CS4442/9542b
Artificial Intelligence II
prof. Olga Veksler

Lecture 6

Machine Learning

Validation
and
Cross-Validation

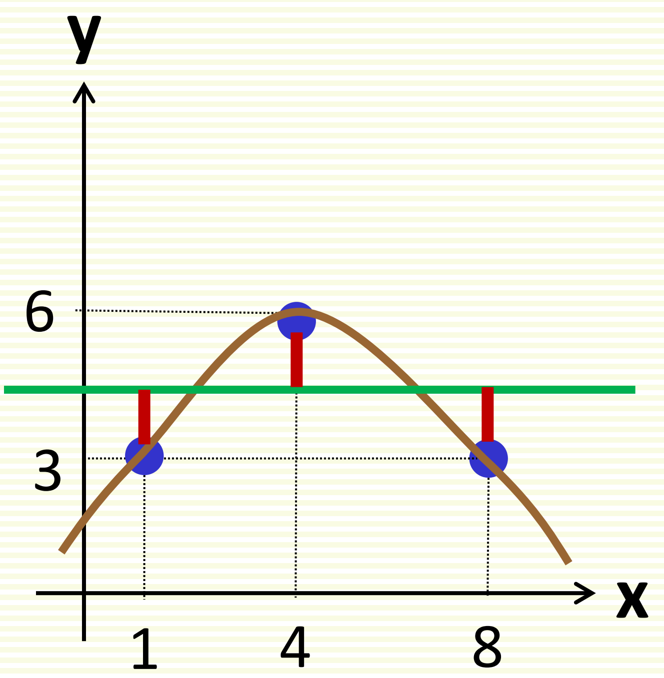
Many slides from Andrew Ng, Andrew Moore

Outline

- Performance evaluation and model selection methods
  - validation
  - cross-validation
    - k-fold
    - Leave-one-out

Regression

- In this lecture, it's convenient to show examples in the context of regression
- In regression, labels $\mathbf{y}^i$ are continuous
- Classification/regression are solved very similarly
- Everything we have done so far transfers to regression with very minor changes
- Error: sum of distances from examples to the fitted model

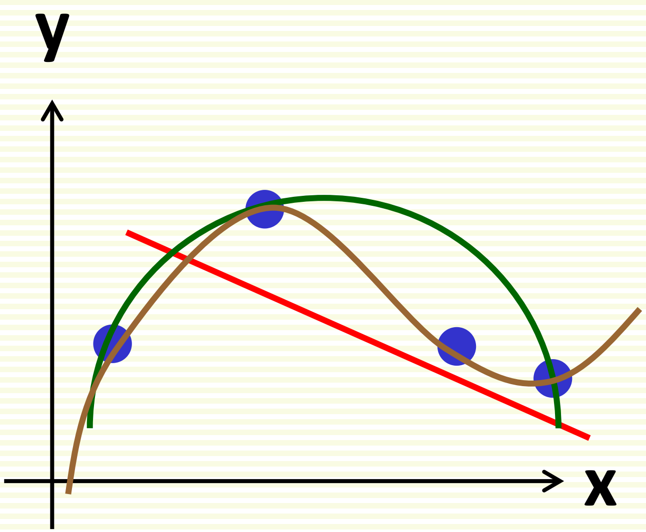


Training/Test Data Split

- Talked about splitting data in training/test sets
  - training data is used to fit parameters
  - test data is used to assess how classifier generalizes to new data
- What if classifier has "non-tunable" (hyper) parameters?
  - a parameter is "non-tunable" if tuning (or training) it on the training data leads to overfitting
  - Examples
    - **k** in kNN classifier
    - **λ** for weight regularization
    - Many hyper-parameters in neural networks
      - number of hidden units in MNN
      - number of hidden layers in MNN
    - etc…

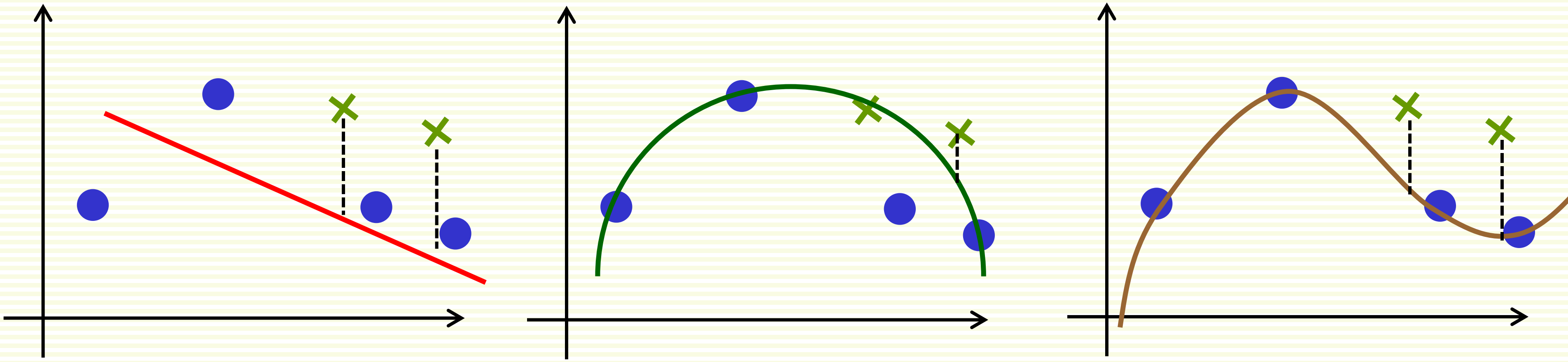
Example of Overfitting

- Want to fit a polynomial machine **f**(**x**,**w**)
- Instead of fixing polynomial degree, make it parameter **d**
  - learning machine **f**(**x**,**w**,**d**)
- Consider just three choices for **d**
  - degree 1
  - degree 2
  - degree 3



- Training error is a bad measure to choose **d**
  - degree 3 is the best according to the training error, but overfits the data

Training/Test Data Split



- What about test error? Seems appropriate
  - degree 2 is the best model according to the test error
- Except what do we report as the test error now?
- Test error should be computed on data that was **not used for training at all**
- Here used "test" data for training, i.e. choosing model

