UVA CS 4774: Machine Learning

Lecture 6: Model Selection

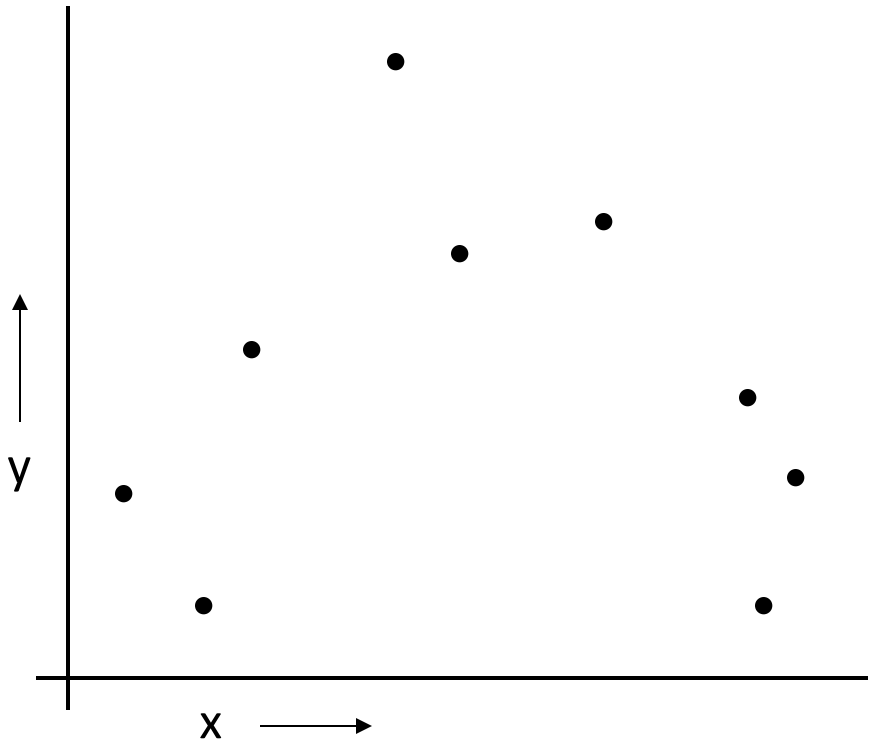
Dr. Yanjun Qi

University of Virginia
Department of Computer Science

Main issues: Model Selection

- How to select the right model type? How to select hyperparameter for a model type?
  - E.g. what polynomial degree d for polynomial regression
  - E.g., where to put the centers for the RBF kernels? How wide?
  - E.g. which basis type? Polynomial or RBF?

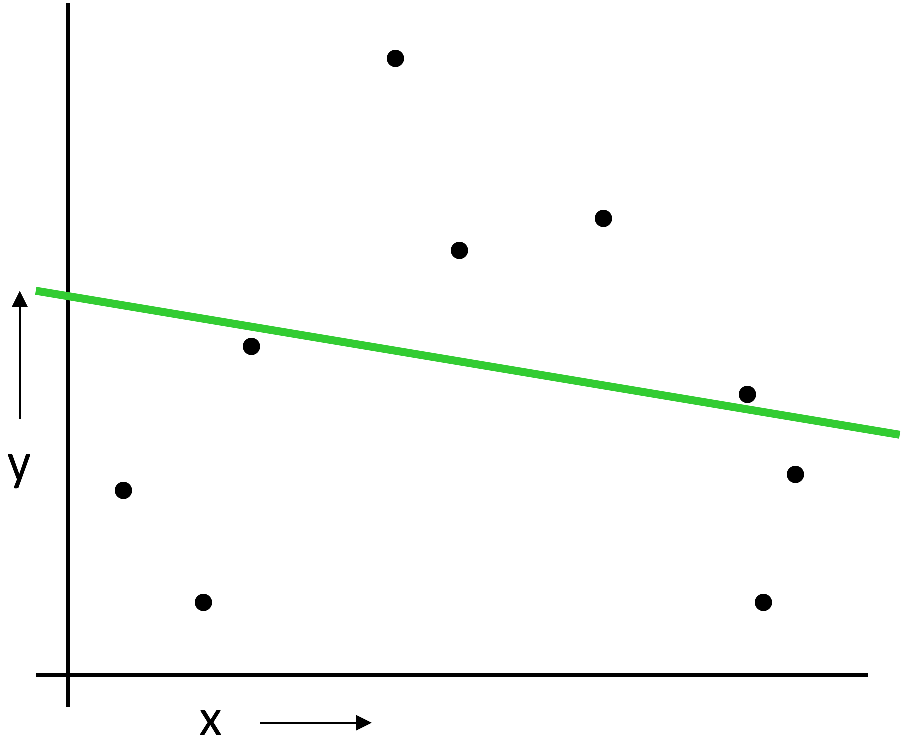
To Avoid: Overfitting or Underfitting



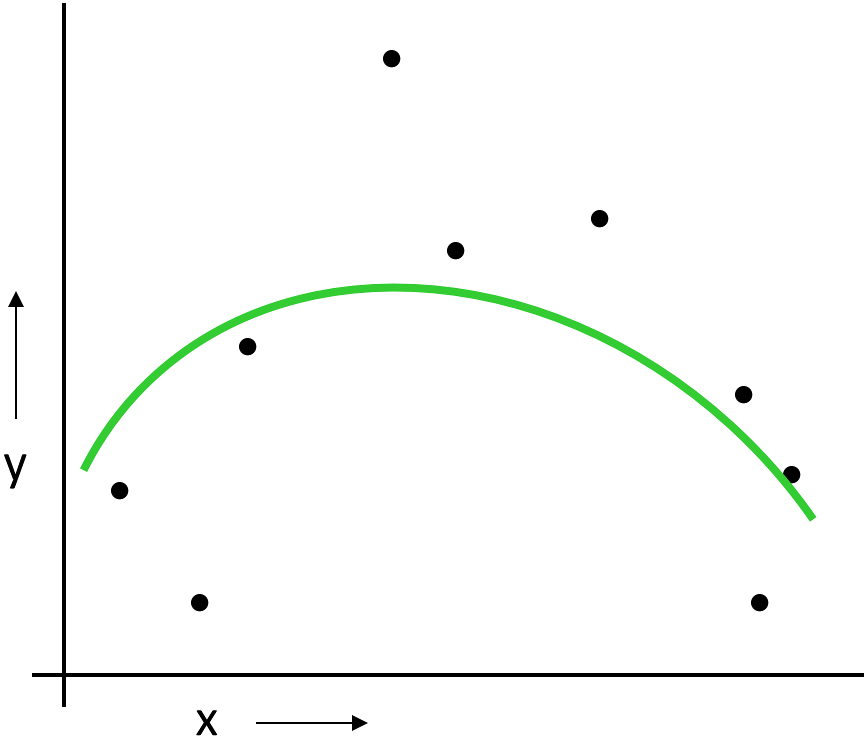
Can we learn a regression f from the data?

Let's consider three methods…

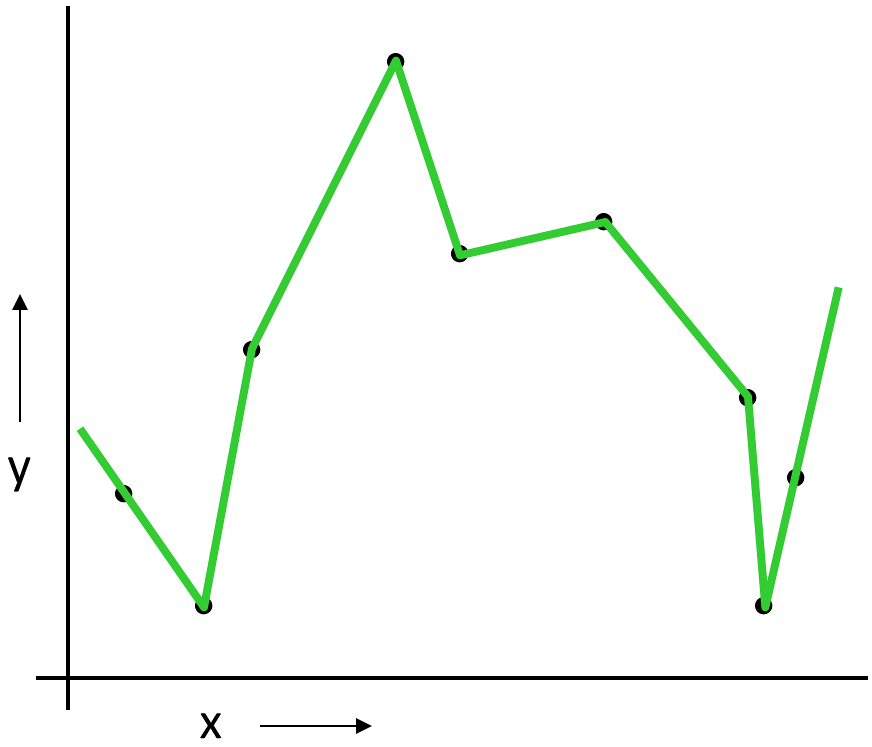
Linear Regression



Quadratic Regression

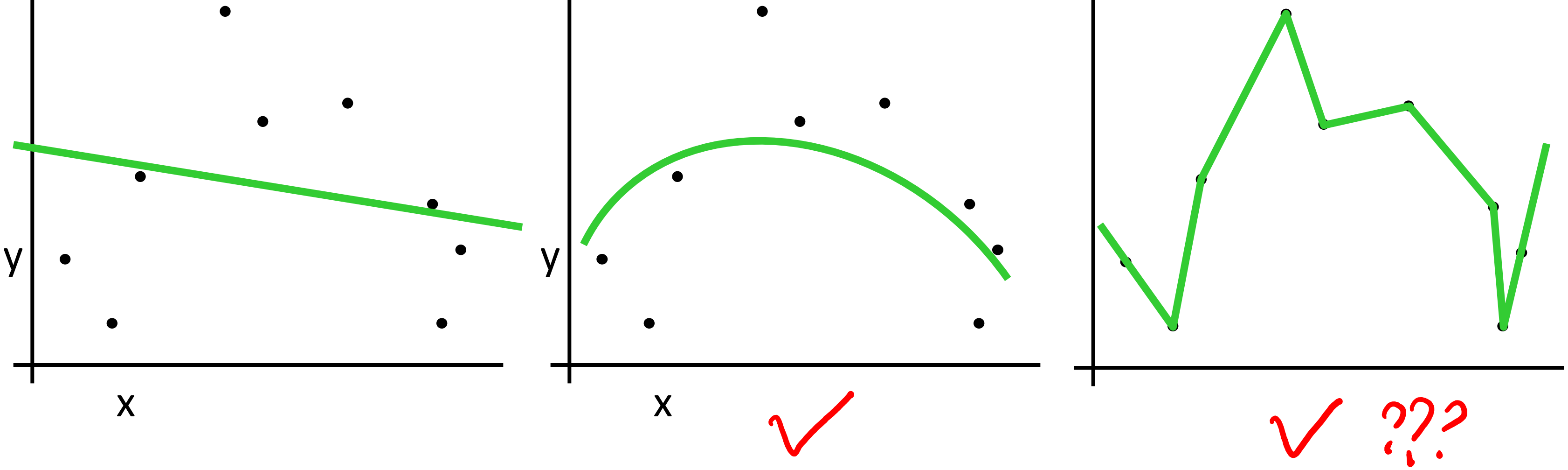


Join-the-dots



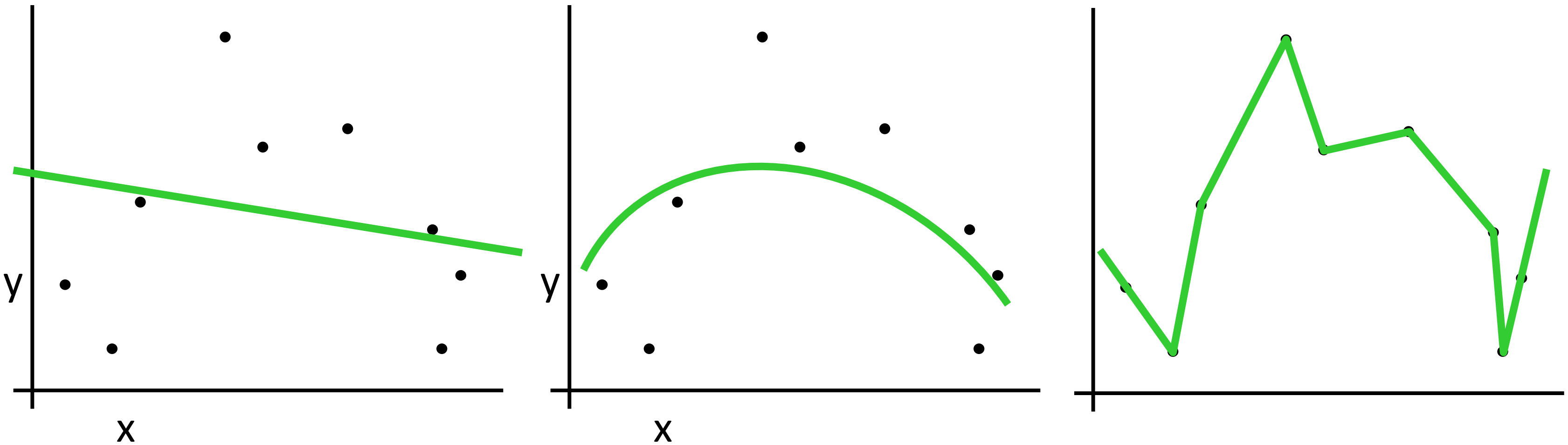
Also known as piecewise linear nonparametric regression if that makes you feel better

Which is best?



Why not choose the method with the best fit to the training data?

What do we really want?

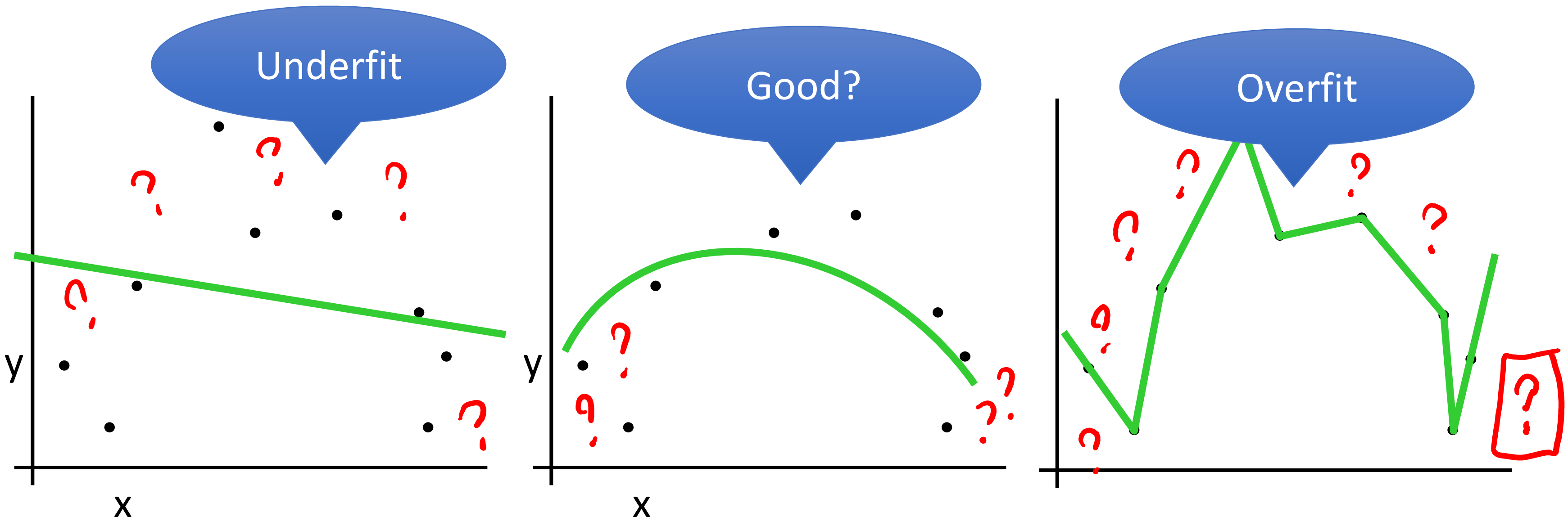


Why not choose the method with the best fit to the data?

