Introduction to Data Science 6

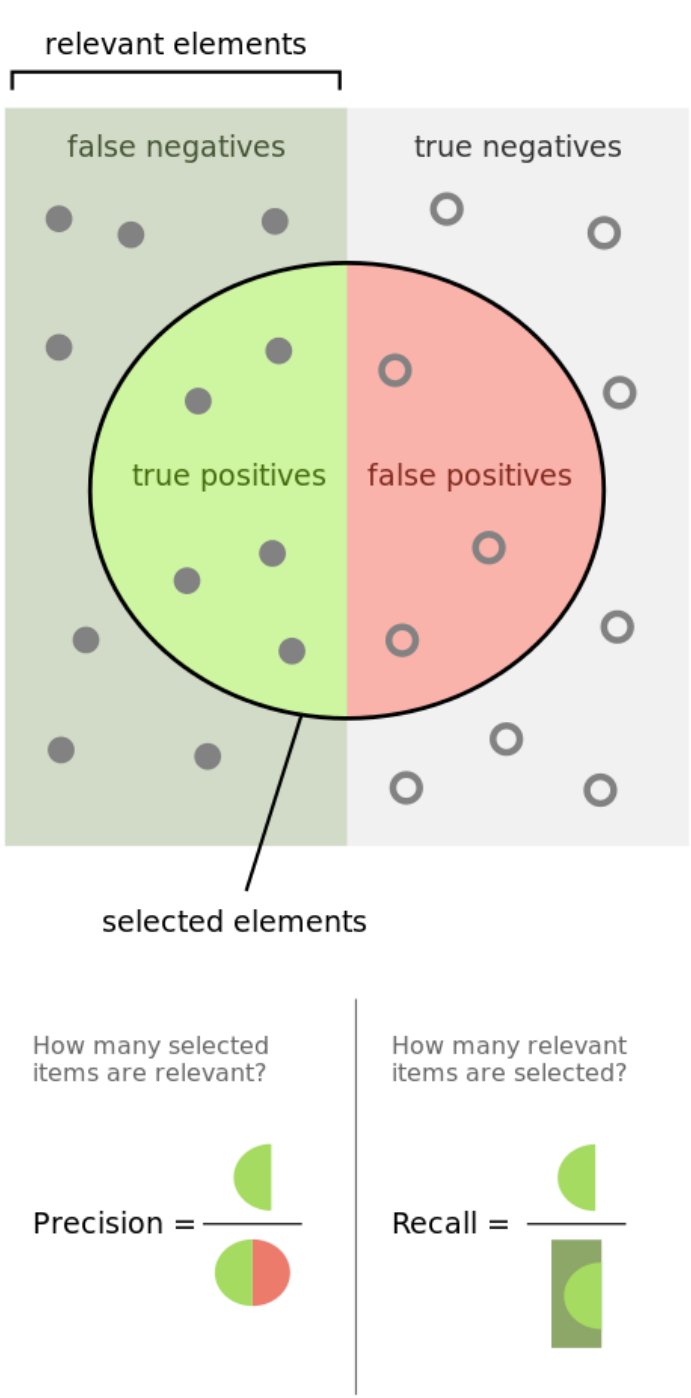
Overview

Precision & Recall (reprise)

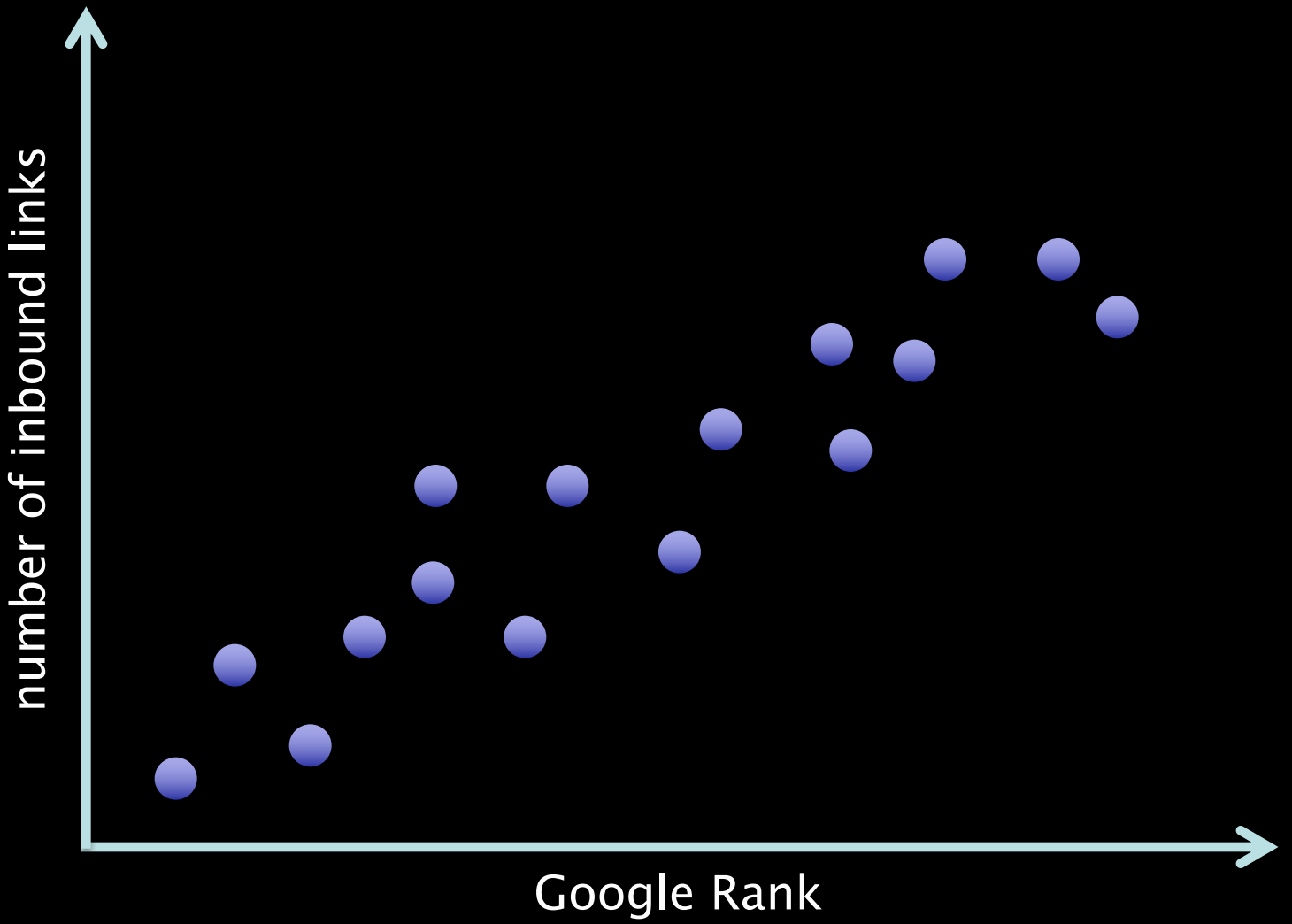
PCA is color blind

3 new classifiers
- Random Decision Forests
- Naive Bayes
- Support Vector Machines

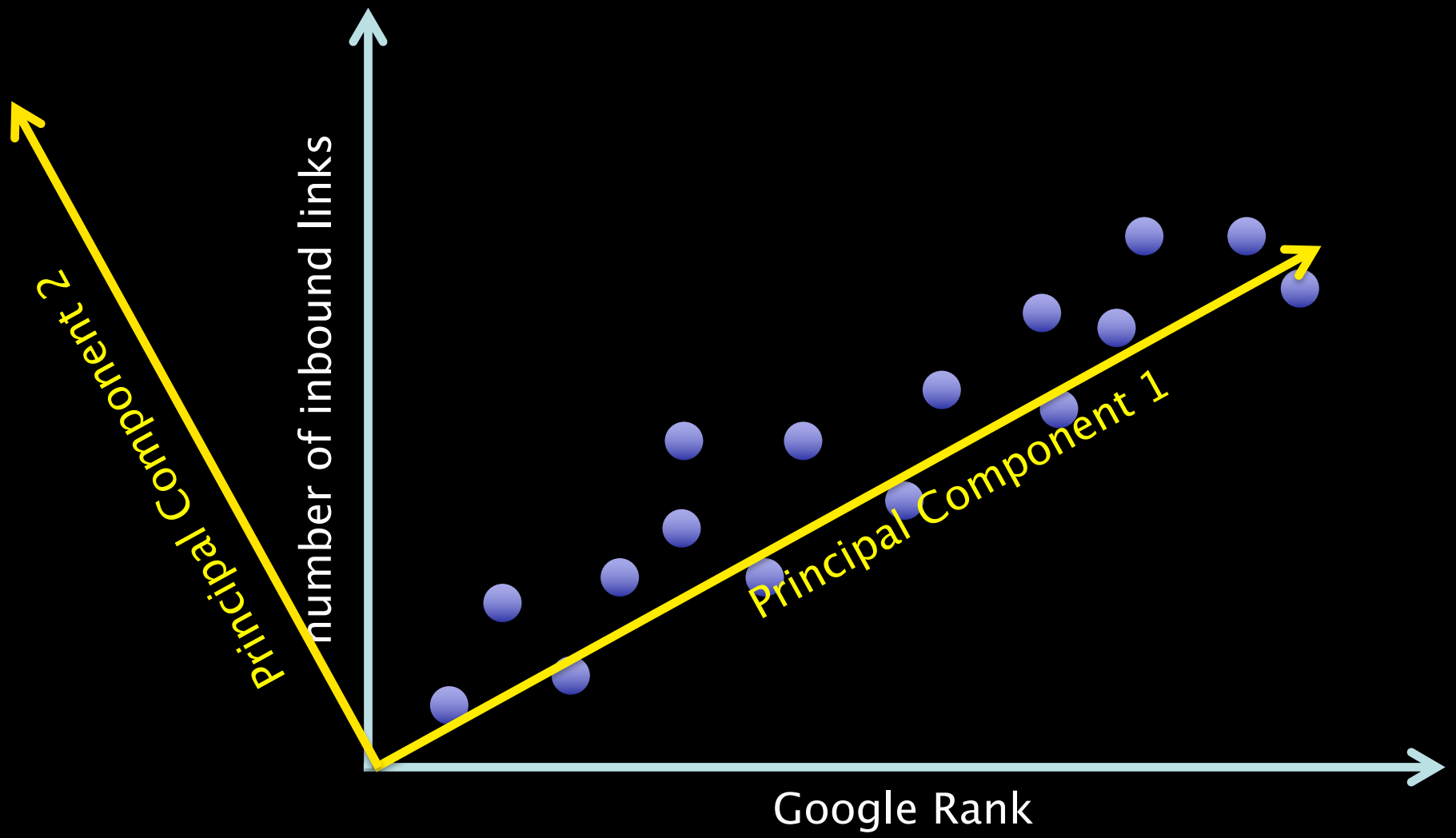
- ***precision*** is the fraction of retrieved instances that are relevant
- ***recall*** is the fraction of relevant instances that are retrieved

