Polynomial Curve Fitting

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Topics

1. Simple Regression Problem
2. Polynomial Curve Fitting
3. Probability Theory of multiple variables
4. Maximum Likelihood
5. Bayesian Approach
6. Model Selection
7. Curse of Dimensionality

x i/p

y → o/p = f(x)

Simple Regression Problem

- Begin discussion on ML by introducing a simple regression problem
  - It motivates a no. of key concepts

training data

weights learned i/p → o/p

function known

- Problem:
  - Observe Real-valued input variable x
  - Use new x to predict value of target variable t
- We consider an artificial example using synthetically generated data
  - Because we know the process that generated the data, it can be used for comparison against a learned model

t - o/p
x - i/p

Synthetic Data for Regression

predict ??

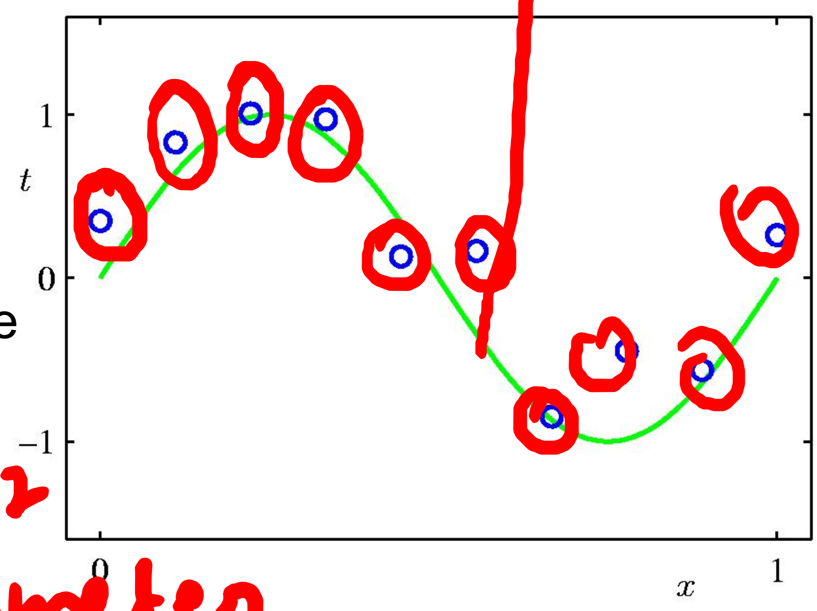
- Data generated from the function $\sin(2\pi\ x)$
  – Where x is the input
- Random noise in target values

A o h → C- B- R-

B o h → C B R

– Dict w_0
– Regularize w_1
– Regularize w_2
→ Parameter

Target Variable



Input Variable

Input values $\{x_n\}$ generated uniformly in range $(0,1)$. Corresponding target values $\{\mathrm{t_n}\}$ Obtained by first computing corresponding values of $\sin\{2\pi x\}$ then adding random noise with a Gaussian distribution with std dev 0.3

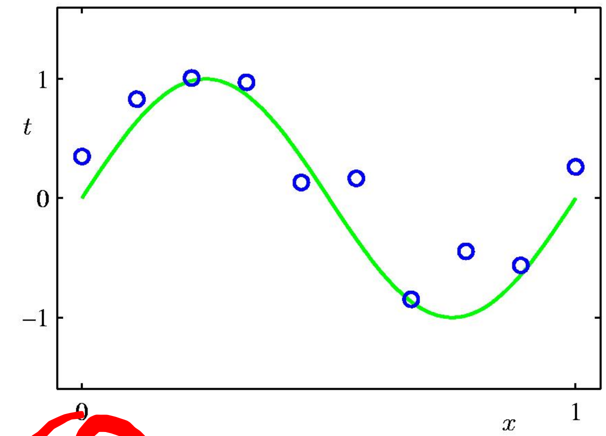
Training Set

N=10

- N observations of x

  $\mathrm{x} = (x_1,..,x_N)^T$ i/p

  $\mathrm{t} = (t_1,..,t_N)^T$ o/p



- Goal is to exploit training set to predict value $\hat{t}$ for some new value $\hat{x}$
- Inherently a difficult problem
- Probability theory provides framework for expressing uncertainty in a precise, quantitative manner
- Decision theory allows us to make a prediction that is optimal according to appropriate criteria

