CS 886
Applied Machine Learning
Introduction Part 2 - Regression, Model Selection, Performance Evaluation

Dan Lizotte

University of Waterloo

9 May 2013

Notation reminder

- Consider a function $J(u_1, u_2, \ldots, u_p) : \mathbb{R}^p \mapsto \mathbb{R}$ (for us, this will usually be an error function)
- The *gradient* $\nabla J(u_1, u_2, \ldots, u_p) : \mathbb{R}^p \mapsto \mathbb{R}^p$ is a function which outputs a vector containing the partial derivatives.
  That is:
$$\nabla J = \left\langle \frac{\partial}{\partial u_1} J, \frac{\partial}{\partial u_2} J, \ldots, \frac{\partial}{\partial u_p} J \right\rangle$$
- If J is differentiable and convex, we can find the global minimum of J by solving $\nabla J = \mathbf{0}$.
- The partial derivative is the derivative along the u_i axis, keeping all other variables fixed.

The Least Squares Solution

- Recalling some multivariate calculus:

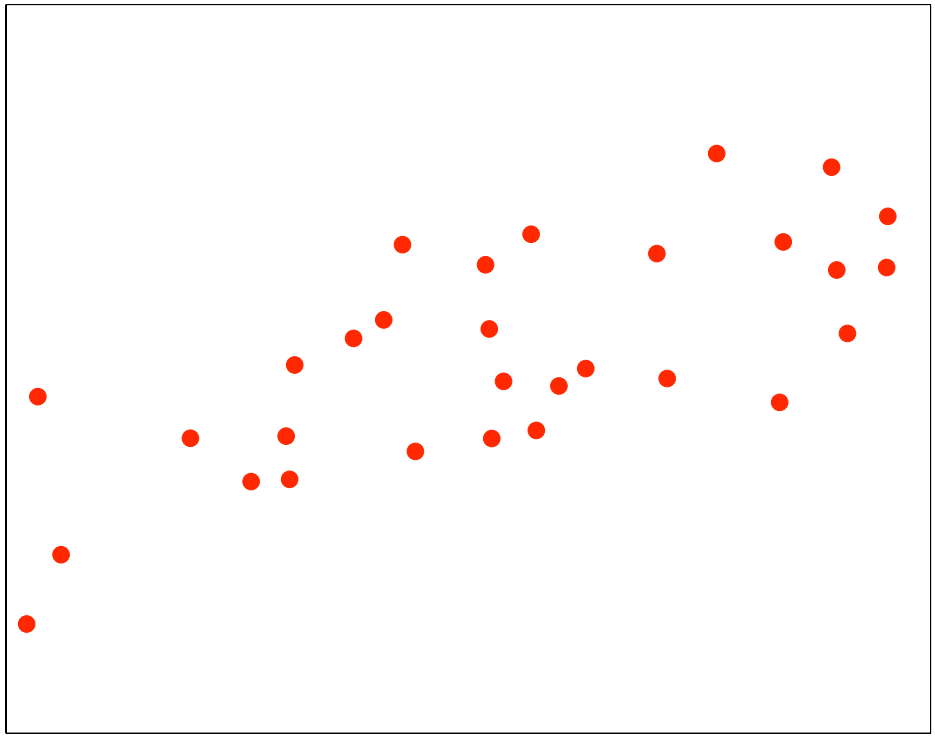
$$\begin{aligned}
\nabla_{\mathbf{w}} J &= \nabla_{\mathbf{w}} (X\mathbf{w} - \mathbf{y})^{\mathsf{T}} (X\mathbf{w} - \mathbf{y}) \\
&= \nabla_{\mathbf{w}} (\mathbf{w}^{\mathsf{T}} X^{\mathsf{T}} X\mathbf{w} - \mathbf{y}^{\mathsf{T}} X\mathbf{w} - \mathbf{w}^{\mathsf{T}} X^{\mathsf{T}} \mathbf{y} + \mathbf{y}^{\mathsf{T}} \mathbf{y}) \\
&= \nabla_{\mathbf{w}} (\mathbf{w}^{\mathsf{T}} X^{\mathsf{T}} X\mathbf{w} - 2\mathbf{y}^{\mathsf{T}} X\mathbf{w} + \mathbf{y}^{\mathsf{T}} \mathbf{y}) \\
&= 2X^{\mathsf{T}} X\mathbf{w} - 2X^{\mathsf{T}} \mathbf{y}
\end{aligned}$$

- Setting gradient equal to zero:

$$\begin{aligned}
2X^{\mathsf{T}} X\mathbf{w} - 2X^{\mathsf{T}} \mathbf{y} &= 0 \\
\Rightarrow X^{\mathsf{T}} X\mathbf{w} &= X^{\mathsf{T}} \mathbf{y} \\
\Rightarrow \mathbf{w} = (X^{\mathsf{T}} X)^{-1} X^{\mathsf{T}} \mathbf{y}
\end{aligned}$$

- The inverse exists if the columns of X are linearly independent.

Example of linear regression



x	y
0.86	2.49
0.09	0.83
-0.85	-0.25
0.87	3.10
-0.44	0.87
-0.43	0.02
-1.10	-0.12
0.40	1.81
-0.96	-0.83
0.17	0.43

Data matrices

$$X = \begin{bmatrix} 1 & 0.86 \\ 1 & 0.09 \\ 1 & -0.85 \\ 1 & 0.87 \\ 1 & -0.44 \\ 1 & -0.43 \\ 1 & -1.10 \\ 1 & 0.40 \\ 1 & -0.96 \\ 1 & 0.17 \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 2.49 \\ 0.83 \\ -0.25 \\ 3.10 \\ 0.87 \\ 0.02 \\ -0.12 \\ 1.81 \\ -0.83 \\ 0.43 \end{bmatrix}$$