Validation data

- Same question when choosing among several classifiers
  - our polynomial degree example can be looked at as choosing among 3 classifiers (degree 1, 2, or 3)
- Solution: split the labeled data into three parts

labeled data

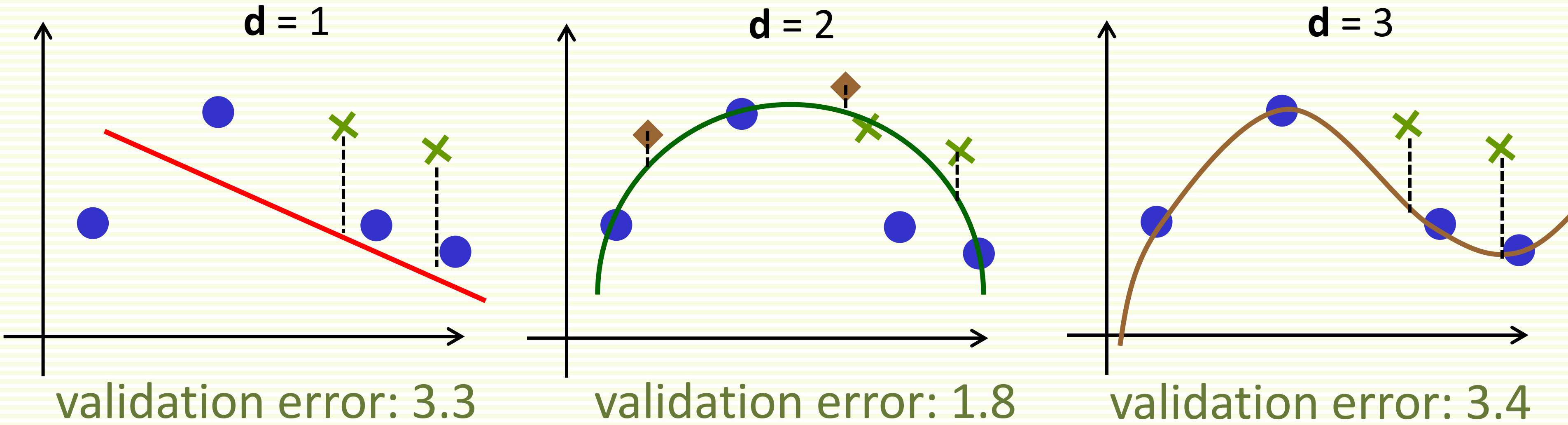
Training ≈60%	Validation ≈20%	Test ≈20%
train tunable parameters **w**	train other parameters, or to select classifier	use **only** to assess final performance

Training/Validation/Test

labeled data

Training ≈60%	Validation ≈20%	Test ≈20%
Training error: computed on training examples	Validation error: computed on validation examples	Test error: computed on test examples

Training/Validation/Test Data



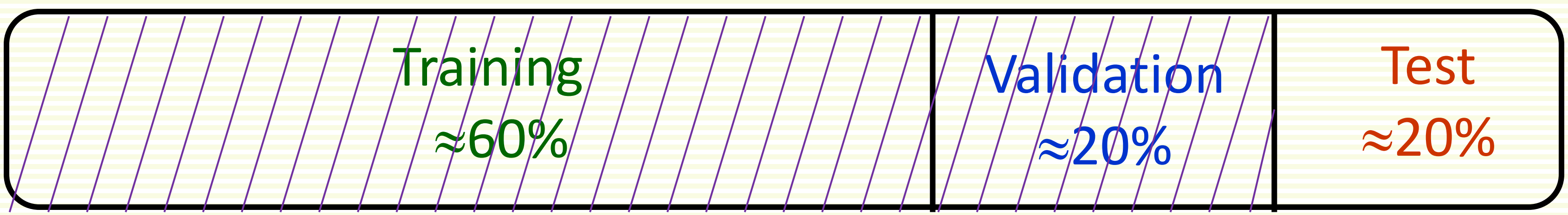
- Training Data
- Validation Data
  - **d** = 2 is chosen
- Test Data
  - 1.3 test error computed for **d** = 2

Training/Validation

labeled data

- After non-tunable parameters are chosen (using validation data), retrain on combined Training+Validation data before computing Test error

labeled data



- The more data to train on, the better is the trained classifier (the more reliable test error)

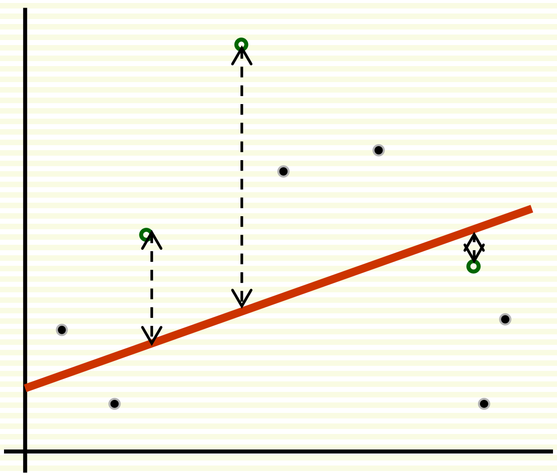
Train/Test/Validation Method

- Good news
  - Very simple
- Bad news:
  - Wastes data
    - in general, the more data we have, the better are the estimated parameters
    - we estimate parameters on 40% less data, since 20% removed for test and 20% for validation data
  - If we have a small dataset our validation set might just be lucky or unlucky

Small Dataset

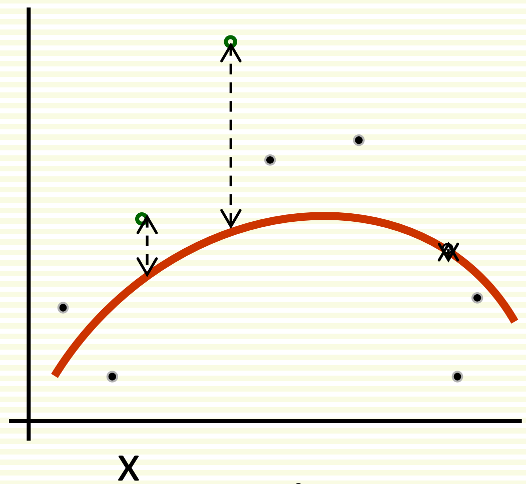
- “Unlucky” validation set:

Linear Model:



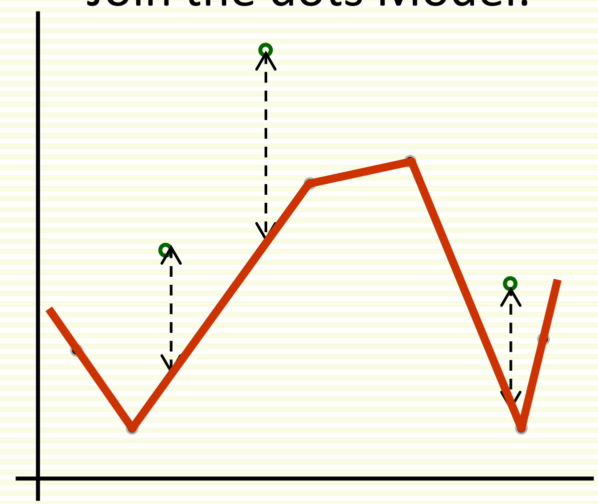
Mean Squared Error = 2.4

Quadratic Model:



Mean Squared Error = 0.9

Join the dots Model:



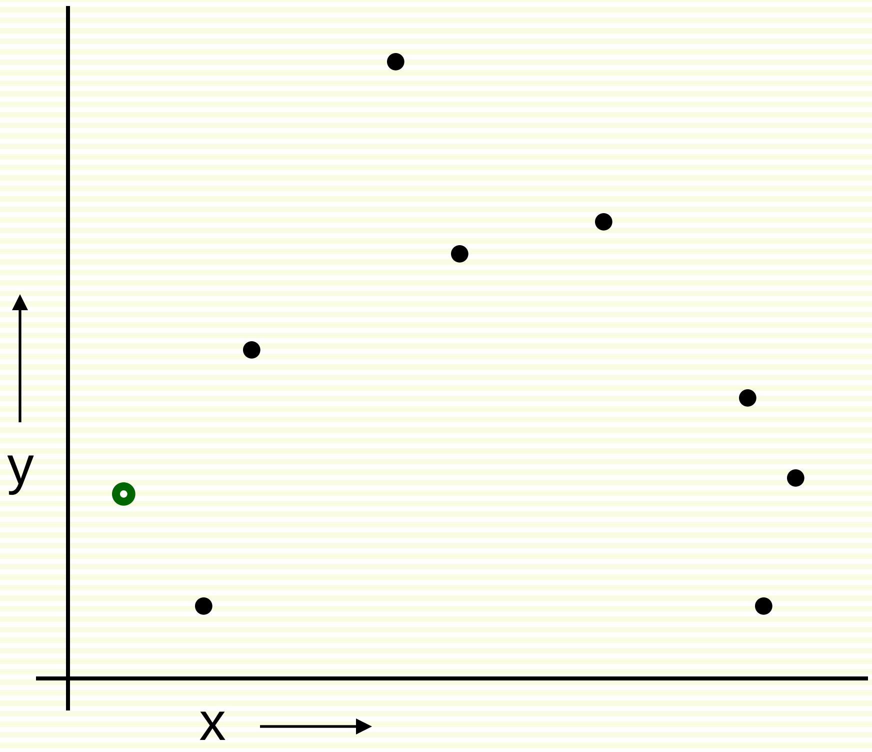
Mean Squared Error = 2.2

Cross Validation

- Create multiple spits of training/validation
- Average results over splits

1	Training	Validation	Test ≈20%	
2	Training	Validation	Training	Test ≈20%
3	Training	Validation	Training	Test ≈20%
4	Validation	Training	Test ≈20%	

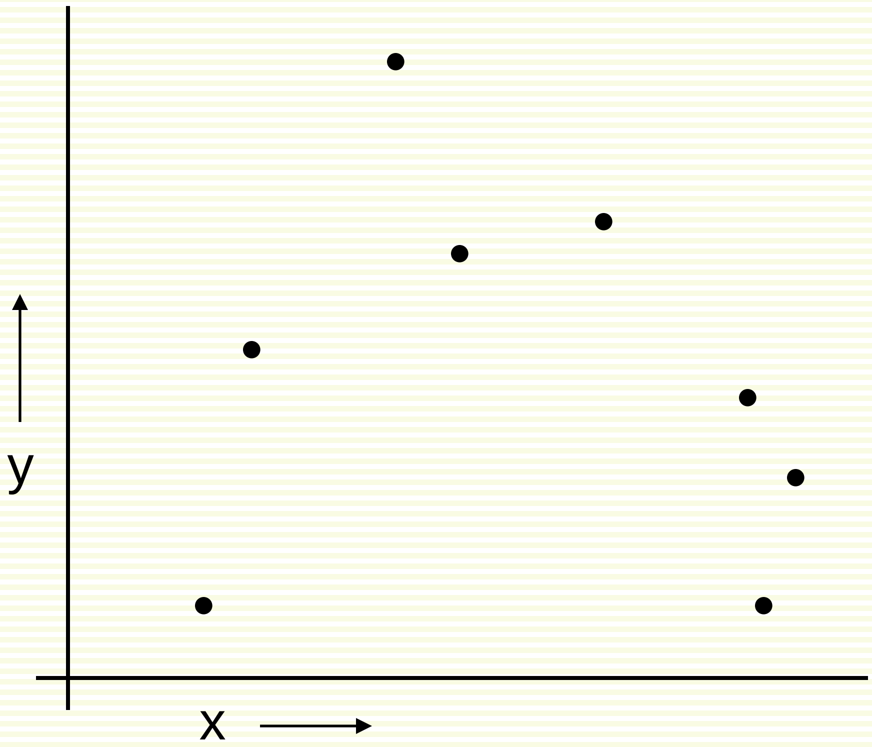
LOOCV (Leave-one-out Cross Validation)



For k=1 to R

1. Let $(\mathbf{x}^k,\mathbf{y}^k)$ be the **k** example

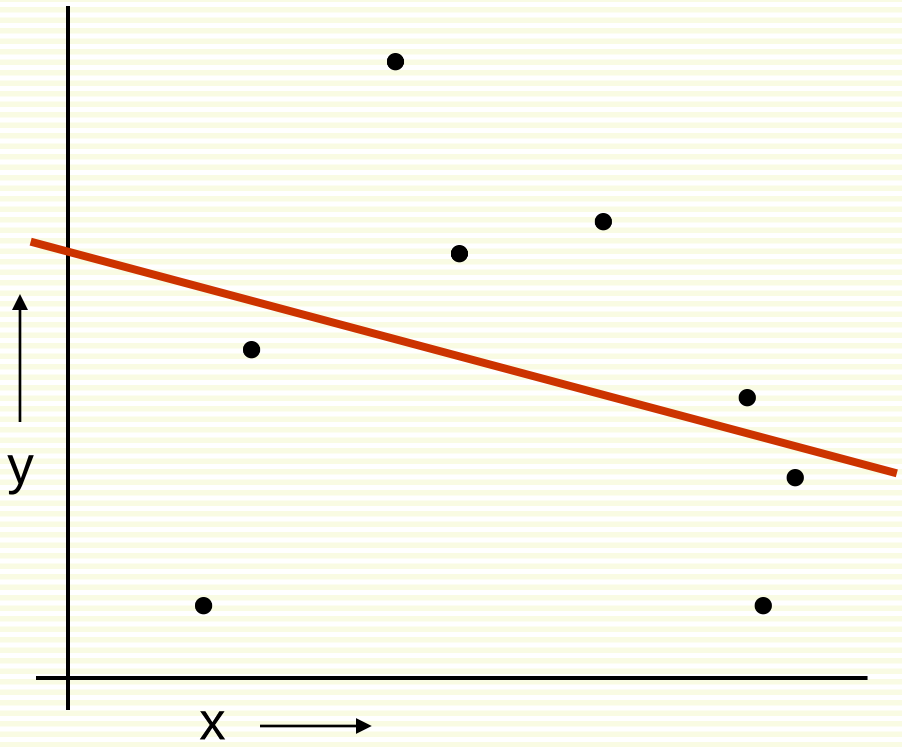
LOOCV (Leave-one-out Cross Validation)



For **k**=1 to **n**

1. Let $(\mathbf{x}^k,\mathbf{y}^k)$ be the **k**th example
2. Temporarily remove $(\mathbf{x}^k,\mathbf{y}^k)$ from the dataset

