UVA CS 6316: Machine Learning

Lecture 5: Non-Linear Regression Models and Model Selection

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Where are we ? ➔ Five major sections of this course

- ❑ Regression (supervised)
- ❑ Classification (supervised)
- ❑ Unsupervised models
- ❑ Learning theory
- ❑ Graphical models

Regression (supervised)

- ❑ Four ways to train / perform optimization for linear regression models
  - ❑ Normal Equation
  - ❑ Gradient Descent (GD)
  - ❑ Stochastic GD
  - ❑ Newton's method

} variations of $\underset{\theta}{\text{argmin}}\ L(\theta)$

- ❑ Supervised regression models
  - ❑ Linear regression (LR)
  - ❑ LR with non-linear basis functions
  - ❑ Locally weighted LR
  - ❑ LR with Regularizations

} variations of f(x)

→ variations of L(θ)

Today ➔ Regression (supervised)

- ❑ ~~Four ways to train / perform optimization for linear regression models~~
  - ~~❑ Normal Equation~~
  - ~~❑ Gradient Descent (GD)~~
  - ~~❑ Stochastic GD~~
  - ~~❑ Newton's method~~

- ~~❑Supervised regression models~~
  - ~~❑Linear regression (LR)~~
  - ❑LR with non-linear basis functions
  - ❑Locally weighted LR
  - ❑LR with Regularizations

Today

- Regression Models Beyond Linear
  - LR with non-linear basis functions
  - Instance-based Regression: K-Nearest Neighbors (later)
  - Locally weighted linear regression (extra)
  - Regression trees and Multilinear Interpolation (later)

LR with non-linear basis functions

- LR does not mean we can only deal with linear relationships

$$\hat{y} = \theta^T \mathbf{x} \quad \Longrightarrow \quad \hat{y} = \theta_0 + \sum_{j=1}^{m} \theta_j \varphi_j(\mathbf{x}) = \theta^T \varphi(\mathbf{x})$$

LR with non-linear basis functions

- We are free to design basis functions (e.g., non-linear features:

Here $\varphi_j(x)$ are fixed basis functions (also define $\varphi_0(x)=1$)

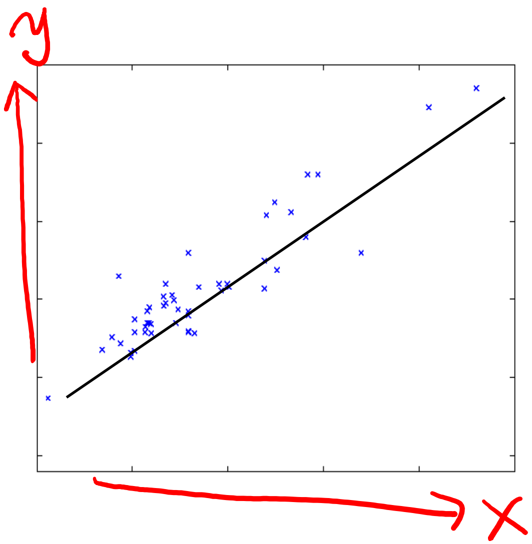
- E.g.: polynomial regression:

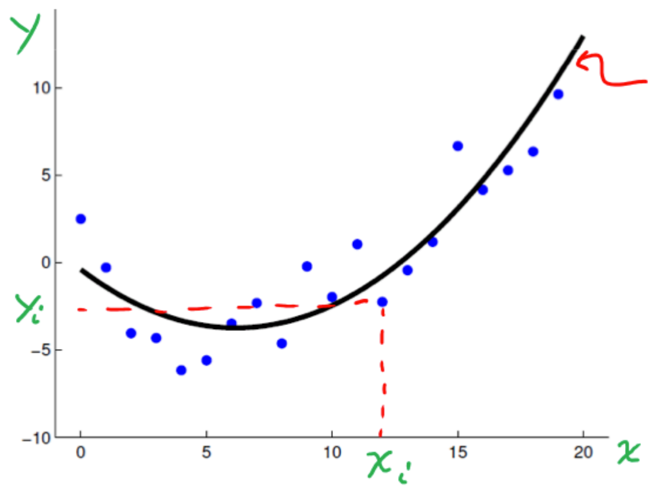
$$\varphi(x) := \left[1, x, x^2\right]^T$$

e.g. (1) polynomial regression

$$\hat{y} = \theta^T \mathbf{x}$$

$$\hat{y} = \theta^T \varphi(\mathbf{x})$$





$= \Theta_0 + x\Theta_1 + x^2\Theta_2$

$$\theta^* = \left(X^T X\right)^{-1} X^T \vec{y}$$

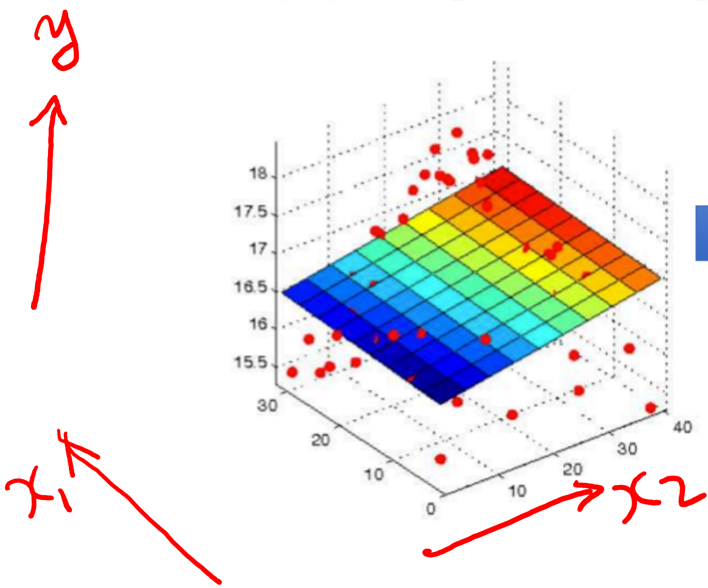
$$\theta^* = \left(\varphi^T \varphi\right)^{-1} \varphi^T \vec{y}$$

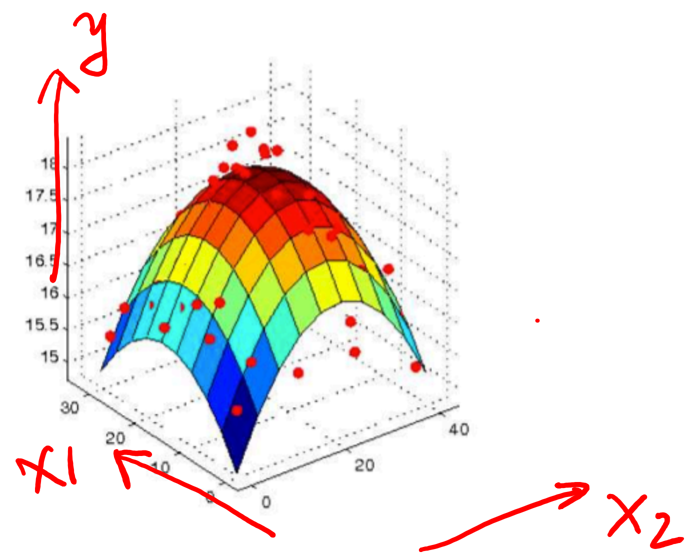
$$\varphi(x) := \left[1, x, x^2\right]^T$$

e.g. (1) polynomial regression

$$\hat{y} = \theta^T \mathbf{x} \quad \Rightarrow \quad \hat{y} = \theta^T \varphi(\mathbf{x})$$

$$\phi(\mathbf{x}) = [1, x_1, x_2] \qquad \phi(\mathbf{x}) = [1, x_1, x_2, x_1^2, x_2^2]$$





KEY: if the bases are given, the problem of learning the parameters is still linear.

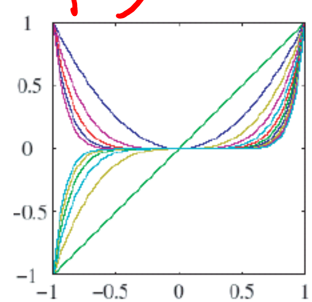
Many Possible Basis functions

- There are many basis functions, e.g.:
  - Polynomial $\varphi_j(x) = x^{j-1}$

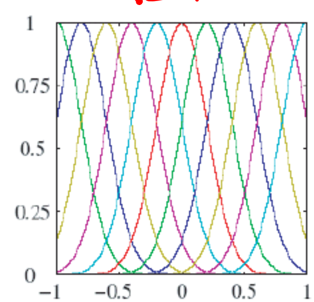
$$\boxed{1,\ x,\ x^2,\ x^3,\ \ldots,\ x^d}$$

  - Radial basis functions $$\phi_j(x) = \exp\left(-\frac{(x-\mu_j)^2}{2s^2}\right)$$
  - Sigmoidal $$\phi_j(x) = \sigma\left(\frac{x-\mu_j}{s}\right)$$
  - Splines,
  - Fourier,
  - Wavelets, etc

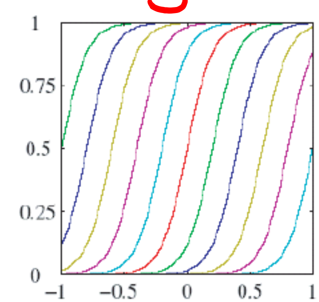
Poly



RBF

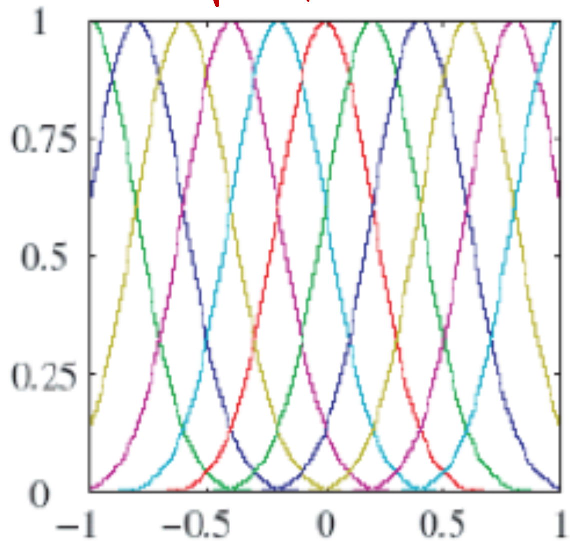


Sigmoid

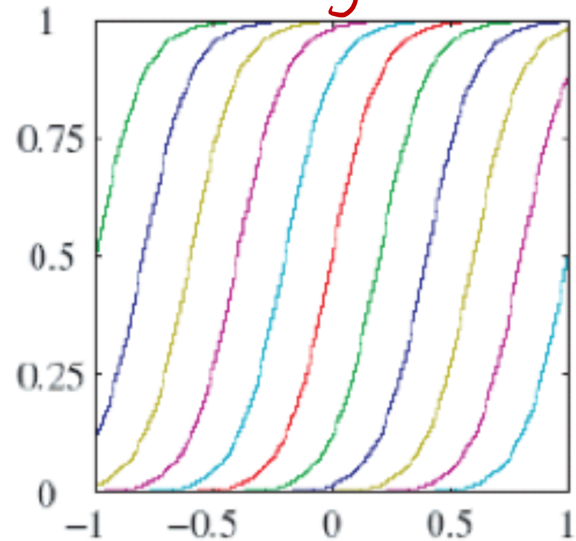


Many Possible Basis functions

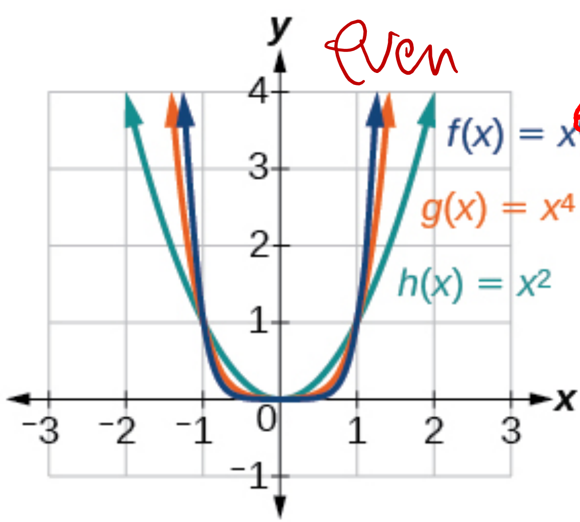
RBF



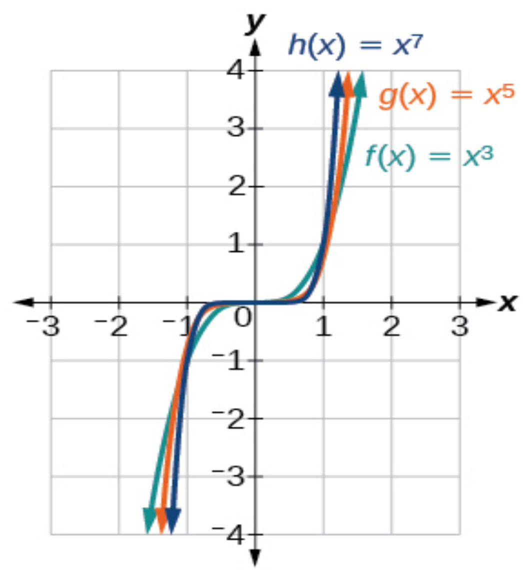
Sigmoid



even



odd



e.g. (2) LR with radial-basis functions

- E.g.: LR with RBF regression:

$$\hat{y} = \theta_0 + \sum_{j=1}^{m} \theta_j \varphi_j(x) = \varphi(x)^T \theta$$

$$\varphi(x) := \left[1, K_{\lambda_1}(x, r_1), K_{\lambda 2}(x, r_2), K_{\lambda_3}(x, r_3), K_{\lambda 4}(x, r_4)\right]^T$$

$$\vec{\theta} = [\theta_0, \theta_1, \theta_2, \theta_3, \theta_4]^T$$

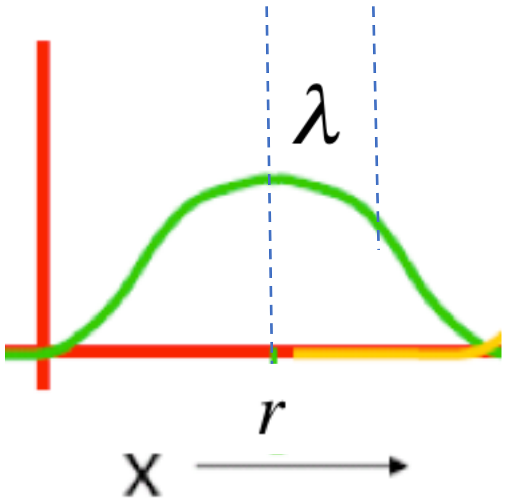
$$\theta^* = \left(\varphi^T \varphi\right)^{-1} \varphi^T \vec{y}$$

