CS60050: Machine Learning

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CROSS-VALIDATION

The test set method

Good news:

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

Bad news:

- What's the downside?

The test set method

Good news:

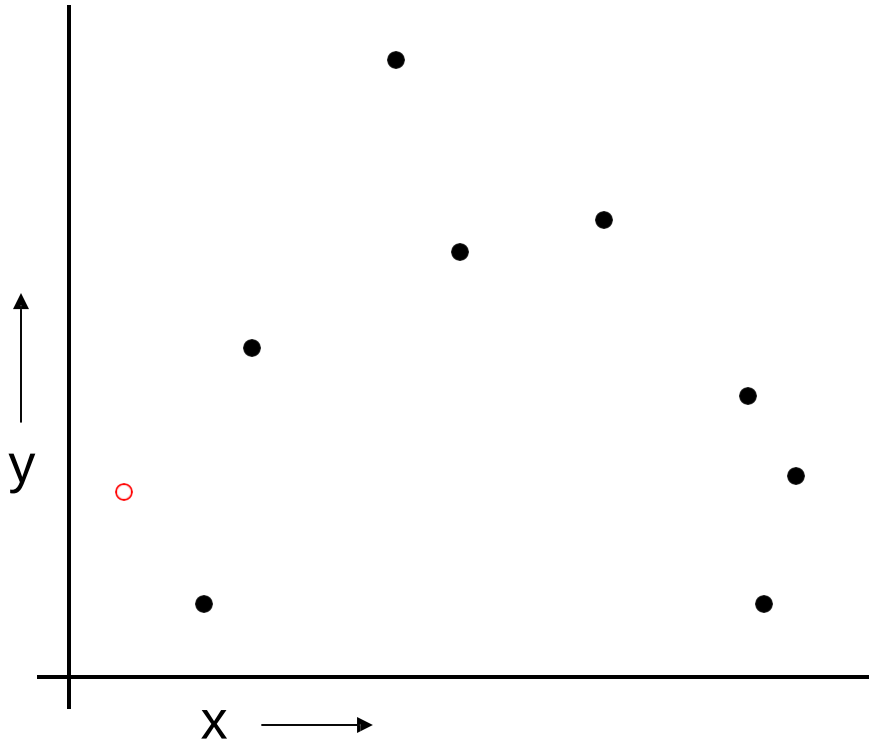
- Very very simple
- Can then simply choose the method with the best test-set score

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 test-set might just be lucky or unlucky

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

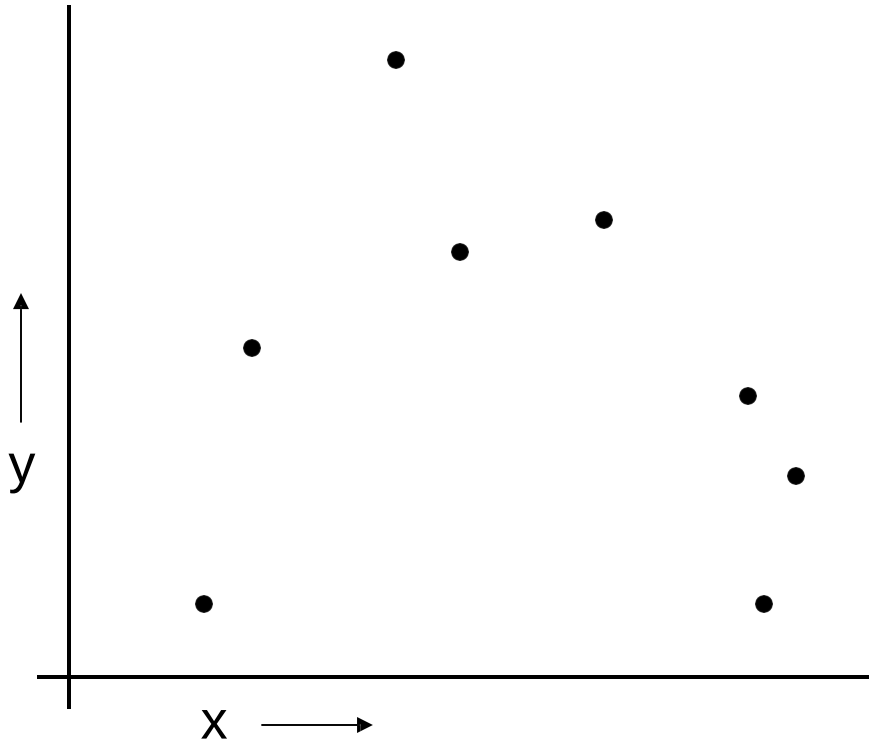
LOOCV (Leave-one-out Cross Validation)