IID { train
test

"How well are you going to predict future data drawn from the same distribution?"

What Model Type / Model Order to Select?



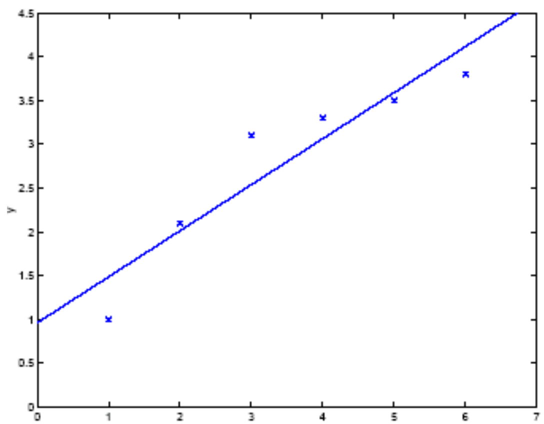
Why not choose the method with the best fit to the data?

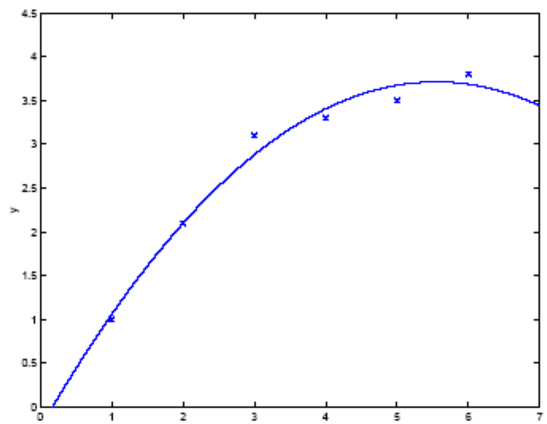
Generalisation: learn function / hypothesis from past data in order to “explain”, “predict”, “model” or “control” new data examples

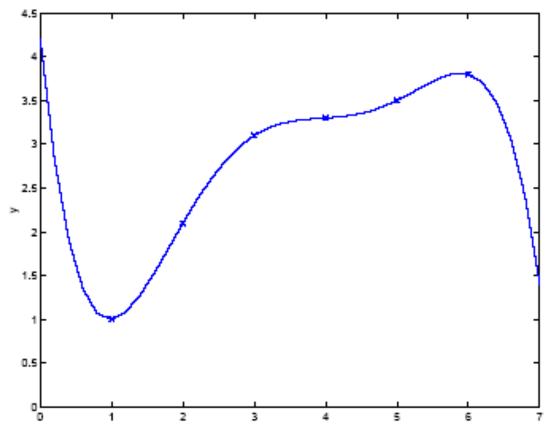
What Model Order to Select?

hyperparameter d

Under fit	Looks good	Over fit
$d=1$	$d=2$	$d=5$







$$y = \theta_0 + \theta_1 x$$

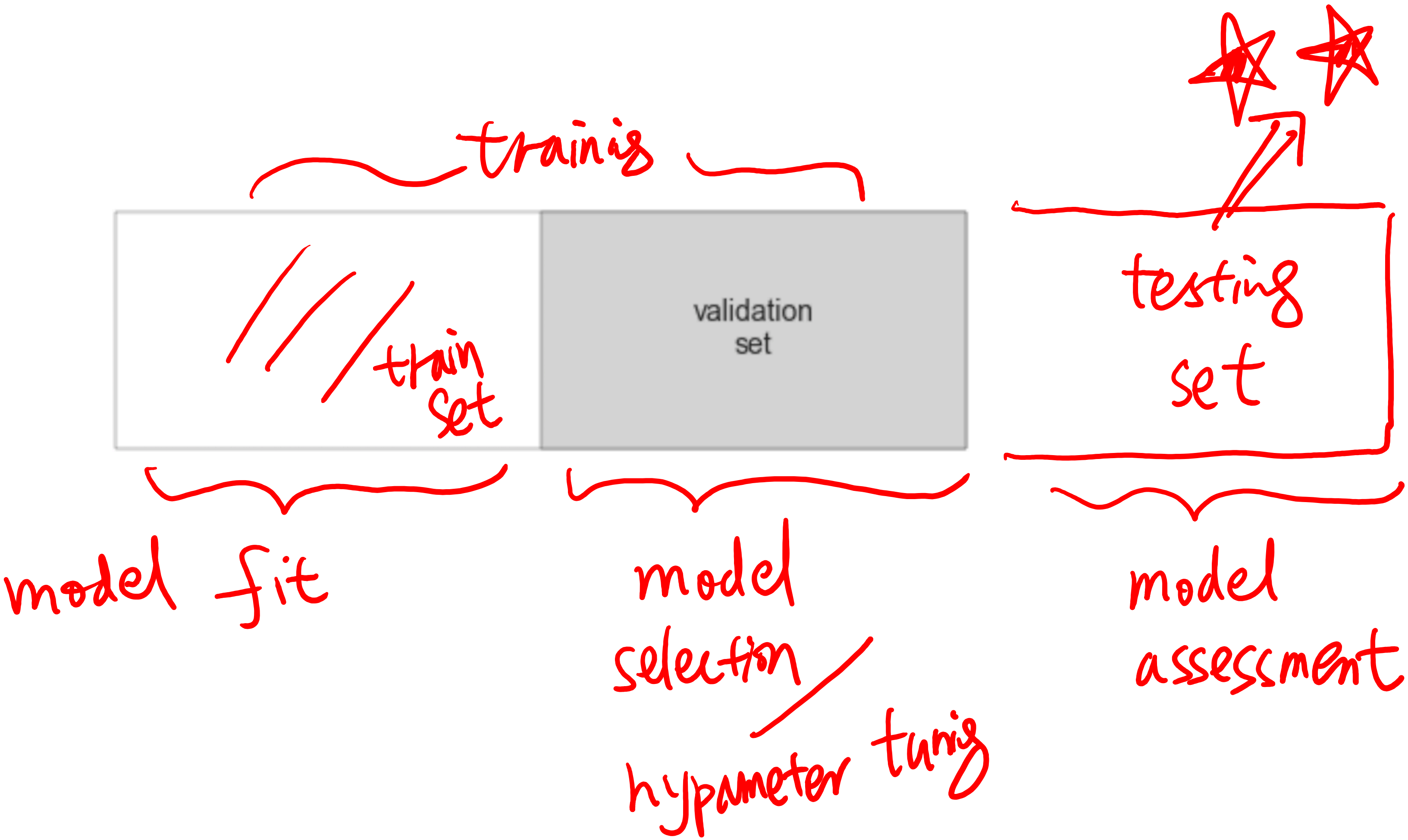
$$y = \theta_0 + \theta_1 x + \theta_2 x^2$$

$$y = \sum_{j=0}^{5} \theta_j x^j$$

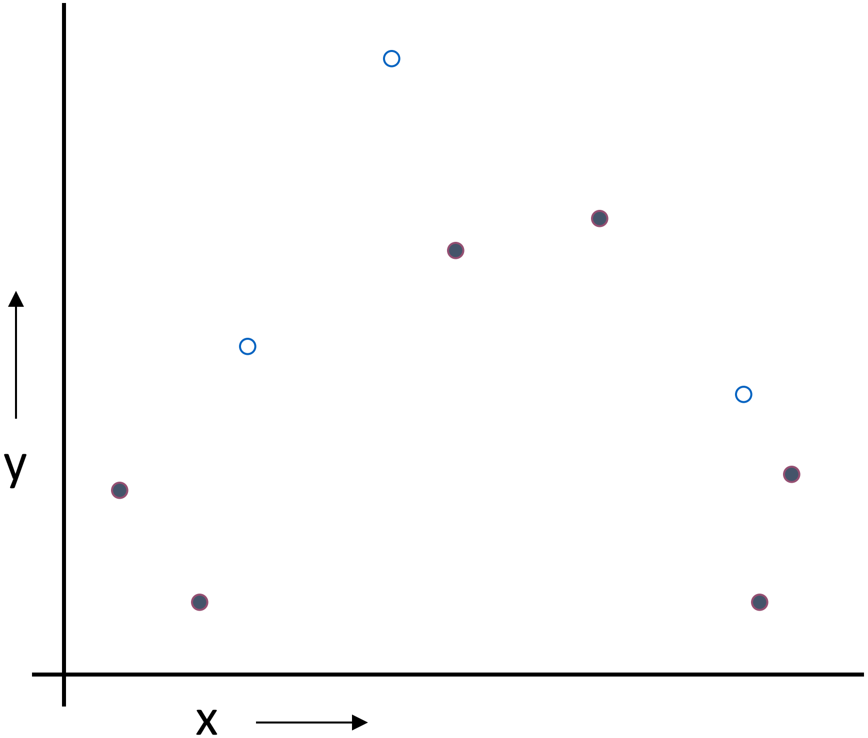
Generalisation: learn function / hypothesis from past data in order to “explain”, “predict”, “model” or “control” new data examples

(a) Train-validation / (b) K-fold Cross Validation /

Choice-I: Train-Validation (Hold m out)



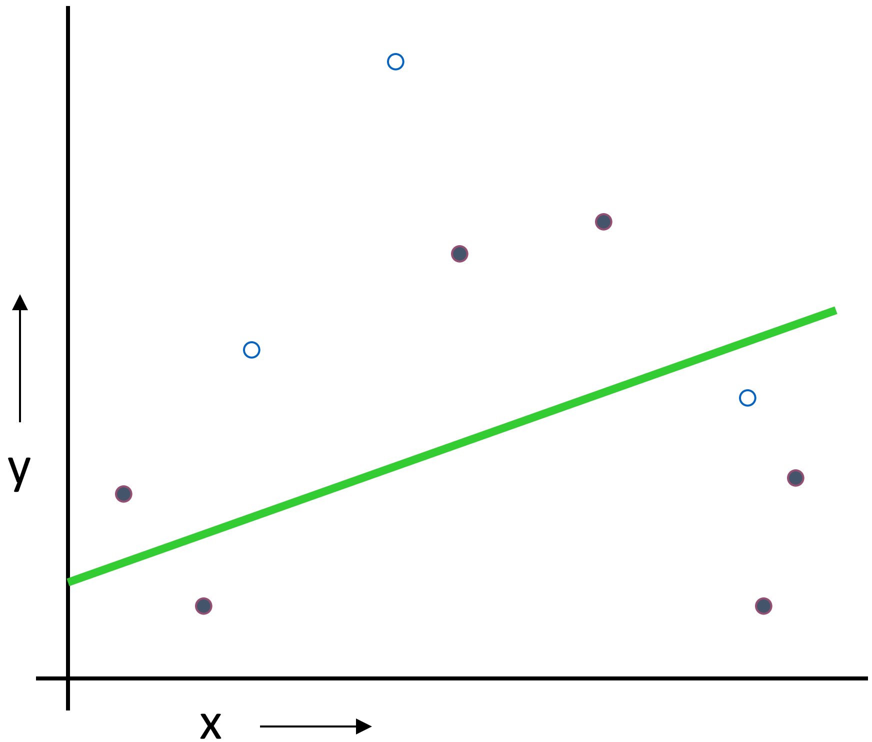
The validation set method



1. Randomly choose some percentage like 30% of the labeled data to be in a validation set
2. The remainder is a training set

Credit: Prof. Andrew Moore

The validation set method

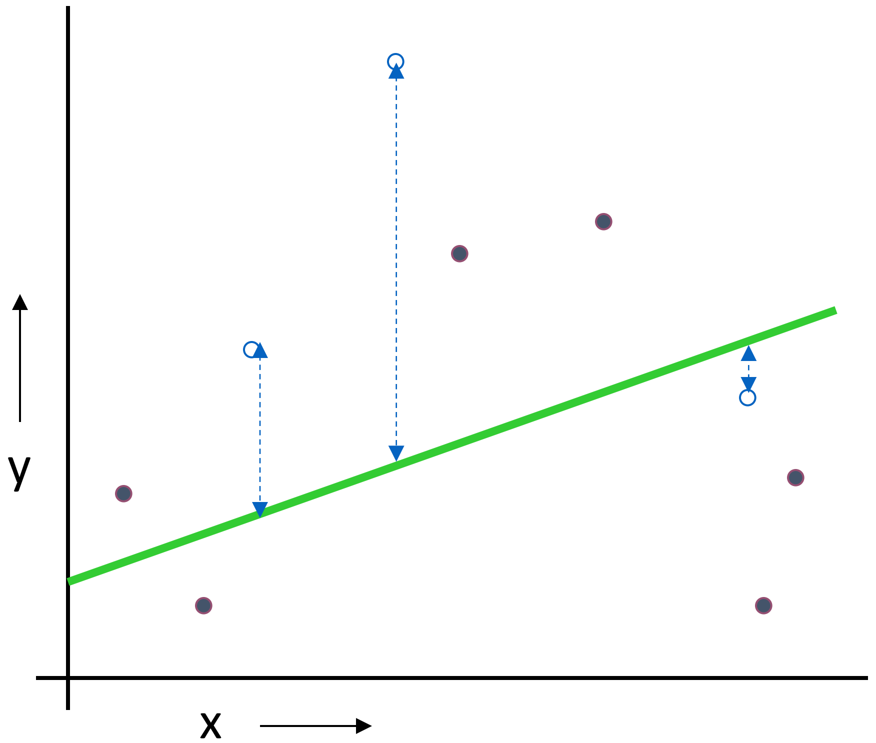


1. Randomly choose some percentage like 30% of the labeled data to be in a validation set
2. The remainder is a training set
3. Perform your regression on the training set

(Linear regression example)

Credit: Prof. Andrew Moore

The validation set method



1. Randomly choose 30% of the data to be in a validation set
2. The remainder is a training set
3. Perform your regression on the training set
4. Estimate your future performance with the validation set

