STAT540
Lecture 18: March 14th 2015

Supervised learning II

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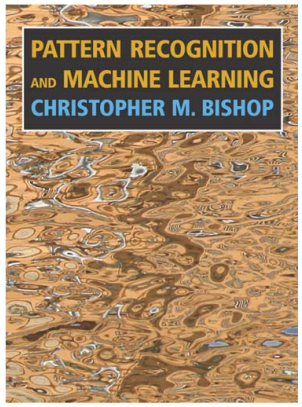
Outline

- Supervised learning
  - General framework
    - Loss function ; global and local minima
    - Complexity of decision boundary
  - Review KNN
  - Support vector machines
    - Linear separability
    - Classification margin
    - Kernels

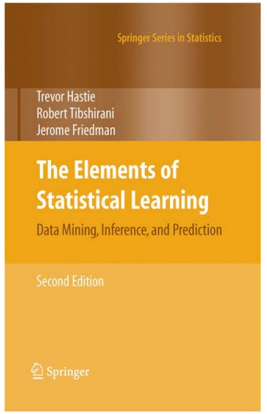
- Complexity and model selection:
  - **Overfitting**
  - Cross-validation

Reading recommendation:

1) Pattern recognition & Machine Learning
by Christopher Bishop



2) The Elements of Statistical Learning
by Hastie, Tibshirani, and Friedman



Components of supervised learning

1. Gather some training data: feature vectors + labels/ outcome.

2. Build/train (i.e., write down) a model that relates the relevant features to the labels/outcome.
   - **Minimize loss/cost function (more generally called objective function)**: fit model parameters based on data to fully specify the model.

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   - Extensively evaluate model using **cross-validation.**

3. Apply the model to new (**test**) data, where you don't have information about labels to make a prediction.

Loss function (more generally we call it objective function)

Linear regression (ordinary least squares):

$$y = f(\vec{x};\theta) = \alpha^T \vec{x} + b$$

Model parameter

Minimize the error on training data!

Objective function $\underset{\alpha,b}{\operatorname{argmin}} \sum_{i=1} (y_i - (b + \alpha^T \vec{x}_i))^2$ Squared error

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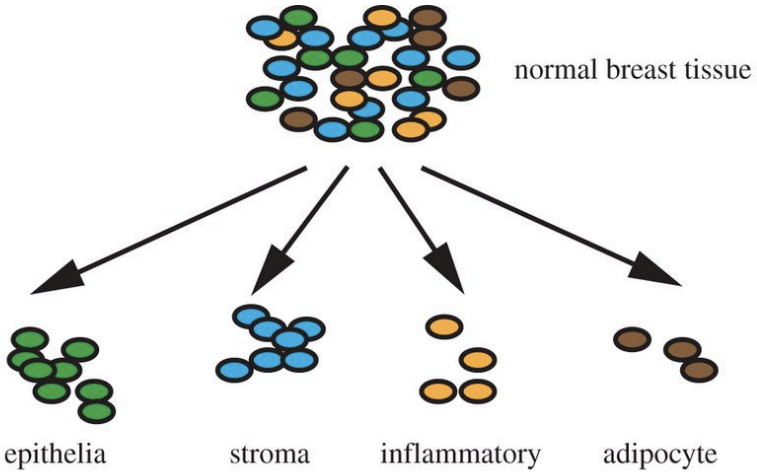
Such that $\alpha_i \geq 0$ For all i

Non-negative least squares (NNLS) for estimating cell type proportions

Objective function $\underset{\alpha,b}{\operatorname{argmin}} \sum_{i=1} (y_i - (b + \alpha^T \vec{x}_i))^2$ Squared error

Such that $\alpha_i \geq 0$



$$y_{i,j} = b + \sum_{d=1}^{D} \alpha_d x_{i,d}$$

Loss function

Linear regression: $y = f(\vec{x};\theta) = \alpha^T \vec{x} + b$

Model parameter

Minimize the error on training data!

$$\underset{\alpha,b}{\operatorname{argmin}} \sum_{i=1} (y_i - (b + \alpha^T \vec{x}_i))^2$$

Squared error

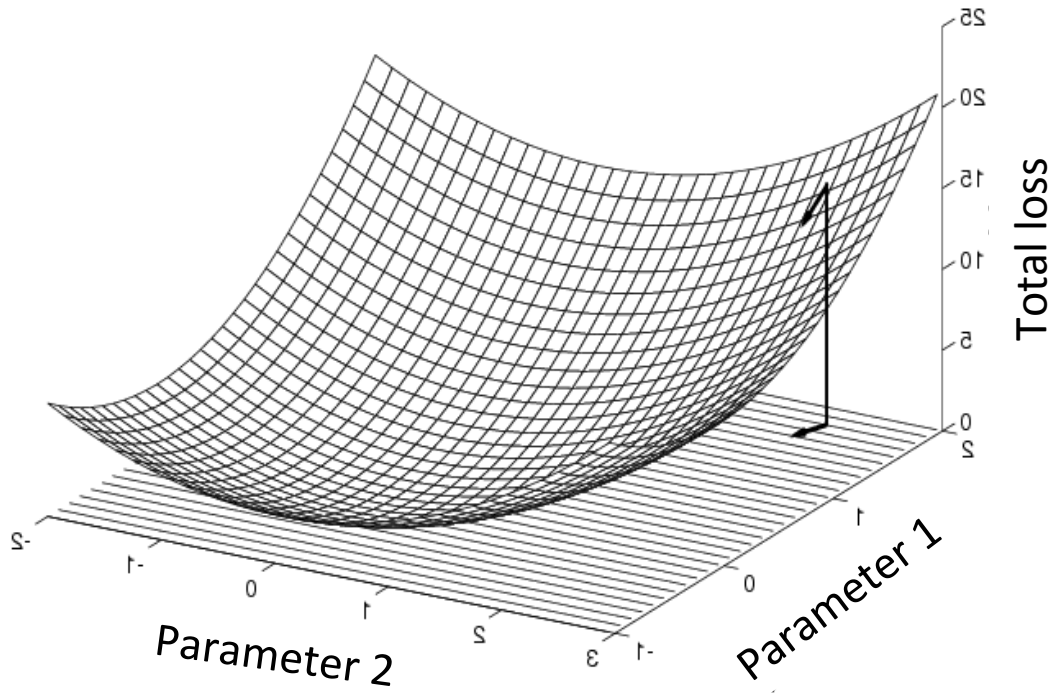
General loss function for classification

