



Pattern recognition

3. Feature selection and extraction

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Some material courtesy of Robert Duin and David Tax

Overview

- Feature extraction:
 - Linear:
 - PCA,
 - Fisher
 - Non-linear
 - MDS
- Feature selection:
 - Criteria
 - search algorithms
 - forward,
 - backward,
 - branch & bound.
- Regularized classifiers:
 - PAM (shrunken centroids)
 - Ridge,
 - LASSO



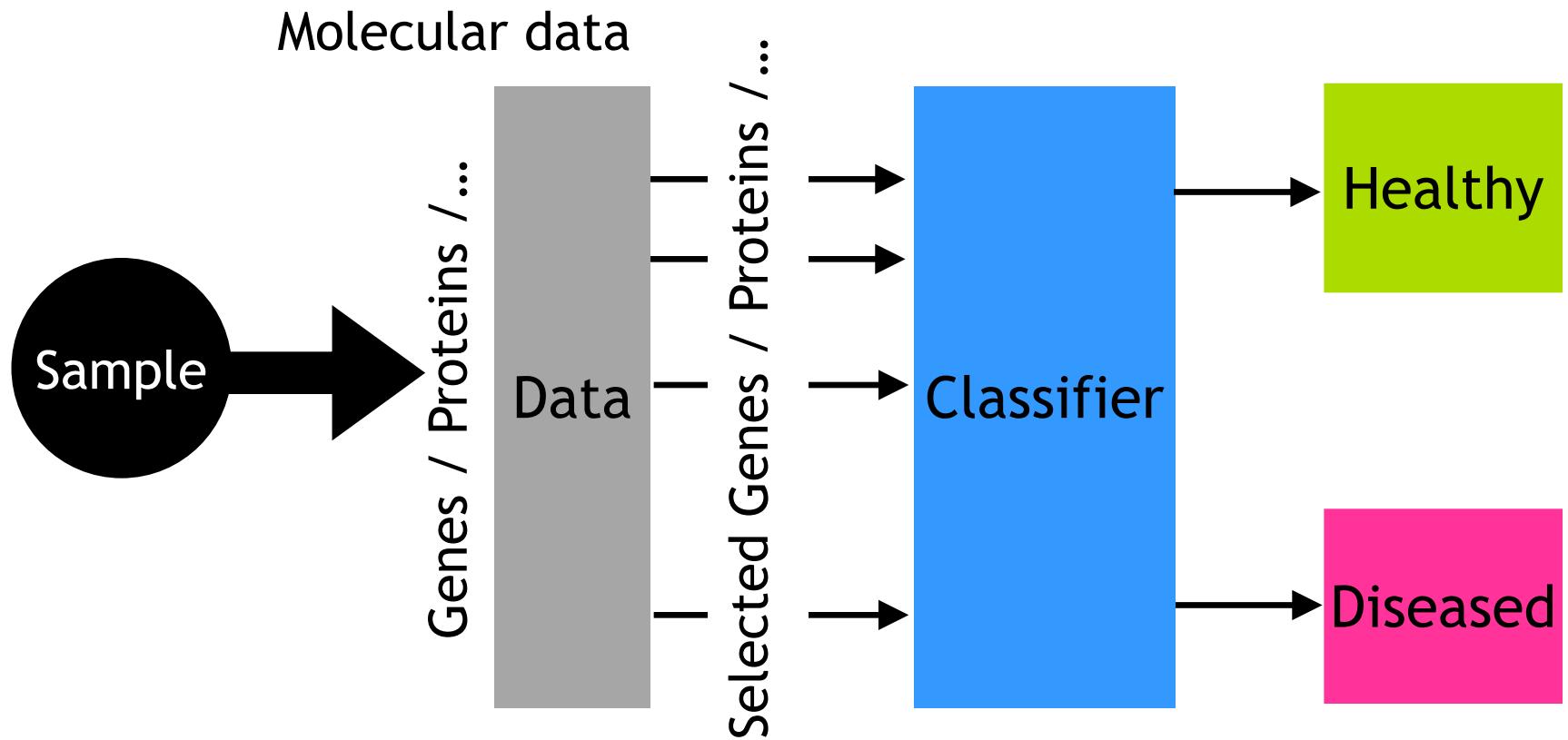
Dimensionality reduction

Aim of Feature Extraction and Selection: reduce dimensionality

Why is reducing dimensionality useful?

1. **Fewer parameters:** faster, easier to estimate - possibly better performance
2. **Explain** which measurements (genes) are useful and which are not (reduce redundancy)
3. **Visualisation**

Example: molecular diagnostic classifiers



Molecular data (e.g. RNAseq data)

- Curse of dimensionality (ratio of # features and # samples):
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 - and **increasing** number of features (number of parameters)
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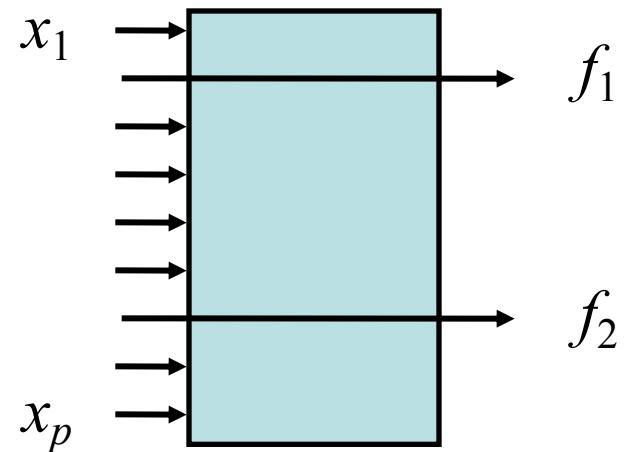
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- For example: nearest mean classifier on Golub data
 - $p = 3051$, $k = 2 \rightarrow$ number of parameters = 6102
 - Number of samples, $n = 38$

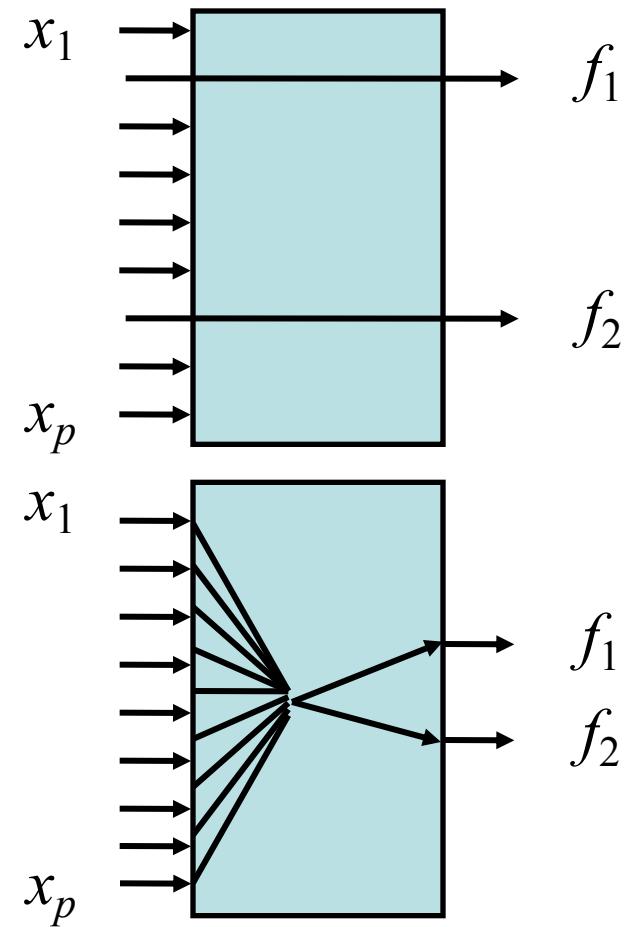
Feature selection vs. extraction

- **Feature selection:**
select d out of p measurements



Feature selection vs. extraction

- **Feature selection:**
select d out of p measurements
- **Feature extraction:**
map p measurements
to d measurements
(e.g. PCA, CCA, LDA, MDS)

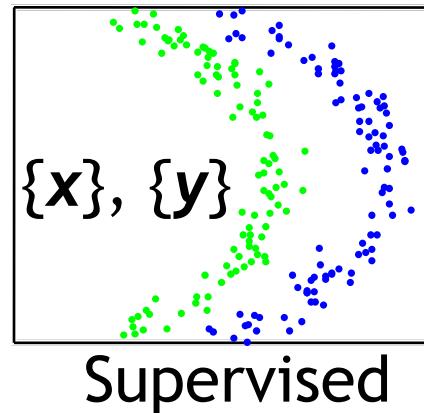
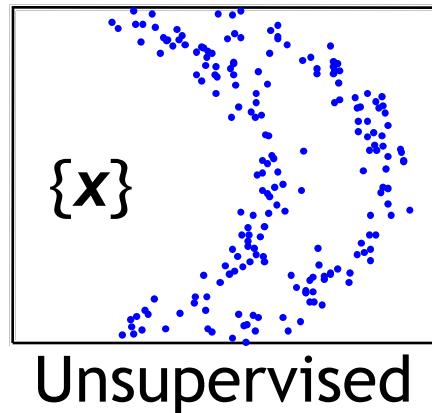


Feature selection v extraction (2)

| | Advantage | Disadvantage |
|-------------------|---------------------|-----------------------|
| Selection | cut in measurements | expensive |
| | easy interpretation | often approximate |
| Extraction | cheap | need all measurements |
| | can be nonlinear | criterion sub-optimal |
| | not axis aligned | |

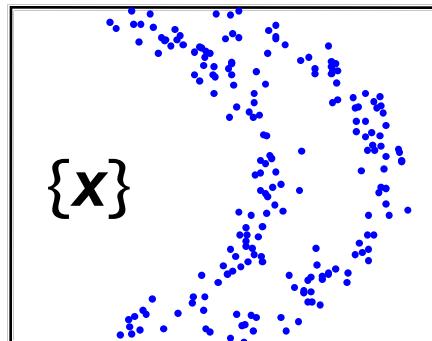
Feature extraction (1)

Main types: supervised/unsupervised

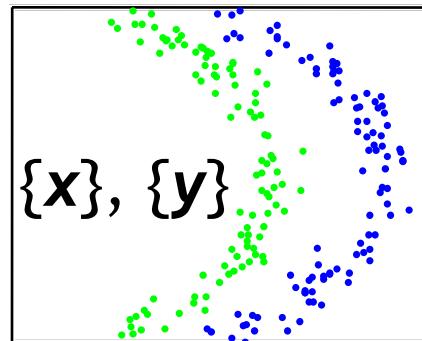


Feature extraction (1)

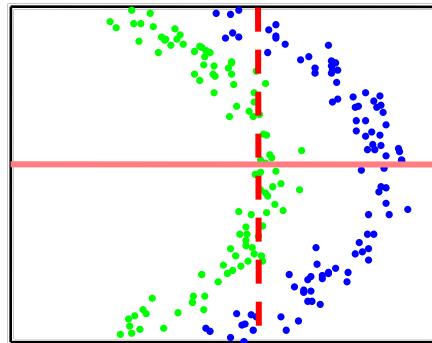
Main types: Linear / Nonlinear



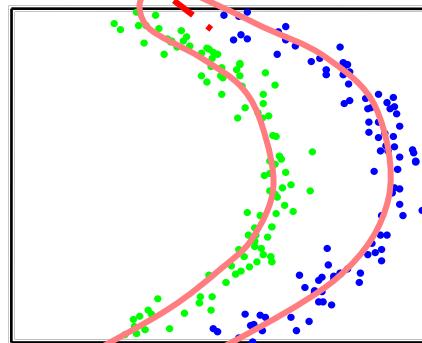
Unsupervised



Supervised



Linear



Nonlinear

Feature extraction (2)

- Subjects:
 - Linear, unsupervised:
 - Principal Component Analysis (PCA)
 - Linear, supervised:
 - Linear Discriminant Analysis (LDA)

Principal component analysis (Unsupervised feature extraction)

- Principal component analysis (PCA, 1901):
find directions in data...
 - which retain as much *variation* as possible
 -

