Reminder:
Multiple Linear Regression

Test-train data split to avoid overfitting

Multiple Linear Regression Model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \ldots \beta_k x_k + \varepsilon$$

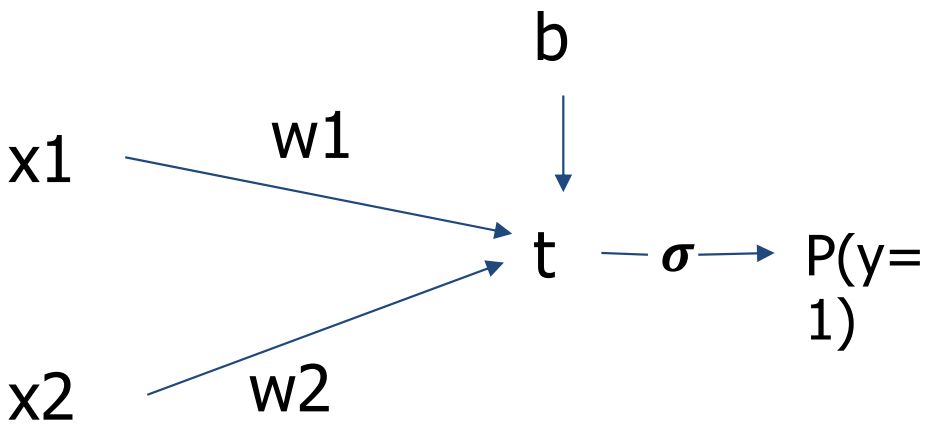
One can also use powers and products of other variables or even non-linear functions like $\exp(x_i)$ or $\log(x_i)$ instead of $x_3, \ldots x_k$.

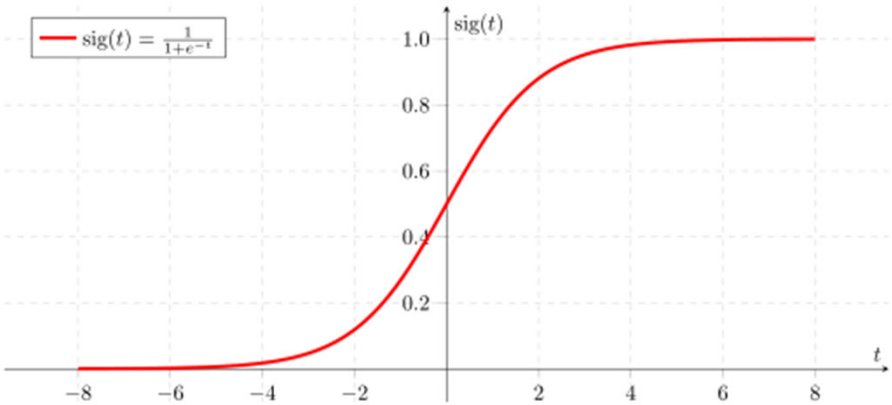
Example: the general two-variable quadratic regression has 6 constants:

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 (x_1)^2 + \beta_4 (x_2)^2 + \beta_5 (x_1 x_2) + \varepsilon$$

Logistic Regression

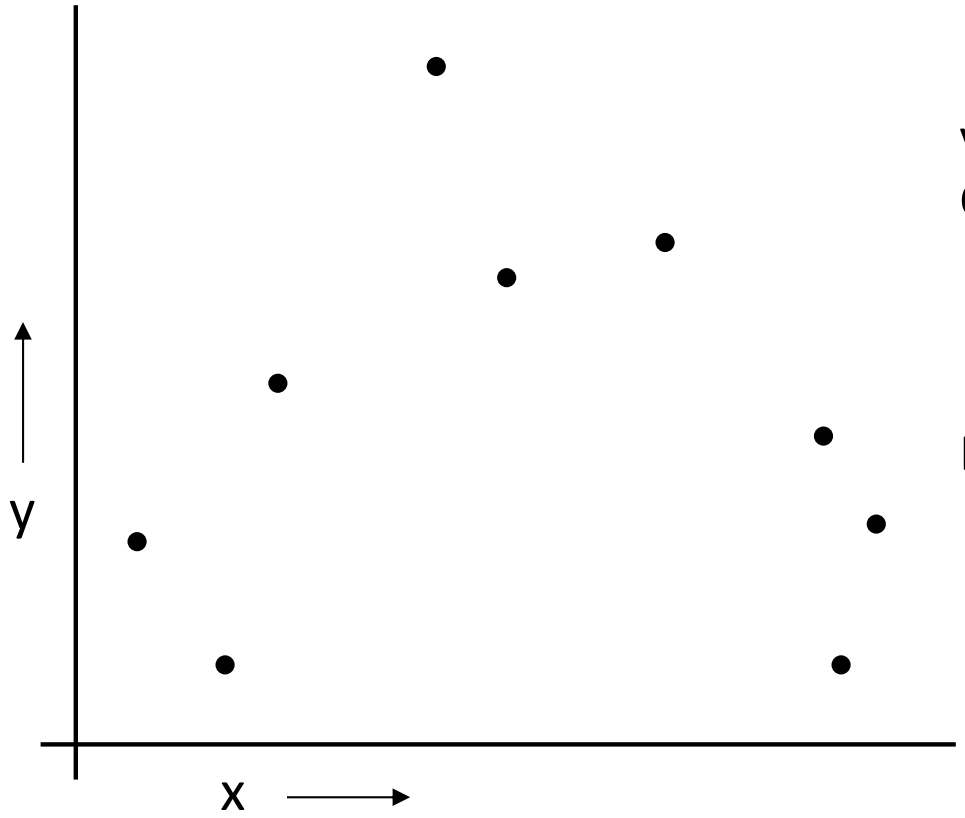
$$P(y=1) = \sigma(x1*w1 + x2*w2 + b)$$





How to know when to stop
adding new variables
or model parameters
in any data fitting algorithm such as
multiple linear regression?