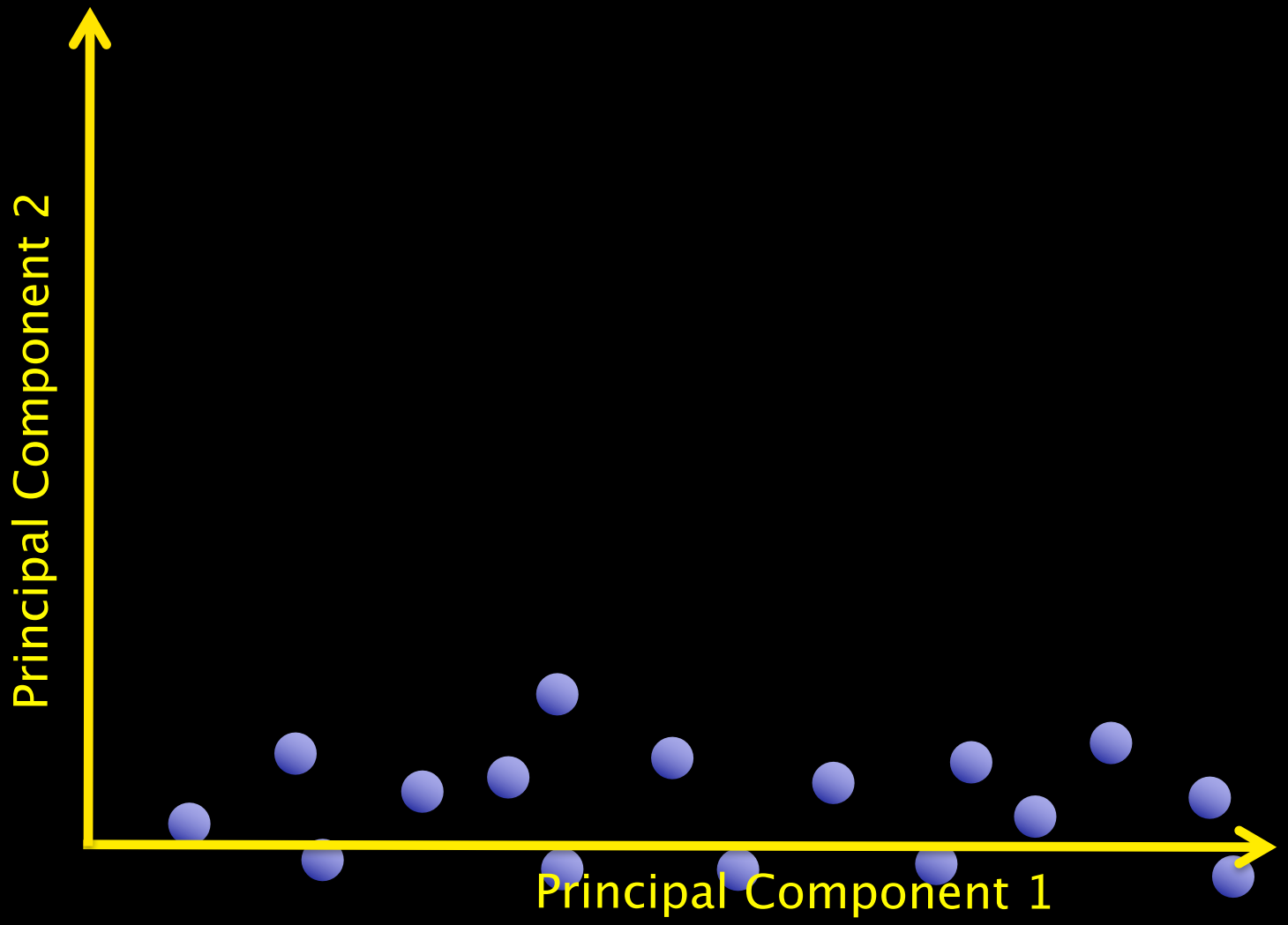


1D structure in 2D feature space



PCA


number of inbound links
Google Rank
Principal Component 1
Principal Component 2


Principal Component 2
Principal Component 1

PCA

Takes 2 features as input

Feature 1: Number of inbound links

Feature 2: Google Rank

… and gives 2 new features as output

Principal Component 1

a  + b 

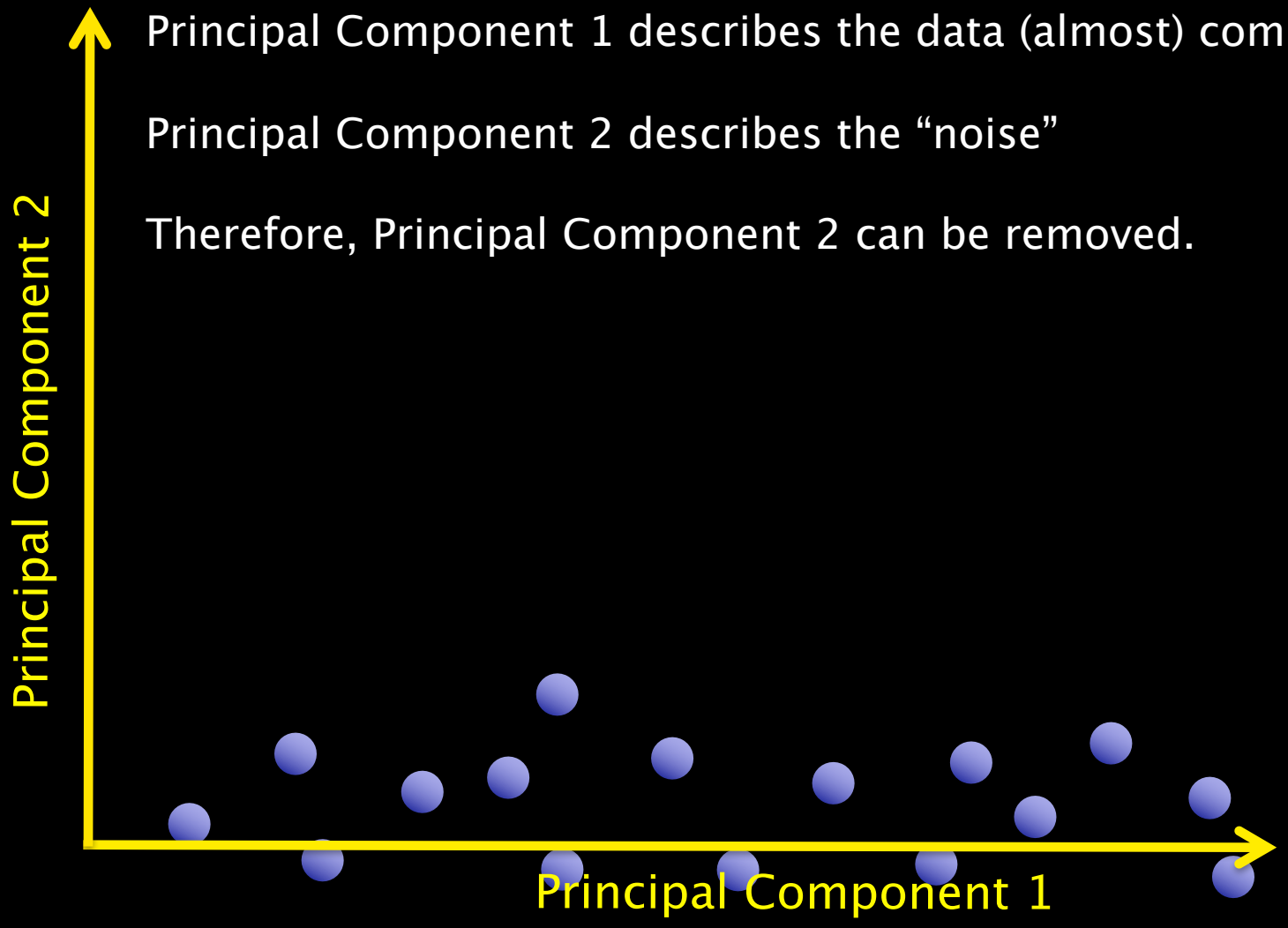
Principal Component 2

c  + d 

Principal Component 1 describes the data (almost) completely

Principal Component 2 describes the “noise”

Therefore, Principal Component 2 can be removed.



PCA + discarding highest PCs

Takes 2 features as input

Feature 1: Number of inbound links

Feature 2: Google Rank

… and gives 1 new feature as output

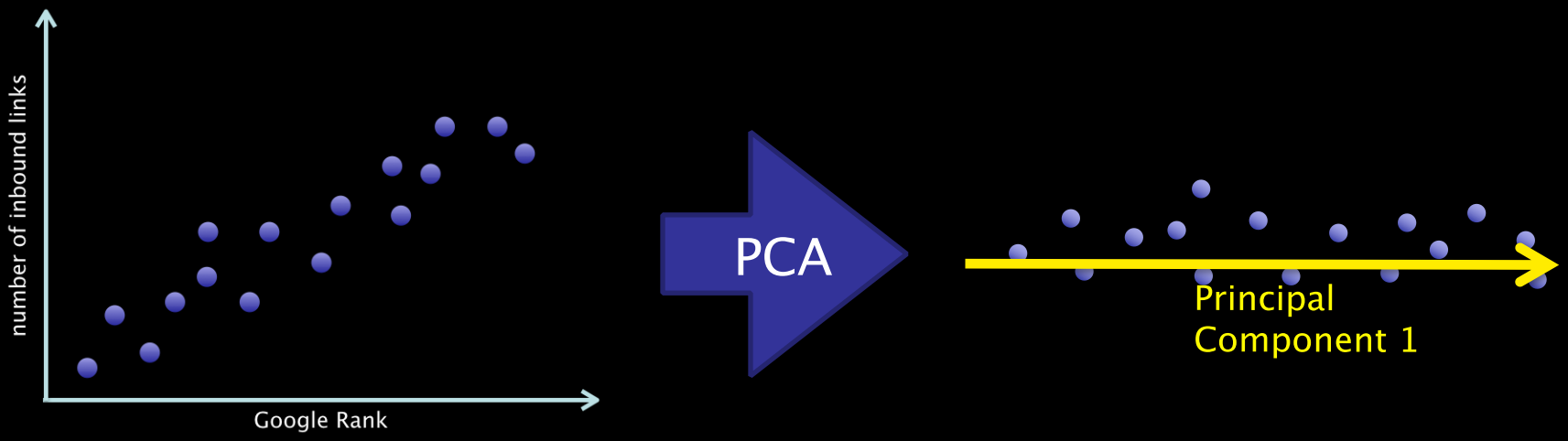
Principal Component 1

a 

+ b 

Dimensionality Reduction

- PCA performs **dimensionality reduction**
- It reduces 2 dimensions (features) to 1



PCA in higher dimensions

For datasets with N features (N>2), PCA rotates the coordinate system in such a way that:

- the projection of the data on the first principal component (new axis) has the largest variance,

- the projection of the data on the second principal component (new axis) has the one-but-largest variance,