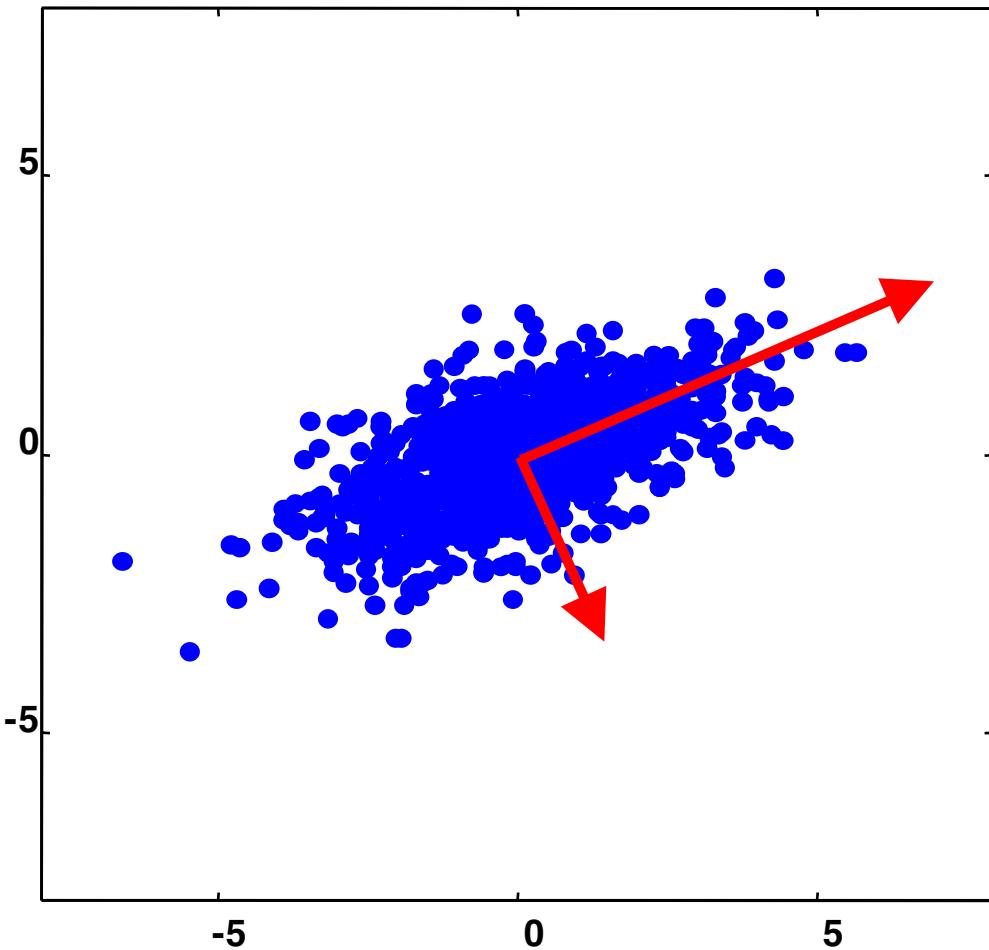
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- Principal component analysis (PCA, 1901):
find directions in data...
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 - which make projected data *uncorrelated*
 - which minimise squared *reconstruction error*

Principal component analysis (Unsupervised feature extraction)



Steps:

1. Center data
2. Compute covariance, C
3. Perform PCA on C

Output:

1. Eigenvectors: $\mathbf{e}_1, \mathbf{e}_2$
2. Eigenvalues: λ_1, λ_2

Reducing dimensions:
Choosing ' d '

Choosing reduced dimensionality

- To choose d inspect the retained variance,

$$\sum_{i=1}^d \lambda_i$$

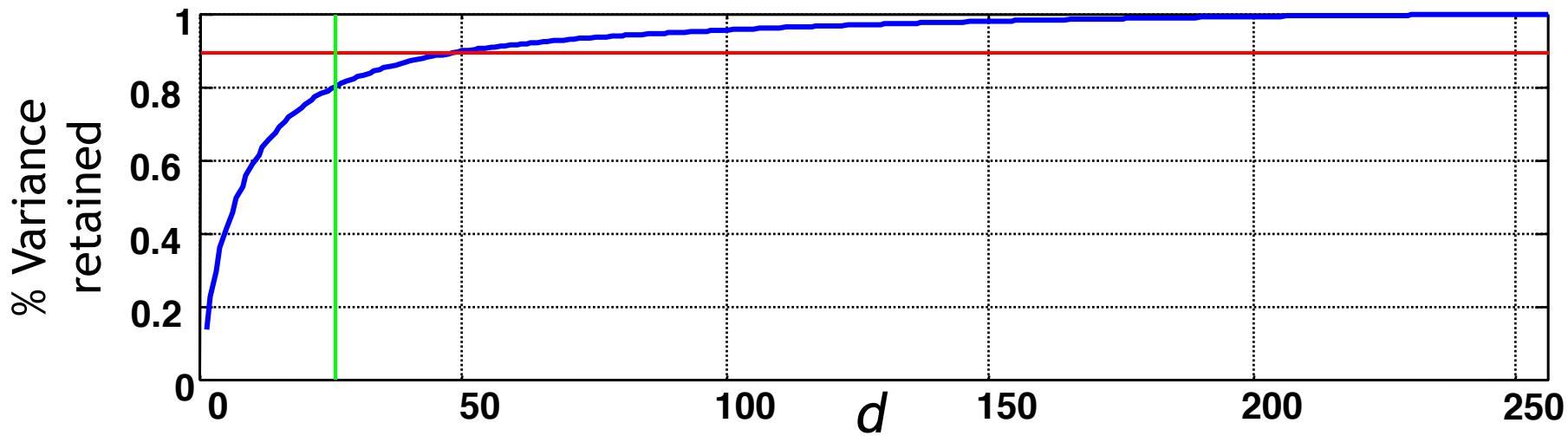
- or the ratio of retained variance,

$$\sum_{i=1}^d \lambda_i \Bigg/ \sum_{j=1}^p \lambda_j$$

- Rule of thumb: Select d for which 80-90% variance is retained
- Reduced dimensionality data set
 - $[\mathbf{x}_1^T; \mathbf{x}_2^T; \dots; \mathbf{x}_d^T] [\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_d]$

PCA example

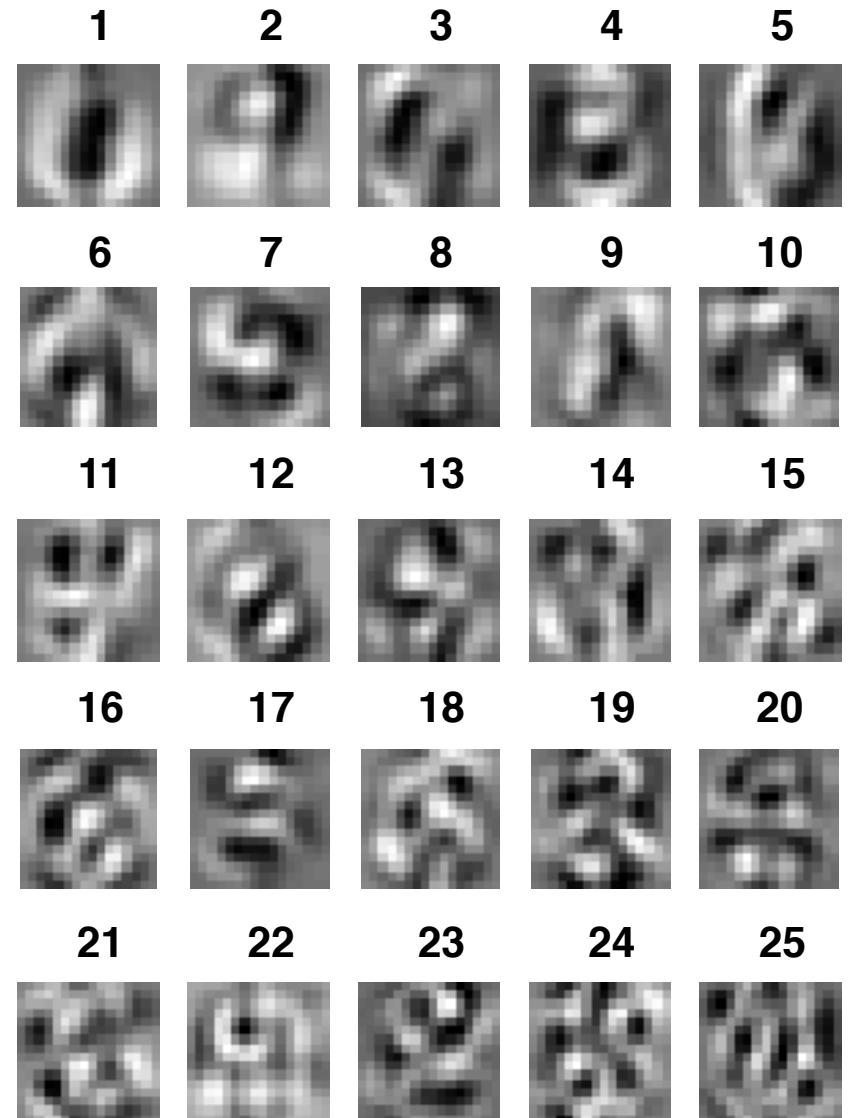
- e.g. NIST digits: 2000 samples, $p = 256$



PCA example (2)

- For image data, principal components can also be interpreted...

most often occurring variations between digits



PCA tips

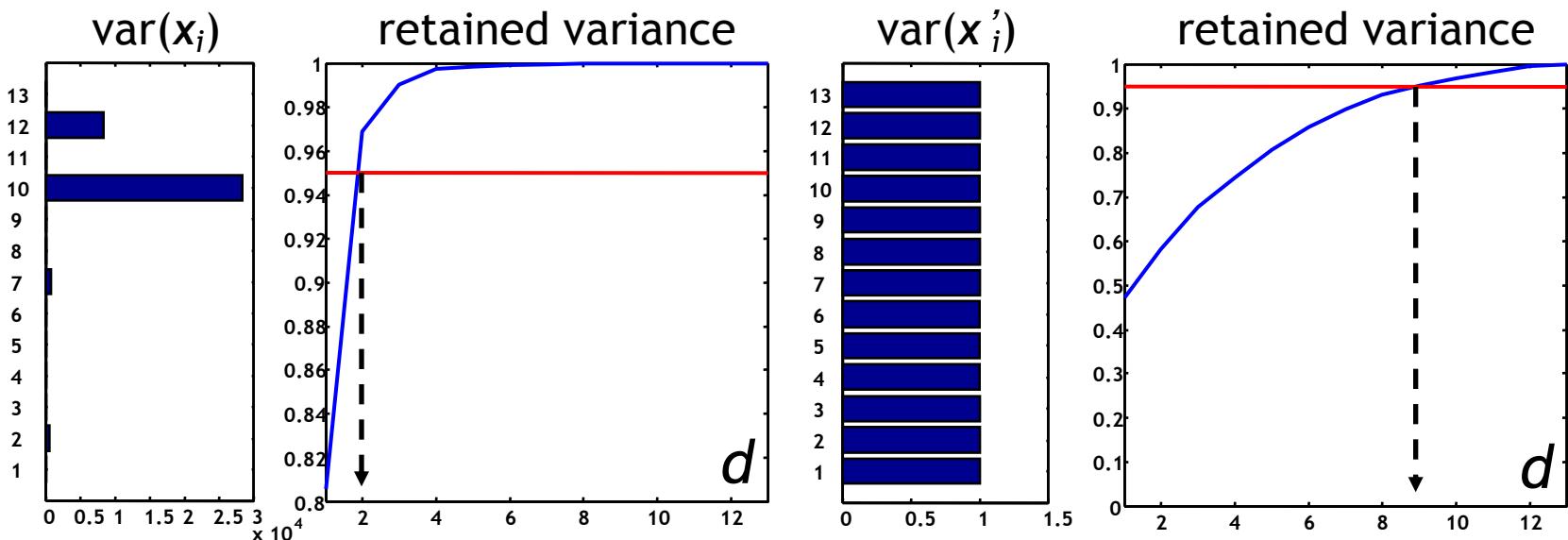
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 $x' \leftarrow (x - \mu)$