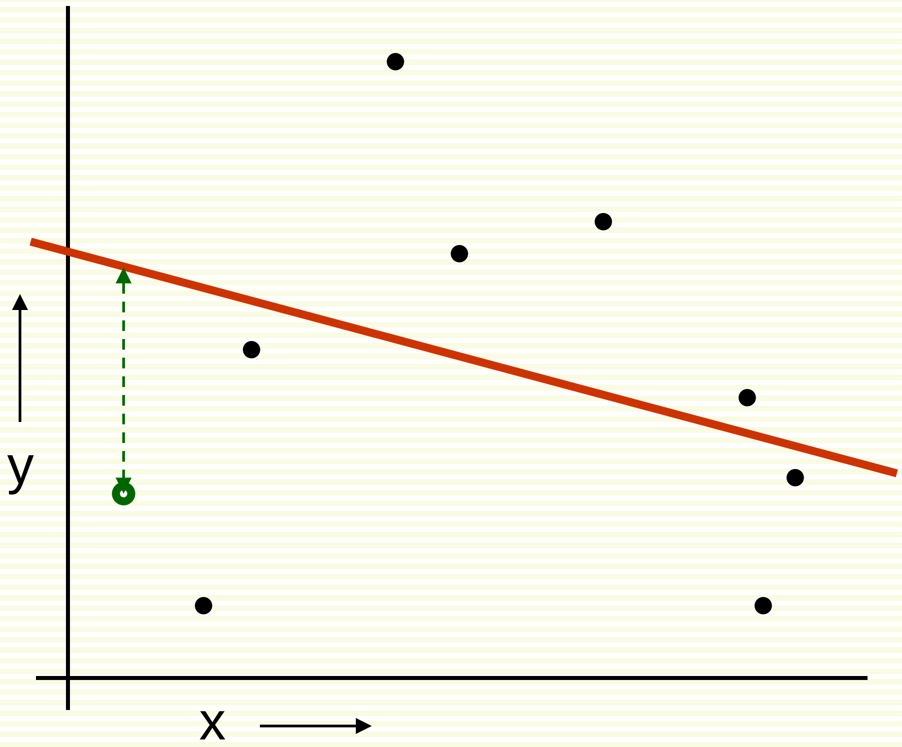
LOOCV (Leave-one-out Cross Validation)



For **k**=1 to **n**

1. Let $(\mathbf{x}^k, \mathbf{y}^k)$ be the **k**th example
2. Temporarily remove $(\mathbf{x}^k, \mathbf{y}^k)$ from the dataset
3. Train on the remaining **n**-1 examples

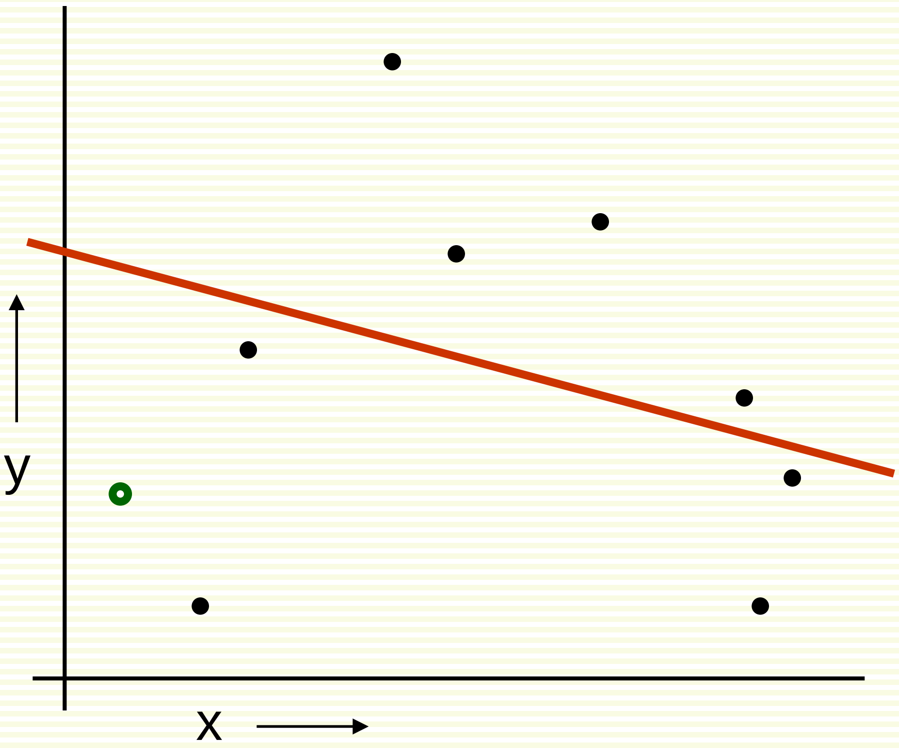
LOOCV (Leave-one-out Cross Validation)



For **k**=1 to **n**

1. Let $(\mathbf{x}^k,\mathbf{y}^k)$ be the **k**th example
2. Temporarily remove $(\mathbf{x}^k,\mathbf{y}^k)$ from the dataset
3. Train on the remaining **n**-1 examples
4. Note your error on $(\mathbf{x}^k,\mathbf{y}^k)$

LOOCV (Leave-one-out Cross Validation)

