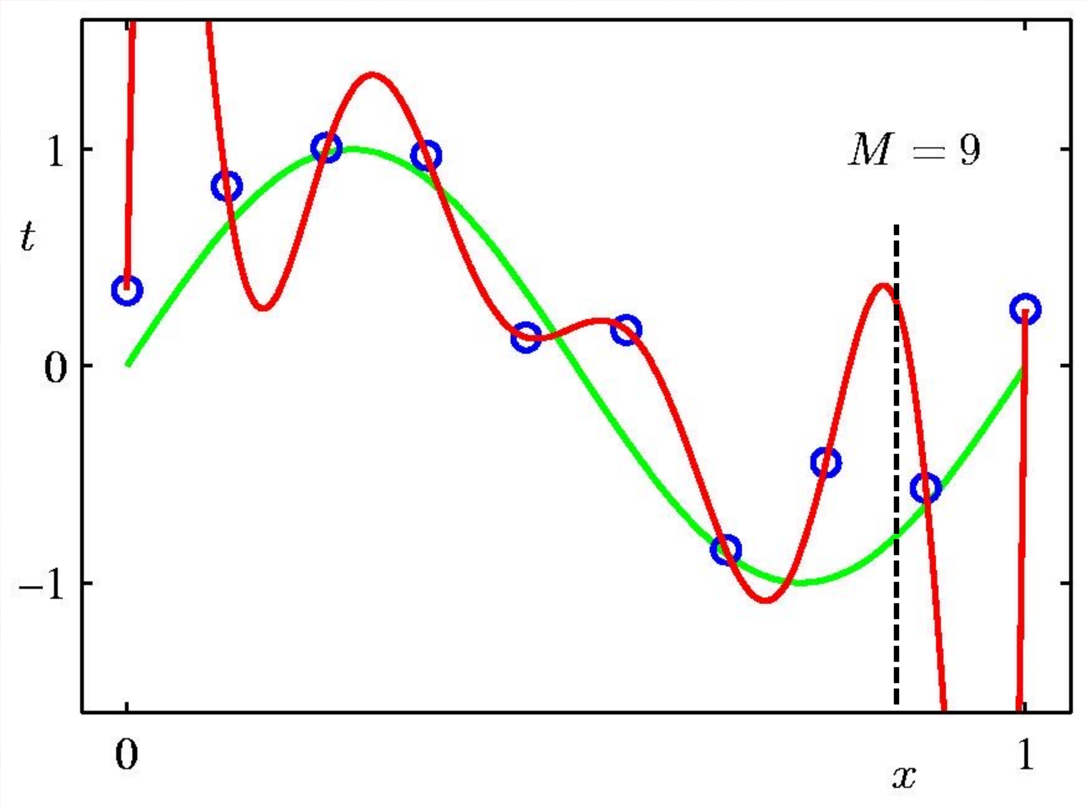
1^{st} Order Polynomial



3^{rd} Order Polynomial



9^{th} Order Polynomial



Polynomial Curve Fitting

- Model Selection: choosing the order M of the polynomial.
  - Best generalization obtained with $M = 3$.
  - $M = 9$ obtains poor generalization, even though it fits training examples perfectly:
    - But $M = 9$ polynomials subsume $M = 3$ polynomials!

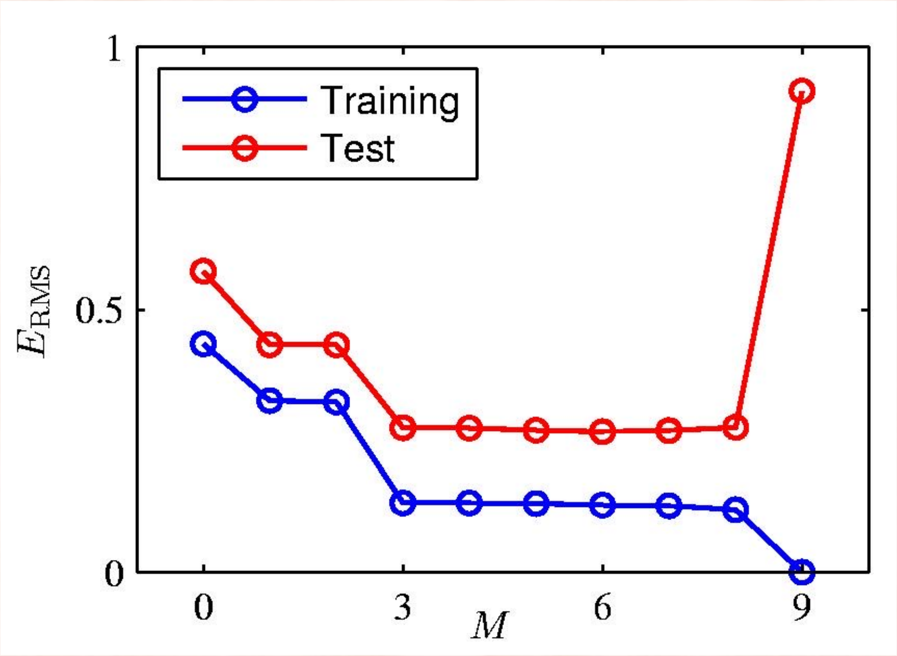
- Overfitting $\equiv$ good performance on training examples, poor performance on test examples.

Overfitting

- Measure fit using the Root-Mean-Square (RMS) error (RMSE):

$$E_{RMS}(\mathbf{w}) = \sqrt{\frac{\sum_n \left(\mathbf{w}^T \mathbf{x}_n - t_n\right)^2}{N}}$$

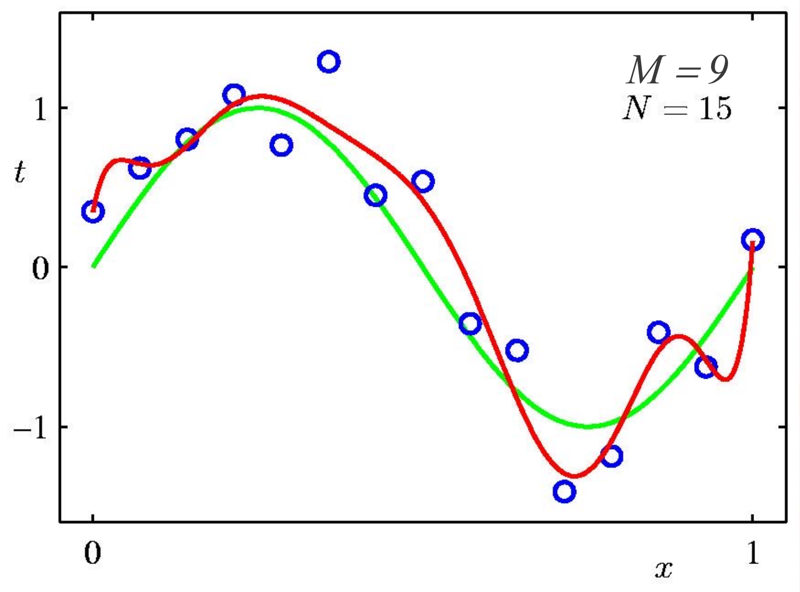
- Use 100 random test examples, generated in the same way:

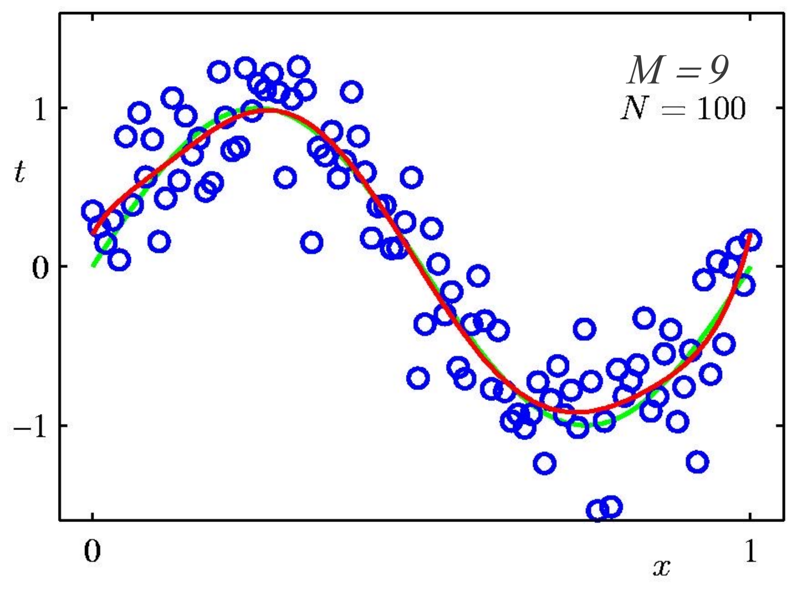


Over-fitting and Parameter Values

	$M = 0$	$M = 1$	$M = 3$	$M = 9$
$w_0^\star$	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

Overfitting vs. Data Set Size





- More training data ⇒ less overfitting.
- What if we do not have more training data?
  - Use **regularization**.

Regularization

- **Parameter norm penalties** (term in the objective).
- Limit parameter norm (constraint).
- Dataset augmentation.
- Dropout.
- Ensembles.
- Semi-supervised learning.
- Early stopping.
- Noise robustness.
- Sparse representations.
- Adversarial training.

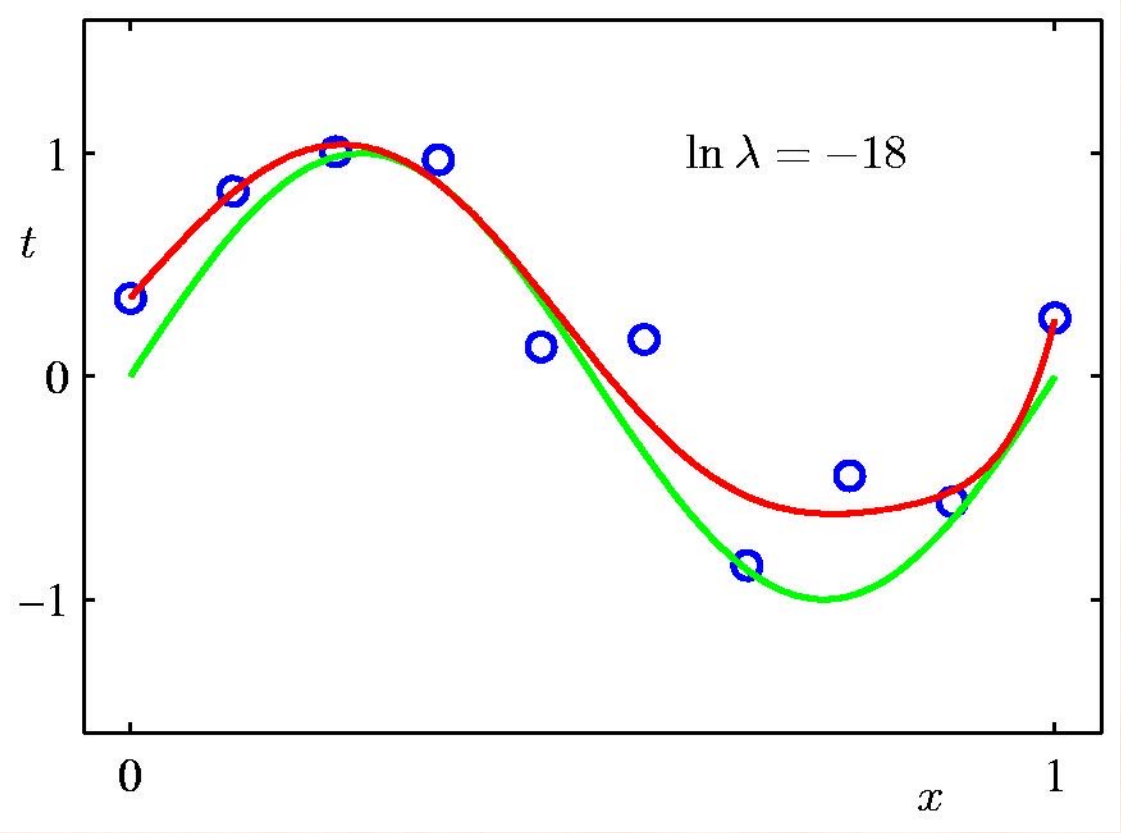
Regularization

- Penalize large parameter values:

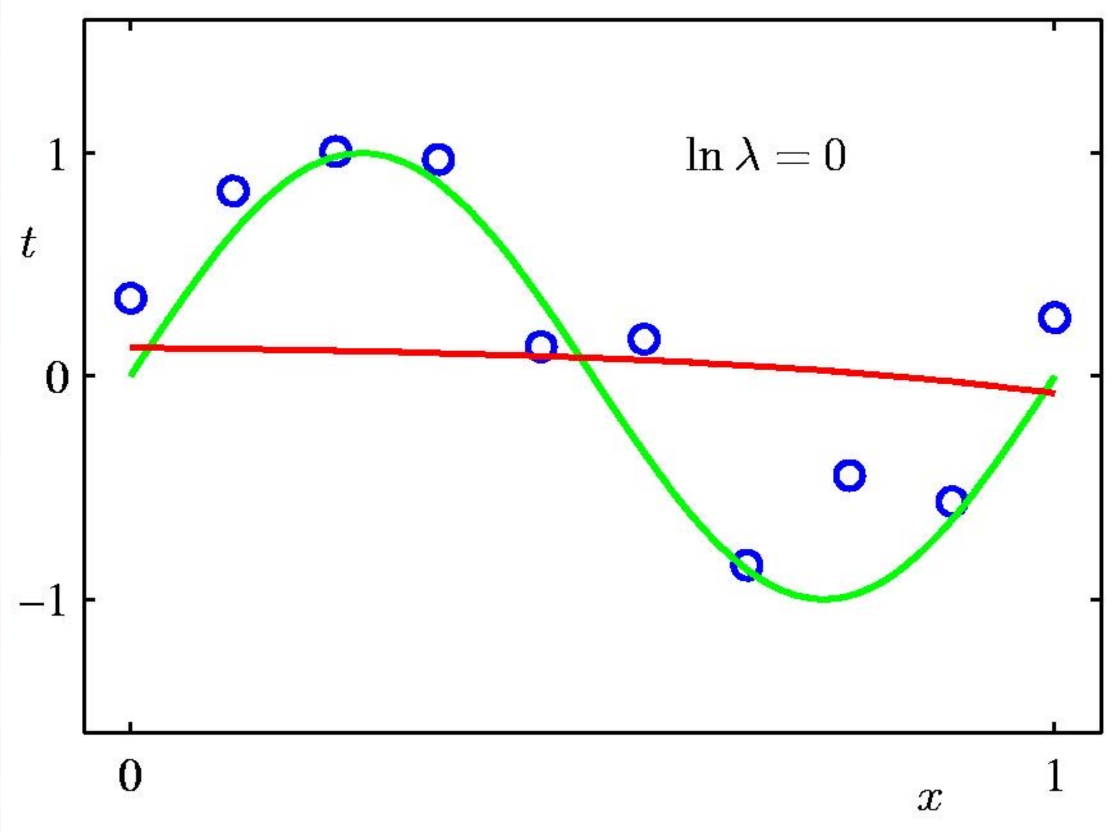
$$J(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N} (h_{\mathbf{w}}(\mathbf{x}_{\mathrm{n}}) - t_n)^2 + \underbrace{\frac{\lambda}{2}\|\mathbf{w}\|^2}_{\textit{regularizer}}$$

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} E(\mathbf{w})$$

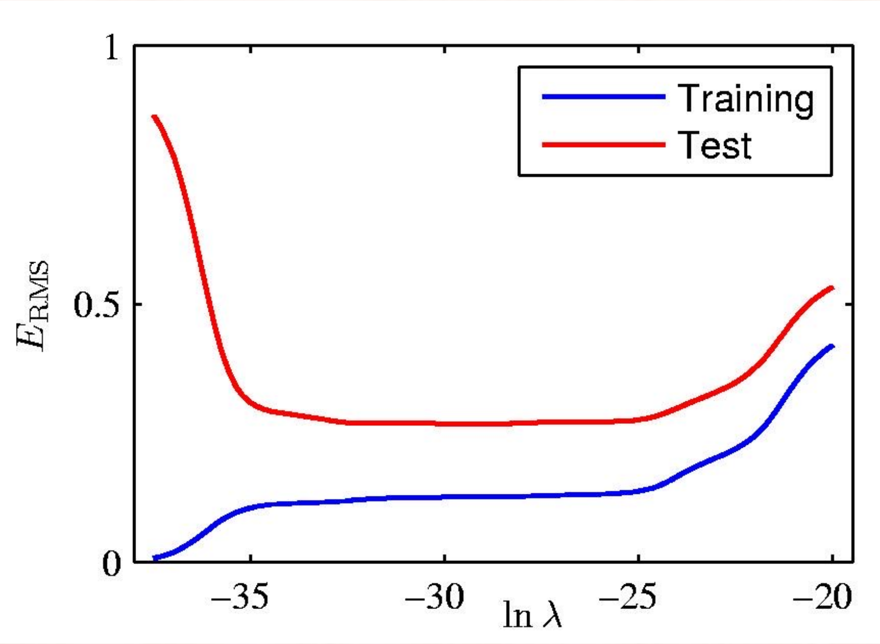
9th Order Polynomial with Regularization



9^{th} Order Polynomial with Regularization



Training & Test error vs. $\ln \lambda$

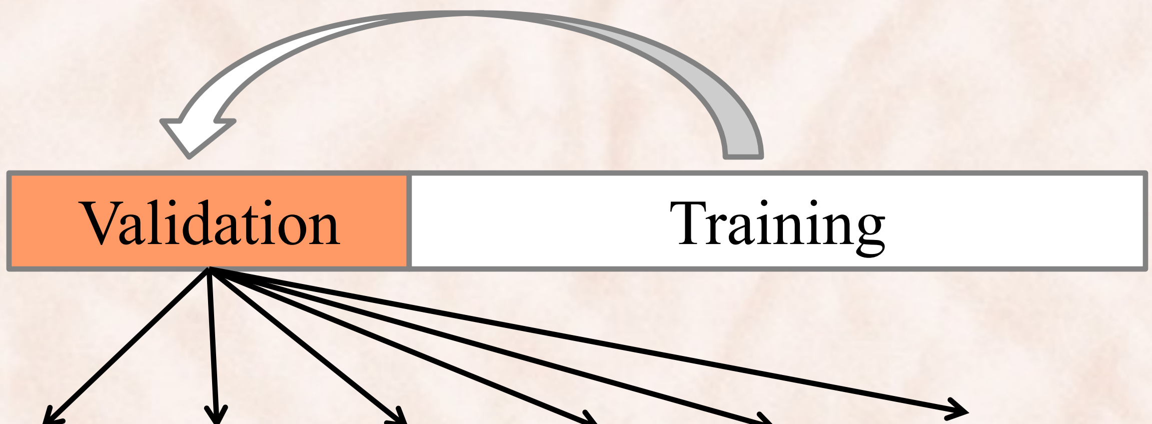


How do we find the optimal value of λ?

Model Selection

- Put aside an independent *validation set*.
- Select parameters giving best performance on validation set.

