STAT540
Lecture 18: March 16th 2015

Supervised learning II

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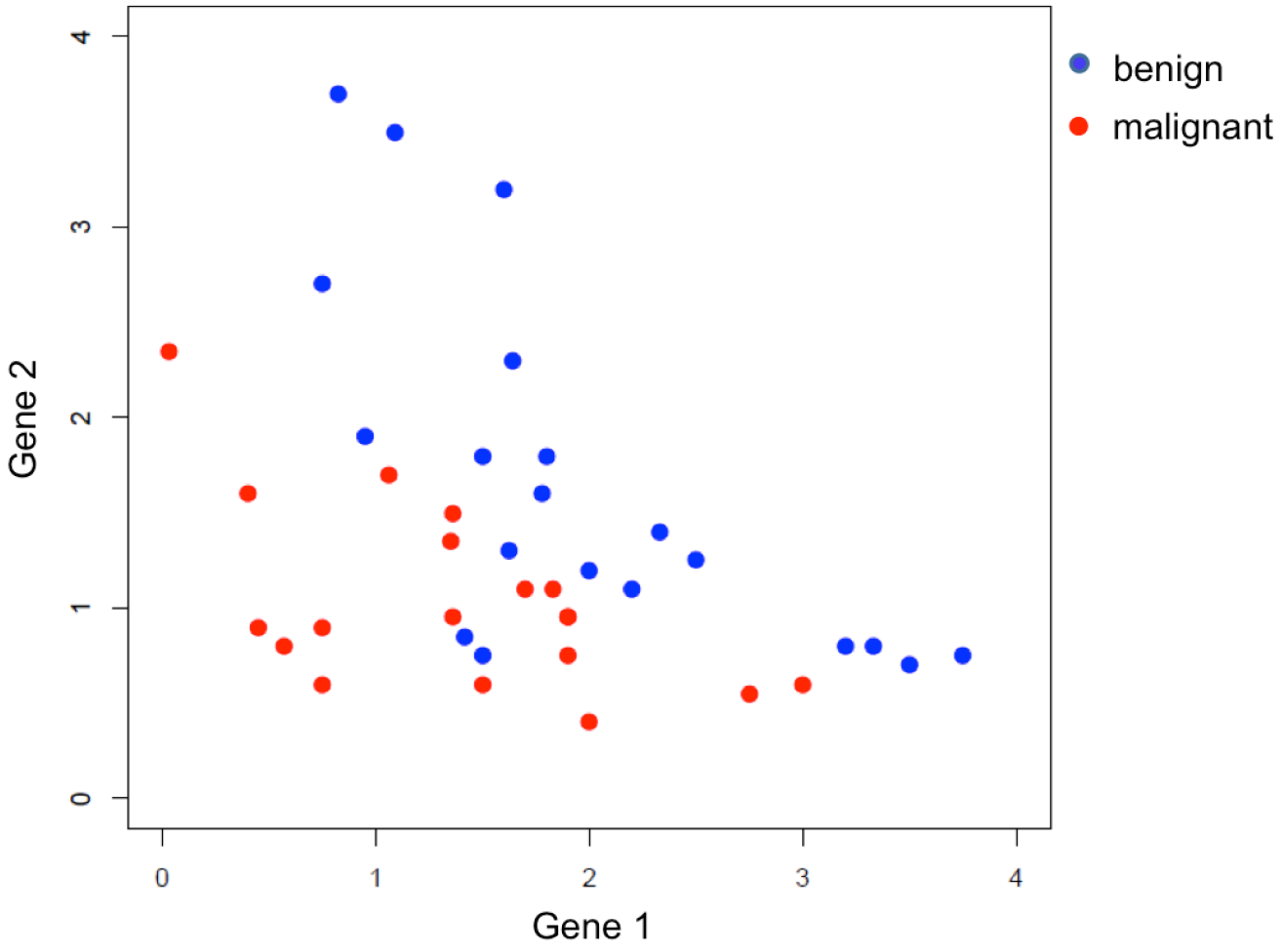
Outline

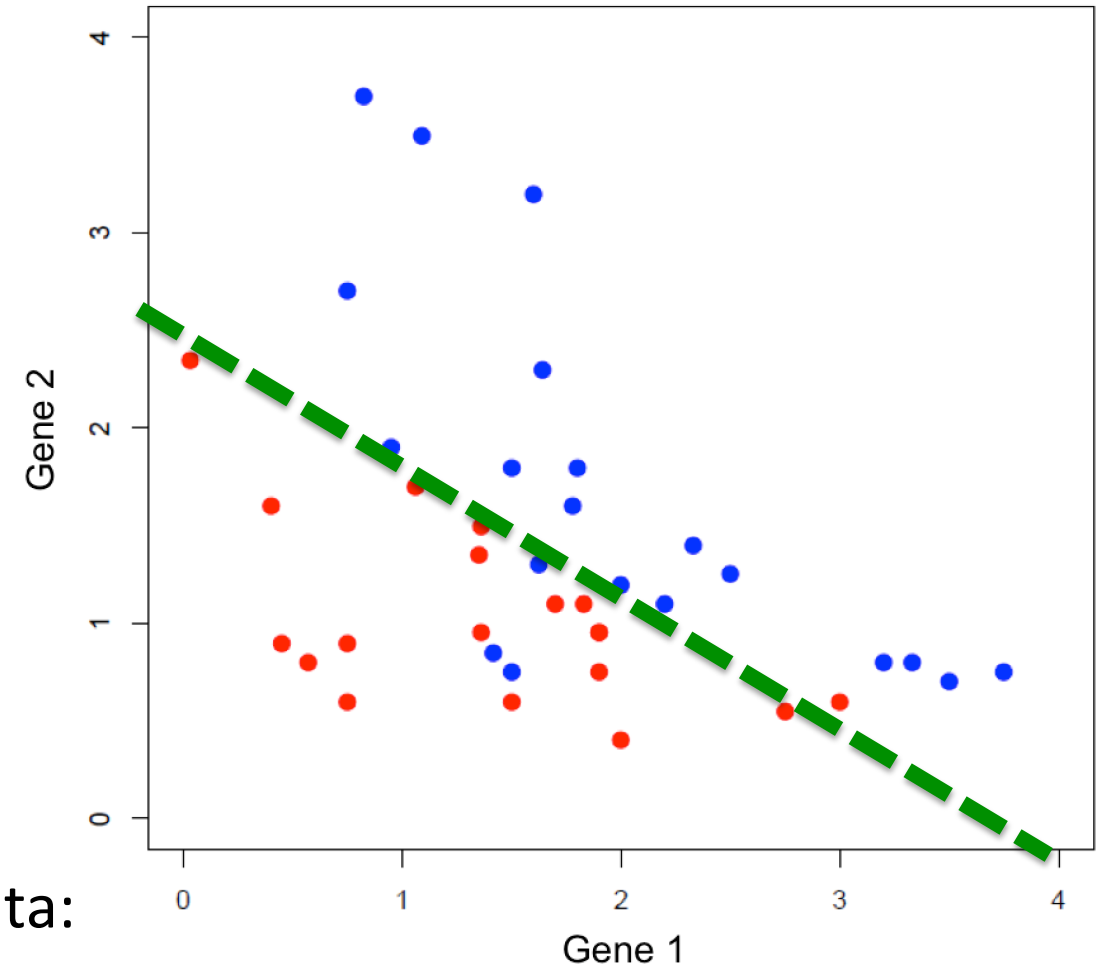
- Binary classification:
  - Logistic regression (linear)
  - Support vector machines ("hyper-linear")