RBF = radial-basis function: a function which depends only on the radial distance from a centre point

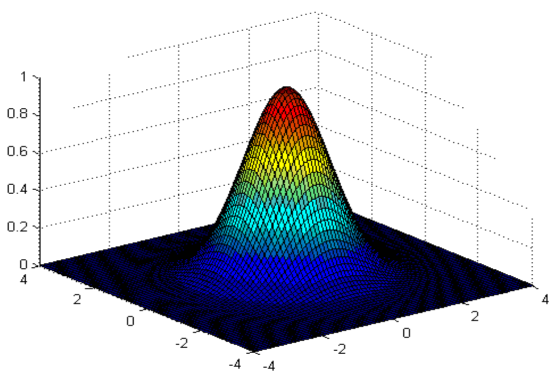
Gaussian RBF →

$$K_\lambda(x,r) = \exp\left(-\frac{(x-r)^2}{2\lambda^2} \right)$$

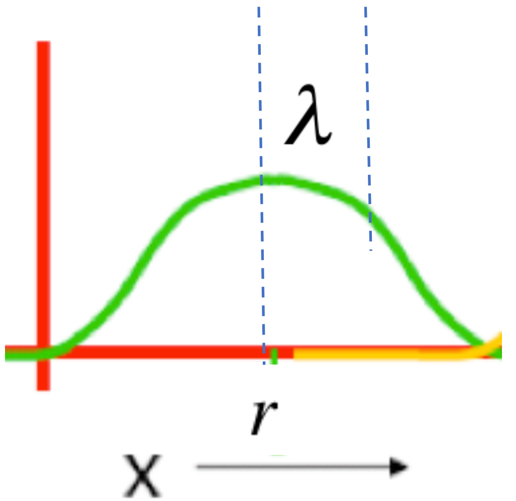
as distance from the center r increases, the output of the RBF decreases



1D case



2D case



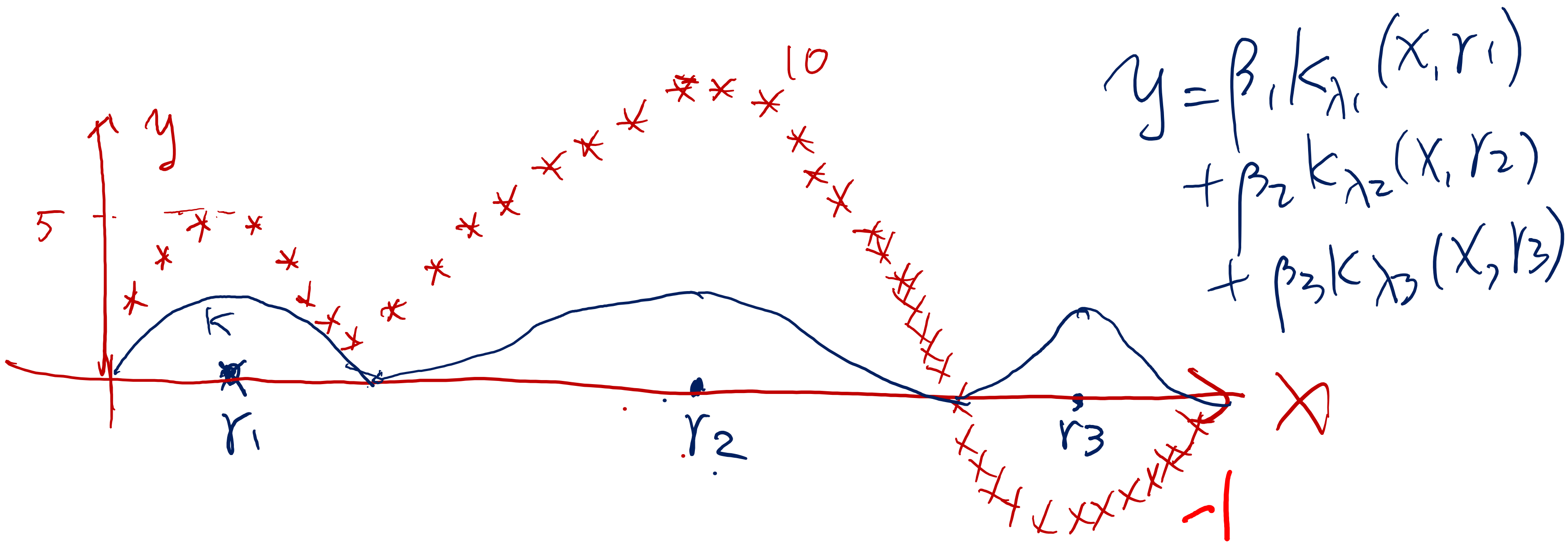
$$K_\lambda(x,r) = \exp\left(-\frac{(x-r)^2}{2\lambda^2}\right)$$

X =	$K_\lambda(x,r) =$
r	1
$r+\lambda$	0.6065307
$r+2\lambda$	0.1353353
$r+3\lambda$	0.0001234098

e.g. another Linear regression with 1D RBF basis functions (assuming 3 predefined centres and width)

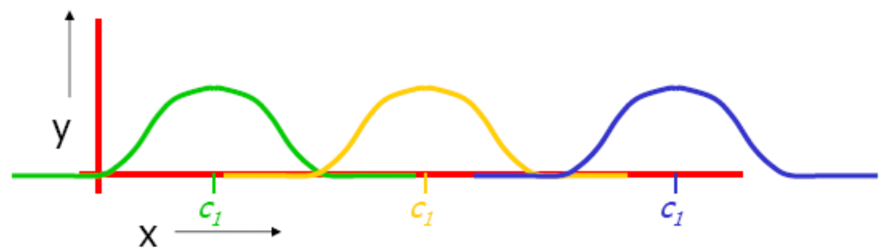
$$\varphi(x) := \left[1, K_{\lambda_1}(x, r_1), K_{\lambda 2}(x, r_2), K_{\lambda_3}(x, r_3) \right]^T$$

$$\theta^* = \left(\varphi^T \varphi \right)^{-1} \varphi^T \vec{y}$$



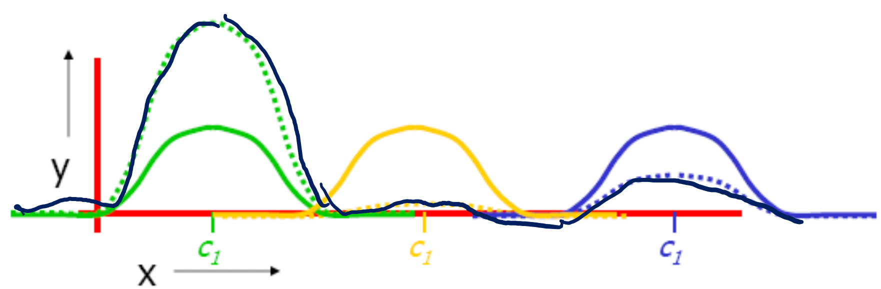
e.g. a LR with 1D RBFs (3 predefined centres and width)

- 1D RBF



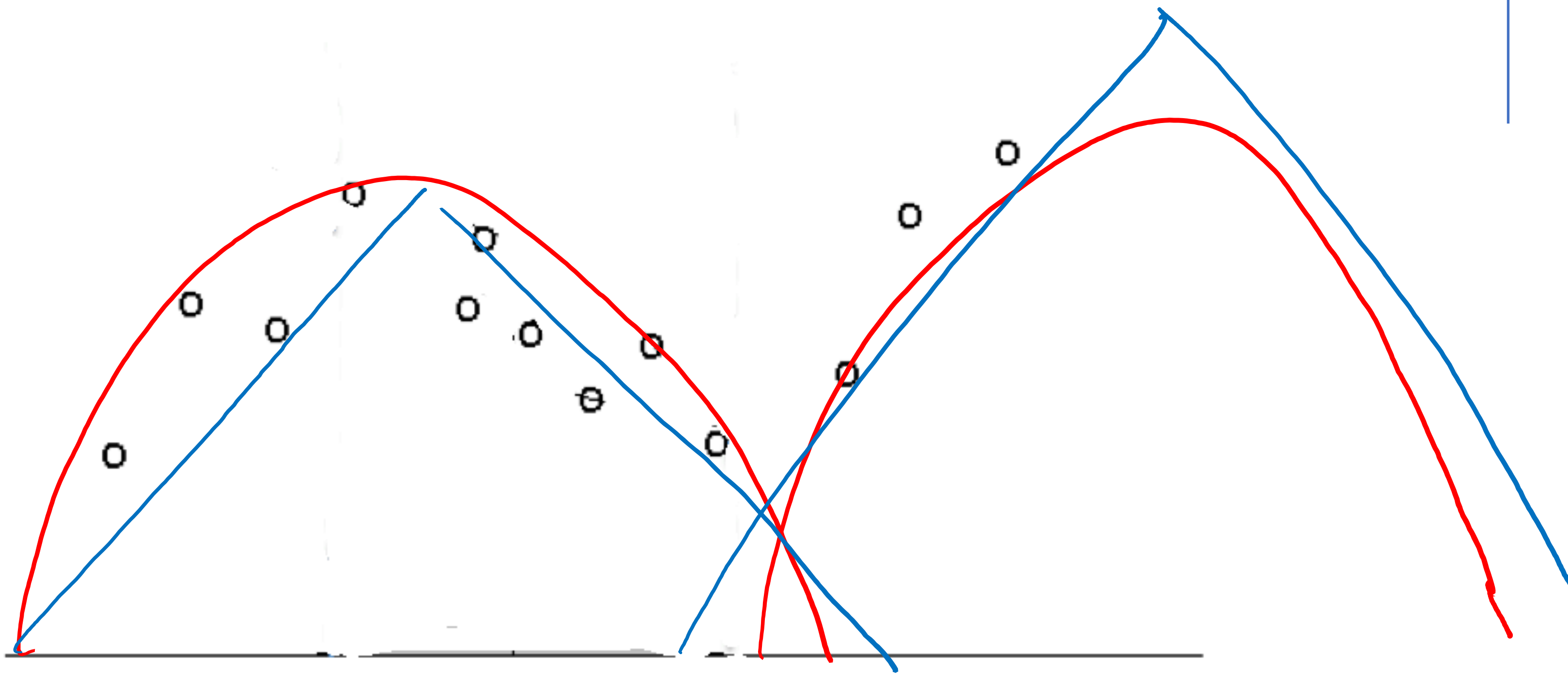
$$y^{est} = \beta_1 \phi_1(x) + \beta_2 \phi_2(x) + \beta_3 \phi_3(x)$$

- After fit:



$$y^{est} = 2\phi_1(x) + 0.05\phi_2(x) + 0.5\phi_3(x)$$

e.g. Even more possible Basis Func?