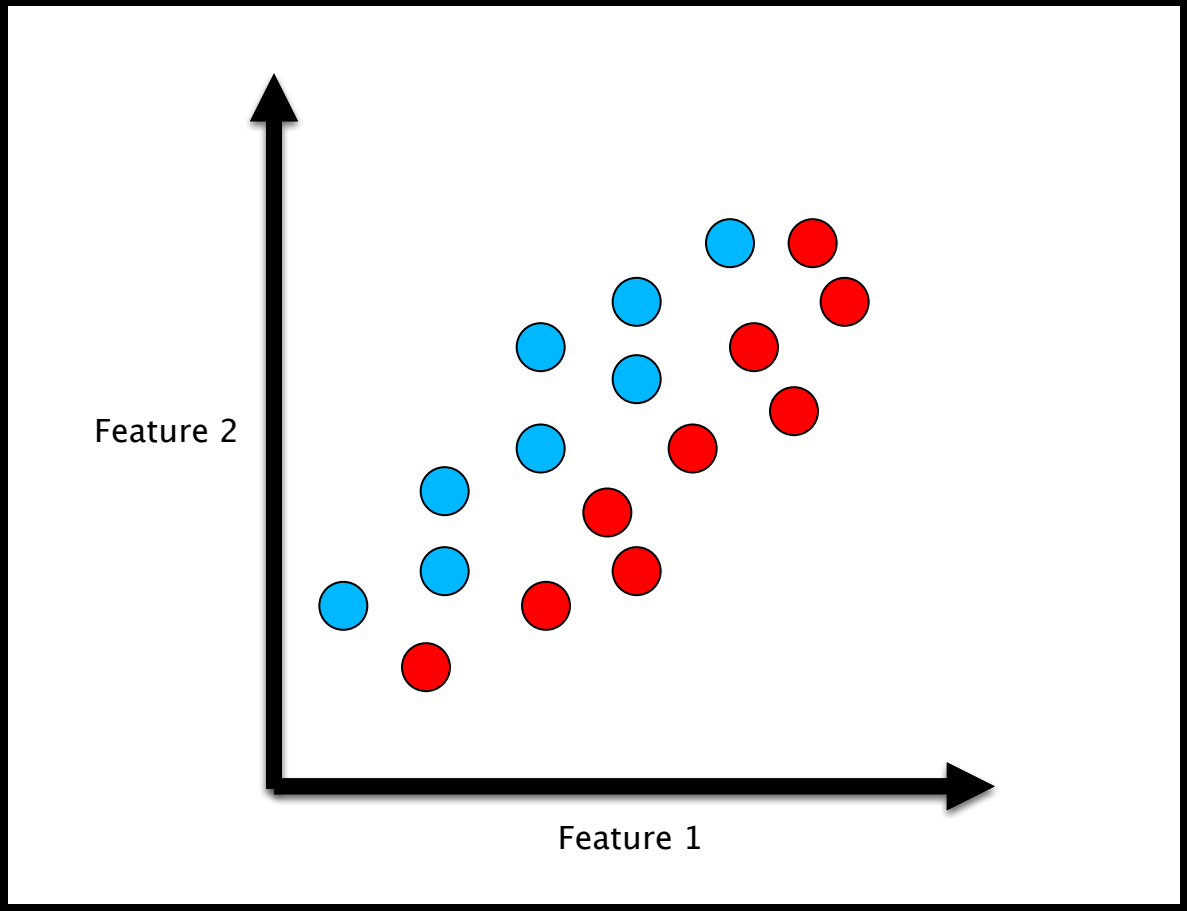
and so forth… (up to N principal components)

If the variation in the data is associated with relevance for classification (or regression), the most relevant features are captured by the first M principal components (and the rest captures noise)

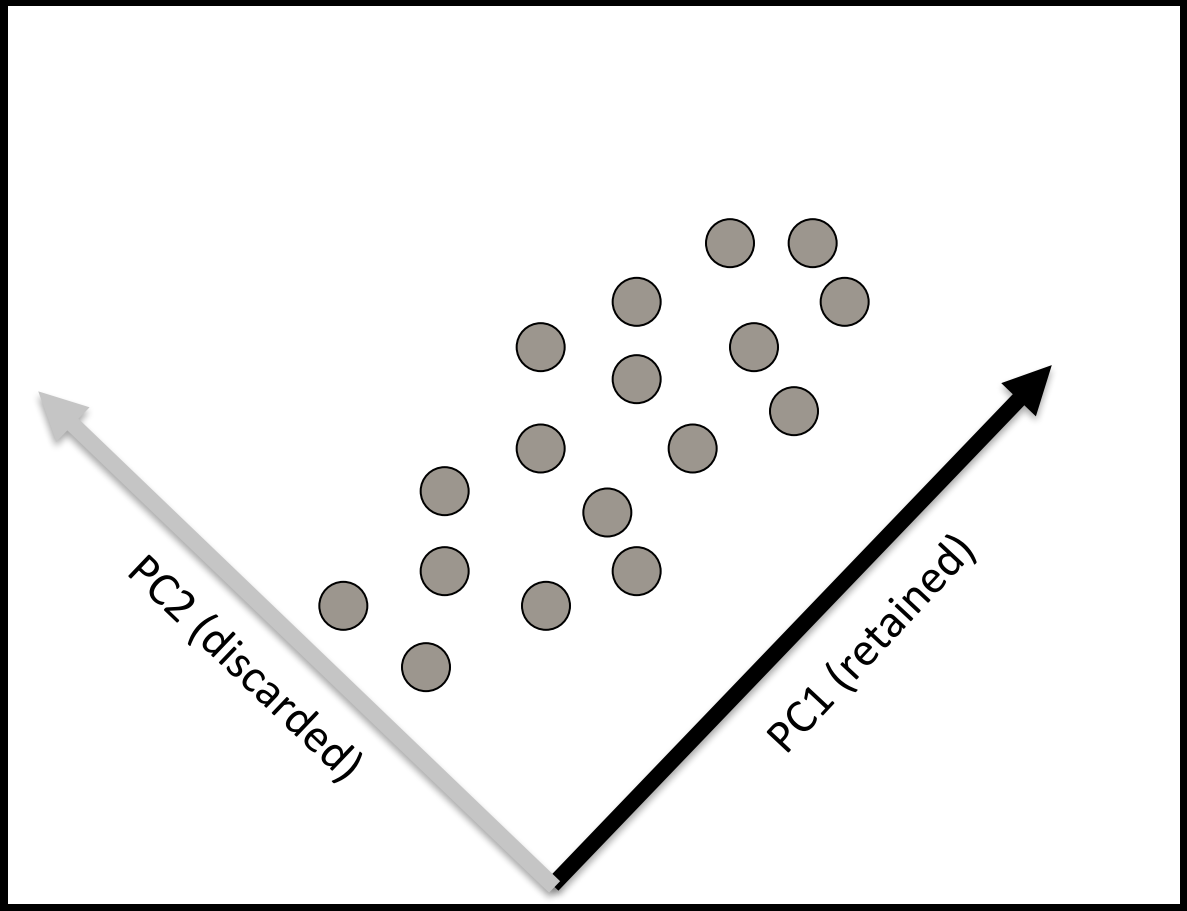
Retaining the first M principal components and throwing away the rest effectively reduces the dimensionality

M is typically much smaller than N, hence “dimensionality reduction”

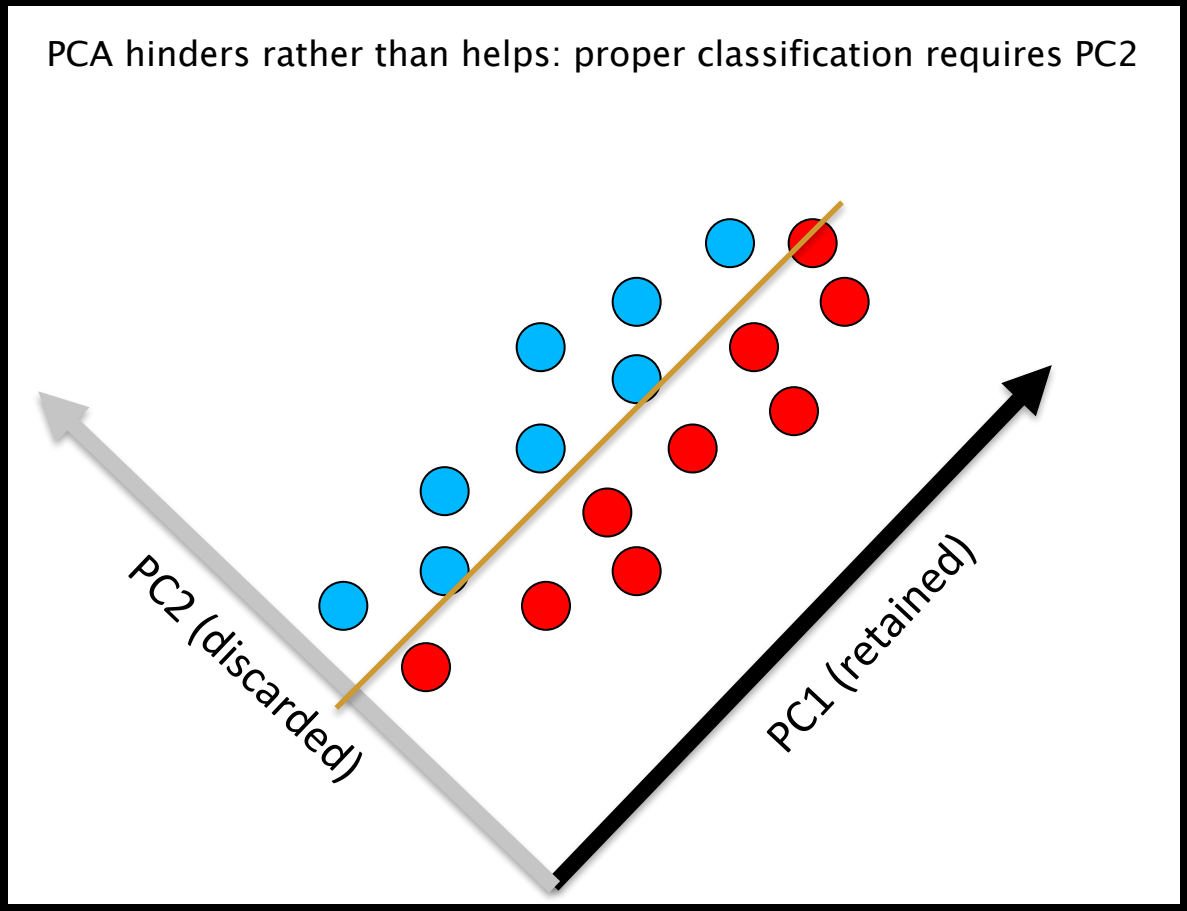
PCA is color blind!



PCA is color blind!



PCA is color blind!