(Linear regression example)
Mean Squared Error = 2.4

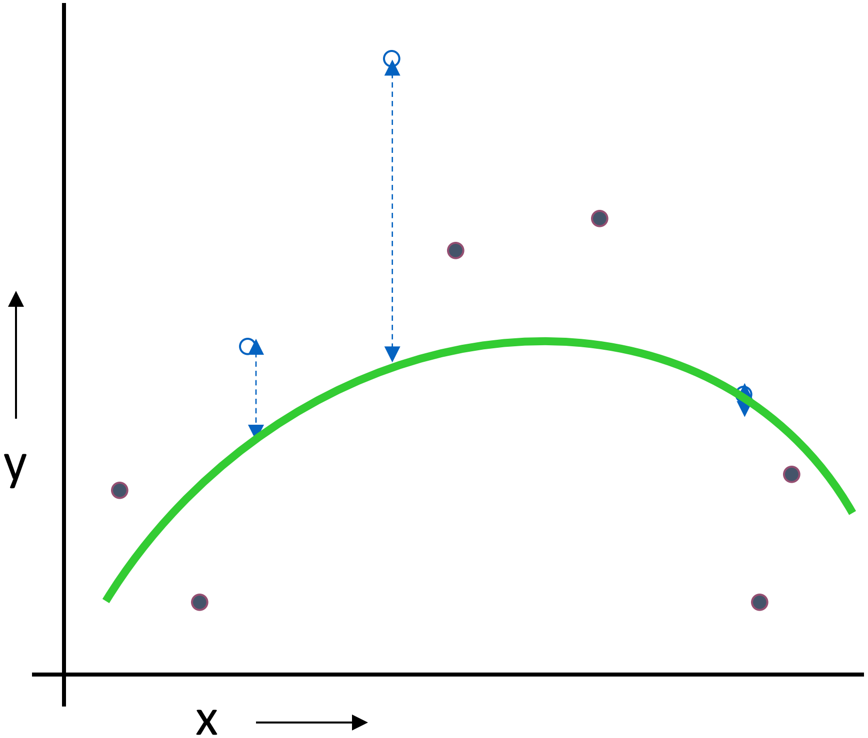
Credit: Prof. Andrew Moore

e.g. for Regression Models

- Mean Squared Error - MSE to report:

$$J_{test} = \frac{1}{m} \sum_{i=n+1}^{n+m} (\mathbf{x}_i^T \theta^* - y_i)^2 = \frac{1}{m} \sum_{i=n+1}^{n+m} \varepsilon_i^2$$

The validation set method

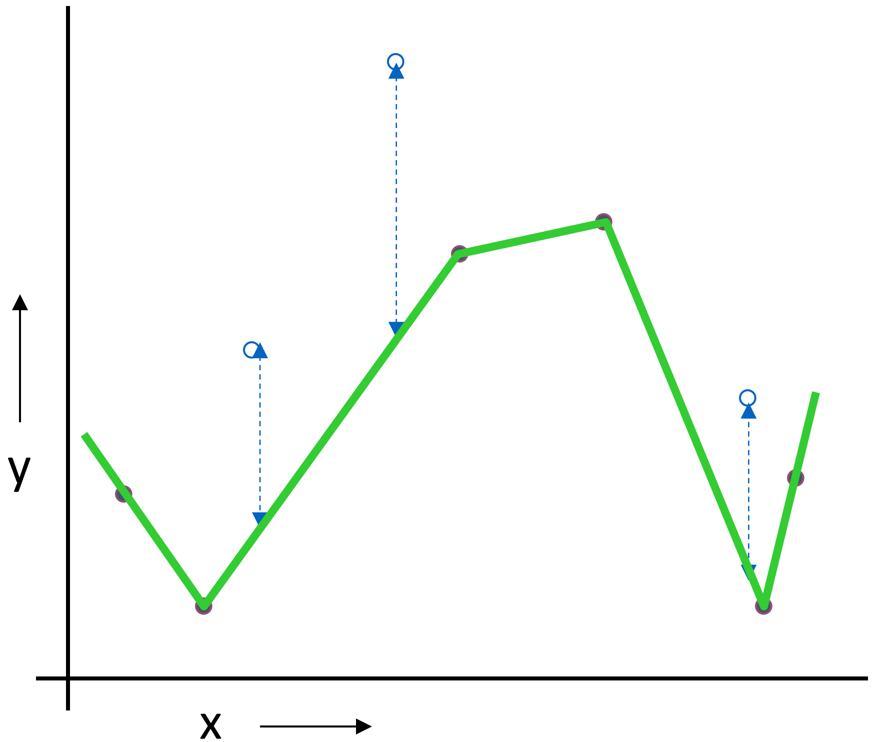


1. Randomly choose 30% of the data to be in a validation set
2. The remainder is a training set
3. Perform your regression on the training set
4. Estimate your future performance with the validation set

(Quadratic regression example)
Mean Squared Error = 0.9

Credit: Prof. Andrew Moore

The validation set method



1. Randomly choose 30% of the data to be in a validation set
2. The remainder is a training set
3. Perform your regression on the training set
4. Estimate your future performance with the validation set

(Join the dots example)
Mean Squared Error = 2.2

Credit: Prof. Andrew Moore

The validation set method

L: Q: D
2.4 0.9 2.2
✓

Good news:

- Very very simple
- Can then simply choose the method with the best validation-set score

Bad news:

- Wastes data: we get an estimate of the best method to apply to 30% less data
- If we don't have much data, our validation-set might just be lucky or unlucky

We say the "validation-set estimator of performance has high variance"

Credit: Prof. Andrew Moore

Choice-II: k-Fold Cross Validation

- Problem of train-validation: in many cases we don’t have enough data to set aside a validation set
- Solution: Each data point is used both as train and validation
- Common types:
  - K-fold cross-validation (e.g. K=5, K=10)
  - Leave-one-out cross-validation (LOOCV, i.e., k=n)

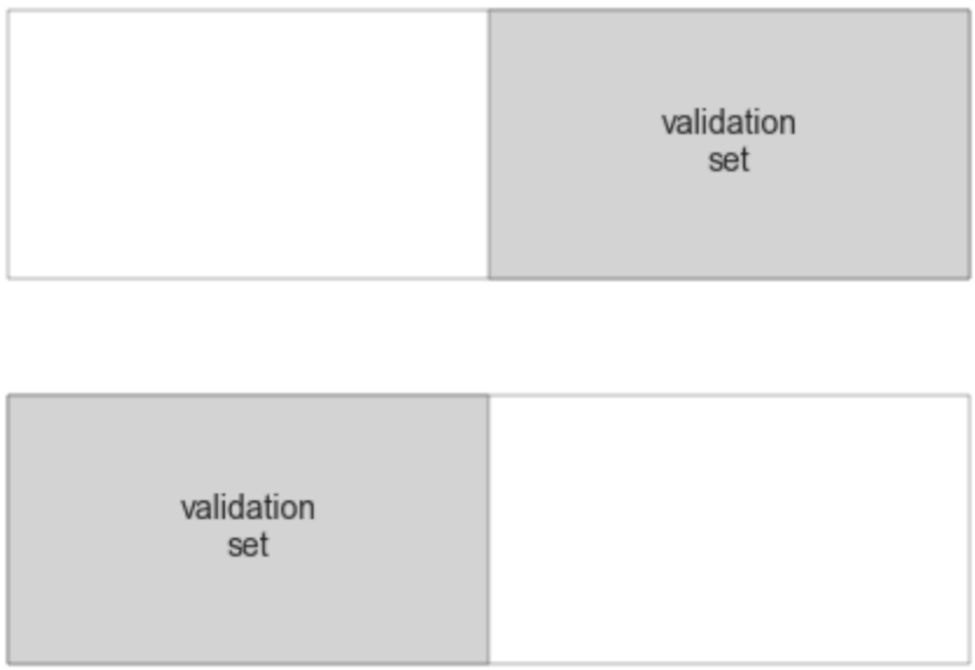
e.g. k=10 folds Cross Validation

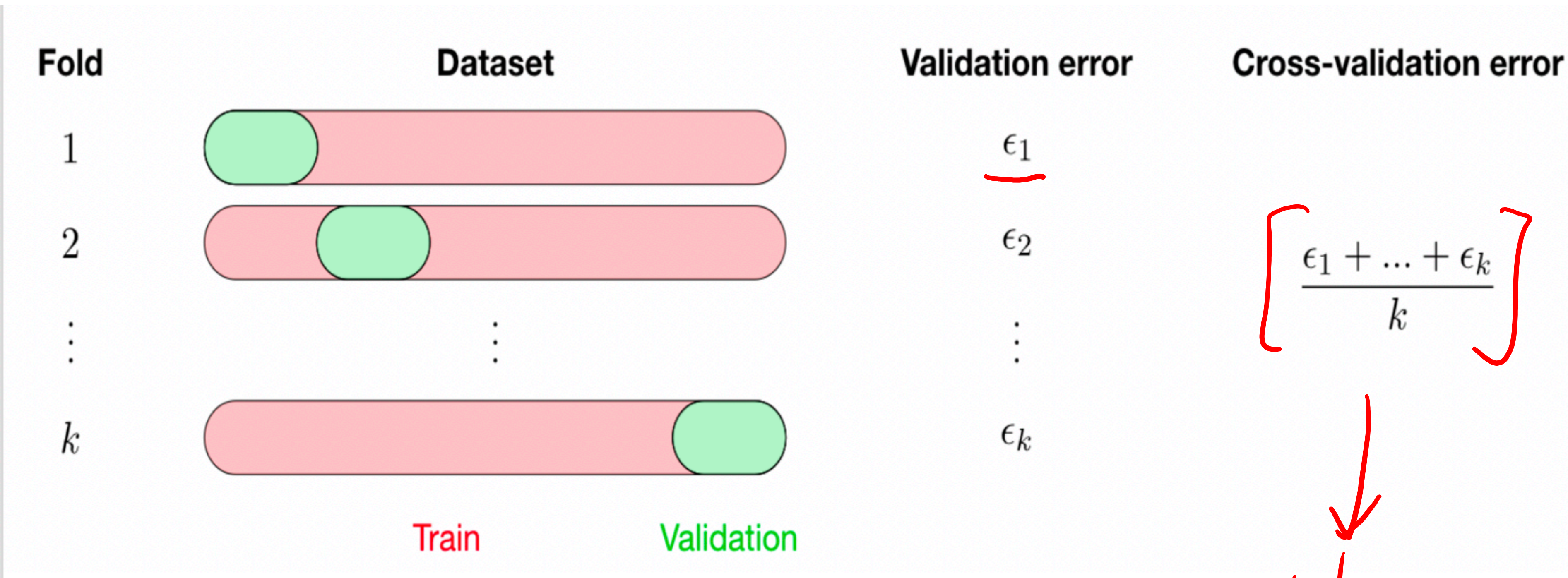
valid

- Divide data into 10 equal pieces
- 9 pieces as training set, the rest 1 as validation set
- Collect the scores from each validation
- We normally use the mean of the scores

model	P1	P2	P3	P4	P5	P6	P7	P8	P9	P10
1	train	train	train	train	train	train	train	train	train	test
2	train	train	train	train	train	train	train	train	test	train
3	train	train	train	train	train	train	train	test	train	train
4	train	train	train	train	train	train	test	train	train	train
5	train	train	train	train	train	test	train	train	train	train
6	train	train	train	train	test	train	train	train	train	train
7	train	train	train	test	train	train	train	train	train	train
8	train	train	test	train	train	train	train	train	train	train
9	train	test	train	train	train	train	train	train	train	train
10	test	train	train	train	train	train	train	train	train	train

e.g. k=2 folds Cross Validation





model selection

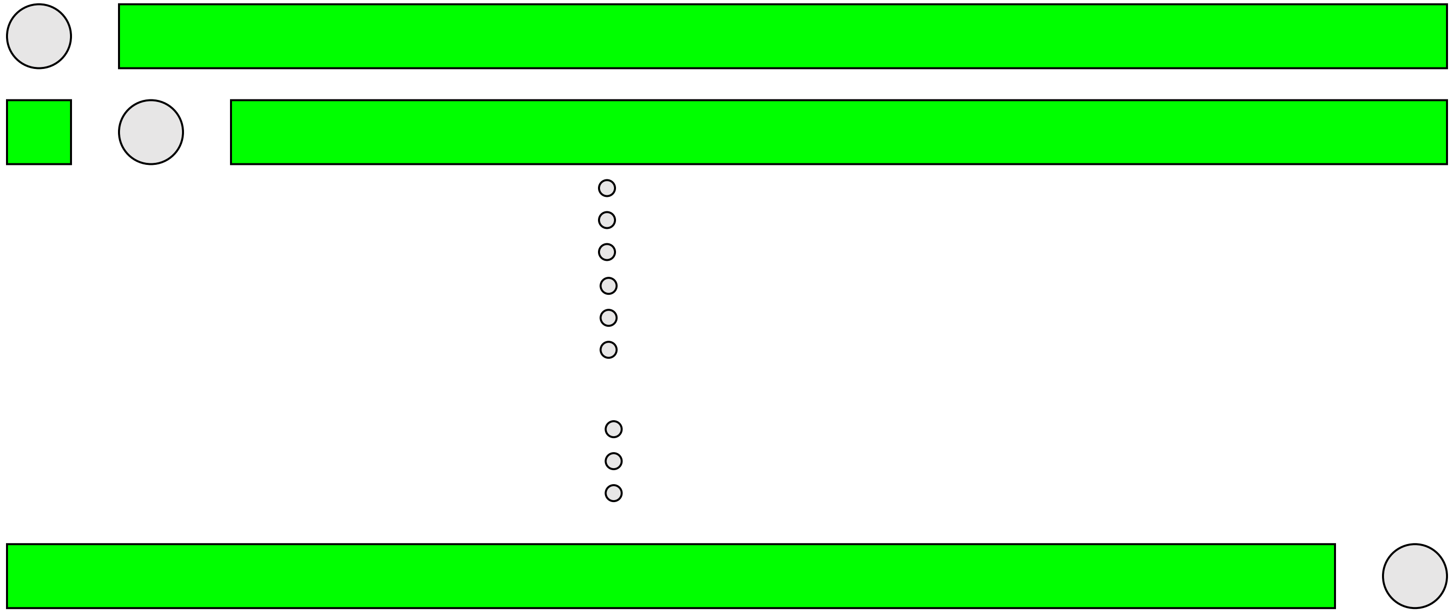
Image Credit: Stanford Machine Learning course

Which K?