For k=1 to R

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

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

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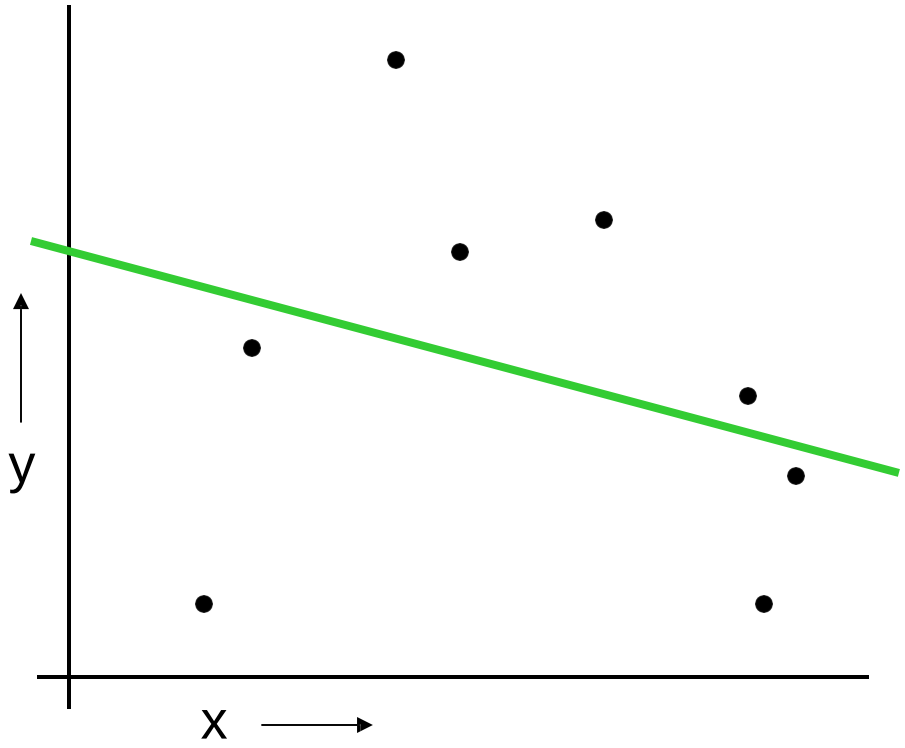

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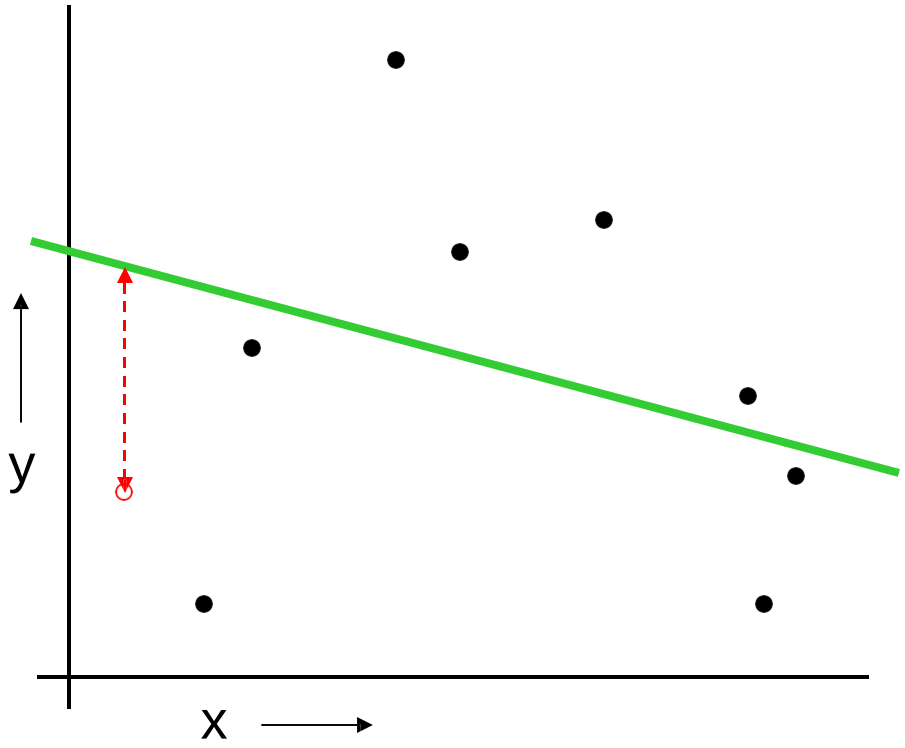

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4. Note your error (x_k,y_k)

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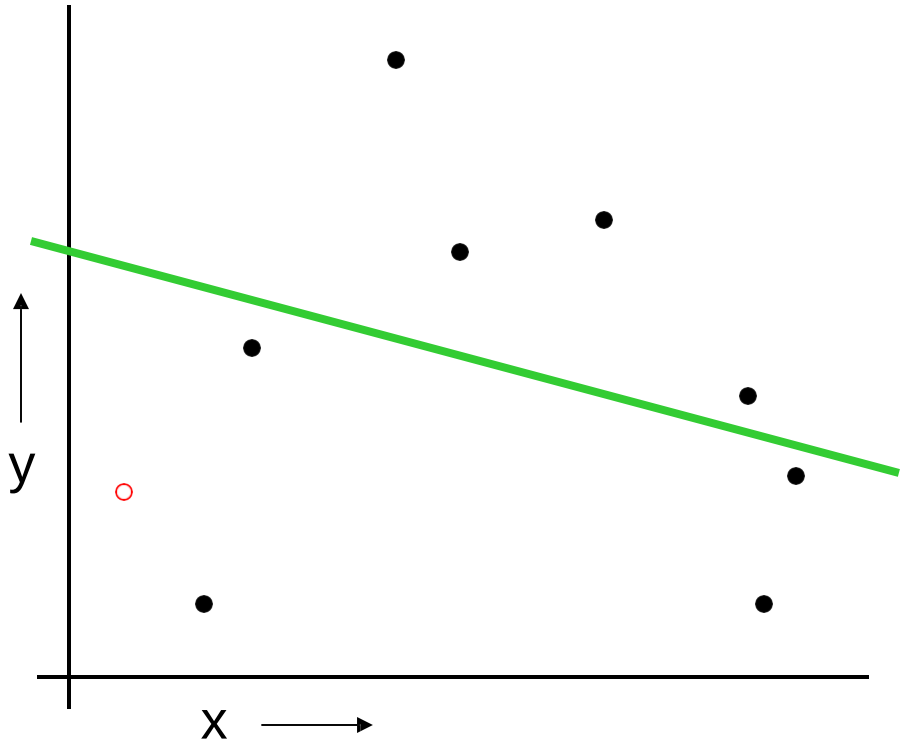