Model $c_i = f(\vec{x}_i;\theta)$

Total loss = $\sum_{i=1}^{n} \text{cost}(c_i, f(\vec{x}_i,\theta))$

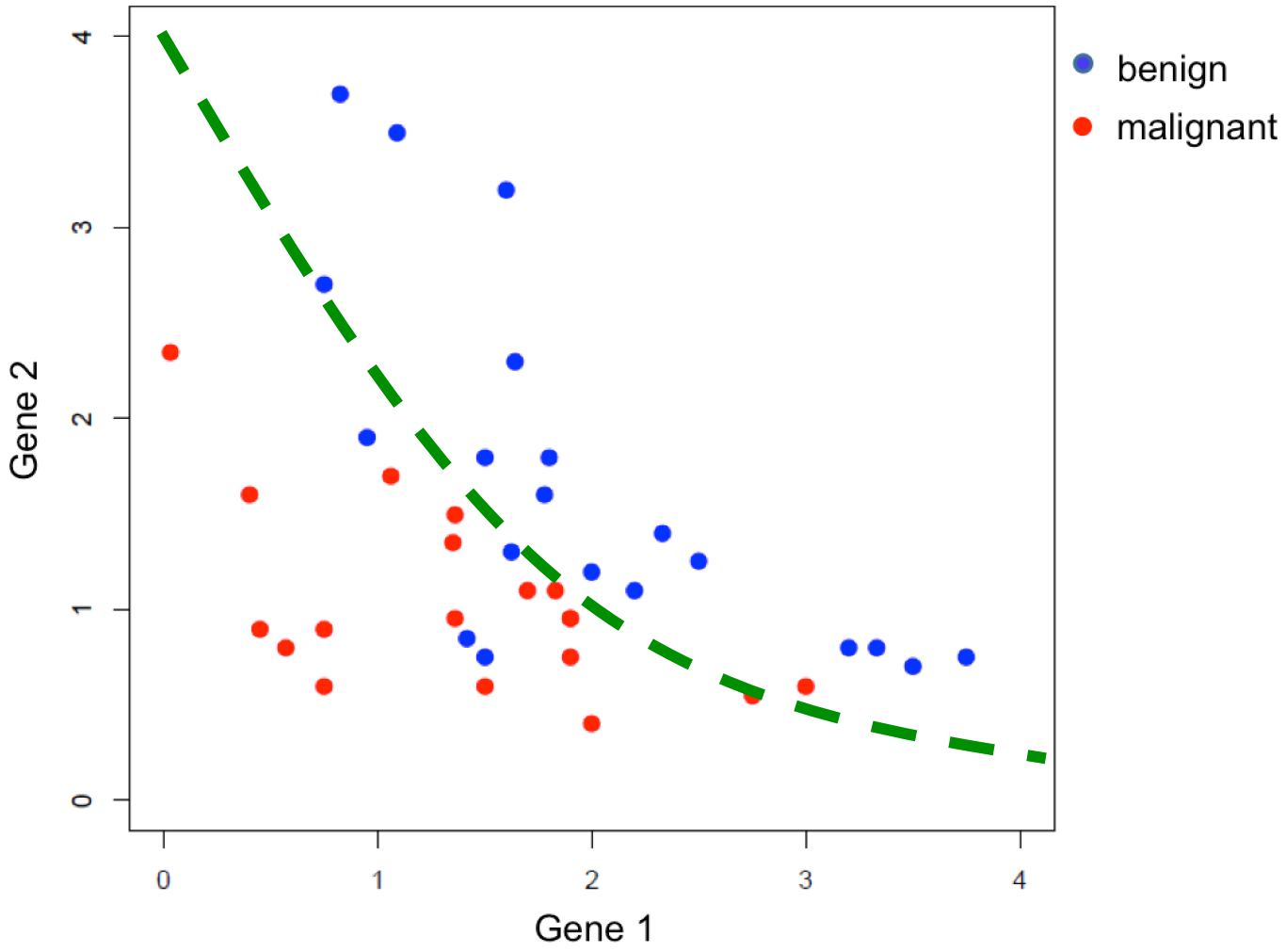
Local vs. global minimum

Concave objective function: one optimal solution (no local minima)



Gradient of the objective function points to the direction of global minimum

Decision boundary



Some example classification methods

Linear/Quadratic discriminant analysis

Naïve Bayes

} Generative approach

Logistic regression

Support vector machines

Neural networks & “Deep Nets”

Decision trees

} Discriminative approach

K-nearest neighbors

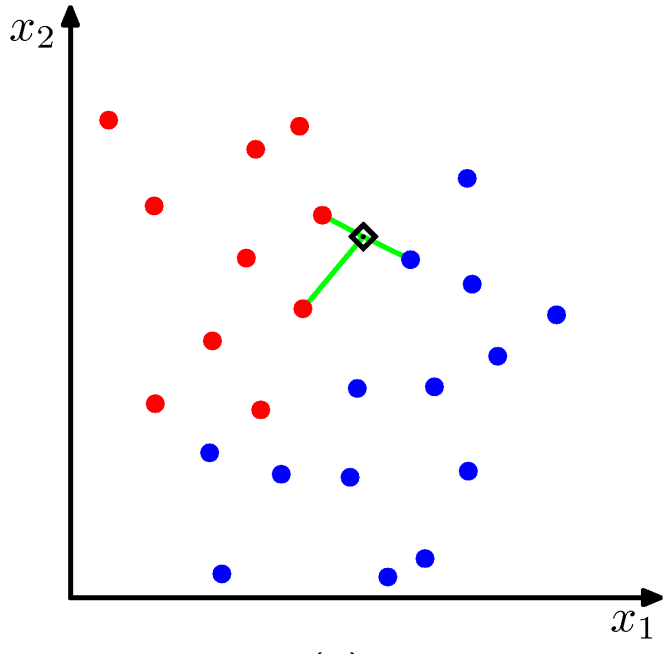
} Nonparametric approach

k-nearest neighbor classifier

One way to define ”near” is to use a fixed predetermined number of neighbours (K)

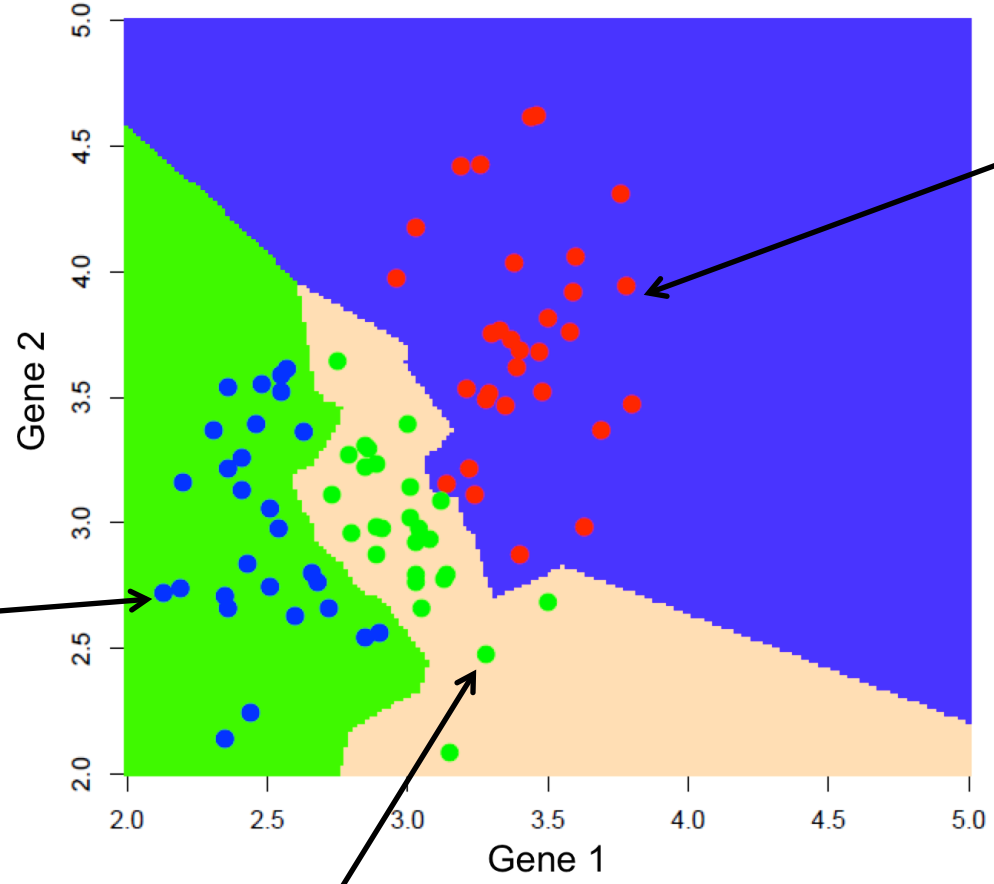
–> count how many points of each class there are among the closest K neighbours to $\boldsymbol{x}$

–> use the majority class as the predicted class



Bishop figure 2.27

1-NN

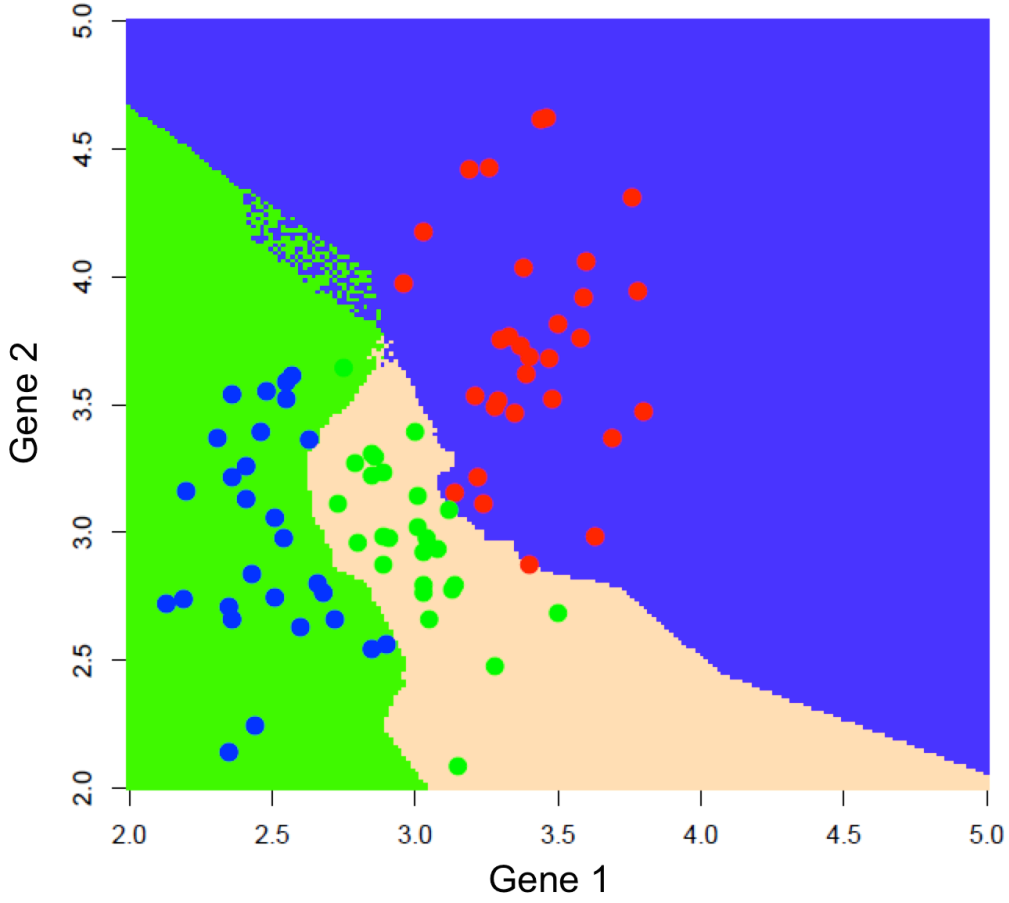


Examples from the "red" class

Examples from the "blue" class

Examples from the "green" class

5-NN



Support Vector Machines (SVMs): history

- Introduced in early 90s by Boser, Guyon, and Vapnik.
-
- Very popular approach for classification.

