COMP 551 - Applied Machine Learning
Lecture 3 – Linear Regression (cont.)

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(with slides and content from Joelle Pineau)

Self-assessment/practice quizzes

- Quiz 0 – Attempt 1 is out and due tonight at11:59pm.
- Quiz 0 – Attempt 2 will be out Thursday at 12am.
- You have one hour to complete it once you begin.
- This week's quizzes do not count towards your grade. They are for self-assessment and practice.
- If you are really struggling or confused by the quiz's this week, it might be worthwhile to wait and take this course in a later semester.
  - (Ideally you should be able to get 100% on your second attempt)

Recall: Linear regression

- The linear regression problem: $f_{\mathbf{w}}(\mathbf{x}) = w_0 + \sum_{j=1:m} w_j x_j$
  where m = the dimension of observation space, i.e. number of features.

- Goal: Find the best linear model (i.e., weights) given the data.
- Many different possible evaluation criteria!

- Most common choice is to find the $\mathbf{w}$ that minimizes:

$$Err(\mathbf{w}) = \sum_{i=1:n} (y_i - \mathbf{w}^T\mathbf{x}_i)^2$$

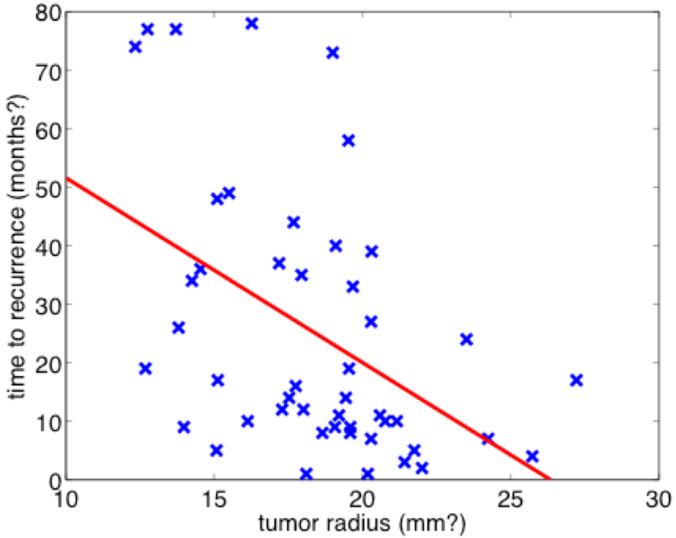
(A note on notation: Here $\mathbf{w}$ and $\mathbf{x}$ are vectors of size $m+1$.)

Is linear regression always easy to solve?

- Recall the least-square solution:
  $$\hat{\mathbf{w}} = (X^T X)^{-1} X^T Y$$
- Assuming for now that X is reasonably small and that we can find a closed-form solution in poly-time.
  - Does this always work (well)?

Is linear regression always easy to solve?

- Recall the least-square solution:
  $\hat{\mathbf{w}} = (X^TX)^{-1} X^T Y$
- Two main failure modes:
  - 1) (X^TX) is **singular**, so the inverse is undefined.
  - 2) A simple linear function is a bad fit… (e.g., figure to the right)



Failure mode 1: Avoiding singularities

- Recall the least-square solution:
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- To have a unique solution, we need $X^T X$ to be nonsingular.
- That means X must have full column rank (i.e. no correlation between features).

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Exercise: What if X does not have full column rank? When would this happen? Design an example. Try to solve it.

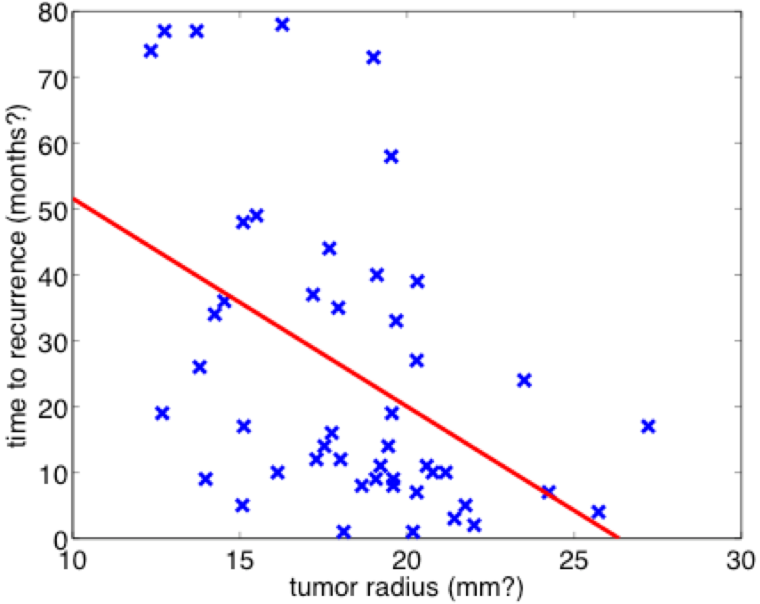
Dealing with difficult cases of $(X^TX)^{-1}$

- Case #1: The weights are not uniquely defined.
  - **Example:** One feature is a linear function of the other, e.g., $X_m = 2X_{m-1} + 2$
  - **Solution:** Re-code or drop some redundant columns of X.