PCA tips

- Ensure data is centered (mean of each feature is zero):
 $x' \leftarrow (x - \mu)$
- PCA is sensitive to scaling
 - length in cm has a much larger variance than length in m
 - best to standardise: $x' \leftarrow (x - \mu) / \sigma$

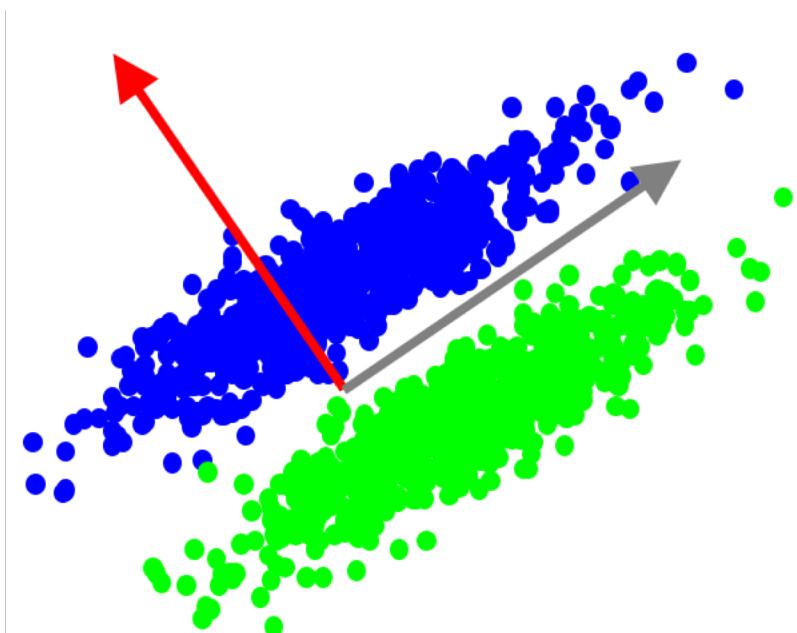
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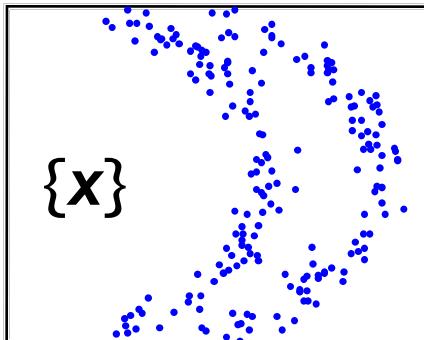
PCA conclusions

- PCA:
 - Is **global** and **linear** (but mixtures can be used)
 - Is **unsupervised** (but we can do PCA on each class)
 - Needs a **lot of data** to estimate Σ well.
- Danger:
criterion is not necessarily related to the goal; might discard important directions

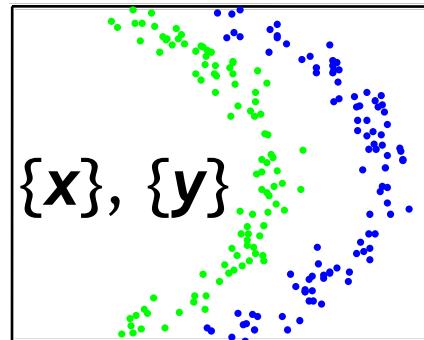


Supervised, linear feature extraction

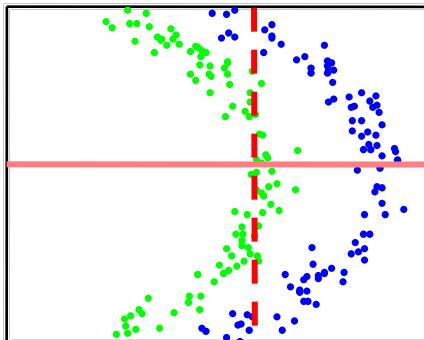
- If class label ω (or y) is given, supervised extraction
- Examples: Fisher mapping; Linear Discriminant Analysis (Day 2)



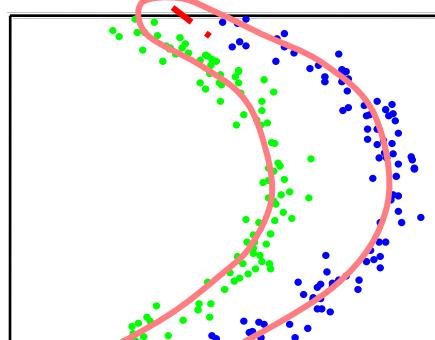
Unsupervised



Supervised



Linear

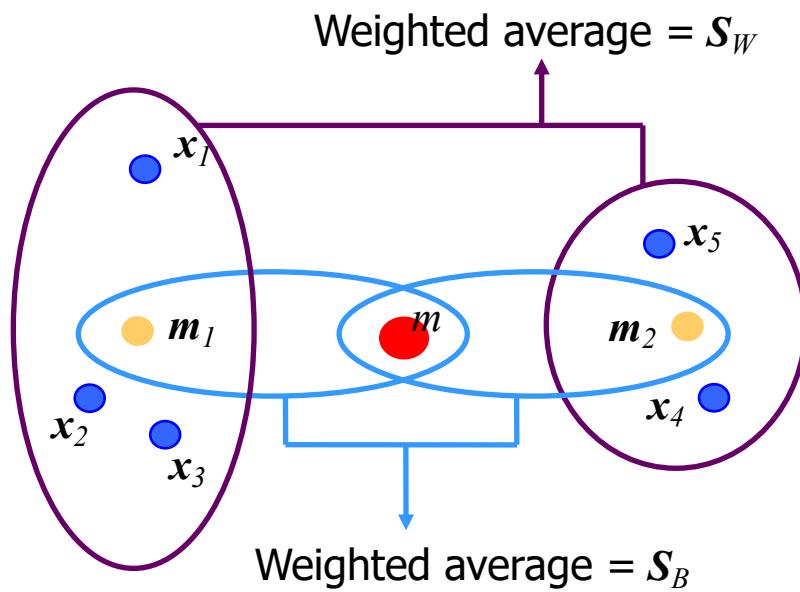


Nonlinear

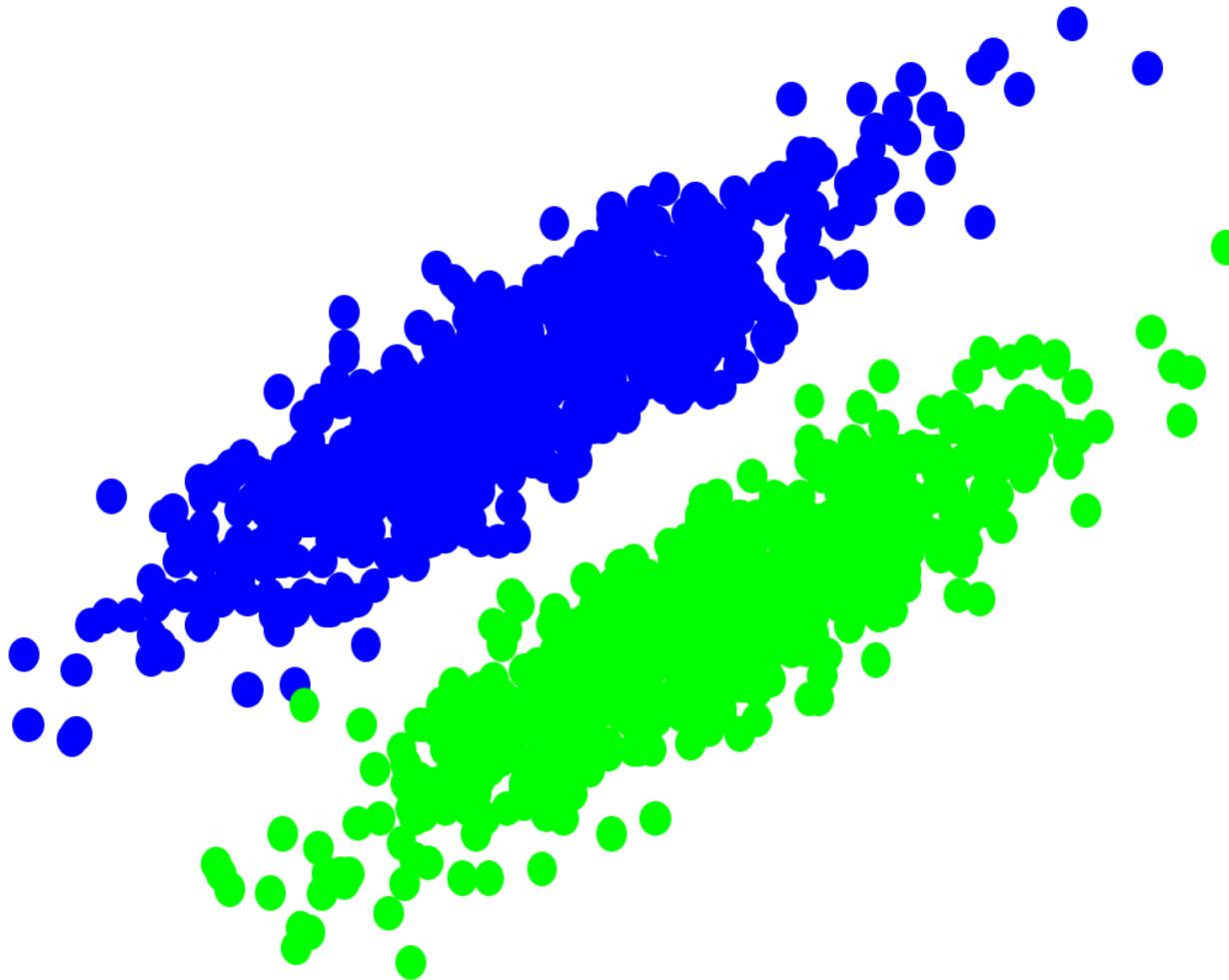
Supervised feature extraction (2)

Within-class and between-class scatter matrices:

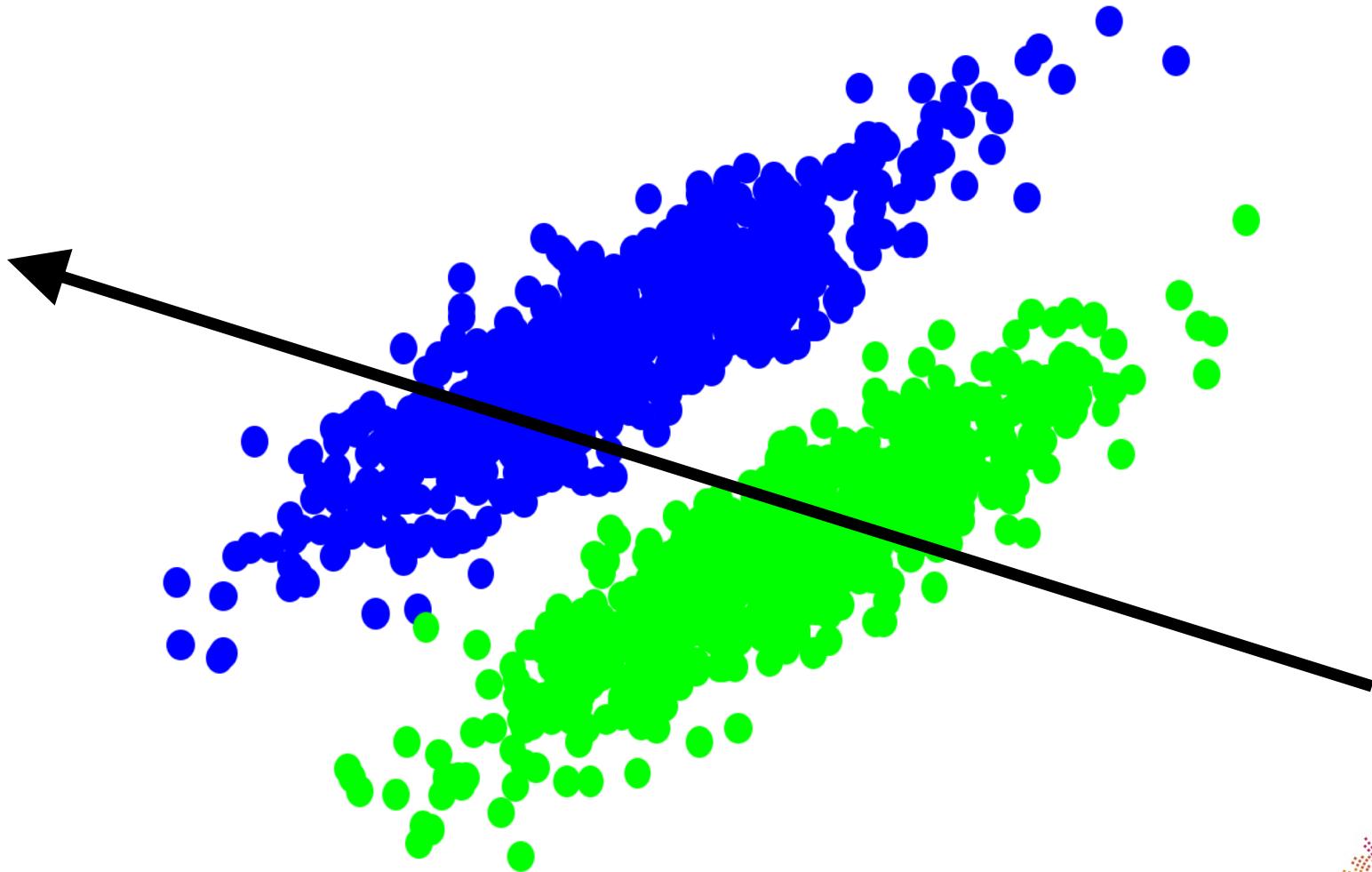
- Within-class: $S_w = \sum_{i=1}^C \frac{n_i}{n} \Sigma_i$
- Between-class: $S_B = \sum_{i=1}^C \frac{n_i}{n} (\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^T$



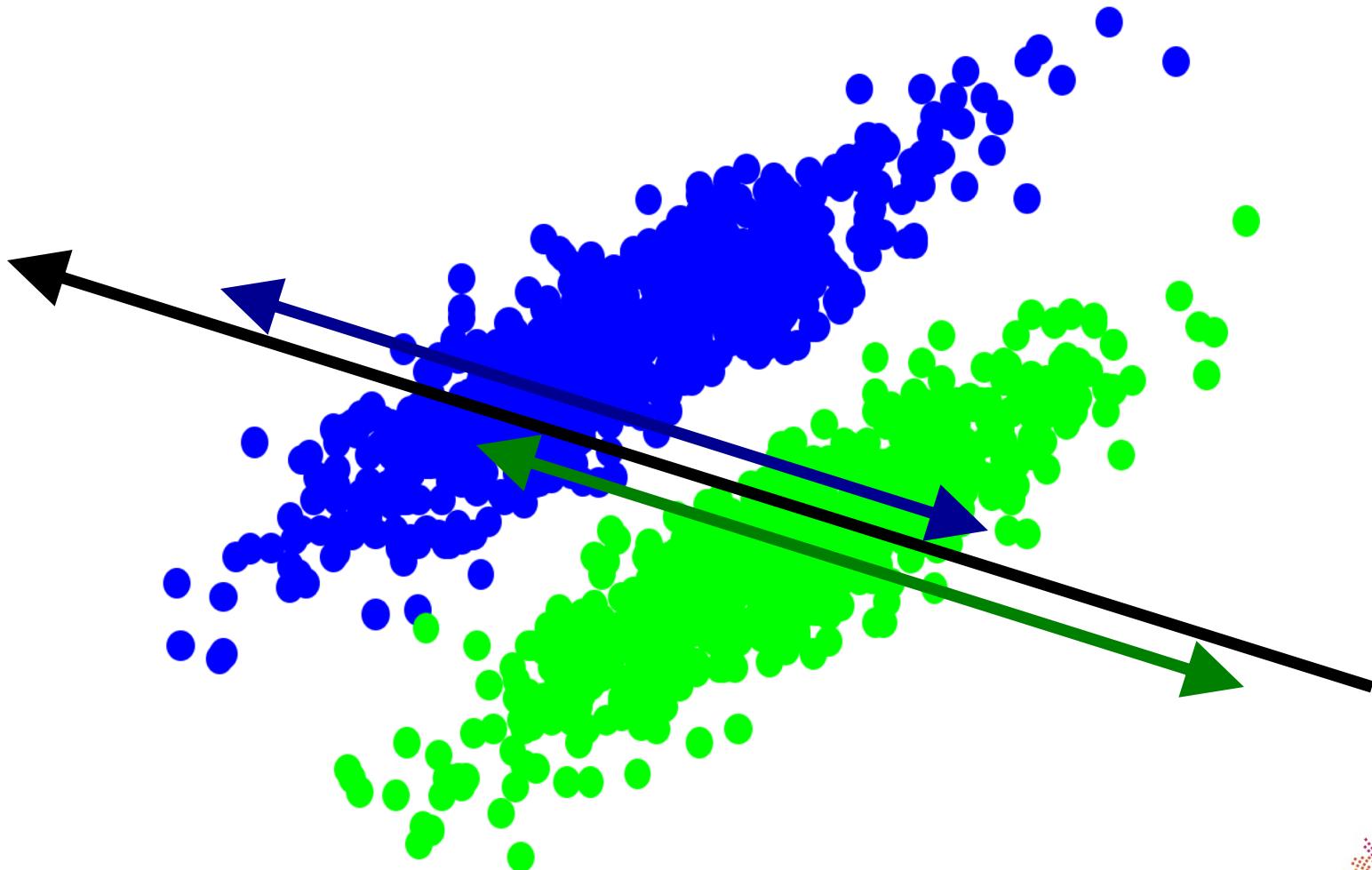
Fisher mapping: finding the direction (subspace) to project onto for the best class separation



Fisher mapping: defining the Fisher criterion

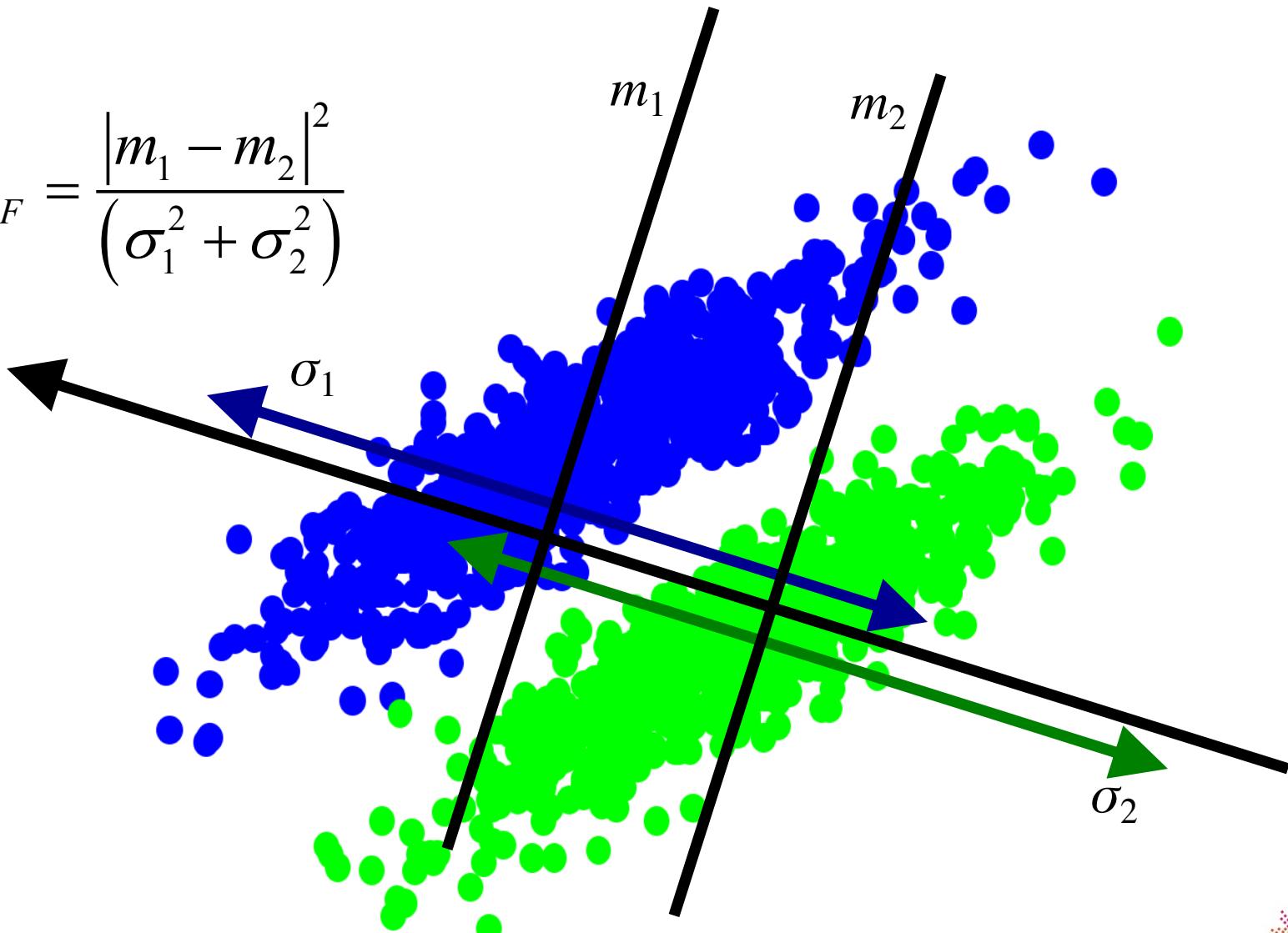


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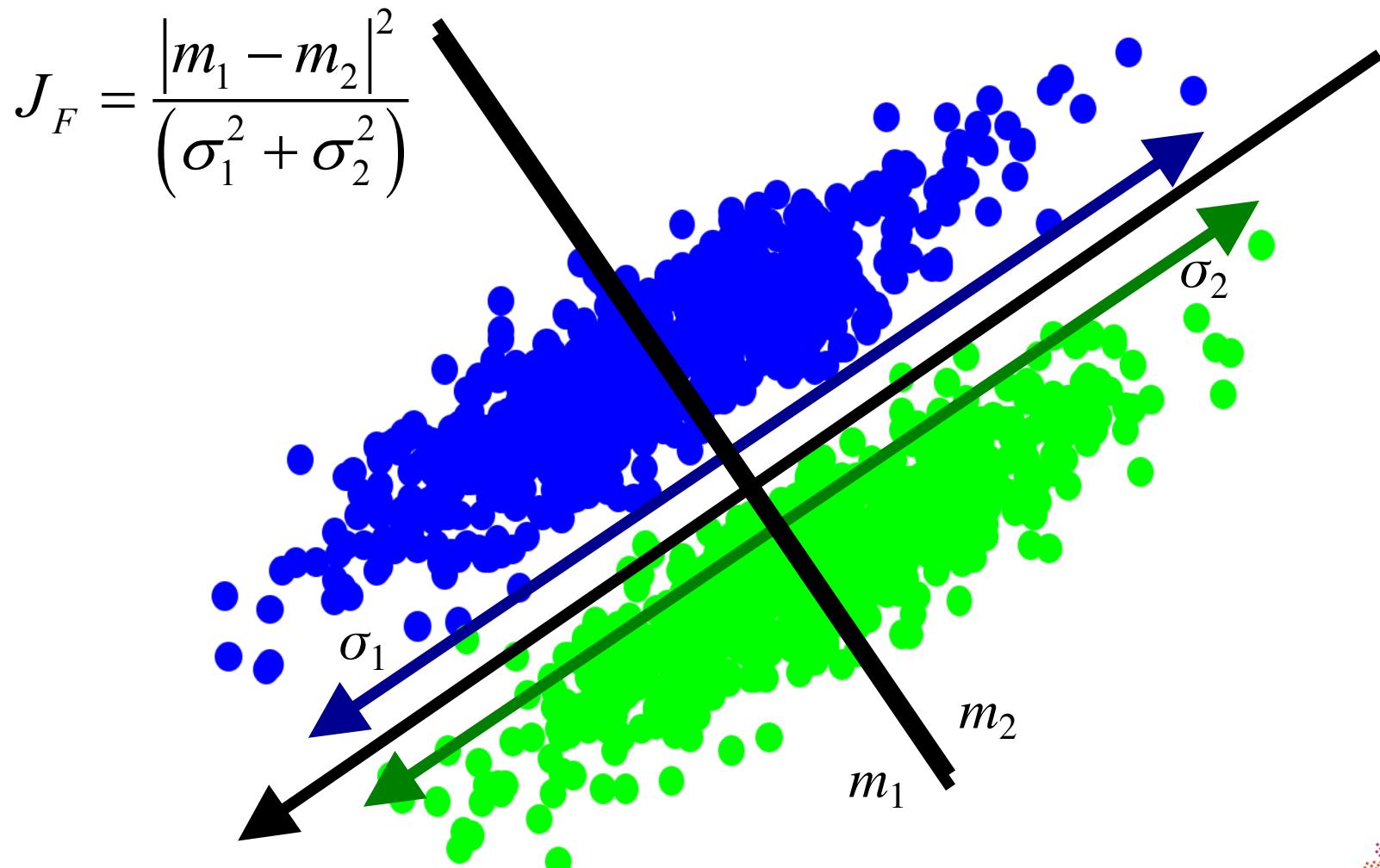