(2) Multivariate Linear Regression with basis Expansion

Task → Representation → Score Function → Search/Optimization → Models, Parameters

Regression → Y = Weighted linear sum of (X basis expansion) → SSE → Linear algebra / GD / SGD → Regression coefficients

$$\hat{y} = \theta_0 + \sum_{j=1}^{m} \theta_j \varphi_j(x) = \varphi(x)^T \theta$$

Two main issues:

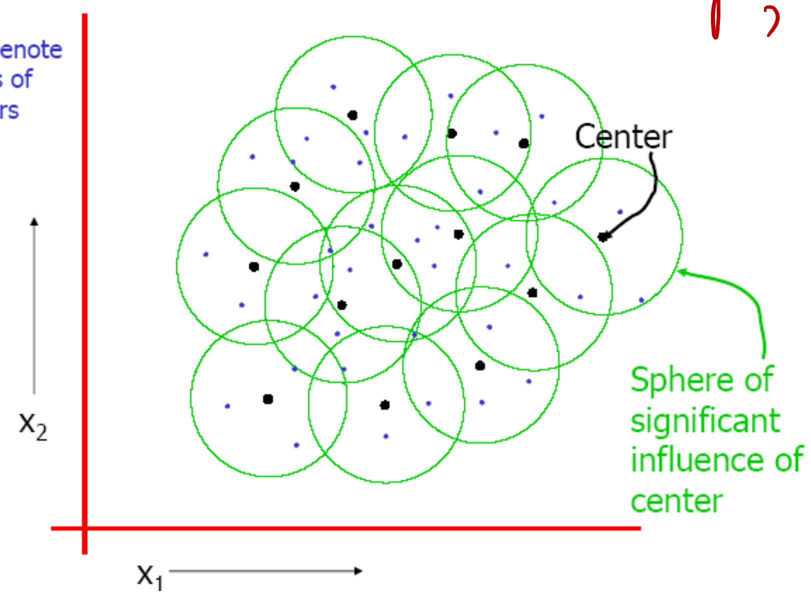
- To Learn the parameter θ^*
  - Almost the same as LR, just ➔ X to $\varphi(x)$
  - Linear combination of basis functions (that can be non-linear)

- How to choose the model order,
  - E.g. what polynomial degree for polynomial regression
  - E.g., where to put the centers for the RBF kernels? How wide?

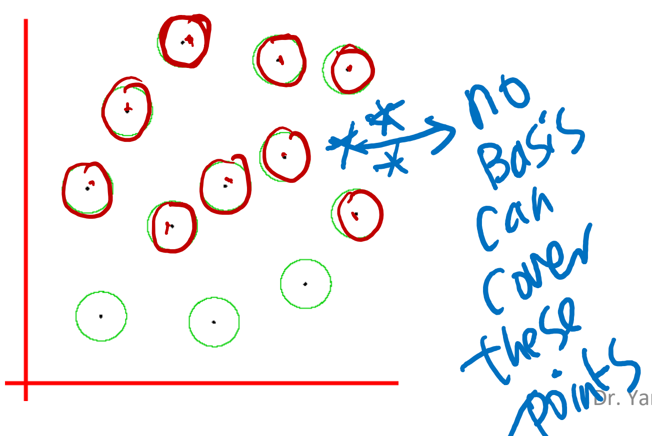
e.g. 2D Good and Bad RBF Basis

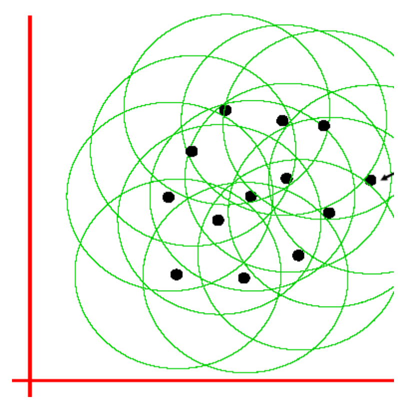
γ, λ

- A good 2D RBF

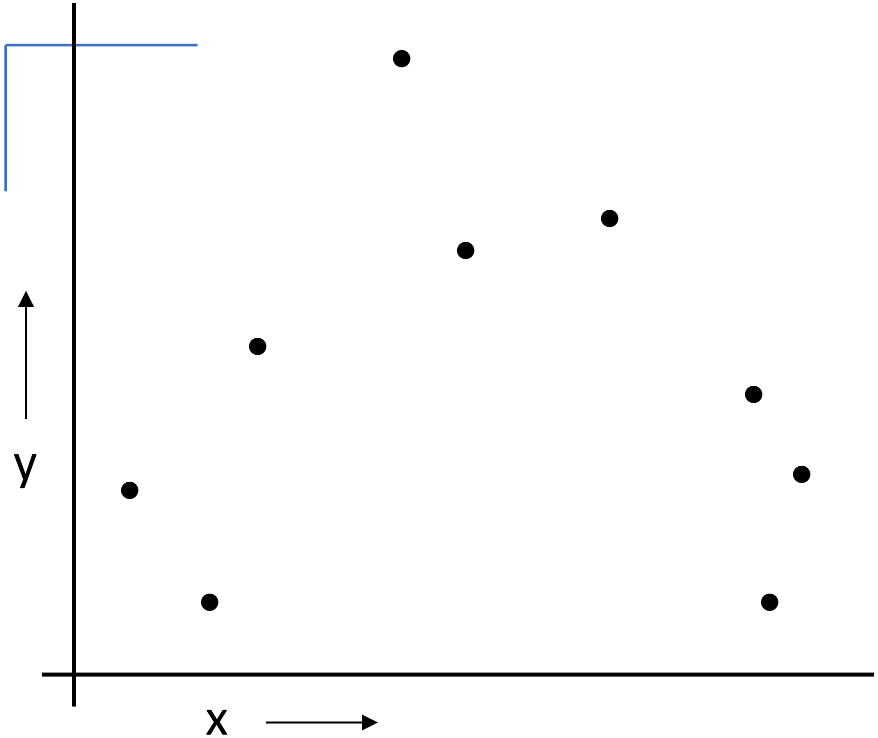


- Two bad 2D RBFs





Issue: Overfitting and Underfitting

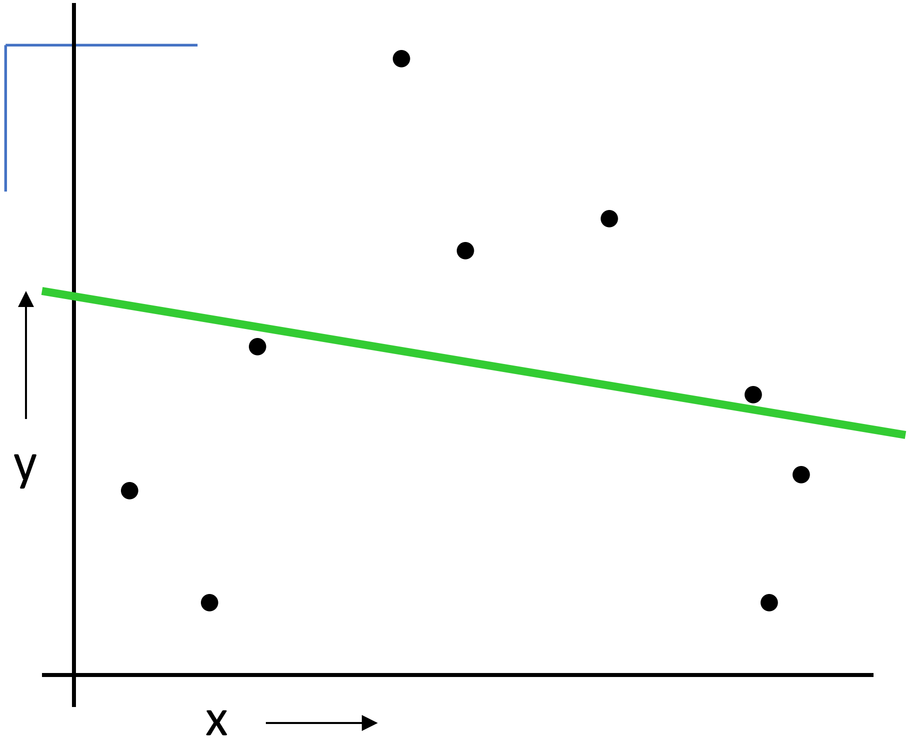


y = f(x) + noise

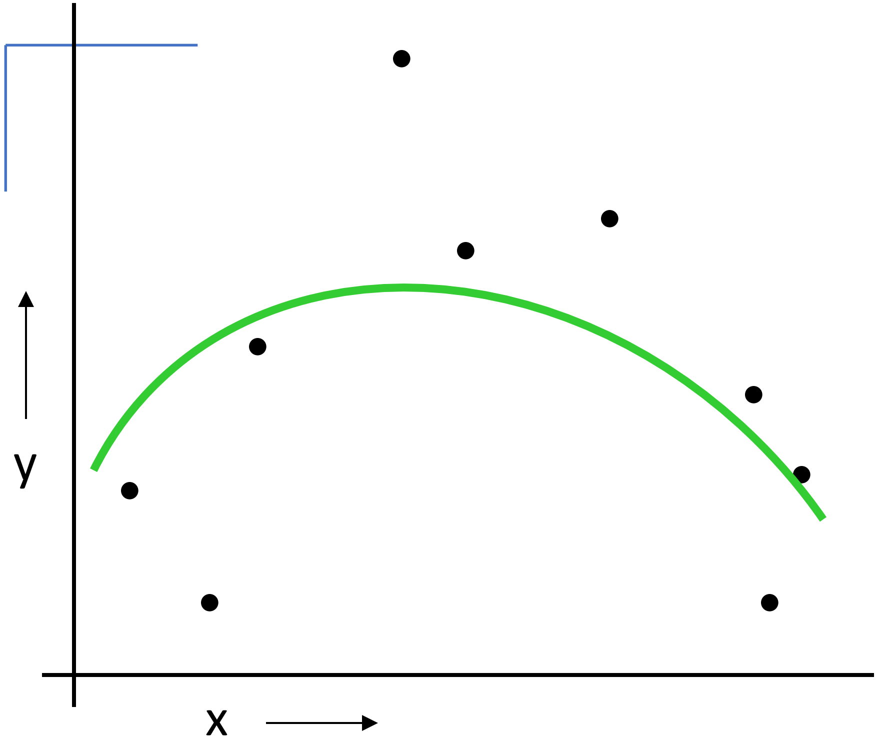
Can we learn a regression f from the data?