- Case #2: The number of features/weights (*m*) exceeds the number of training examples (*n*).
  - **Solution:** Reduce the number of features using various techniques (to be studied later.)

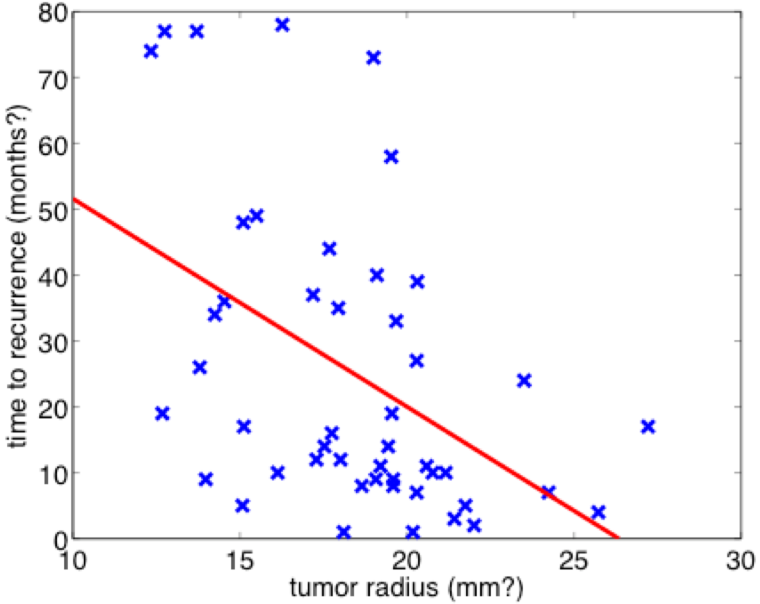
Failure mode 2: When linear is a bad fit

- This function looks complicated, and a linear hypothesis does not seem very good.
- What should we do?



Failure mode 2: When linear is a bad fit

- This function looks complicated, and a linear hypothesis does not seem very good.
- What should we do?
  - *Pick a better function?*
  - *Use more features?*
  - *Get more data?*



Input variables for linear regression

- Original quantitative variables $X_1, \ldots, X_m$

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- Numeric coding of qualitative variables, e.g. $X_{m+1} = 1$ if X_i is true and 0 otherwise.

In all cases, we can add $X_{m+1}, \ldots, X_{m+k}$ to the list of original variables and perform the linear regression.

Variable coding is not always straightforward!

- Suppose we have a categorical variable with four possible values: $\mathrm{X_{cat}} = \{\mathrm{blue, red, green, yellow}\}$
  - How do we encode this?

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    - Careful… this can lead to singularities, since these four variables will be perfectly correlated. I.e., if we know X_{cat} is not $\{\text{red}, \text{green}, \text{yellow}\}$ then it must be blue!
  - Solution 2: Three separate binary variables for $\{\text{red}, \text{green}, \text{yellow}\}$ with the blue category represented by the intercept.
    - This is a better solution!

Variable coding is not always straightforward!

- What about if our input is just raw text (or images)…?
- We need to get creative! E.g.,
  - word counts
  - average word length
  - number of words per sentence
  - etc…

Variable coding is not always straightforward!

- What about if our input is just raw text (or images)…?
- We need to get creative! E.g.,
  - word counts
  - average word length
  - number of words per sentence
  - etc…
- This is called feature design, and it will be a recurring theme throughout the course!

Input variables for linear regression

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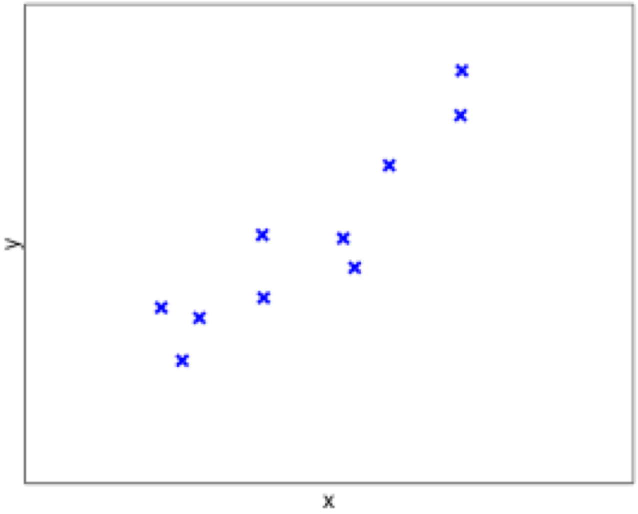
In all cases, we can add $X_{m+1}, \ldots, X_{m+k}$ to the list of original variables and perform the linear regression.