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

Binary classification task



The decision boundary



$$y_i = \{0,1\}$$

Training data:

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

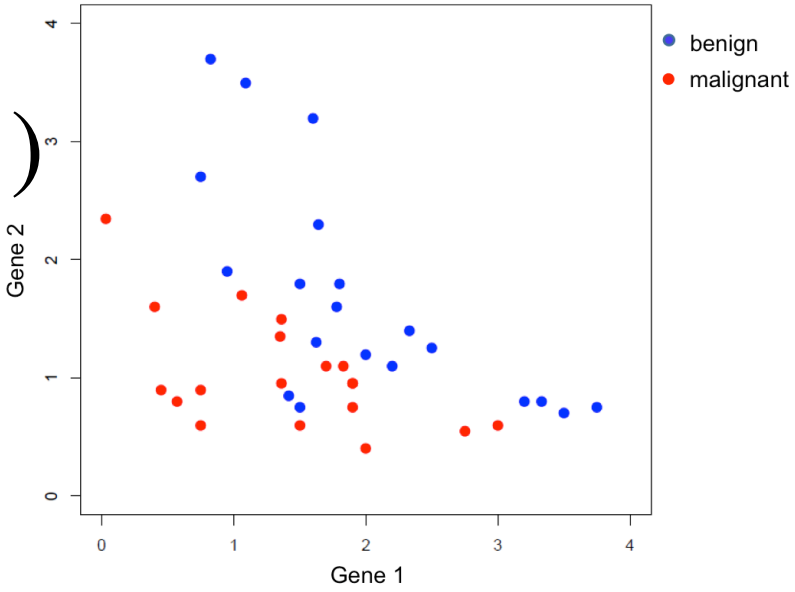
Linear Disciminant Analysis

(by Fisher in 1936)

- Assume that gene 1 and gene 2 are normally distributed in each class

$$p(\vec{x}_i \mid y_k) \sim N(\vec{x}_i \mid \mu_k, \Sigma_k)$$

Conditional probability of data, given class



Linear Disciminant Analysis

Posterior probability of class

Prior class probability

$$\frac{p(y_i = 0 \mid \vec{x}_i)}{p(y_i = 1 \mid \vec{x}_i)} > 1 \Leftrightarrow \log\left(\frac{N(\vec{x}_i \mid \mu_1, \Sigma\ )p(y_i = 0)}{N(\vec{x}_i \mid \mu_2, \Sigma)p(y_i = 1)}\right) > 0$$

Linear Disciminant Analysis

Posterior probability of class

Prior class probability

$$\frac{p(y_i = 0 \mid \vec{x}_i)}{p(y_i = 1 \mid \vec{x}_i)} > 1 \Leftrightarrow \log\left(\frac{N(\vec{x}_i \mid \mu_1, \Sigma)\, p(y_i = 0)}{N(\vec{x}_i \mid \mu_2, \Sigma)\, p(y_i = 1)}\right) > 0$$

$$\Leftrightarrow \vec{a}^T \vec{x}_i + b > 0$$

where

$$\vec{a} = \Sigma^{-1}(\mu_1 - \mu_2)$$

$$b = (\mu_1 - \mu_2)^T \Sigma^{-1}(\mu_1 - \mu_2) - \log\left(\frac{p(y_i = 0)}{p(y_i = 1)}\right)$$

Logistic regression

Log odds

$$\log\left(\frac{p(y_i = 0 \mid \vec{x}_i)}{p(y_i = 1 \mid \vec{x}_i)}\right) = \log\left(\frac{p(y_i = 0 \mid \vec{x}_i)}{1 - p(y_i = 0 \mid \vec{x}_i)}\right) = \vec{a}^T \vec{x}_i + b$$

Derive the maximum likelihood estimate (MLE) for the parameters (*a* and *b*)

Logistic regression (cont'd)

Derive the maximum likelihood estimate (MLE) for the parameters (*a* and *b*):

- We need to write down the likelihood of the data, given our models/parameters

Data Likelihood

$$L(D \mid \theta) = \prod_{i=1}^{n} p(y_i \mid \vec{x}_i, \theta)$$

IID Samples

Logistic regression (cont'd)