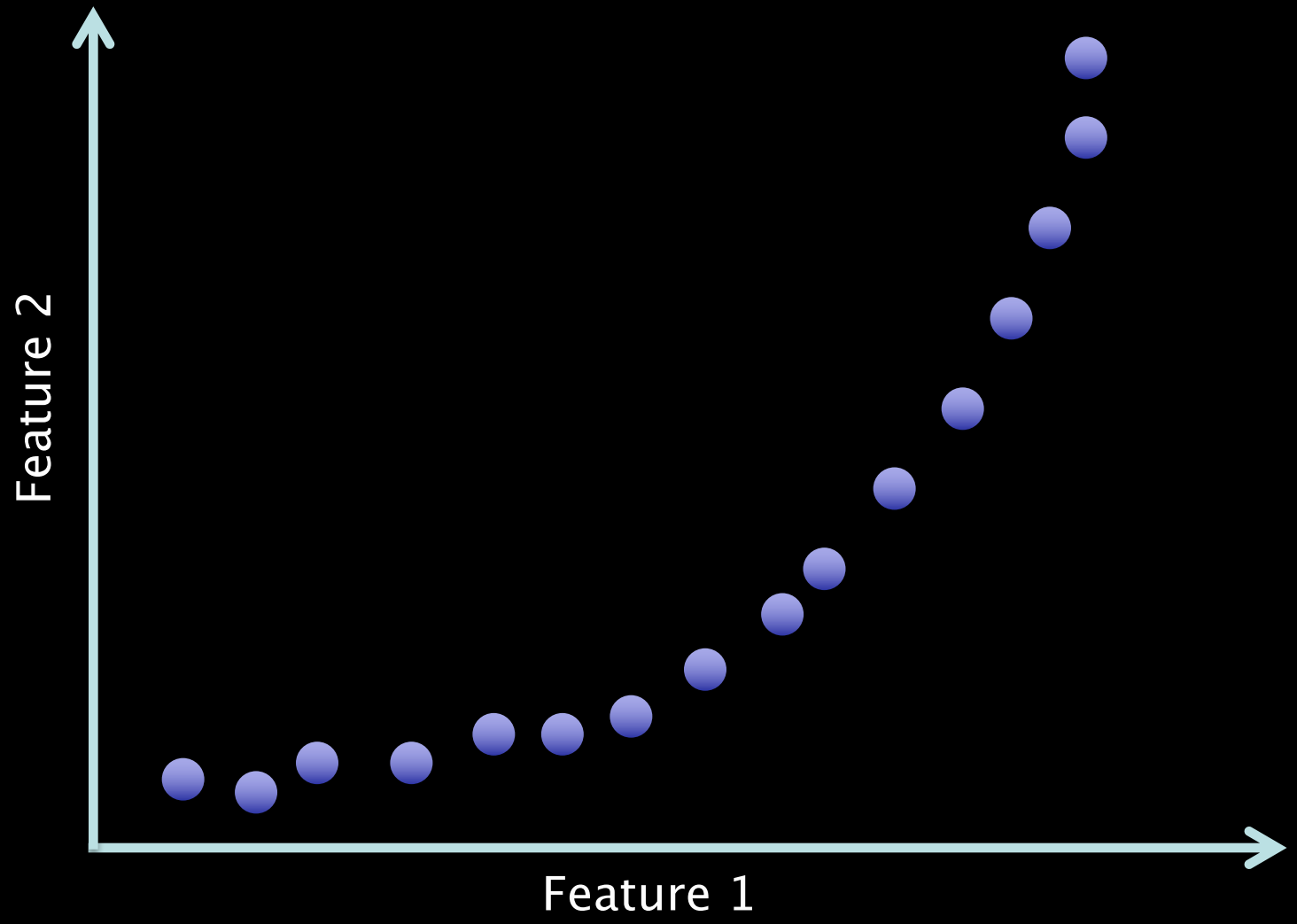


PCA is a “linear” method

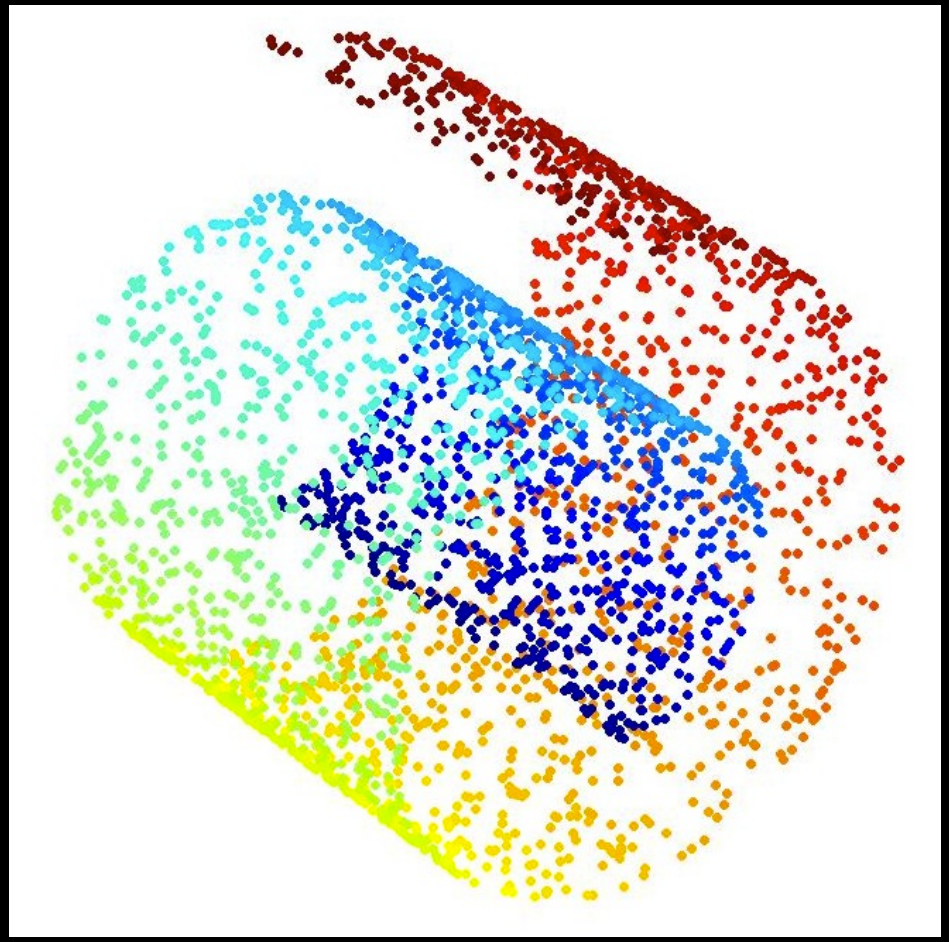
Another reason why PCA is not beneficial to the classification/regression is that it relies on “linear” (straight) data relations

It cannot deal with nonlinear (curved) data relations

1D curved structure in 2D feature space

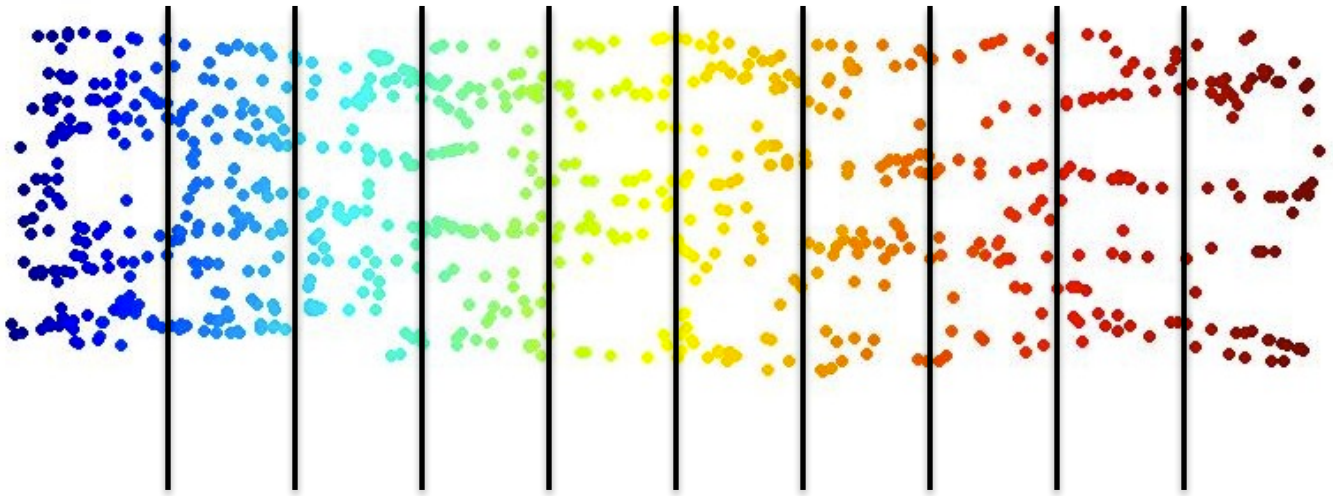


The Swiss Roll dataset



Data points in 3D (hard to classify)

A problem PCA cannot deal with

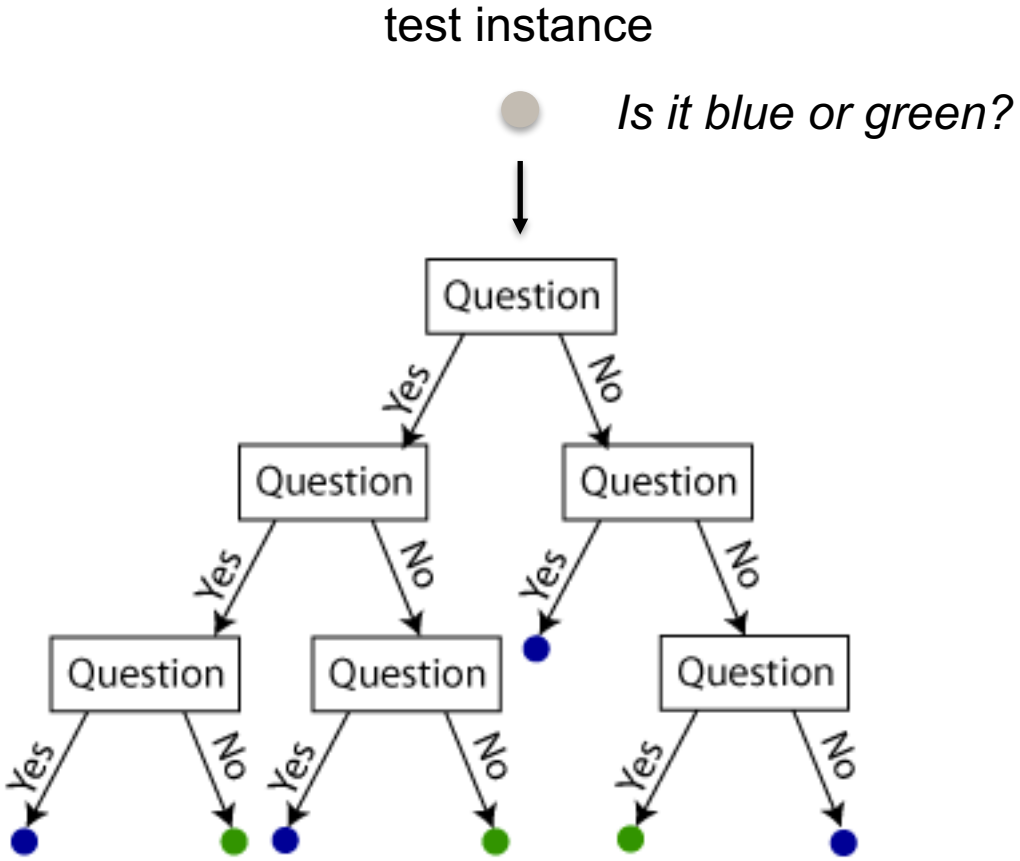


Unfolded data points in 2D (easy to classify)