Ex: Linear regression with polynomial terms

$$f_w(x) \quad = \quad w_0 + w_1\,x + w_2\,x^2$$



$$X = \begin{array}{c} \begin{array}{ccc} x^2 & x & \end{array} \\ \begin{bmatrix} 0.75 & 0.86 & 1 \\ 0.01 & 0.09 & 1 \\ 0.73 & -0.85 & 1 \\ 0.76 & 0.87 & 1 \\ 0.19 & -0.44 & 1 \\ 0.18 & -0.43 & 1 \\ 1.22 & -1.10 & 1 \\ 0.16 & 0.40 & 1 \\ 0.93 & -0.96 & 1 \\ 0.03 & 0.17 & 1 \end{bmatrix} \end{array} \qquad Y = \begin{bmatrix} 2.49 \\ 0.83 \\ -0.25 \\ 3.10 \\ 0.87 \\ 0.02 \\ -0.12 \\ 1.81 \\ -0.83 \\ 0.43 \end{bmatrix}$$

Data matrices

$$X^T X =$$

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

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

Data matrices

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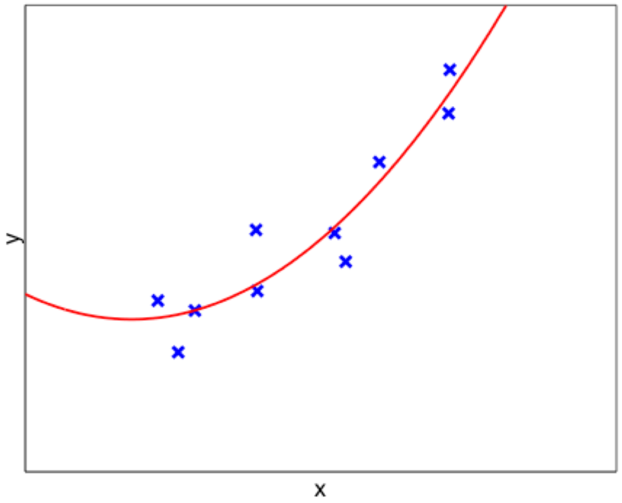
$$= \begin{bmatrix} 3.60 \\ 6.49 \\ 8.34 \end{bmatrix}$$

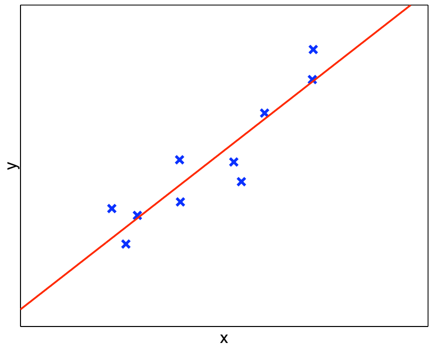
Solving the problem

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

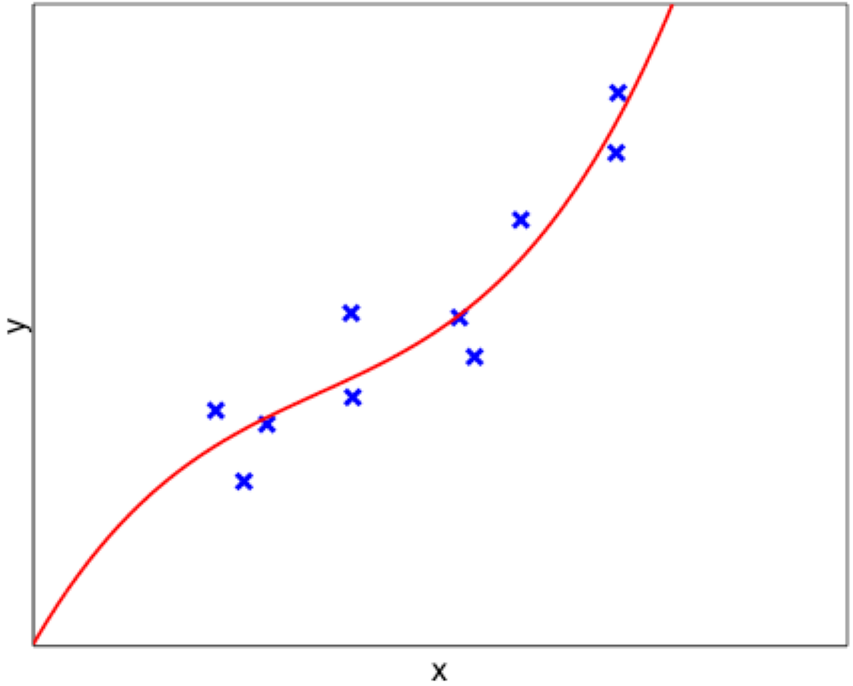
So the best order-2 polynomial is $y = 0.68x^2 + 1.74x + 0.73$.