To find the MLE, we need to know: $p(y_i \mid \vec{x}_i) \text{ for } y_i = \{0,1\}$

$$\log\left(\frac{p(y_i = 0 \mid \vec{x}_i)}{1 - p(y_i = 0 \mid \vec{x}_i)}\right) = \vec{a}^T \vec{x}_i + b$$

Logistic regression

To find the MLE, we need to know: $p(y_i \mid \vec{x}_i)$ for $y_i = \{0,1\}$

$$\log\left(\frac{p(y_i = 0 \mid \vec{x}_i)}{1 - p(y_i = 0 \mid \vec{x}_i)}\right) = \vec{a}^T \vec{x}_i + b$$

$$p(y_i = 0 \mid \vec{x}_i) = \frac{e^{\vec{w}^T \vec{x}_i}}{1 + e^{\vec{w}^T \vec{x}_i}}$$

$$p(y_i = 1 \mid \vec{x}_i) = \frac{1}{1 + e^{\vec{w}^T \vec{x}_i}}$$

W=[b a]
x_i=[1 x_i]

Logistic regression: MLE

Data likelihood

$$L(D \mid \theta) = \prod_{i=1}^{n} p(y_i \mid \vec{x}_i)$$

$$p(y_i \mid \vec{x}_i) = \begin{cases} p(y_i = 0 \mid \vec{x}_i) = \dfrac{e^{\vec{w}^T \vec{x}_i}}{1 + e^{\vec{w}^T \vec{x}_i}} & \text{if } y_i = 0 \\ p(y_i = 1 \mid \vec{x}_i) = \dfrac{1}{1 + e^{\vec{w}^T \vec{x}_i}} & \text{if } y_i = 1 \end{cases}$$

Logistic regression: MLE

Data Likelihood

Note: Mathematical convenience

$$L(D \mid \theta) = \prod_{i=1}^{n} p(y_i \mid \vec{x}_i, \theta)$$

$$= \prod_{i=1}^{n} p(y_i = 0 \mid \vec{x}_i)^{1-y_i} \, p(y_i = 1 \mid \vec{x}_i)^{y_i}$$

Logistic regression: MLE

$$L(D;w) = \prod_{i=1}^{n} p(y_i = 0 \mid \vec{x}_i)^{1-y_i}\, p(y_i = 1 \mid \vec{x}_i)^{y_i} = \prod_{i=1}^{n} \left(\frac{1}{1+e^{(\vec{w}^T \vec{x}_i)}}\right)^{y_i} \left(\frac{e^{(\vec{w}^T \vec{x}_i)}}{1+e^{(\vec{w}^T \vec{x}_i)}}\right)^{1-y_i}$$

$$\text{argmax}_w \; \text{L}(D;w)$$

What does it mean? For all possible w's, find the one that maximizes the likelihood.

Logistic regression: MLE

$$L(D \mid \theta) = \prod_{i=1}^{n} p(y_i = 0 \mid \vec{x}_i)^{1-y_i} \, p(y_i = 1 \mid \vec{x}_i)^{y_i} = \prod_{i=1}^{n} \left(\frac{1}{1 + e^{(\vec{w}^T \vec{x}_i)}}\right)^{y_i} \left(\frac{e^{(\vec{w}^T \vec{x}_i)}}{1 + e^{(\vec{w}^T \vec{x}_i)}}\right)^{1-y_i}$$

$$\text{argmax}_w \; \text{L}(D; w) = \text{argmin}_w \; -\text{L}(D; w) = \text{argmin}_w \; -\log \text{L}(D; w)$$

What does it mean? For all possible w's, find the one that maximizes the likelihood.

Logistic regression: MLE

MLE

$$\text{argmin}_W \; -L(D;w)$$

$$= \text{argmin}_W - \sum_{i=1}^{n} y_i \log \frac{1}{1+e^{y_i(\vec{w}^T\vec{x}_i)}} + (1-y_i)\log \frac{e^{y_i(\vec{w}^T\vec{x}_i)}}{1+e^{y_i(\vec{w}^T\vec{x}_i)}}$$

Final objective function

Optimization problem

f(w)

$$\text{argmin}_W - \sum_{i=1}^{n} y_i \log \frac{1}{1+e^{(\vec{w}^T \vec{x}_i)}} + (1-y_i) \log \frac{e^{(\vec{w}^T \vec{x}_i)}}{1+e^{(\vec{w}^T \vec{x}_i)}}$$

- We need to differentiate the objective function wrt *w* to get the gradient for *w.*
- Differentiating the objective function reveals that there is no *closed-form* solution for *w.*
- We can use an iterative procedure (e.g., gradient descent) to find the optimal *w.*

Optimization problems & gradient descent

- Consider the likelihood function f(w): need to find w that minimizes the likelihood function.

- No-closed form solution for w: numerical methods that update the solution *w* at each
  - Gradient descent, conjugate gradient, Newtwon method