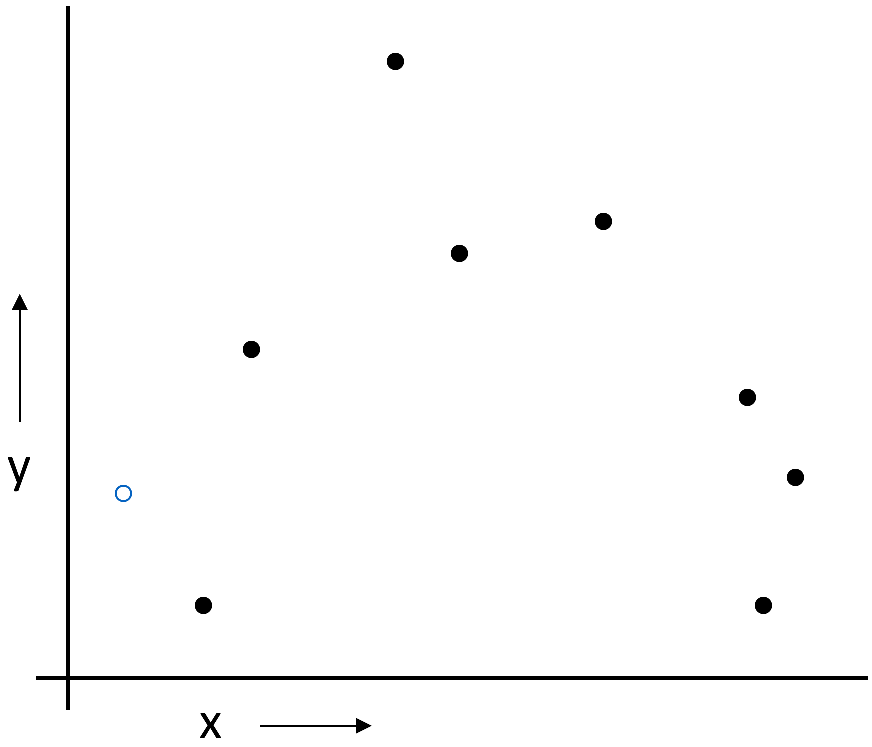
Leave-one-out / LOOCV:

(k=n-fold cross validation)

n is num. of data samples



LOOCV (Leave-one-out Cross Validation)

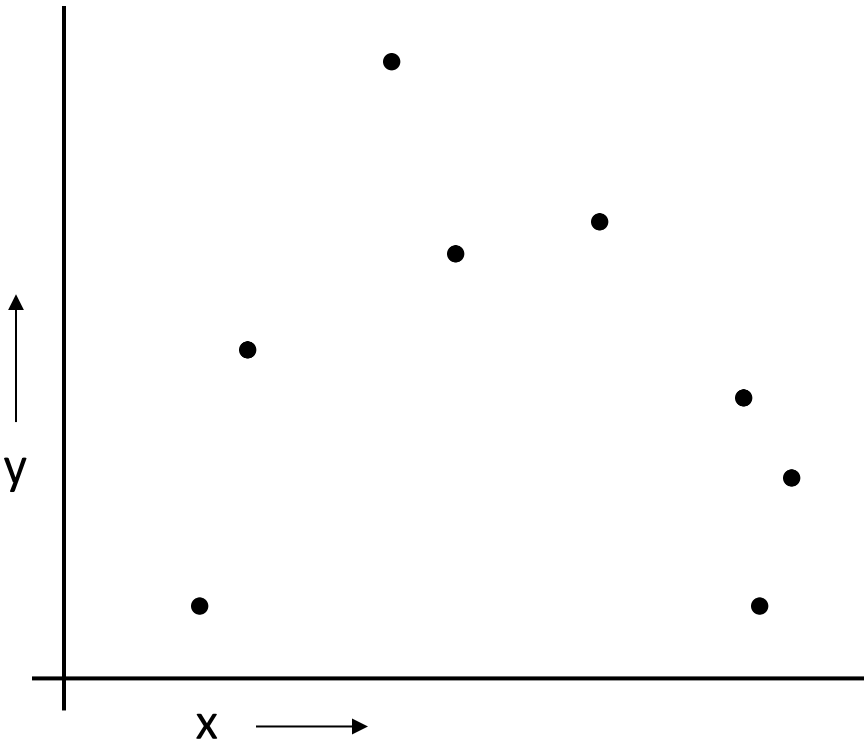


For k=1 to n

1. Let (x_k, y_k) be the k^{th} record

Credit: Prof. Andrew Moore

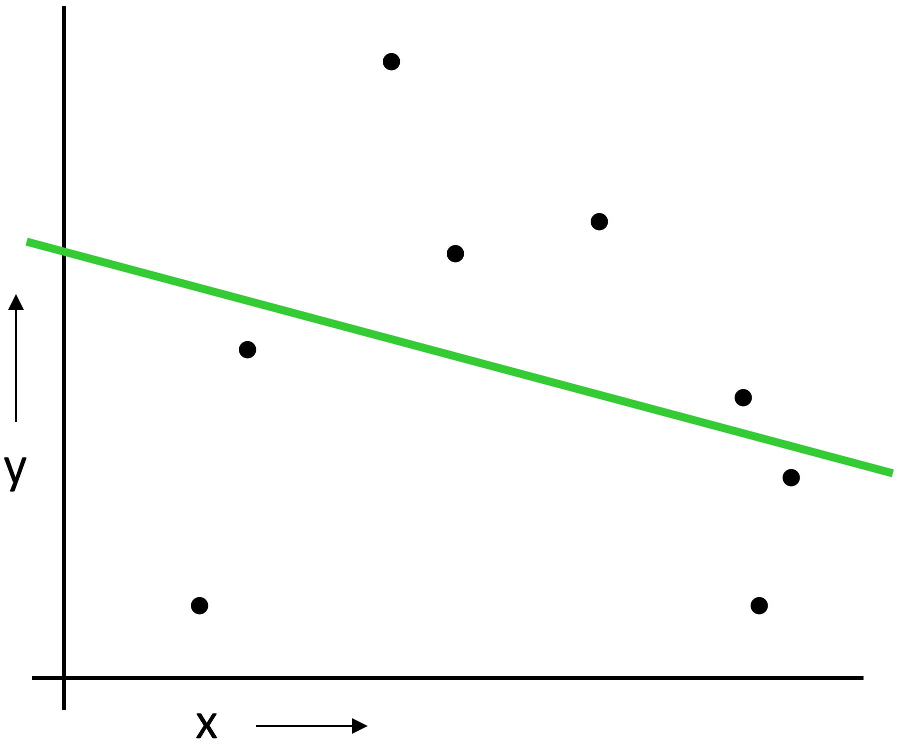
LOOCV (Leave-one-out Cross Validation)



For k=1 to n

1. Let (x_k, y_k) be the k^{th} record
2. Temporarily remove (x_k, y_k) from the dataset

LOOCV (Leave-one-out Cross Validation)

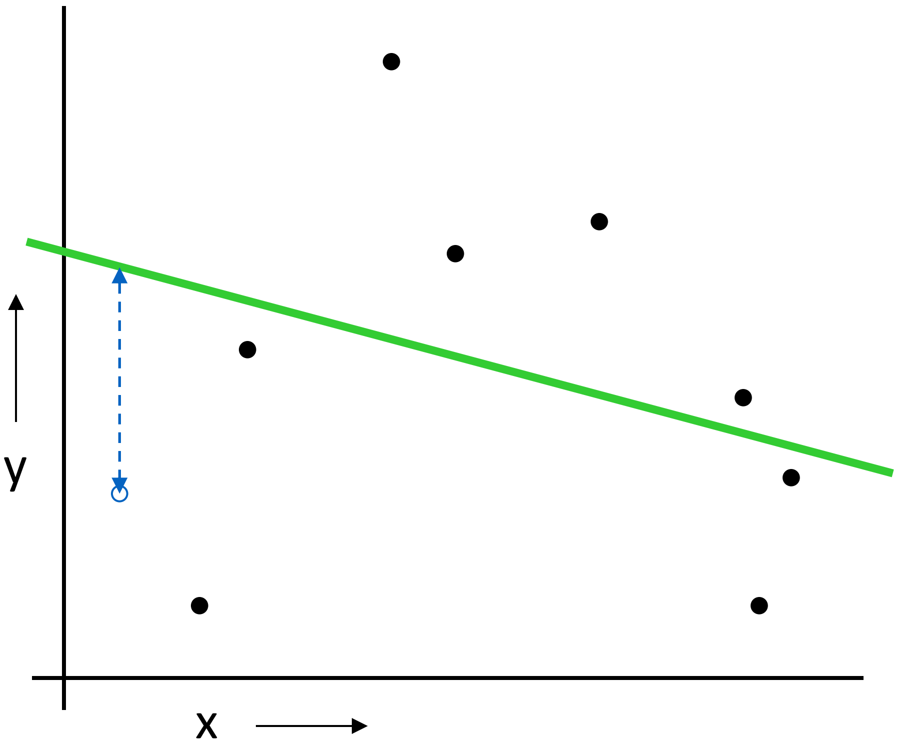


For k=1 to n

1. Let (x_k, y_k) be the k^{th} record
2. Temporarily remove (x_k, y_k) from the dataset
3. Train on the remaining n-1 datapoints

Credit: Prof. Andrew Moore

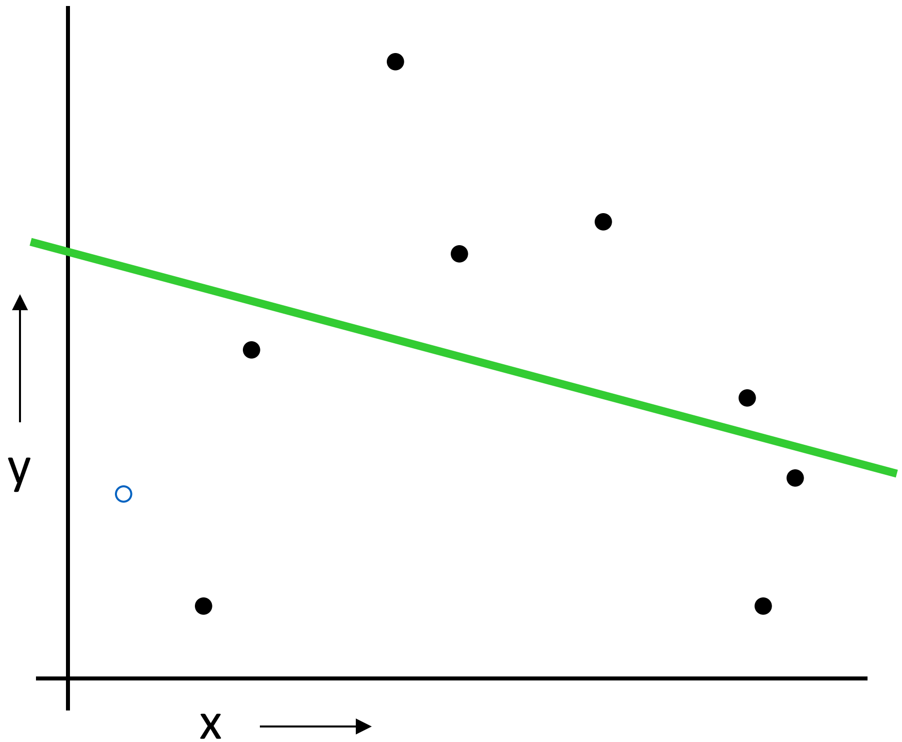
LOOCV (Leave-one-out Cross Validation)



For k=1 to n

1. Let (x_k,y_k) be the k^{th} record
2. Temporarily remove (x_k,y_k) from the dataset
3. Train on the remaining R-1 datapoints
4. Note your error (x_k,y_k)

LOOCV (Leave-one-out Cross Validation)

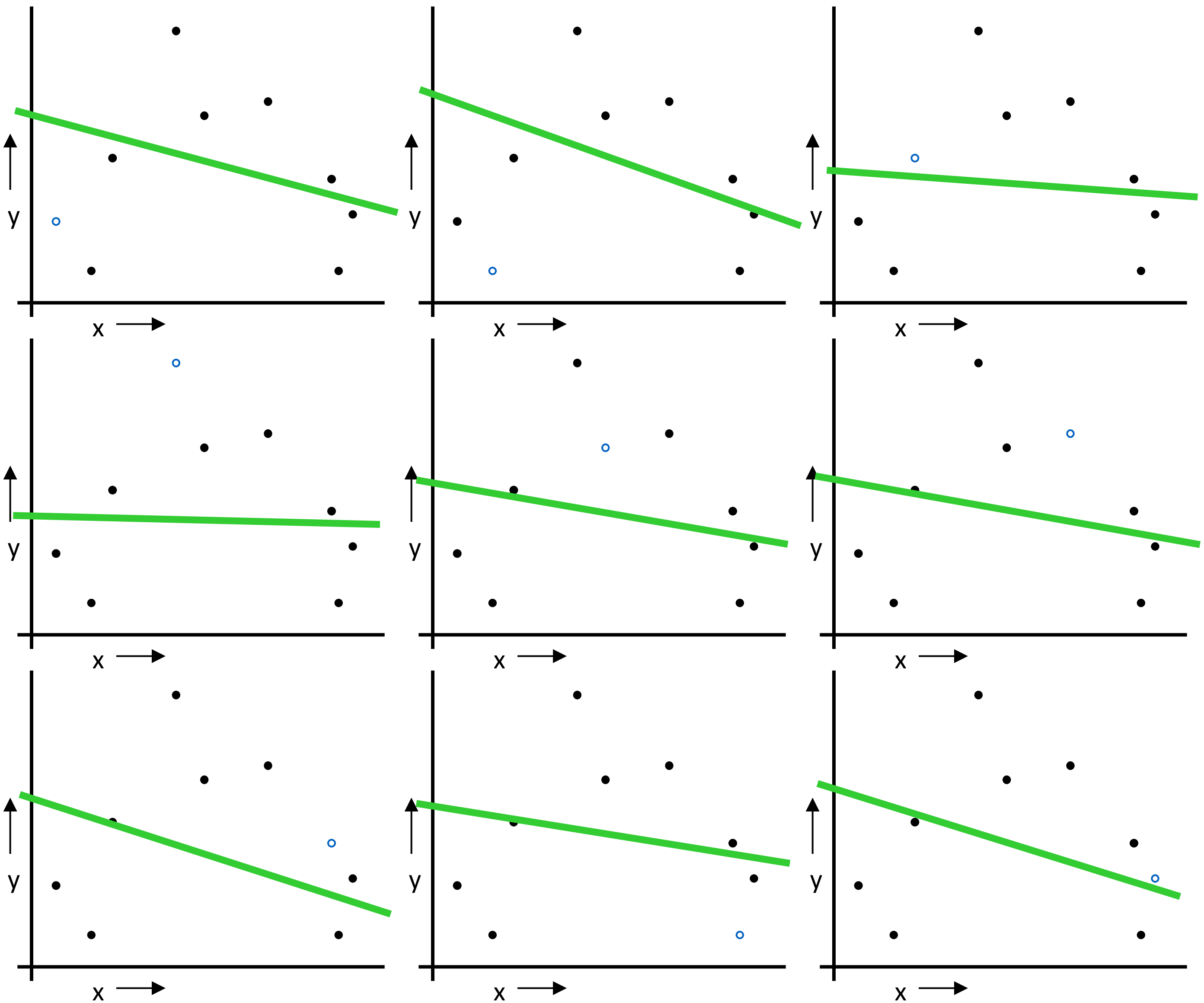


For k=1 to R

1. Let (x_k,y_k) be the k^{th} record
2. Temporarily remove (x_k,y_k) from the dataset
3. Train on the remaining R-1 datapoints
4. Note your error (x_k,y_k)

When you've done all points, report the mean error.