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When you've done all points, report the mean error.

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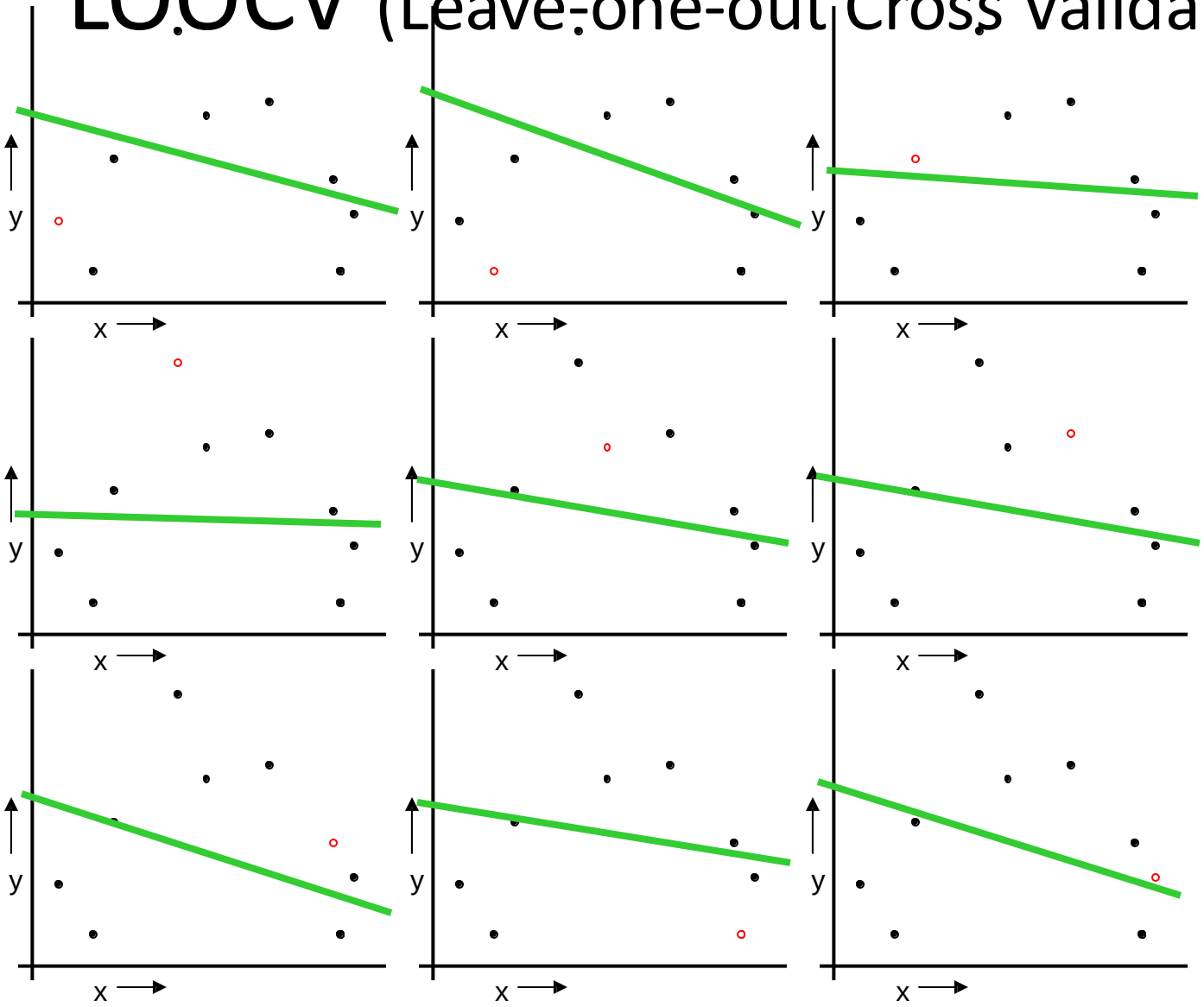