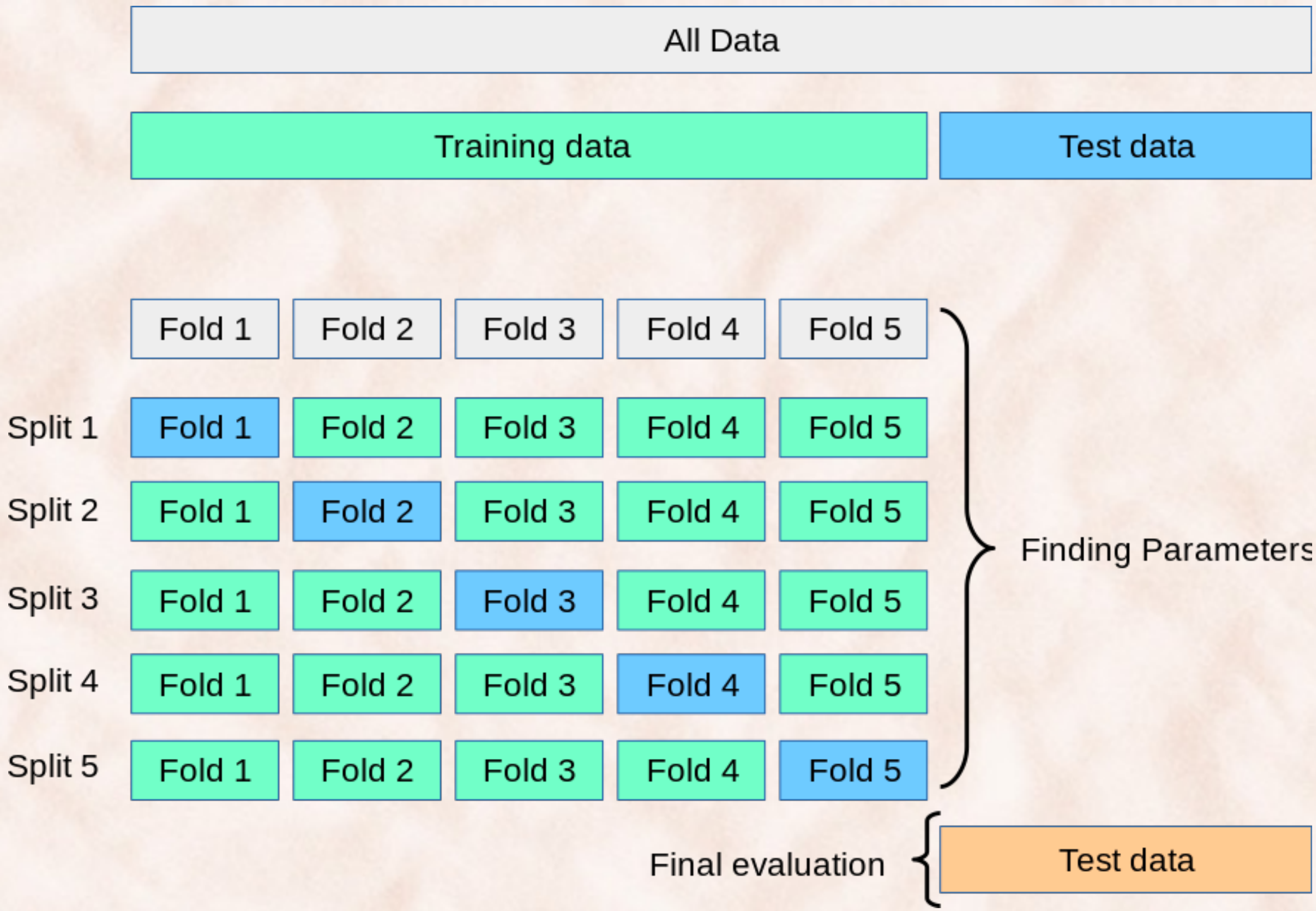
$$\ln \lambda \in \{-40, -35, -30, -25, -20, -15\}$$



$\ln \lambda$	-40	-35	-30	-25	-20	-15
E_{RMS}	1.05	0.30	0.25	0.27	0.52	0.55

K-fold Cross-Validation

https://scikit-learn.org/stable/modules/cross_validation.html



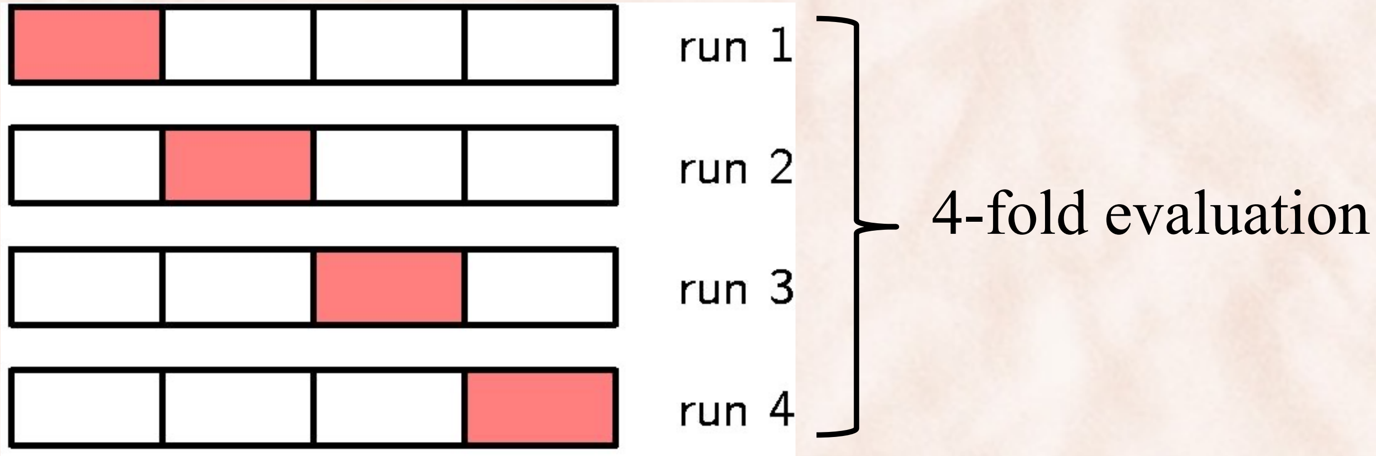
K-fold Cross-Validation

- Split the training data into K folds and try a wide range of tunning parameter values:
  - split the data into K folds of roughly equal size
  - iterate over a set of values for λ
    - iterate over k = 1, 2, ..., K
      - use all folds except k for training
      - validate (calculate test error) in the k-th fold
    - error[λ] = average error over the K folds
  - choose the value of λ that gives the smallest error.

https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LassoCV.html

Model Evaluation

- K-fold evaluation:
  - randomly partition dataset in K equally sized subsets $P_1, P_2, \ldots P_k$
  - for each fold i in {1, 2, …, k}:
    - test on P_i, train on $P_1 \cup \ldots \cup P_{i-1} \cup P_{i+1} \cup \ldots \cup P_k$
  - compute average error/accuracy across K folds.