3 new classifiers…

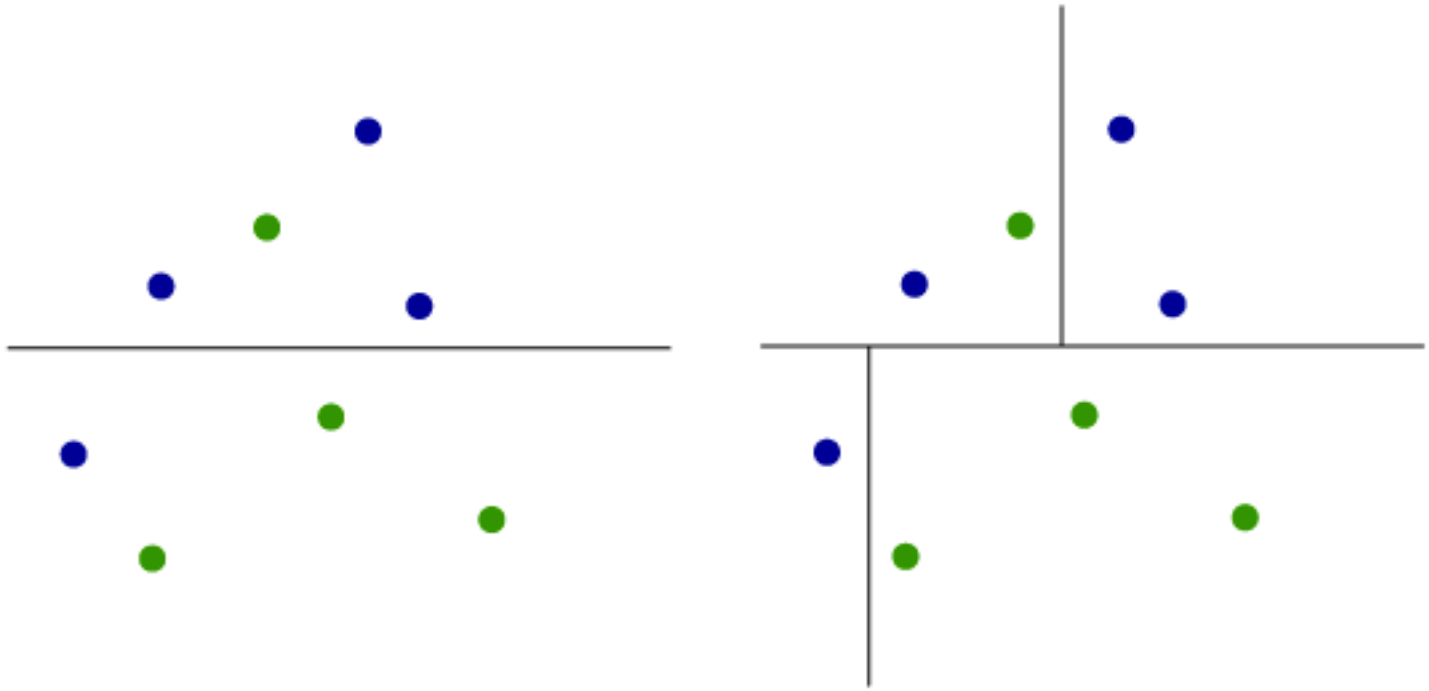
1. Random Decision Forests

Recall: decision tree



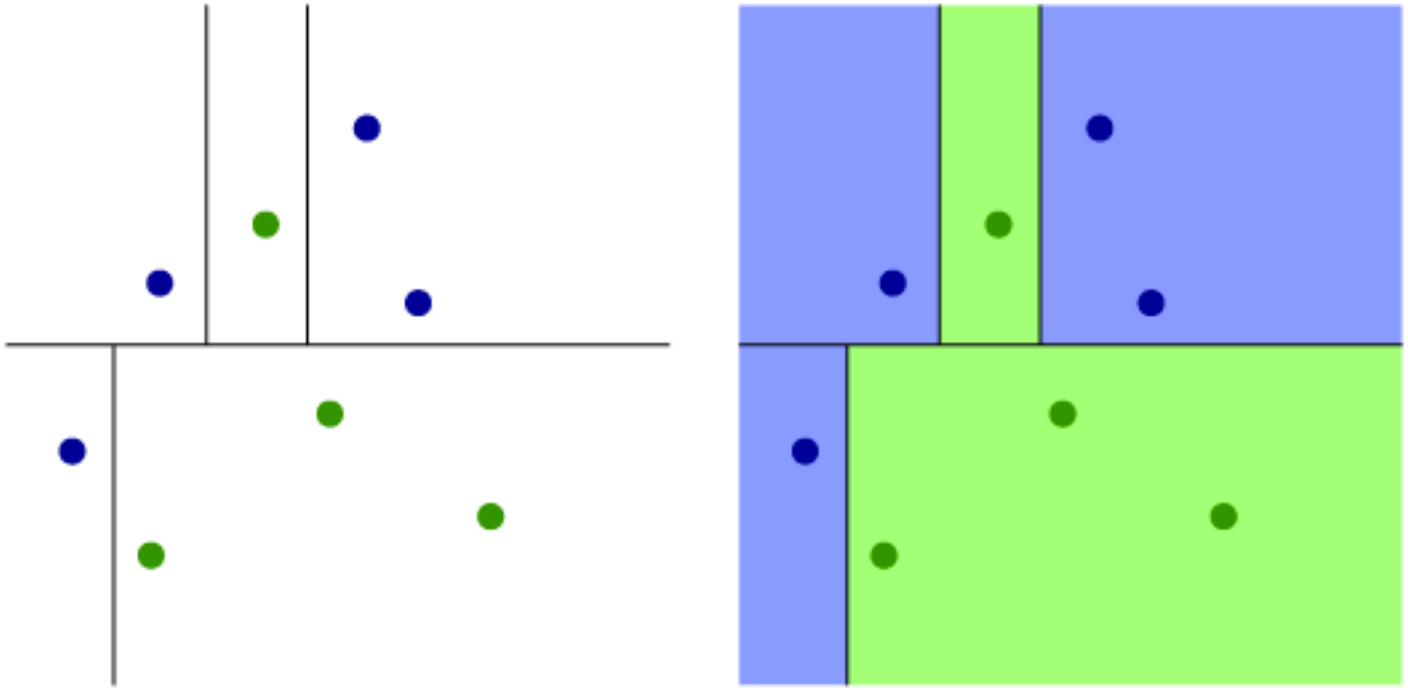
Reproduced from: https://shapeofdata.wordpress.com/2013/07/02/decision-trees/

Each test (node) adds a decision boundary



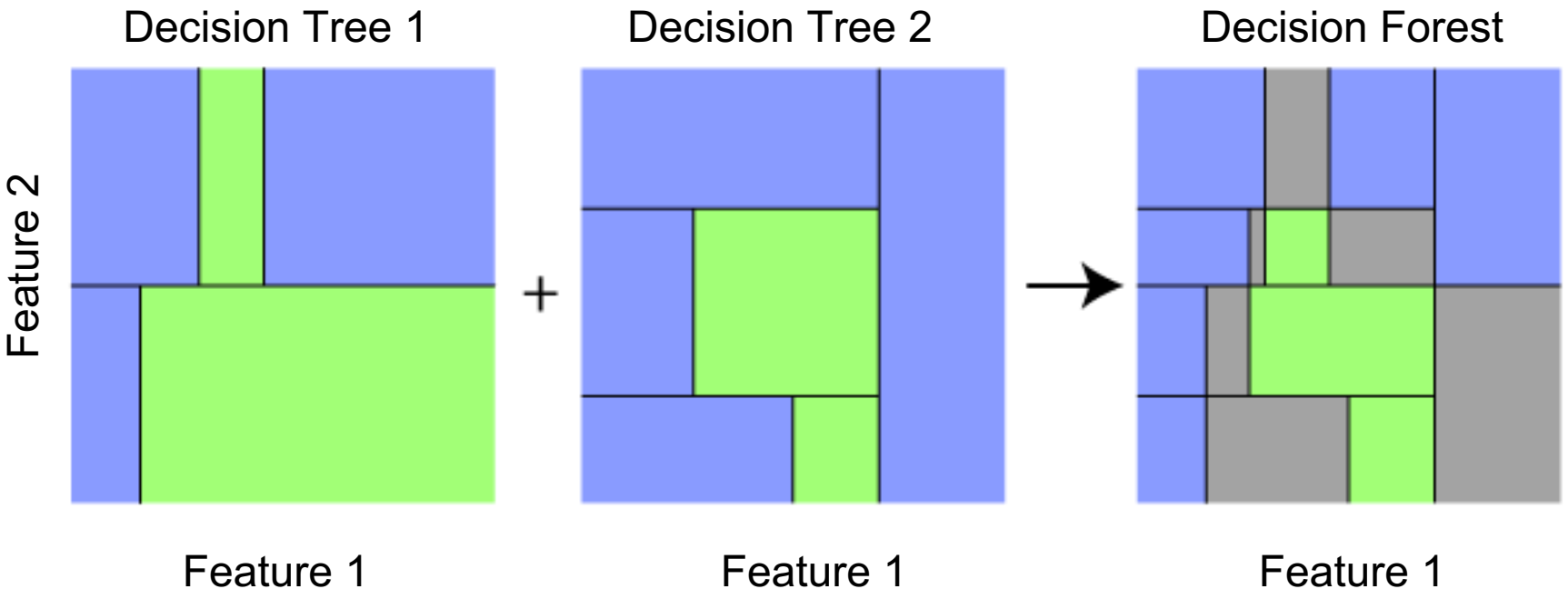
Reproduced from: https://shapeofdata.wordpress.com/2013/07/02/decision-trees/

Adding another node/decision boundary



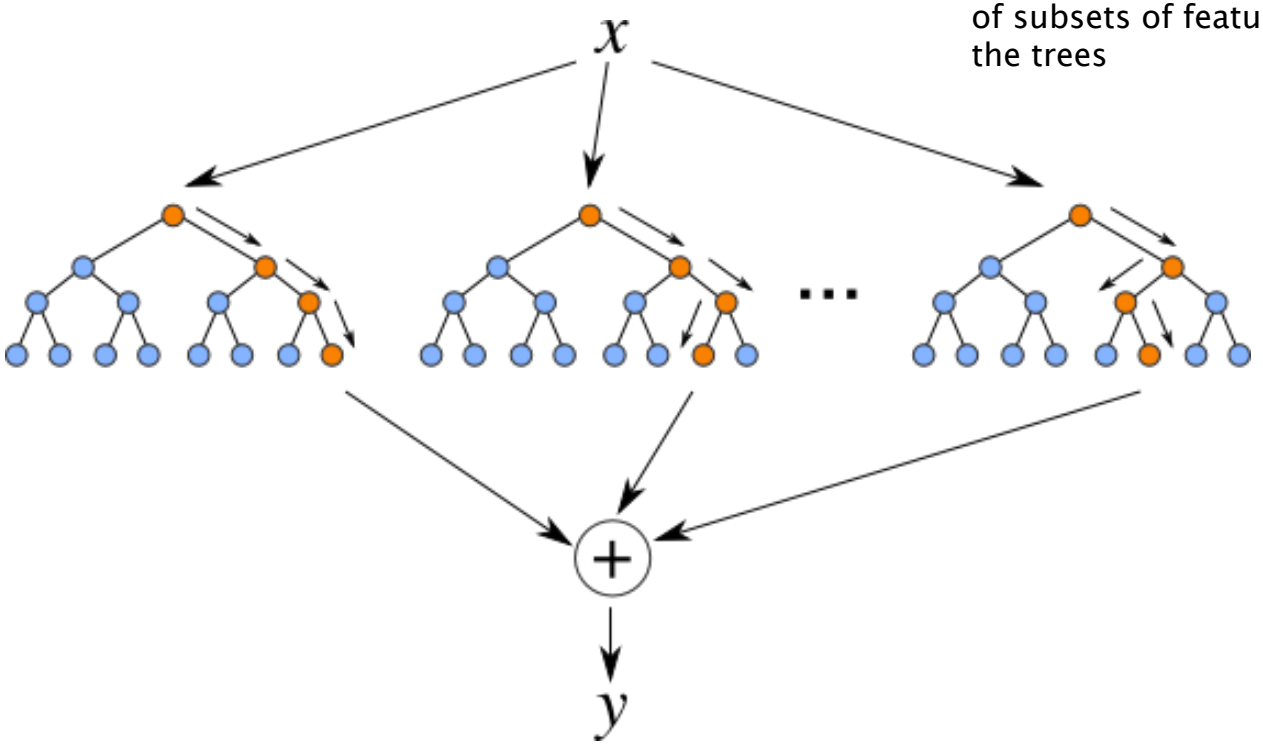
Reproduced from: https://shapeofdata.wordpress.com/2013/07/02/decision-trees/

Decision Forests: from one tree to many



Classification and Regression with Random Decision Forests

RDFs: random distribution of subsets of features over the trees



Classification: y = the mode of the classes outputted by the trees.
Regression: y = the mean of the values outputted by the trees.