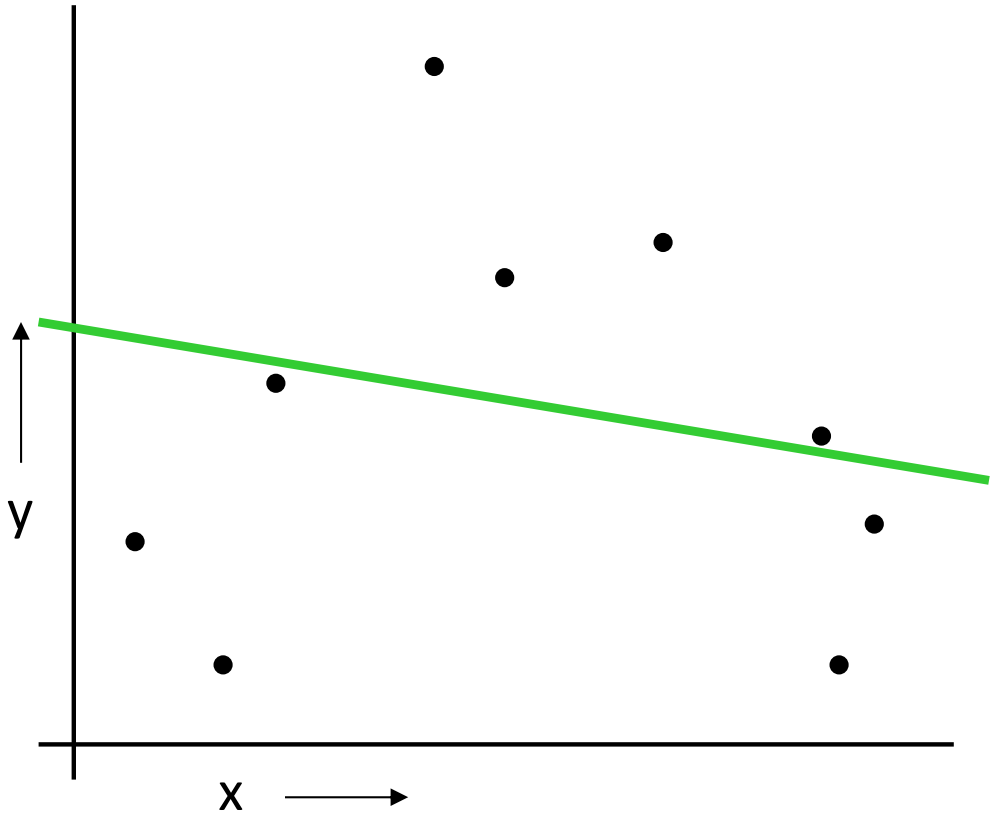
A Regression Problem



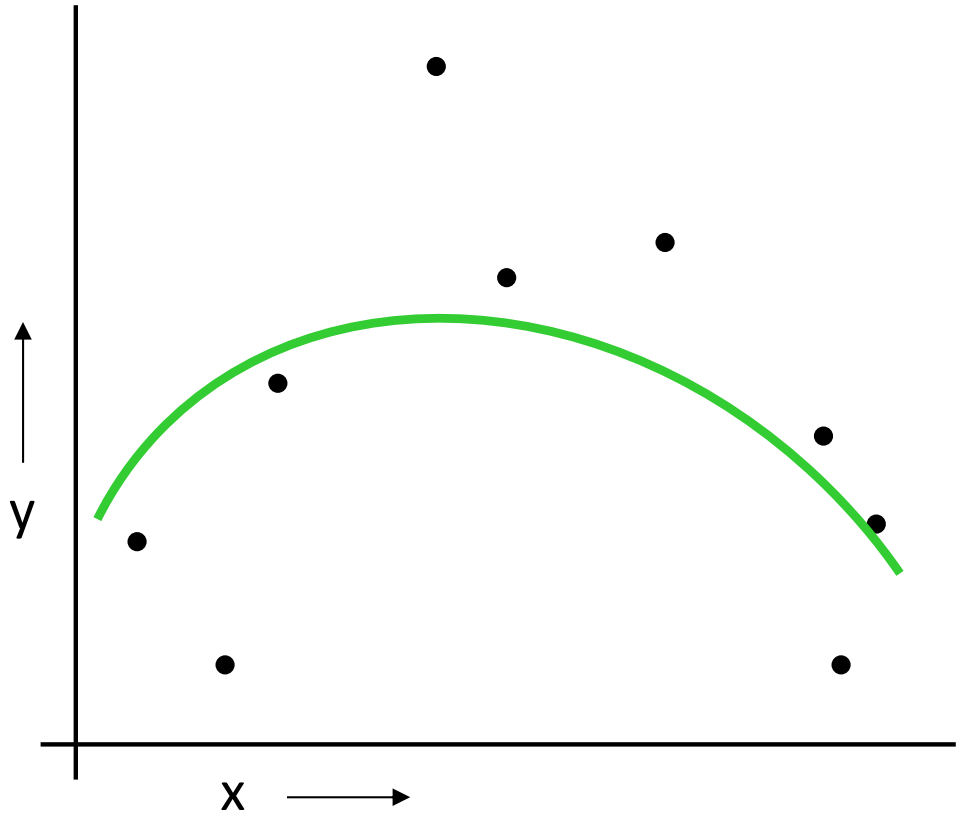
y = f(x) + noise
Can we learn f from this data?