- Update form: $w^{(k)} \leftarrow w^{(k-1)} - \gamma \nabla f(w)$

Magnitude/length of step in the direction of gradient

Gradient descent for logistic regression

Simple *for loop* for fining the optimal value of w

$W^{new} = \boldsymbol{0}$

$W^{old} = \boldsymbol{0}$

While $||w^{new} - w^{old}||_2 > e$

$$w^{old} = w^{new}$$

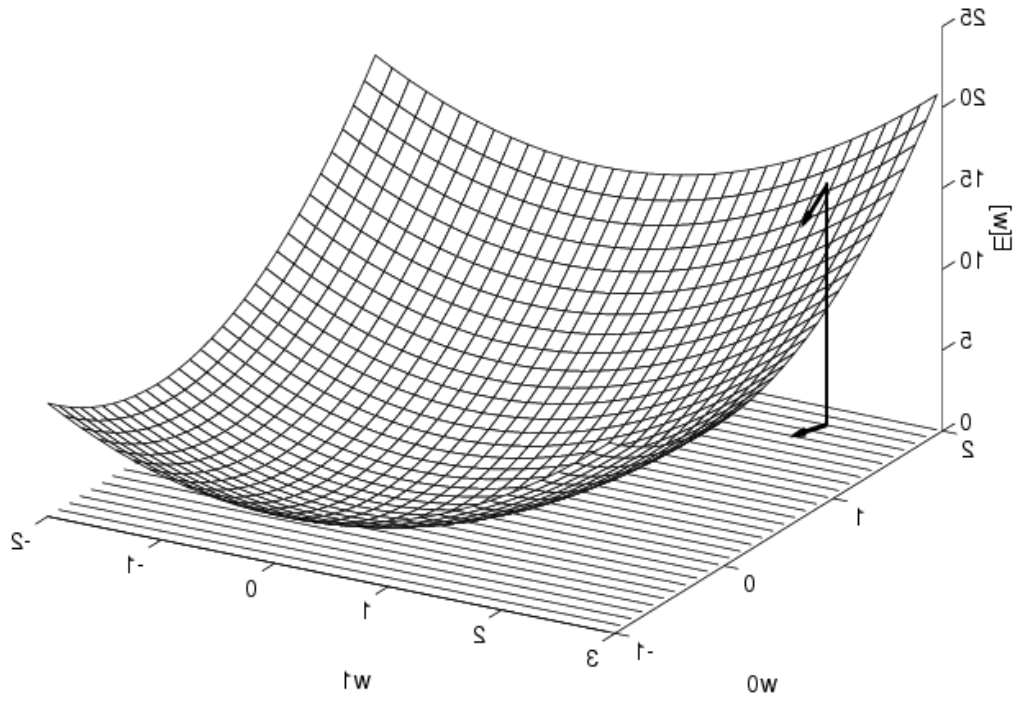
$$w^{new} \leftarrow w^{old} - \gamma \nabla f(w)$$

Summary: logistic regression

- Defined a model for quantifying data likelihood
- Simplify the likelihood if possible
- Write down an optimization problem for optimizing data likelihood given parameters
  - Use gradient descent or other more sophisticated numerical methods for estimating model parameters.

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

Support Vector Machines (SVMs)

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

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:

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

$y_i = \{-1, 1\}$ 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: $K(\vec{x}_i, \vec{x}_j) = \exp(-\frac{\| \vec{x}_i - \vec{x}_j \|}{\sigma})$

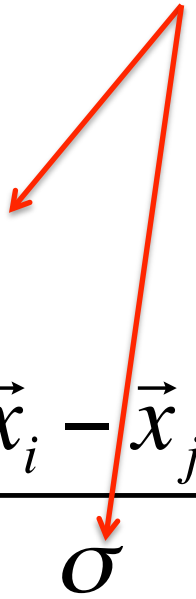
Examples of kernels

Parameters you can tune

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

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

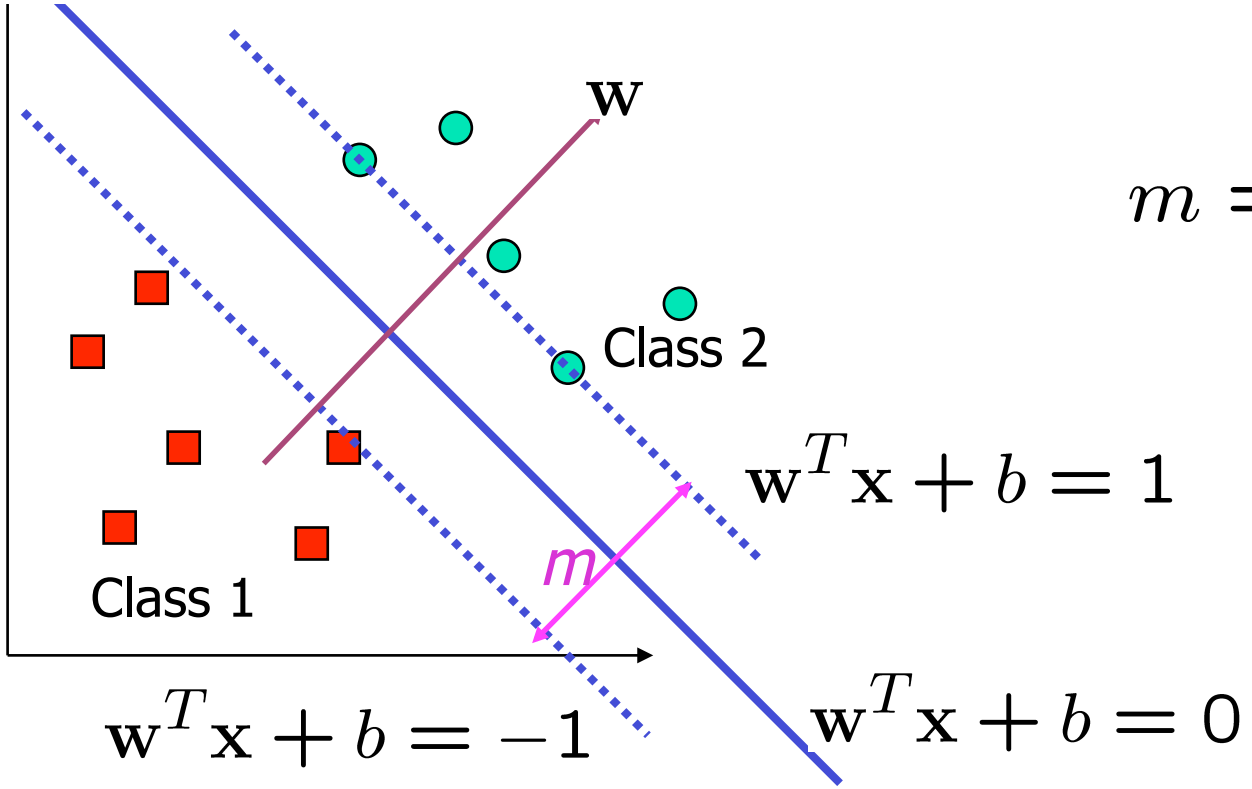
Gaussian kernel: $K(\vec{x}_i, \vec{x}_j) = \exp(-\frac{\| \vec{x}_i - \vec{x}_j \|}{\sigma})$