Let's consider three methods…

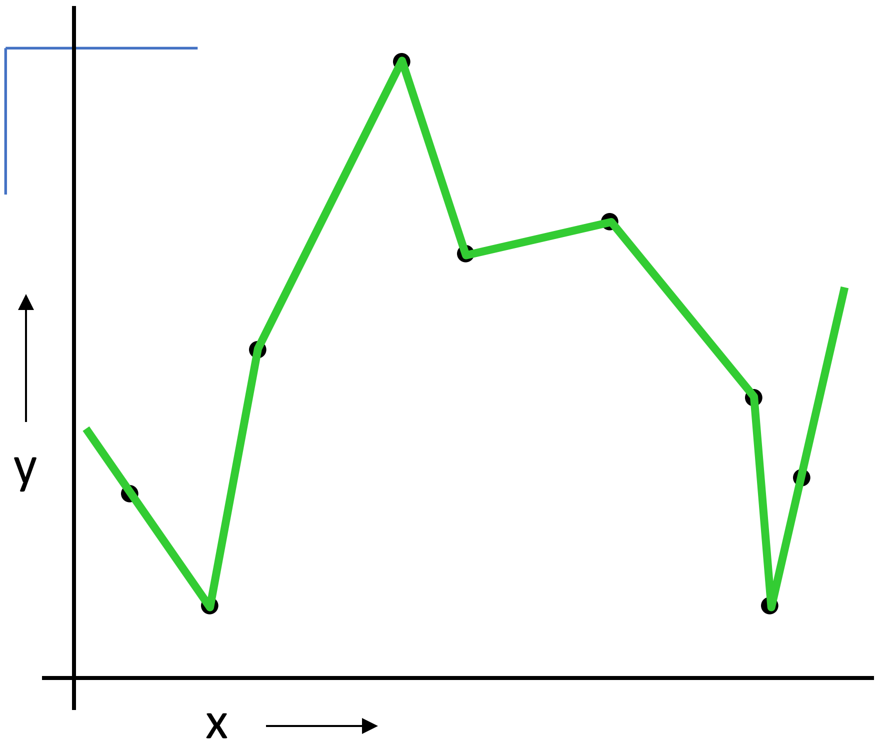
Linear Regression



Quadratic Regression

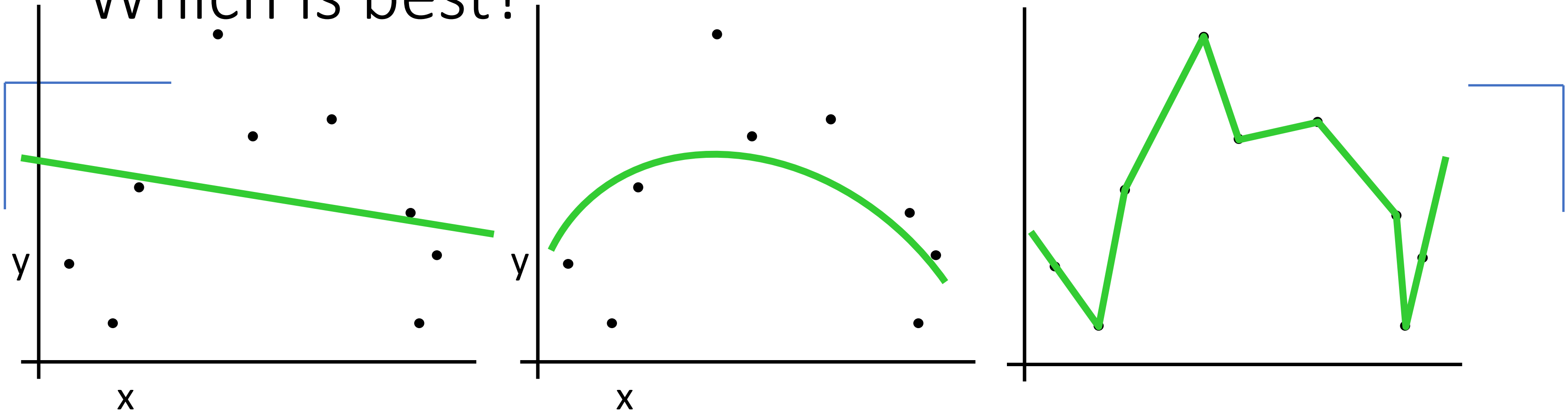


Join-the-dots



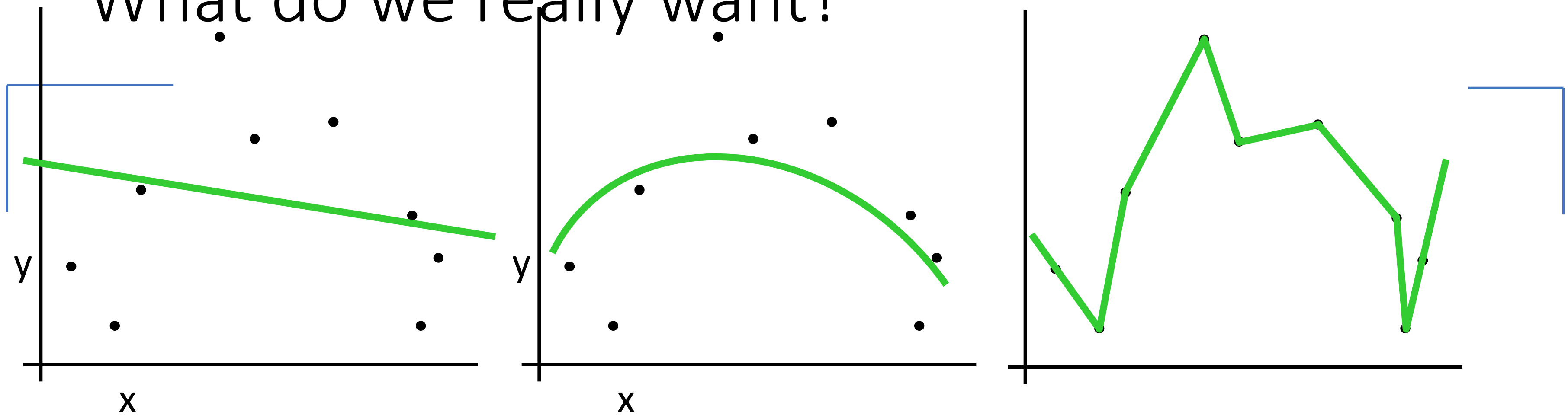
Also known as piecewise linear nonparametric regression if that makes you feel better

Which is best?



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

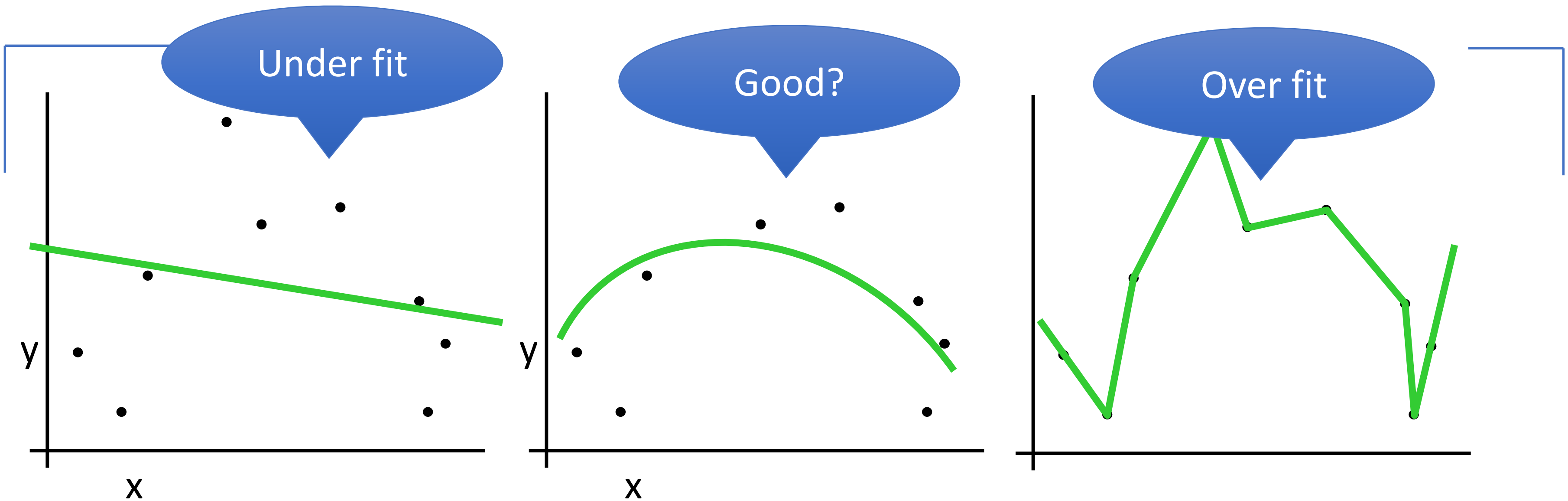
What do we really want?



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

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

What do we really want?



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

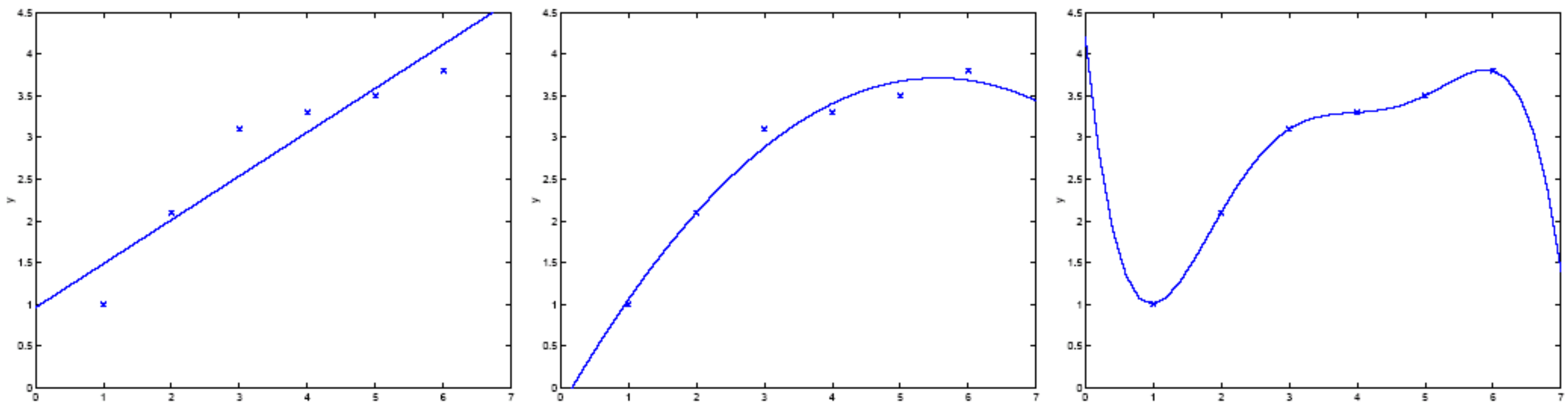
“How well are you going to predict future data drawn from the same distribution?”

Issue: Overfitting and underfitting

Under fit

Looks good

Over fit



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

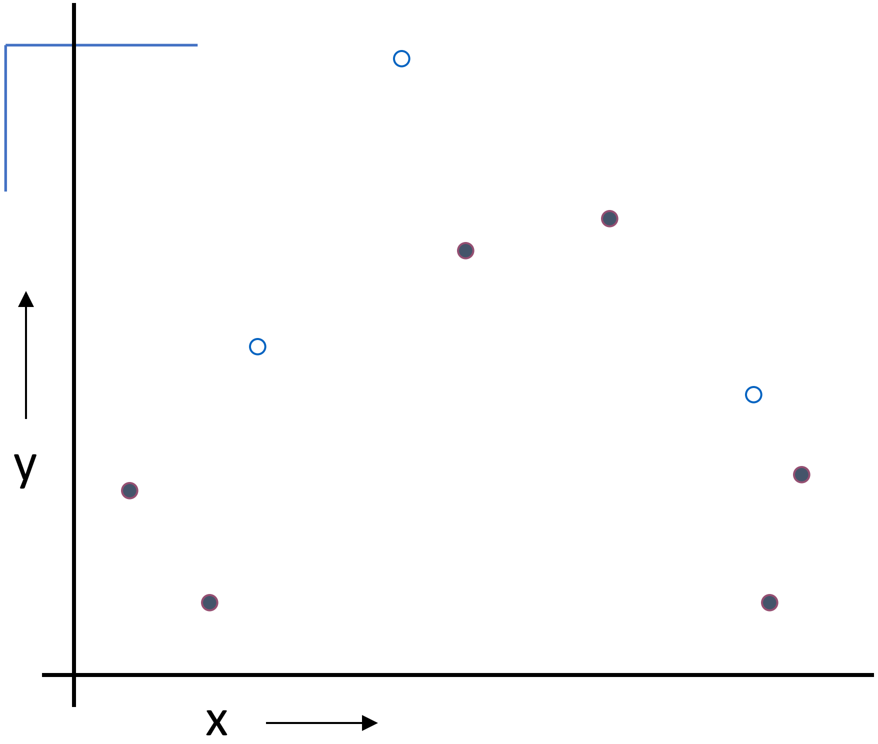
$$y = \theta_0 + \theta_1 x + \theta_2 x^2$$

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

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

K-fold Cross Validation / Train-Test /

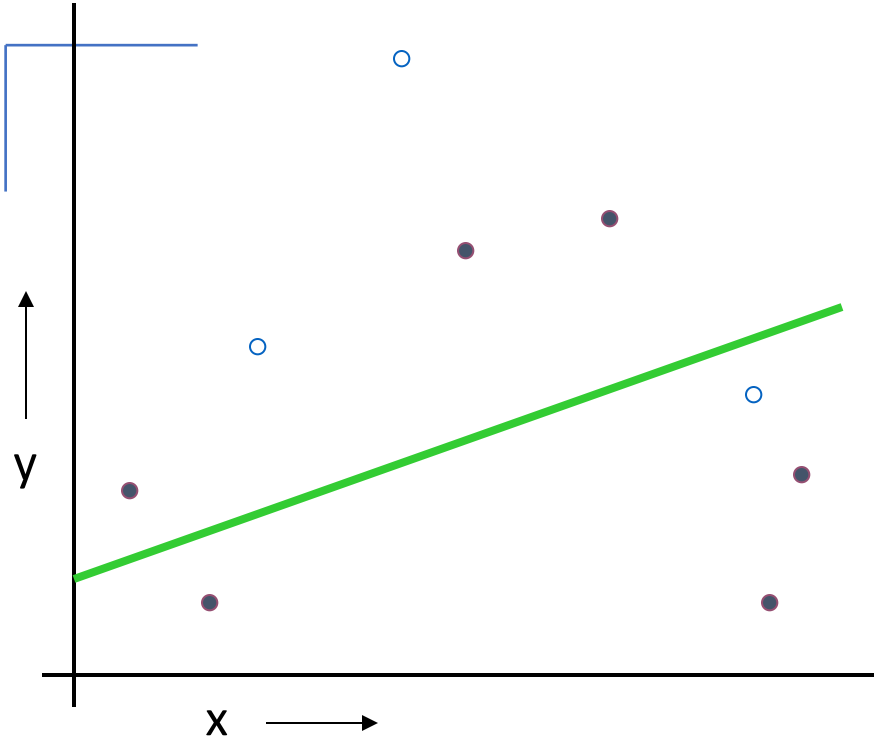
The test set method



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

Credit: Prof. Andrew Moore

The test set method



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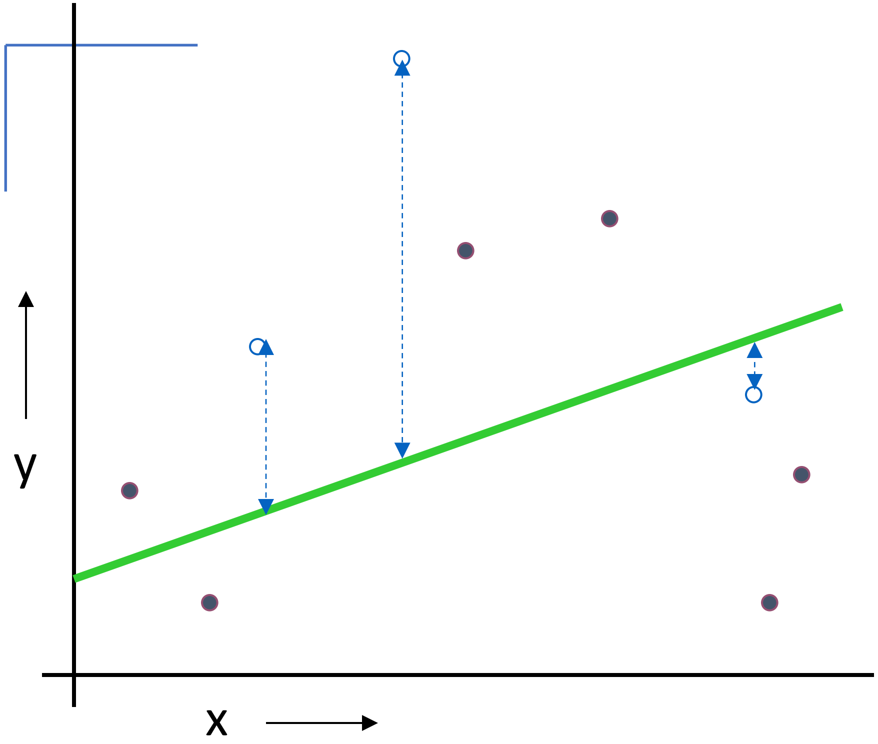
3. Perform your regression on the training set

(Linear regression example)

Credit: Prof. Andrew Moore

The test set method



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

(Linear regression example)
Mean Squared Error = 2.4

Credit: Prof. Andrew Moore

Evaluation:
e.g. train / test split as follows

training dataset

$$\mathbf{X}_{train} = \begin{bmatrix} -- & \mathbf{x}_1^T & -- \\ -- & \mathbf{x}_2^T & -- \\ \vdots & \vdots & \vdots \\ -- & \mathbf{x}_n^T & -- \end{bmatrix} \qquad \vec{y}_{train} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

test dataset

$$\mathbf{X}_{test} = \begin{bmatrix} -- & \mathbf{x}_{n+1}^T & -- \\ -- & \mathbf{x}_{n+2}^T & -- \\ \vdots & \vdots & \vdots \\ -- & \mathbf{x}_{n+m}^T & -- \end{bmatrix} \qquad \vec{y}_{test} = \begin{bmatrix} y_{n+1} \\ y_{n+2} \\ \vdots \\ y_{n+m} \end{bmatrix}$$

Testing MSE Error to report:

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

In Homework, when we ask for plots of training error, we ask for the MSE per-sample train errors; Because it is comparable to test MSE error.