$X^\top X$

$$X^\top X =$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0.86 & 0.09 & -0.85 & 0.87 & -0.44 & -0.43 & -1.10 & 0.40 & -0.96 & 0.17 \end{bmatrix} \times \begin{bmatrix} 1 & 0.86 \\ 1 & 0.09 \\ 1 & -0.85 \\ 1 & 0.87 \\ 1 & -0.44 \\ 1 & -0.43 \\ 1 & -1.10 \\ 1 & 0.40 \\ 1 & -0.96 \\ 1 & 0.17 \end{bmatrix}$$

$$= \begin{bmatrix} 10 & -1.39 \\ -1.39 & 4.95 \end{bmatrix}$$

$X^T\mathbf{y}$

$$X^T\mathbf{y} =$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0.86 & 0.09 & -0.85 & 0.87 & -0.44 & -0.43 & -1.10 & 0.40 & -0.96 & 0.17 \end{bmatrix} \times \begin{bmatrix} 2.49 \\ 0.83 \\ -0.25 \\ 3.10 \\ 0.87 \\ 0.02 \\ -0.12 \\ 1.81 \\ -0.83 \\ 0.43 \end{bmatrix}$$

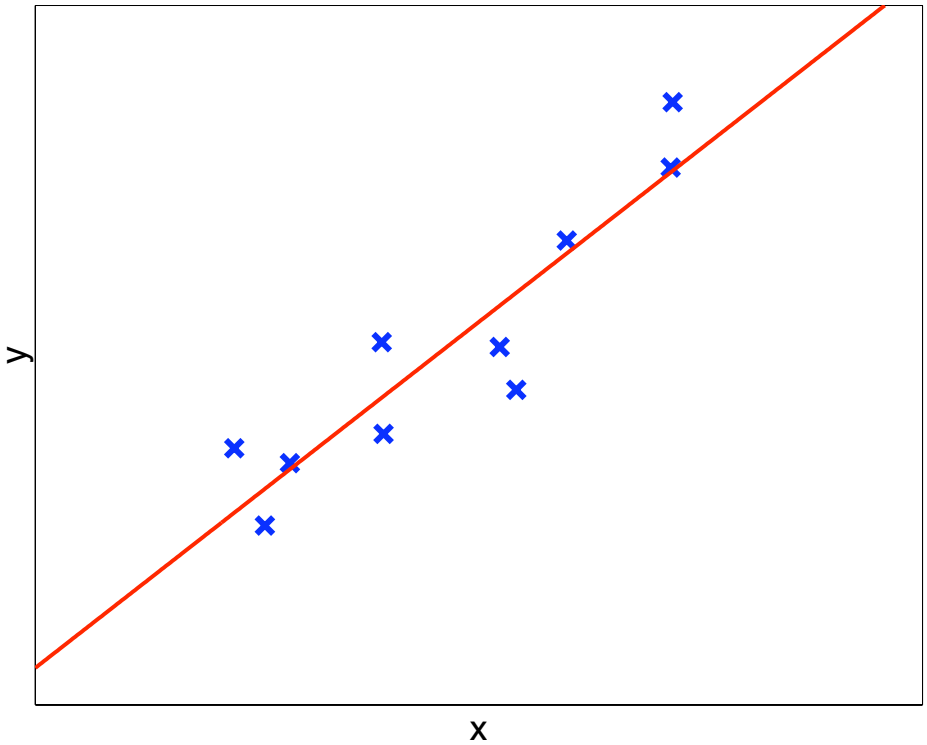
$$= \begin{bmatrix} 8.34 \\ 6.49 \end{bmatrix}$$

Solving for **w**

$$\mathbf{w} = (X^\top X)^{-1} X^\top \mathbf{y} = \begin{bmatrix} 10 & -1.39 \\ -1.39 & 4.95 \end{bmatrix}^{-1} \begin{bmatrix} 8.34 \\ 6.49 \end{bmatrix} = \begin{bmatrix} 1.05 \\ 1.60 \end{bmatrix}$$

So the best fit line is $y = 1.05 + 1.60x$.

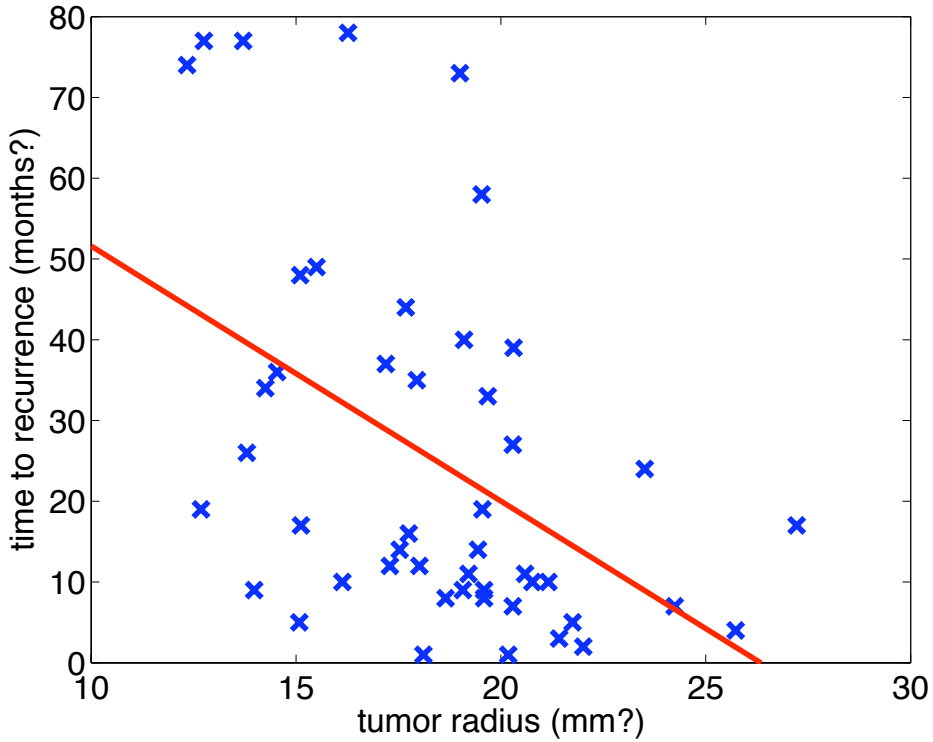
Data and line $y = 1.05 + 1.60x$



Linear regression summary

- The optimal solution (minimizing sum-squared-error) can be computed in polynomial time in the size of the data set.
- The solution is $\mathbf{w} = (X^{\mathsf{T}}X)^{-1}X^{\mathsf{T}}\mathbf{y}$, where X is the data matrix augmented with a column of ones, and $\mathbf{y}$ is the column vector of target outputs.
- A very rare case in which an analytical, exact solution is possible

Predicting recurrence time based on tumor size



Is linear regression enough?