Random Decision Forests

The complexity of RDFs is determined by the number of trees (and their depths)

In some decision forests trees are induced on the same complete set of features

In random decision forests, trees are induced on randomly selected subsets of features

2. Naive Bayes Classifier

Bayes's rule

- Data (**d**)
- Hypotheses (h_i)
- Evidence

- Bayes' rule:

$$P(h_i|\mathbf{d}) = \alpha P(\mathbf{d}|h_i)P(h_i)$$

"P(h|**d**)" should be read as: the probability that h is true, given **d**

Reading the Bayes equation

$$P(h_i|\mathbf{d}) = \alpha P(\mathbf{d}|h_i)P(h_i)$$

POSTERIOR LIKELIHOOD PRIOR

multiplication constant

New observations update your beliefs

$$P(h_i|\mathbf{d}) = \alpha P(\mathbf{d}|h_i)P(h_i)$$

You encounter a person with long hair and try to determine the probability of the person being female

PRIOR = 0.5 (both genders are equally likely)

LIKELIHOOD = P(long hair | female)

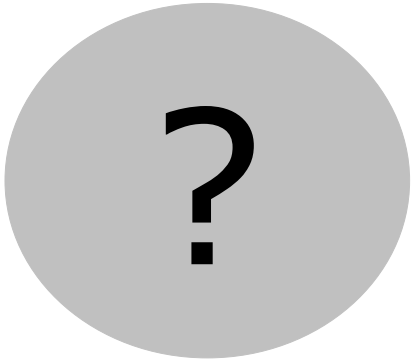
POSTERIOR probability updates the future prior (e.g., flower power)

Example (adapted from Russell & Norvig)

Five types of candy bags

h_1: 100% cherry
h_2: 75% cherry + 25% lime
h_3: 50% cherry + 50% lime
h_4: 25% cherry + 75% lime
h_5: 100% lime

Which one is it?



Candy in two flavors

Bayesian prediction

- Given a new opaque bag of candy
- H denotes the type of bag (h1,h2,h3,h4,h5)
- **d** denotes all observations of cherry and lime
- TASK: predict the flavour of the next piece of candy

- In Bayesian learning: Calculate the probability of each hypothesis, given the observations (data)

$$P(h_i|\mathbf{d}) = \alpha P(\mathbf{d}|h_i)P(h_i)$$

Calculating Likelihoods

h_1: 100% cherry
h_2: 75% cherry + 25% lime
h_3: 50% cherry + 50% lime
h_4: 25% cherry + 75% lime
h_5: 100% lime

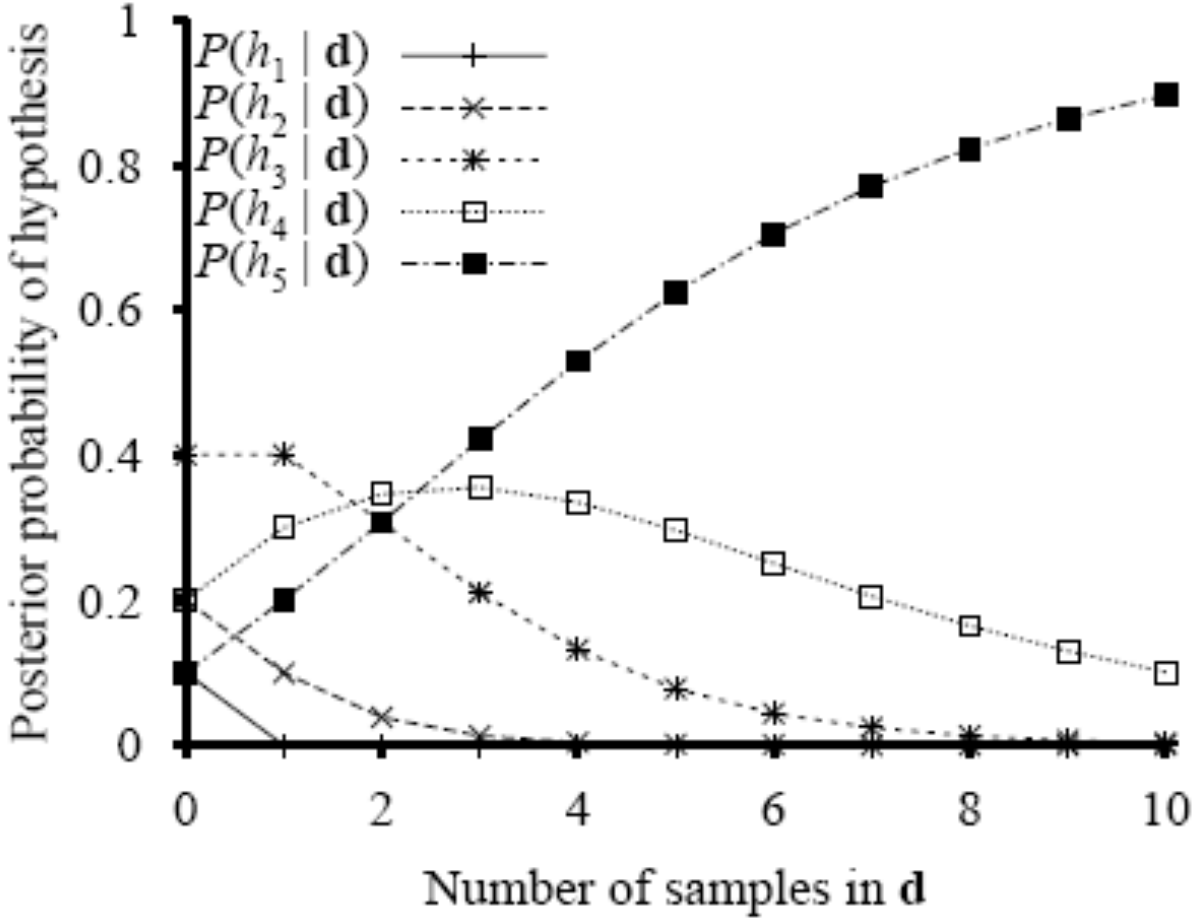
- With each observation, the likelihood is computed according to

  P(d|h) = P(cherry|h) x P(lime|h) <— assuming independence

- In case the bag is all lime (h5) and the first 10 observations are lime, than

  $P(d|h3) = 0.5^{10}$ and $P(d|h5) = 1^{10}$

Development of the posterior probabilities (h5 is the true hypothesis, all observations are 'lime')



maximum likelihood

Naive Bayes Classifier

- Given a dataset with two classes (Dem,Rep) and three features (A,B,C), compute

  $P(Dem|data) = P(Dem)\ P(A|Dem) \times P(B|Dem) \times P(C|Dem)$
  $P(Rep|data) = P(Rep)\ P(A|Rep) \times P(B|Rep) \times P(C|Rep)$

- IF $P(Dem|data) > P(Rep|data)$
  THEN Classification is Dem
  ELSE Classification is Rep

maximum likelihood

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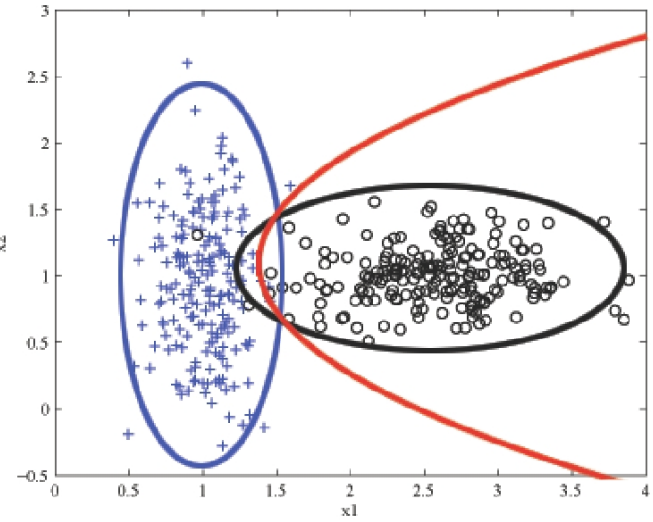
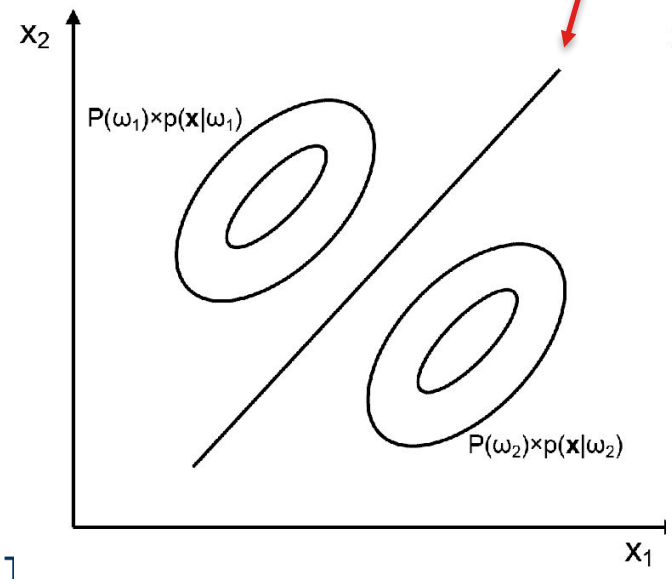
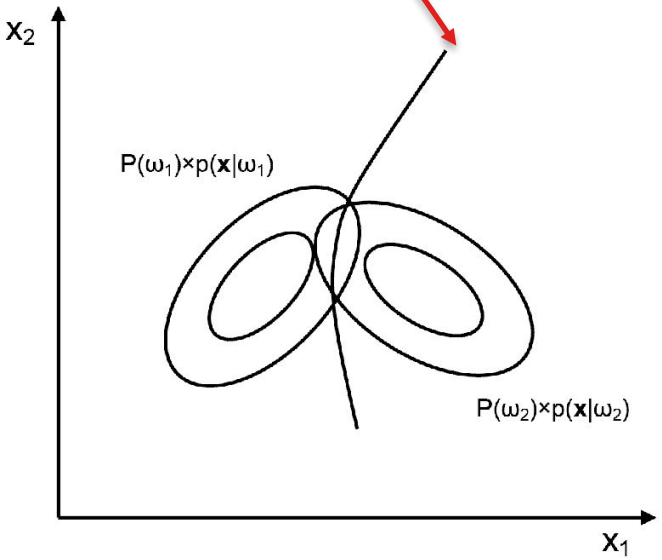
Naive Bayes decision boundaries



probabilities for black and blue classes are equal

can be straight or curved





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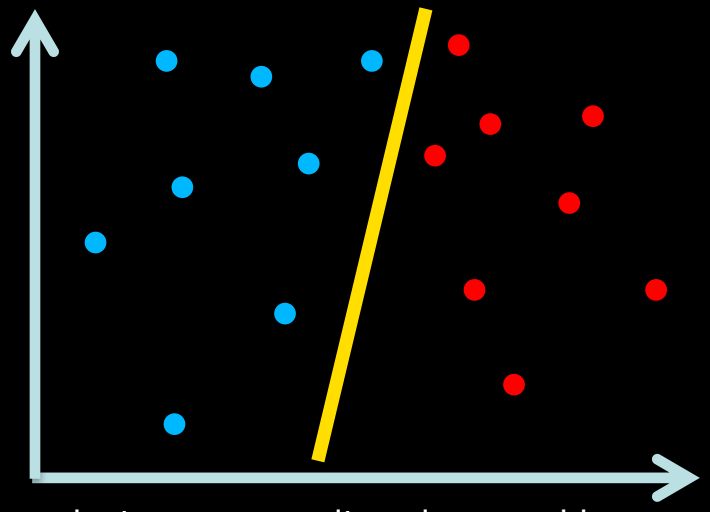
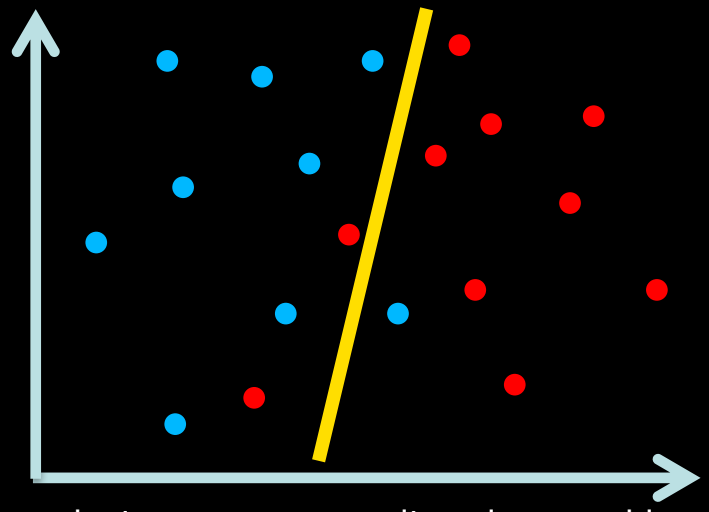
3. Support Vector Machines a.k.a. Kernel Machines