LOOCV for Linear Regression



For k=1 to n

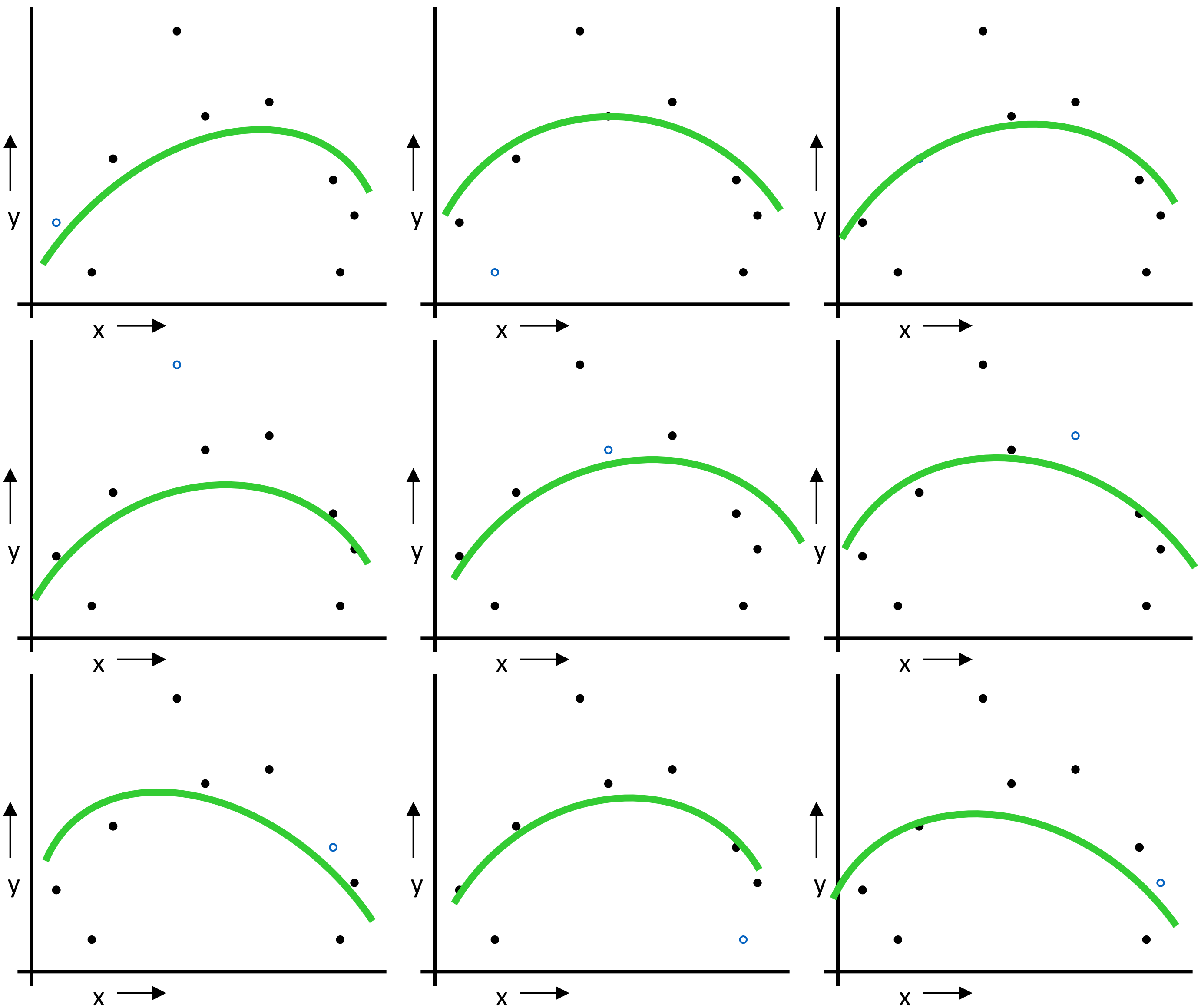
1. Let (x_k,y_k) be the k^{th} record
2. Temporarily remove (x_k,y_k) from the dataset
3. Train on the remaining n-1 datapoints
4. Note your error (x_k,y_k)

When you've done all points, report the mean error.

$MSE_{LOOCV} = 2.12$

Credit: Prof. Andrew Moore

LOOCV for Quadratic Regression



For k=1 to n

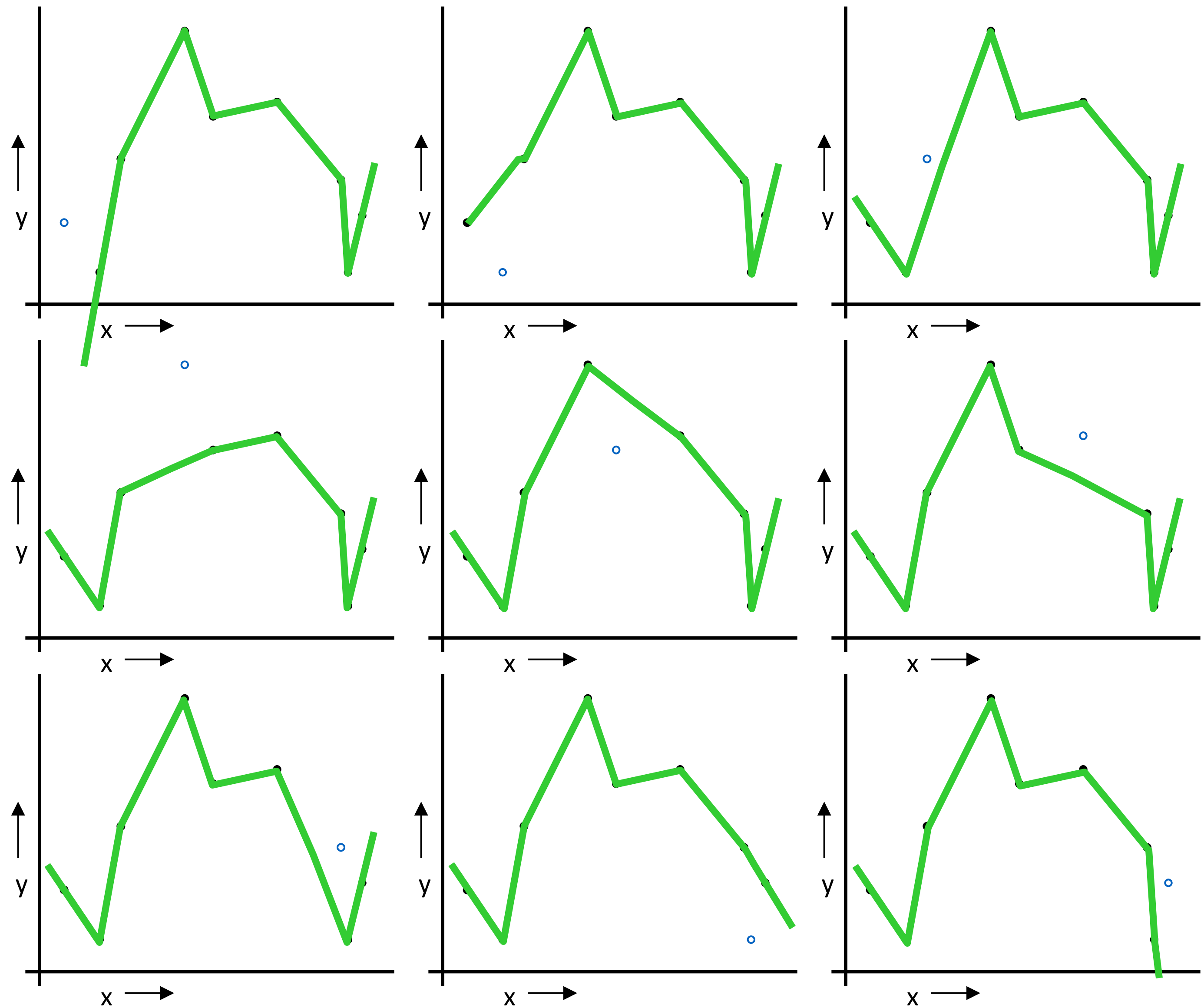
1. Let (x_k,y_k) be the k^{th} record
2. Temporarily remove (x_k,y_k) from the dataset
3. Train on the remaining n-1 datapoints
4. Note your error (x_k,y_k)

When you've done all points, report the mean error.

$MSE_{LOOCV}=0.962$

Credit: Prof. Andrew Moore

LOOCV for Join The Dots



For k=1 to n

1. Let (x_k,y_k) be the k^{th} record
2. Temporarily remove (x_k,y_k) from the dataset
3. Train on the remaining n-1 datapoints
4. Note your error (x_k,y_k)

When you've done all points, report the mean error.

MSE_{LOOCV}=3.33

Credit: Prof. Andrew Moore

Which kind of Cross Validation?

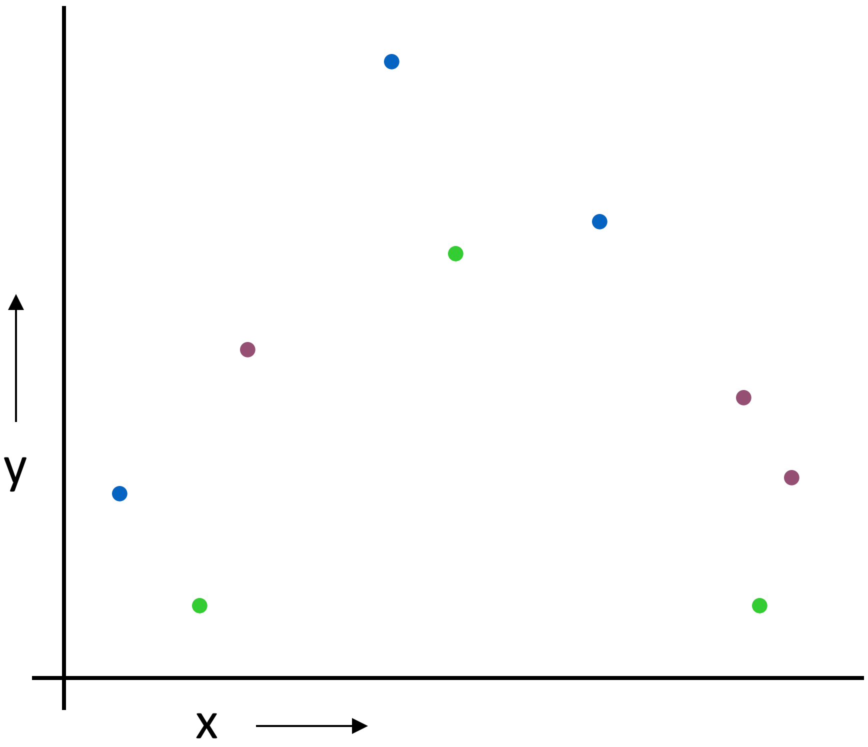
	Downside	Upside
validation-set	Variance: unreliable estimate of future performance	Cheap
Leave-one-out	Expensive. Has some weird behavior	Doesn’t waste data

..can we get the best of both worlds?

Credit: Prof. Andrew Moore

k-fold Cross Validation

Randomly break the dataset into k partitions (in our example we'll have k=3 partitions colored Purple Green and Blue)

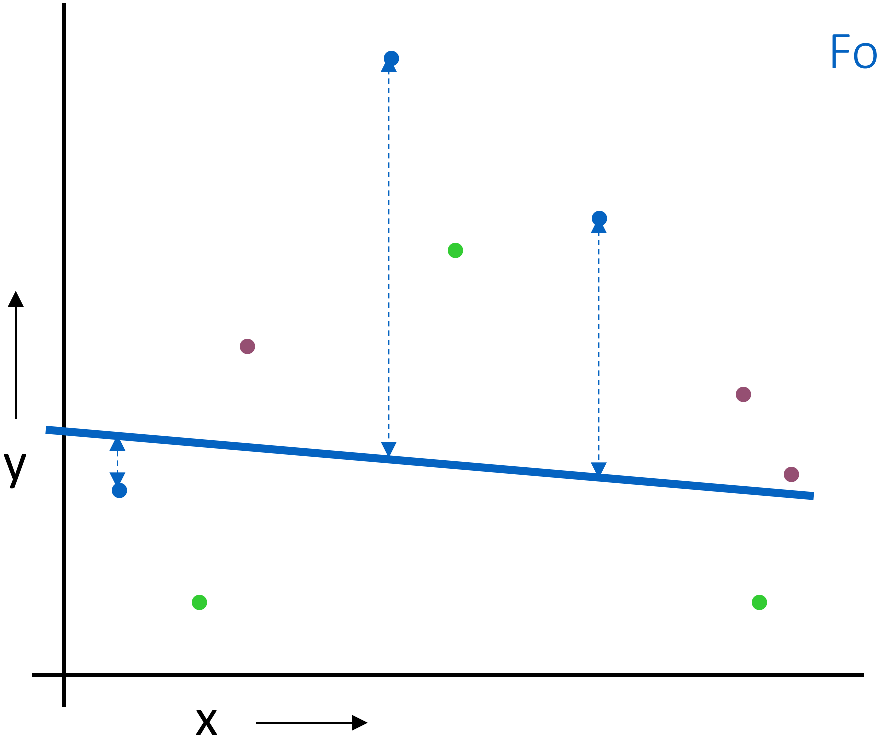


Credit: Prof. Andrew Moore

k-fold Cross Validation

Randomly break the dataset into k partitions (in our example we'll have k=3 partitions colored Purple Green and Blue)

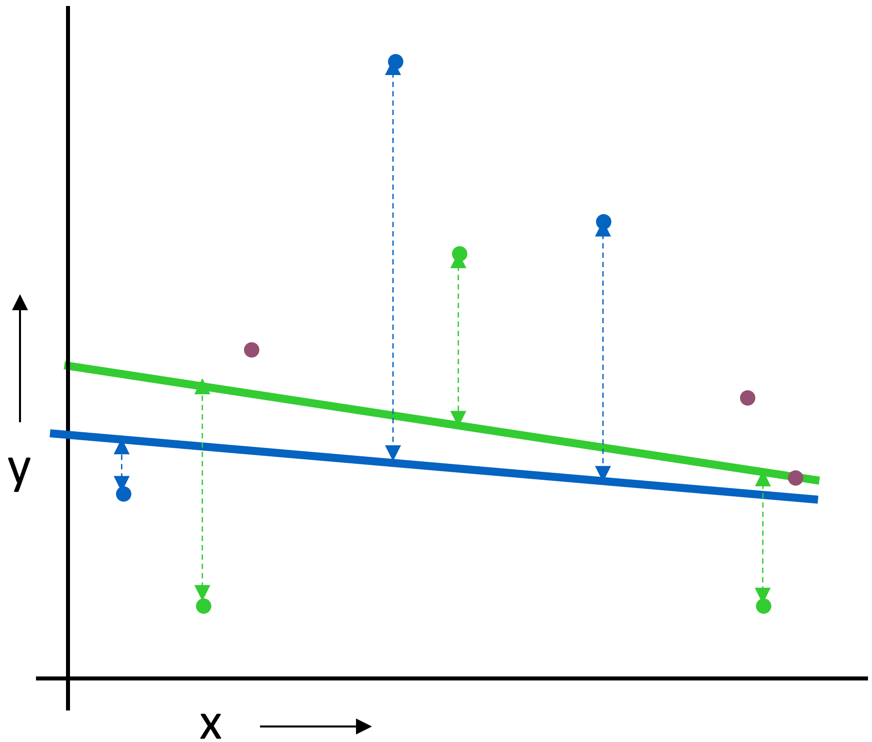
For the blue partition: Train on all the points not in the blue partition. Find the validation-set sum of errors on the blue points.



Credit: Prof. Andrew Moore

k-fold Cross Validation

Randomly break the dataset into k partitions (in our example we'll have k=3 partitions colored Purple Green and Blue)

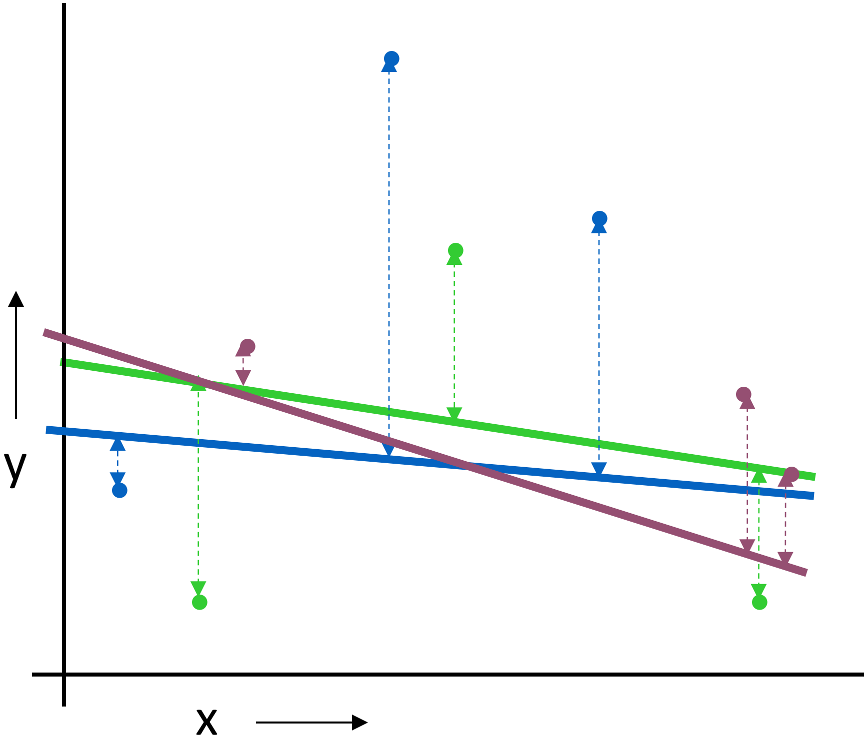


- For the blue partition: Train on all the points not in the red partition. Find the validation-set sum of errors on the red points.
- For the green partition: Train on all the points not in the green partition. Find the validation-set sum of errors on the green points.