Let's consider three methods…

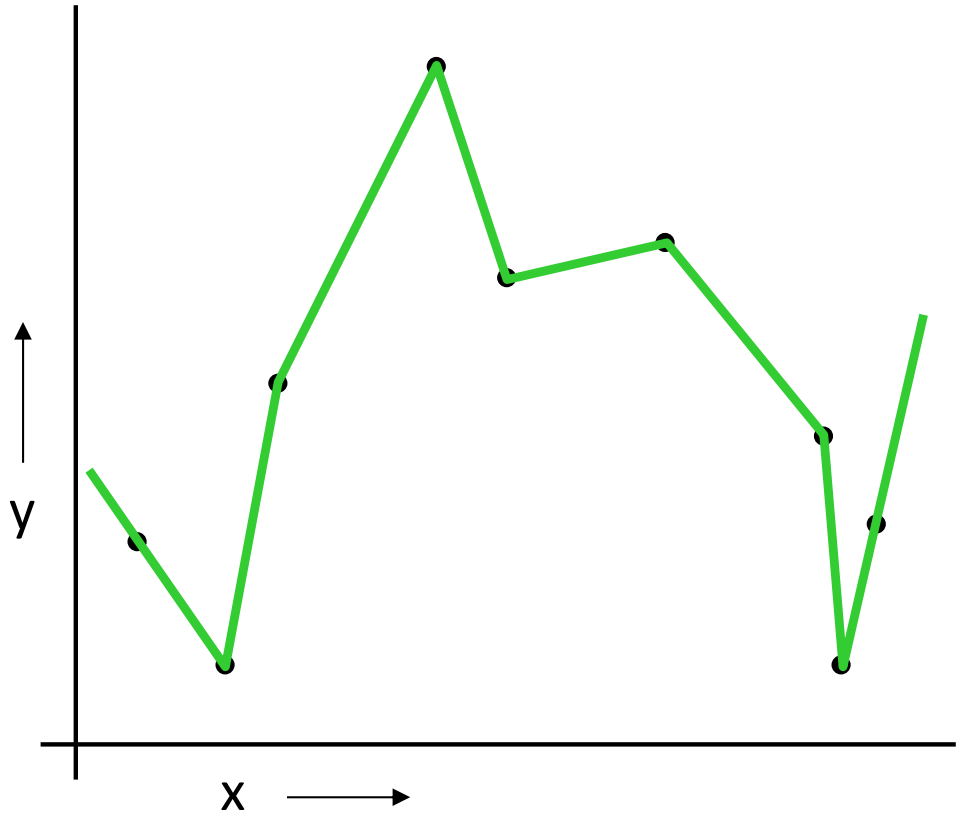
Single Variable Linear Regression



2-variable Linear Regression with x and x^2

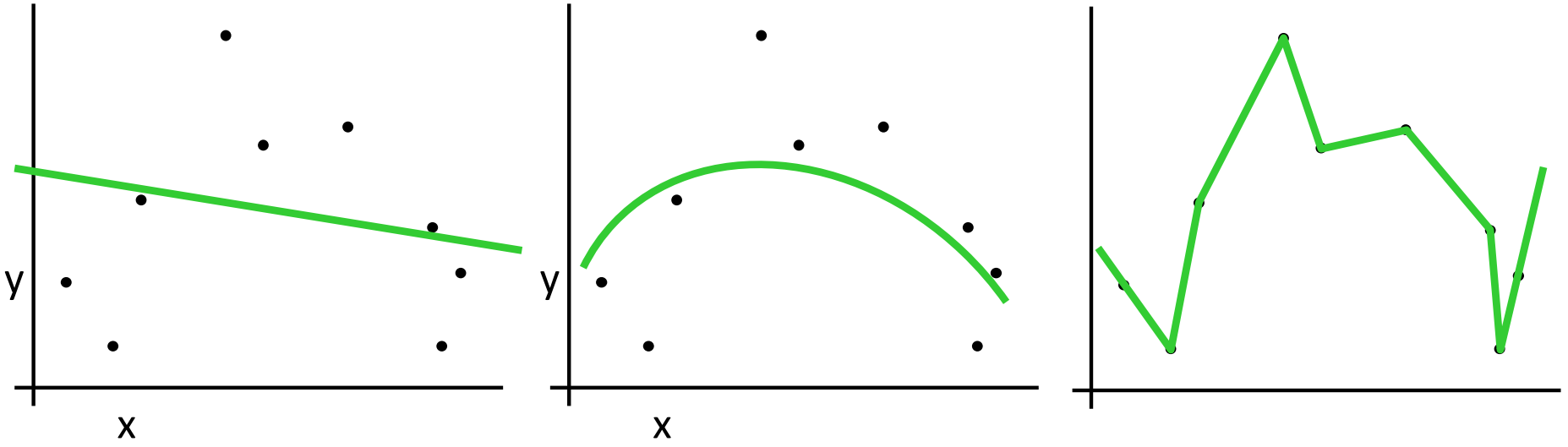


Join-the-dots



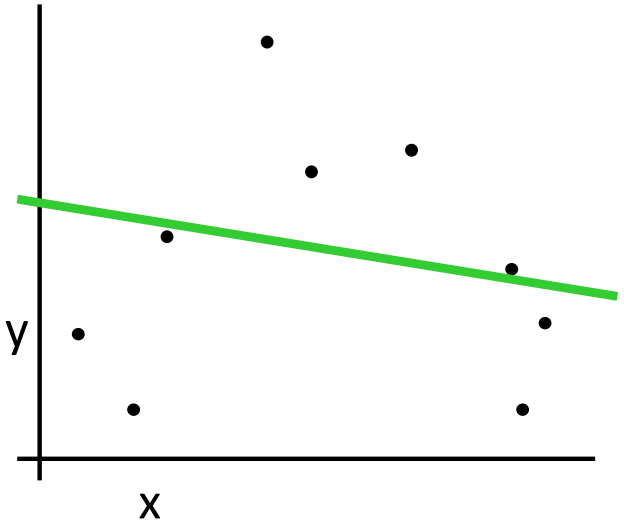
Also known as piecewise linear nonparametric regression if that makes you feel better

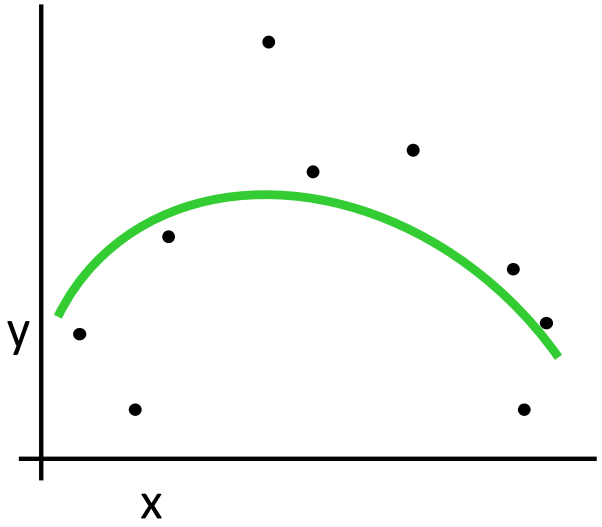
Which is best?

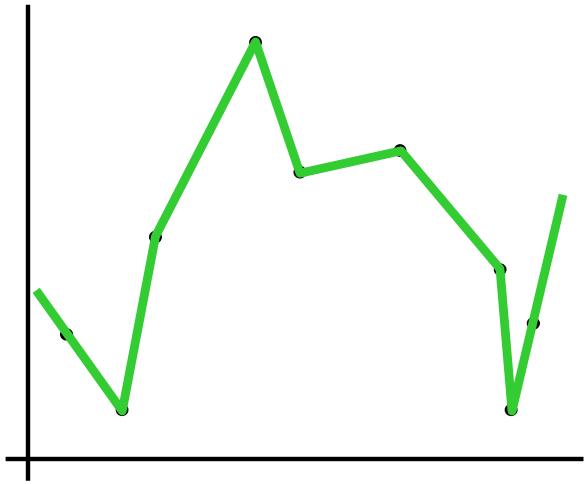


Why not choose the method with the best fit to the data?

What do we really want?



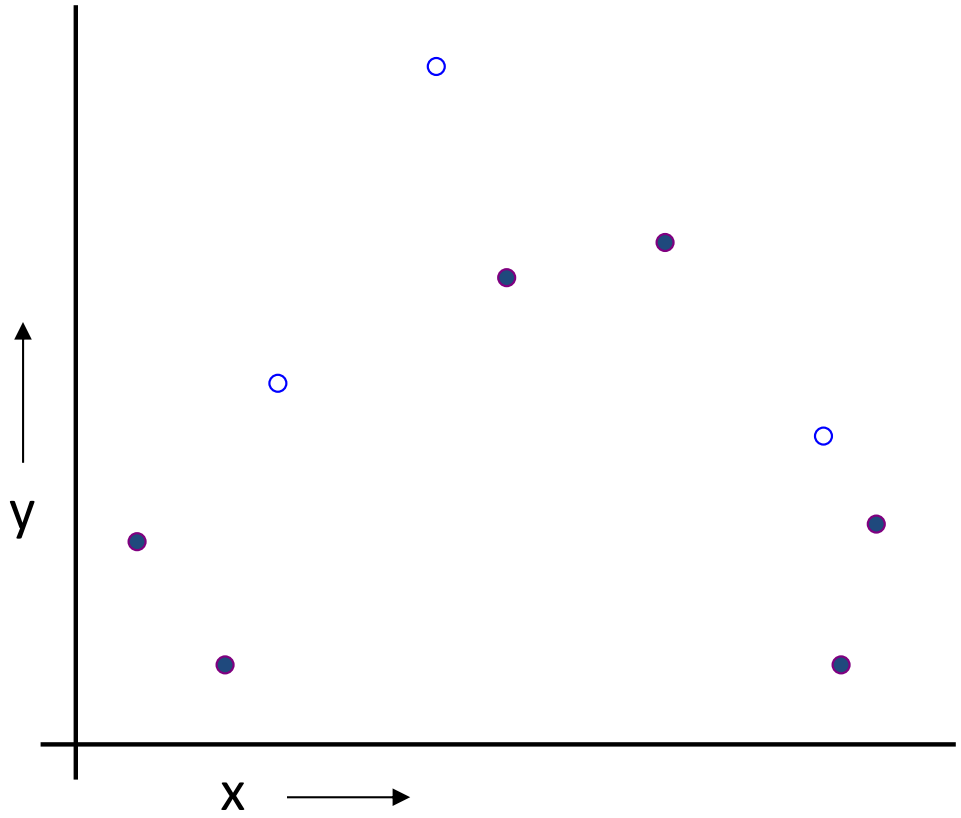




Why not choose the method with the best fit to the data?