Data Generation:
$\mathrm{N} = 10$
Spaced uniformly in range $[0,1]$
Generated from $\sin(2\pi x)$ by adding small Gaussian noise
Noise typical due to unobserved variables

A Simple Approach to Curve Fitting

finite   mapping

- Fit the data using a *polynomial function*   nth order

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

  - where M is the order of the polynomial
- Is higher value of M better? We'll see shortly!
- Coefficients $w_0 ,\ldots w_M$ are collectively denoted by vector $\mathbf{w}$
- It is a nonlinear function of x, but a linear function of the unknown parameters $\mathbf{w}$
- Have important properties and are called Linear Models

Error Function

x - fixed

N - Sample

- We can obtain a fit by minimizing an error function
  - Sum of squares of the errors between the predictions $y(x_n, \mathbf{w})$ for each data point x_n and target value t_n

Actual

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

Predicted

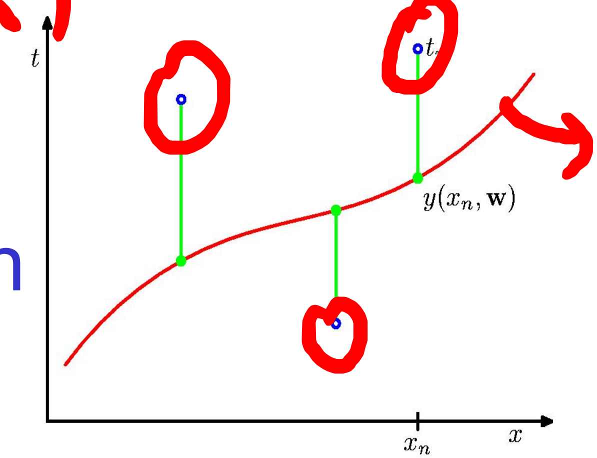
  - Factor ½ included for later convenience

$(y - t_n)$

$(t_n - y)$

- Solve by choosing value of w for which small as possible

Red line is best polynomial fit



$\frac{1}{2}\frac{d}{dx}(x^2) = \frac{2x}{2} = x$

Minimization of Error Function

1st — 11/12th Class

- Error function is a quadratic in coefficients w
- Thus derivative with respect to coefficients will be linear in elements of w
- Thus error function has a unique solution which can be found in closed form
  – Unique minimum denoted w^*
- Resulting polynomial is $y(x,\mathrm{w}^*)$

Set of Simultaneous linear equations

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

Details

Since $y(x,\mathrm{w}) = \sum_{j=0}^{M} w_j x^j$

$$\frac{\partial E(\mathrm{w})}{\partial w_i} = \sum_{n=1}^{N}\{y(x_n,\mathrm{w}) - t_n\}x_n^i$$

$$0 = \sum_{n=1}^{N}\{\sum_{j=0}^{M} w_j x_n^j - t_n\}x_n^i$$

Setting equal to zero

$$\sum_{n=1}^{N}\sum_{j=0}^{M} w_j x_n^{i+j} = \sum_{n=1}^{N} t_n x_n^i$$

Set of M+1 equations (i=0,..,M) over M+1 variables are solved to get elements of w^*

Solving Simultaneous equations

- $A\mathbf{w}=\mathbf{b}$

  where A is $N \times (M+1)$: Design Matrix

  $\mathbf{w}$ is $(M+1) \times 1$: set of weights to be determined

  $\mathbf{b}$ is $N \times 1$: Target values

- Can be solved using matrix inversion

  $\mathbf{w}=A^{-1}\mathbf{b}$

- Or by using Gaussian elimination

$w = A^{-1} b$

unstable

$A \Rightarrow |\det A| = 0$

$O(n^3)$

Solving Linear Equations

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 \\ \vdots \quad\quad \vdots \quad\quad\quad \vdots \quad &\quad \vdots \\ a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n &= b_m \end{aligned}$$

$$x_1 \begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{m1} \end{bmatrix} + x_2 \begin{bmatrix} a_{12} \\ a_{22} \\ \vdots \\ a_{m2} \end{bmatrix} + \cdots + x_n \begin{bmatrix} a_{1n} \\ a_{2n} \\ \vdots \\ a_{mn} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