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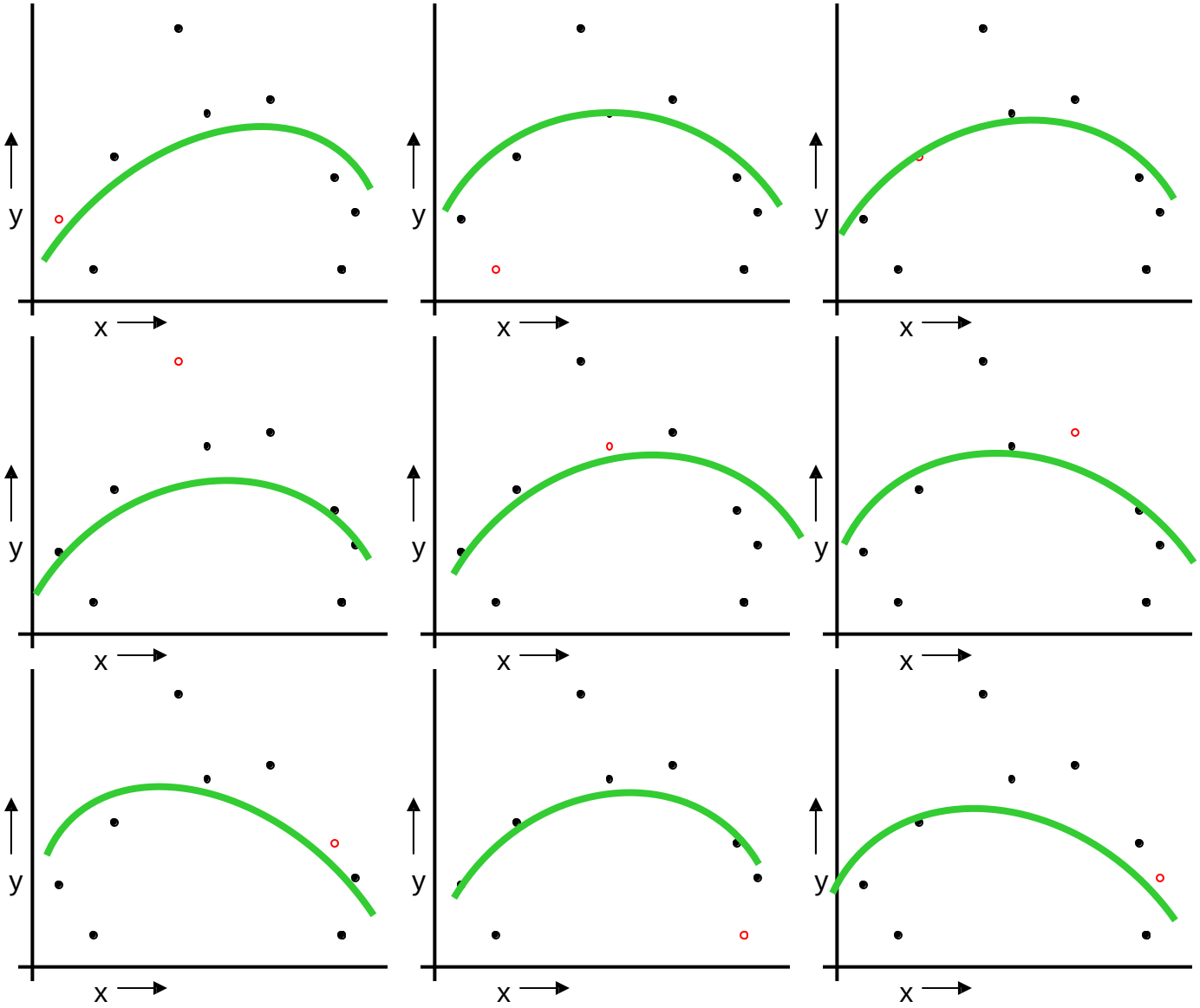
$$MSE_{LOOCV} = 2.12$$