Learning SVMs

- Choose a kernel function
  - How? black art or CV
- Choose the support vectors
  - How? Side effect of learning the "weights" $\vec{\alpha}$
- Choose the weights
  - Write down an objective function that maximizes the margin (primal form → dual form gives you the "weights")

Maximizing the margin



$$m = \frac{2}{||\mathbf{w}||}$$

Note Distance between point and hyperplane:

$$\frac{|\mathbf{x}_i \cdot \mathbf{w} + b|}{\|\mathbf{w}\|}$$

Finding the maximum margin hyperplane

- Maximize margin $2/\|\mathbf{w}\|$
- Correctly classify all training data:

$$\begin{cases} \mathbf{x}_i \text{ positive } (y_i = 1): & \mathbf{x}_i \cdot \mathbf{w} + b \geq 1 \\ \mathbf{x}_i \text{ negative } (y_i = -1): & \mathbf{x}_i \cdot \mathbf{w} + b \leq -1 \end{cases}$$

Finding the maximum margin hyperplane

- Maximize margin $2/\|\mathbf{w}\|$
- Correctly classify all training data:

$$\begin{cases} \mathbf{x}_i \text{ positive } (y_i = 1): & \mathbf{x}_i \cdot \mathbf{w} + b \geq 1 \\ \mathbf{x}_i \text{ negative } (y_i = -1): & \mathbf{x}_i \cdot \mathbf{w} + b \leq -1 \end{cases}$$

***Quadratic optimization problem*:**

Minimize $\frac{1}{2} \| \mathbf{w} \|$

Subject to $y_i(\mathbf{w} \cdot \boldsymbol{x}_i + b) \geq 1$ for all $(\boldsymbol{x_i}, y_i)$

Solving the SVM Optimization Problem

Find **w** and b such that
argmin_w **||w||**
Such that for all $(\mathbf{x}_i, y_i)$, i=1..n : $y_i (\mathbf{w}^T\mathbf{x}_i + b) \geq 1$

- Need to optimize a *quadratic* function subject to *linear* constraints.
- The solution involves constructing a *dual problem* where a *Lagrange multiplier* α_i is associated with every inequality constraint in the primal (original) problem:

Find $\alpha_1 \ldots \alpha_n$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x}_i^T\mathbf{x}_j$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $\alpha_i \geq 0$ for all α_i

Solving the SVM Optimization Problem

- Dual problem:

Find $\alpha_1 \ldots \alpha_n$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $\alpha_i \geq 0$ for all α_i

Linear Kernel function

"support vector" weights

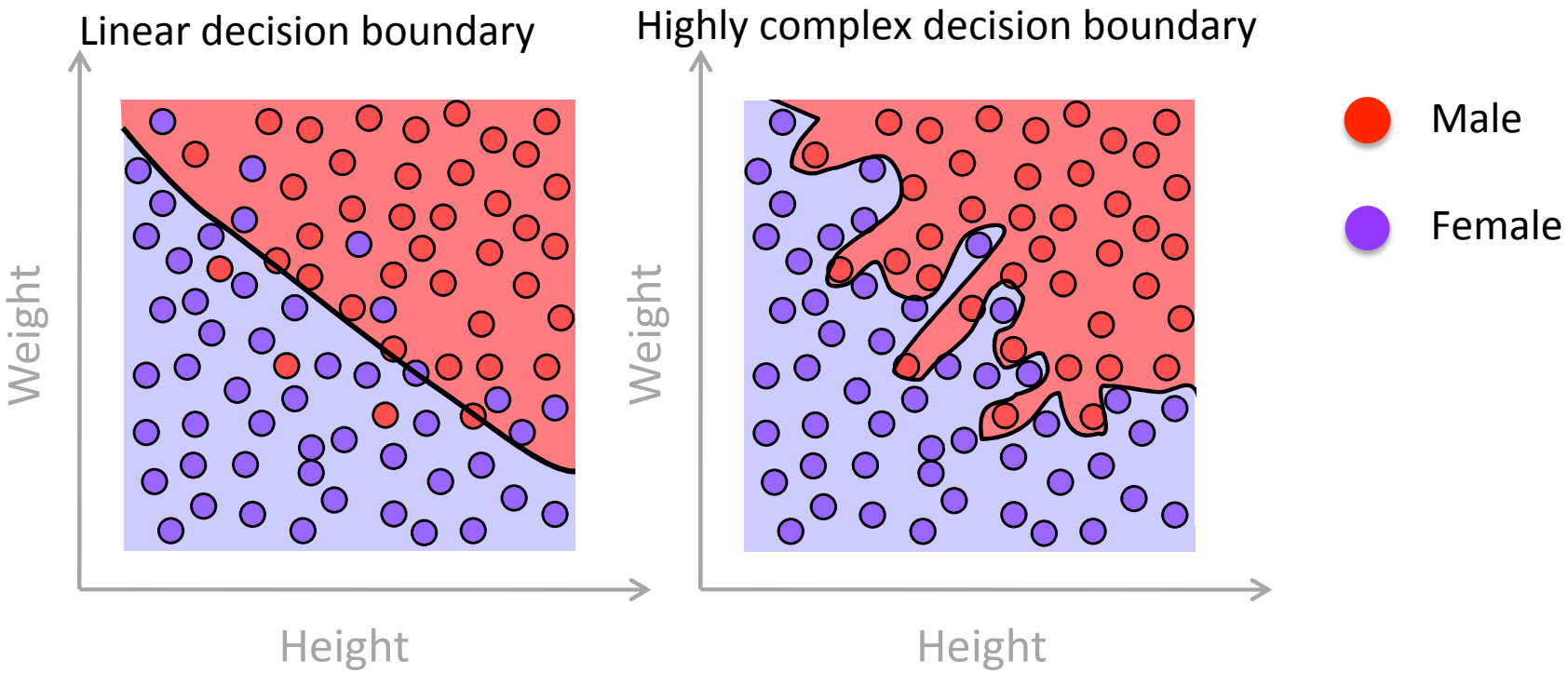
$$K(\vec{x}_i, \vec{x}_j) = \vec{x}_i^T \vec{x}_j$$