1. Matrix Formulation: $A\mathbf{x}=\mathbf{b}$
Solution: $\mathbf{x}=A^{-1}\mathbf{b}$

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

Here $m=n=M+1$

2. Gaussian Elimination followed by back-substitution

$$\begin{aligned} x + 3y - 2z &= 5 \\ 3x + 5y + 6z &= 7 \\ 2x + 4y + 3z &= 8 \end{aligned}$$

$L_2-3L_1 \to L_2$ $\quad$ $L_3-2L_1 \to L_3$ $\quad$ $-L_2/4 \to L_2$

$$\left[\begin{array}{ccc|c} 1 & 3 & -2 & 5 \\ 3 & 5 & 6 & 7 \\ 2 & 4 & 3 & 8 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & 3 & -2 & 5 \\ 0 & -4 & 12 & -8 \\ 2 & 4 & 3 & 8 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & 3 & -2 & 5 \\ 0 & -4 & 12 & -8 \\ 0 & -2 & 7 & -2 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & 3 & -2 & 5 \\ 0 & 1 & -3 & 2 \\ 0 & -2 & 7 & -2 \end{array}\right]$$

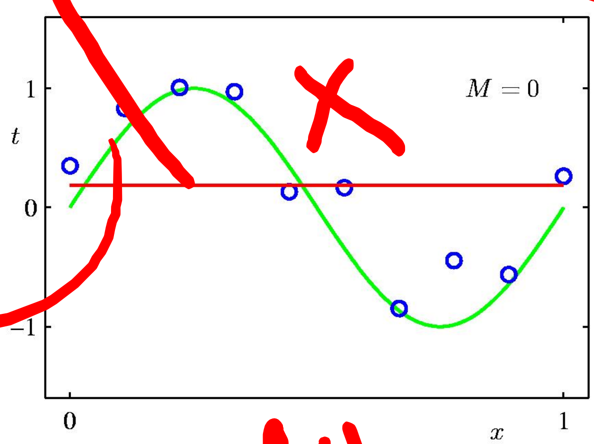
$$\sim \left[\begin{array}{ccc|c} 1 & 3 & -2 & 5 \\ 0 & 1 & -3 & 2 \\ 0 & 0 & 1 & 2 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & 3 & -2 & 5 \\ 0 & 1 & 0 & 8 \\ 0 & 0 & 1 & 2 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & 3 & 0 & 9 \\ 0 & 1 & 0 & 8 \\ 0 & 0 & 1 & 2 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & 0 & 0 & -15 \\ 0 & 1 & 0 & 8 \\ 0 & 0 & 1 & 2 \end{array}\right]$$

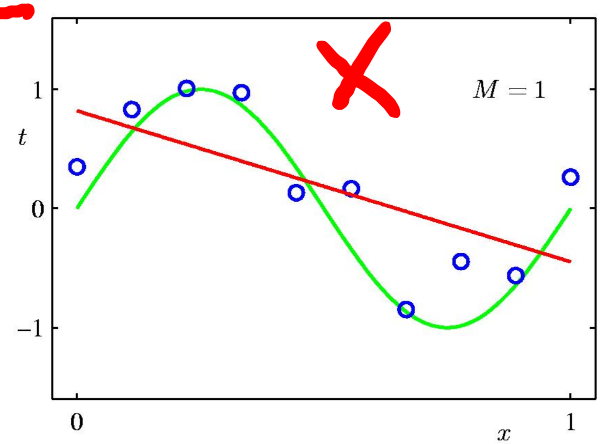
Choosing the order of M

Predicted

- Model Comparison or Model Selection
- Red lines are best fits with
  - $M = 0,1,3,9$ and $N=10$