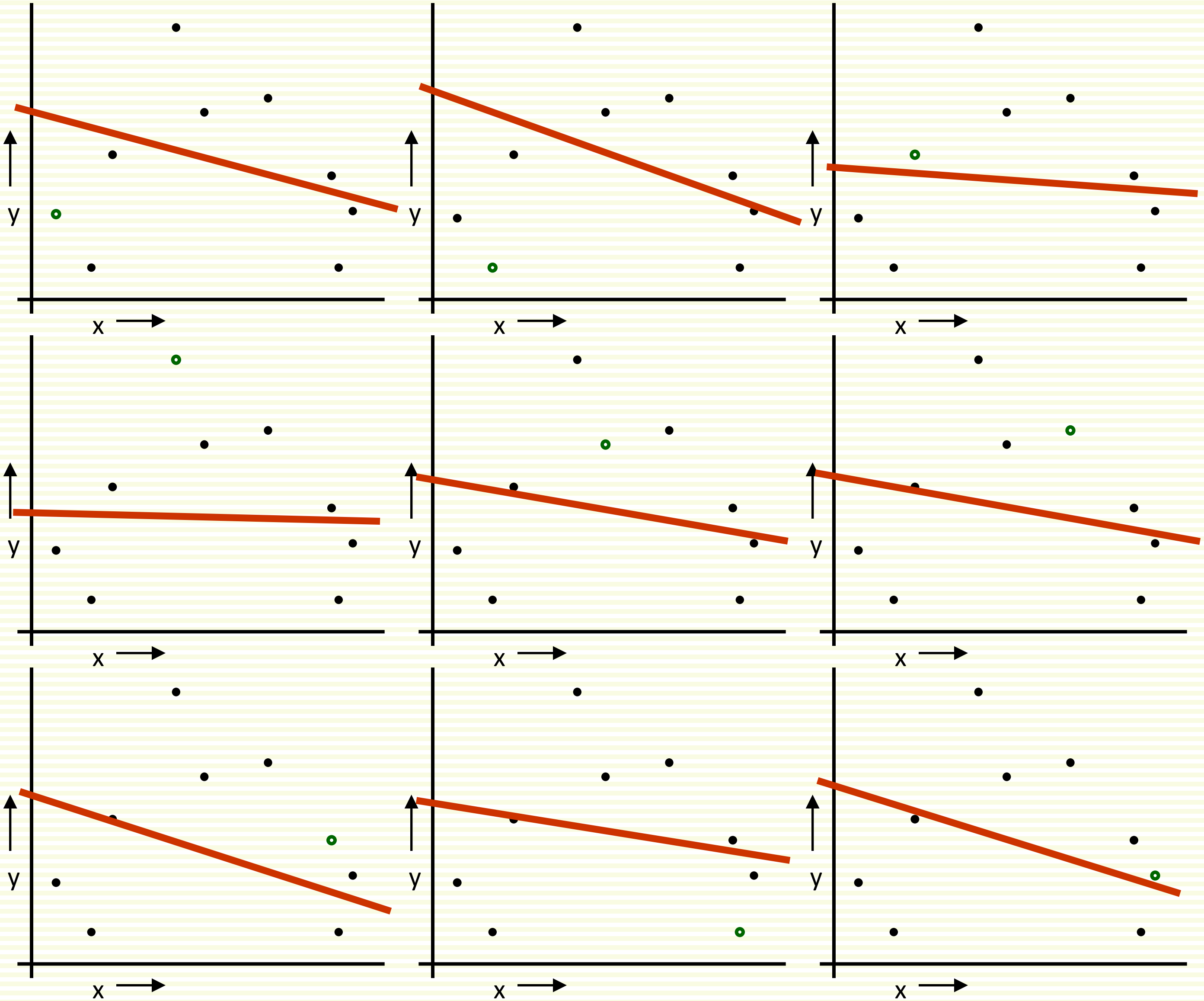


For **k**=1 to **n**

1. Let $(\mathbf{x}^k, \mathbf{y}^k)$ be the **k**th example
2. Temporarily remove $(\mathbf{x}^k, \mathbf{y}^k)$ from the dataset
3. Train on the remaining **n**-1 examples
4. Note your error on $(\mathbf{x}^k, \mathbf{y}^k)$

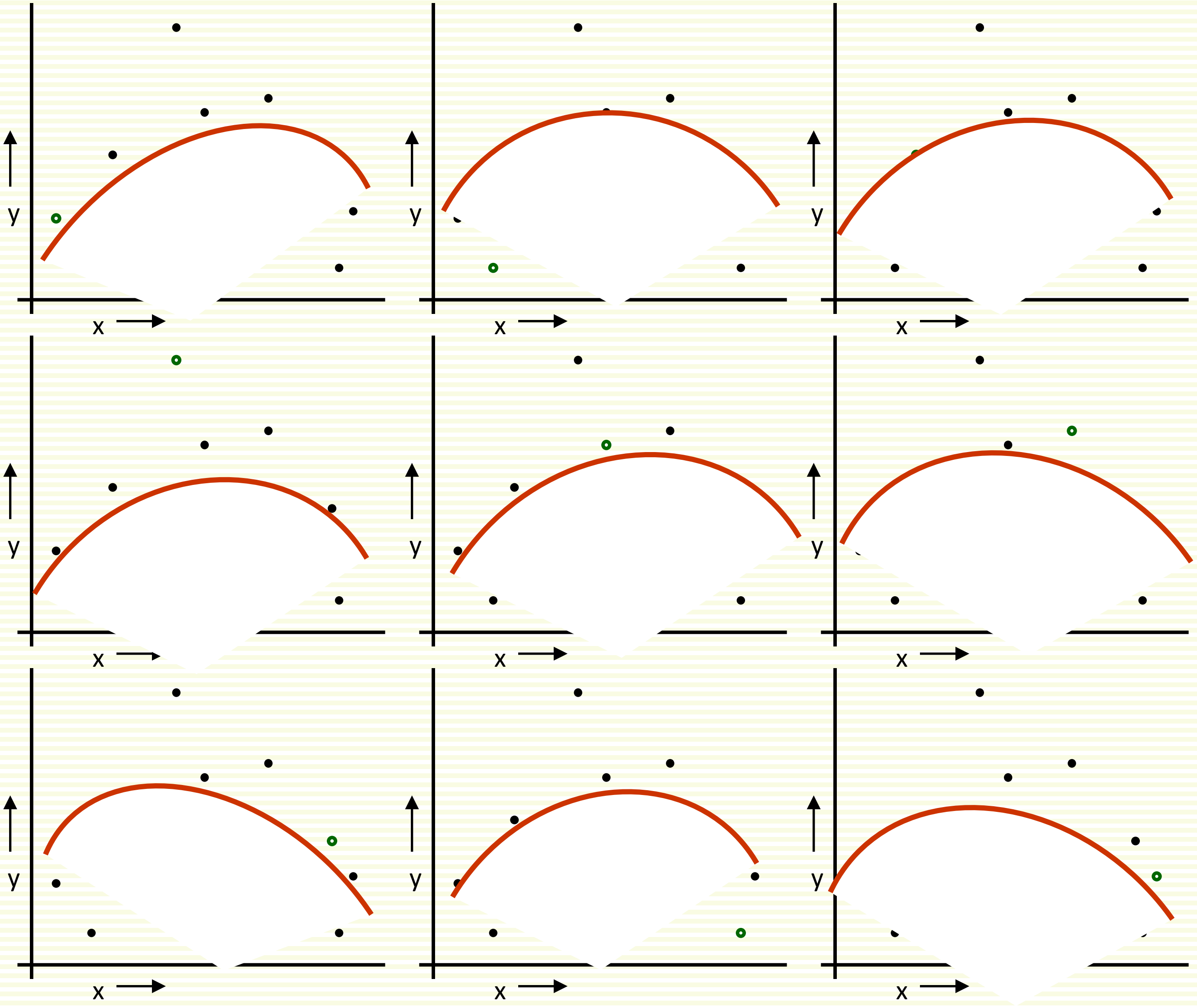
When you've done all points, report the mean error

LOOCV (Leave-one-out Cross Validation)