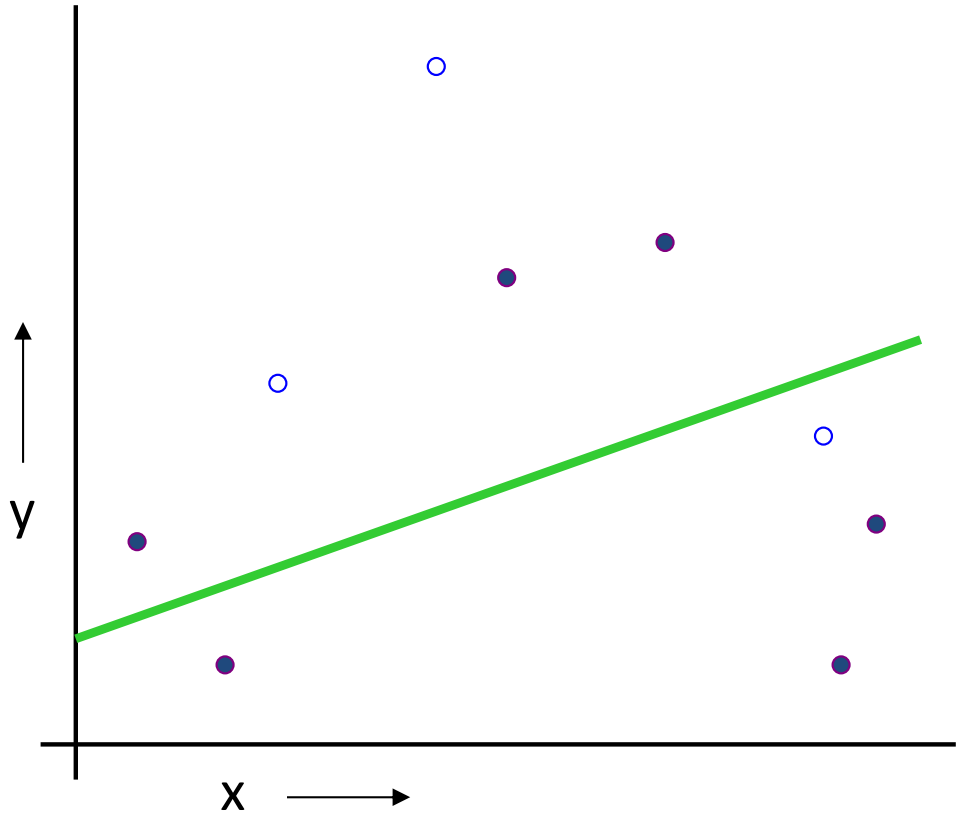
"How well are you going to predict future data drawn from the same distribution?"

The test set method



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

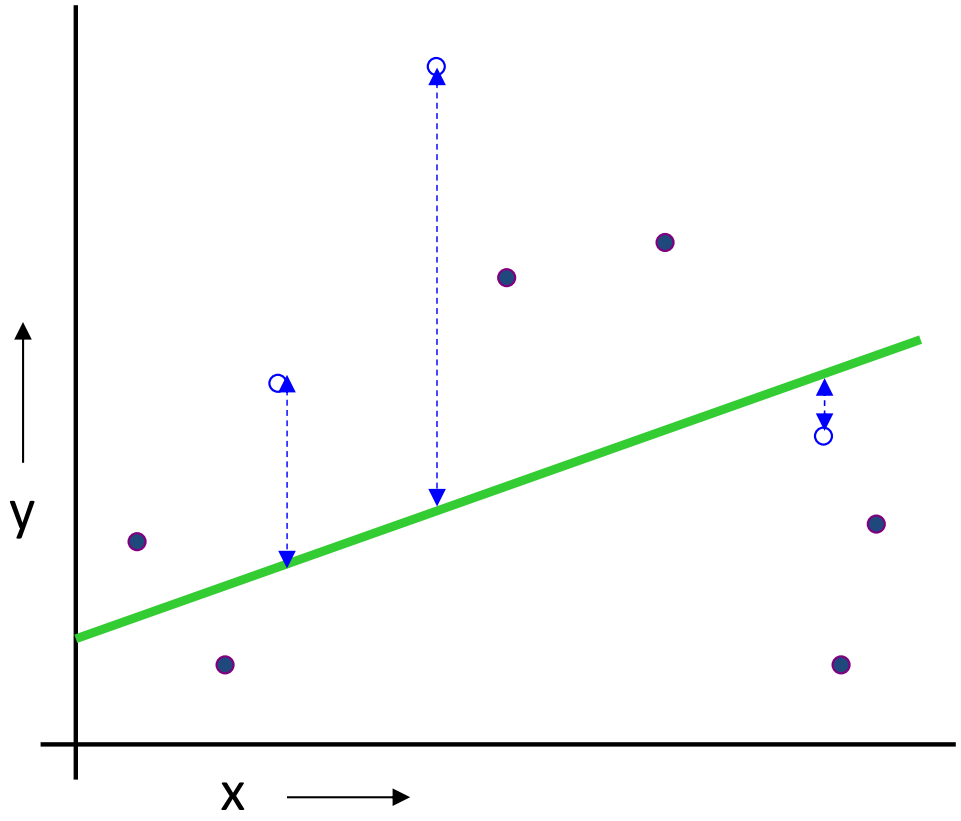
The test set method



(Linear regression example)