Credit: Prof. Andrew Moore

k-fold Cross Validation

Randomly break the dataset into k partitions (in our example we'll have k=3 partitions colored Purple Green and Blue)



For the red partition: Train on all the points not in the red partition. Find the validation-set sum of errors on the red points.

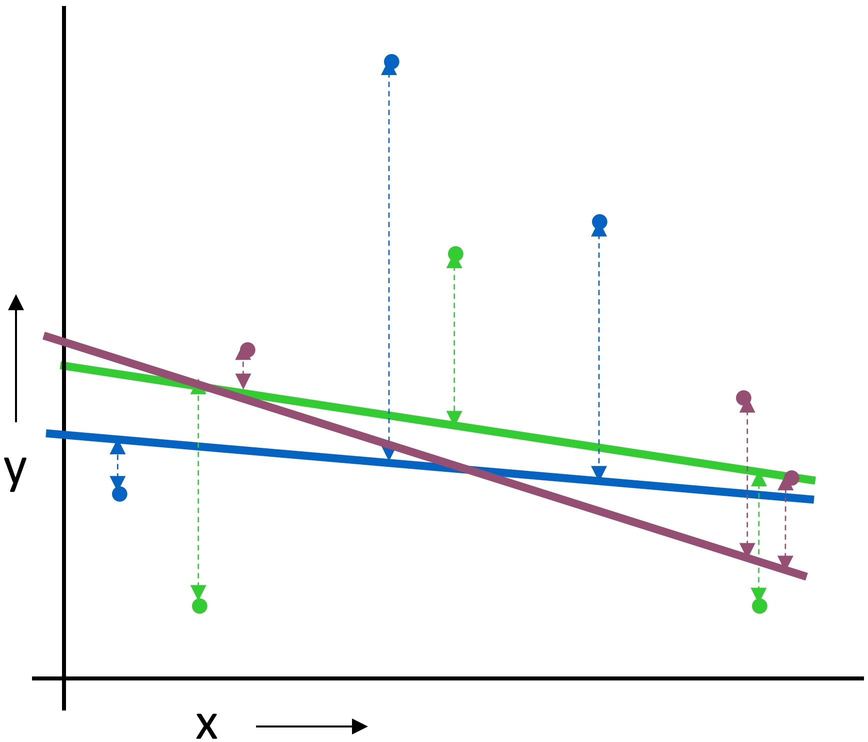
For the green partition: Train on all the points not in the green partition. Find the validation-set sum of errors on the green points.

For the purple partition: Train on all the points not in the purple partition. Find the validation-set sum of errors on the purple points.

Credit: Prof. Andrew Moore

k-fold Cross Validation

Randomly break the dataset into k partitions (in our example we'll have k=3 partitions colored Purple Green and Blue)



Linear Regression $MSE_{3FOLD}=2.05$

For the red partition: Train on all the points not in the red partition. Find the validation-set sum of errors on the red points.

For the green partition: Train on all the points not in the green partition. Find the validation-set sum of errors on the green points.

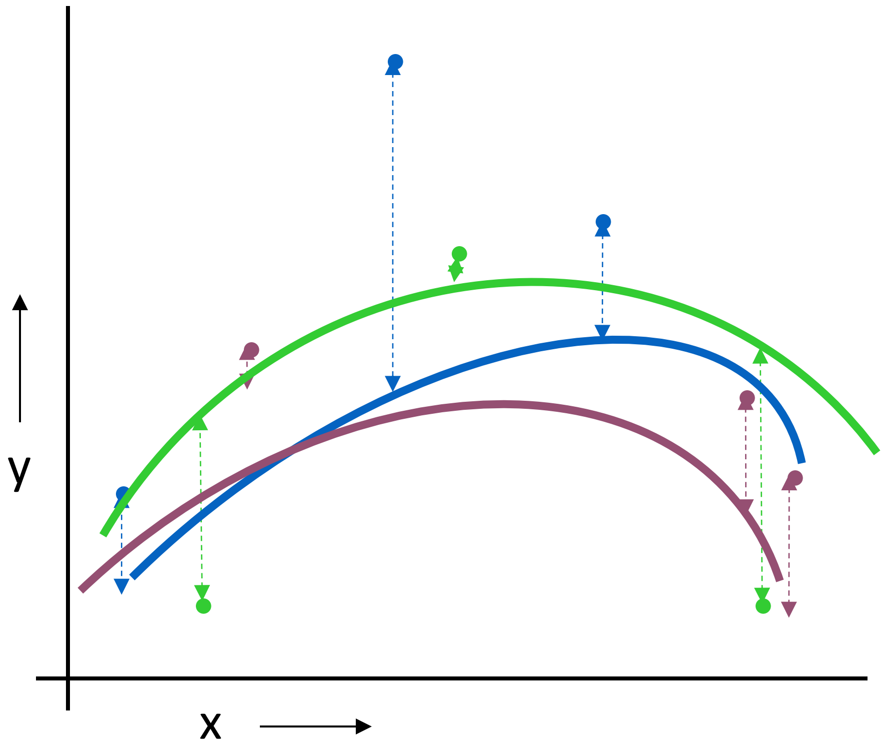
For the purple partition: Train on all the points not in the purple partition. Find the validation-set sum of errors on the purple points.

Then report the mean error

Credit: Prof. Andrew Moore

k-fold Cross Validation

Randomly break the dataset into k partitions (in our example we'll have k=3 partitions colored Purple Green and Blue)



Quadratic Regression $MSE_{3FOLD}=1.11$

For the red partition: Train on all the points not in the red partition. Find the validation-set sum of errors on the red points.

For the green partition: Train on all the points not in the green partition. Find the validation-set sum of errors on the green points.

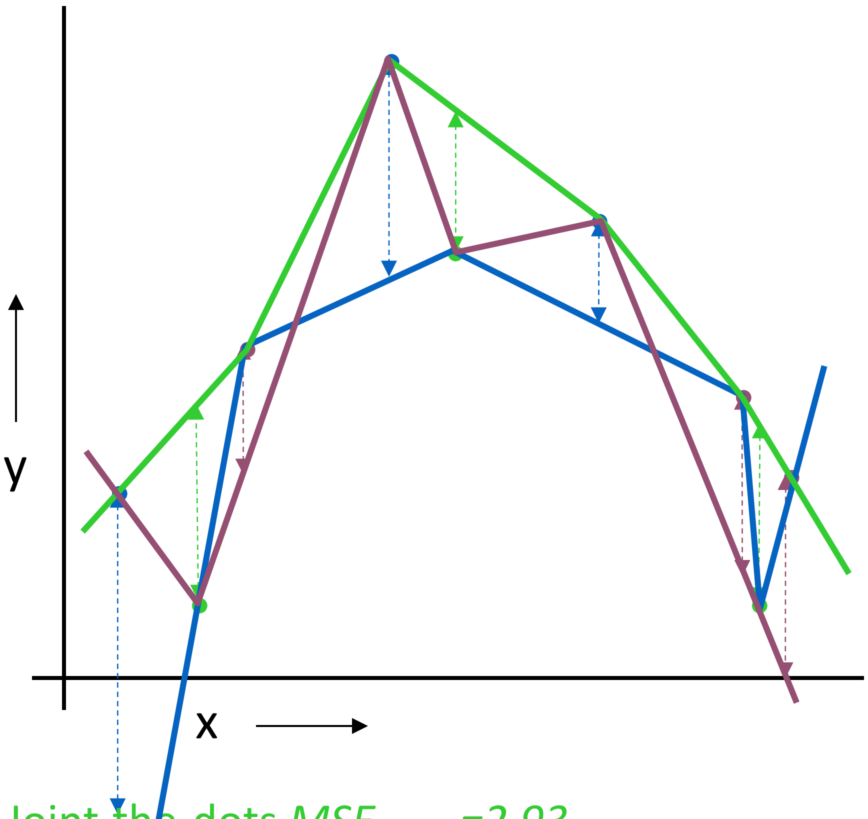
For the purple partition: Train on all the points not in the purple partition. Find the validation-set sum of errors on the purple points.

Then report the mean error

Credit: Prof. Andrew Moore

k-fold Cross Validation

Randomly break the dataset into k partitions (in our example we'll have k=3 partitions colored Purple Green and Blue)



Joint-the-dots $MSE_{3FOLD}=2.93$

For the red partition: Train on all the points not in the red partition. Find the validation-set sum of errors on the red points.

For the green partition: Train on all the points not in the green partition. Find the validation-set sum of errors on the green points.

For the blue partition: Train on all the points not in the blue partition. Find the validation-set sum of errors on the blue points.

Then report the mean error

Credit: Prof. Andrew Moore

Which kind of Cross Validation?

	Downside	Upside
validation -set	Variance: unreliable estimate of future performance	Cheap
Leave-one-out	Expensive. Has some weird behavior	Doesn't waste data
10-fold	Wastes 10% of the data. 10 times more expensive than validation set	Only wastes 10%. Only 10 times more expensive instead of n times.
3-fold	Wastier than 10-fold. More Expensive than validation set style	better than validation-set
n-fold	Identical to Leave-one-out	

CV-based Model Selection

- We're trying to decide which algorithm/model/ hyperpara to use.
- We train/learn/fit each model and make a table…

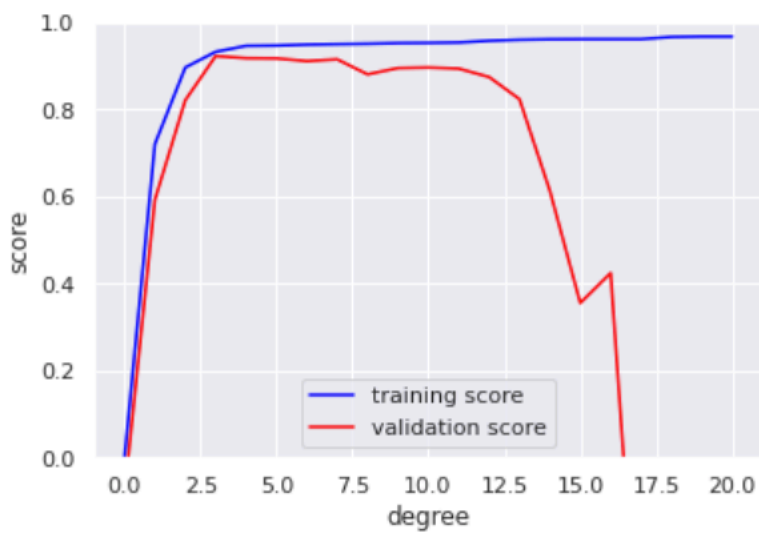
i	f_i	TRAINERR	k-FOLD-CV-ERR	Choice
1	f_1			
2	f_2			
3	f_3			YEAH!!!!
4	f_4			
5	f_5			
6	f_6			

Credit: Prof. Andrew Moore

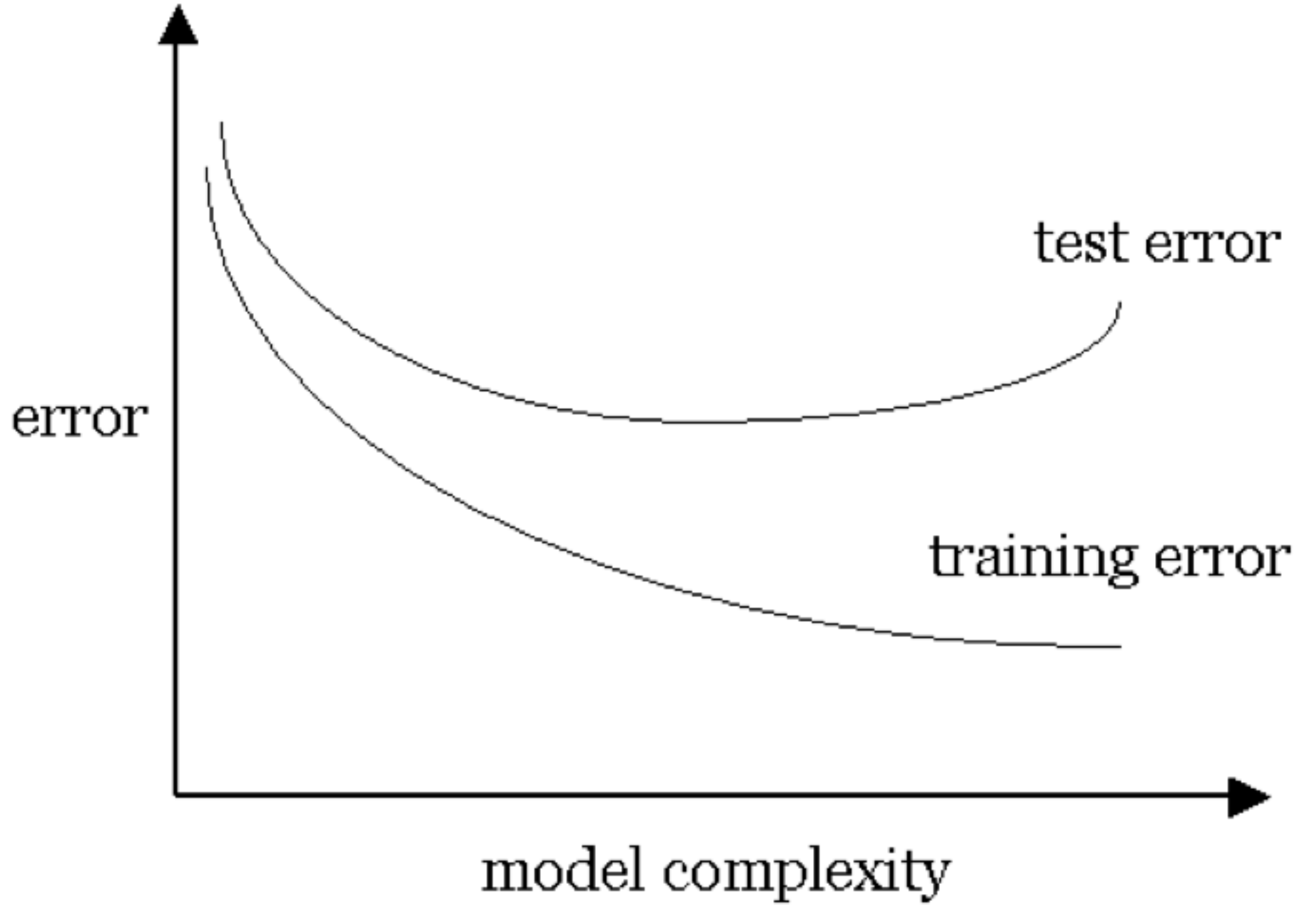
I will code-run: https://colab.research.google.com/drive/1MFy_6da9zL4yqGXTZg80My_2KACo0pY8#scrollTo=T-a0H80OQgHD