- Linear regression should be the **first thing** you try for real-valued outputs!
- ...but it is sometimes not expressive enough.[1]
- Two possible solutions:
  1. Explicitly transform the data, i.e. create additional features
     - Add cross-terms, higher-order terms
     - More generally, apply a transformation of the inputs from $\mathcal{X}$ to some other space $\mathcal{X}'$, then do linear regression in the transformed space
  2. Use a different hypothesis class
- Idea (1) and idea (2) are two views of the strategy. Today we focus on the first approach

[1] Problems can also occur if $X^\top X$ is not invertible.

Polynomial fits

- Suppose we want to fit a higher-degree polynomial to the data. (E.g., $y = w_0 + w_1 x_1 + w_2 x_1^2$.)
- Suppose for now that there is a single input variable $x_{i,1}$ per training sample.
- How do we do it?

Answer: Polynomial regression

- Given data: $(x_{1,1}, y_1), (x_{1,2}, y_2), \ldots, (x_{1,n}, y_n)$.
- Suppose we want a degree-d polynomial fit.
- Let $\mathbf{y}$ be as before and let

$$X = \begin{bmatrix} 1 & x_{1,1} & x_{1,1}^2 & \cdots & x_{1,1}^d \\ 1 & x_{1,2} & x_{1,2}^2 & \cdots & x_{1,2}^d \\ \vdots & & \vdots & \vdots & \vdots \\ 1 & x_{1,n} & x_{1,n}^2 & \cdots & x_{1,n}^d \end{bmatrix}$$

- We are **making up features** to add to our design matrix
- Solve the linear regression $X\mathbf{w} \approx \mathbf{y}$.

Example of quadratic regression: Data matrices

$$X = \begin{bmatrix} 1 & 0.86 & 0.75 \\ 1 & 0.09 & 0.01 \\ 1 & -0.85 & 0.73 \\ 1 & 0.87 & 0.76 \\ 1 & -0.44 & 0.19 \\ 1 & -0.43 & 0.18 \\ 1 & -1.10 & 1.22 \\ 1 & 0.40 & 0.16 \\ 1 & -0.96 & 0.93 \\ 1 & 0.17 & 0.03 \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 2.49 \\ 0.83 \\ -0.25 \\ 3.10 \\ 0.87 \\ 0.02 \\ -0.12 \\ 1.81 \\ -0.83 \\ 0.43 \end{bmatrix}$$

$X^\top X$

$$X^\top X =$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0.86 & 0.09 & -0.85 & 0.87 & -0.44 & -0.43 & -1.10 & 0.40 & -0.96 & 0.17 \\ 0.75 & 0.01 & 0.73 & 0.76 & 0.19 & 0.18 & 1.22 & 0.16 & 0.93 & 0.03 \end{bmatrix} \times \begin{bmatrix} 1 & 0.86 & 0.75 \\ 1 & 0.09 & 0.01 \\ 1 & -0.85 & 0.73 \\ 1 & 0.87 & 0.76 \\ 1 & -0.44 & 0.19 \\ 1 & -0.43 & 0.18 \\ 1 & -1.10 & 1.22 \\ 1 & 0.40 & 0.16 \\ 1 & -0.96 & 0.93 \\ 1 & 0.17 & 0.03 \end{bmatrix}$$

$$= \begin{bmatrix} 10 & -1.39 & 4.95 \\ -1.39 & 4.95 & 1.64 \\ 4.95 & 1.64 & 4.11 \end{bmatrix}$$

$X^T\mathbf{y}$

$$X^T\mathbf{y} =$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0.86 & 0.09 & -0.85 & 0.87 & -0.44 & -0.43 & -1.10 & 0.40 & -0.96 & 0.17 \\ 0.75 & 0.01 & 0.73 & 0.76 & 0.19 & 0.18 & 1.22 & 0.16 & 0.93 & 0.03 \end{bmatrix} \times \begin{bmatrix} 2.49 \\ 0.83 \\ -0.25 \\ 3.10 \\ 0.87 \\ 0.02 \\ -0.12 \\ 1.81 \\ -0.83 \\ 0.43 \end{bmatrix}$$

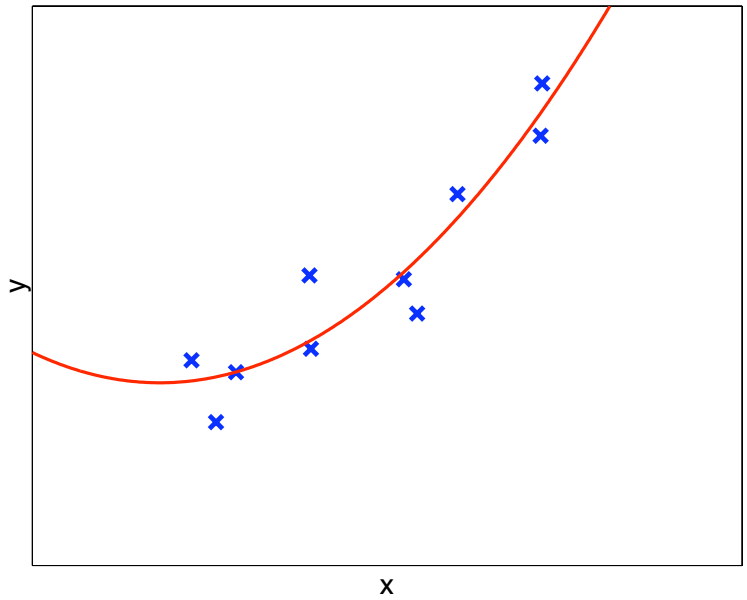
$$= \begin{bmatrix} 8.34 \\ 6.49 \\ 3.60 \end{bmatrix}$$