Fisher mapping (Fisher criterion)

$$J_F = \frac{|m_1 - m_2|^2}{(\sigma_1^2 + \sigma_2^2)}$$

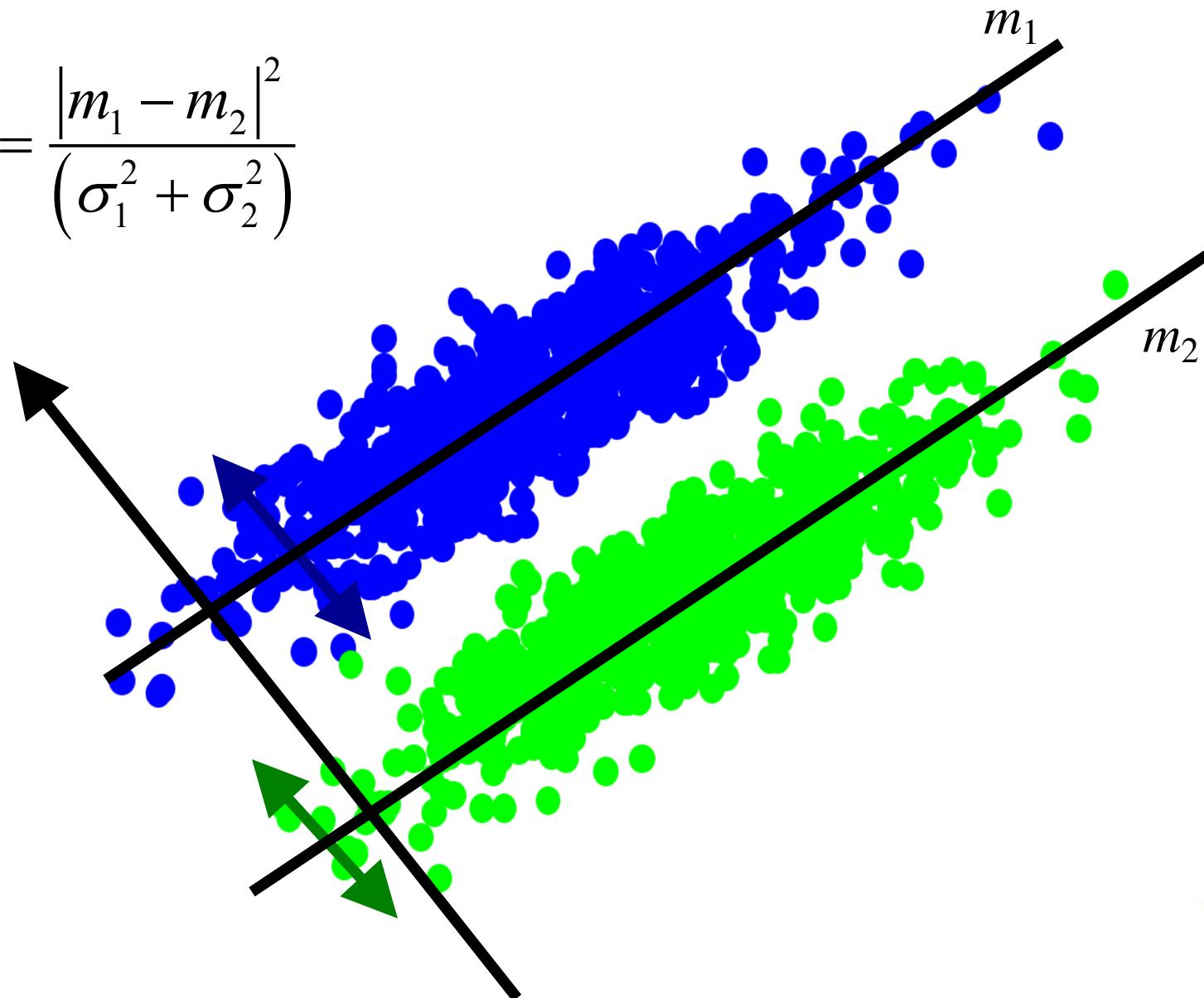


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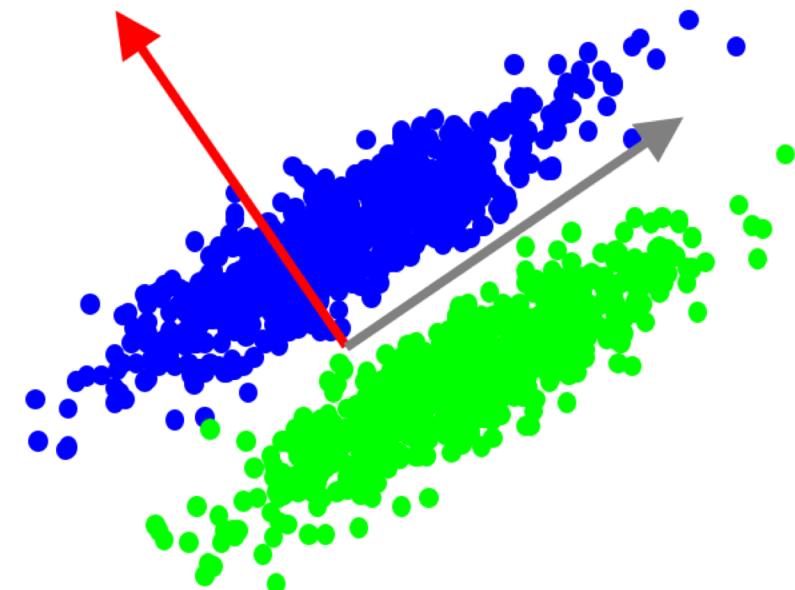


Fisher mapping

- Find basis vector a_1 for $\{x\}$ such that in the projections, the classes are maximally separated
- Choose a_1 to maximise Fisher criterion:

$$J_F(a_1) = \frac{a_1^T S_B a_1}{a_1^T S_W a_1}$$

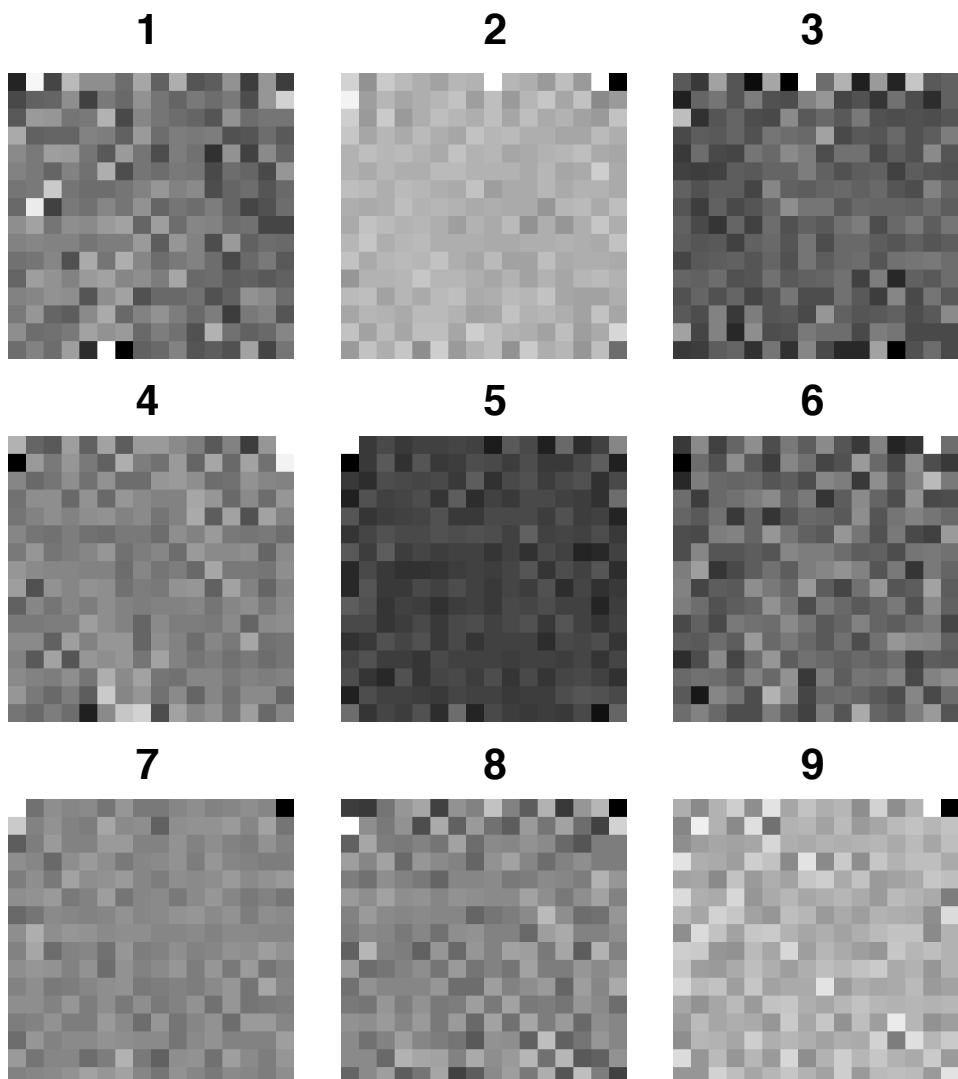
- Maximize between class variance
Minimize within class variance



- Solution:
 - eigen-analysis on $S_W^{-1}S_B$
 - select $c-1$ (# classes - 1) dimensions for final classifier
(allows linear separation of classes)