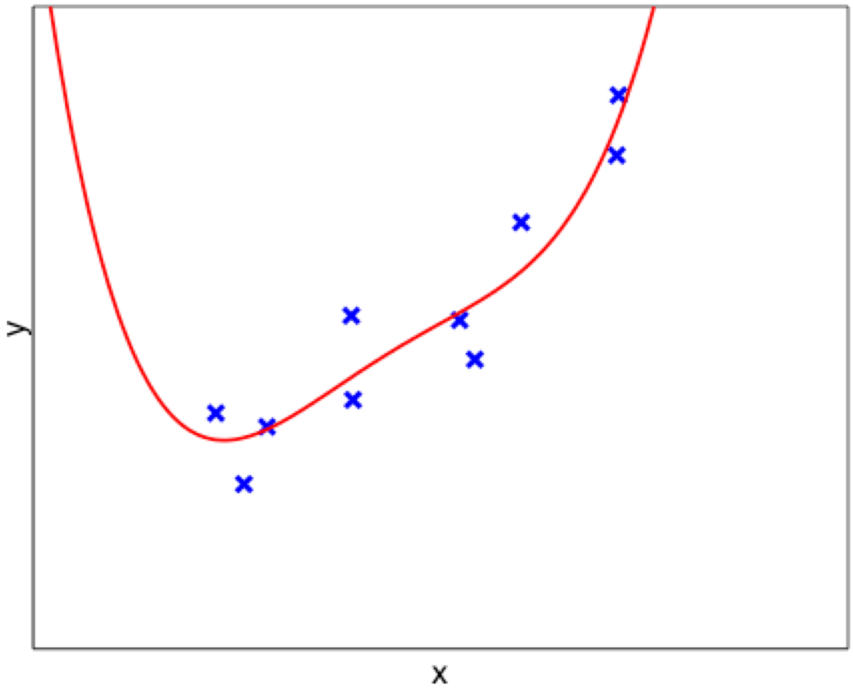
Compared to $y = 1.6x + 1.05$ for the order-1 polynomial.



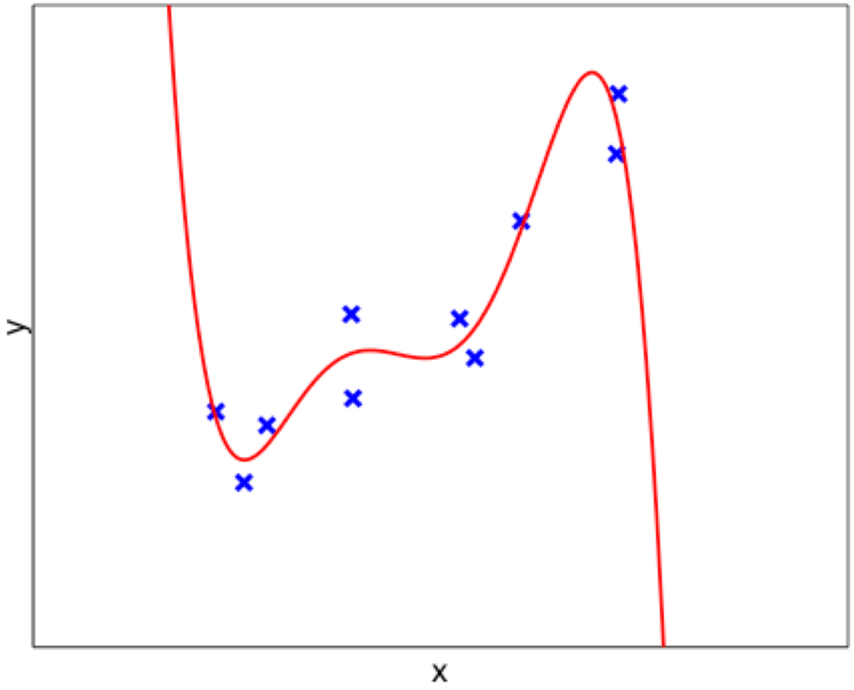
Order-3 fit: Is this better?