Solving for **w**

$$\mathbf{w} = (X^\mathsf{T}X)^{-1}X^\mathsf{T}\mathbf{y} = \begin{bmatrix} 10 & -1.39 & 4.95 \\ -1.39 & 4.95 & 1.64 \\ 4.95 & 1.64 & 4.11 \end{bmatrix}^{-1} \begin{bmatrix} 3.60 \\ 6.49 \\ 8.34 \end{bmatrix} = \begin{bmatrix} 0.73 \\ 1.74 \\ 0.68 \end{bmatrix}$$

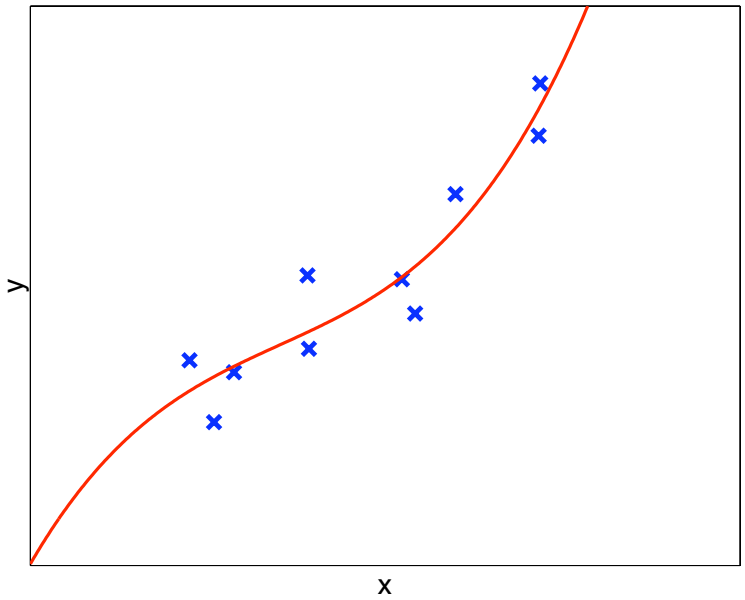
So the best order-2 polynomial is $y = 0.73 + 1.74x + 0.68x^2$.

Data and curve $y = 0.68x^2 + 1.74x + 0.73$



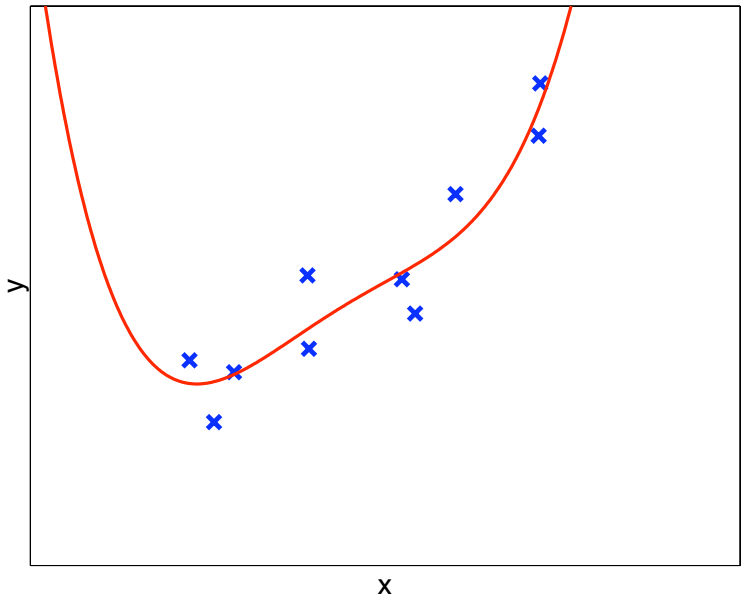
Is this a better fit to the data?

Order-3 fit



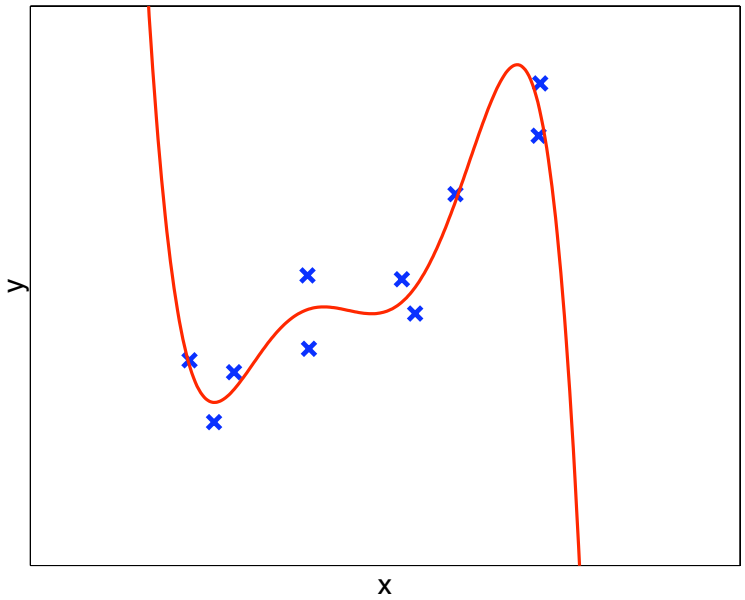
Is this a better fit to the data?