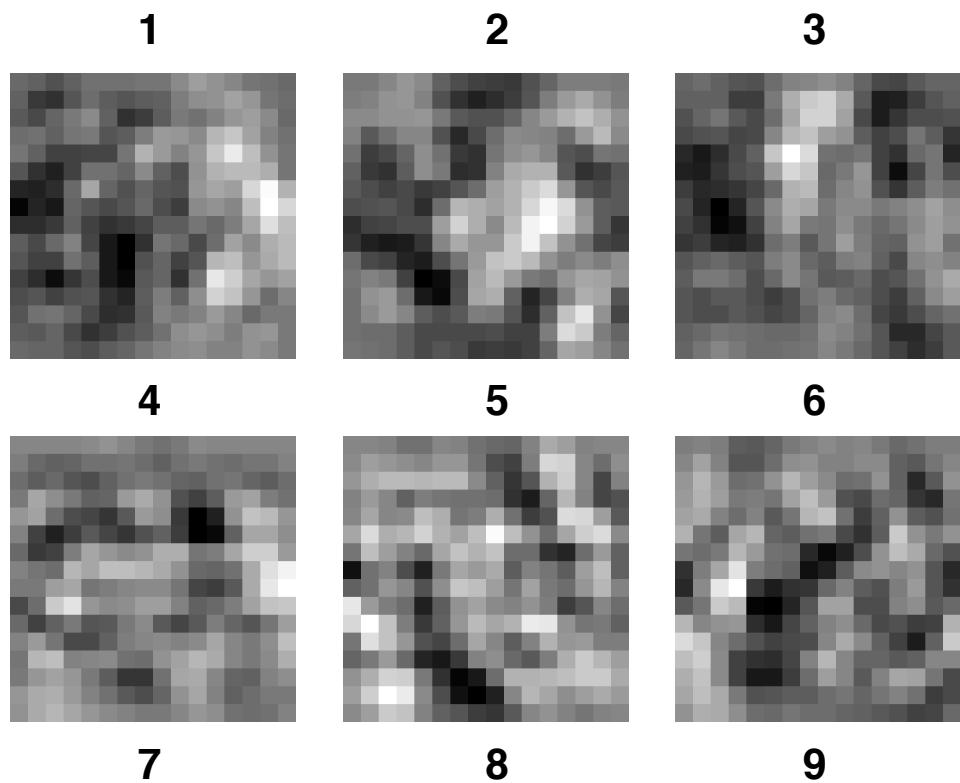
Fisher mapping (3)

- Map down to a maximum of $c - 1$ dimensions
- Example: NIST digits



Fisher mapping (4)

- To avoid fitting noise, can do PCA first
- If system underdetermined ($n \leq p$), first doing PCA is required, otherwise matrix inversion results in singularity

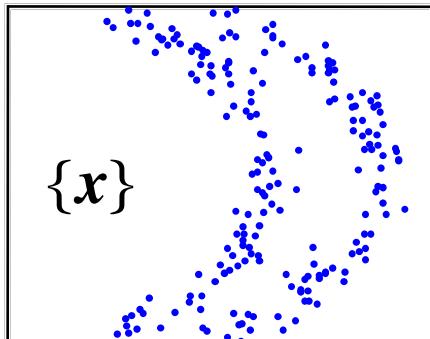


Recapitulation

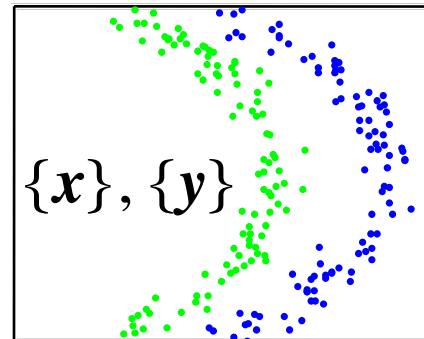
- Discussed:
 - Linear feature extraction
 - Unsupervised: Principal Component Analysis (PCA)
 - Supervised: Fisher mapping

Feature extraction

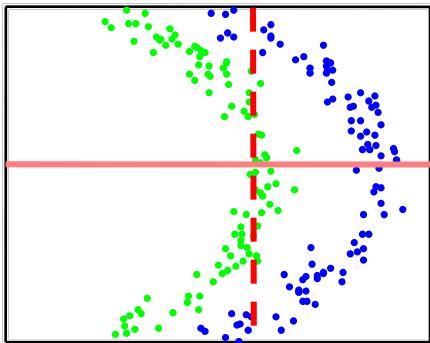
- Main types:



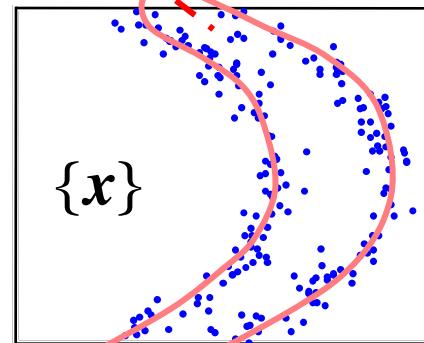
Unsupervised



Supervised



Linear



Nonlinear, unsupervised

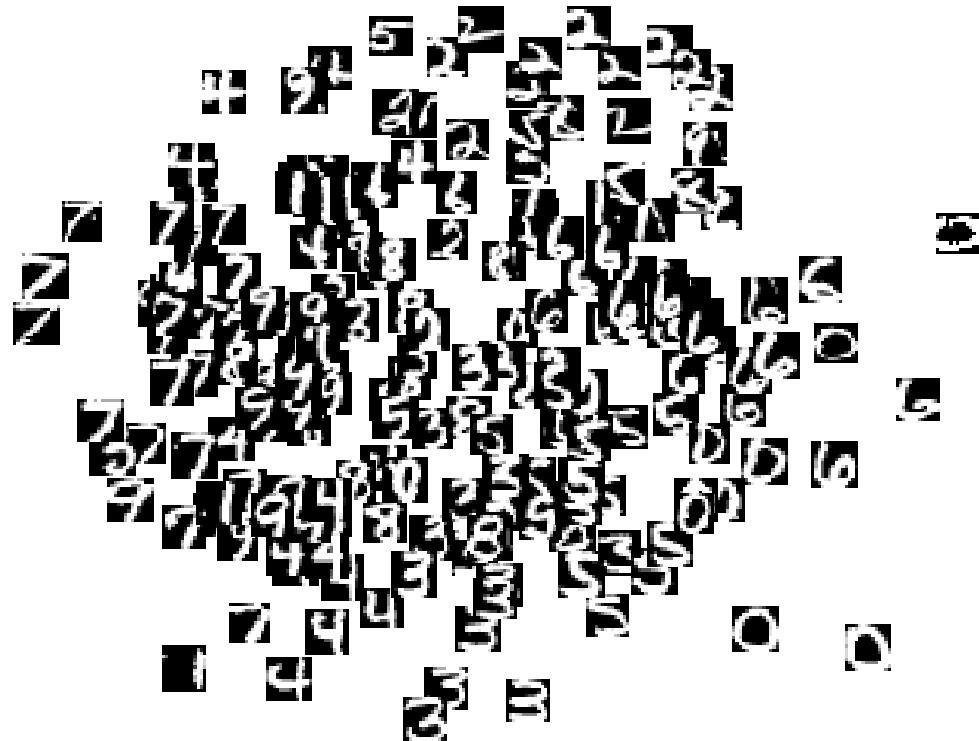
Nonlinear, unsupervised feature extraction

- Multidimensional scaling (MDS):
 - Nonlinear:
 - Sammon mapping
 - t-SNE

Nonlinear feature extraction (3)

Example: embedding

- Find new representation such that distances between samples are preserved as well as possible

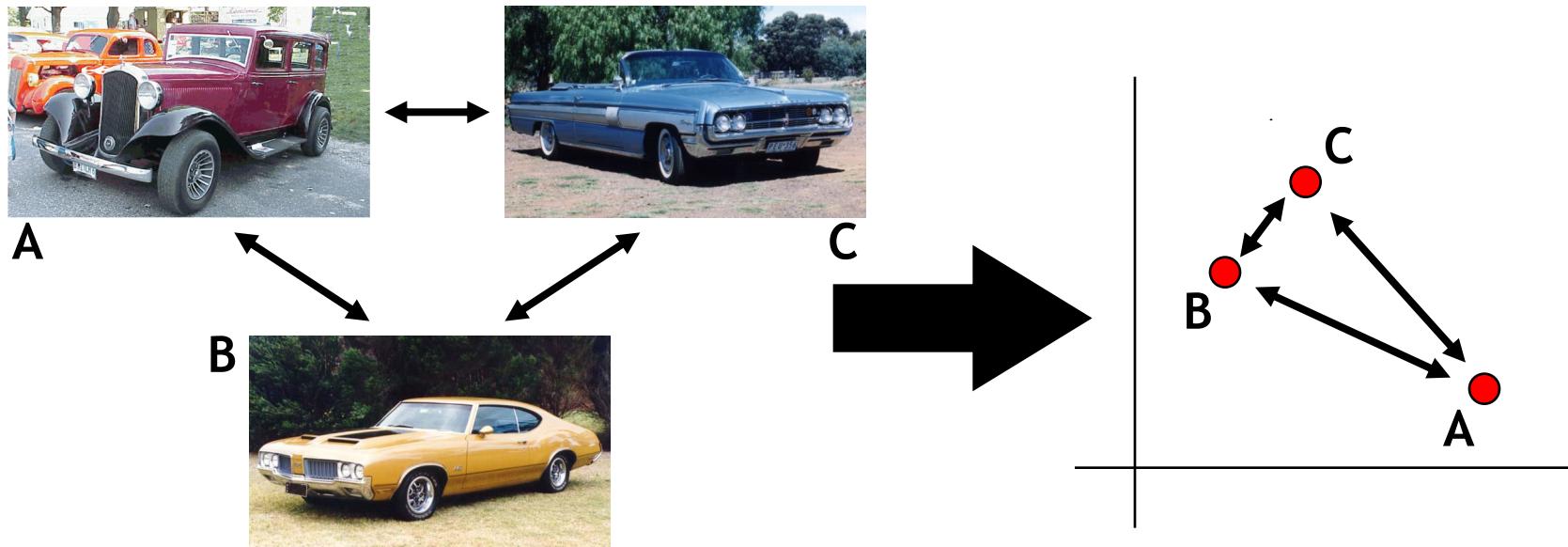


Multidimensional scaling (MDS)

- Criterion: preserve all inter-sample distances
- Needed: $n \times n$ distance matrix between all samples
- Map samples to a new (lower dimensional) space

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 - easy to introduce nonlinearity
- Algorithms should find:
 - new, low-dimensional coordinates for each object
 - the number of dimensions to embed the data in

MDS: Non-linear mappings (5)

- d_{ij} : distance $\|x_i - x_j\|$ in original space ($? - \text{dimensional}$)
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$$Stress(y) = \frac{1}{\sum \sum d_{ij}^{(q+2)}} \sum_i \sum_{j>i} d_{ij}^q (\delta_{ij} - d_{ij})^2$$

- weight factor $q = ..., -2, -1, 0, 1, 2, ...$
 $q > 0$: emphasise large distances
 $q < 0$: de-emphasise large distances (smalled more important)

Sammon mapping: $q = -1$

MDS: Non-linear mappings (6)

- **Procedure:**

- Initialize positions of samples in lower dimensional space (y_i)
- Compute stress