LOOCV for Quadratic Regression



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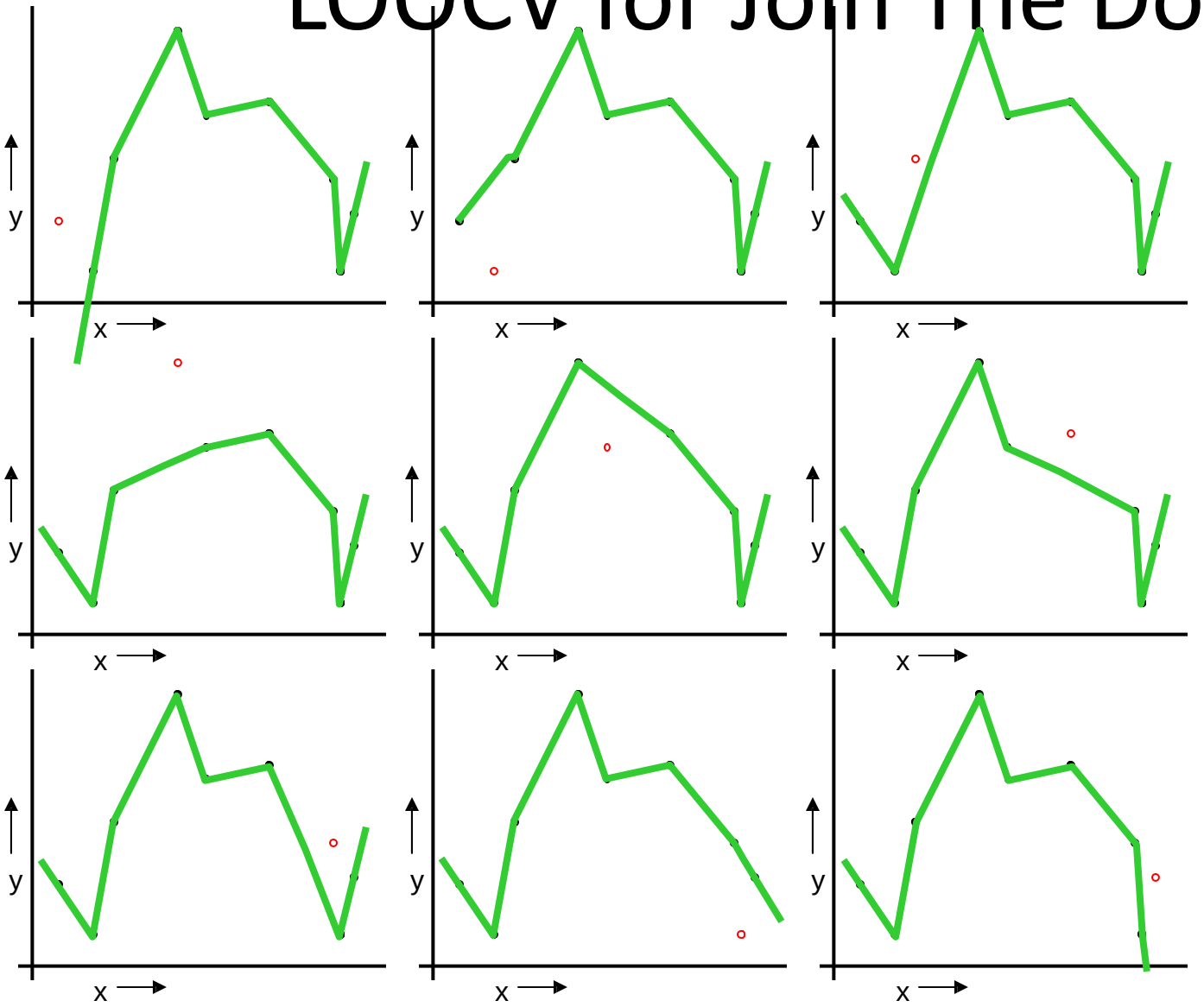
$MSE_{LOOCV} = 0.962$

LOOCV for Join The Dots



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

$MSE_{LOOCV} = 3.33$

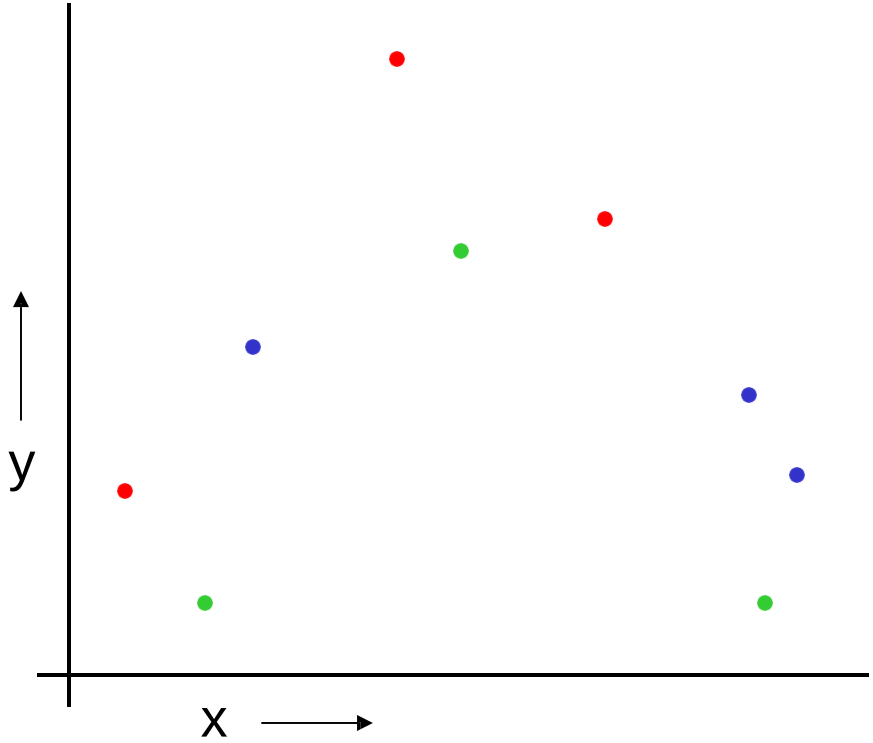
Which kind of Cross Validation?