- Can be applied to binary classification problem and problems with more than two classes.

- Empirically has had good performance in many different fields (bioinformatics, text and image recognition)

Support Vector Machines (SVMs): two novel ideas

1. Define the decision boundary by maximizing the classification *margin*

2. SVMs kernel trick: make linear model work in non-linear setting.
   – Input-output relationships may not be linear

Review of notation: binary classification

- Given training data $\{(\vec{x}_1, c_1), \ldots, (\vec{x}_n, c_n)\}, \;\; c_i \in \{-1, +1\}$

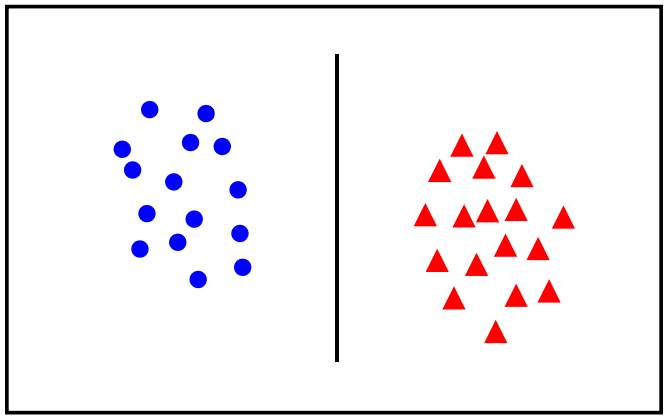
- Goal: learn a classifier $f(\vec{x}_i)$ such that

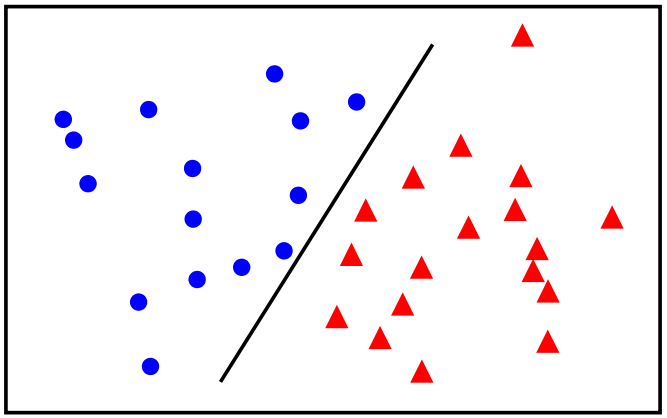
$$f(\vec{x}_i) = \begin{cases} \geq 0 & \text{if } c_i = +1 \\ < 0 & \text{if } c_i = -1 \end{cases}$$