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

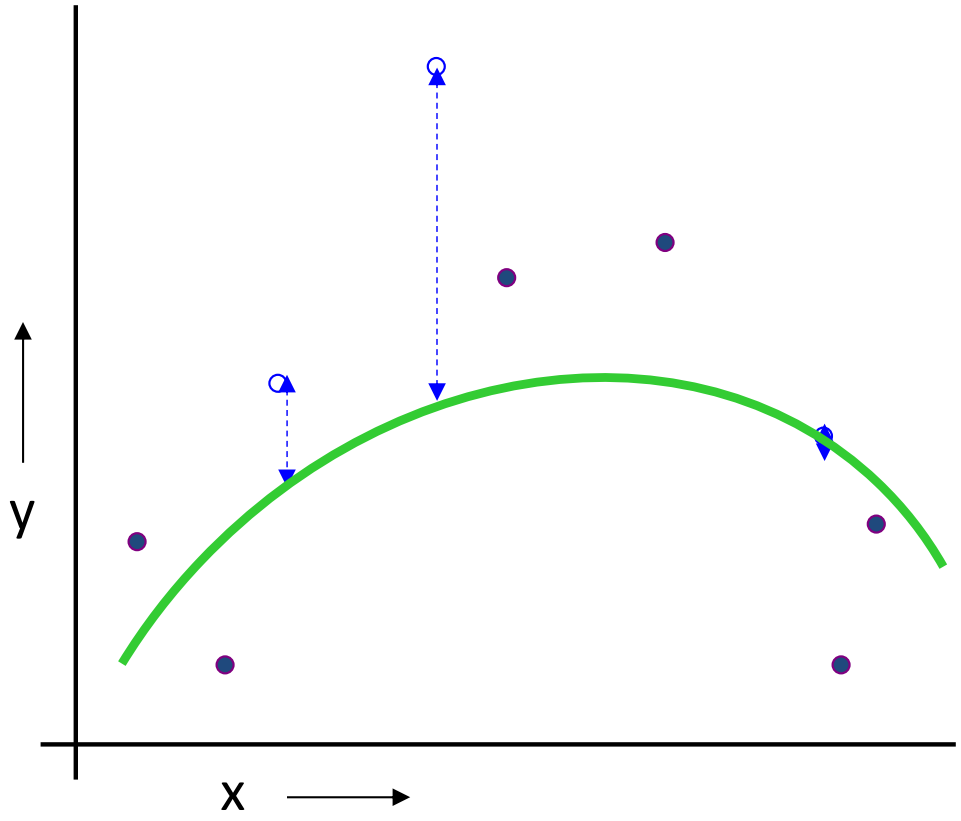
The test set method



(Linear regression example)
Mean Squared Error = 2.4

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

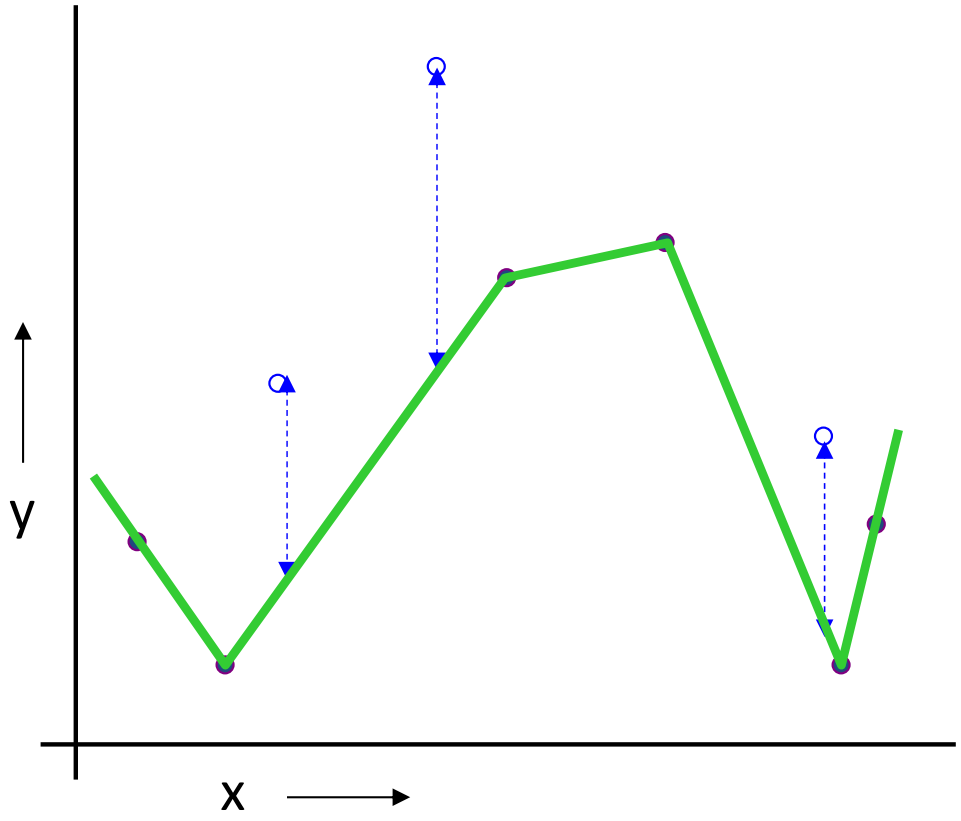
The test set method



(Quadratic regression example)
Mean Squared Error = 0.9

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

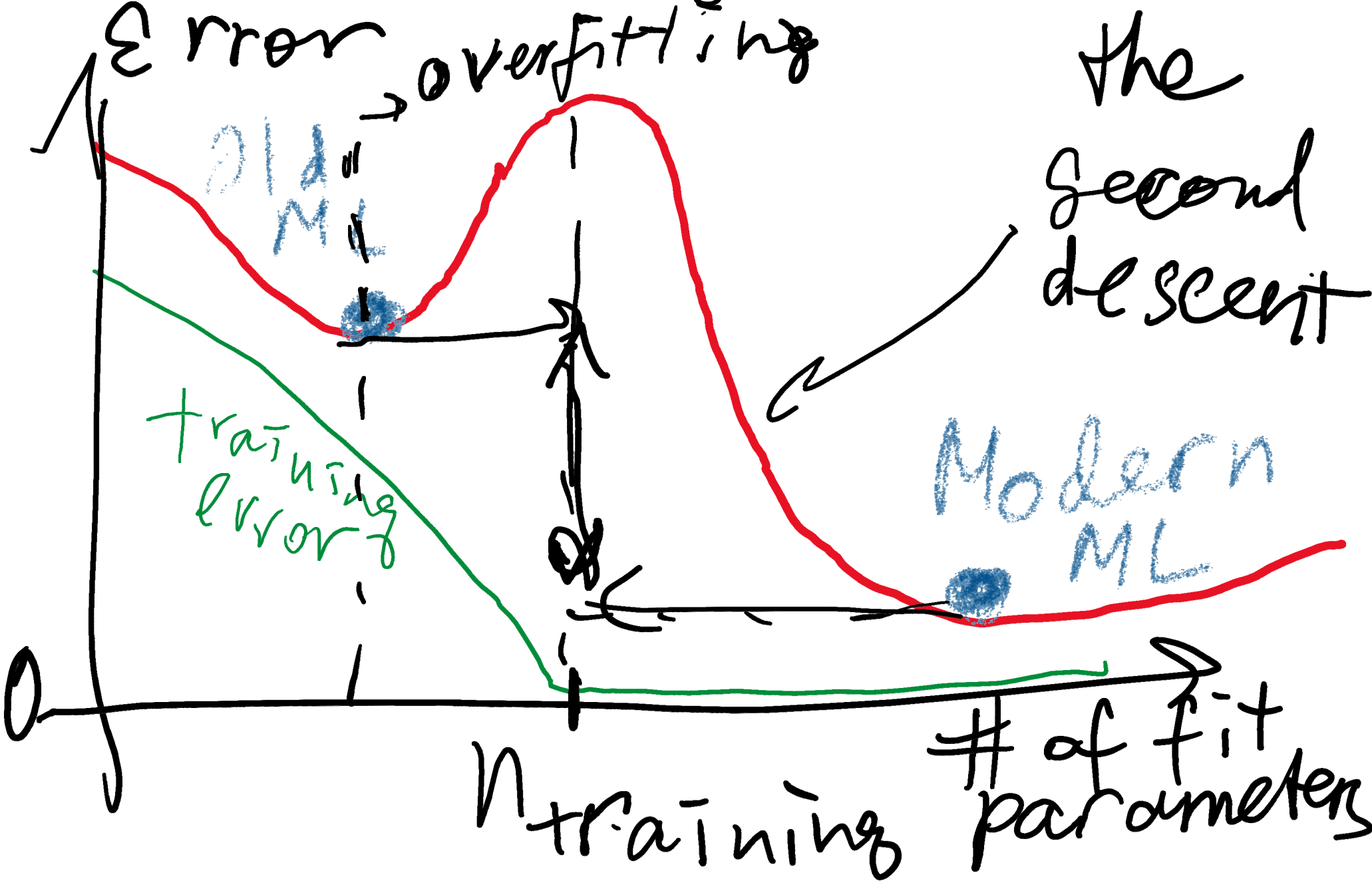
The test set method



(Join the dots example)
Mean Squared Error = 2.2

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

Double descend- the main reason modern Machine Learning works so well



R^2 and Adjusted R^2

The **coefficient of multiple determination R^2**

$$R^2 = \frac{SS_R}{SS_T} = 1 - \frac{SS_E}{SS_T}$$

The **adjusted R^2** is

$$R^2_{\text{adj}} = 1 - \frac{SS_E/(n-p)}{SS_T/(n-1)} \qquad (12\text{-}23)$$

$\approx 1 - \frac{\hat{\sigma}^2}{S_y^2}$

- The adjusted R^2 statistic penalizes adding terms to the MLR model.
- It can help guard against overfitting (including regressors that are not really useful)

How to know where to stop adding variables?

- Adding new variables x_i to MLR
  watch the adjusted R^2

- Once the adjusted R^2
  no longer increases = stop.
  Now you did the best you can.

Credit: XKCD comics

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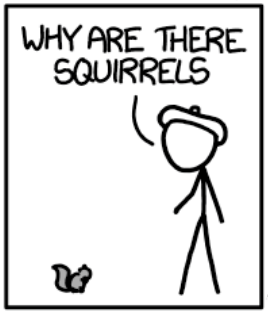

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WHEEL OF FORTUNE

Matlab exercise #1: “Wheel of Fortune”

- Each group gets a pair of genes that are known to be correlated.
- Each group also gets a random pair of genes selected by the “Wheel of Fortune”. They may or may not be correlated
- Download (log-transformed) expression_table.mat
- Run command fitlm(x,y) on assigned and random pairs