Order-4 fit



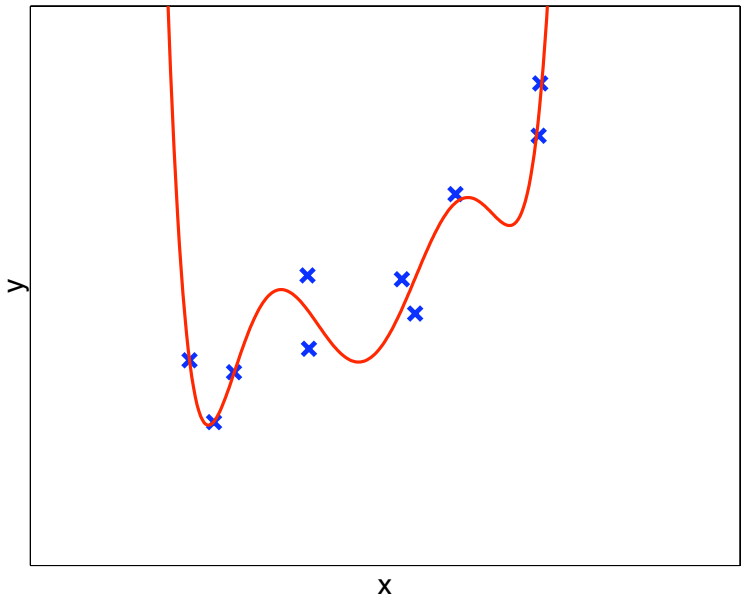
Is this a better fit to the data?

Order-5 fit



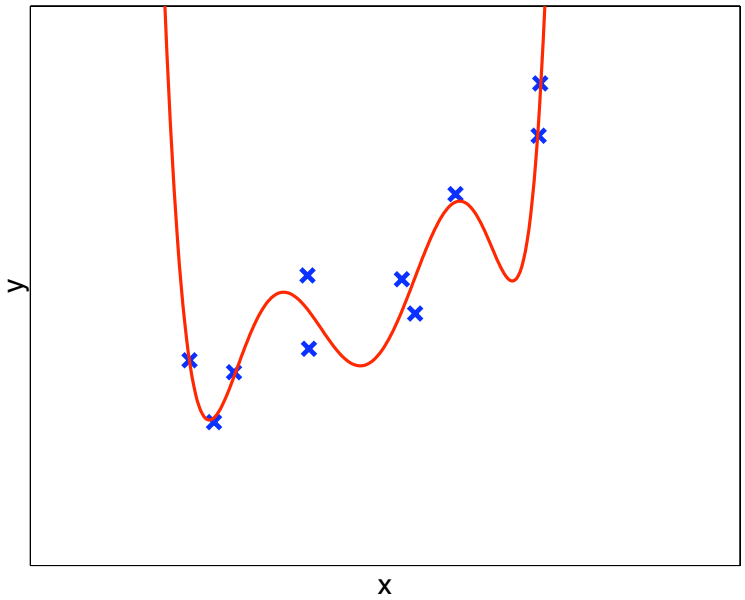
Is this a better fit to the data?

Order-6 fit



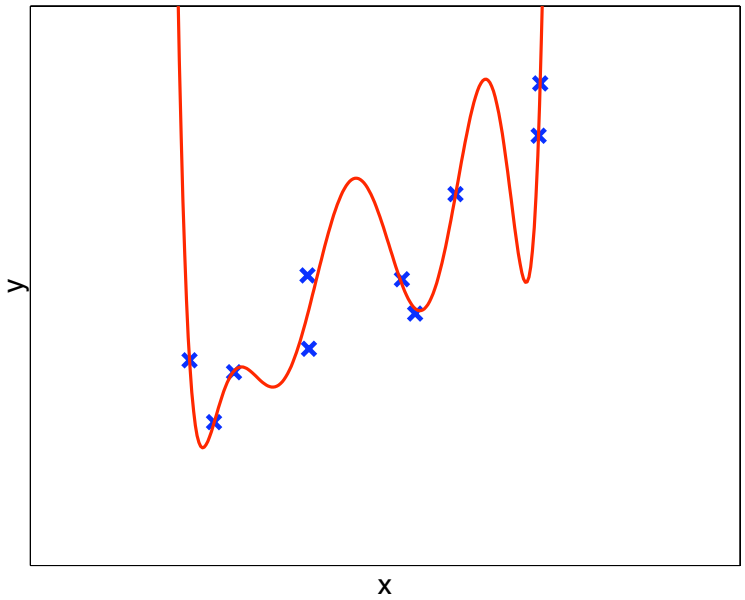
Is this a better fit to the data?

Order-7 fit



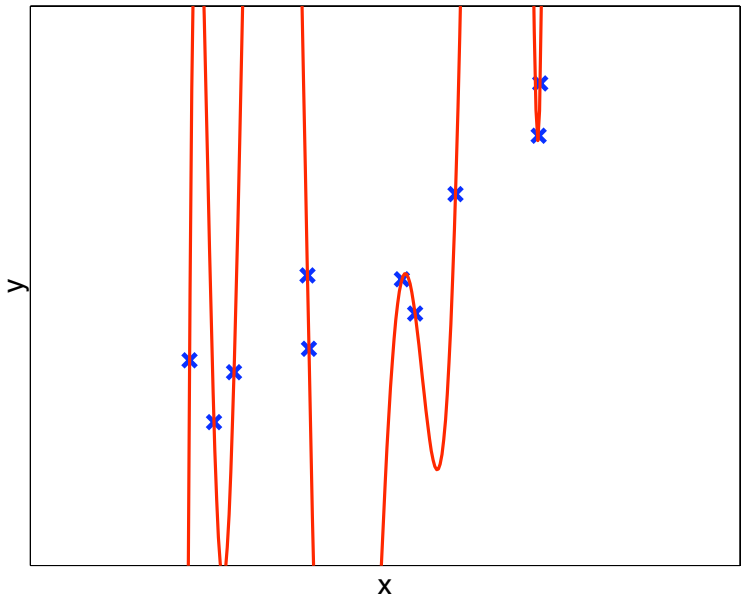
Is this a better fit to the data?