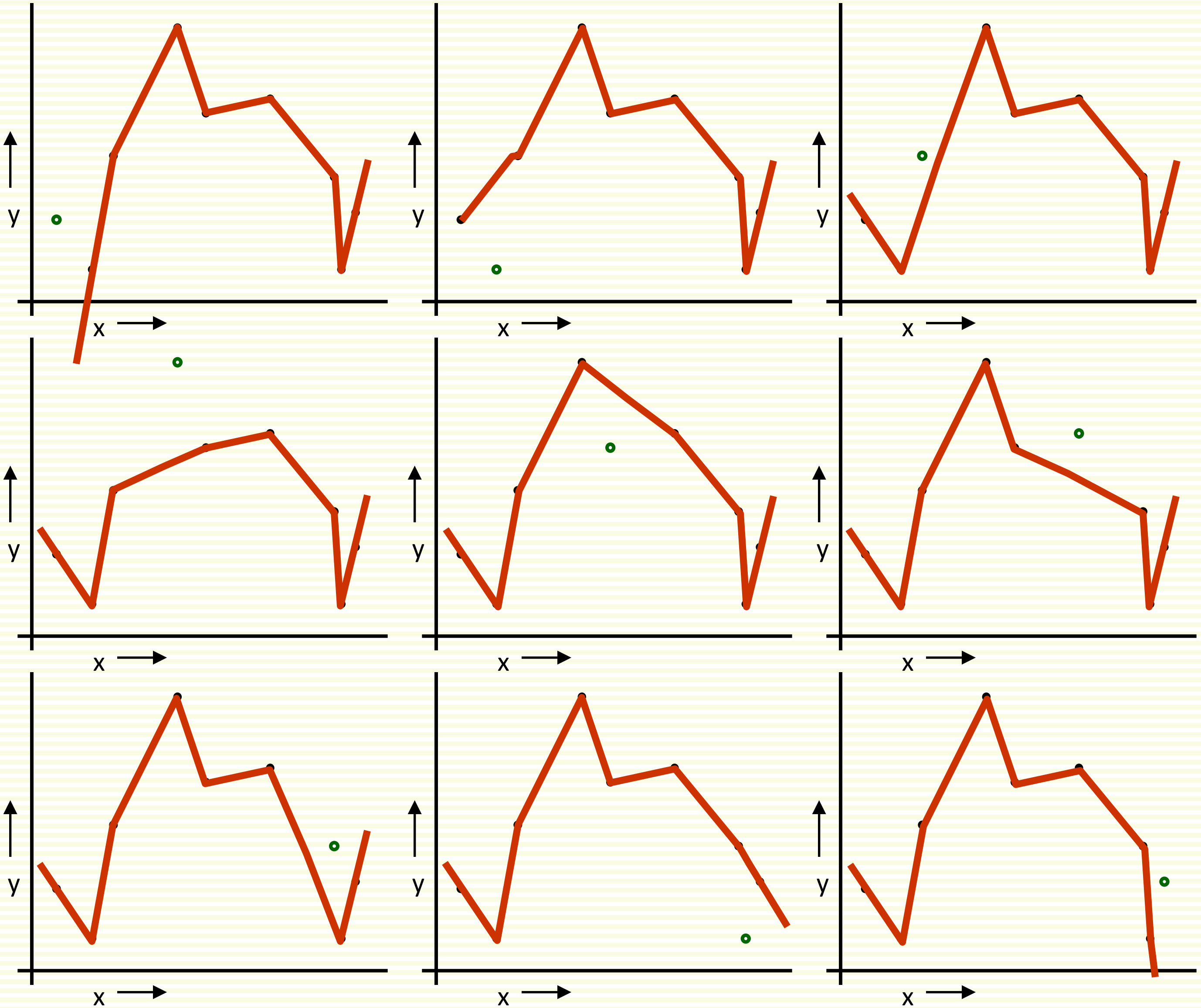
$MSE_{LOOCV} = 2.12$

LOOCV for Quadratic Regression



MSE_{LOOCV}
$= 0.962$

LOOCV for Join The Dots



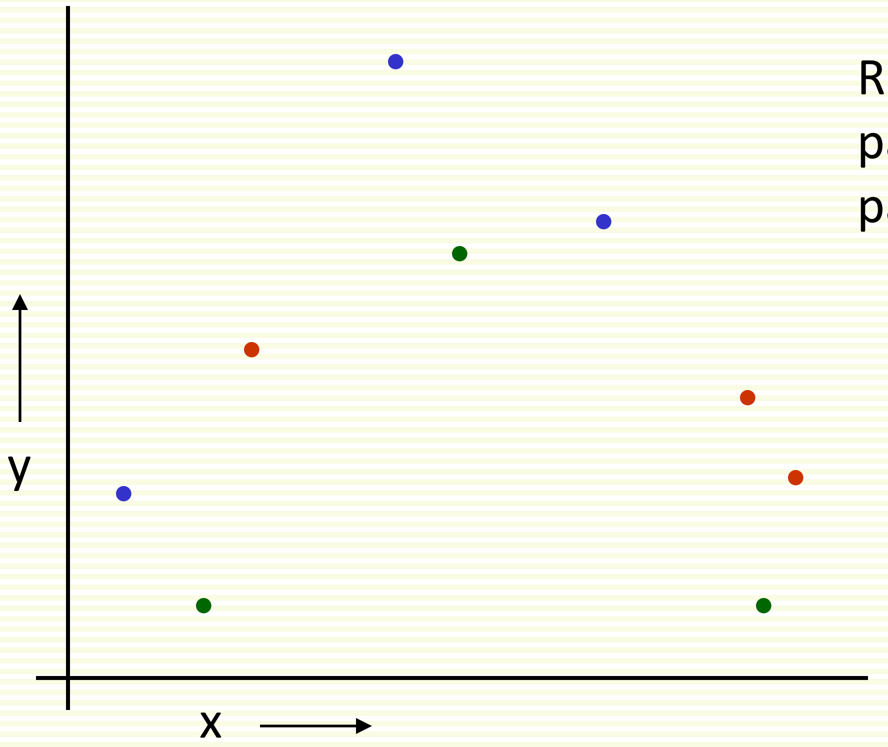
MSE_{LOOCV}
$=3.33$

Which kind of Cross Validation?

	Downside	Upside
Validation-set	may give unreliable estimate of future performance	cheap
Leave-one-out	expensive	doesn't waste data

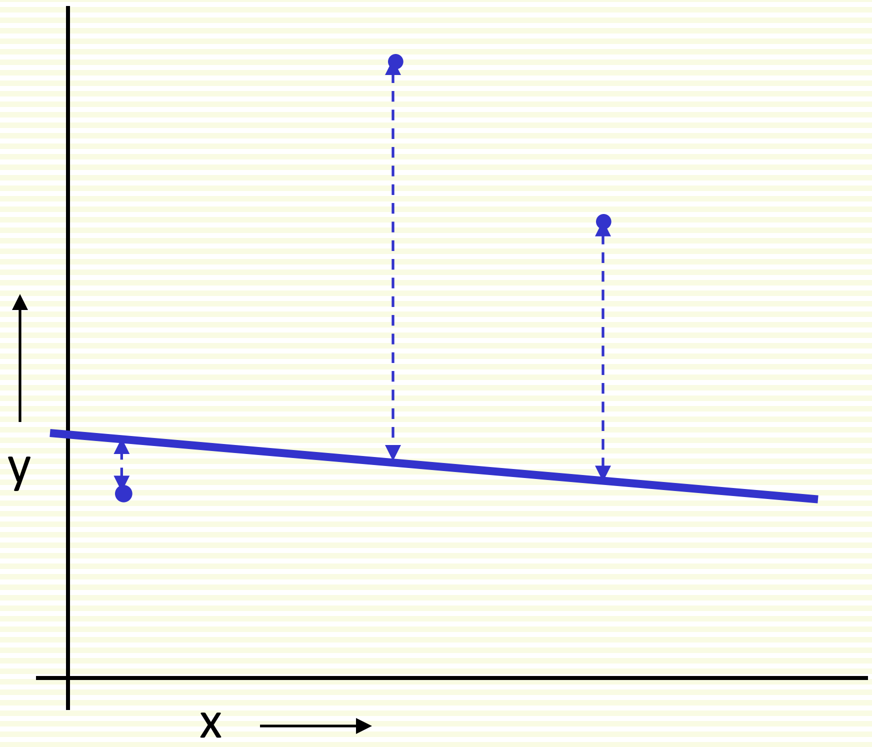
- Can we get the best of both worlds?