Adapted from:
https://colab.research.google.com/github/jakevdp/PythonDataScienceHandbook/blob/master/notebooks/05.03-Hyperparameters-and-Model-Validation.ipynb
https://scikit-learn.org/stable/modules/learning_curve.html

```
[21] from sklearn.model_selection import validation_curve

     degree = np.arange(0, 21)
     train_score, val_score = validation_curve(PolynomialRegression(), X, y,
                                               'polynomialfeatures__degree', degree, cv=7)

     plt.plot(degree, np.median(train_score, 1), color='blue', label='training score')
     plt.plot(degree, np.median(val_score, 1), color='red', label='validation score')
     plt.legend(loc='best')
     plt.ylim(0, 1)
     plt.xlabel('degree')
     plt.ylabel('score');
```

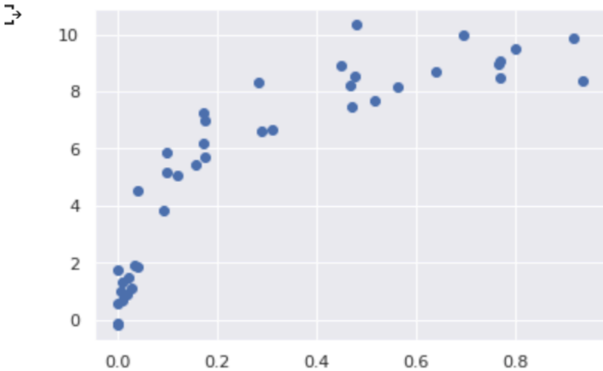


A Plot for Model Selection

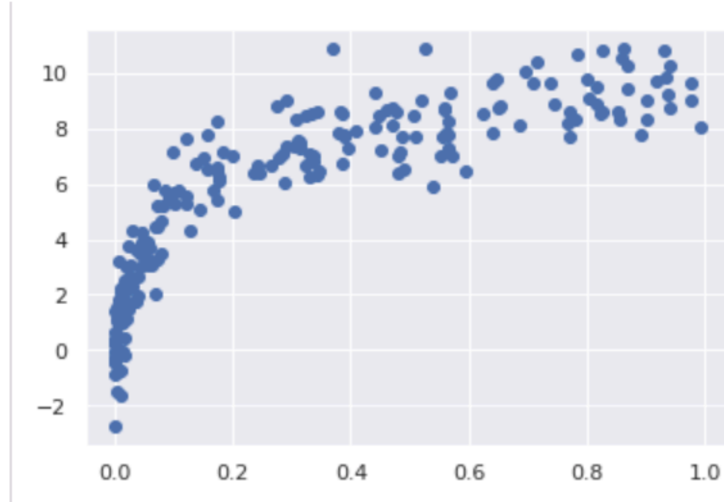


k-CV on train to choose model and hyperparameter / then a separate test set to assess future performance

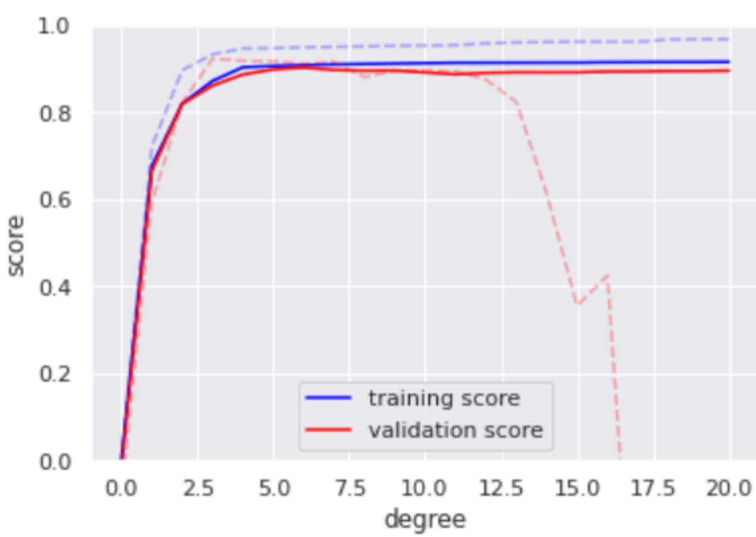
```
X, y = make_data(40)
plt.scatter(X, y);
```




```
X2, y2 = make_data(200)
plt.scatter(X2.ravel(), y2);
```



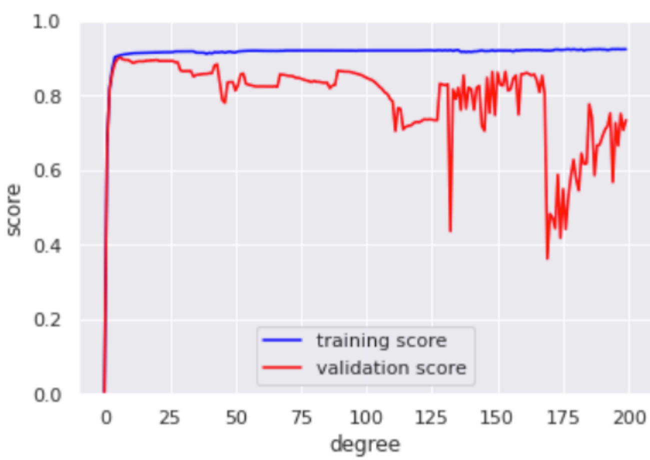

```
plt.plot(degree, np.median(train_score2, 1), color='blue'
plt.plot(degree, np.median(val_score2, 1), color='red', l
plt.plot(degree, np.median(train_score, 1), color='blue',
plt.plot(degree, np.median(val_score, 1), color='red', al
plt.legend(loc='lower center')
plt.ylim(0, 1)
plt.xlabel('degree')
plt.ylabel('score');
```



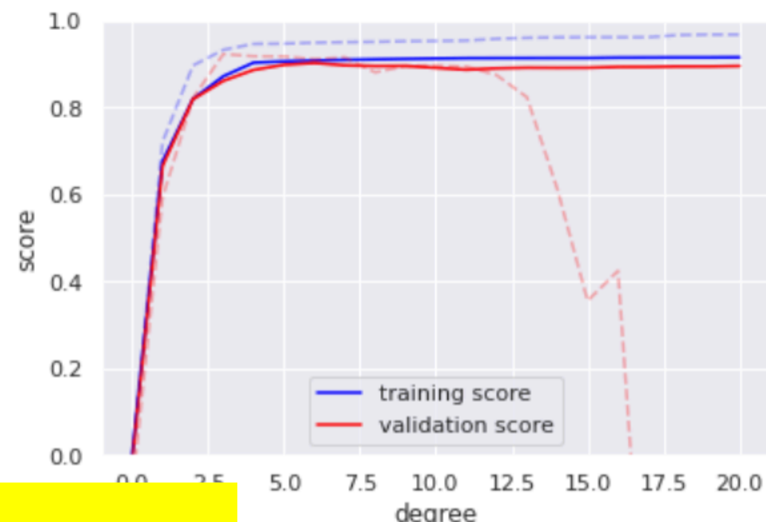
Behavior of the validation curve:

- the model complexity
- the number of training points

```python
X2, y2 = make_data(200)

degree = np.arange(200)
train_score2, val_score2 = validation_curve(PolynomialR
                                            'polynomial

plt.plot(degree, np.median(train_score2, 1), color='blu
plt.plot(degree, np.median(val_score2, 1), color='red',
plt.legend(loc='lower center')
plt.ylim(0, 1)
plt.xlabel('degree')
plt.ylabel('score');
```




```python
X2, y2 = make_data(200)
degree = np.arange(21)
train_score2, val_score2 = validation_curve(PolynomialReg
                                            'polynomialfe

plt.plot(degree, np.median(train_score2, 1), color='blue'
plt.plot(degree, np.median(val_score2, 1), color='red', l
plt.plot(degree, np.median(train_score, 1), color='blue',
plt.plot(degree, np.median(val_score, 1), color='red', al
plt.legend(loc='lower center')
plt.ylim(0, 1)
plt.xlabel('degree')
plt.ylabel('score');
```



Interesting Relation between

- the right range of model complexity
- the number of training points

Another plot of the training/validation score with respect to the size of the training set is known as a *learning curve.*

The general behavior we would expect from a learning curve is this:

•A model of a given complexity will *overfit* a small dataset: this means the training score will be relatively high, while the validation score will be relatively low.

•A model of a given complexity will *underfit* a large dataset: this means that the training score will decrease, but the validation score will increase.

•A model will never, except by chance, give a better score to the validation set than the training set: this means the curves should keep getting closer together but never cross.

https://colab.research.google.com/github/jakevdp/PythonDataScienceHandbook/blob/master/notebooks/05.03-Hyperparameters-and-Model-Validation.ipynb

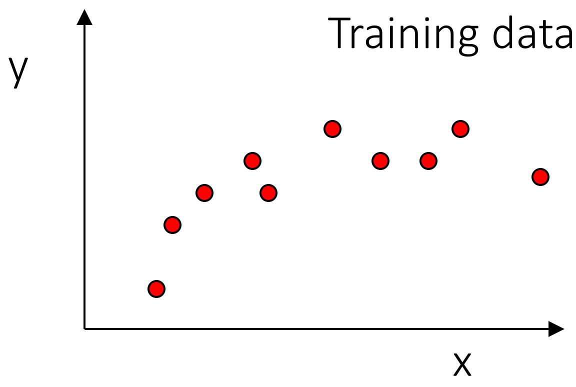
References

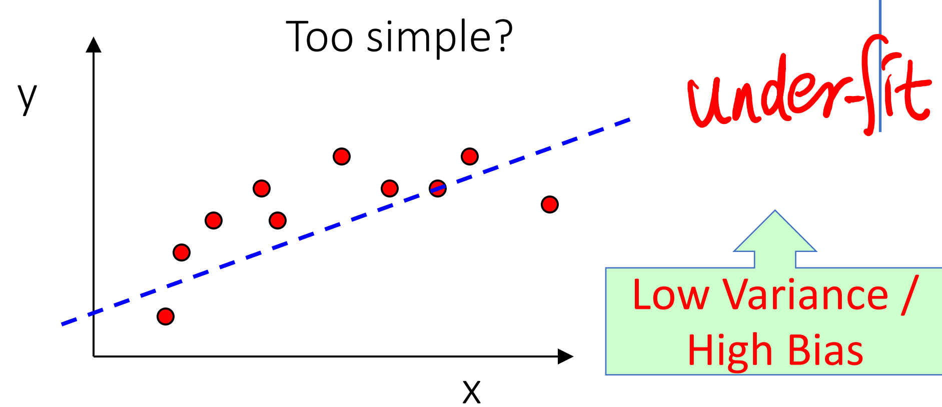
- Big thanks to Prof. Eric Xing @ CMU for allowing me to reuse some of his slides

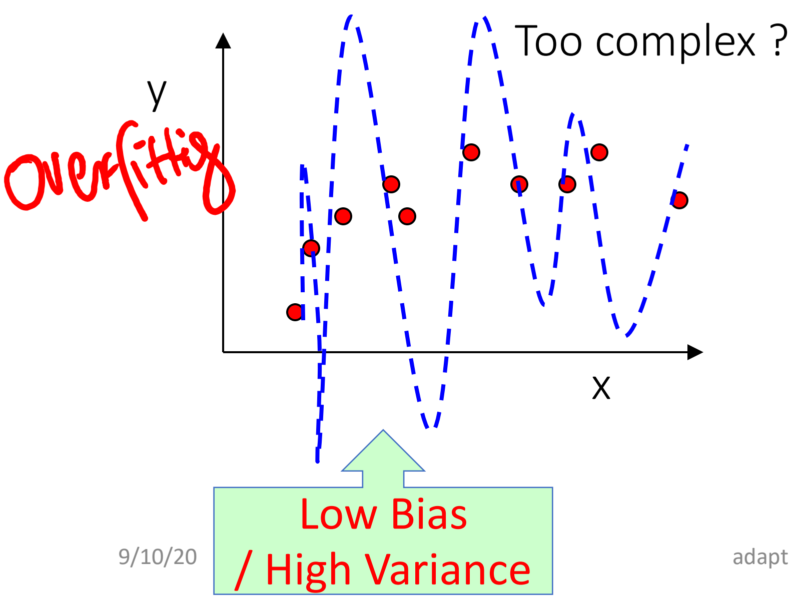
❑ Prof. Nando de Freitas's tutorial slide

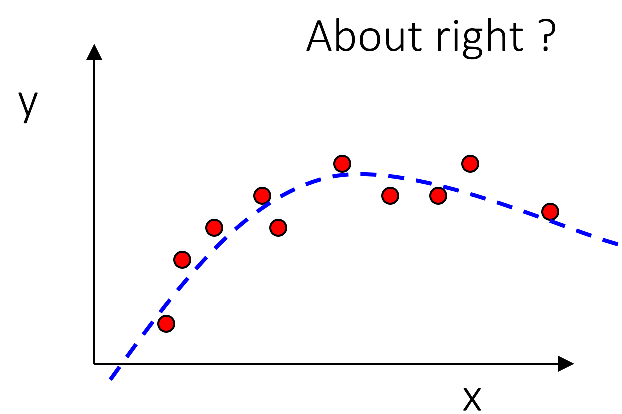
❑ Prof. Andrew Moore's slides @ CMU

Later: Complexity versus Goodness of Fit









What ultimately matters: GENERALIZATION

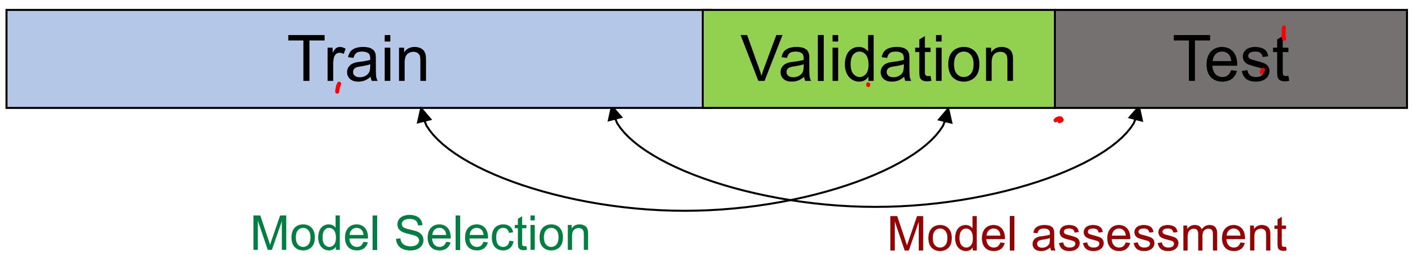
Later: Model Selection and Assessment

- Model Selection
  - Estimating performances of different models to choose the best one

- Model Assessment
  - Having chosen a model, estimating the <u>prediction error</u> on new data

Model Selection and Assessment

- When Data Rich Scenario: Split the dataset



- When Insufficient data to split into 3 parts
  - Approximate validation step analytically
    - AIC, BIC, MDL, SRM
  - Efficient reuse of samples
    - Cross validation, bootstrap