Order-8 fit



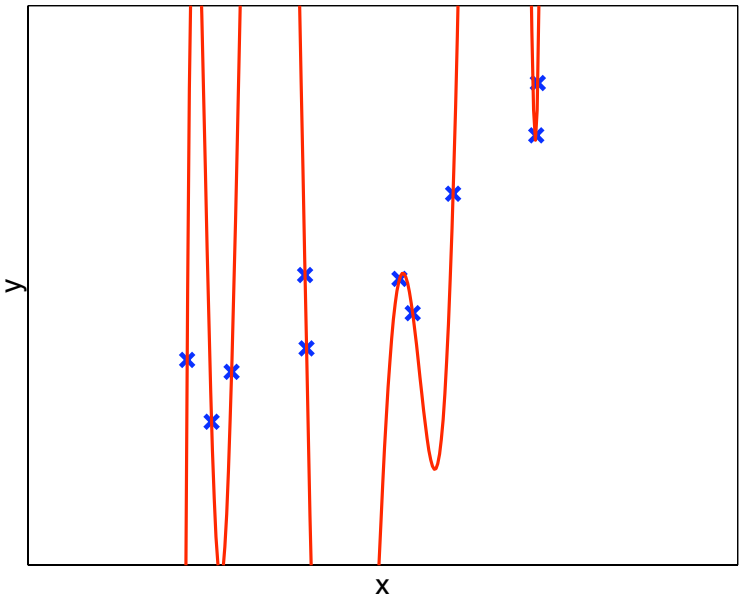
Is this a better fit to the data?

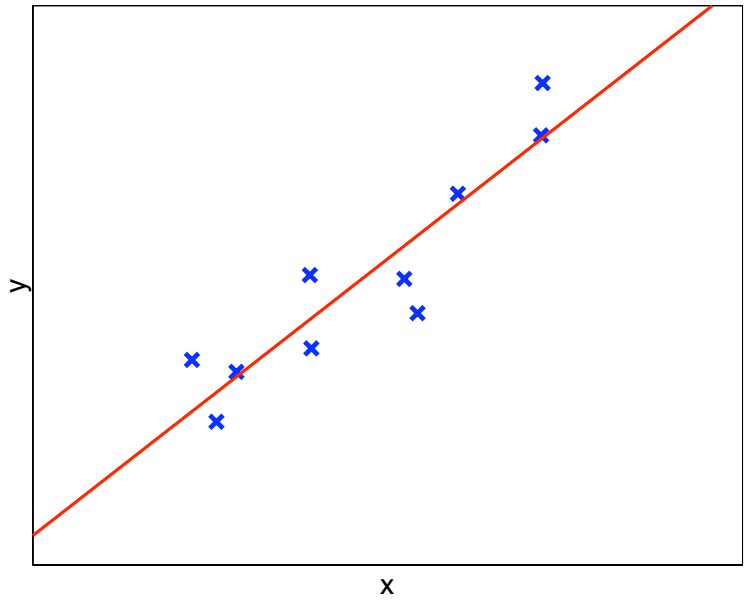
Order-9 fit



Is this a better fit to the data?

Evaluating Performance





Which do you prefer and why?

Fits the data we have right now

Fits data we will see in the future

Performance of a Fixed Hypothesis

- Assume that data $(\mathbf{x}, y)$ are drawn from some fixed, unknown probability distribution $P(\mathbf{x}, y)$
- Given a hypothesis h, (which could have come from anywhere), its *generalization error* is:

$$J_h^* = \mathbb{E}[L(h(\mathbf{x}), y)]$$

- We don't have access to $P(\mathbf{x}, y)$, but if we have access to a *test set* of data, we can compute the *test error*

$$\hat{J}_h^* = \frac{1}{n} \sum_{i=1}^{n} L(h(\mathbf{x}_i), y_i)$$

- $\hat{J}_h^*$ is an *unbiased* estimate of J_h^* **so long as the** $(\mathbf{x}_i, y_i)$ **do not influence** h**.** Can use $\hat{J}_h^*$ to get a confidence interval for J_h^*.

Test Error: The Gold Standard

$$\hat{J}_h^* = \frac{1}{n}\sum_{i=1}^{n} L(h(\mathbf{x}_i), y_i)$$

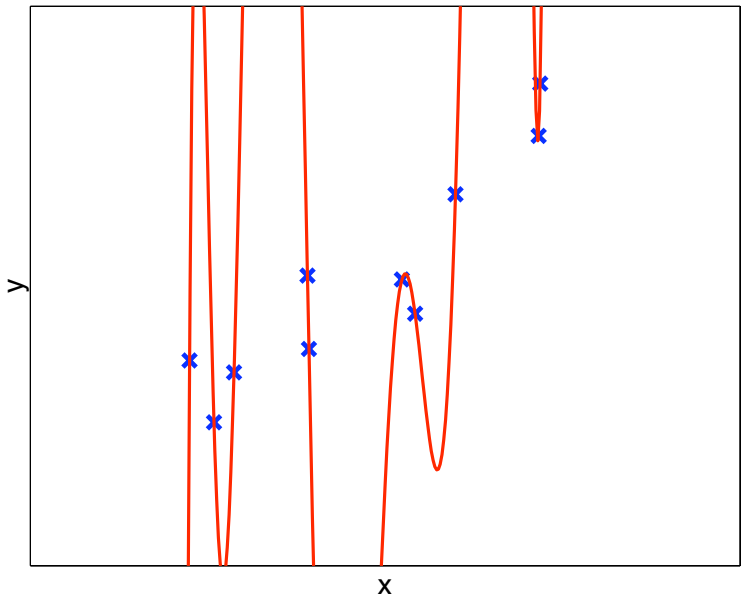
- $\hat{J}_h^*$ is an *unbiased* estimate of J_h^* **so long as the** $(\mathbf{x}_i, y_i)$ **do not influence** h**.** Can use $\hat{J}_h^*$ to get a confidence interval for J_h^*.
- Gives a strong statistical guarantee about the true performance of our system, *if we didn't use the test data to choose h.*
- Note we can write training error for hypothesis class $\mathcal{H}$ as

$$\hat{J}_{\mathcal{H}} = \min_{h' \in \mathcal{H}} \frac{1}{n}\sum_{i=1}^{n} L(h'(\mathbf{x}_i), y_i)$$

- Obviously, for any data set, $\hat{J}_{\mathcal{H}} \leq \hat{J}_h^*$.