SVMs summary

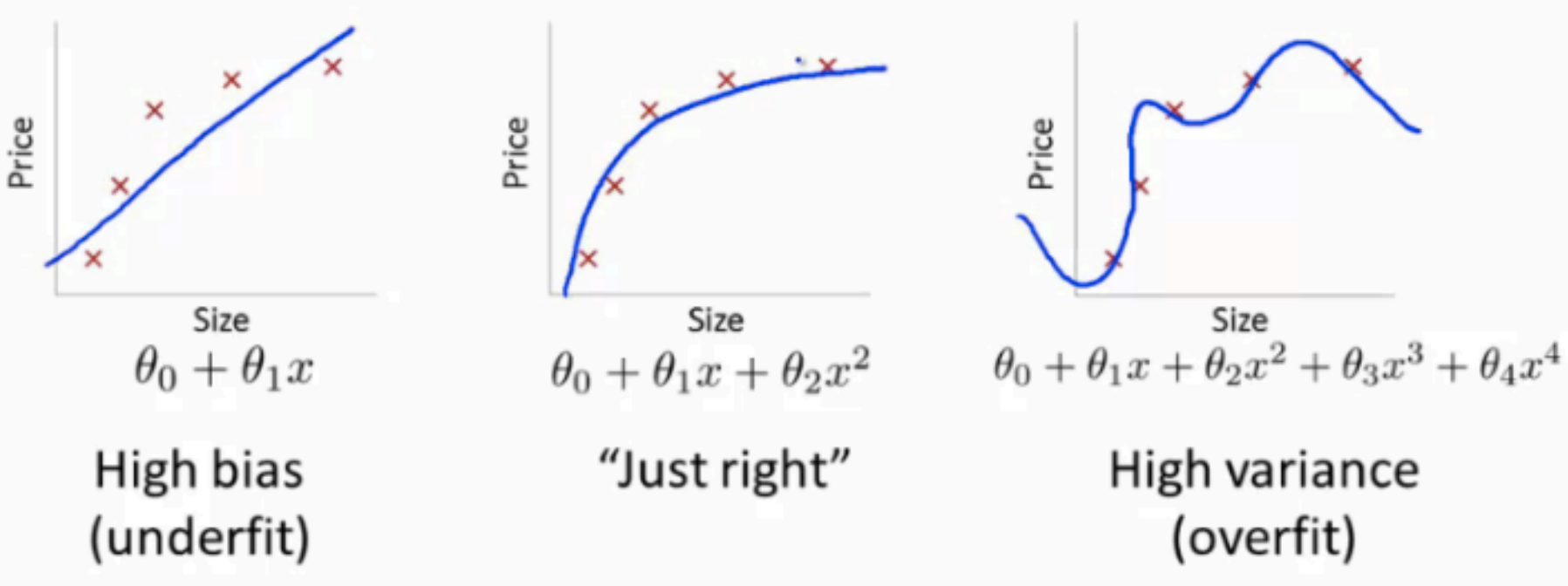
- Pros
  - Lots of publically available software.
  - Kernel based framework is very powerful, flexible.
  - Works well in practice, but need to have good number of training examples.
- Cons
  - Need to define suitable kernel (not hard to do, just use linear kernel).
  - Hard optimization problem: training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

Overfitting

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



Overfitting example: polynomial of degree k for k={1,..,4} (regression problem)