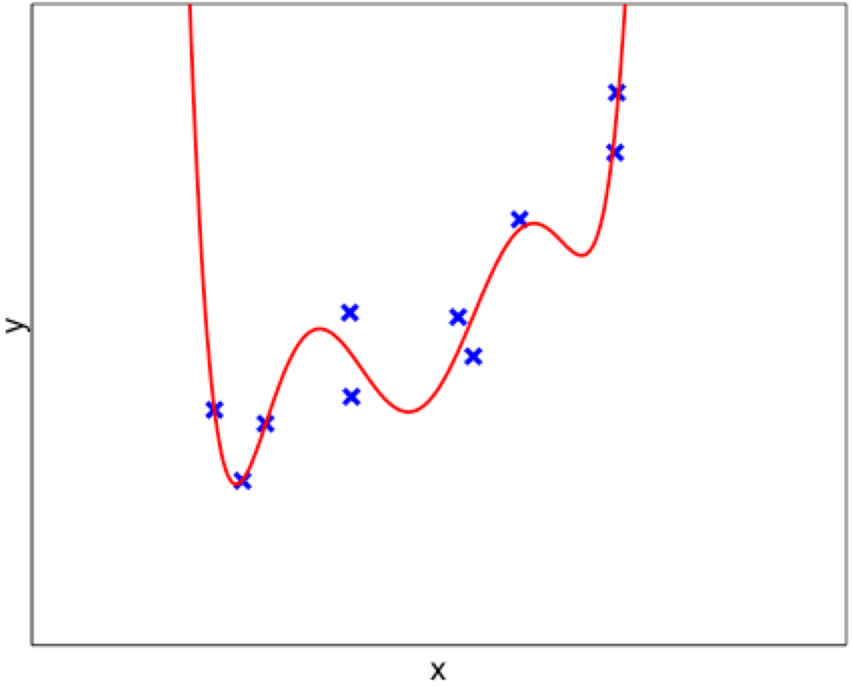
Order-4 fit



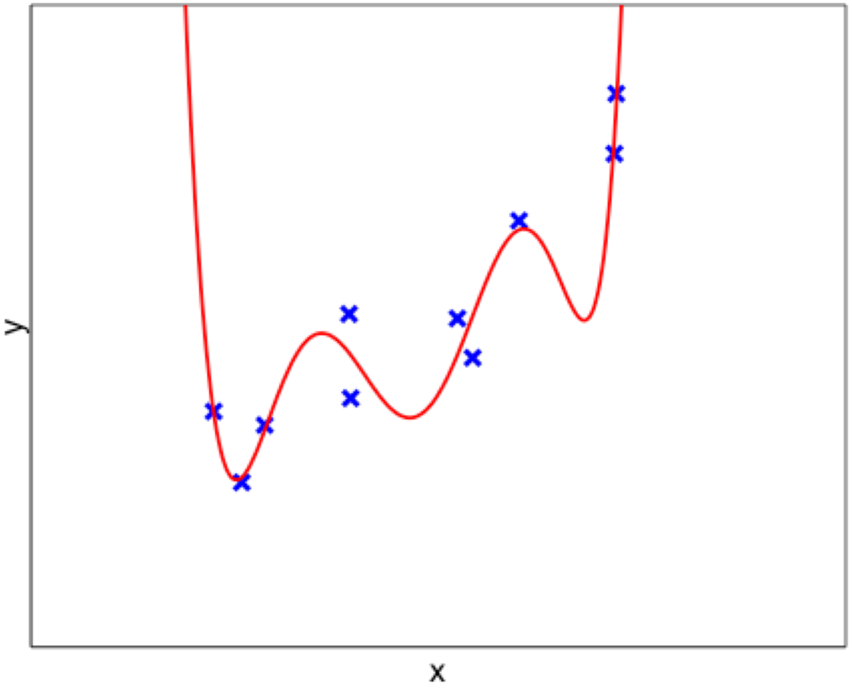
Order-5 fit



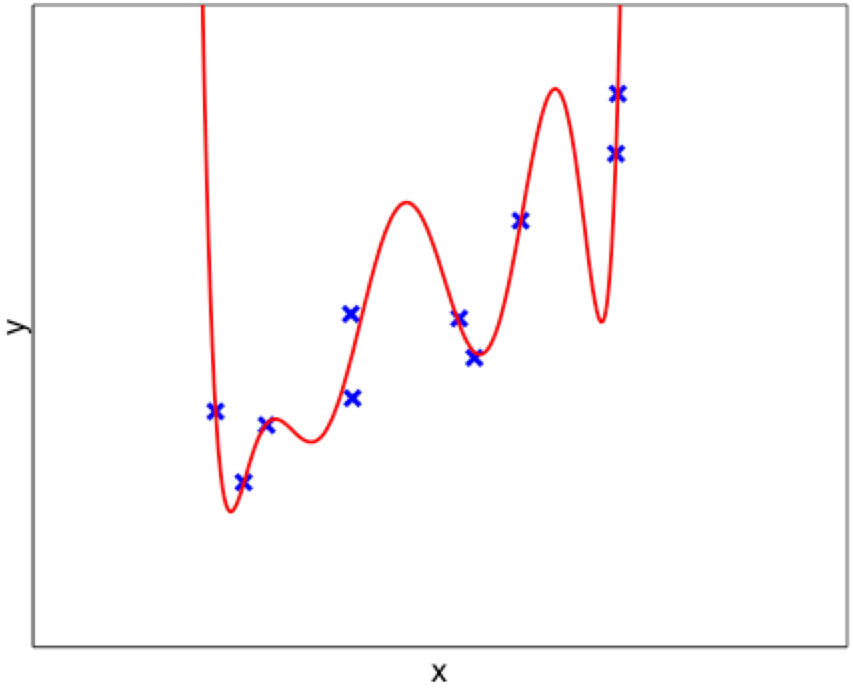
Order-6 fit



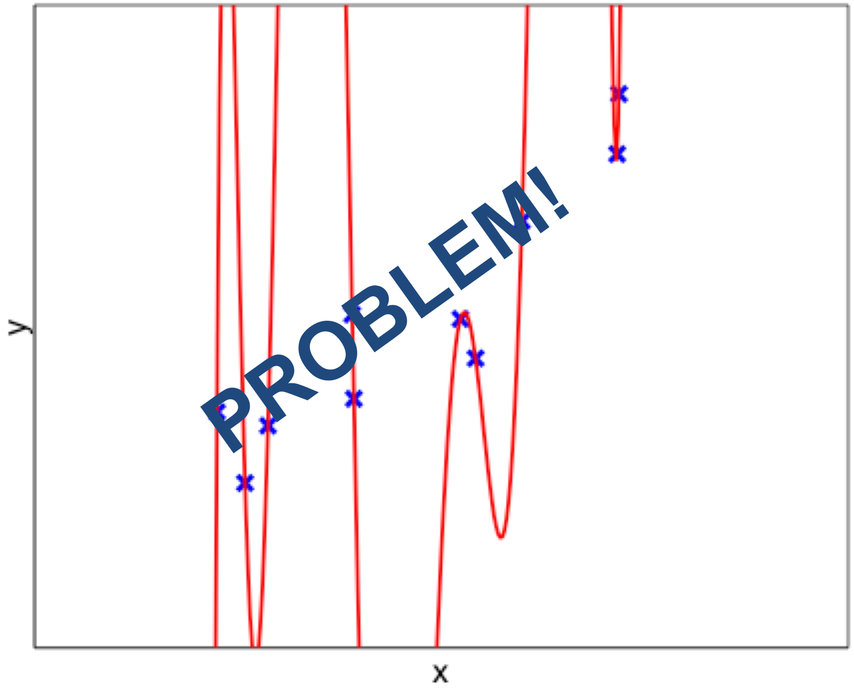
Order-7 fit



Order-8 fit



Order-9 fit



This is overfitting!

- We can find a hypothesis that explains perfectly the training data, but <u>does not generalize</u> well to new data.
- **In this example:** we have a lot of parameters (weights), so the model matches the data points exactly,

  but is wild everywhere else.
- A <u>very important</u> problem in machine learning.

Overfitting

- Every hypothesis has a **true** error measured on all possible data items we could ever encounter (e.g. $f_w(\mathbf{x}_i) - y_i$).

- Since we don't have all possible data, in order to decide what is a good hypothesis, we measure error over the training set.