- Record β_0, β_1, R^2, P-value of the slope β_1 and write them on the blackboard
- Validate Matlab result for R^2 using your own calculations
- Look up gene names (see gene_description in your workspace) and write down a brief description of biological functions of genes. Does their correlation make biological sense?

Correlated pairs

plausible biological connection based

on short description

1, 6 g1=1994; g2=188;

2, g1=2872; g2=1269;

3, g1=1321; g2=10;

4, g1= 886; g2=819;

5, g1=2138; g2=1364;

no obvious biological common function

```
g1=1+floor(rand.*3000); g2=1+floor(rand.*3000);
disp([g1, g2])
```

Random pairs

```
>> g1=floor(3000.*rand)+1; g2=floor(3000.*rand)+1;
disp([g1,g2]);
```

```
>> g1=floor(3000.*rand)+1; g2=floor(3000.*rand)+1;
disp([g1,g2]);
```

```
>> g1=floor(3000.*rand)+1; g2=floor(3000.*rand)+1;
disp([g1,g2]);
```

```
>> g1=floor(3000.*rand)+1; g2=floor(3000.*rand)+1;
disp([g1,g2]);
```

Matlab code

- load expression_table.mat
- g1=2907; g2=288;
- x=exp_t(g1,:)'; y=exp_t(g2,:)';
- figure; plot(x,y,'ko');
- lm=fitlm(x,y)
- y_fit=lm.Fitted;
- hold on; plot(x,lm.Fitted,'r-');
- SST=sum((y-mean(y)).^2);
- SSR=sum((y_fit-mean(y)).^2);
- SSE=sum((y-y_fit).^2);
- R2=SSR./SST
- disp([gene_names(g1), gene_names(g2)]);
- disp(gene_description(g1)); disp(gene_description (g2));

Credit: XKCD comics

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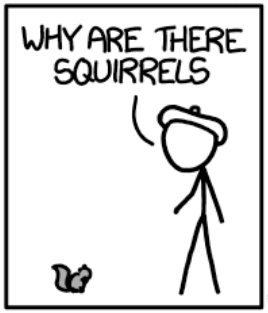

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Matlab exercise on #2 on MLR

- Every group works with
  g0=2907; g1=1527; g2=2629; g3=2881;
  g4=1144; g5=1066;
- Compute Multiple Linear Regression (MLR):
  where
  y=exp_t (g0); x1= exp_t (g1); x2= exp_t (g2);
- How much better the MLR did compared to the Single Linear Regression (SLR)?
- Continue increasing the number of genes in x until R_adj starts to decrease