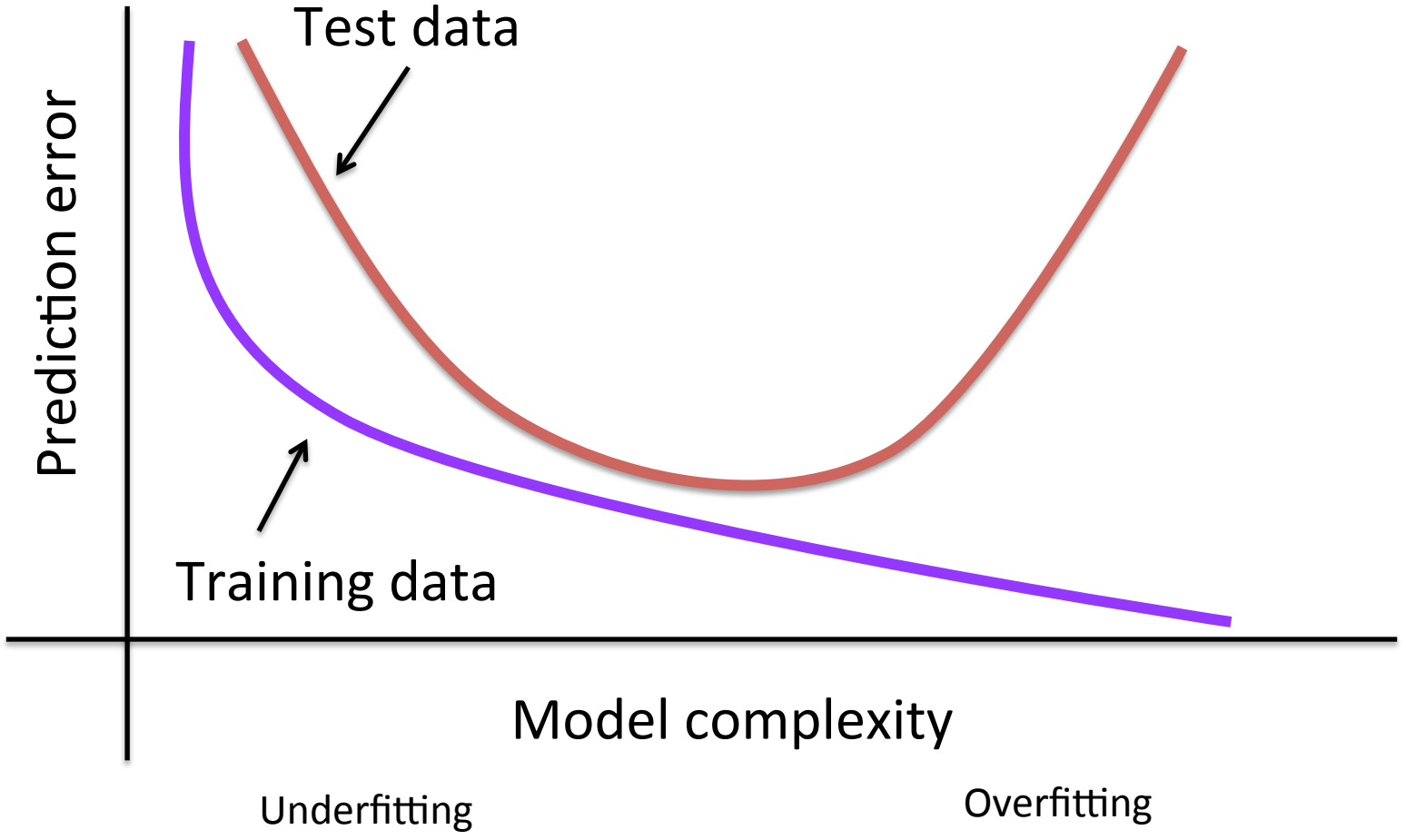
Ockam's Razor

William of Ockham (1285-1349) Principle of Parsimony:

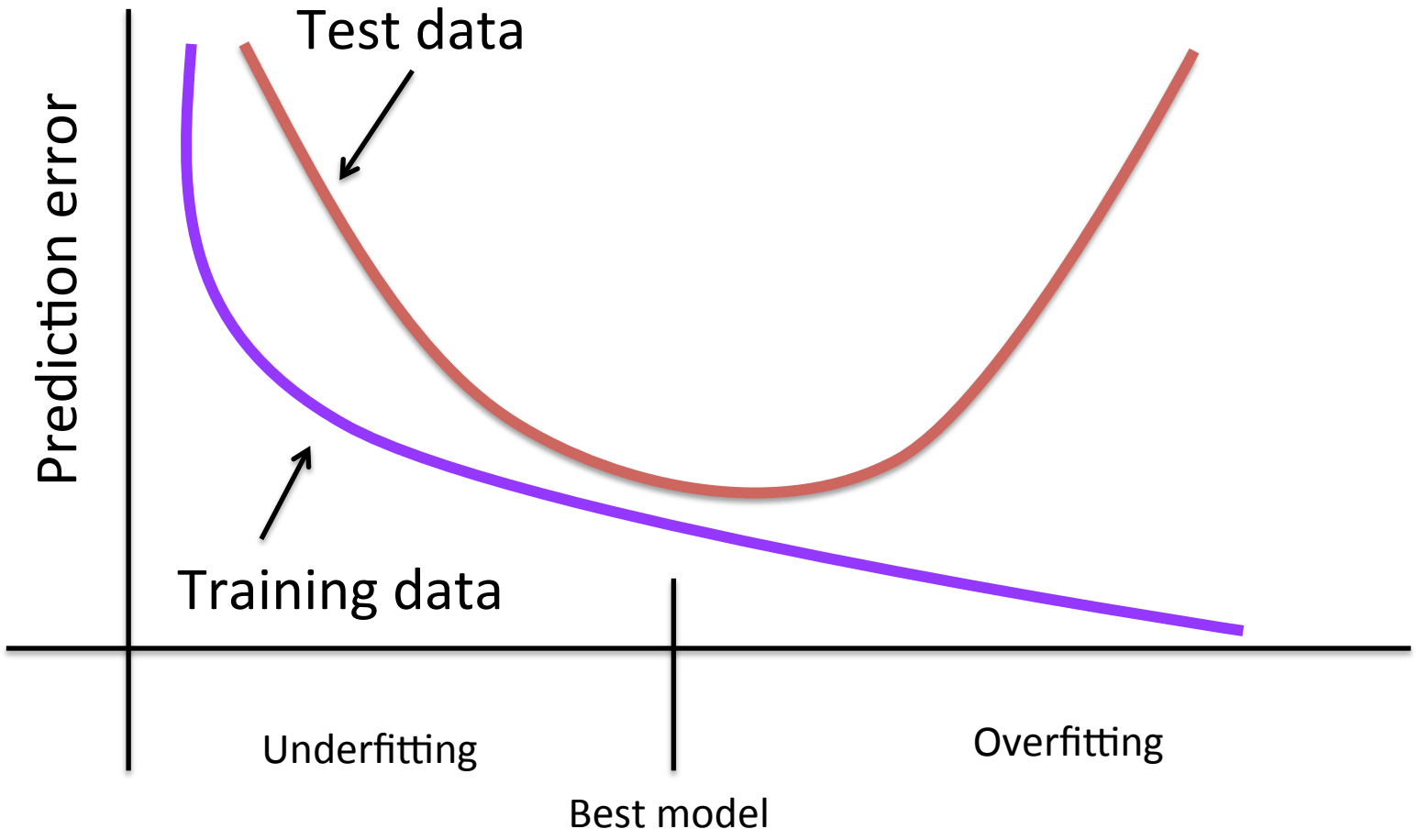
"One should not increase, beyond what is necessary, thenumber of entities required to explain anything."

Alternatively: seek the simplest explanation.