Multiple Linear Regression

- *Q*: What if the raw feature is insufficient for good performance?
  - Example: house prices depend not only on *floor size*, but also number of *bedrooms*, *age*, *location*, …

- *A*: Use **Multiple Linear Regression**.

Multiple Linear Regression

- Polynomial curve fitting:

  $\mathbf{x} = [1, x, x^2, \ldots, x^M]^T$

  $\quad = [x_0, x_1, \ldots, x_M]^T$

  $h(x) = h(\mathbf{x},\mathbf{w}) = \mathbf{w}^T\mathbf{x}$

- **Multiple linear regression**:

  $\mathbf{x} = [x_0, x_1, \ldots, x_M]^T$

  $h(x) = h(\mathbf{x},\mathbf{w}) = \mathbf{w}^T\mathbf{x}$

- Training examples: $(\mathbf{x}^{(1)},t_1), (\mathbf{x}^{(2)},t_2), \ldots (\mathbf{x}^{(N)},t_N)$

Multiple Linear Regression

- **Learning** = minimize the Sum-of-Squares error function:

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} J(\mathbf{w}) \qquad J(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N}\left(h_{\mathbf{w}}(\mathbf{x}^{(n)}) - t_n\right)^2$$

- Computing the gradient $\nabla J(\mathbf{w})$ and setting it to zero:

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

- Solving for $\mathbf{w}$ yields $\mathbf{w} = \underbrace{\left(\mathrm{X}^{\mathrm{T}}\mathrm{X}\right)^{-1}\mathrm{X}^{\mathrm{T}}}_{\text{The Moore-Penrose pseudo-inverse of X.}}\mathbf{t}$
  - Prove it.

Normal Equations

- Solution is $\mathbf{w} = \left(\mathrm{X}^{\mathrm{T}}\mathrm{X}\right)^{-1}\mathrm{X}^{\mathrm{T}}\mathbf{t}$

- X is the data matrix, or the **design matrix**:

$$X = \begin{pmatrix} \mathbf{x}^{(1)^{\mathrm{T}}} \\ \mathbf{x}^{(2)^{\mathrm{T}}} \\ \dots \\ \dots \\ \mathbf{x}^{(N)^{\mathrm{T}}} \end{pmatrix} = \begin{pmatrix} x_0^{(1)} & x_1^{(1)} & \dots & x_M^{(1)} \\ x_0^{(2)} & x_1^{(2)} & \dots & x_M^{(2)} \\ & & \dots & \\ & & \dots & \\ x_0^{(N)} & x_1^{(N)} & \dots & x_M^{(N)} \end{pmatrix}$$

For poly fit:

$$\begin{pmatrix} 1 & x_1 & x_1^2 & \dots & x_1^M \\ 1 & x_2 & x_2^2 & \dots & x_2^M \\ & & \dots & & \\ & & \dots & & \\ 1 & x_N & x_N^2 & \dots & x_N^M \end{pmatrix}$$

- $\mathbf{t} = [t_1, t_2, \dots, t_{\mathrm{N}}]^{\mathrm{T}}$ is the vector of labels.

Ridge Regression

- Multiple linear regression with L2 regularization:

$$J(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N} (h_{\mathbf{w}}(\mathbf{x}_{\mathrm{n}}) - t_n)^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} J(\mathbf{w})$$

- Solution is $\mathbf{w} = \left(\lambda N\mathbf{I} + \mathrm{X}^{\mathrm{T}}\mathrm{X}\right)^{-1}\mathrm{X}^{\mathrm{T}}\mathbf{t}$
  - Prove it.

Regularization: Ridge vs. Lasso

- Ridge regression:

$$J(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N} (h_{\mathbf{w}}(\mathbf{x}_{\mathrm{n}}) - t_n)^2 + \frac{\lambda}{2}\sum_{j=1}^{M} w_j^2$$

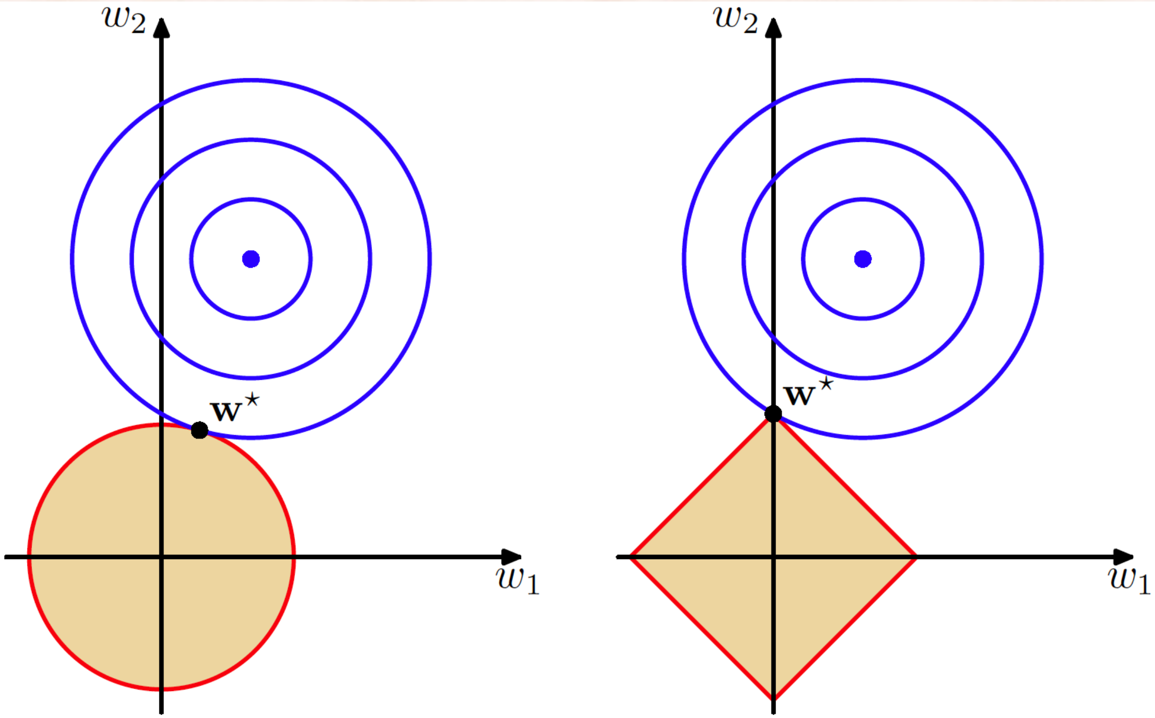
- Lasso:

$$J(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N} (h_{\mathbf{w}}(\mathbf{x}_{\mathrm{n}}) - t_n)^2 + \frac{\lambda}{2}\sum_{j=1}^{M} |w_j|$$

  – If λ is sufficiently large, some of the coefficients w_j are driven to 0 => *sparse* model.