K-Fold Cross Validation



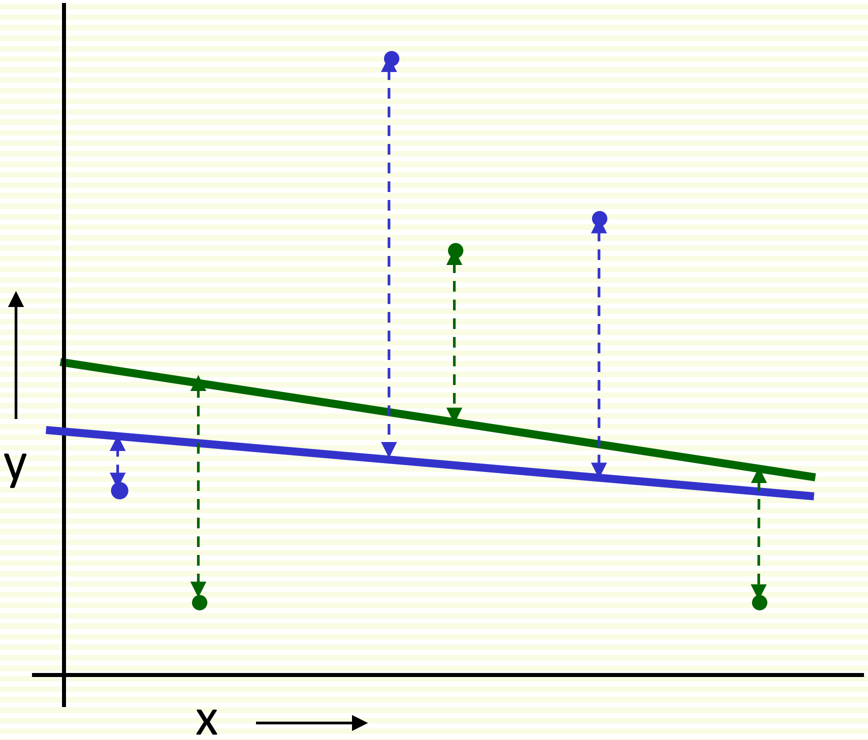
Randomly break the dataset into k partitions in this example we'll have k=3 partitions colored Red Green and Blue)

K-Fold Cross Validation



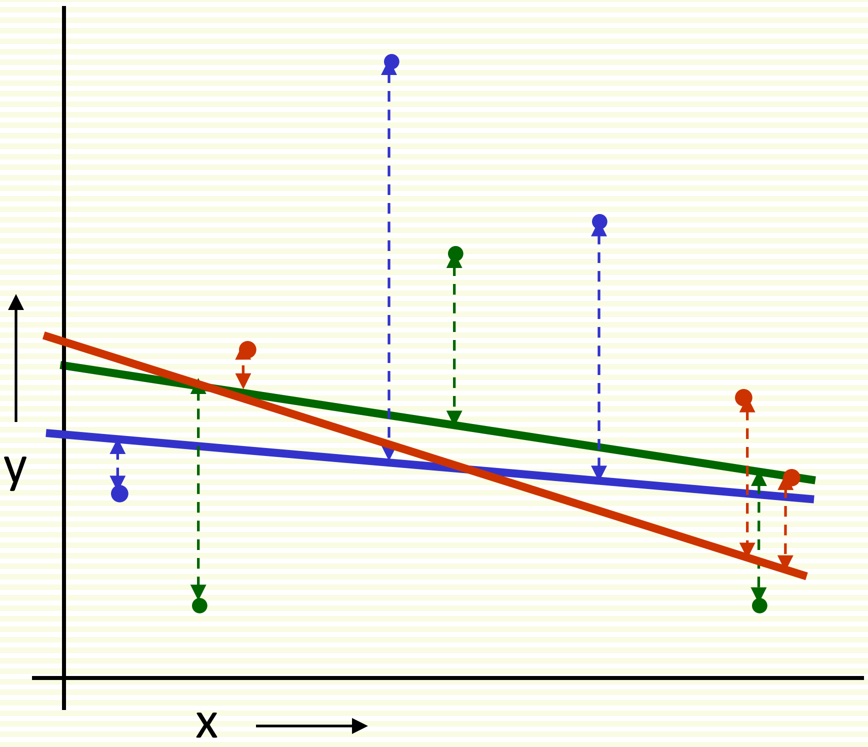
- Randomly break the dataset into k partitions
- in example have k=3 partitions colored red green and blue
- For the blue partition: train on all points not in the blue partition. Find test-set sum of errors on blue points

K-Fold Cross Validation



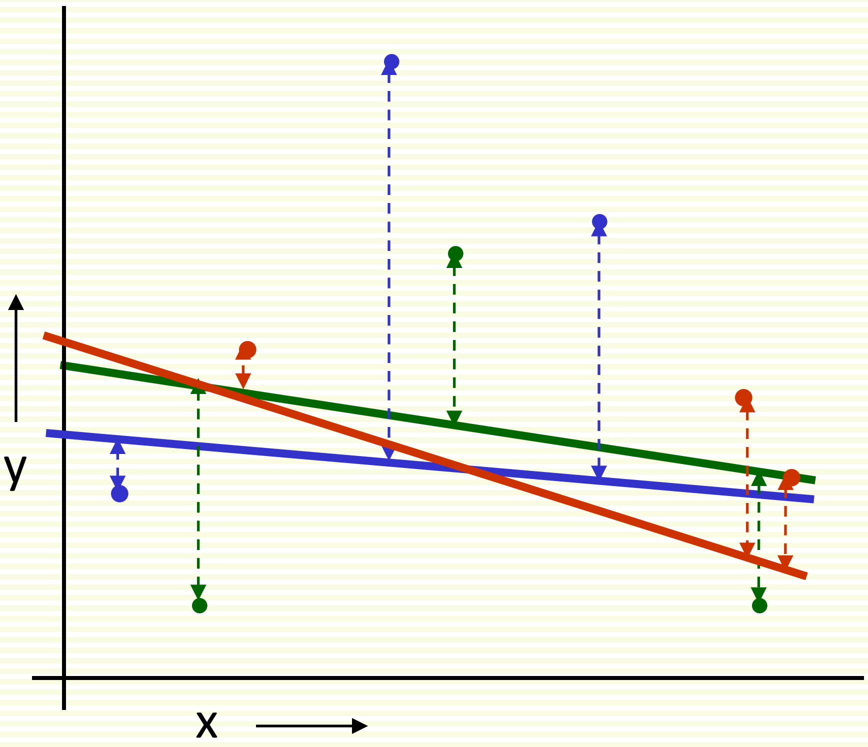
- Randomly break the dataset into k partitions
- in example have k=3 partitions colored red green and blue
- For the blue partition: train on all points not in the blue partition. Find sum of errors on blue points
- For the green partition: train on all points not in green partition. Find sum of errors on green points

K-Fold Cross Validation



- Randomly break the dataset into k partitions
- in example have k=3 partitions colored red green and blue
- For the blue partition: train on all points not in the blue partition. Find sum of errors on blue points
- For the green partition: train on all points not in green partition. Find sum of errors on green points
- For the red partition: train on all points not in red partition. Find sum of errors on red points