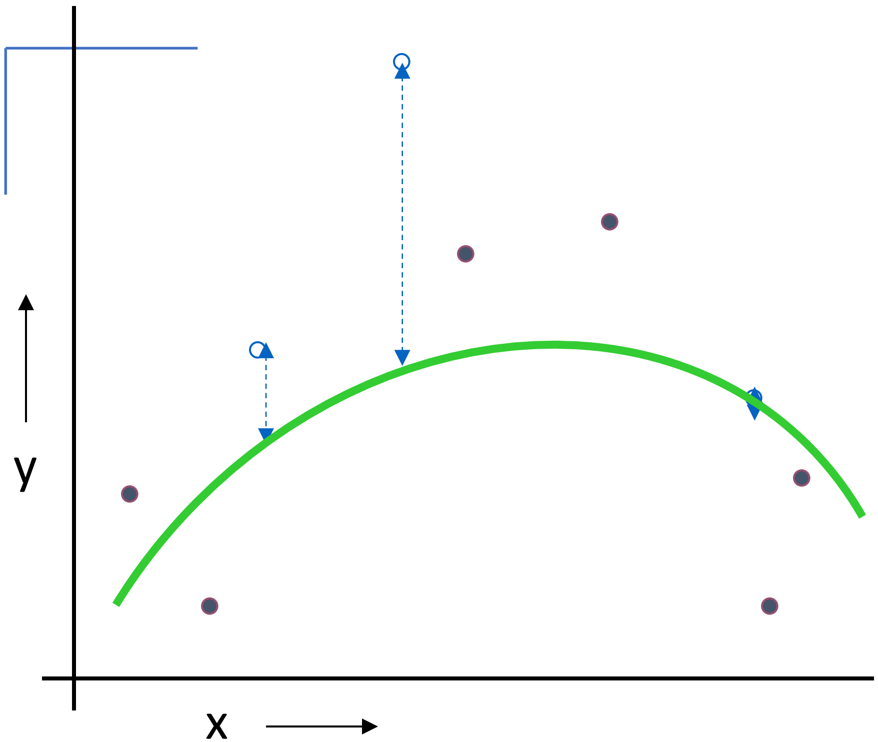
- Train MSE Error to observe:

$$J_{train-MSE} = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i{}^T\theta^* - y_i)^2$$

In many situations, visualizing Train-MSE can be helpful to understand the behavior of your method, e.g., the influence of the hyper parameter you chose……

In Homework, when we ask for plots of training error, we ask for the MSE per-sample train errors; Because it is comparable to test MSE error.

The test set method

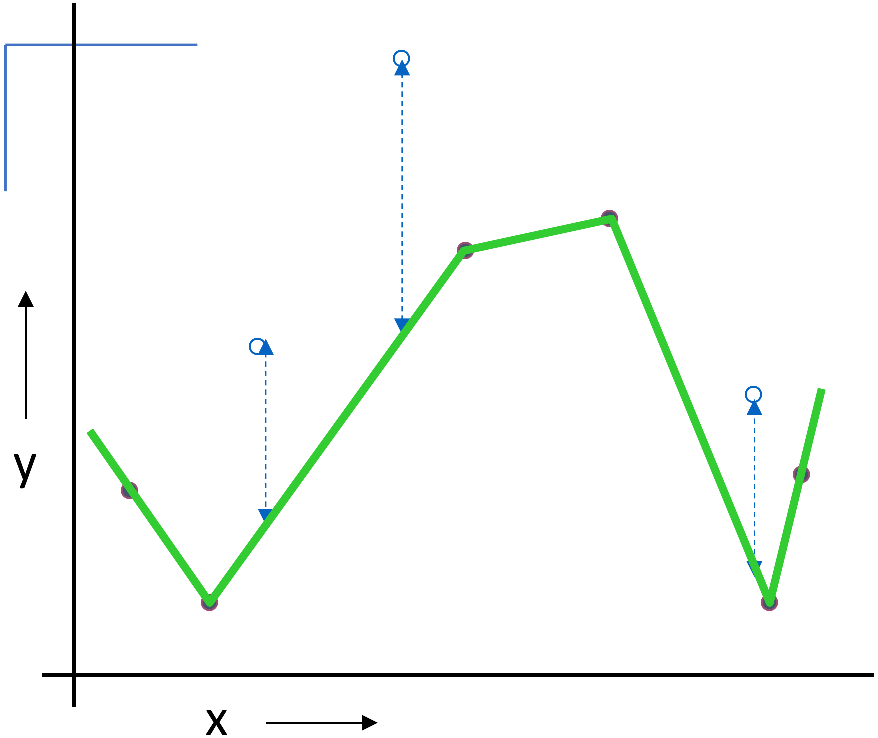


1. Randomly choose 30% of the data to be in a test set
2. The remainder is a training set
3. Perform your regression on the training set
4. Estimate your future performance with the test set

(Quadratic regression example)
Mean Squared Error = 0.9

Credit: Prof. Andrew Moore

The test set method



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

(Join the dots example)
Mean Squared Error = 2.2

Credit: Prof. Andrew Moore

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?

Credit: Prof. Andrew Moore

The test set method

Good news:

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

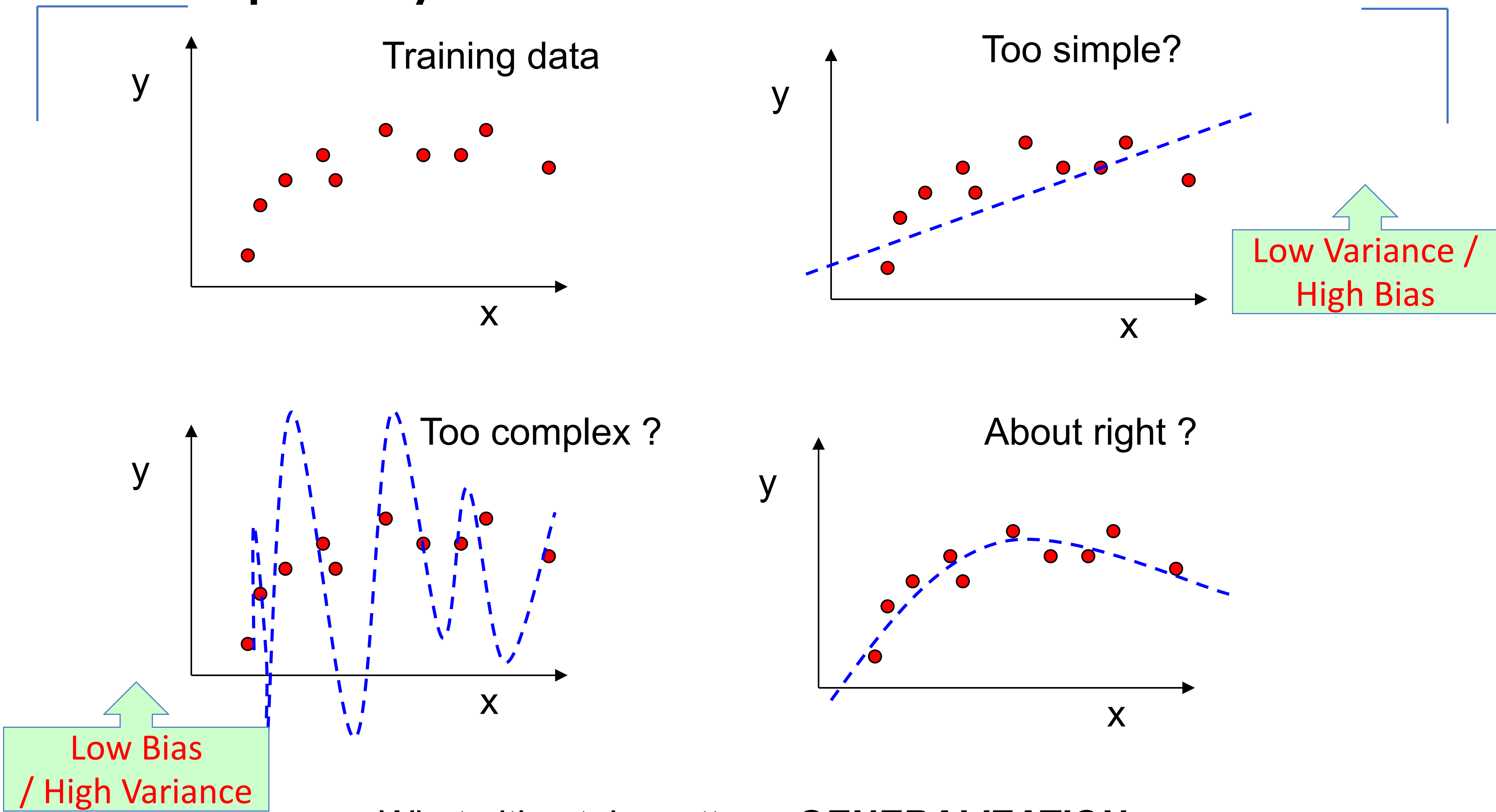
Bad news:

- 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"

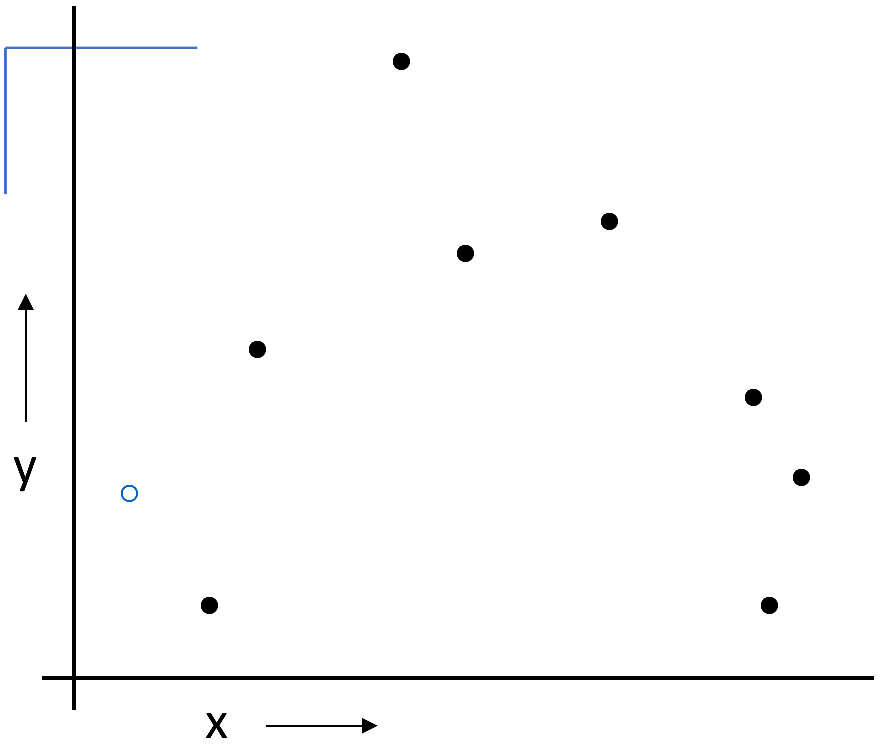
Credit: Prof. Andrew Moore

Regression: Complexity versus Goodness of Fit



What ultimately matters: ***GENERALIZATION***

LOOCV (Leave-one-out Cross Validation)