- Note: $f(\vec{x}_i) c_i > 0$ for correct classification of example *i*

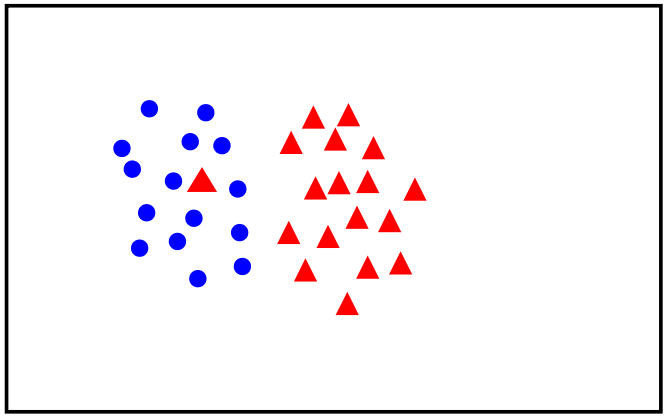
Linear separability

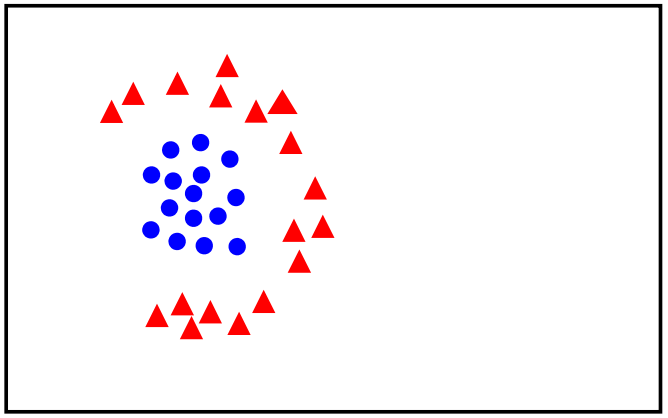
linearly separable





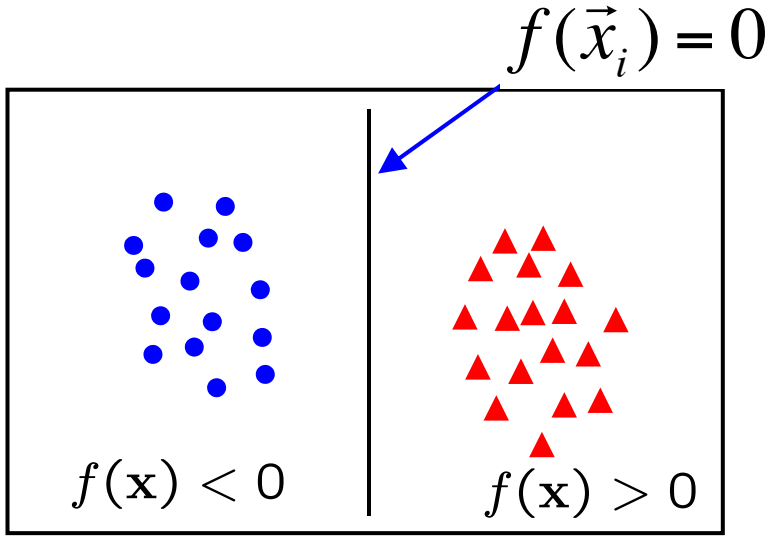
not linearly separable



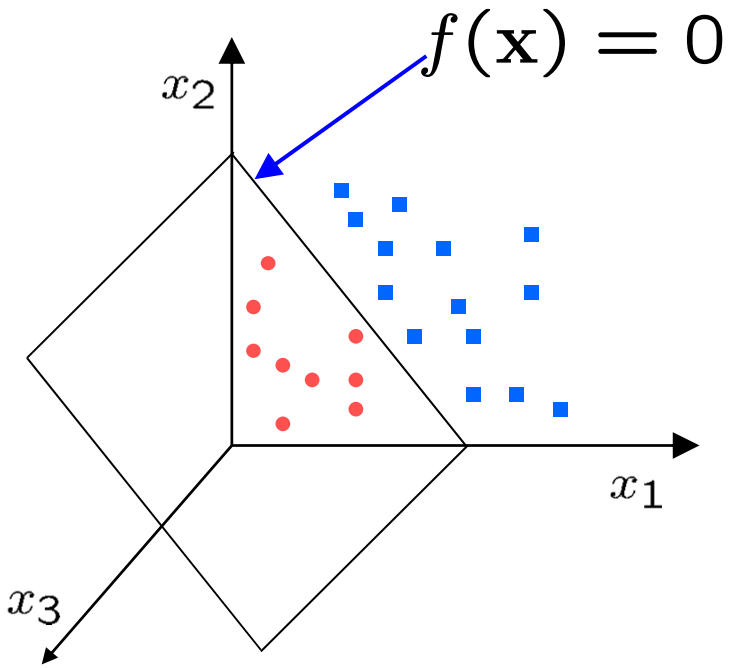


Linear classifier

$$f(\vec{x}) = \vec{w}^T \vec{x} + b$$

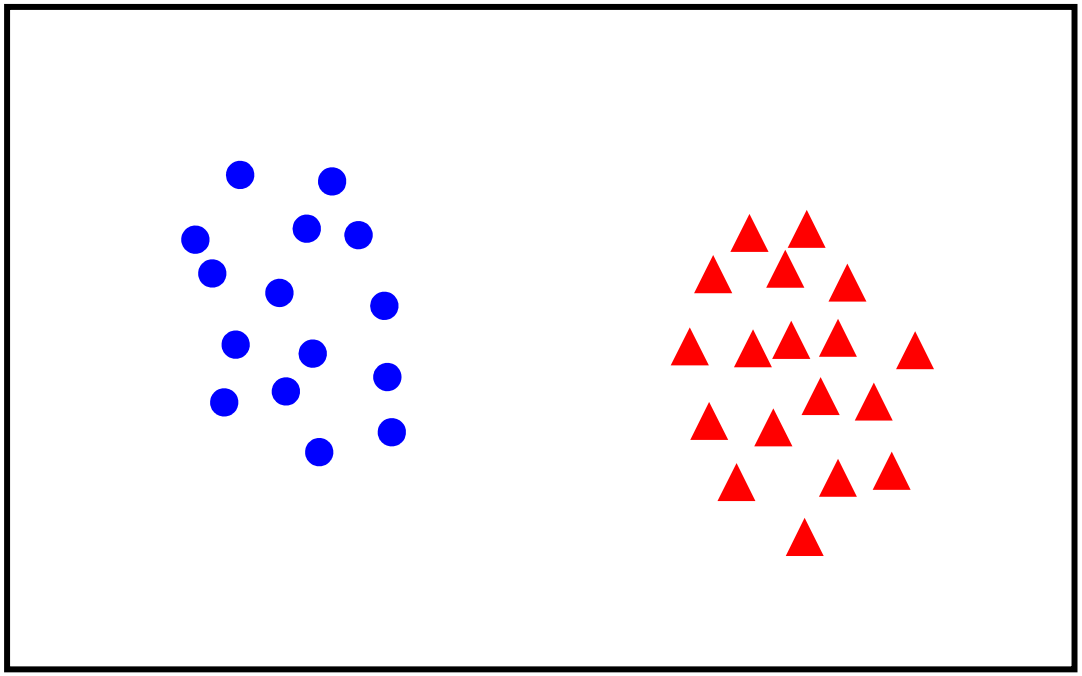


Linear classifier in 3D



- In 3D the decision boundary is a plane
- in nD the decision boundary is a hyperplane

What's the best linear decision boundary?



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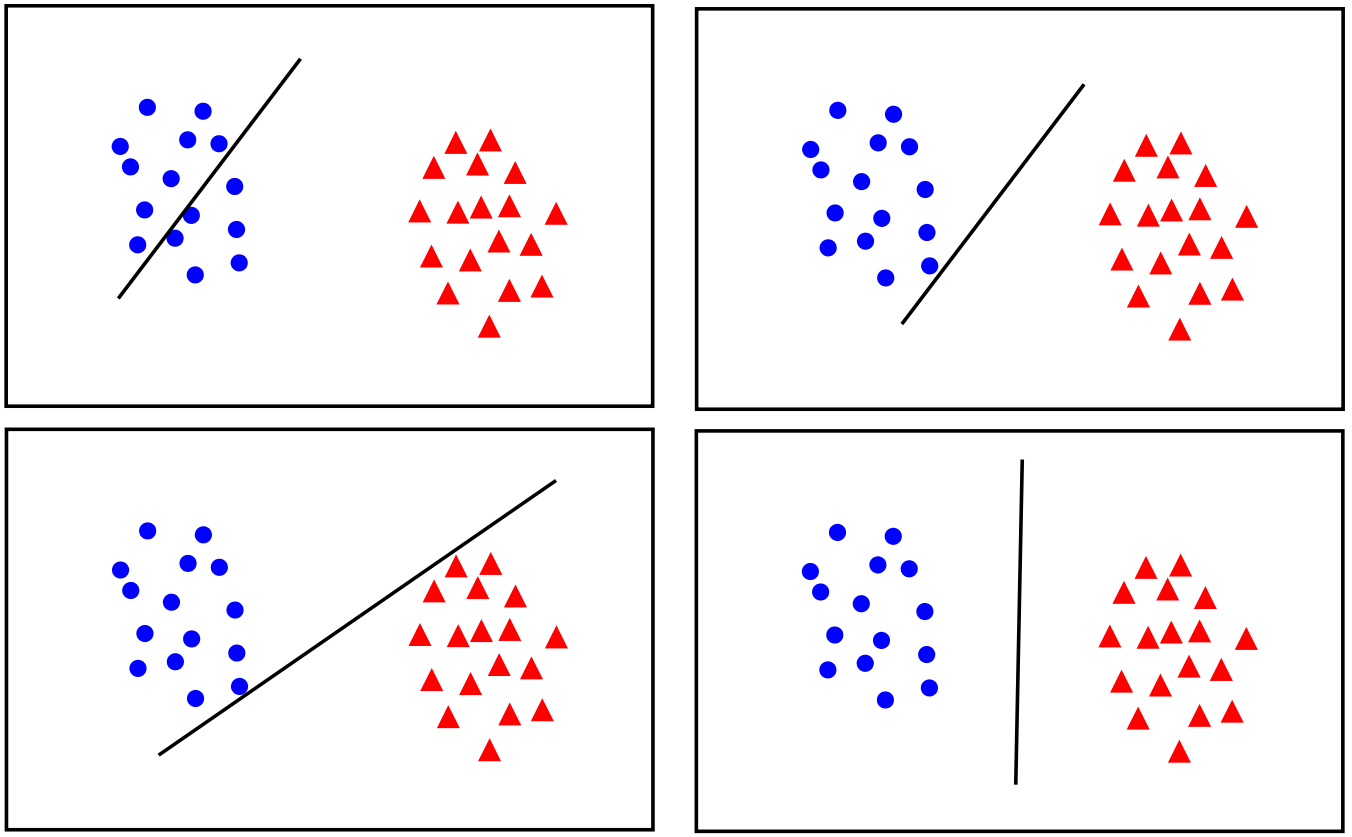
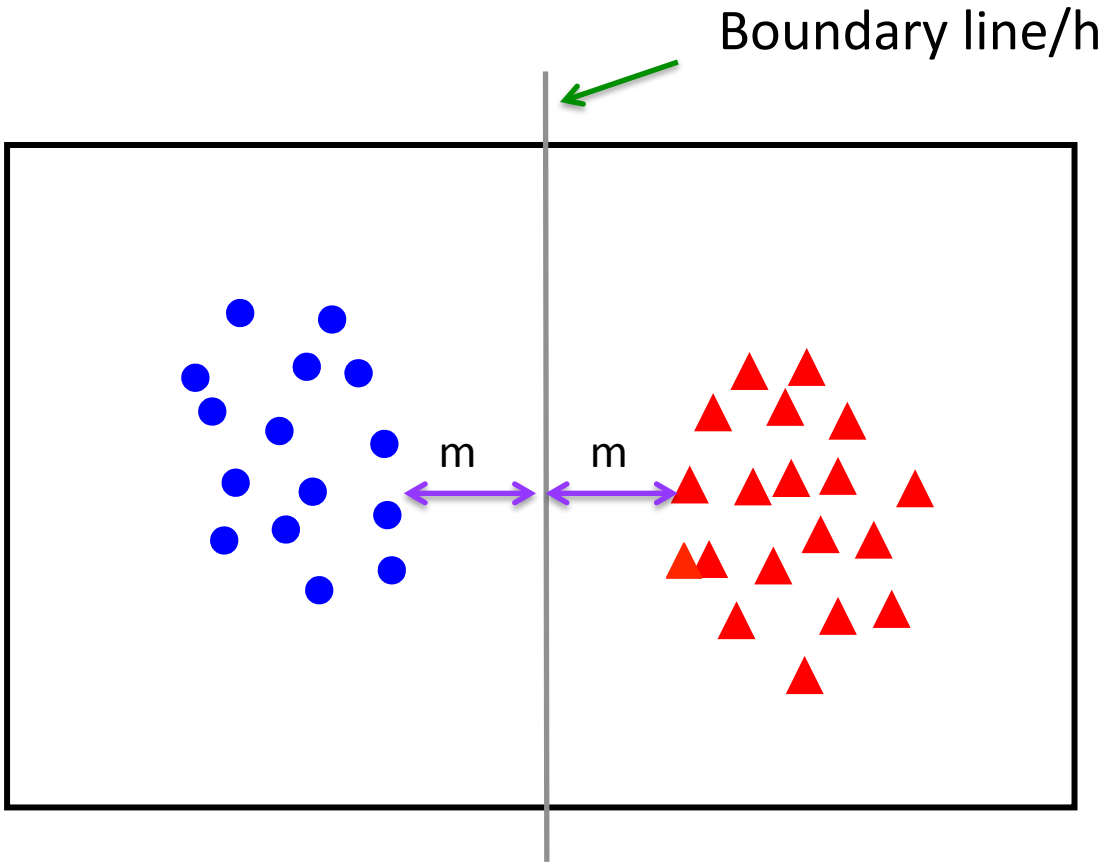