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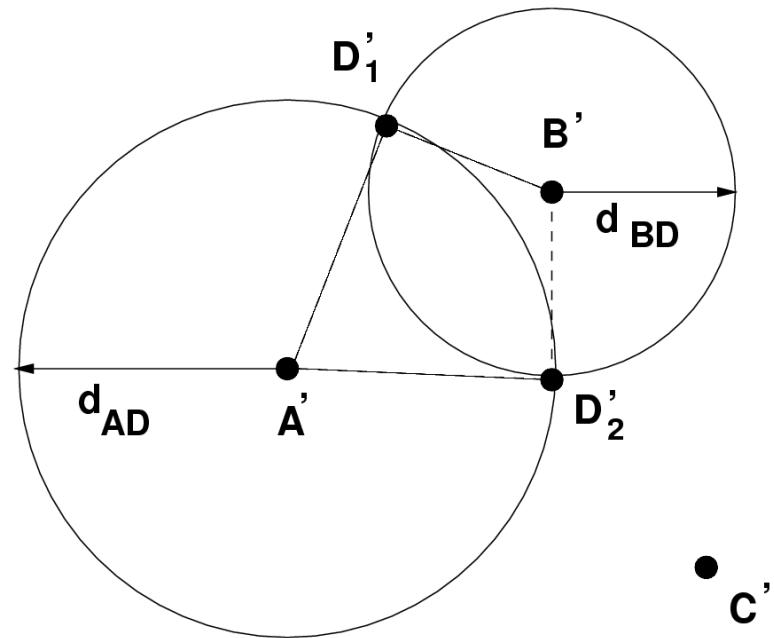
- Compute derivative of the stress with respect to positions of samples in new space
- Adapt the positions of samples in lower dimensional space

$$y' = y - \alpha \frac{\partial Stress(y)}{\partial y}$$

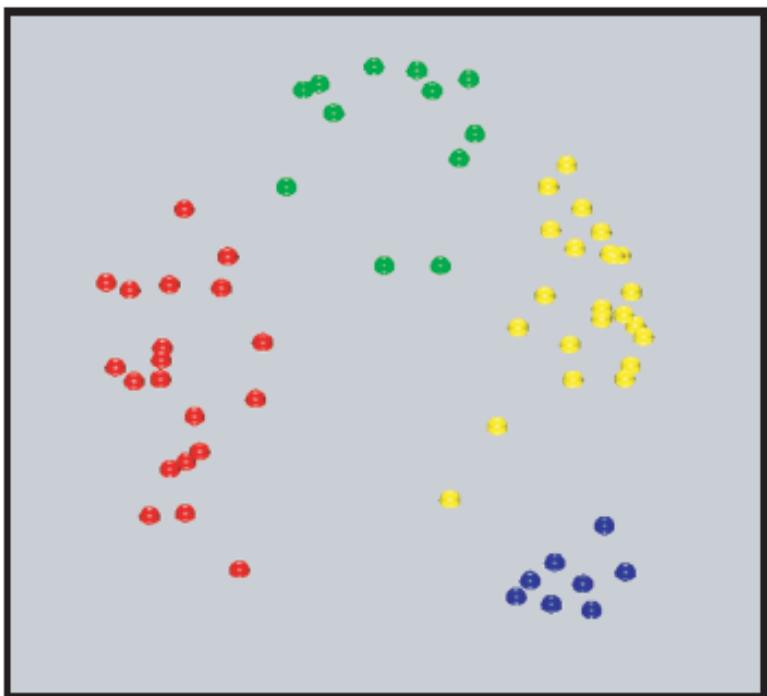
- Repeat till convergence (positions of samples do not change)

Embedding new points

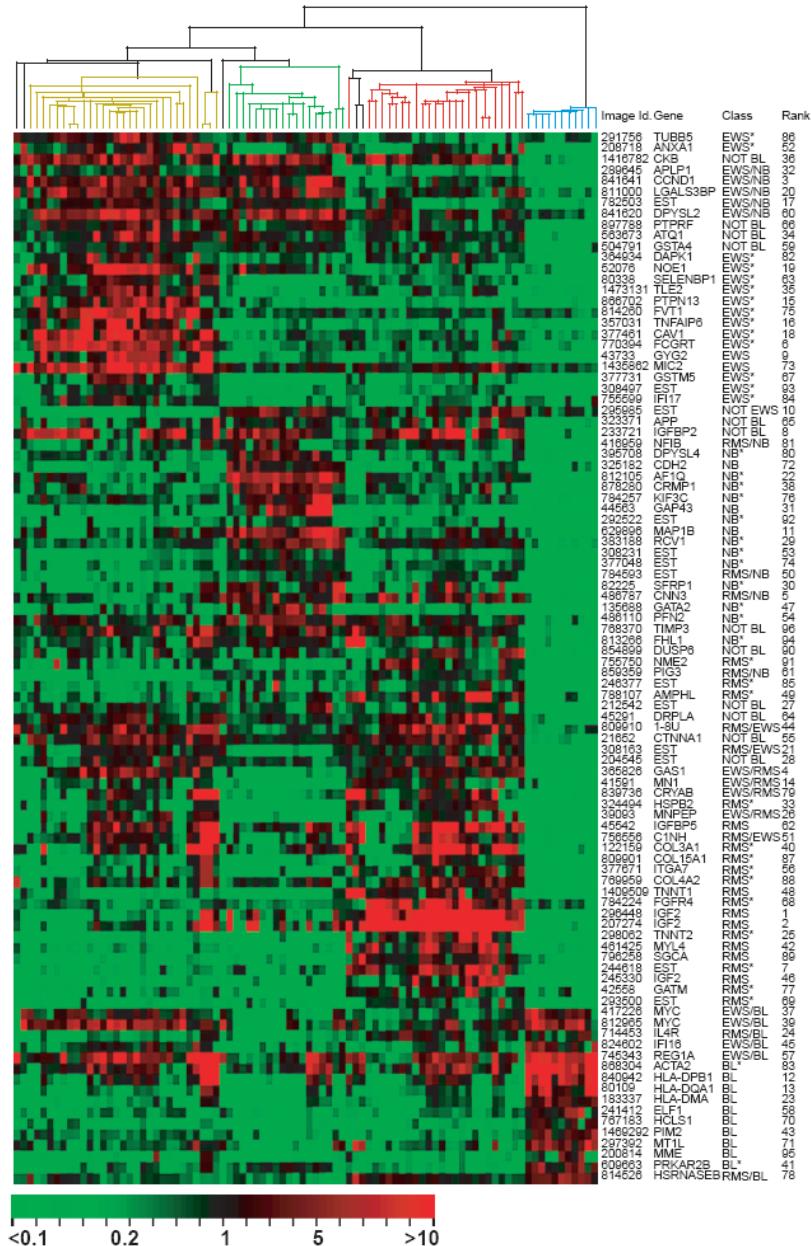
- Problematic: re-run entire algorithm...
- Sub-optimal solution: triangulation
 - Embed new point D
 - D has A and B as neighbors in original space
 - Preserve distance to two embedded neighbours A' , B' exactly
 - Use C' to decide which of the two candidates D_1' , D_2' to use



MDS example

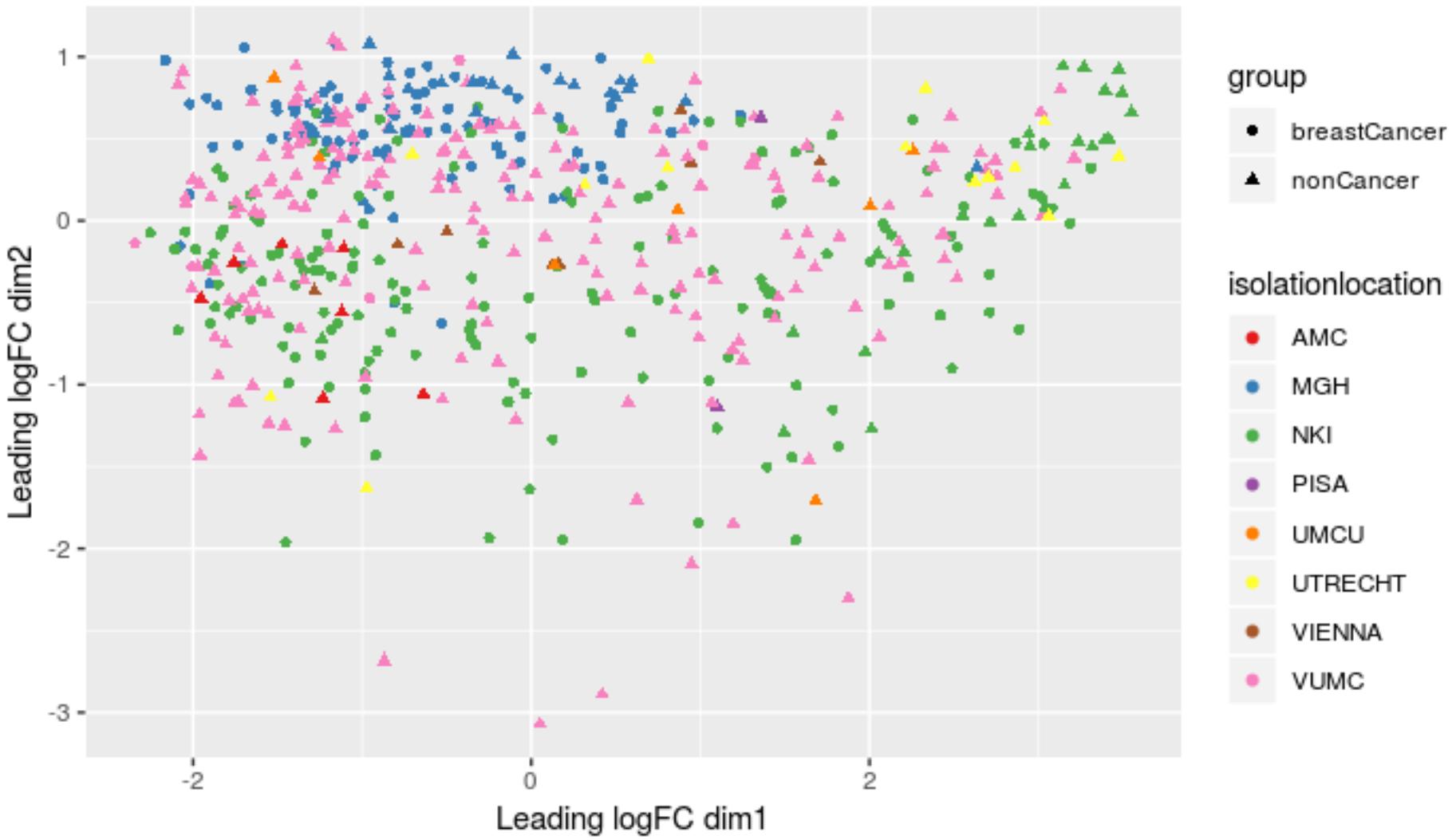


- Neuroblastoma (NB)
- Rhabdomyosarcoma (RMS)
- Burkitt lymphoma (BL)
- Ewing family of tumors (EWS),



Khan et al, Nature Medicine, 2001

MDS Example: detecting batch effects



t-SNE (t-distributed stochastic neighbor embedding) (van der Maaten et al, 2008)

- **Definitions:**

- A **data point** is a point x_i in the original data space R^D
- A **map point** is a point y_i in the map space R^2
- This space will contain our final representation of the dataset
- Every map point represents one of the data points.

t-SNE (3)

- **How do we choose the positions of the map points?**
 - We want to conserve the structure of the data
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- Similarity of data points
 - Let $|x_i - x_j|$ be the Euclidean distance between two data points
 - The conditional similarity between the two data points is:

$$p_{j|i} = \frac{\exp(-|x_i - x_j|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-|x_i - x_k|^2 / 2\sigma_i^2)}$$

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Convert a *dissimilarity*
(Euclidean distance)
to a *similarity*

- This represents the likelihood of x_j given x_i
- Assuming a Gaussian distribution around x_i with variance σ_i^2

t-SNE (4)

- The conditional similarity between the two data points is:

$$p_{j|i} = \frac{\exp(-|x_i - x_j|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-|x_i - x_k|^2 / 2\sigma_i^2)}$$

- σ_i^2 is different for every point
 - * dense areas are given a smaller variance
 - * sparse areas are given a larger variance
- Similarity is symmetrized form:

$$p_{ij} = (p_{j|i} + p_{i|j})/2N$$

t-SNE (5)