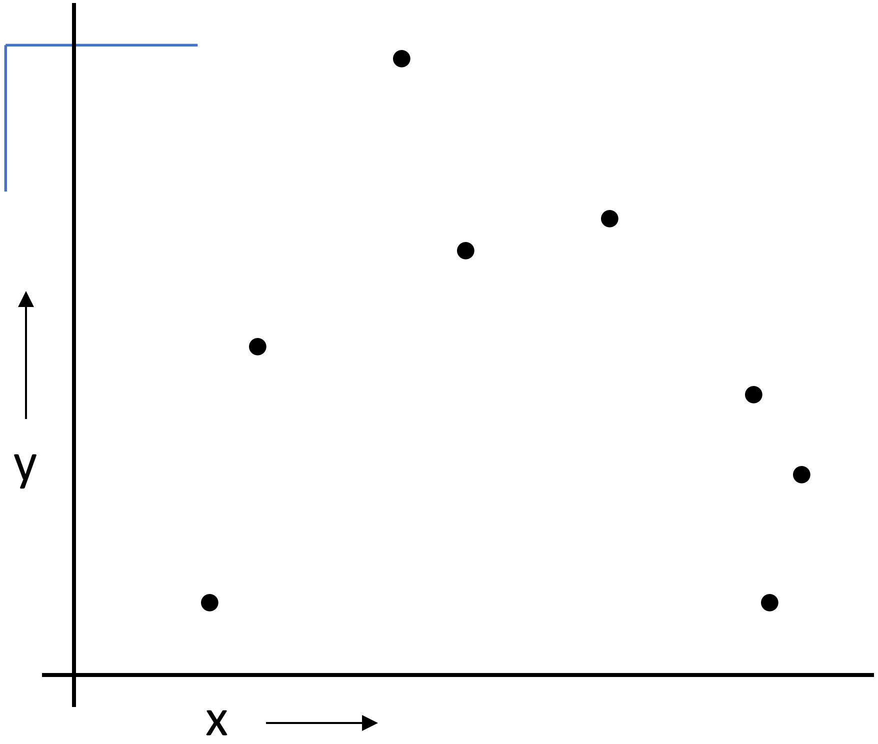


For k=1 to n

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

Credit: Prof. Andrew Moore

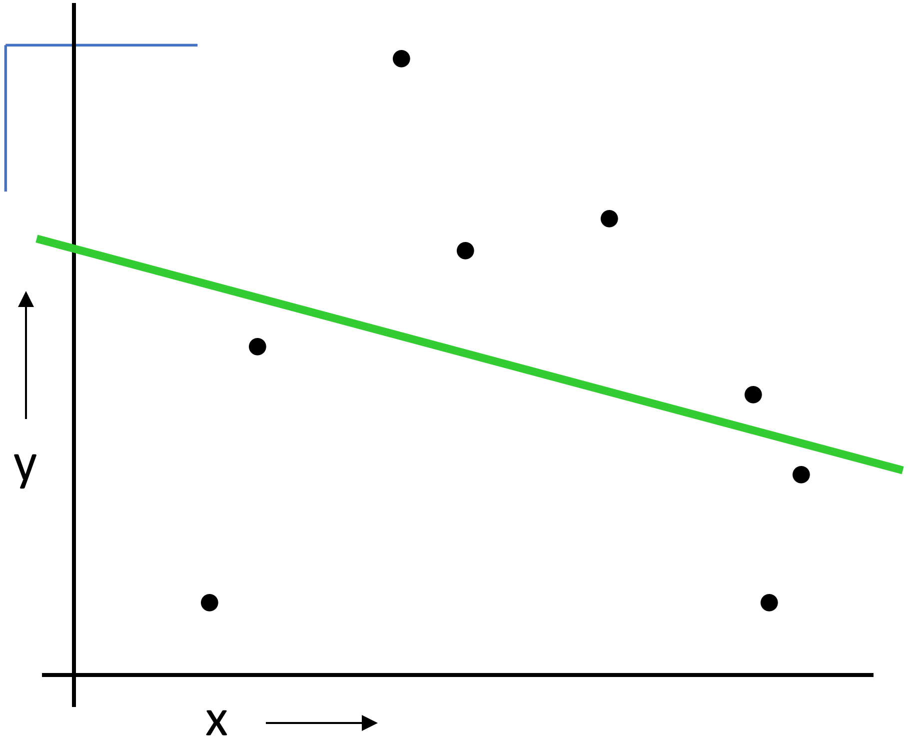
LOOCV (Leave-one-out Cross Validation)



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)

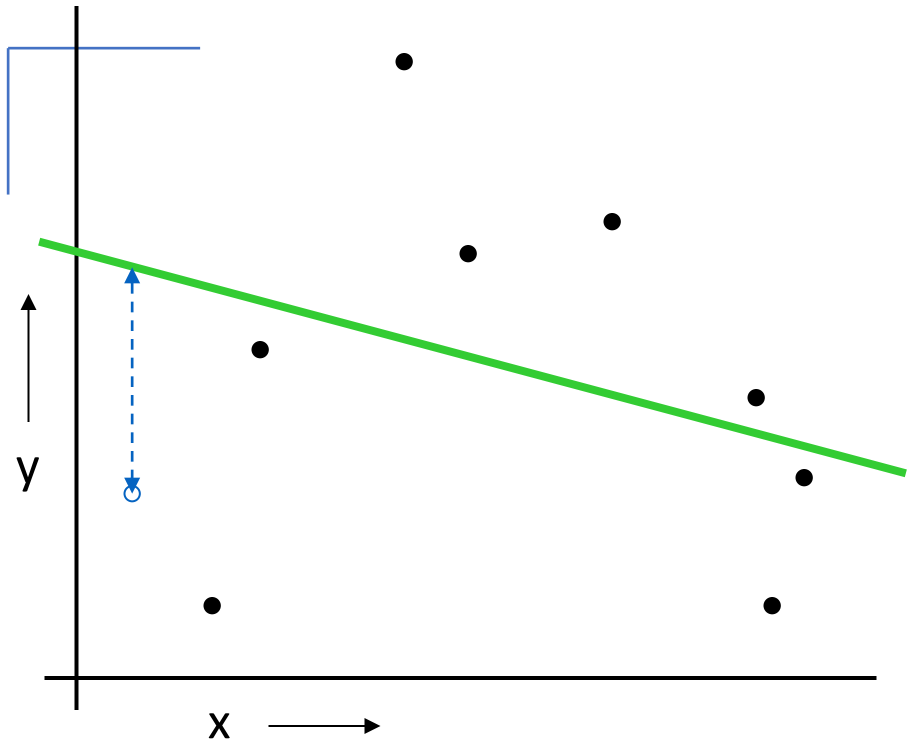


For k=1 to n

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 R-1 datapoints

Credit: Prof. Andrew Moore

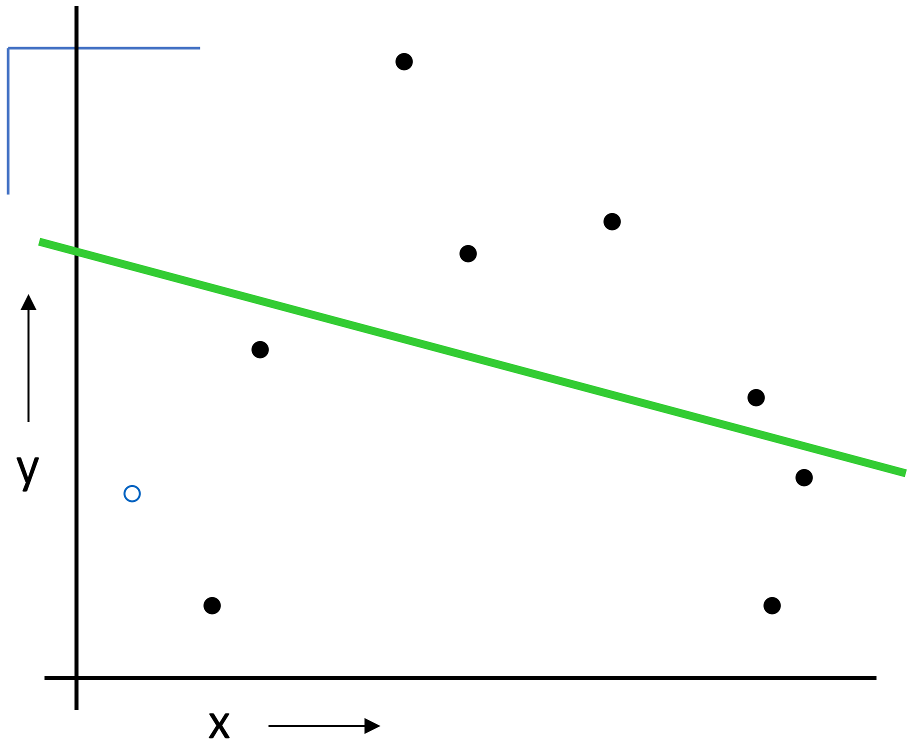
LOOCV (Leave-one-out Cross Validation)



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)

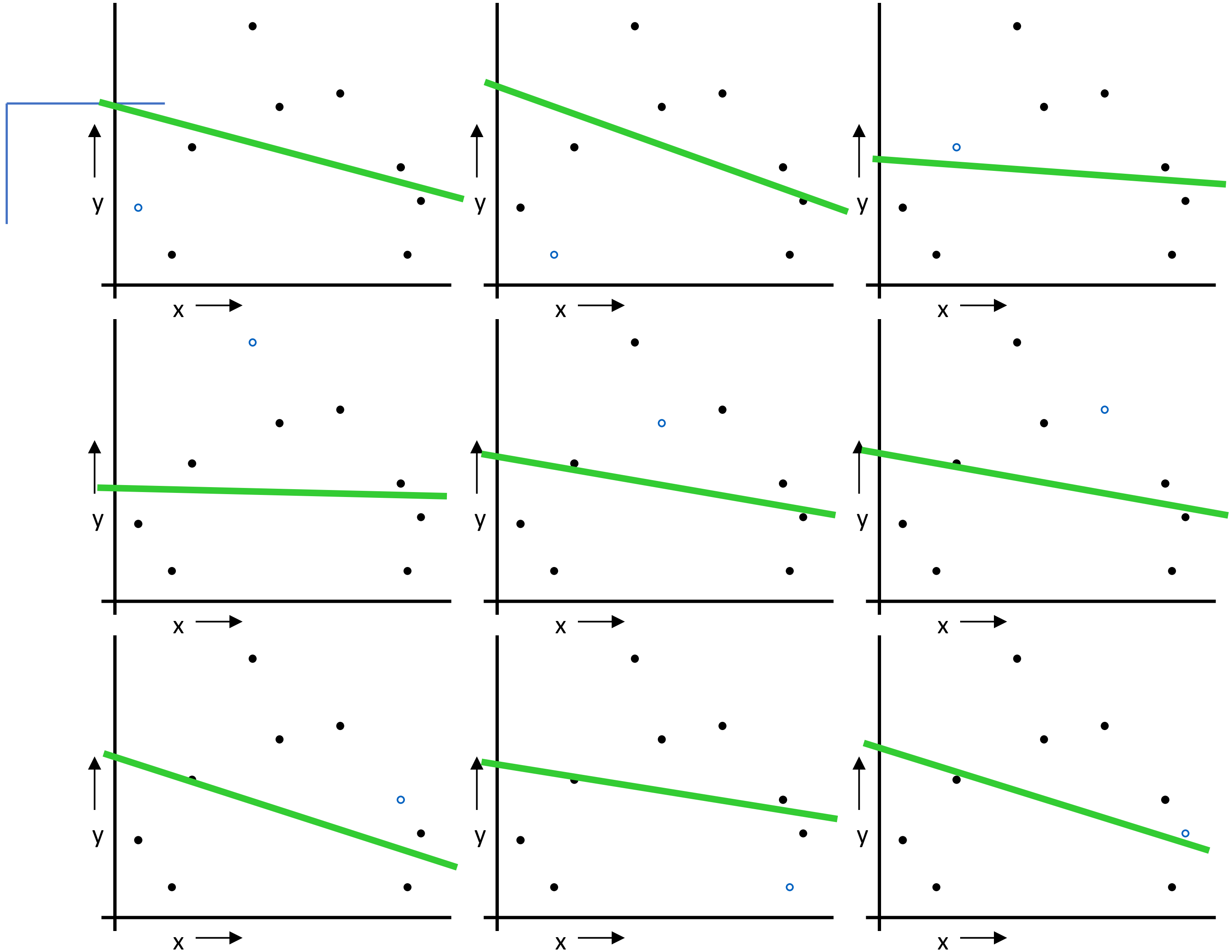


For k=1 to R

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 (Leave-one-out Cross Validation)