Simplest SVM

- Linear SVM
- Places a straight line between the classes (simplest model)

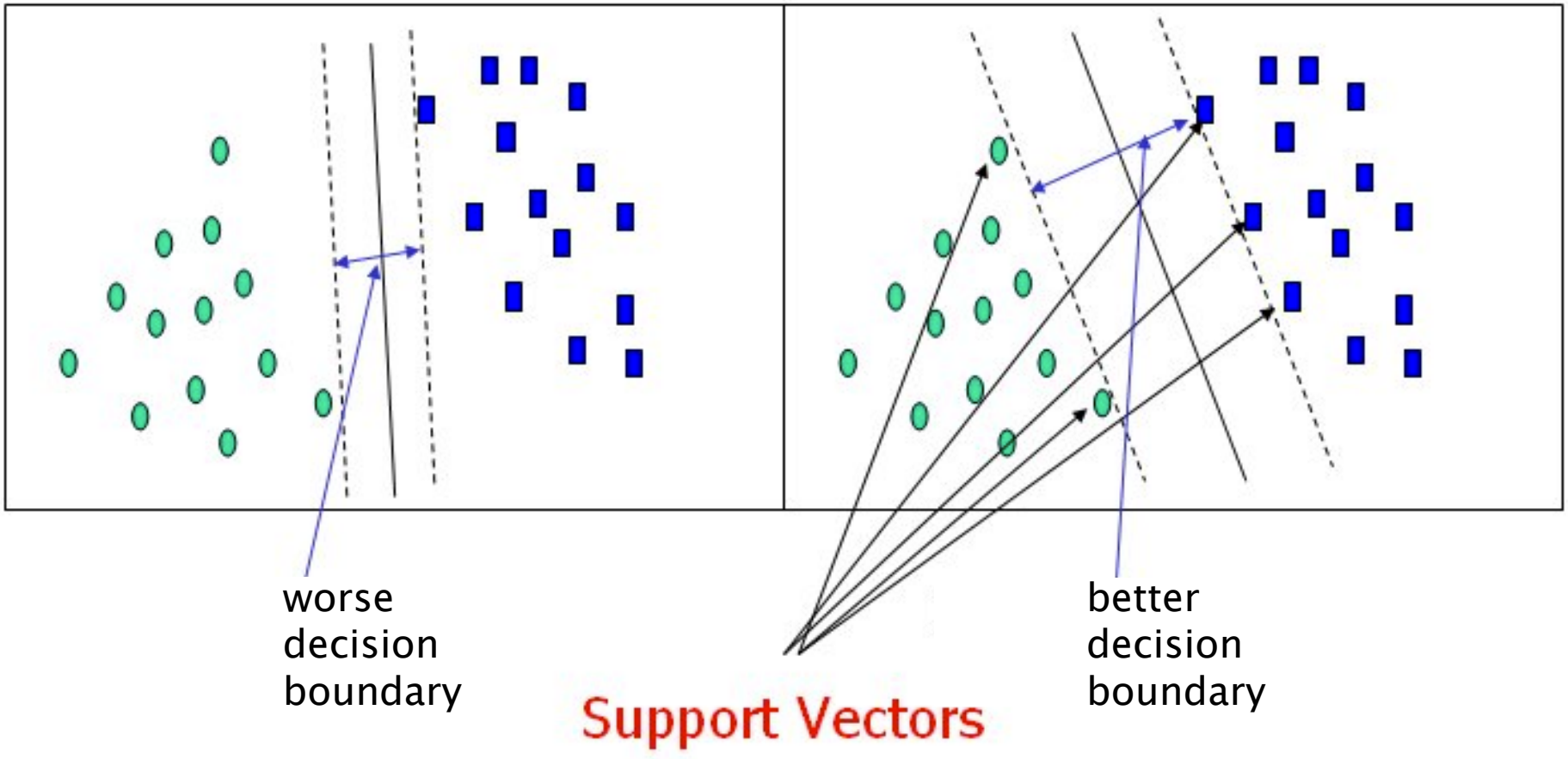


the instances are linearly separable

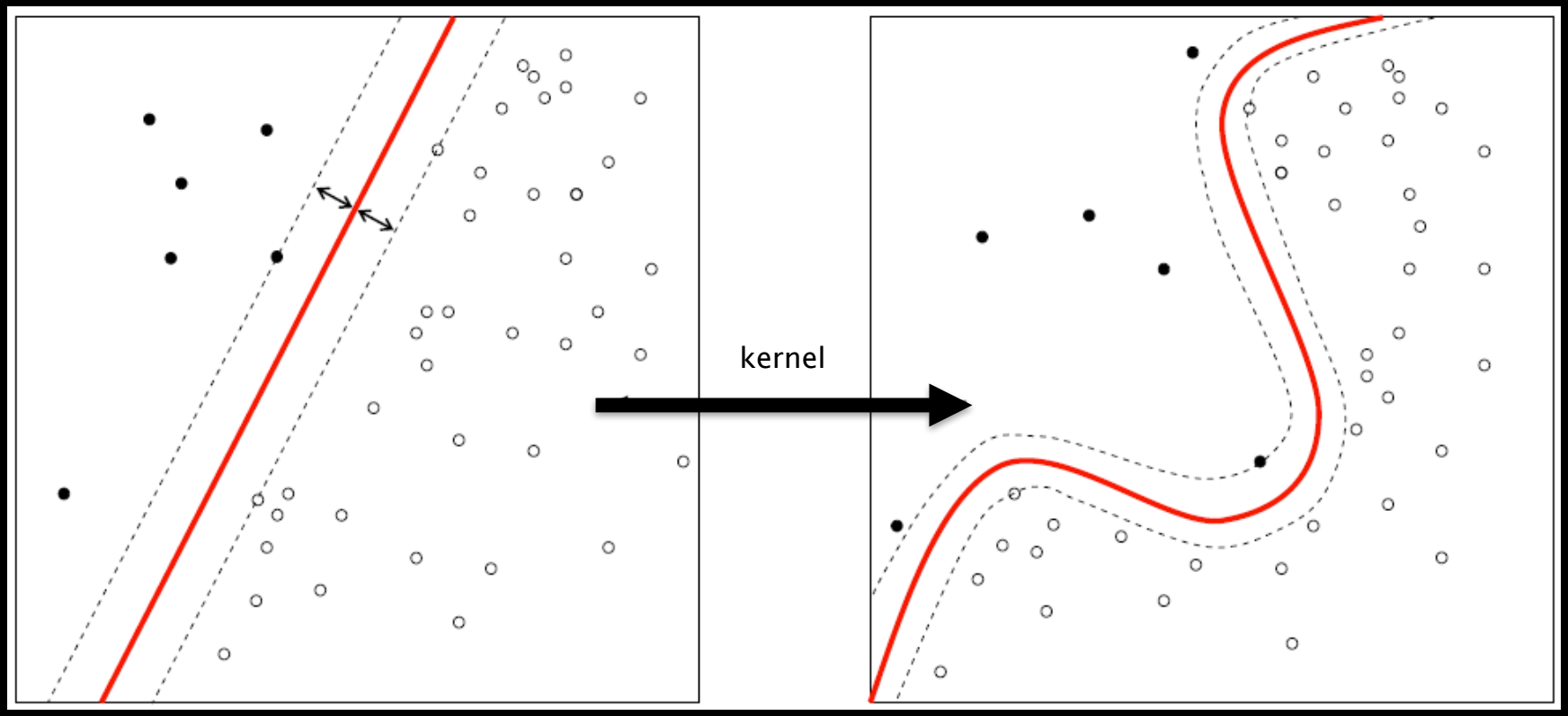


the instances are **not** linearly separable

Why “Support Vector Machine”?