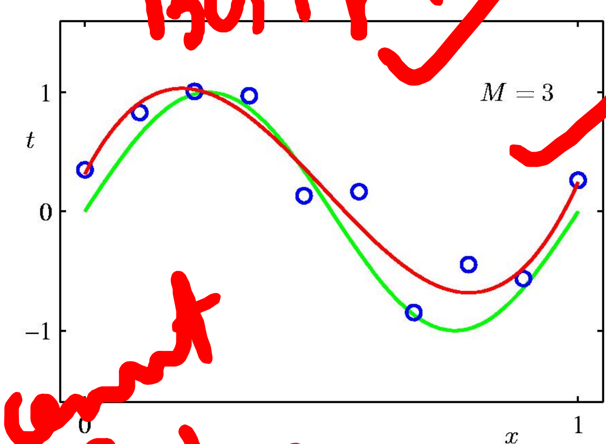
$y(x, w) = w_0 + w_1 x^1 + w_2 x^2 + \dots + w_M x^M$



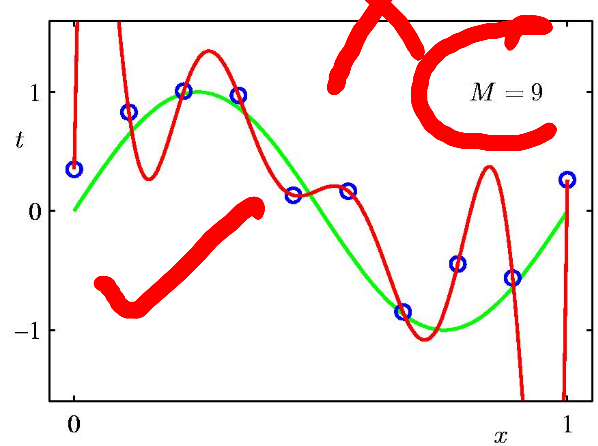


← Poor representations of $\sin(2\pi x)$

Best fit



← Best Fit to $\sin(2\pi x)$



Over Fit
Poor representation of $\sin(2\pi x)$

Placement c 9pil A, B → clam same exam in test 100%

100 Students - 20, 20, 20, 20, 20 K-fold Validation

Generalization Performance

- Consider separate *test* set of 100 points - y - F
- For each value of M evaluate

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

$$\boxed{y(x,\mathbf{w}^*) = \sum_{j=0}^{M} w_j^* x^j}$$

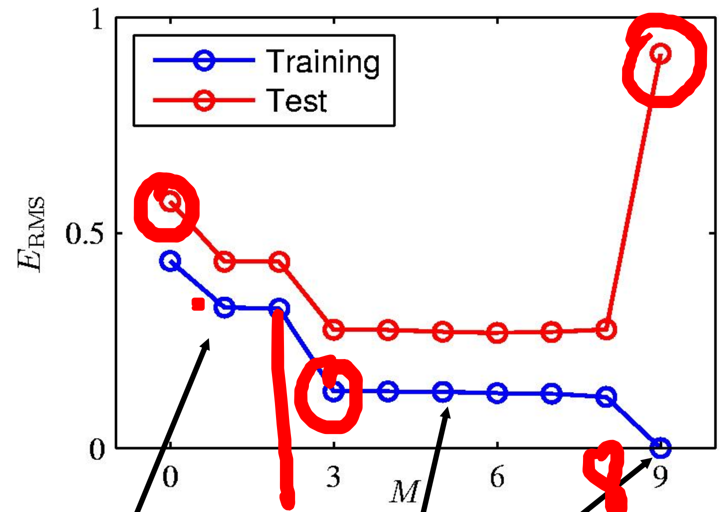
for training data and test data

- Use RMS error

$$E_{RMS} = \sqrt{2E(\mathbf{w}^*)\,/\,N}$$

  – Division by N allows different sizes of N to be compared on equal footing
  – Square root ensures E_{RMS} is measured in same units as t

overfit



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8

Poor due to Inflexible polynomials

Small Error

M=9 means ten degrees of freedom. Tuned exactly to 10 training points (wild oscillations in polynomial)

Values of Coefficients w^* for different polynomials of order M

w0   w0, 1   w0, 1, 2, 3

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

10^{5-6}

overfitting

As M increases magnitude of coefficients increases
At $M=9$ finely tuned to random noise in target values