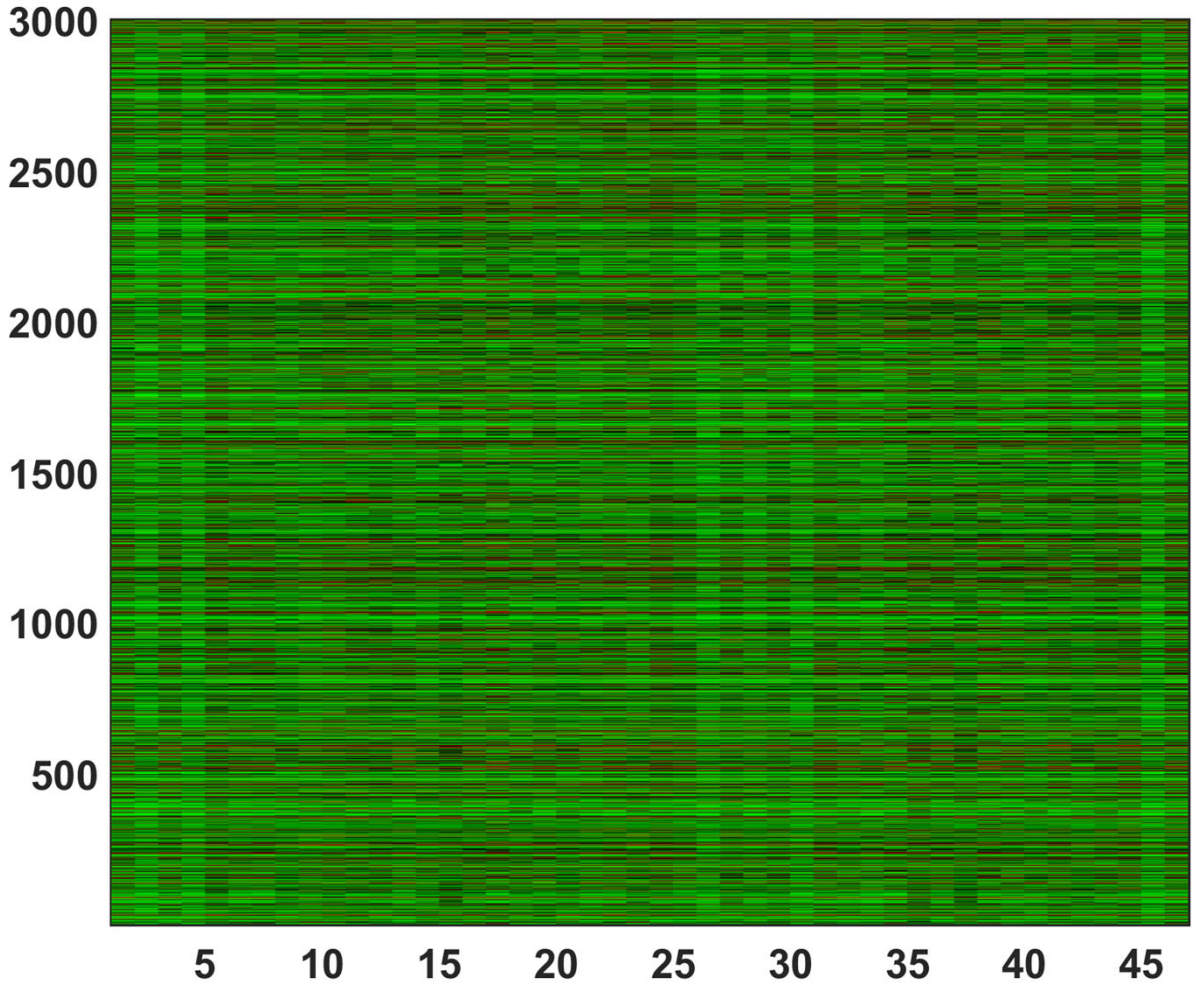
How I did it

```
g0=2907; g1=1527; g2=2629; g3=2881;g4=1144; g5=1066;
y=exp_t(g0,:)';
%% first use one x to predict y
x=exp_t(g1,:)';
figure; plot(x,y,'ko')
lm=fitlm(x,y)
y_fit=lm.Fitted;
hold on;
plot(x,lm.Fitted,'r-');
%% now use 2 x's to predict y
x=[exp_t(g1,:)', exp_t(g2,:)'];
lm2=fitlm(x,y)
y_fit=lm2.Fitted;
hold on; plot(x(:,1),y_fit,'gd');
%% now use m x's to predict y
corr_matrix=corr(exp_t');
g0=2907;
[u v]=sort(corr_matrix(g0,:),'descend');
x=[exp_t(v(2:m+1),:)'];
lm3=fitlm(x,y)
y_fit=lm3.Fitted;
plot(x(:,1),y_fit,'s');
```

Clustering analysis of gene expression data

Chapter 11 in
Jonathan Pevsner,
Bioinformatics and Functional Genomics,
3rd edition
(Chapter 9 in 2nd edition)

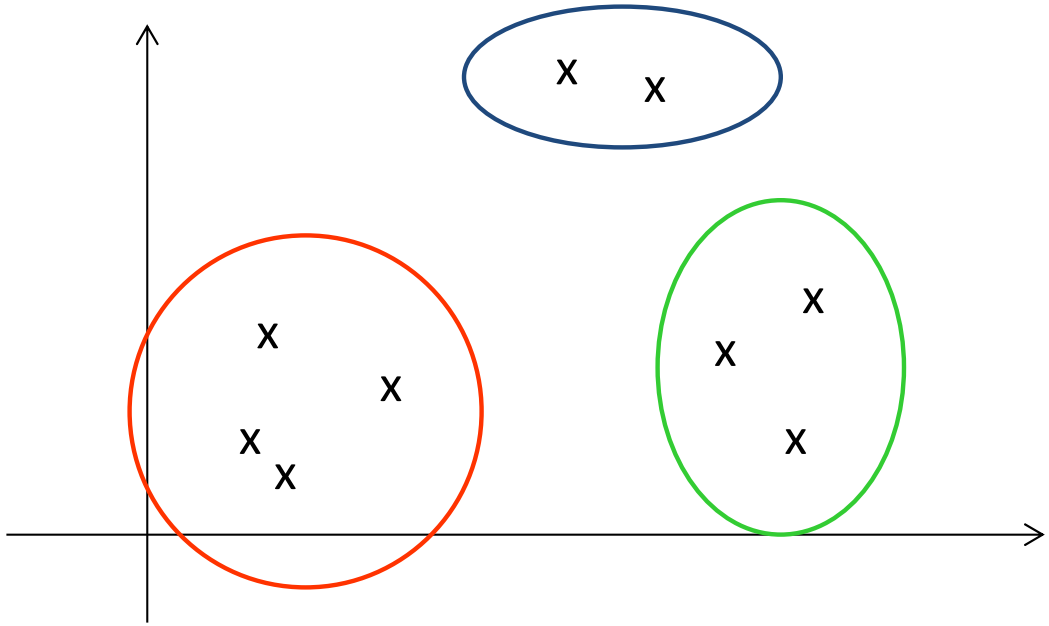
How to find the entire groups of mutually correlated genes if you have many genes and many samples?



Clustering to the rescue!

What is clustering?

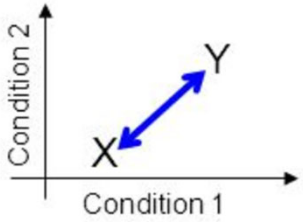
- The goal of clustering is to
  - group data points that are close (or **similar**) to each other
  - Usually, one needs to identify such groups (or clusters) in an **unsupervised** manner
  - Sometimes one takes into account **prior information** (Bayesian methods)
- Need to define some distance d_{ij} between objects i and j
- Clustering is easy in 2 dimensions but hard in 3000 dimensions -> need to somehow reduce dimensionality



How to define the distance?

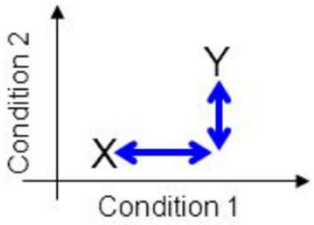
- Euclidean distance:
  - Most commonly used distance
  - Sphere shaped cluster
  - Corresponds to the geometric distance into the multidimensional space

$$d(X,Y) = \sqrt{\sum_i (x_i - y_i)^2}$$



- City Block (Manhattan) distance:
  - Sum of differences across dimensions
  - Less sensitive to outliers
  - Diamond shaped clusters