For k=1 to n

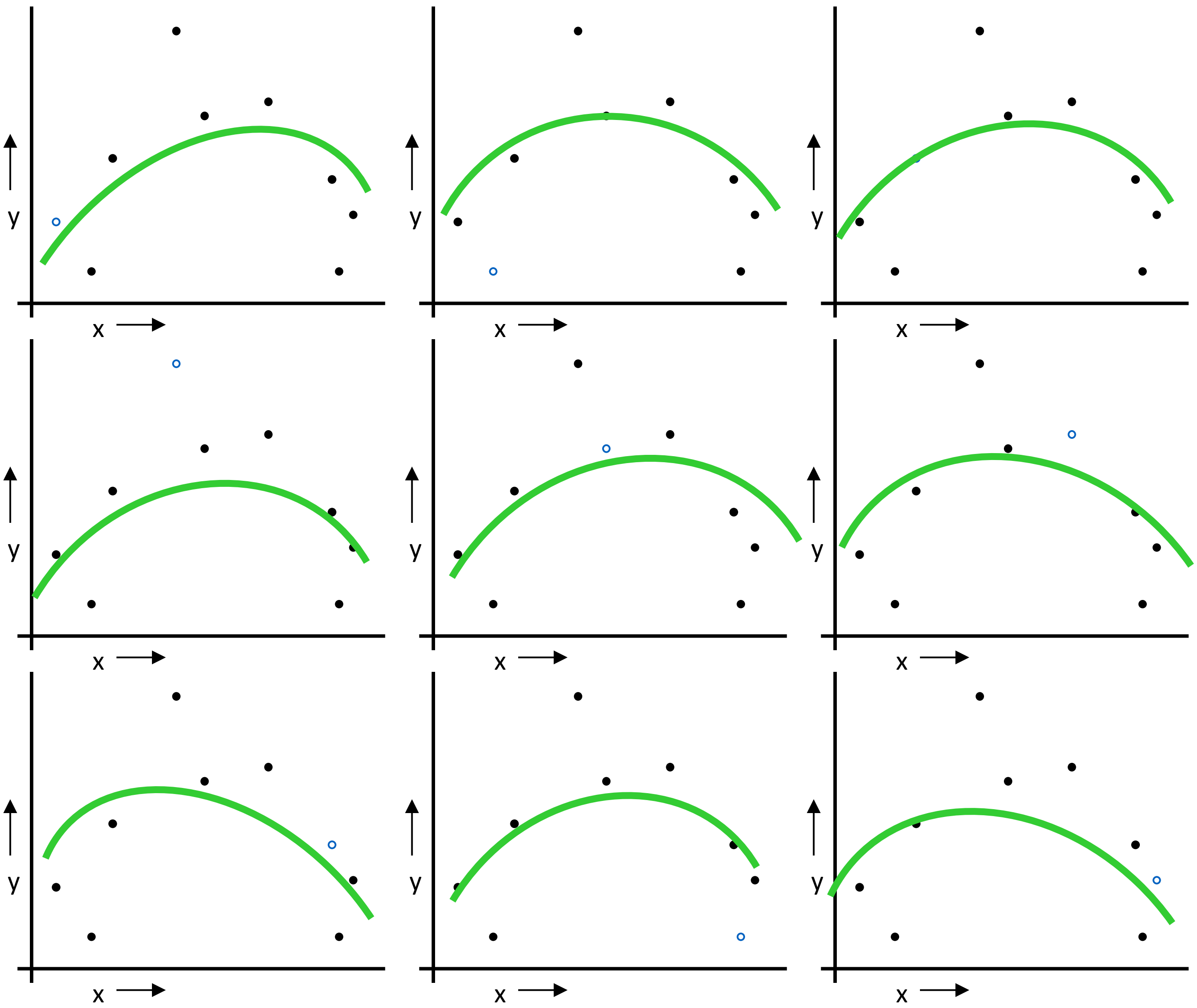
1. Let (x_k, y_k) be the k^{th} record
2. Temporarily remove (x_k, y_k) from the dataset
3. Train on the remaining R-1 datapoints
4. Note your error (x_k, y_k)

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

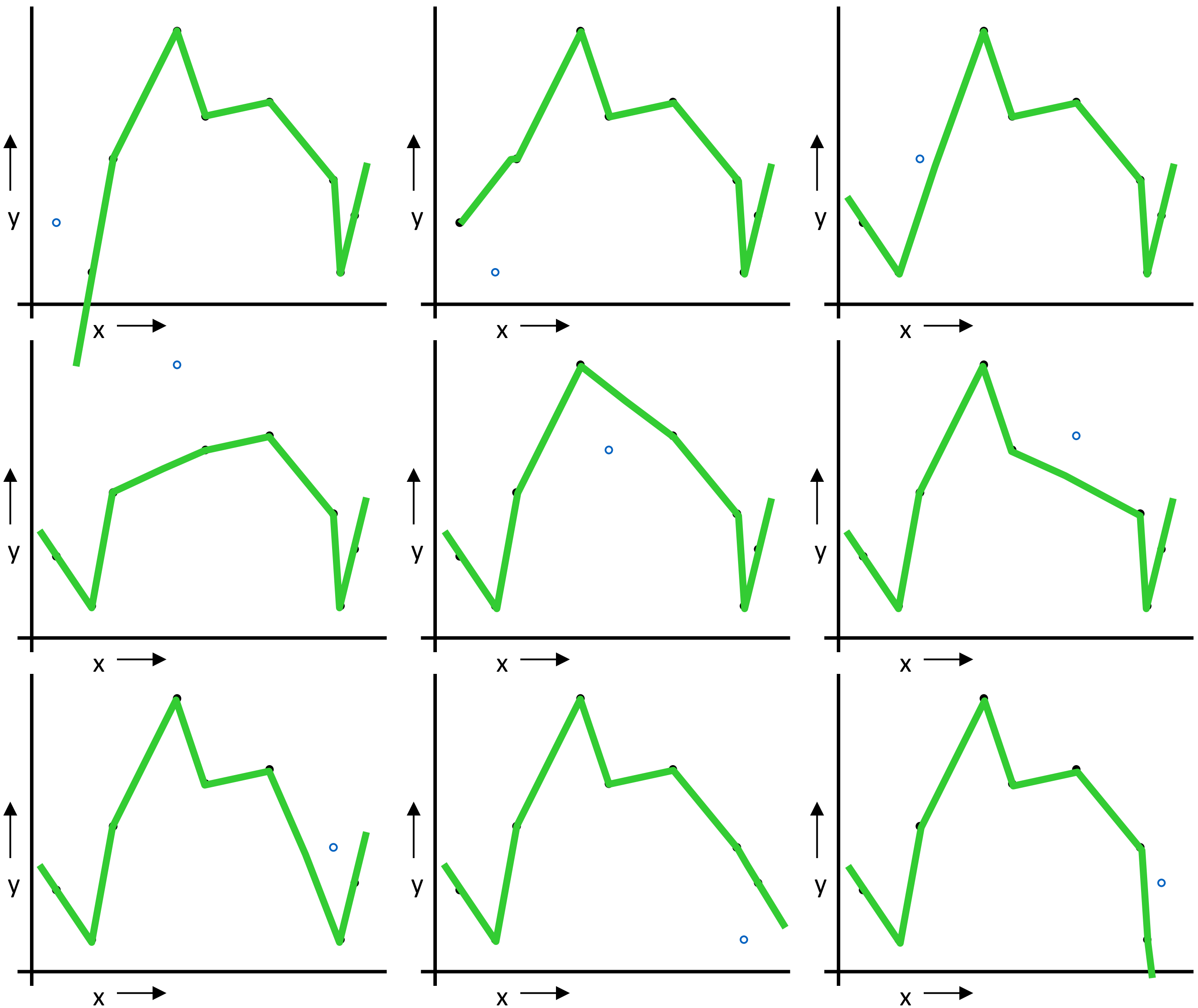
1. Let (x_k, y_k) be the k^{th} record
2. Temporarily remove (x_k, y_k) from the dataset
3. Train on the remaining R-1 datapoints
4. Note your error (x_k, y_k)

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 R-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**
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?

Credit: Prof. Andrew Moore

Make sure that the train/test/validation folds are indeed independent samples.

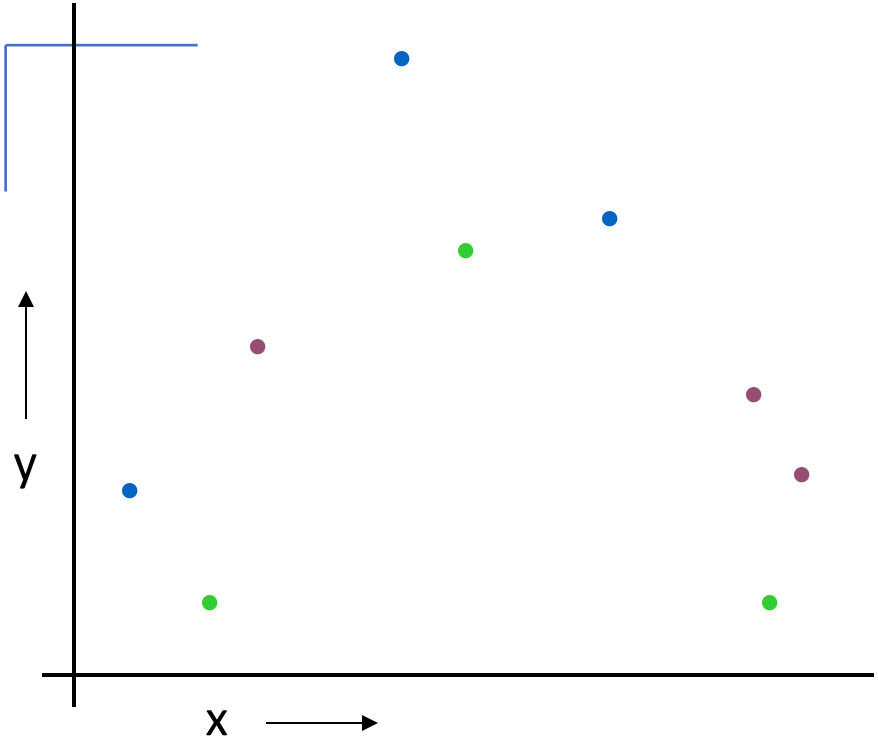
e.g. By k=10 fold Cross Validation

- Divide data into 10 equal pieces
- 9 pieces as training set, the rest 1 as test set
- Collect the scores from the diagonal
- 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

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)

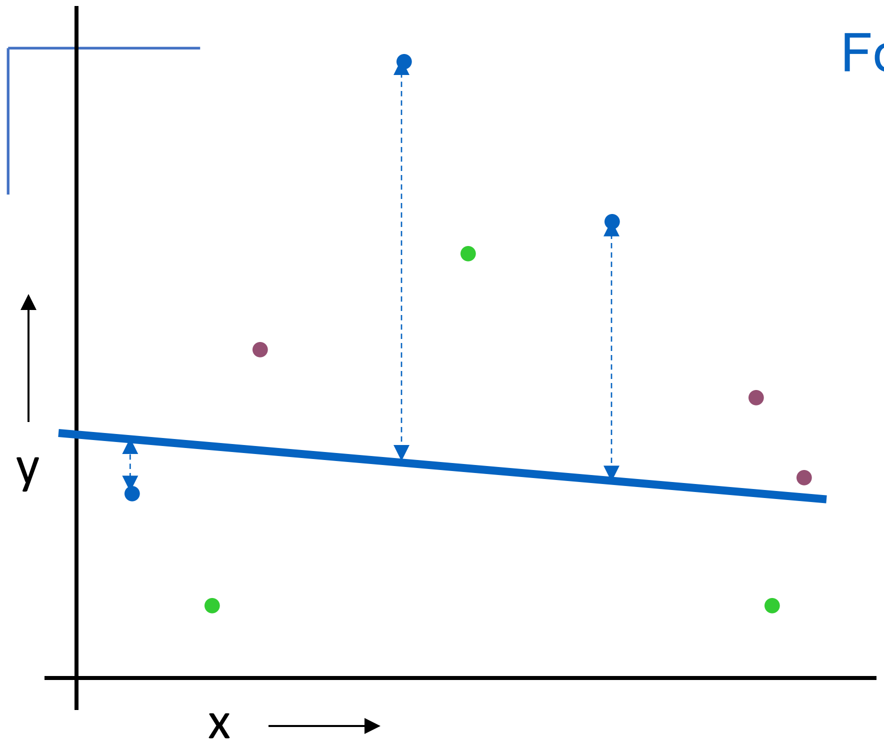


Credit: Prof. Andrew Moore

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)

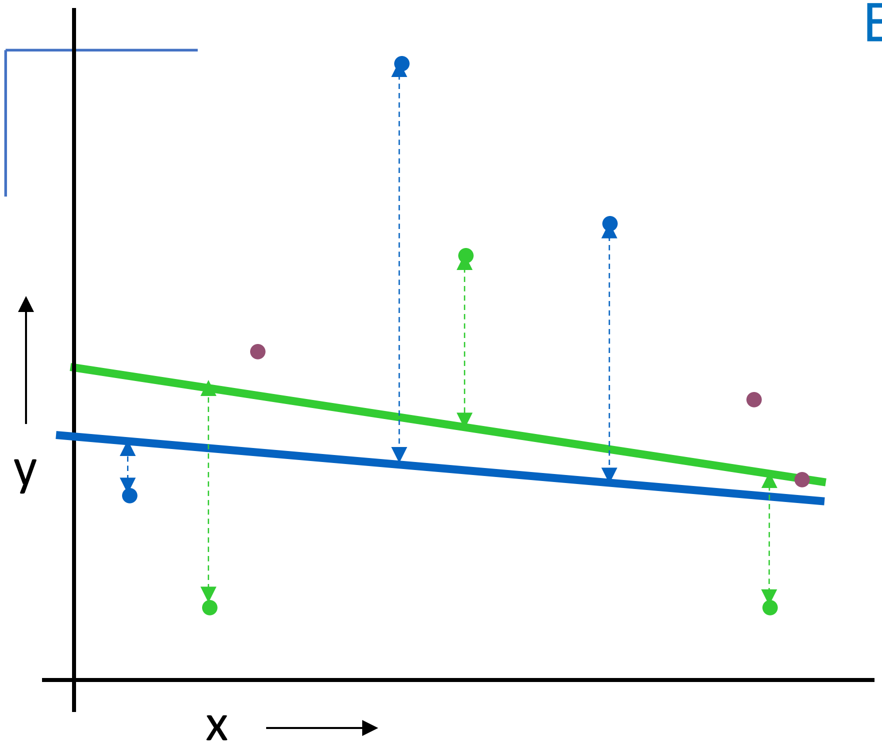
For the blue partition: Train on all the points not in the blue partition. Find the test-set sum of errors on the blue points.