	Downside	**Upside**
Test-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?

k-fold Cross Validation

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



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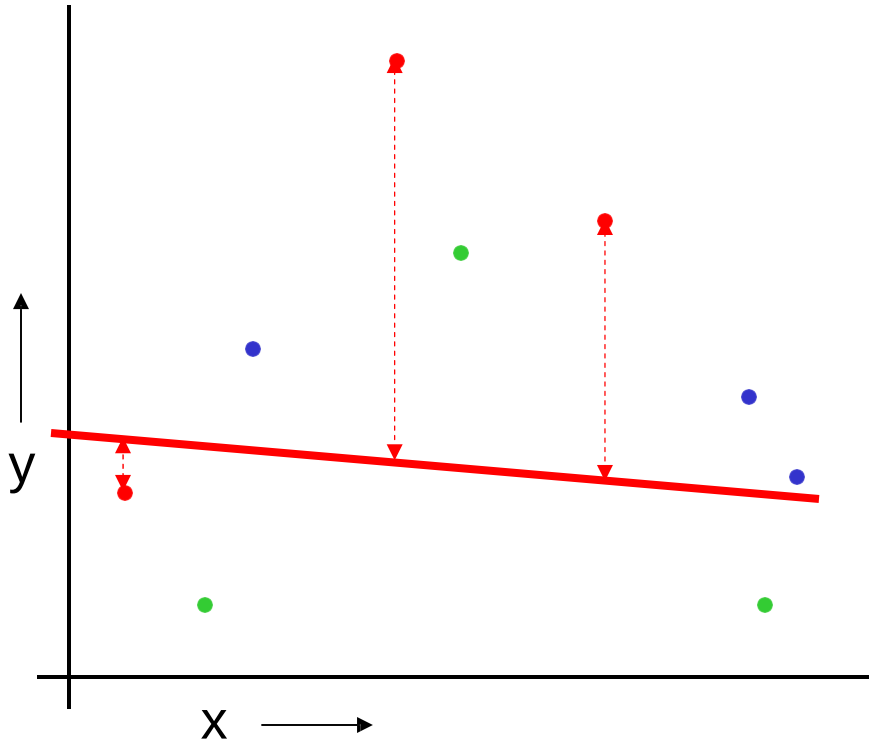
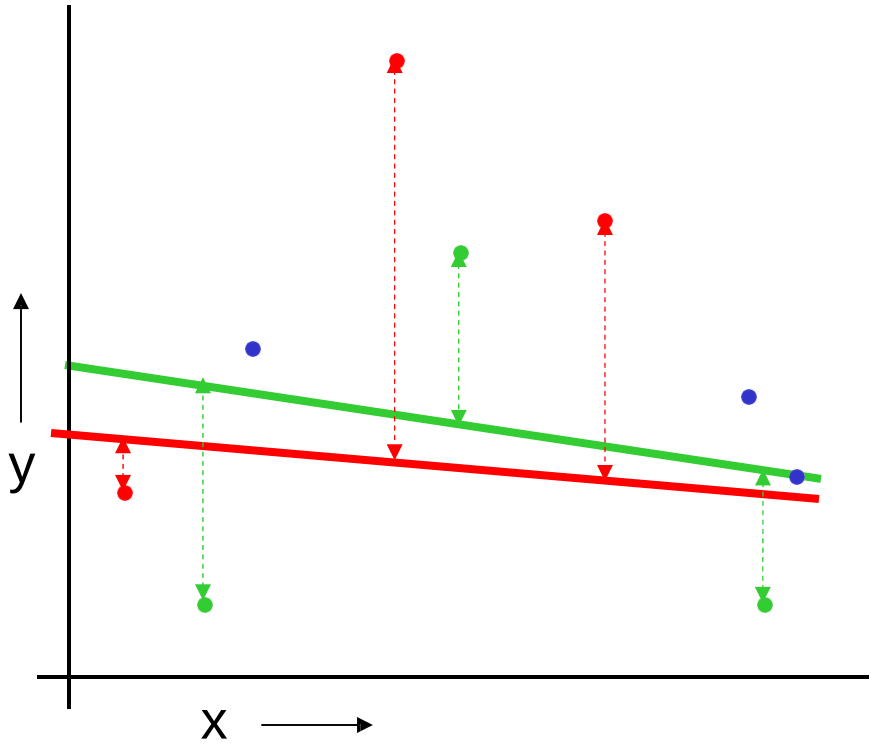


Randomly break the dataset into k partitions (in our example we'll have k=3 partitions colored Red Green and Blue)