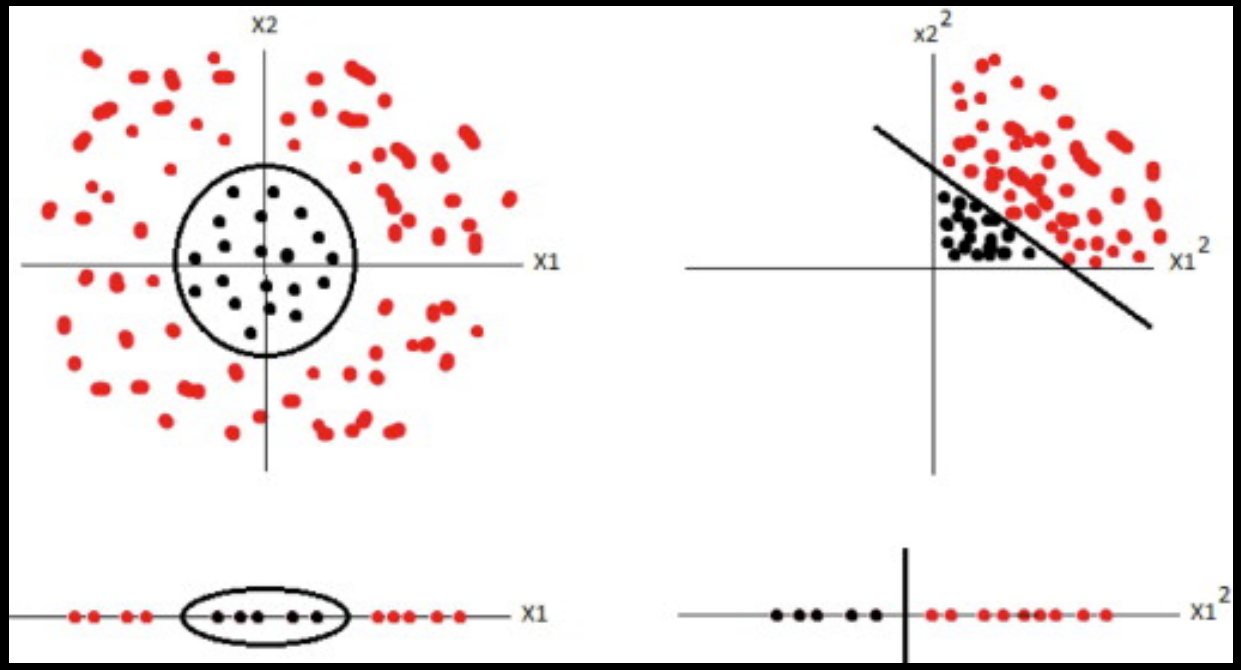


SVMs can make more complex decision boundaries by using kernels



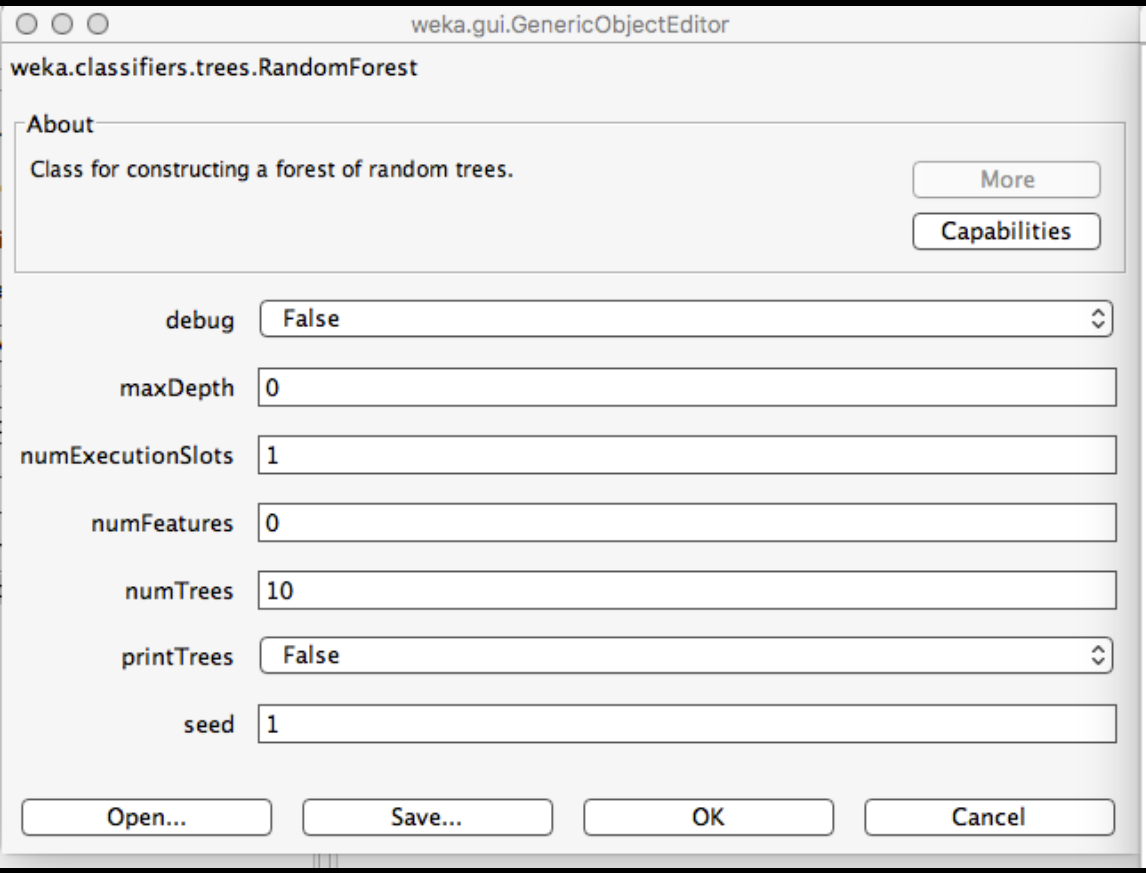
Kernel

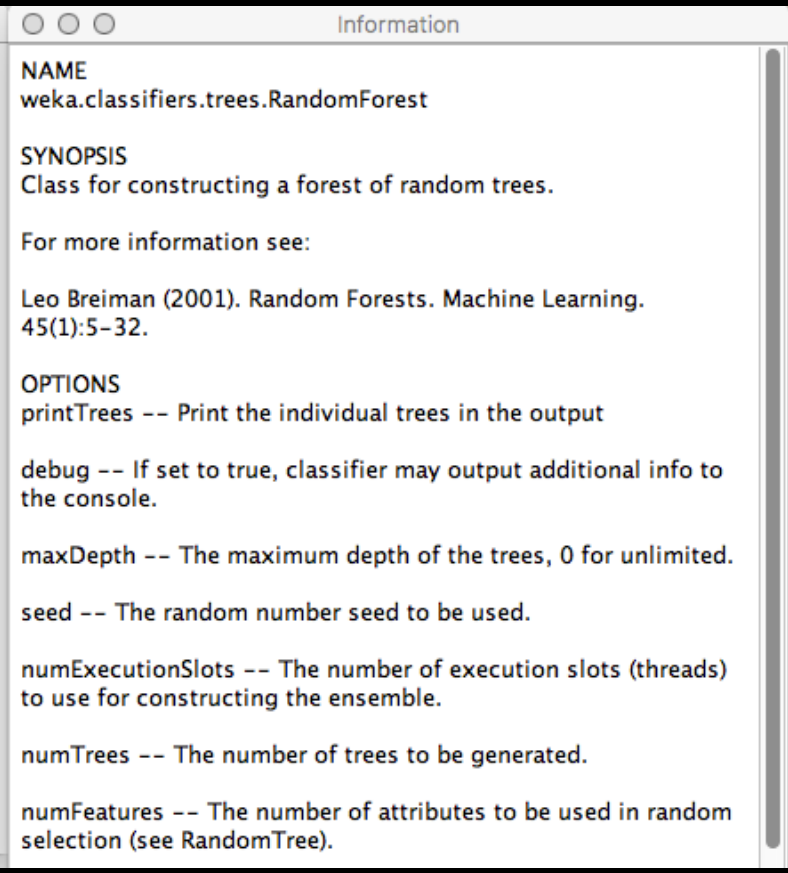
- A kernel performs a mathematical operation on instances in two classes that are **not** linearly separable, so that they do become linearly separable



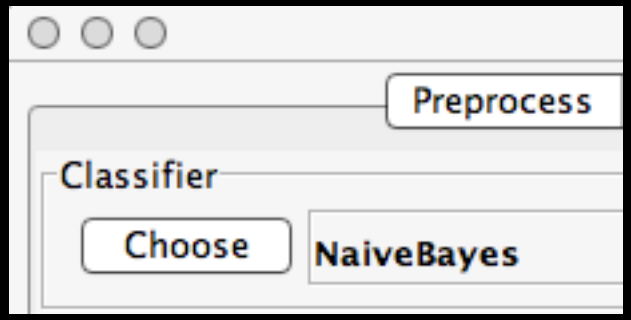
WEKA

Random Decision Forests in WEKA

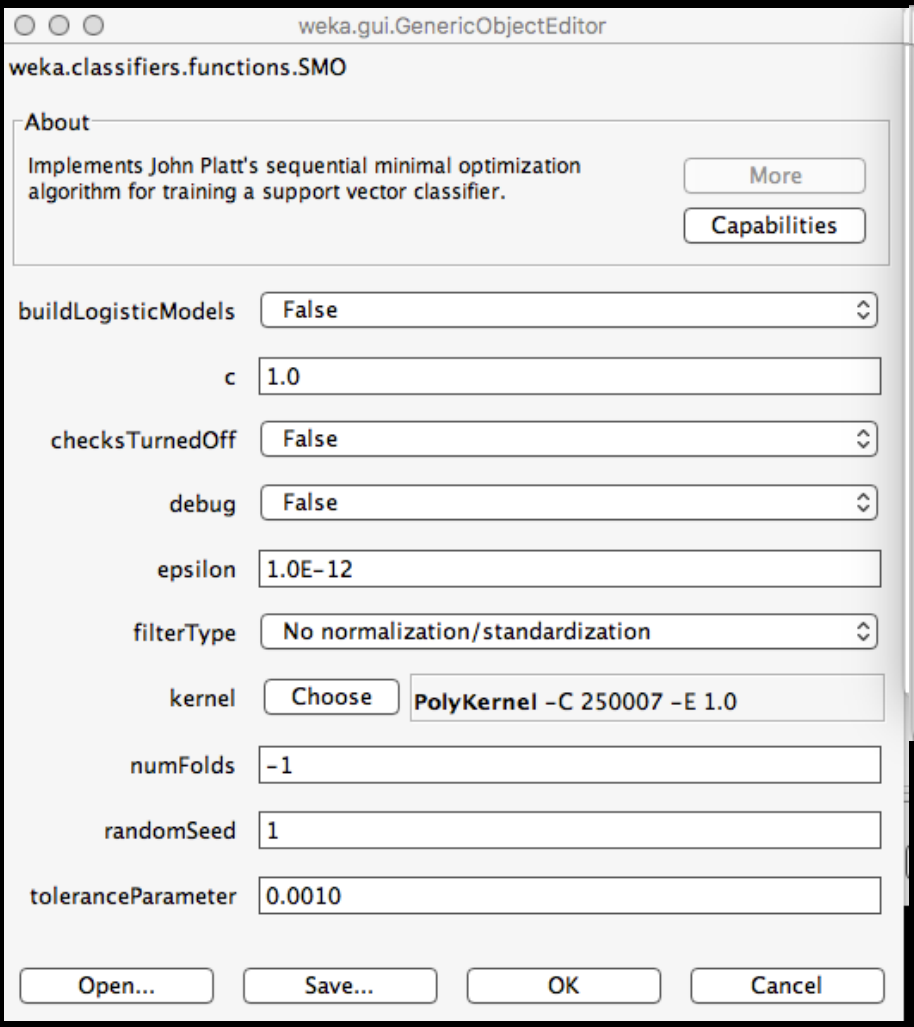


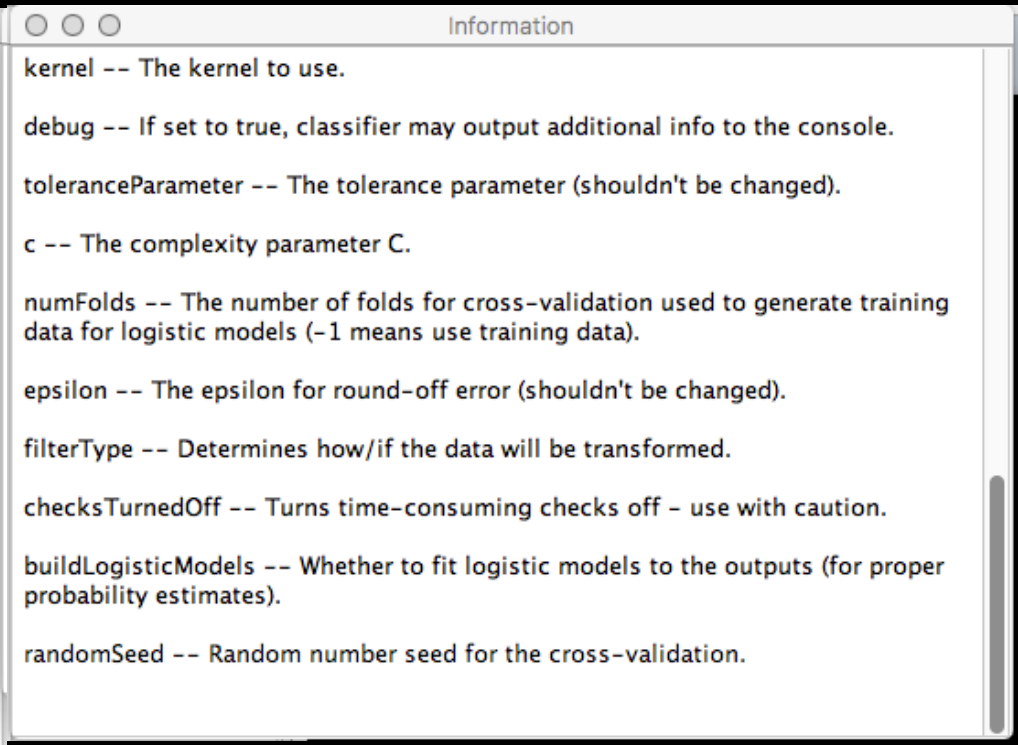


Naive Bayes in WEKA



SVM (SMO) in WEKA





(There is also a LibSVM version.)

Suggested Reading

WEKA book

Kernel methods: Section 6.4, pp. 223–229

Naive Bayes: Section 4.2, pp. 90–99

Please note that these sections contain many equations.