$$d(X,Y) = \sum_i |x_i - y_i|$$



The Canberra distance metric is calculated in R by

$$\sum \left(\frac{|x_i - y_i|}{|x_i + y_i|} \right).$$

Correlation coefficient distance

$$d(X,Y) = 1 - \rho(X,Y) = 1 - \frac{Cov(X,Y)}{\sqrt{(Var(X) \cdot Var(Y)}}$$

Common types of clustering algorithms

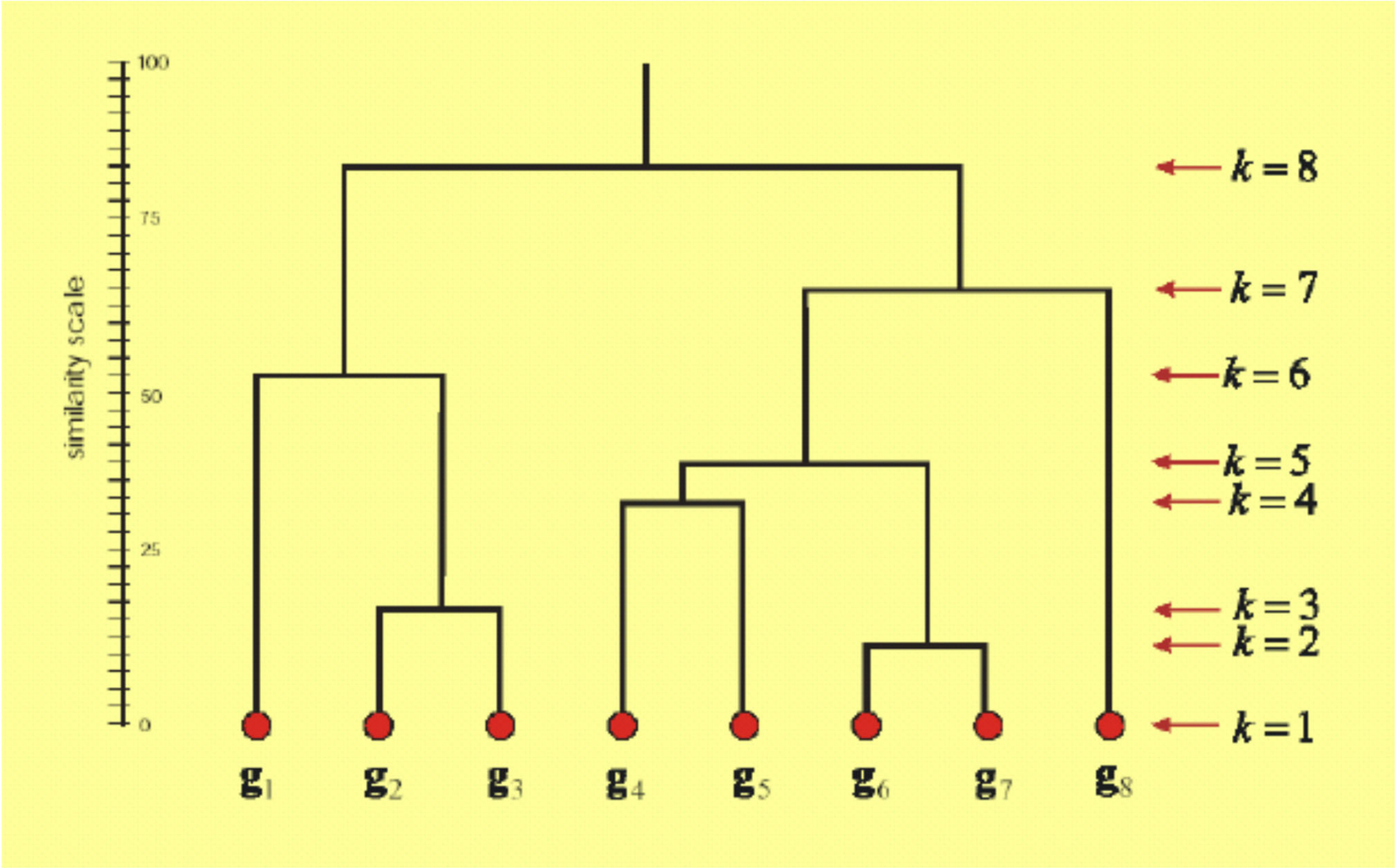
- Hierarchical if one doesn't know in advance the # of clusters
  - Agglomerative: start with N clusters and gradually merge them into 1 cluster
  - Divisive: start with 1 cluster and gradually break it up into N clusters
- Non-hierarchical algorithms
  - K-means clustering:
    - Iteratively apply the following two steps:
    - Calculate the centroid (center of mass) of each cluster
    - Assign each to the cluster to the nearest centroid
  - Principal Component Analysis (PCA)
    - plot pairs of top eigenvectors of the covariance matrix $Cov(X_i, X_j)$ and uses visual information to group

Hierarchical clustering

UPGMA algorithm

- Hierarchical agglomerative clustering algorithm
- **UPGMA** = Unweighted Pair Group Method with Arithmetic mean
- Iterative algorithm:
- Start with a pair with the smallest d(X,Y)
- Cluster these two together and replace it with their arithmetic mean (X+Y)/2
- Recalculate all distances to this new “cluster node”
- Repeat until all nodes are merged

Output of UPGMA algorithm



Clustering in Matlab

Choices of distance metrics in clustergram(… 'RowPDistValue' …, 'ColumnPDistValue' …,)

Metric	Description
'euclidean'	Euclidean distance (default).
'seuclidean'	Standardized Euclidean distance. Each coordinate difference between rows in X is scaled by dividing by the corresponding element of the standard deviation S=nanstd(X). To specify another value for S, use D=pdist(X,'seuclidean',S).
'cityblock'	City block metric.
'minkowski'	Minkowski distance. The default exponent is 2. To specify a different exponent, use D = pdist(X,'minkowski',P), where P is a scalar positive value of the exponent.
'chebychev'	Chebychev distance (maximum coordinate difference).
'mahalanobis'	Mahalanobis distance, using the sample covariance of X as computed by nancov. To compute the distance with a different covariance, use D = pdist(X,'mahalanobis',C), where the matrix C is symmetric and positive definite.
'cosine'	One minus the cosine of the included angle between points (treated as vectors).
'correlation'	One minus the sample correlation between points (treated as sequences of values).
'spearman'	One minus the sample Spearman's rank correlation between observations (treated as sequences of values).
'hamming'	Hamming distance, which is the percentage of coordinates that differ.
'jaccard'	One minus the Jaccard coefficient, which is the percentage of nonzero coordinates that differ.
custom distance function	A distance function specified using @: D = pdist(X,@distfun) A distance function must be of form d2 = distfun(XI,XJ) taking as arguments a 1-by-*n* vector XI, corresponding to a single row of X, and an *m*2-by-*n* matrix XJ, corresponding to multiple rows of X. distfun must accept a matrix XJ with an arbitrary number of rows. distfun must return an *m*2-by-1 vector of distances d2, whose *k*th element is the distance between XI and XJ(k,:).

Choices of hierarchical clustering algorithm in clustergram(…'linkage',…)

`X`	Matrix with two or more rows. The rows represent observations, the columns represent categories or dimensions.
`method`	Algorithm for computing distance between clusters.

Method	Description
`'average'`	Unweighted average distance (UPGMA)
`'centroid'`	Centroid distance (UPGMC), appropriate for Euclidean distances only
`'complete'`	Furthest distance
`'median'`	Weighted center of mass distance (WPGMC), appropriate for Euclidean distances only
`'single'`	Shortest distance
`'ward'`	Inner squared distance (minimum variance algorithm), appropriate for Euclidean distances only
`'weighted'`	Weighted average distance (WPGMA)

Default: `'single'`