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

k-fold Cross Validation

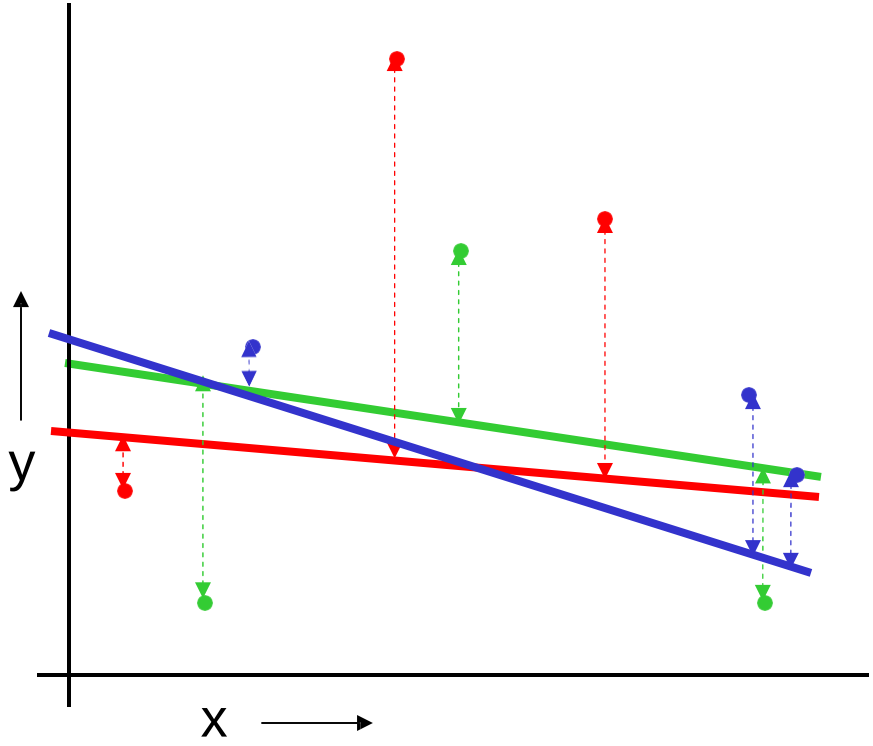


Randomly break the dataset into k partitions (in our example we'll have k=3 partitions colored Red Green and Blue)

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

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

k-fold Cross Validation



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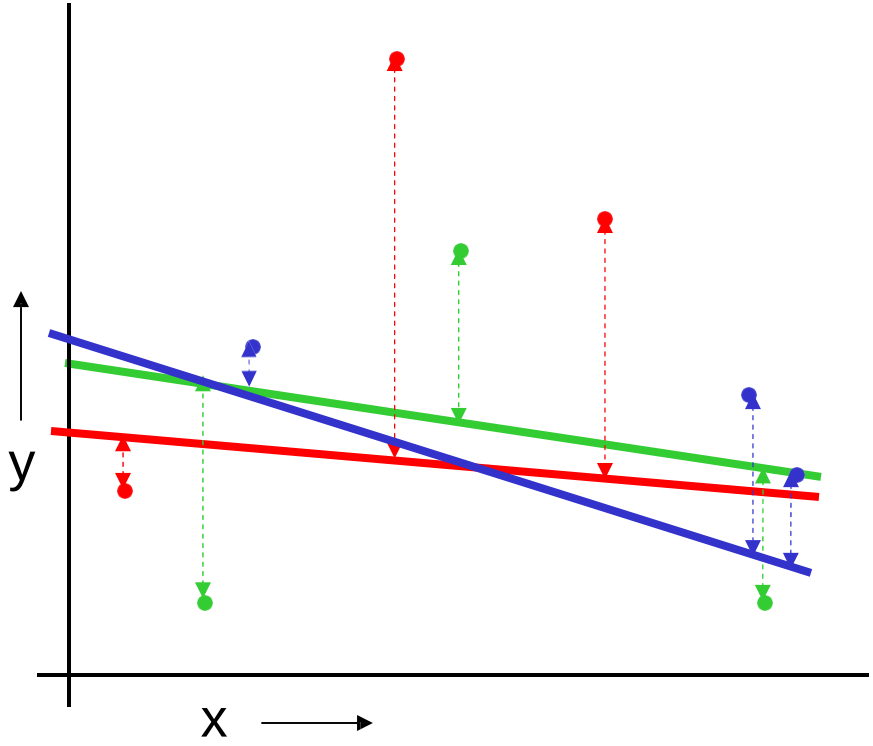
k-fold Cross Validation



Linear Regression

$MSE_{3FOLD}=2.05$

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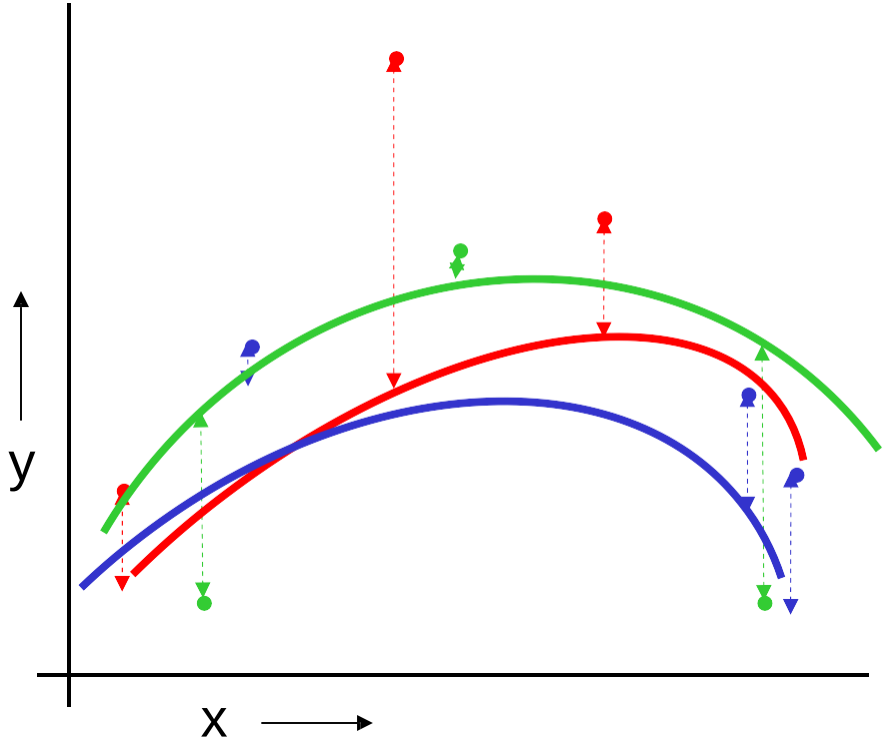
For the blue partition: Train on all the points not in the blue partition. Find the test-set sum of errors on the blue points.