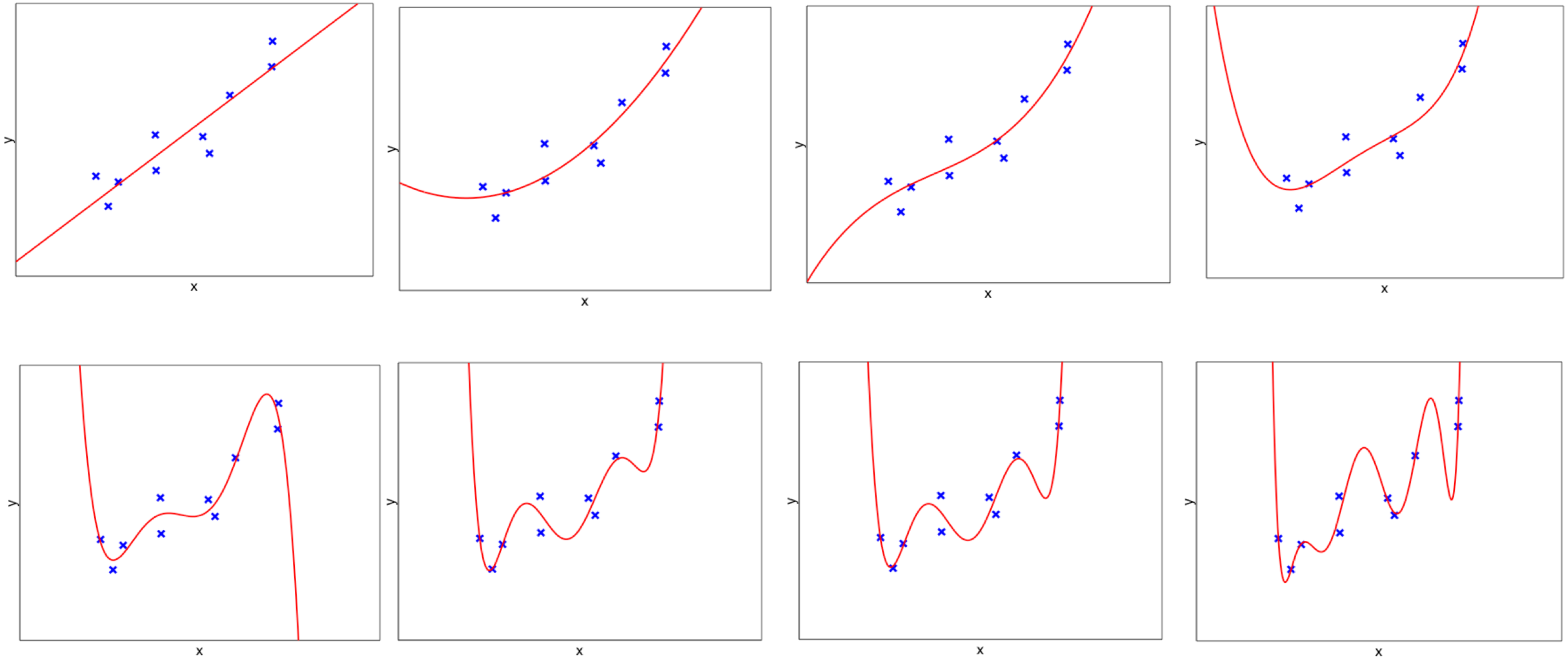
- Formally: Suppose we compare hypotheses f_1 and f_2.
  - Assume f_1 has lower error on the training set.
  - If f_2 has lower true error, then our algorithm is overfitting.

Generalization

- In machine learning our goal is to develop models that **generalize.**
- With lots of parameters it is easy to perfectly fit a training set!
  - For example, if my model has more parameters than there are training points, then the model can just memorize the training data!
- Performing well on **previously unseen data** (i.e., generalization) is the real challenge.
- But how do we evaluate generalization?

Overfitting

Which hypothesis has the lowest true error?



Evaluating on held out data

- Partition your data into a training set, validation set, and test set.
  - The proportions in each set can vary.

- Training set is used **to fit a model** (find the best hypothesis in the class).

- Validation set is used for **model selection,** i.e., to estimate true error and compare hypothesis classes. (E.g., compare different order polynominals).

- Test set is **what you report the final accuracy on.**

Evaluating on held out data

Training set =

Validation set =

Test set =

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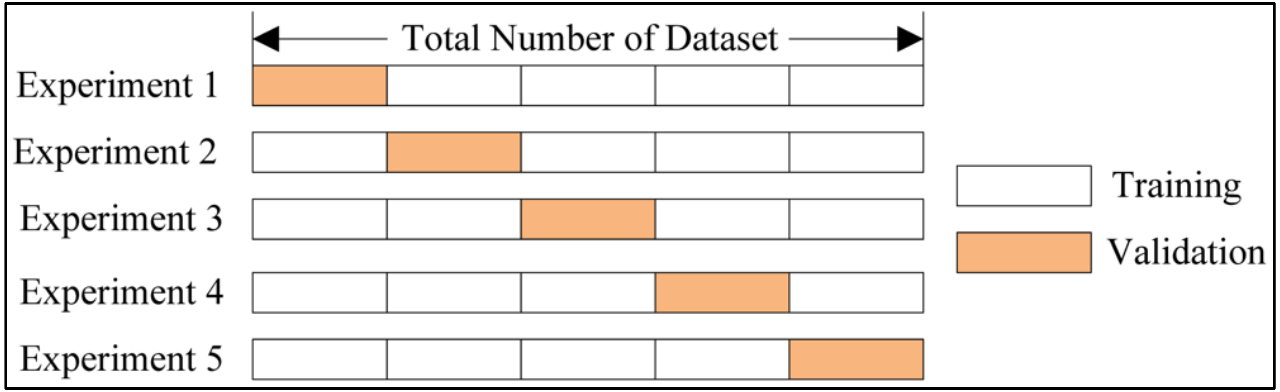
Validation set vs. test set