Model Selection (Hyperparameter Tuning) Model Assessment Pipelines in HW2

- (1) train / Validation / test

- (2) k-CV on train to choose hyperparameter / then test

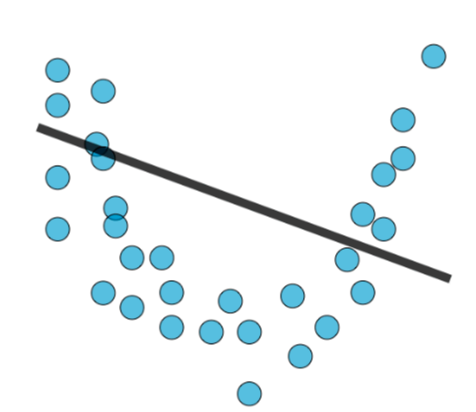
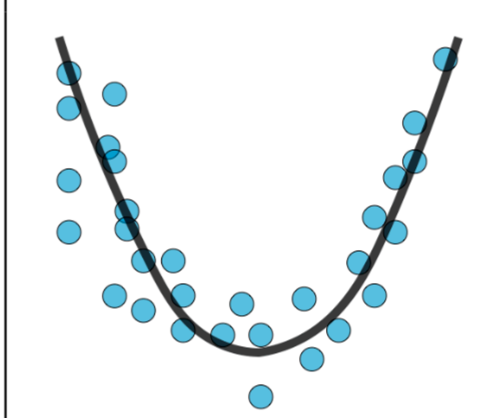
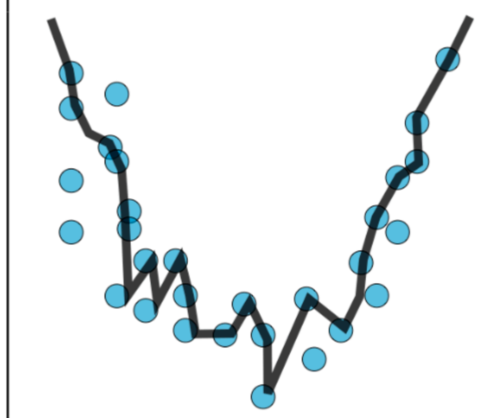
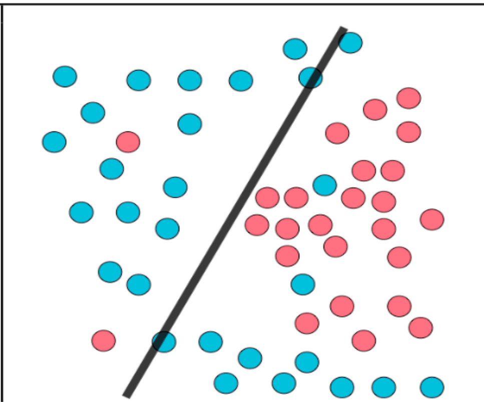
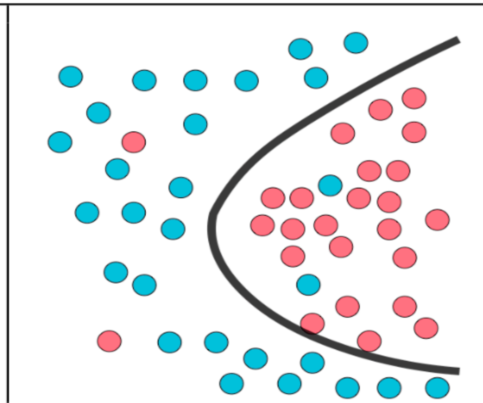
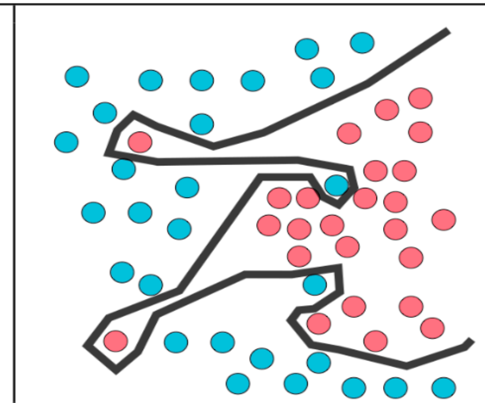
need to make assumptions that are able to generalize

- **Underfitting:** model is too "simple" to represent all the relevant characteristics
  - High bias and low variance
  - High training error and high test error
- **Overfitting:** model is too "complex" and fits irrelevant characteristics (noise) in the data
  - Low bias and high variance
  - Low training error and high test error

A Gentle Touch of Bias - Variance Tradeoff

(More details … Later)

Slide credit: L. Lazebnik

	Underfitting	Just right	Overfitting
Symptoms	- High training error - Training error close to test error - High bias	- Training error slightly lower than test error	- Low training error - Training error much lower than test error - High variance
Regression			
Classification			
Remedies	- Complexify model - Add more features - Train longer		- Regularize - Get more data - Feature selection

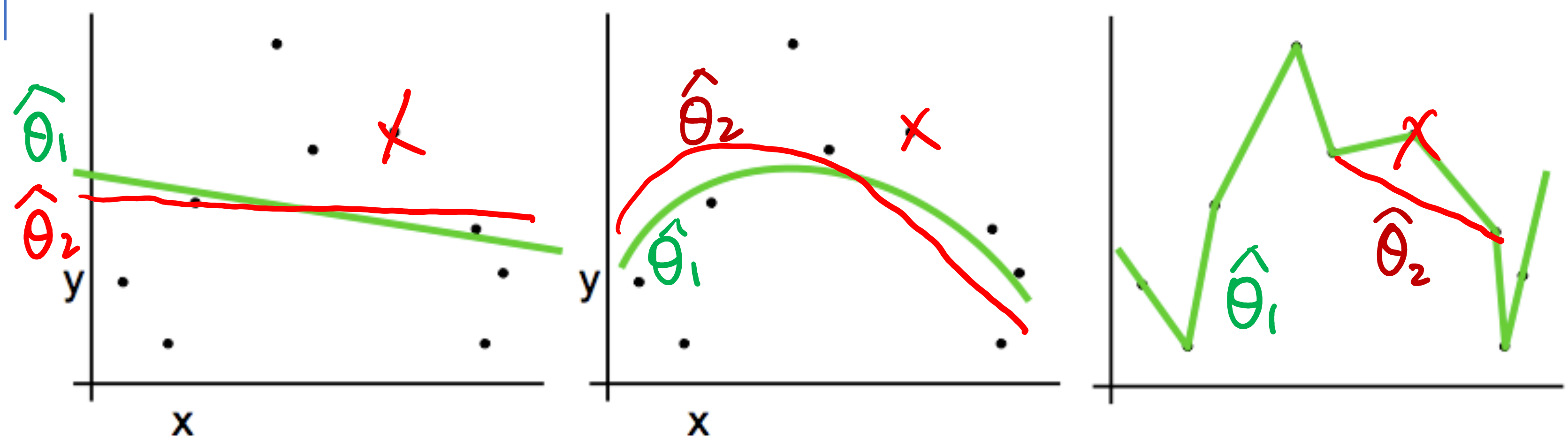
Credit: Stanford Machine Learning

need to make assumptions that are able to generalize

- Components
  - **Bias:** how much the average model over all training sets differ from the true model?
    - Error due to inaccurate assumptions/simplifications made by the model
  - **Variance:** how much models estimated from different training sets differ from each other

Slide credit: L. Lazebnik

Randomness of Train Set
=> Variance of Models, e.g.,

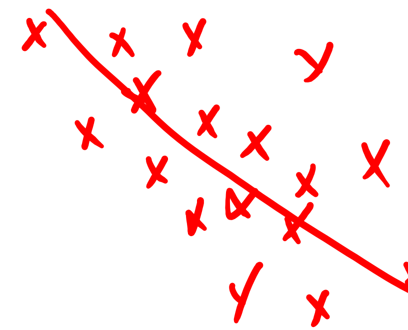


e.g. removing one training sample

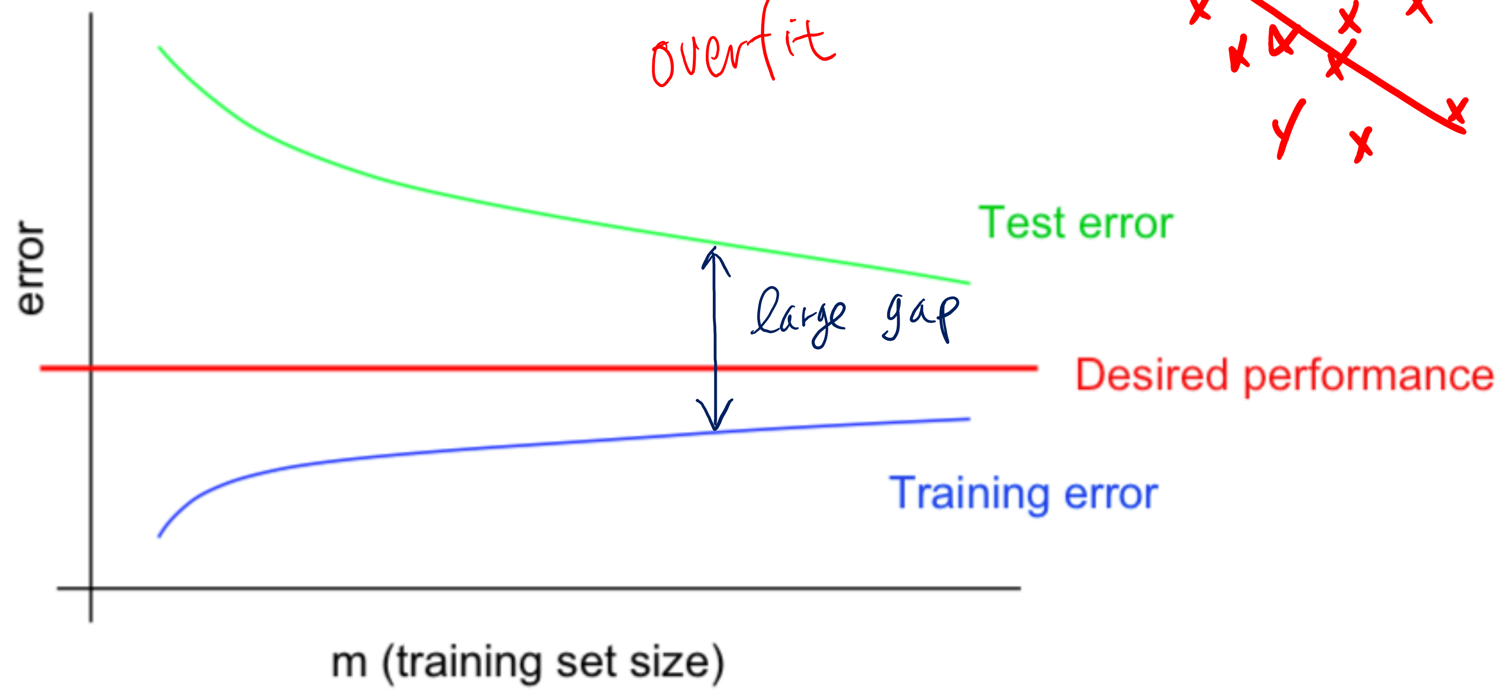
model complexity ↗ ⇒ model variance ↗

(1) Overfitting / High variance / Model too Complex

Typical learning curve for high variance:



overfit



- Test error still decreasing as m increases. Suggests larger training set will help.
- Large gap between training and test error.
- Low training error and high test error

Slide credit: A. Ng

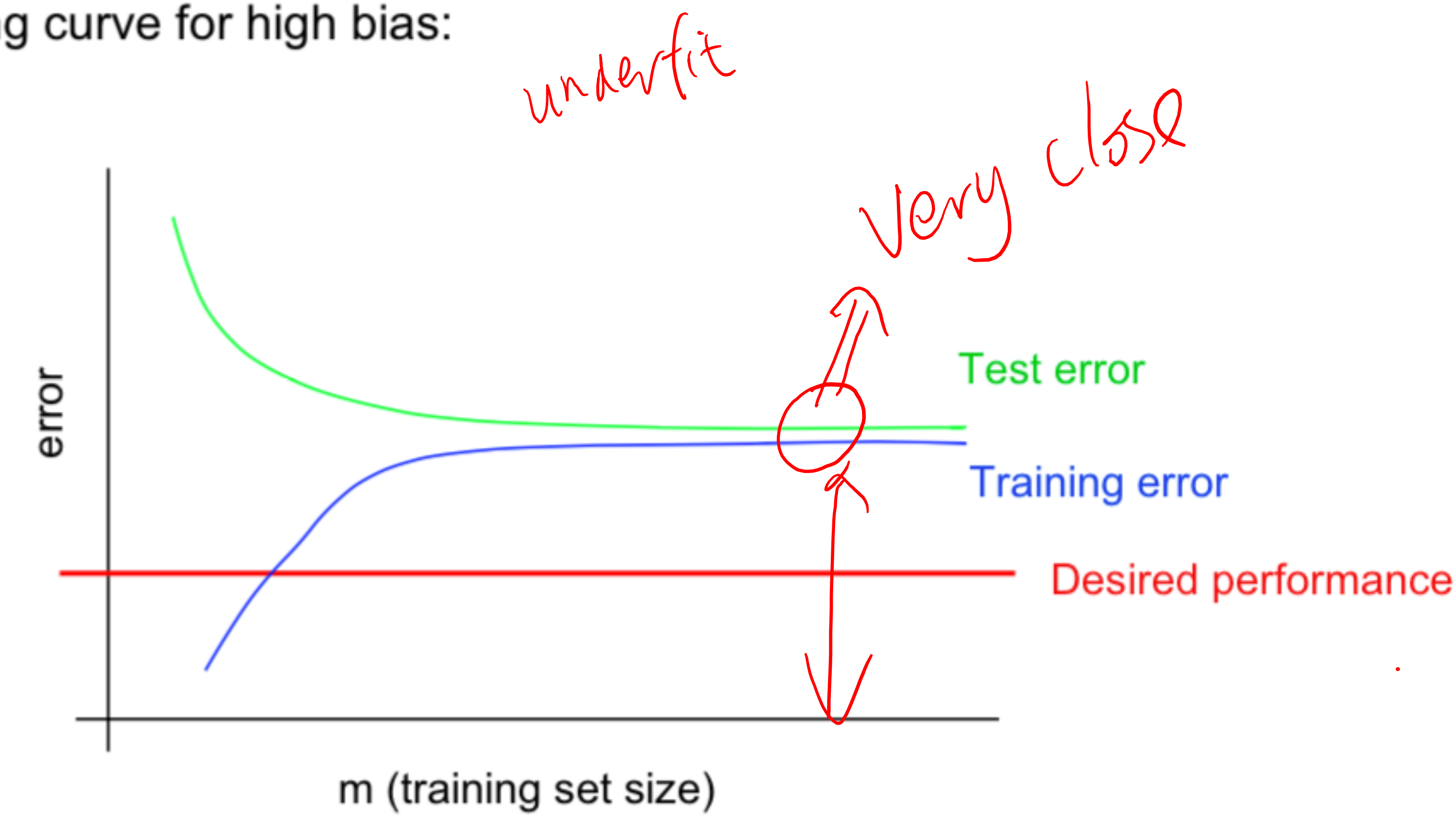
How to reduce Model High Variance?

- Choose a simpler classifier
  - More Bias
- Regularize the parameters
  - More Bias
- Get more training data
- Try smaller set of features
  - More Bias

Slide credit: D. Hoiem

(2) Underfitting / High bias / Model too Simple

Typical learning curve for high bias:



- Even training error is unacceptably high.
- Small gap between training and test error.

High training error and high test error

Slide credit: A. Ng

How to reduce Model High Bias ?

- E.g.
  - Get additional features
  - Try more complex learner