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)

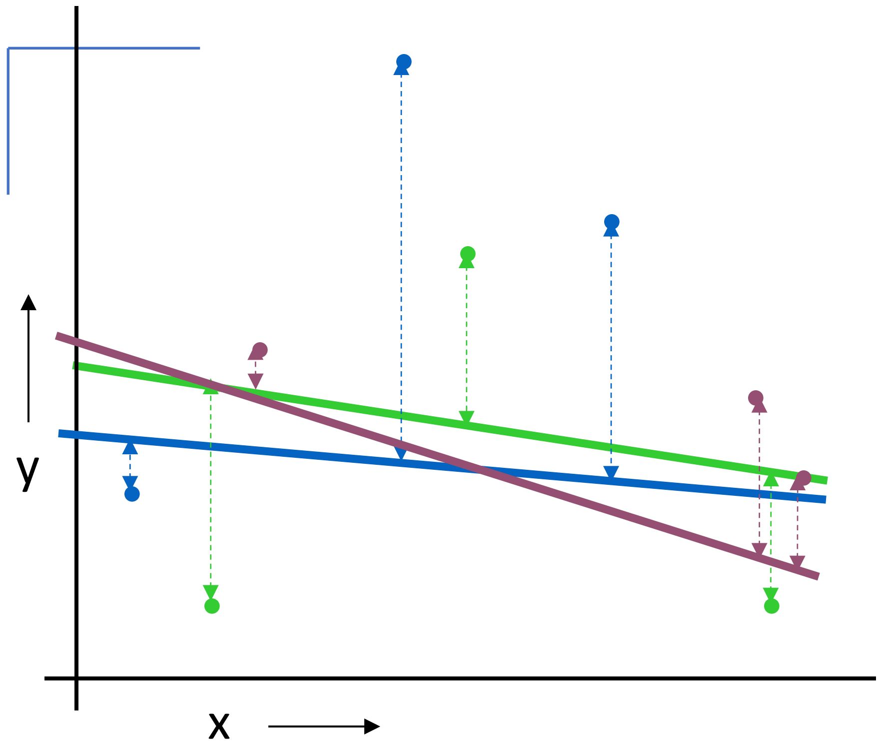


For the red partition: Train on all the points not in the red partition. Find the test-set sum of errors on the red points.

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.

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)

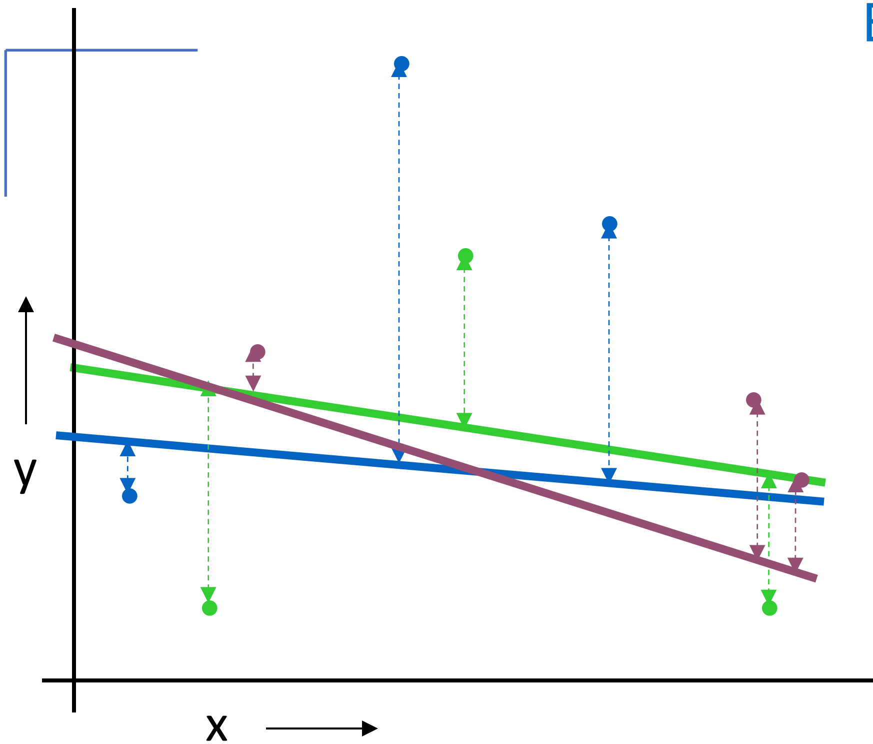
For the red partition: Train on all the points not in the red partition. Find the test-set sum of errors on the red points.

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.

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

Credit: Prof. Andrew Moore

k-fold Cross Validation



Linear Regression $MSE_{3FOLD}=2.05$

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

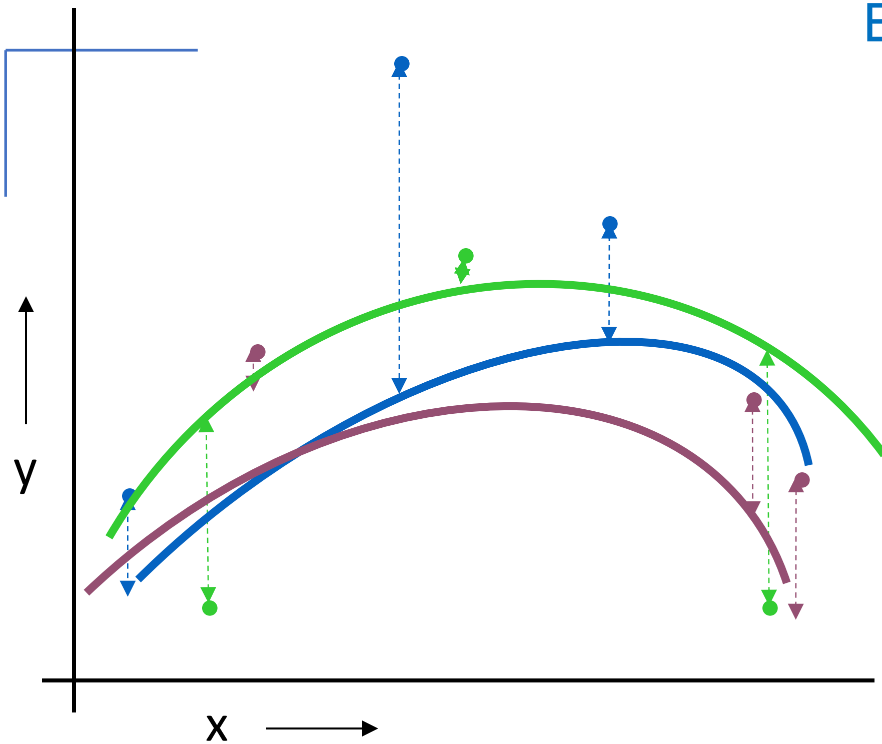
- For the red partition: Train on all the points not in the red partition. Find the test-set sum of errors on the red points.
- For the green partition: Train on all the points not in the green partition. Find the test-set sum of errors on the green points.
- For the purple partition: Train on all the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

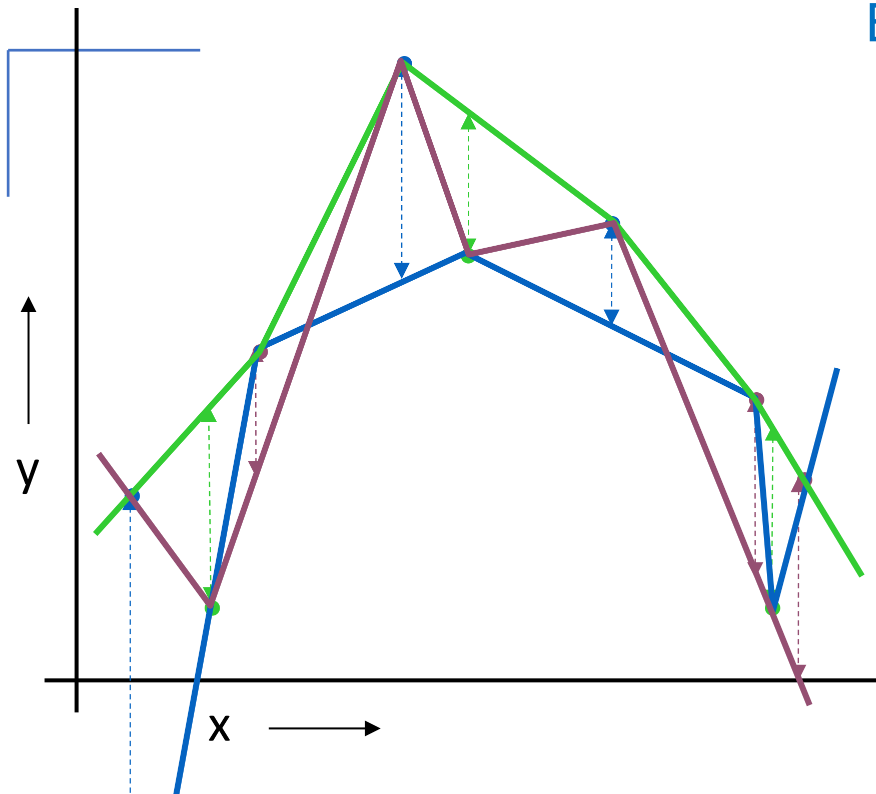
For the green partition: Train on all the points not in the green partition. Find the test-set sum of errors on the green points.

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

Then report the mean error

Credit: Prof. Andrew Moore

k-fold Cross Validation



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

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 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.
- 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

Credit: Prof. Andrew Moore

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	better than test-set
n-fold	Identical to Leave-one-out	

CV-based Model Selection

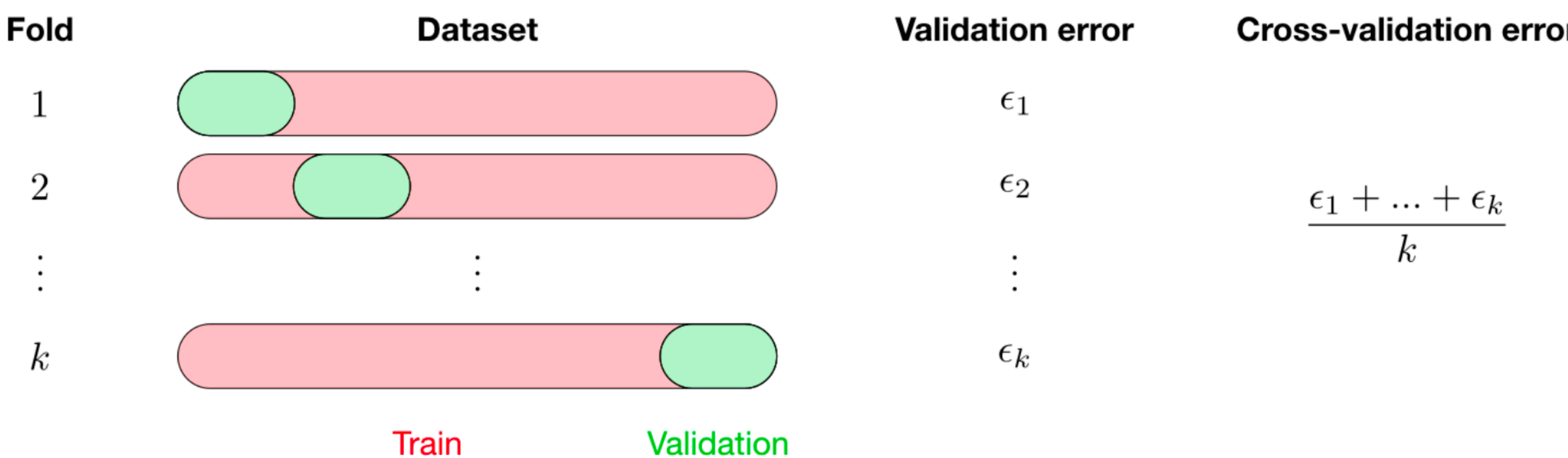
- We're trying to decide which algorithm to use.
- We train each machine and make a table…

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

Credit: Prof. Andrew Moore

k-fold	Leave-p-out
- Training on $k-1$ folds and assessment on the remaining one - Generally $k=5$ or 10	- Training on $n-p$ observations and assessment on the p remaining ones - Case $p=1$ is called leave-one-out

The most commonly used method is called k-fold cross-validation and splits the training data into k folds to validate the model on one fold while training the model on the $k-1$ other folds, all of this k times. The error is then averaged over the k folds and is named cross-validation error.



Credit: Stanford Machine Learning course

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