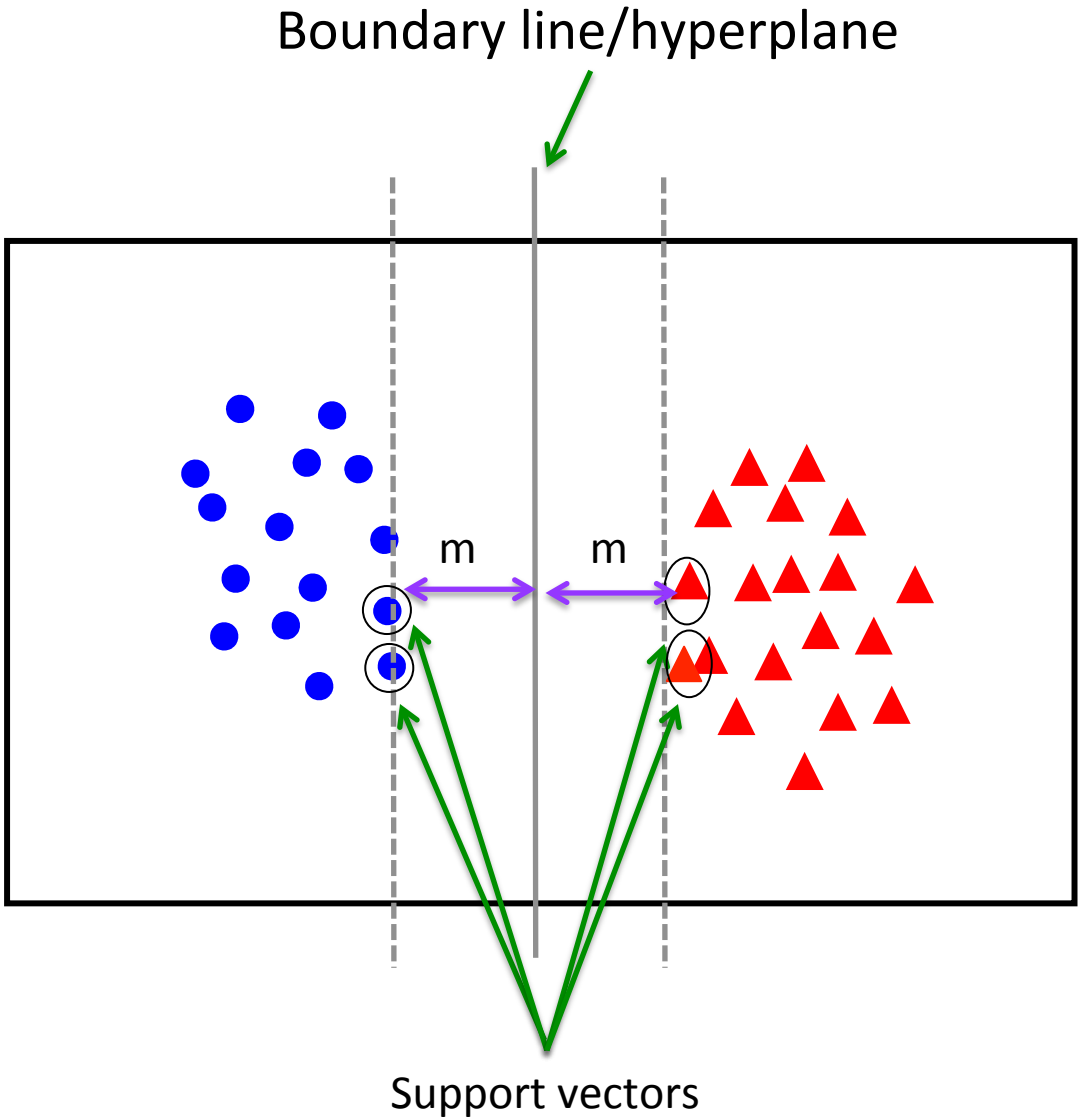
What's the best linear decision boundary?

- One that has the largest distance (margin) to the nearest training data points of any class.



m is the "margin"

What's the best linear decision boundary?



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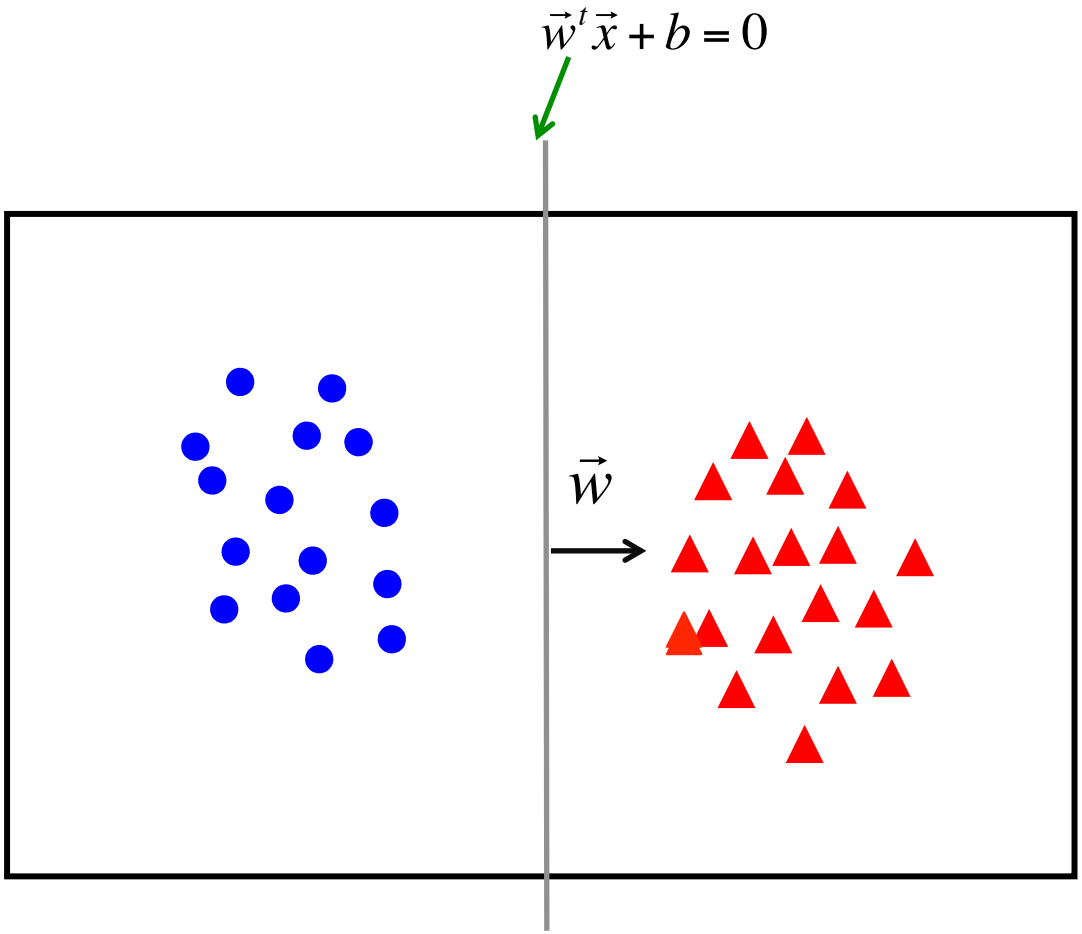