Regularization: Ridge vs. Lasso

Figure 3.4 Plot of the contours of the unregularized error function (blue) along with the constraint region (3.30) for the quadratic regularizer $q = 2$ on the left and the lasso regularizer $q = 1$ on the right, in which the optimum value for the parameter vector $\mathbf{w}$ is denoted by $\mathbf{w}^{\star}$. The lasso gives a sparse solution in which $w_1^{\star} = 0$.



Regularization

- Regularization alleviates overfitting when using models with high capacity (e.g. high degree polynomials):
  - Want high capacity because we do not know how complicated the data is.

- *Q*: Can we achieve high capacity when doing curve fitting without using high degree polynomials?

- *A*: Use piecewise polynomial curves.
  - Example: **Cubic spline smoothing**.

Cubic Spline Smoothing

- **Cubic spline smoothing** is a regularized version of cubic spline interpolation.
  - Cubic spline interpolation: given n points $\{(x_i, y_i)\}$, connect adjacent points using cubic functions S_i, requiring that the spline and its first and second derivative remain continuous at all points:

$$S_i(x) = a_i(x-x_i)^3 + b_i(x-x_i)^2 + c_i(x-x_i) + d_i, \forall x \in [x_i, x_{i+1}]$$

  - **Cubic spline smoothing**: the spline S = $\{S_i\}$ is allowed to deviate from the data points and has low curvature => constrained optimization problem with objective:

$$L = \sum_{i=1}^{n} \frac{w_i}{Z}(S_i(x_i) - y_i)^2 + \frac{\lambda}{x_n - x_1} \int_{x_1}^{x_n} |S''(x)|^2 dx$$

$$w_i = \begin{cases} C, & \text{if } (x_i, y_i) \text{ is a significant local optima} \\ 1, & \text{otherwise} \end{cases}$$

Cubic Spline Smoothing

http://ace.cs.ohio.edu/~razvan/papers/icmla11.pdf

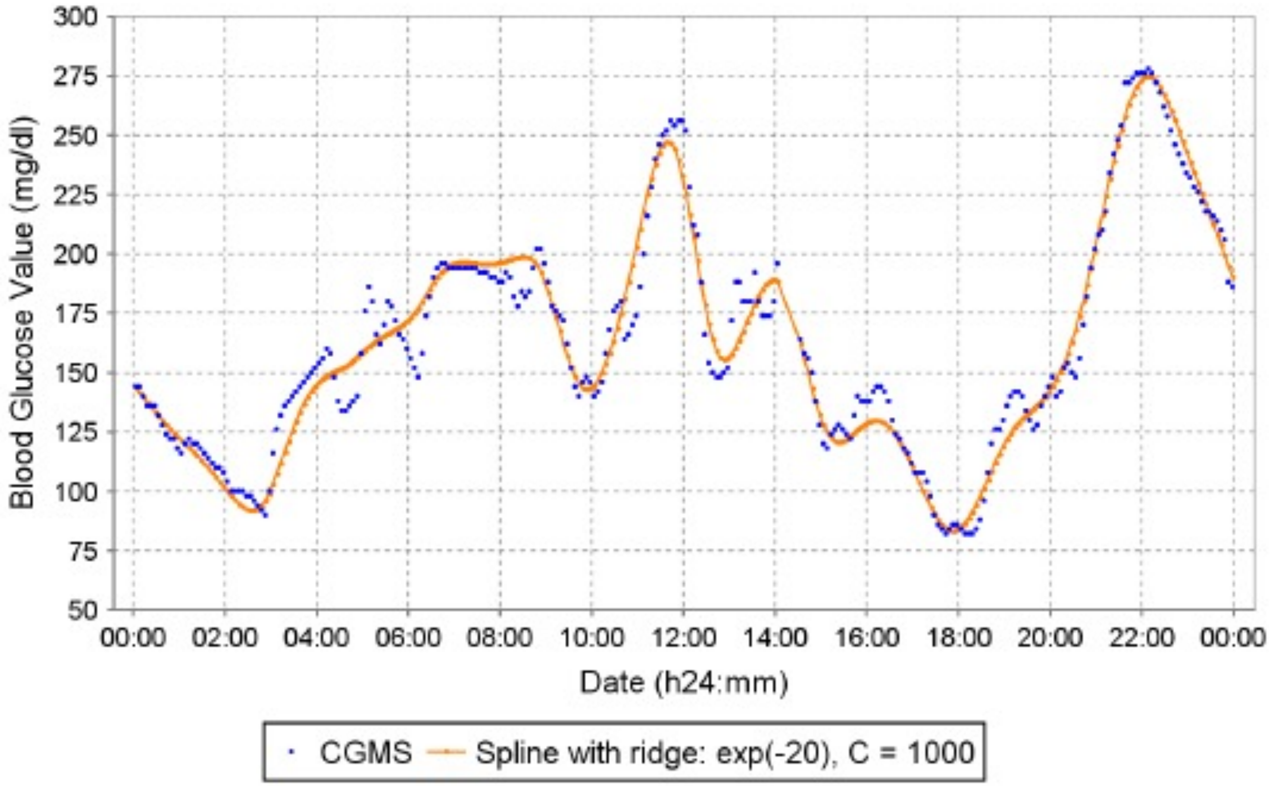
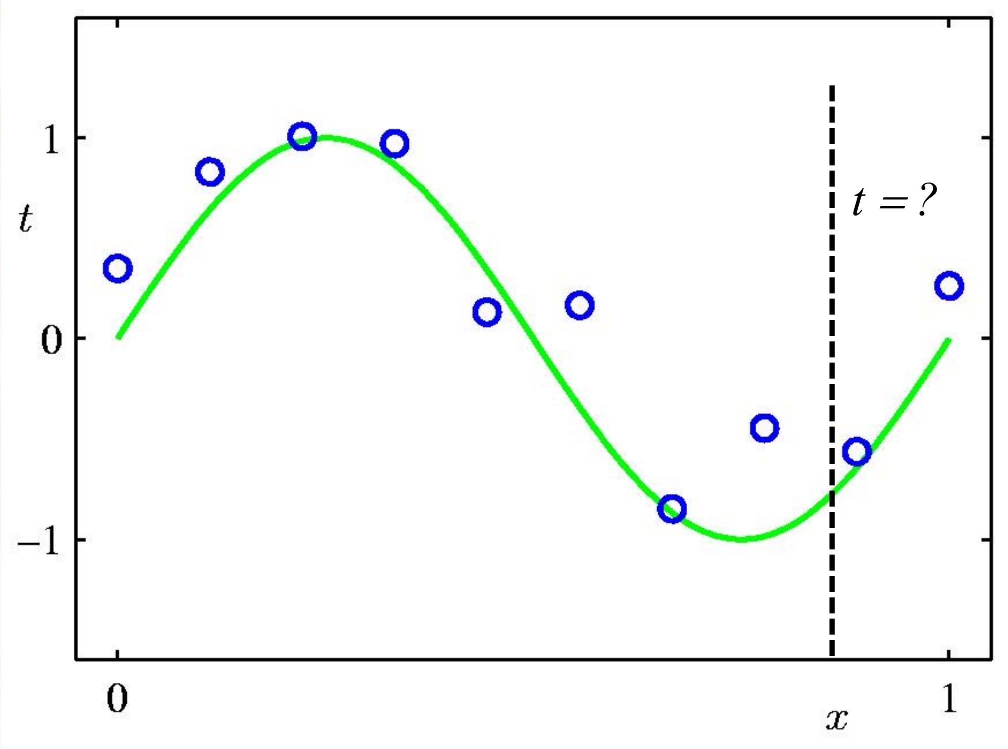