$N = 10$ sambler $M = 9$

Increasing Size of Data Set

$M \downarrow$

$M=9$

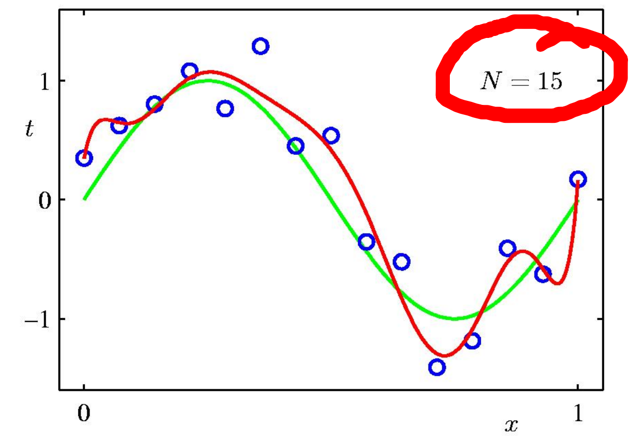
$N \uparrow$

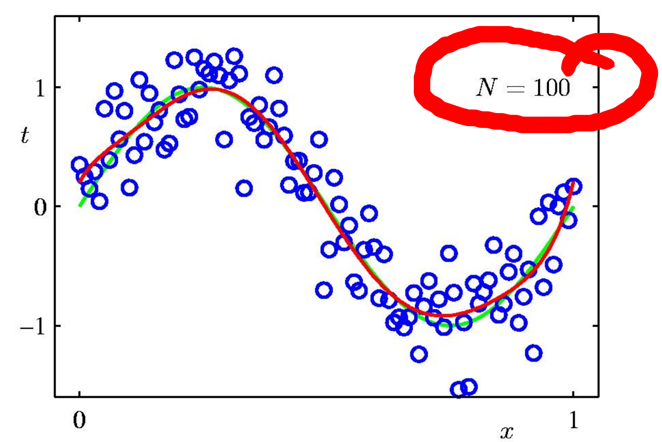
N=15, 100

- For a given model complexity overfitting problem is less severe as size of data set increases
- Larger the data set, the more complex we can afford to fit the data

thumb rule

- Data should be no less than 5 to 10 times adaptive parameters in model





Least Squares is case of Maximum Likelihood

- Unsatisfying to limit the number of parameters to size of training set
- More reasonable to choose model complexity according to problem complexity
- Least squares approach is a specific case of maximum likelihood
  - Over-fitting is a general property of maximum likelihood
- Bayesian approach avoids over-fitting problem
  - No. of parameters can greatly exceed no. of data points
  - Effective no. of parameters adapts automatically to size of data set

Regularization of Least Squares

- Using relatively complex models with data sets of limited size

M=9 , N=10

- Add a penalty term to error function to discourage coefficients from reaching large values

w_0 - 10

w_0 - 3

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

where

$$||\,\mathrm{w}^2\,|| \equiv w^T w = w_0^{\,2} + w_1^{\,2} + .. + w_M^{\,2}$$

w_4 - 0.0 - -

- λ determines relative importance of regularization term to error term
- Can be minimized exactly in closed form
- Known as *shrinkage* in statistics