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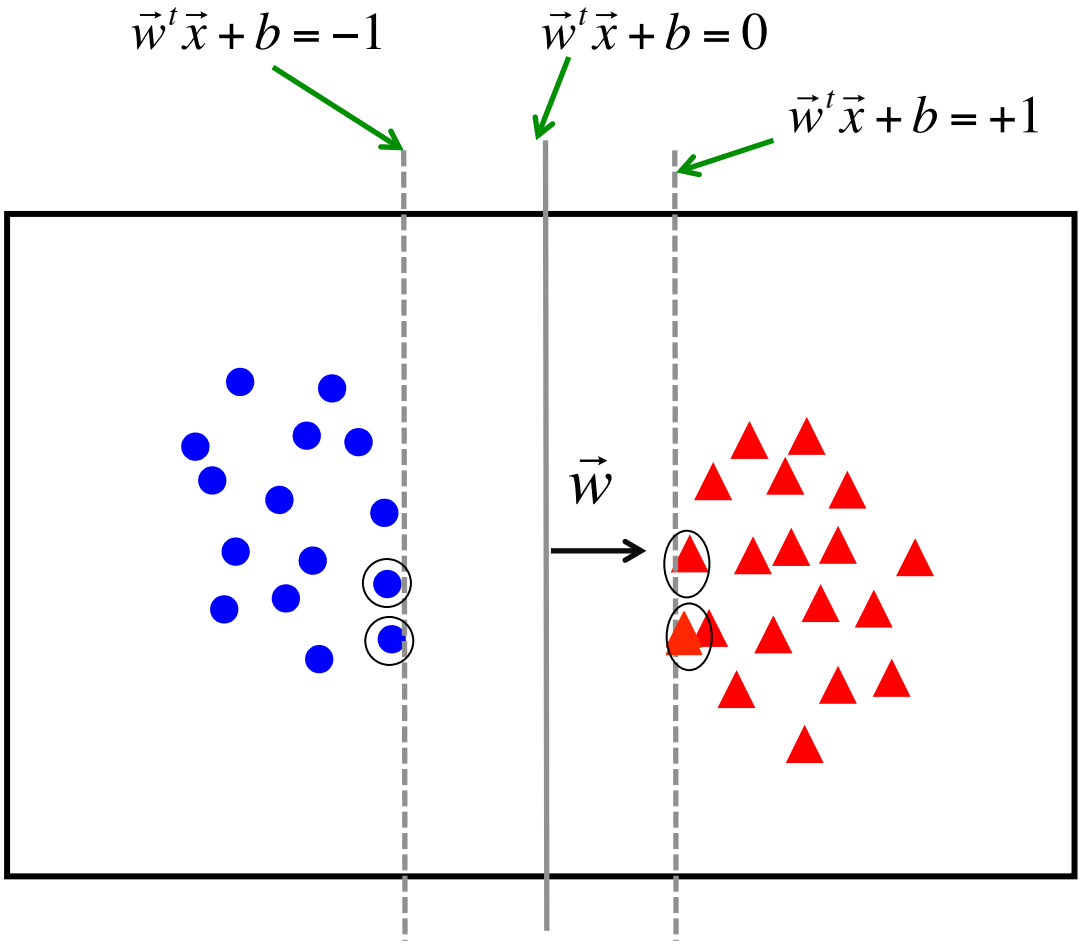
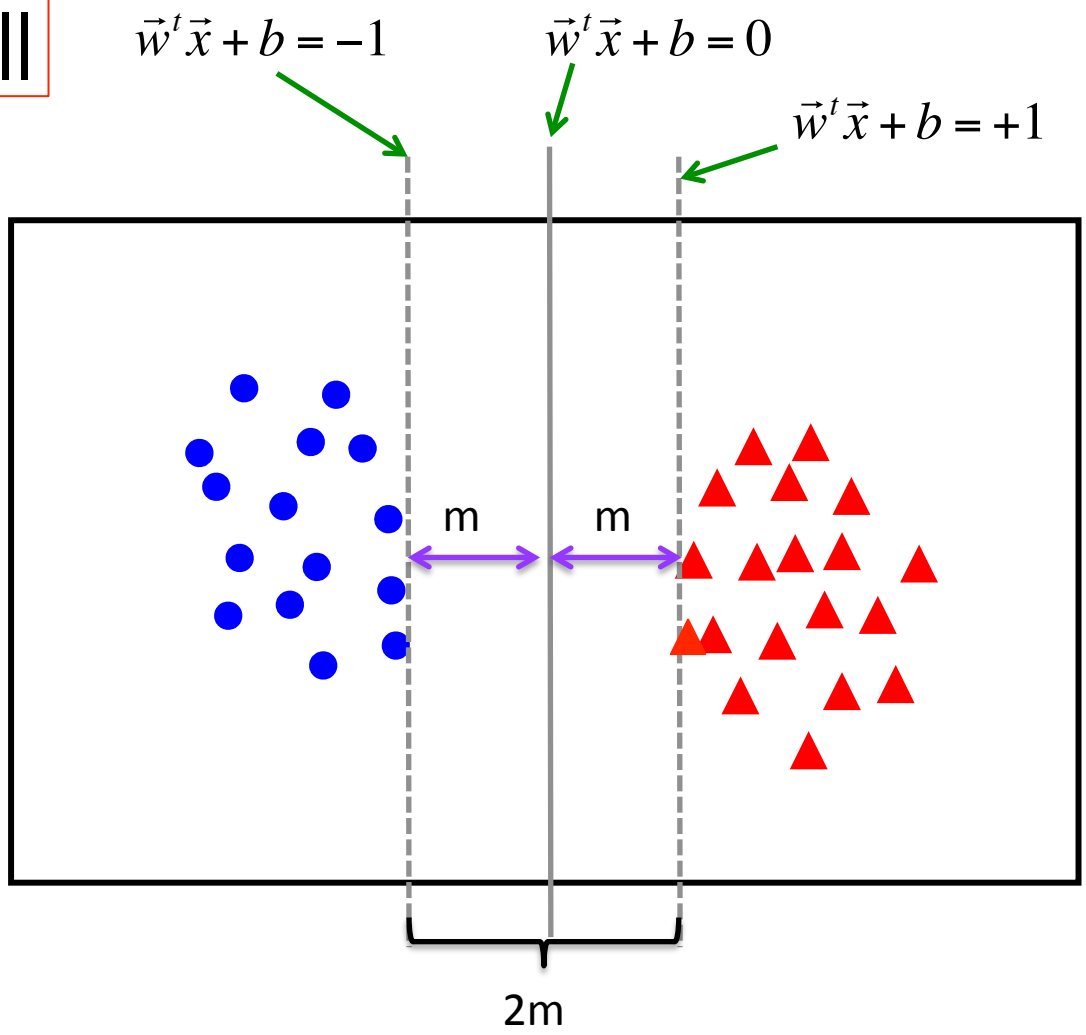


What's the best linear decision boundary?

$$m = \frac{1}{\| \vec{w} \|}$$



Finding the maximum margin hyperplane

- Maximize margin $2m = \frac{2}{\| \vec{w} \|}$

- Correctly classify all training data:

$$\begin{cases} \vec{w}^t \vec{x}_i + b \geq -1 & \text{if } c_i = -1 \\ \vec{w}^t \vec{x}_i + b \geq +1 & \text{if } c_i = +1 \end{cases}$$

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***Quadratic optimization problem*:**

Maximize $\frac{2}{\| \vec{w} \|}$

such that $c_i(\vec{w}^t \vec{x}_i + b) \geq +1$ for all i

Solving the SVM Optimization Problem

- Long story short … you can derive the "dual" of the SVM optimization problem, and then you realize:

$$\underset{\alpha_1,\ldots,\alpha_n}{\operatorname{argmax}} \sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j c_i c_j \vec{x}_i^{\,t} \vec{x}_j$$

$$\text{such that} \quad \sum_{i=1}^{n} \alpha_i c_i = 0 \;\; ; \alpha_i \geq 0$$

Solving the SVM Optimization Problem

$$\underset{\alpha_1,\ldots,\alpha_n}{\text{argmax}} \sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j c_i c_j \vec{x}_i^{t}\vec{x}_j$$

$$\text{such that} \quad \sum_{i=1}^{n}\alpha_i c_i = 0 \quad ; \alpha_i \geq 0$$

$$f(\vec{x}_i) = \text{sign}(\sum_j \alpha_j c_j (\vec{x}_i . \vec{x}_j))$$

Solving the SVM Optimization Problem

Similarity between examples i and j

$$f(\vec{x}_i) = \text{sign}(\sum_j \alpha_j c_j (\vec{x}_i . \vec{x}_j))$$

Replace $\vec{x}_i \vec{x}_j$ by a potentially non-linear similarity function

$$\text{similarity}(\vec{x}_i, \vec{x}_j) = K(\vec{x}_i, \vec{x}_j)$$

What is a support vector machine?

1. A subset of training examples (**support vectors**)
2. A vector of weights for the support vectors ($\vec{\alpha}$)
3. A similarity function: K($\mathbf{x}_1$,$\mathbf{x}_2$) (**kernel** function)

Predicting class labels for example x_i:

$$f(\vec{x}_i) = \text{sign}(\sum_j \alpha_j c_j K(\vec{x}_i, \vec{x}_j))$$

$c_i = \{-1, 1\}$ We are switching to -1,1 class labels for mathematical convenience

(Thanks to P. Domingos for slides)

Examples of kernels

Linear kernel: $K(\vec{x}_i, \vec{x}_j) = \vec{x}_i^T \vec{x}_j$

Polynomial kernel: $K(\vec{x}_i, \vec{x}_j) = (\vec{x}_i^T \vec{x}_j)^d$

Gaussian kernel: $K(\vec{x}_i, \vec{x}_j) = \exp(-\frac{\| \vec{x}_i - \vec{x}_j \|}{\sigma})$

Examples of kernels

Parameters you can tune

Linear kernel: $K(\vec{x}_i, \vec{x}_j) = \vec{x}_i^T \vec{x}_j$

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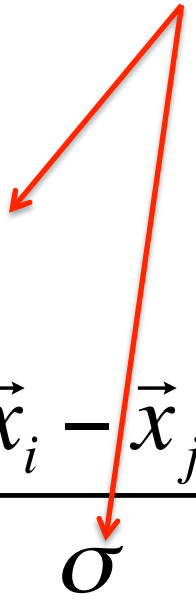

SVMs summary

- Pros
  - Lots of publically available software.
  - Kernel based framework is very powerful, flexible.
  - Works well in practice, but need to have good number of training examples.
- Cons
  - Need to define suitable kernel (not hard to do, just use linear kernel).
  - Hard optimization problem: training could take a long time depending on size of your problem.