- Validation set is used **compare different models during development.**
  - Compare hypothesis/model classes. E.g., should I use a first- or second-order polynomial fit?
  - Compare hyperparameters (i.e., a parameter that is **not** learned but that could impact performance). E.g., what learning rate should I use?
- Test set is used **evaluate the final performance of your model** (e.g., compare between research groups).
- Why separate them? If you try too many models or hyperparameter settings, you might start to overfit the validation set! (A kind of "meta"-overfitting).

k-fold cross validation

- Instead of just one validation set, we can evaluate on many splits!
  - Consider k partitions of the training/non-test data (usually of equal size).
  - Train with $k\text{-}1$ subsets, validate on k^{th} subset. Repeat k times.
  - Average the prediction error over the k rounds/folds.



Source: *http://stackoverflow.com/questions/31947183/how-to-implement-walk-forward-testing-in-sklearn*

(increases computation time by a factor of k)

Leave-one-out cross validation

- Let $k = n$, the size of the training set

- For each model / hyperparameter setting,
  - Repeat n times:
    - Set aside *one instance* $<x_i, y_i>$ from the training set.
    - Use all other data points to find $\mathbf{w}$ (optimization).
    - Measure prediction error on the held-out $<x_i, y_i>$.
  - Average the prediction error over all n subsets.

- Choose the setting with lowest estimated true prediction error.

Generalization: test vs. train error

- Overly simple model:
  - High training error and high test error.
- Overly complex model:
  - Low training error but high test error.

[From Hastie et al. textbook]

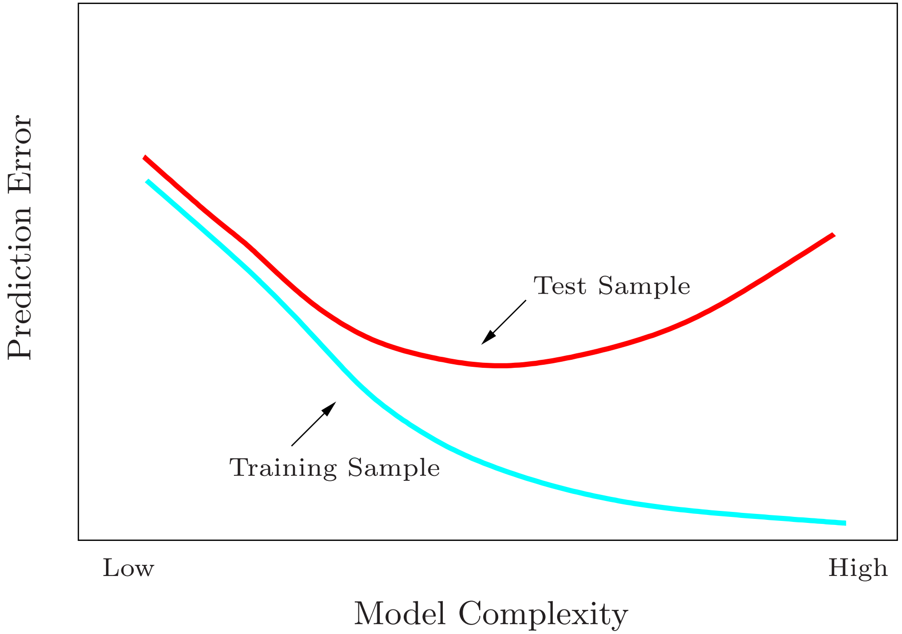


FIGURE 2.11. *Test and training error as a function of model complexity.*

Traditional statistics vs. machine learning

- <u>Traditional statistics:</u> how can we accurately estimate the effect of $\mathbf{x}$ on $\mathbf{y}$?

- <u>Machine learning:</u> how can we design a function that predicts $\mathbf{x}$ from $\mathbf{y}$ and generalizes to unseen data?

Recap: Evaluating on held out data

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What you should know

- Linear regression (hypothesis class, error function, algorithm).
- How linear regression can fail
- Gradient descent method (algorithm, properties).
- Train vs. validation vs. test sets.
- The notion of generalization.