K-Fold Cross Validation

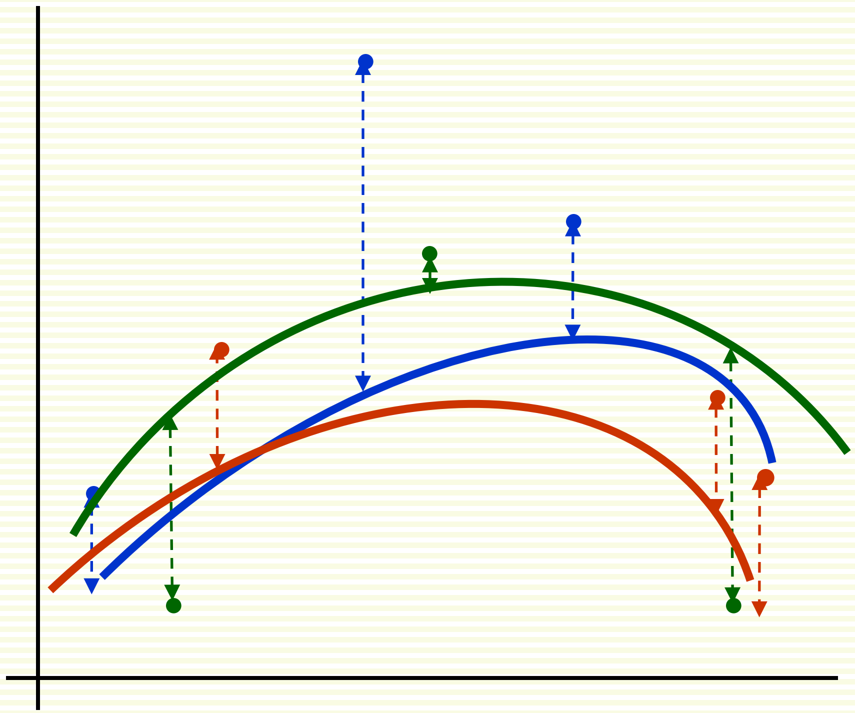


Linear Regression

MSE_{3FOLD}=2.05

- Randomly break the dataset into k partitions
- in example have k=3 partitions colored red green and blue
- For the blue partition: train on all points not in the blue partition. Find sum of errors on blue points
- For the green partition: train on all points not in green partition. Find sum of errors on green points
- For the red partition: train on all points not in red partition. Find sum of errors on red points
- Report the mean error

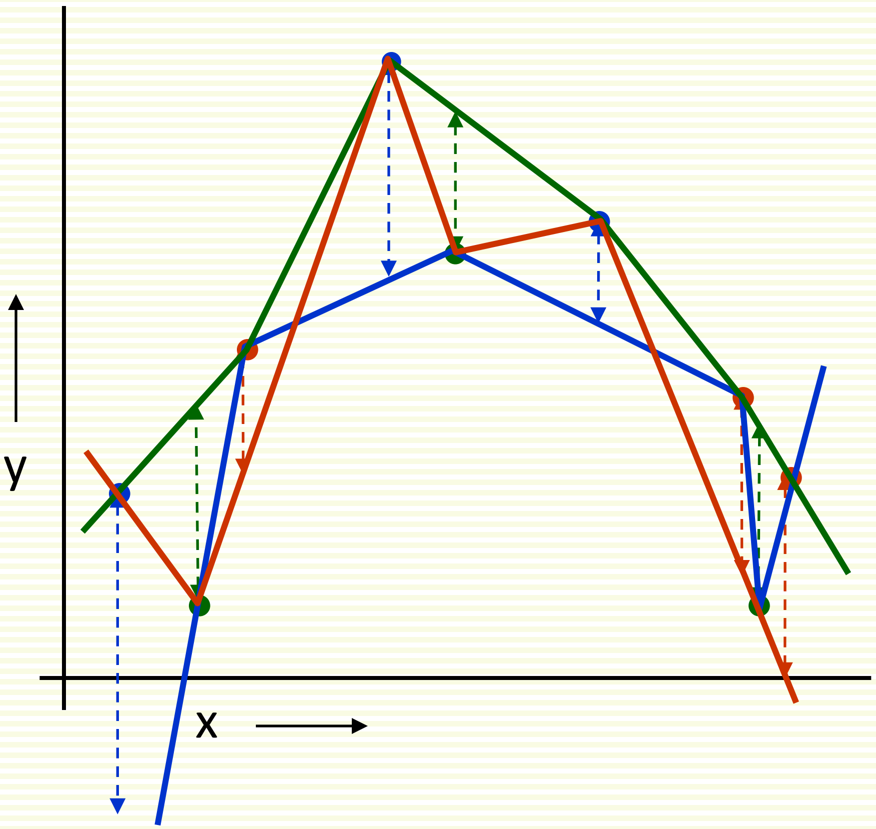
K-Fold Cross Validation



Quadratic Regression
MSE_{3FOLD}=1.11

- Randomly break the dataset into k partitions
- in example have k=3 partitions colored red green and blue
- For the blue partition: train on all points not in the blue partition. Find sum of errors on blue points
- For the green partition: train on all points not in green partition. Find sum of errors on green points
- For the red partition: train on all points not in red partition. Find sum of errors on red points
- Report the mean error

K-Fold Cross Validation



Joint-the-dots

MSE_{3FOLD}= 2.93

- Randomly break the dataset into k partitions
- in example have k=3 partitions colored red green and blue
- For the blue partition: train on all points not in the blue partition. Find sum of errors on blue points
- For the green partition: train on all points not in green partition. Find sum of errors on green points
- For the red partition: train on all points not in red partition. Find sum of errors on red points
- Report the mean error

Which kind of Cross Validation?

	Downside	Upside
Validation-set	may give unreliable estimate of future performance	cheap
Leave-one-out	expensive	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	wastes more data than 10-fold, more expensive than validation set	slightly better than validation-set
N-fold	Identical to Leave-one-out	

CV-based Model Selection

- We're trying to decide which algorithm to use.
- We train each machine and make a table…

f_i	Training Error	10-FOLD-CV Error	Choice
f_1			
f_2			
f_3			⌦
f_4			
f_5			
f_6			

CV-based Model Selection

- Example: Choosing “k” for a k-nearest-neighbor regression.
- Step 1: Compute LOOCV error for six different model classes:

Algorithm	Training Error	10-fold-CV Error	Choice
k=1			
k=2			
k=3			
k=4			⌧
k=5			
k=6			

- Step 2: Choose model that gave best CV score
- Train it with all the data, and that’s the final model you’ll use

CV-based Model Selection

- Why stop at **k**=6?
  - No good reason, except it looked like things were getting worse as K was increasing
- Are we guaranteed that a local optimum of K vs LOOCV will be the global optimum?
  - No, in fact the relationship can be very bumpy
- What should we do if we are depressed at the expense of doing LOOCV for **k** = 1 through 1000?
  - Try: **k**=1, 2, 4, 8, 16, 32, 64, … ,1024
  - Then do hillclimbing from an initial guess at **k**

Cross Validation Notes

- After we chose non-tunable parameters/classifiers, retrain chosen classifier on all training data

Training	Validation	Test ≈20%		$\lambda = 0.1$
Training	Validation	Training	Test ≈20%	$\lambda = 0.2$
Training	Validation	Training	Test ≈20%	$\lambda = 0.3$
Validation	Training	Test ≈20%		$\lambda = 0.4$

- Based on 4-fold cross validation error, suppose **λ = 0.3** is the best
- Retrain classifier with $\lambda = 0.3$ on all training data now

Training	Test ≈20%

Cross Validation Notes

- Should still have separate Test set, not touched during cross-validation

- Sometime report just CV-results, no separate Test data
- Common practice, but should be aware that extensive use of CV could overfit to the data