Fig. 3. Cubic spline smoothing with $\lambda = e^{-20}$ and $C = 1000$.

Polynomial Curve Fitting (Revisited)



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

parameters   *features*

Generalization: Basis Functions as Features

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

- Typically $\varphi_0(\mathbf{x}) = 1$, so that w_0 acts as a bias.

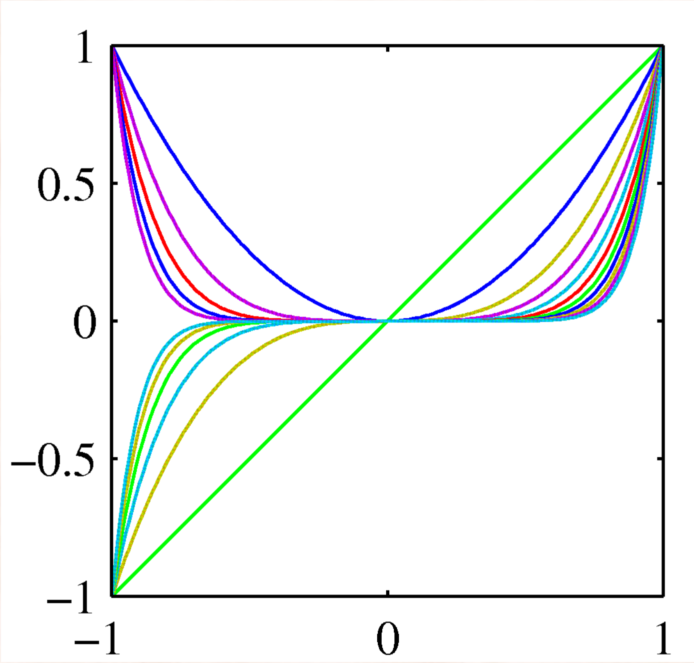
- In the simplest case, use linear basis functions : $\varphi_d(\mathbf{x}) = x_d$.

Linear Basis Function Models (1)

- Polynomial basis functions:

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

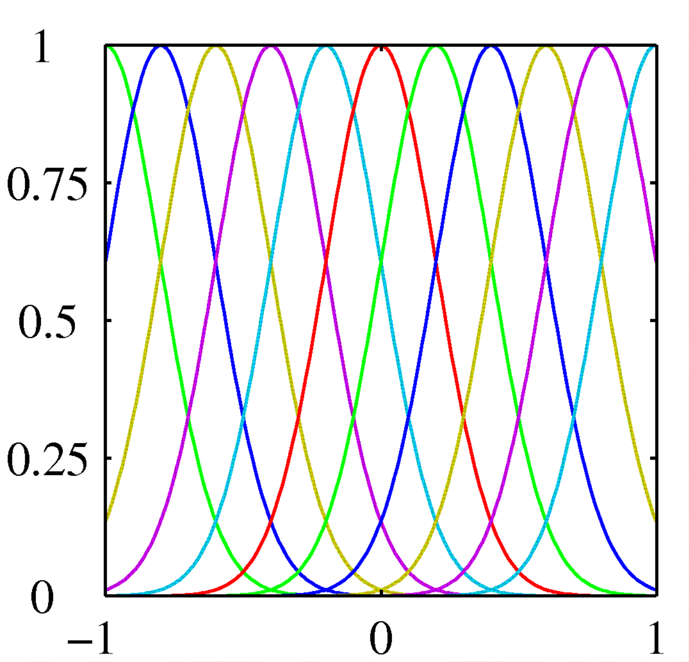
- Global behavior:
  - a small change in x affect all basis functions.



Linear Basis Function Models (2)

- Gaussian basis functions:

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



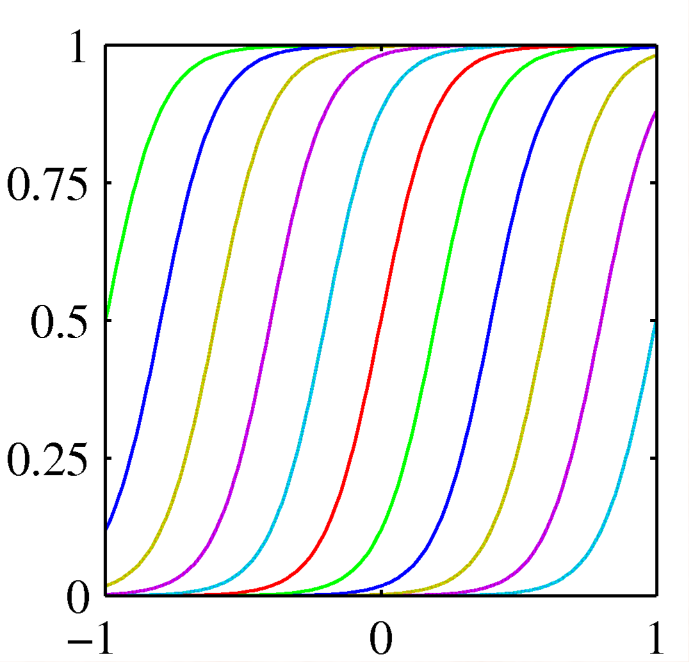
- Local behavior:
  - a small change in x only affects nearby basis functions.
  - μ_j and s control location and scale (width).