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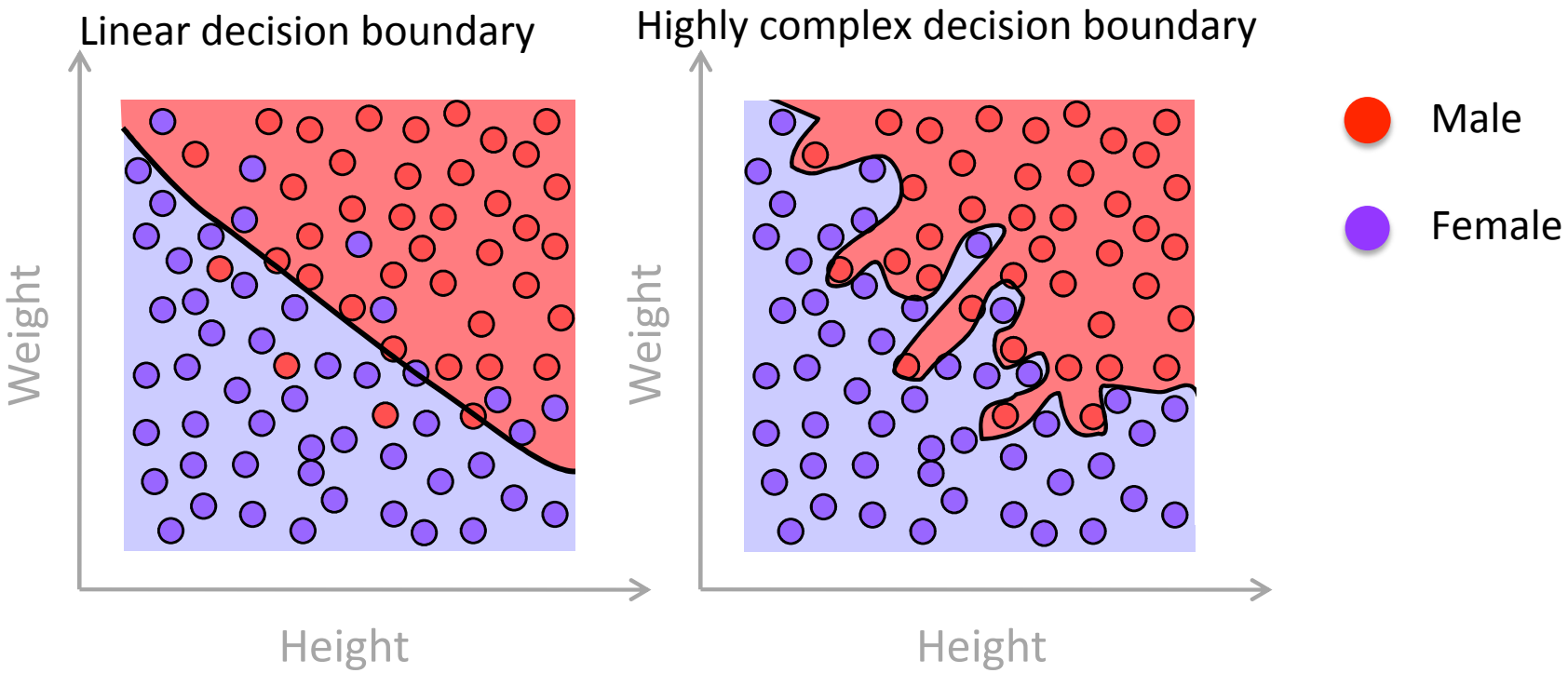
- Supervised learning
  - General framework
    - Loss function ; global and local minima
    - Complexity of decision boundary
  - Review KNN
  - Support vector machines
    - Linear separability
    - Classification margin
    - Kernels

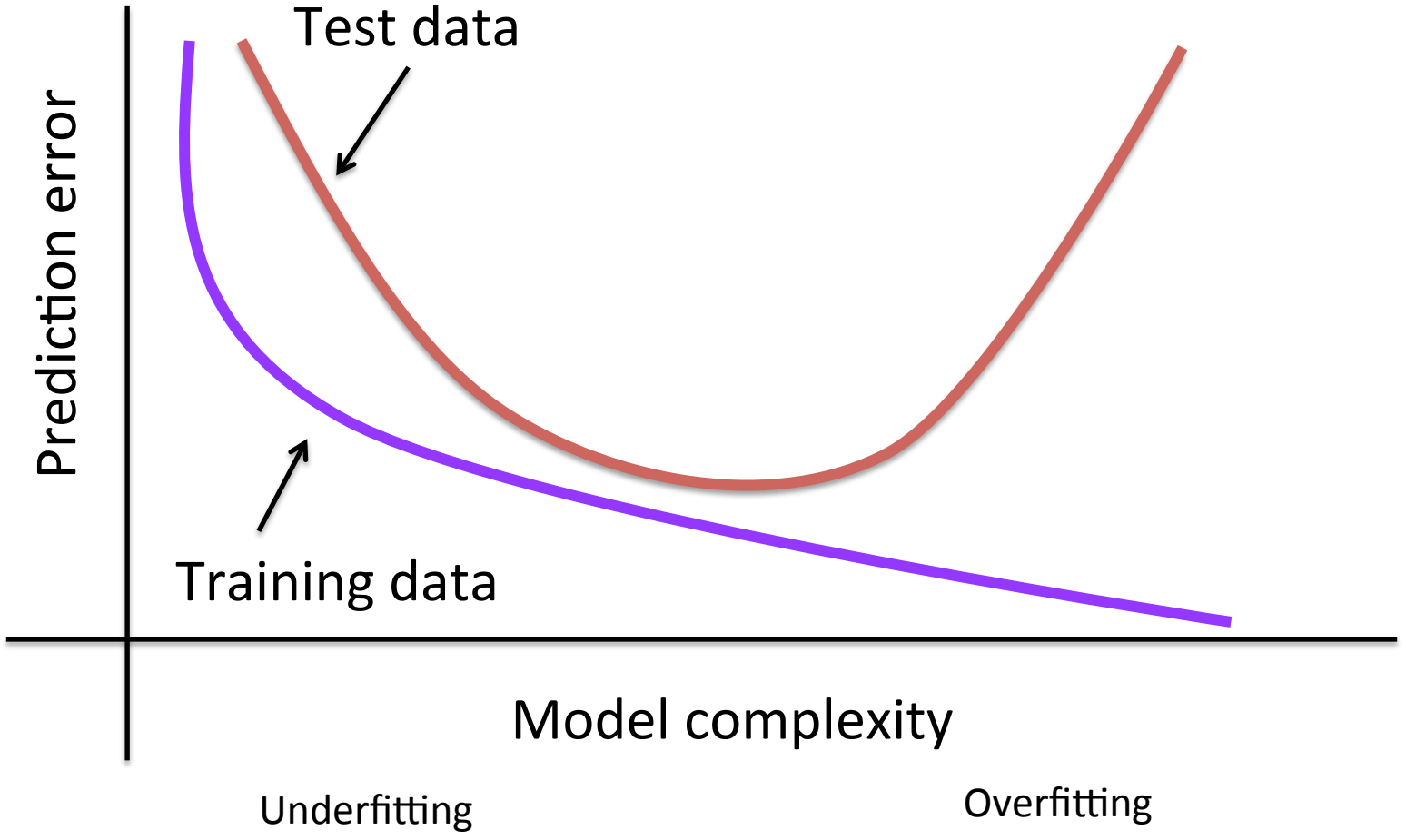
- Complexity and model selection:
  - **Overfitting**
  - Cross-validation

Overfitting

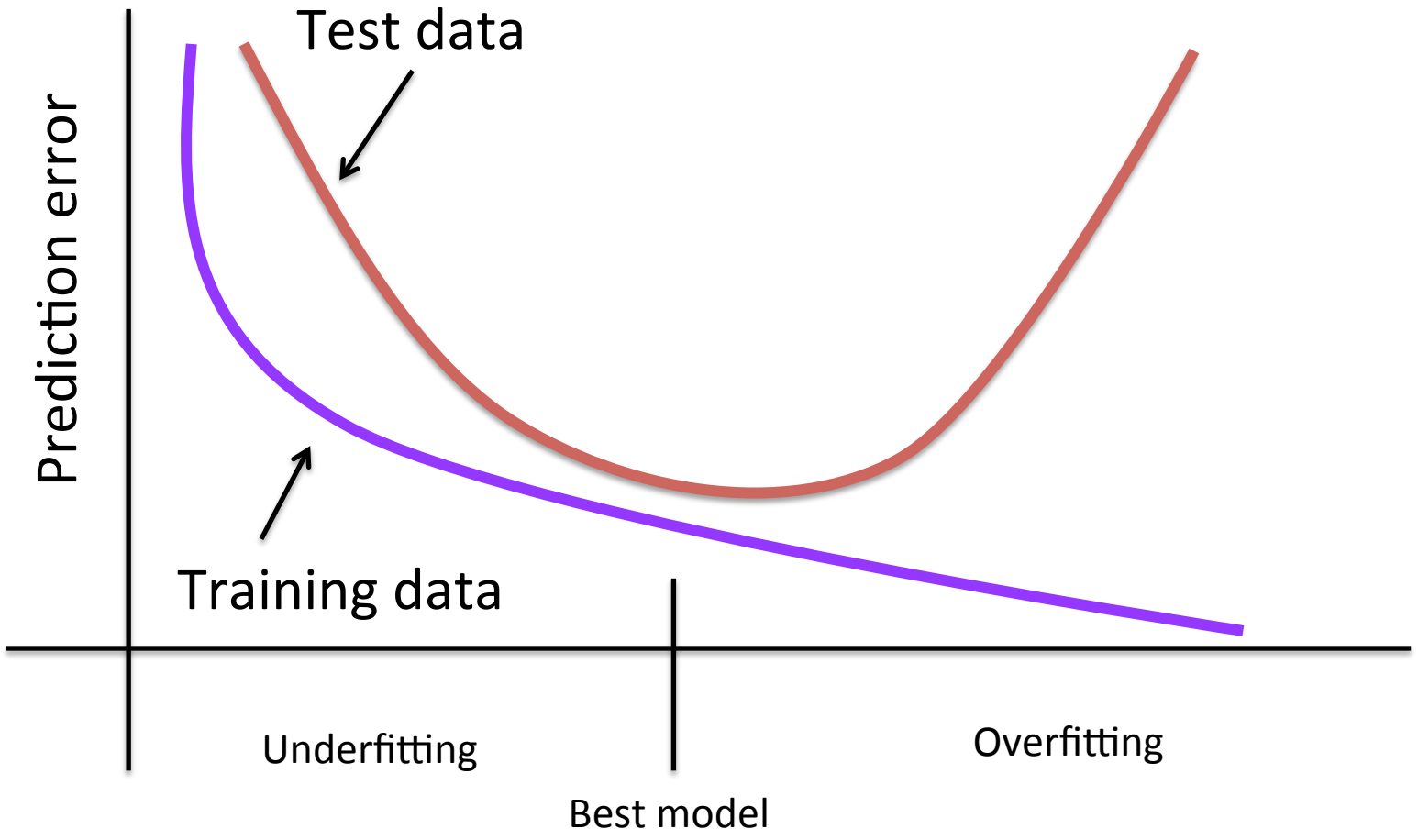
If we allow very complicated predictors, we could overfit the training data:



Error and model complexity



Error and model complexity



How can we determine the optimal complexity? model selection

- **Cross-validation**
- Complexity regularization
  - Variable selection
  - Variable penalization
- Information criteria (AIC and BIC)

Hold-out method

- We would like to pick a model with lowest **generalization** error.

- Simple idea. Find some "validation" data. Train model on training data, measure performance of the model on validation data.

Training data

$$D_T = \{(\vec{x}_1, y_1), \ldots, (\vec{x}_n, y_n)\}$$

Validation data

$$D_V = \{(\vec{x}_1, y_1), \ldots, (\vec{x}_n, y_n)\}$$

Hold-out method

- Model that generalizes: low validation error

- Problems:
  - What if we don't have some validation data put aside?
  - Validation error could be misleading, what if we got unlucky on the split of training/validation data?

Cross-validation (CV)

- K-fold cross-validation:
  1. Create k partition (folds) of input data
  2. Set aside data in one of the data subsets (fold) for validation
  3. Train model on all but the held-out fold
  4. Measure cross-validation (CV) error using data from the left-out fold:

$$\text{CV Error}_i = \frac{1}{n_i} \sum_{j \in T_i} L(y_j, \hat{y}_{j(-i)})$$

  5. Repeat leaving out for all folds and measure average error

$$\text{CV Error} = \frac{1}{k} \sum_{i=1}^{k} \text{CV Error}_i$$

Example: 4-fold cross-validation

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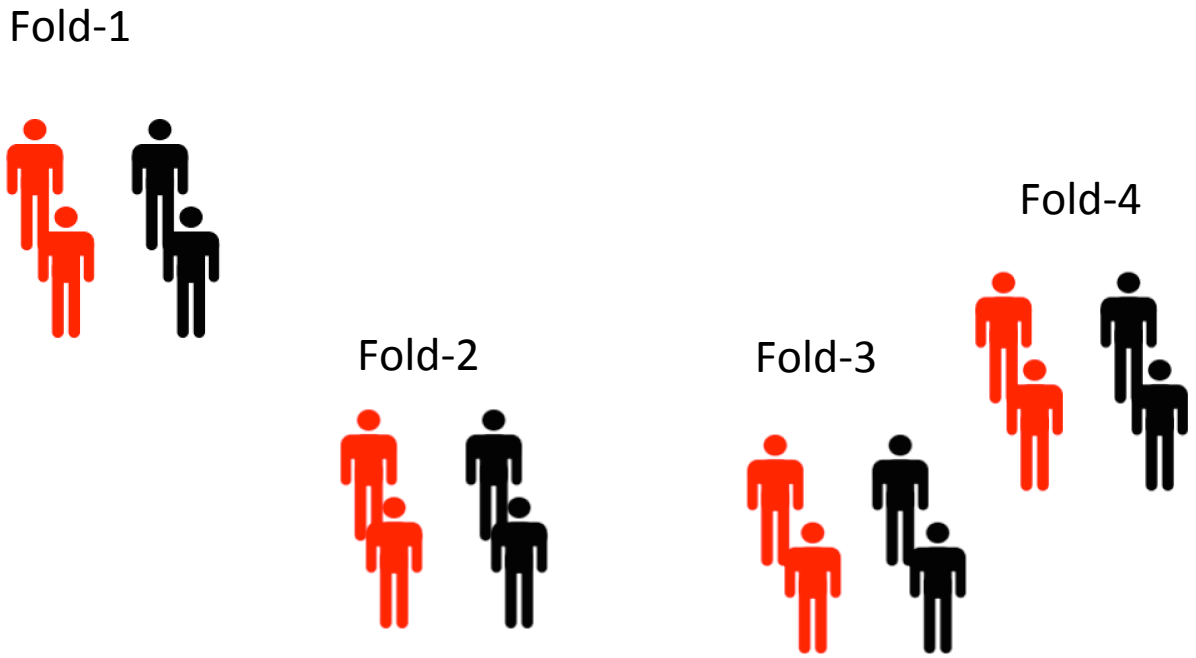
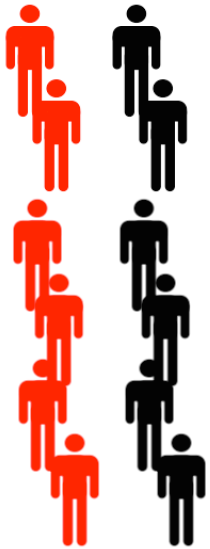


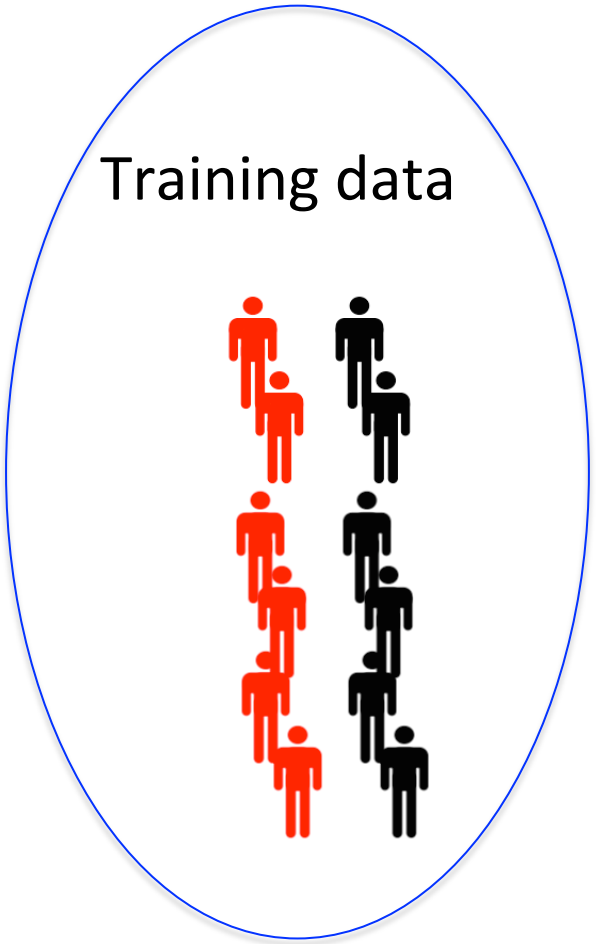
Example: 4-fold cross-validation

Training data



Validation data

Example: 4-fold cross-validation



Validation data

Use model to predict class labels for validation fold

Build (train) a model

$$\text{CV\_Error}_i = \frac{1}{n_i} \sum_{j \in T_i} L(y_j, \hat{y}_{j(-i)})$$

K-fold cross-validation

- k can range from 2 to n:
  - Larger k:
    - Variance of true error will be high
    - Computational time will be large
    + More data to fit model parameters
  - Smaller k:
    + reduced computation time
    + variance of error estimate is small
    - Less data to fit model parameters
- n-fold CV is called “Leave-One-Out” CV
- In practice:
  - Lower k is more reliable, eg., 3-fold CV is standard.

Concluding remarks

- Supervised learning:
  - Write down a model → objective function
  - Algebraically simplify model/objective as much as possible
  - Write down the optimization problem: solve for parameters

  (highly recommend doing the above, and program your own logistic regression function)
- Overfitting:
  - Constantly think about it!
  - Overfitting can severely delude you about the accuracy of your model

- Cross-validation:
  - Good fist-pass solution for tuning parameters, finding the "right" model
  - But could be computationally very expensive
  - Serious assumption: test and training data are independent (this may not always be the case, especially due to systematic artifacts in genomics)