Problem 1 with Training Error

Training error $\hat{J}_{\mathcal{H}}$ systematically underestimates generalization error J_h^*

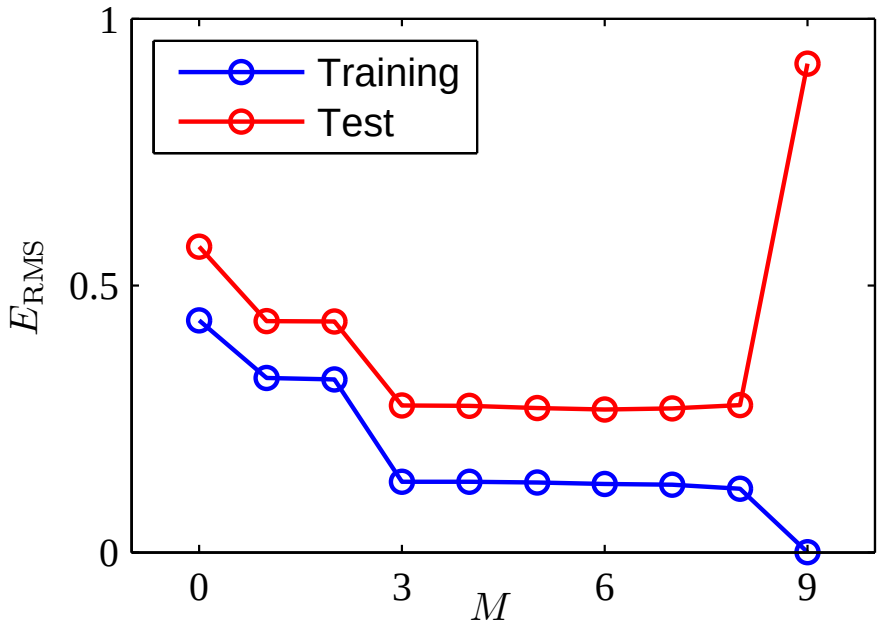


- Training error of the degree-9 polynomial is 0.
- Training error of the degree-9 polynomial *on any set of 10 points* is 0.
- The more complex the model and the smaller the training set, the worse this is.

Problem 2 with Training Error

Smaller training error does not mean smaller generalization error.

- Suppose $\mathcal{H}_1$ is the space of all linear functions, $\mathcal{H}_2$ is the space of all quadratic functions. Note $\mathcal{H}_1 \subset \mathcal{H}_2$.
- Let $h_1 = \arg\min_{h' \in \mathcal{H}_1} \hat{J}^*_{h'}$ and $h_2 = \arg\min_{h' \in \mathcal{H}_2} \hat{J}^*_{h'}$
- We **must** have $\hat{J}^*_{h_2} \leq \hat{J}^*_{h_1}$, *but we may have* $J^*_{h_2} > J^*_{h_1}$.



Training error is no good for choosing the hypothesis class.

Fix the problems with Training Error?

1. Training error $\hat{J}_{\mathcal{H}}$ underestimates generalization error J_h^*
   - If you really want a good estimate of J_h^*, you need a **test set**
   - (But new stat methods can produce a CI using training error)
   - Could report test error, then deploy whatever you train on the whole data. (Probably won't be worse.)
2. Smaller training error does not mean smaller generalization error.
   - Known as **overfitting**
   - Hypothesis class choice problem is called *model selection*
   - A **validation set** can be used for this. Train on the training set using each proposed hypothesis class, evaluate each on the validation set, choose the one with lowest *validation* error

Training, Model Selection, and Error Estimation

- A general procedure for estimating the true error of a specific learned hypothesis using model selection
- The data is randomly partitioned into three subsets:
  - A *training set* used only to find the parameters $\mathbf{w}$
  - A *validation set* used to find the right hypothesis class (e.g., the degree of the polynomial)
  - A *test set* used to report the prediction error of the algorithm
- The test set *must be disjoint from training and validation*!
- Can generate standard confidence intervals for the test error of the learned hypothesis

Problems with the Single-Partition Approach

- Pros:
  - Measures what we want. Performance of the actual learned hypothesis.
- Cons:
  - Why don't we use all the data we have? Is it rational to "throw away" data that could have been used for training/model selection?
  - Can produce a high-variance estimate, especially for classification. (actually the bigger concern) "What if I get a weird test/train/validation set 'by accident?' "
  - For a test set of size 100, with 60 correct classifications, 95% C.I. for actual accuracy is $(0.497, 0.698)$.

k-fold cross-validation

- Divide the instances into k disjoint partitions or folds
- Loop through the partitions $i = 1...k$:
  - Partition i is for testing (i.e., estimating the performance of the algorithm after learning is done)
  - Partition $(i \mod k) + 1$ is for validation (e.g., choosing the hypothesis class or the parameters of the learning algorithm)
  - The rest are used for training (e.g., choosing the specific hypothesis within the class)
- *Report average error on the testing partitions*
- You should also compute and report standard error based on the testing errors on the different folds
- Magic number: $k = 10$
- To deploy at the end of the day, train on all the data using your chosen hypothesis class. If you want to estimate its error, go get more data.