Linear Basis Function Models (3)

- Sigmoidal basis functions:

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

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



- Local behavior:
  - a small change in x only affect nearby basis functions.
  - μ_j and s control location and scale (slope).

Solving Linear Regression using Maximum Likelihood

Least Squares <=> Maximum Likelihood (1)

- Assume observations from a deterministic function y with added Gaussian noise ϵ:

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

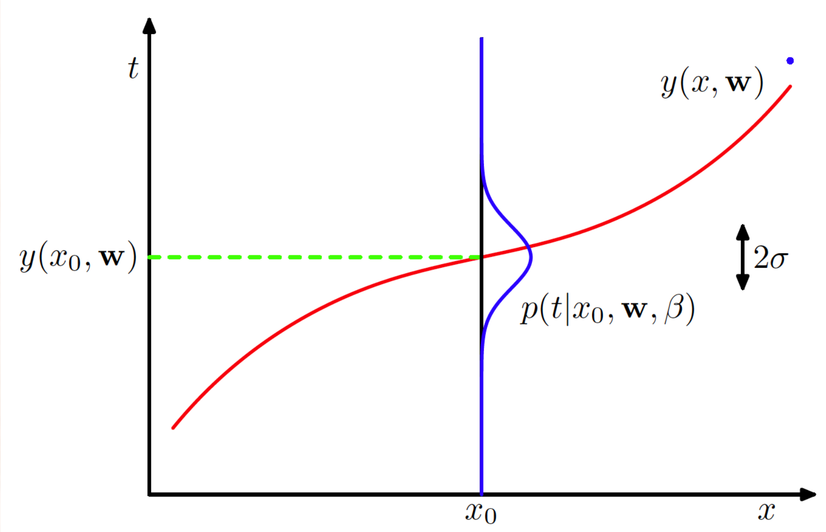
where $p(\epsilon|\beta) = \mathcal{N}(\epsilon|0, \beta^{-1})$

$$= \frac{\sqrt{\beta}}{\sqrt{2\pi}}\, e^{-\beta\frac{\epsilon^2}{2}}$$

which is the same as saying:

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

$$= \frac{\sqrt{\beta}}{\sqrt{2\pi}}\, e^{-\beta\frac{(t-y(\mathbf{x},\mathbf{w}))^2}{2}}$$



Least Squares <=> Maximum Likelihood (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 i.i.d inputs $\mathbf{X} = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$ and targets $\mathbf{t} = [t_1, ..., t_N]^T$, we obtain the *likelihood* function:

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

Least Squares <=> Maximum Likelihood (2)

- Taking the logarithm, we get the *log-likelihood* function:

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

where

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

- $E_D(\mathbf{w})$ is the sum-of-squares error!

Least Squares <=> Maximum Likelihood (3)

- Minimizing square error <=> maximizing likelihood:

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} E_D(\mathbf{w}) = \mathbf{w}_{ML} = \arg\max_{\mathbf{w}} \ln p(\mathbf{t} \mid \mathbf{w}, \beta)$$

- How do we find **w** (and β)?

Least Squares <=> Maximum Likelihood (4)

- 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

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

where

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

Least Squares <=> Maximum Likelihood (5)

- Minimizing square error <=> maximizing likelihood:

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} E_D(\mathbf{w}) = \mathbf{w}_{ML} = \arg\max_{\mathbf{w}} \ln p(\mathbf{t} \mid \mathbf{w}, \beta)$$

- Maximizing with respect to w gives:

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

- Maximizing with respect to β gives:

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

Regularized Least Square

- 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:

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

which is minimized by:

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

λ is called the *regularization coefficient*.

Regularized Least Square <=> Maximum A Posteriori (MAP)

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

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

- We also have the **likelihood** function:

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

- Bayes to combine prior with the likelihood => **posterior**:

$$p(\mathbf{w}|\mathbf{t}) = \frac{p(\mathbf{t}|\mathbf{w})p(\mathbf{w})}{p(\mathbf{t})}$$

$$p(\mathbf{w}|\mathrm{X}, \mathbf{t}, \alpha, \beta) = \frac{p(\mathbf{t}|\mathbf{w}, \mathrm{X}, \beta)p(\mathbf{w}|\alpha)}{p(\mathbf{t}|\mathrm{X}, \alpha, \beta)} \propto p(\mathbf{t}|\mathbf{w}, \mathrm{X}, \beta)p(\mathbf{w}|\alpha)$$

Regularized Least Square <=> Maximum A Posteriori (MAP)

- Taking the logarithm of the posterior distribution:

$$\ln p(\mathbf{w} \mid \mathbf{t}) = -\frac{\beta}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^T\varphi(x_n)\}^2 - \frac{\alpha}{2}\mathbf{w}^T\mathbf{w} + const$$

- The MAP estimate of w is:

$$\begin{aligned}
\mathbf{w}_{MAP} &= \arg\max_{\mathbf{w}} \ \ln p(\mathbf{w} \mid \mathbf{t}) \\
&= \arg\max_{\mathbf{w}} \ -\frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^T\varphi(x_n)\}^2 - \frac{\boxed{\alpha/\beta}}{2}\mathbf{w}^T\mathbf{w} \\
&= \arg\min_{\mathbf{w}} \ \frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^T\varphi(x_n)\}^2 + \frac{\boxed{\lambda}}{2}\mathbf{w}^T\mathbf{w} \\
&= \arg\min_{\mathbf{w}} \ E_D(\mathbf{w}) + E_W(\mathbf{w})
\end{aligned}$$

Regularized Least Square <=> Maximum A Posteriori (MAP)

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

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

- We also have the **likelihood** function:

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

- Using Bayes and results for marginal and conditional Gaussian distributions, gives the **posterior**

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

$$\boxed{\hat{\mathbf{w}} = \mathbf{m}_N = \left(\frac{\alpha}{\beta}\mathbf{I} + \Phi^T\Phi\right)^{-1} \Phi^T\mathbf{t} = (\lambda\mathbf{I} + \Phi^T\Phi)^{-1}\Phi^T\mathbf{t}}$$

Supplemental Readings

- PRML:
  - Section 1.1 (Polynomial curve fitting).
  - Section 1.2 (up to and including 1.2.5).
  - Section 3.1.4 (Regularized least squares).