Then report the mean error

k-fold Cross Validation



Quadratic Regression

$MSE_{3FOLD}=1.11$

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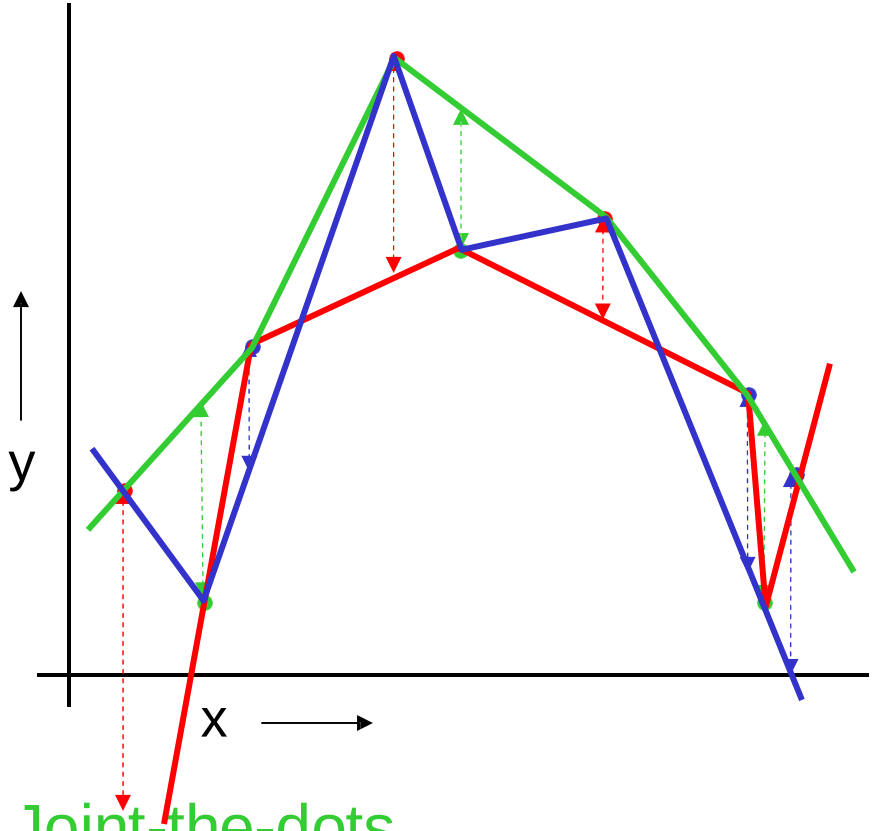
Then report the mean error

k-fold Cross Validation



Joint-the-dots

$MSE_{3FOLD}=2.93$

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Which kind of Cross Validation?

	Downside	Upside
Test-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 test set	Only wastes 10%. Only 10 times more expensive instead of R times.
3-fold	Wastier than 10-fold. Expensivier than test set	Slightly better than test-set
R-fold	Identical to Leave-one-out	

CV-based Model Selection

- Example: Choosing number of hidden units in a one-hidden-layer neural net.
- Step 1: Compute 10-fold CV error for six different model classes:

Algorithm	TRAINERR	10-FOLD-CV-ERR	Choice
0 hidden units			
1 hidden units			
2 hidden units			⊠
3 hidden units			
4 hidden units			
5 hidden units			

- Step 2: Whichever model class gave best CV score: train it with all the data, and that's the predictive model you'll use.

CV-based Model Selection

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

Algorithm	TRAINERR	10-fold-CV-ERR	Choice
K=1			
K=2			
K=3			
K=4			⊠
K=5			
K=6			

- Step 2: Whichever model class gave best CV score: train it with all the data, and that’s the predictive model you’ll use.

CV-based Model Selection

- Can you think of other decisions we can ask Cross Validation to make for us, based on other machine learning algorithms in the class so far?
  - Degree of polynomial in polynomial regression
  - Whether to use full, diagonal or spherical Gaussians in a Gaussian Bayes Classifier.
  - The Kernel Width in Kernel Regression
  - The Kernel Width in Locally Weighted Regression
  - The Bayesian Prior in Bayesian Regression

These involve choosing the value of a real-valued parameter. What should we do?

Idea One: Consider a discrete set of values (often best to consider a set of values with exponentially increasing gaps, as in the K-NN example).

Idea Two: Compute $\frac{\partial \text{LOOCV}}{\partial \text{Parameter}}$ and then do gradianet descent.