Cross Validation [HTF 7.12]

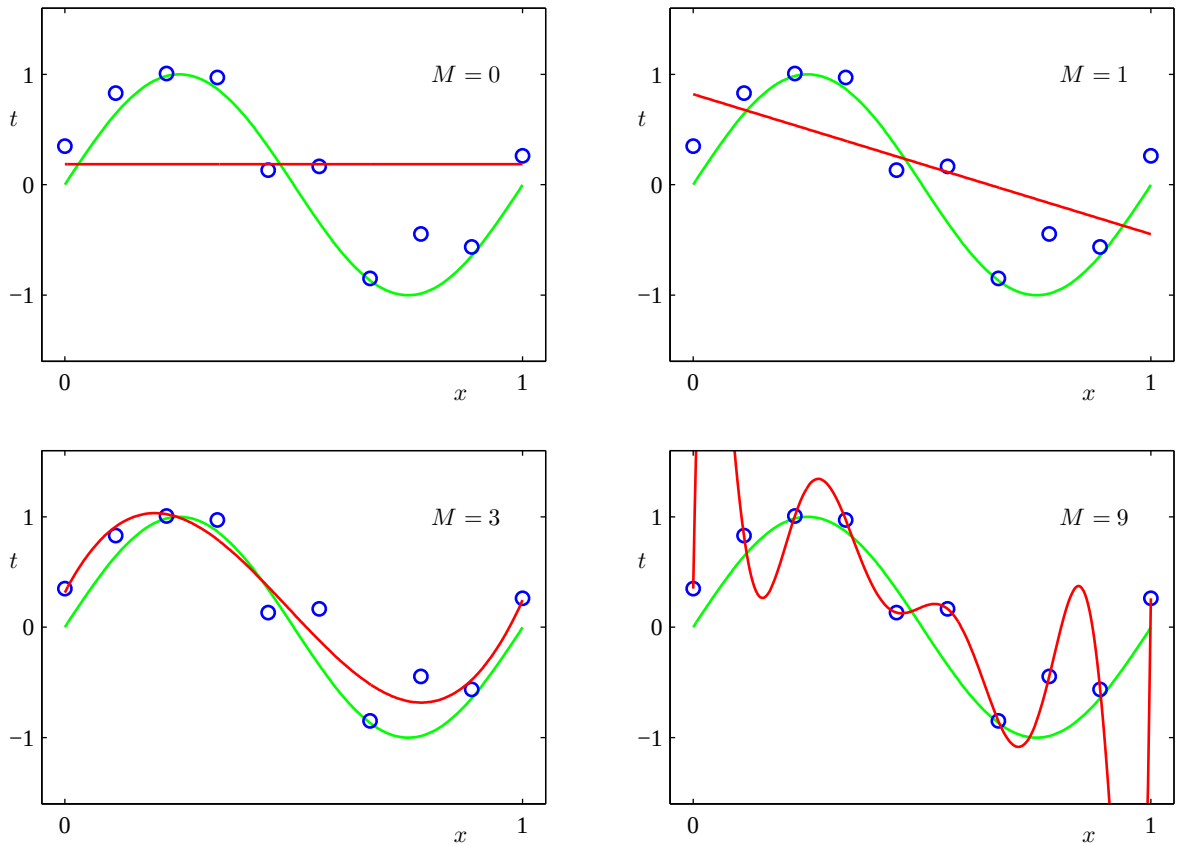
- Error on each test fold is an unbiased estimate of generalization error of a hypothesis *trained on the rest of the data*
- It is an **average of error estimates for k different hypotheses**
- They're similar: Each was trained on a slightly different dataset from the same distribution
- CV estimate approximately unbiased for the *expected generalization error*
  1. Draw many datasets of size n
  2. Train on each one (maybe split for validation; doesn't matter)
  3. Average the true generalization error of each of the hypotheses
- **This is not the generalization error of the hypothesis learned from the data we actually have.**
- More like an evaluation of the learning method.

Cross Validation

- Not exactly what we want, but close
- Standard errors are usually shown (i.e. standard deviation of test errors) but cannot[2] be used to produce valid confidence intervals
- Well-accepted

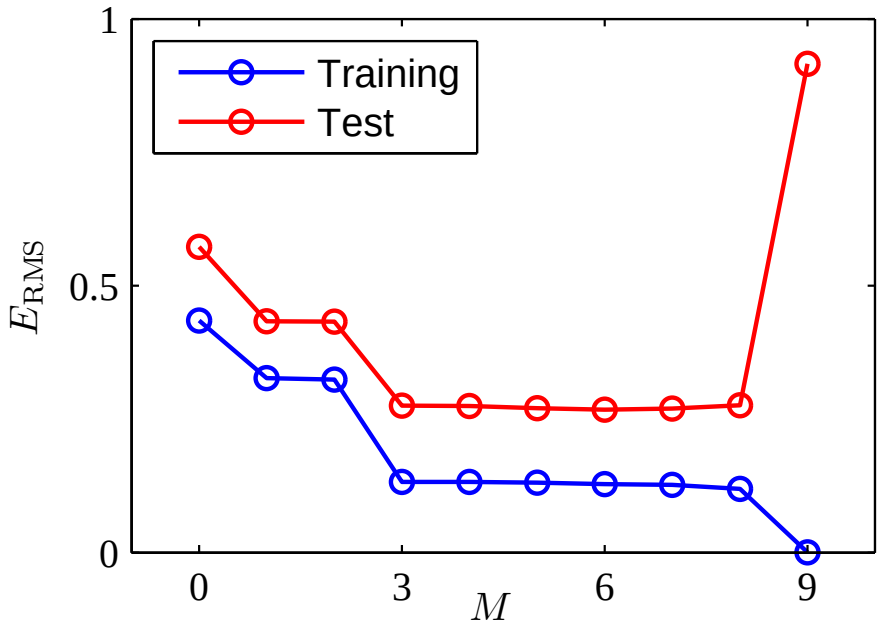
[2] easily: "Some progress has been made on constructing confidence intervals around cross-validation estimates, but this is considered a difficult problem." - Wikipedia. The WP CV article is pretty good.

Summary: Overfitting



- The higher the degree of the polynomial M, the more degrees of freedom, and the more capacity to "overfit" the training data
- Typical overfitting means that error on the training data is very low, but error on new instances is high

Summary: Overfitting



- The training error decreases with the degree of the polynomial M, i.e. *the complexity (size) of the hypothesis class*
- Generalization error decreases at first, then starts increasing
- Set aside a *validation set* helps us find a good hypothesis class
- We then can report unbiased error estimate, using a *test set*, **untouched during both parameter training and validation**
- Cross-validation is a lower-variance but possibly biased version of this approach. It is standard.