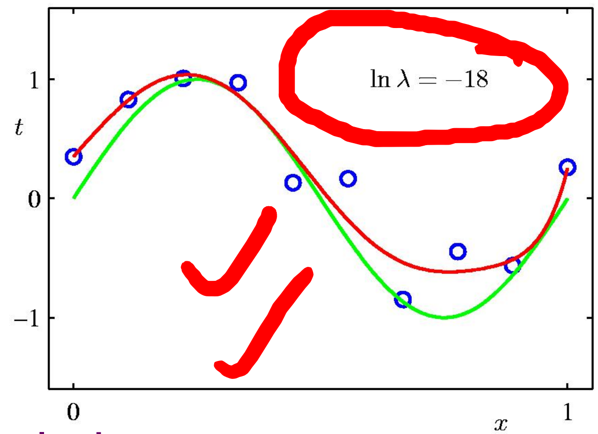
  Weight decay in neural networks

$0 < \lambda < 1$

Effect of Regularizer $\ln \lambda = 0$

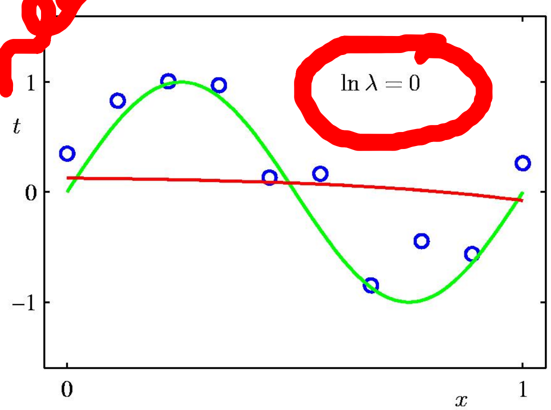
M=9 polynomials using regularized error function

Optimal



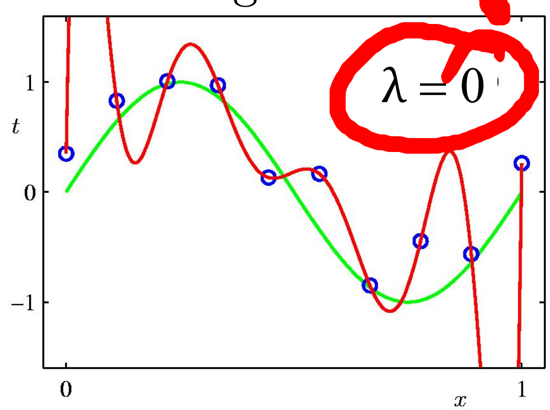
Not learned

Large Regularizer



overfitted

No Regularizer



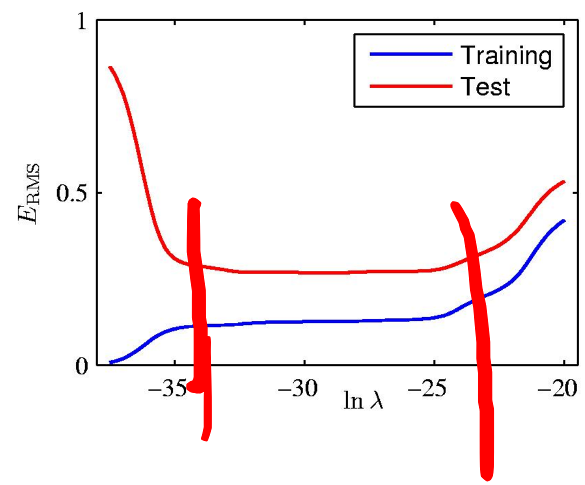
No Regularizer $\lambda = 0$

Large Regularizer $\lambda = 1$

	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
$w_0^\star$	0.35	0.35	0.13
$w_1^\star$	232.37	4.74	-0.05
$w_2^\star$	-5321.83	-0.77	-0.06
$w_3^\star$	48568.31	-31.97	-0.05
$w_4^\star$	-231639.30	-3.89	-0.03
$w_5^\star$	640042.26	55.28	-0.02
$w_6^\star$	-1061800.52	41.32	-0.01
$w_7^\star$	1042400.18	-45.95	-0.00
$w_8^\star$	-557682.99	-91.53	0.00
$w_9^\star$	125201.43	72.68	0.01

Impact of Regularization on Error

- λ controls the complexity of the model and hence degree of over-fitting
  - Analogous to choice of M
- Suggested Approach:
- Training set
  - to determine coefficients $\mathbf{w}$
  - For different values of (M or λ)
- Validation set (holdout)
  - to optimize model complexity (M or λ)



$M=9$ polynomial

Summary of Curve Fitting

- Partitioning data into *training set* (to determine coefficients $\mathbf{w}$) and a separate *validation set* (or *hold-out* set) to optimize model complexity M or λ
- More sophisticated approaches are not as wasteful of training data
- More principled approach is based on probability theory
- Classification is a special case of regression where target value is discrete values