Error and model complexity



Error and model complexity



How can we determine the optimal complexity? model selection

- Hold-out method
- 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 partition (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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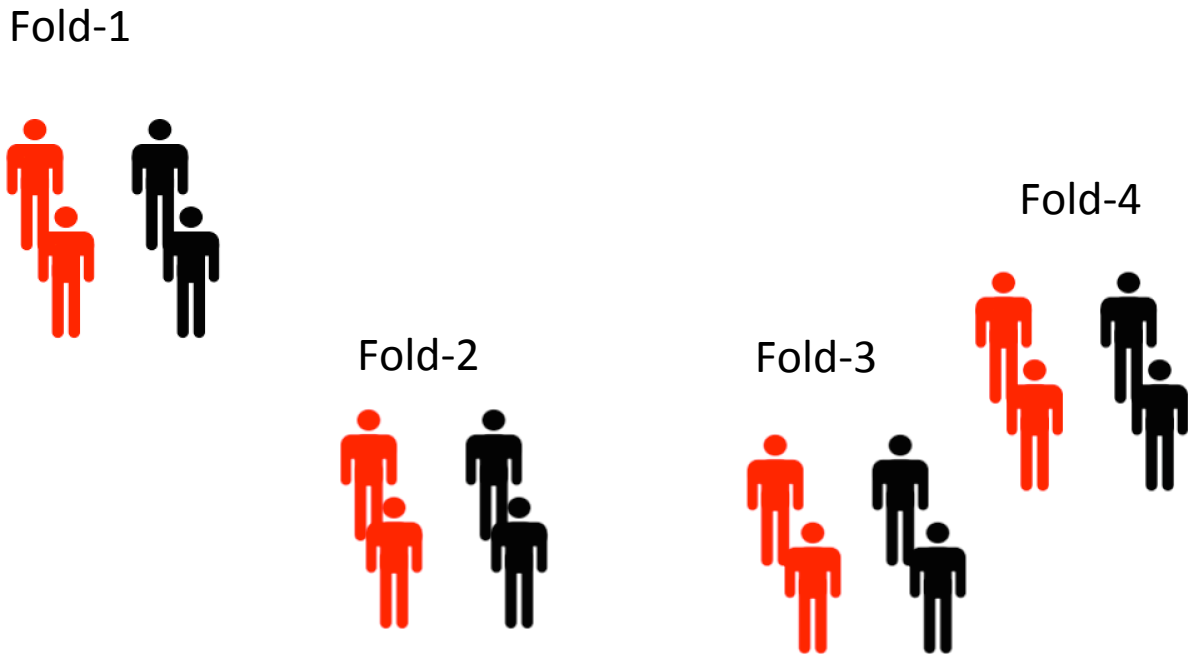
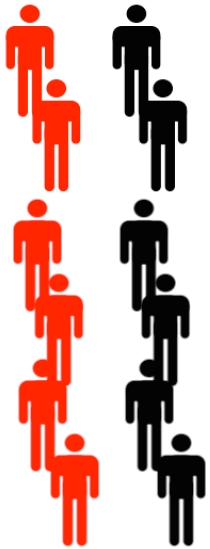


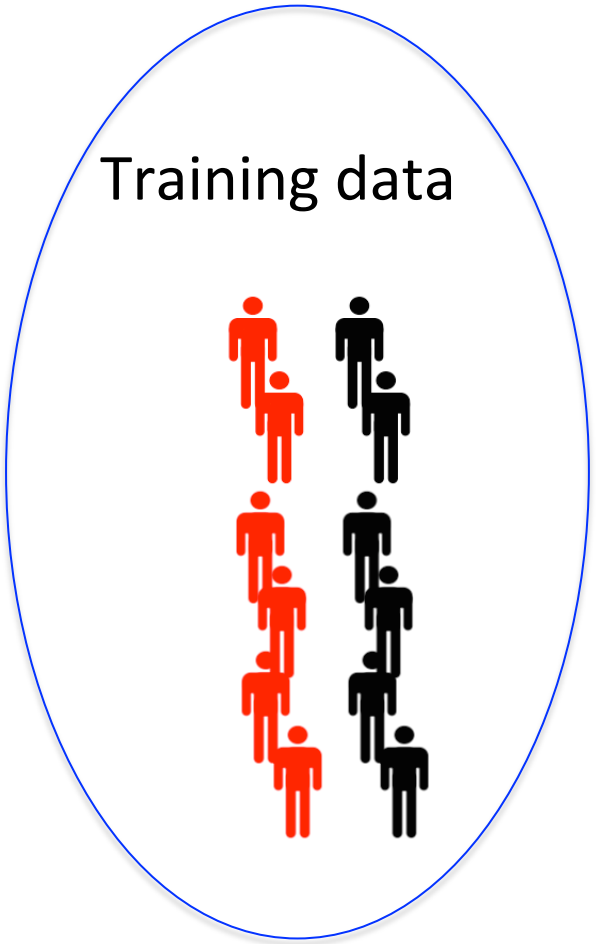
Example: 4-fold cross-validation

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
    + bias of error estimate will be small
  - Smaller k:
    + reduced computation time
    + variance of error estimate is small
    - Bias of error estimate is large
- N-fold CV is called “Leave-One-Out” CV
- In practice:
  - Lower k is more reliable, eg., 3-fold CV is standard.

How do we measure error on validation/test set?

continuous response

Examples:

- Squared error loss

$$L(\boldsymbol{y}, \hat{\boldsymbol{y}}) = \|\boldsymbol{y} - \hat{\boldsymbol{y}}\|_2^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

- Absolute error loss

$$L(\boldsymbol{y}, \hat{\boldsymbol{y}}) = \|\boldsymbol{y} - \hat{\boldsymbol{y}}\|_1 = \sum_{i=1}^{n} |y_i - \hat{y}_i|$$

Binary response/labels

- True positive (TP)
- True negative (TN)
- False positive (?Type I error?) (FP)
- False negative (?Type II error?) (FN)

- Accuracy (TP + TN)/N (=1-error rate)
- Sensitivity: TP/(TP+FN) (recall)
- Specificity: TN/(TN + FP)

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)