- **Similarity of map points:**

- Let $|y_i - y_j|$ be the Euclidean distance between the map points

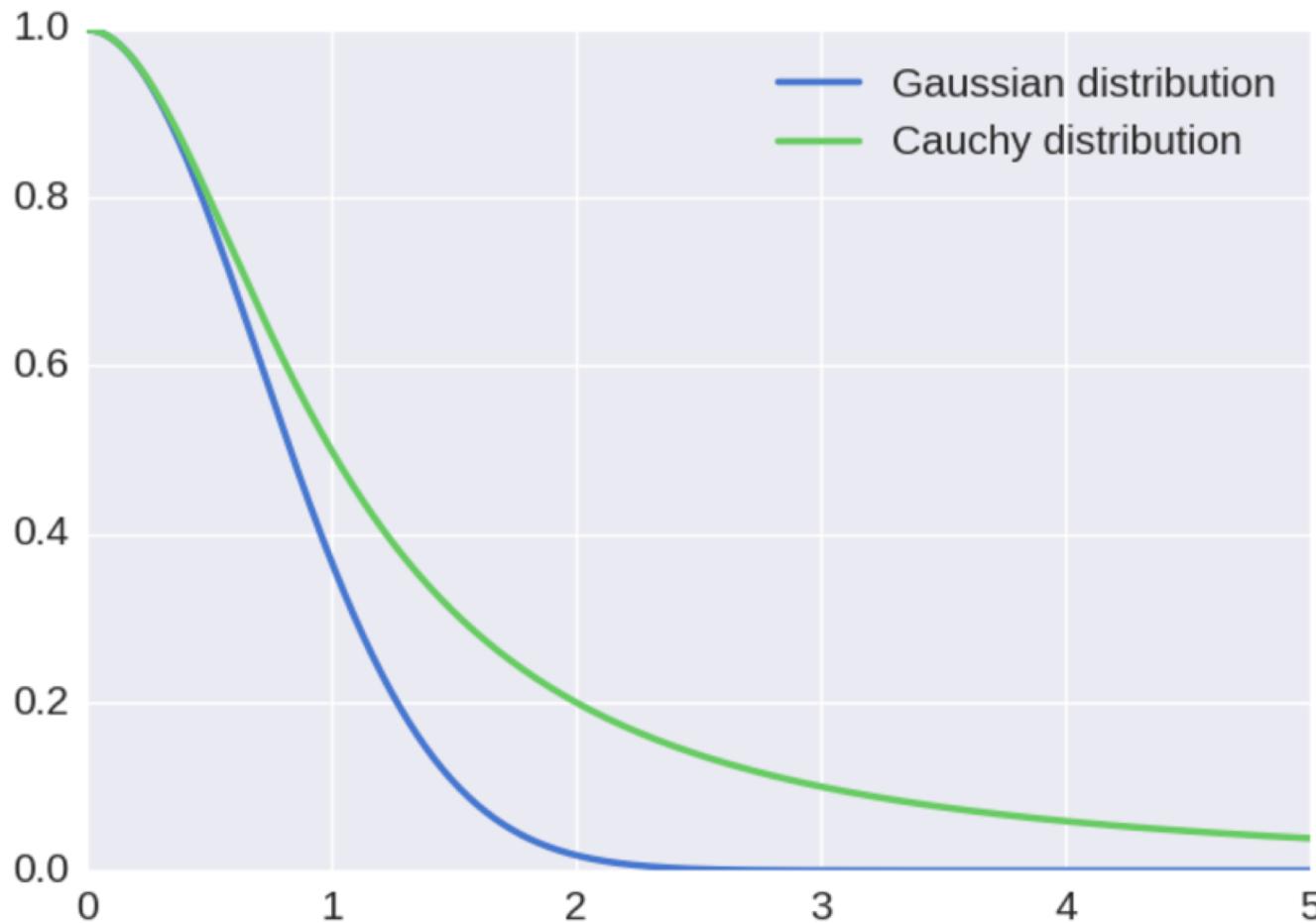
$$q_{ij} = \frac{f(|y_i - y_j|)}{\sum_{k \neq i} f(|y_i - y_k|)}$$

with

$$f(z) = 1/(1 + z^2)$$

- Same as for the data points, but different distribution:
 - t-Student with one degree of freedom, or Cauchy distribution

t-SNE (10): Cauchy and Gaussian distribution



t-SNE (6)

- How do we choose the positions of the map points?
 - Data similarity matrix (p_{ij}) is fixed
 - Map similarity matrix (q_{ij}) depends on the map points
 - Get two matrices as similar as possible
 - Idea: similar data points yield similar map points

t-SNE (7)

- **Algorithm**

- Minimizing the Kullback-Leibler divergence between p_{ij} and q_{ij} :

$$KL(P, Q) = \sum_{i,j} p_{ij} \log(p_{ij}/q_{ij})$$

- $KL(P, Q)$ measures the distance between our two distributions

t-SNE (7)

- **Algorithm**

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$$KL(P, Q) = \sum_{i,j} p_{ij} \log(p_{ij}/q_{ij})$$

- $KL(P, Q)$ measures the distance between our two distributions
 - To minimize this score, we perform a gradient descent
 - The gradient can be computed analytically:

$$\frac{\partial KL(P, Q)}{\partial y_i} = 4 \sum_j (p_{ij} - q_{ij}) f(|y_i - y_j|)$$

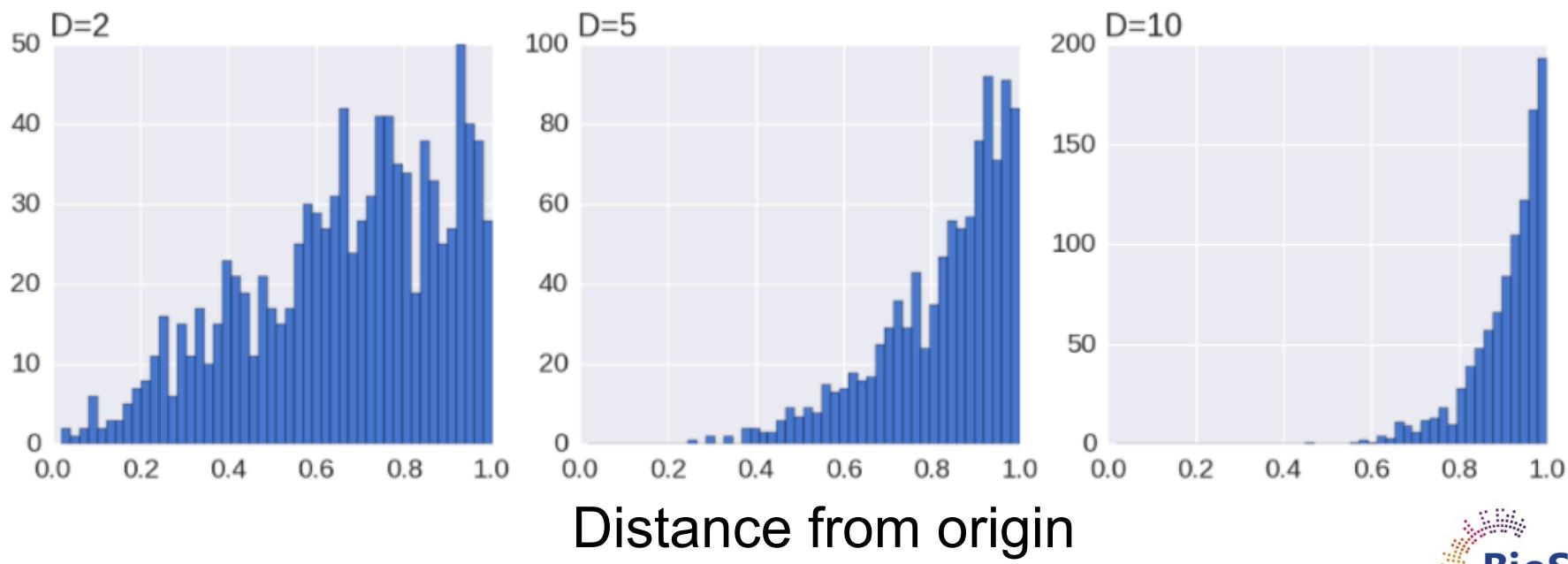
where $f(z) = z/(1 + z^2)$

- The gradient expresses the sum of all spring forces applied to map point i .

t-SNE (8)

- Why the t-Student distribution?

- The volume of the N -dim. ball of radius r scales as r^N
- For large N , random points are close to the surface, not in center



t-SNE (9)

- Why the t-Student distribution?

- We go from high dimensionality to low dimensionality
- If we use the same distribution in data and map space
- There is an imbalance in the distribution of the distances of a point's neighbors.
- As distances are so different between a high-D and low-D space
- Yet, t-SNE tries to reproduce the same distances in the two spaces
- Result: excess of 'attraction forces' (gradient) that move map space points
- t-SNE compensates this by the heavier tail of the t-distribution in low-D
- Larger distances in low-D get more weight so match high-D

t-SNE (10)

- Setting σ_i
 - Unlikely that a single value of σ_i is optimal
 - Density of datapoints varies
 - * In dense regions a smaller value
 - * In sparse regions a larger value
 - σ_i induces a probability distribution, P_i , across all datapoints
 - This distribution's entropy increases as σ_i increases
 - t-SNE searches for the σ_i such that P_i has the specified *perplexity* (J):

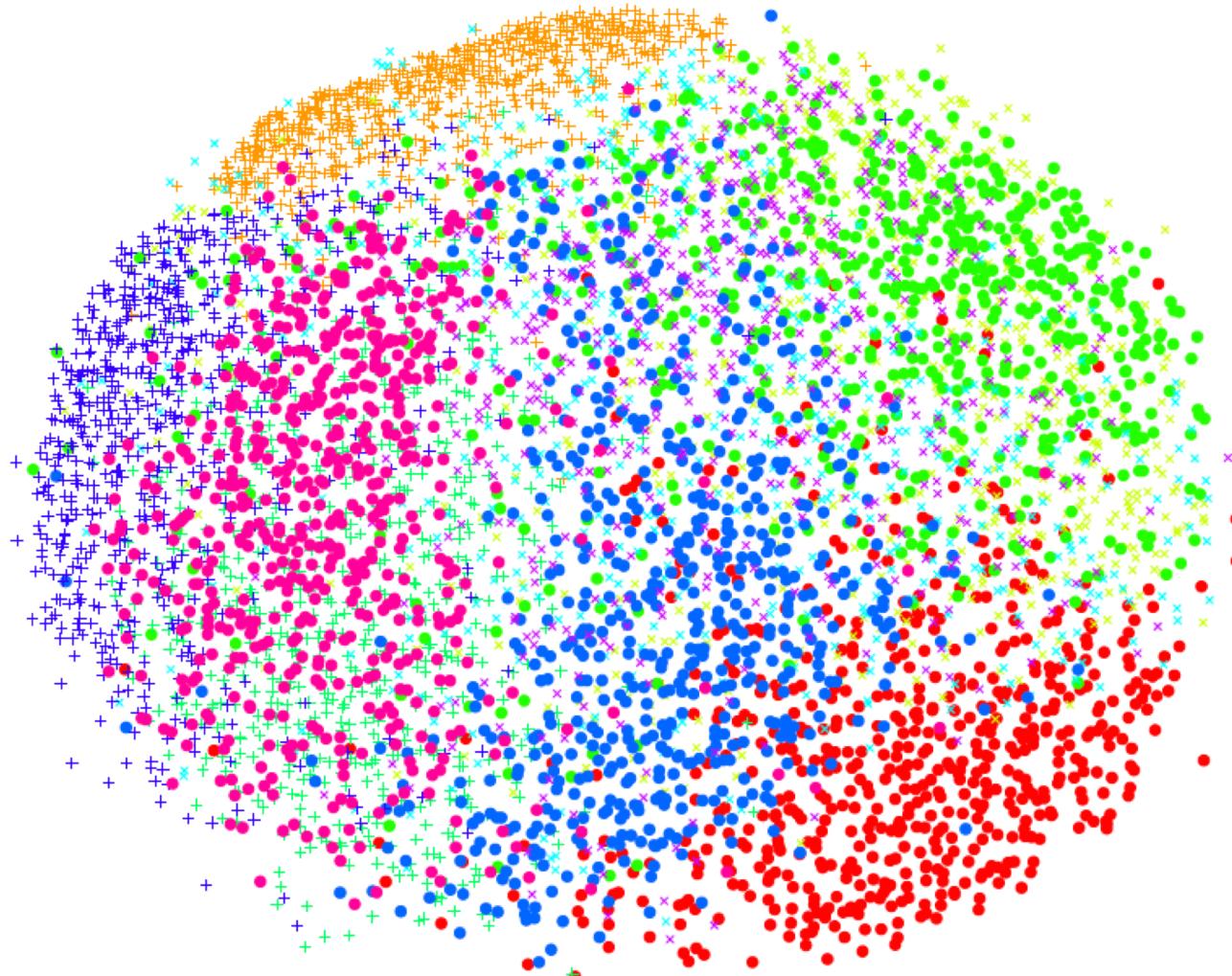
$$J(P_i) = 2^{H(P_i)}$$

- where $H(P_i)$ is the Shannon entropy of P_i in bits:

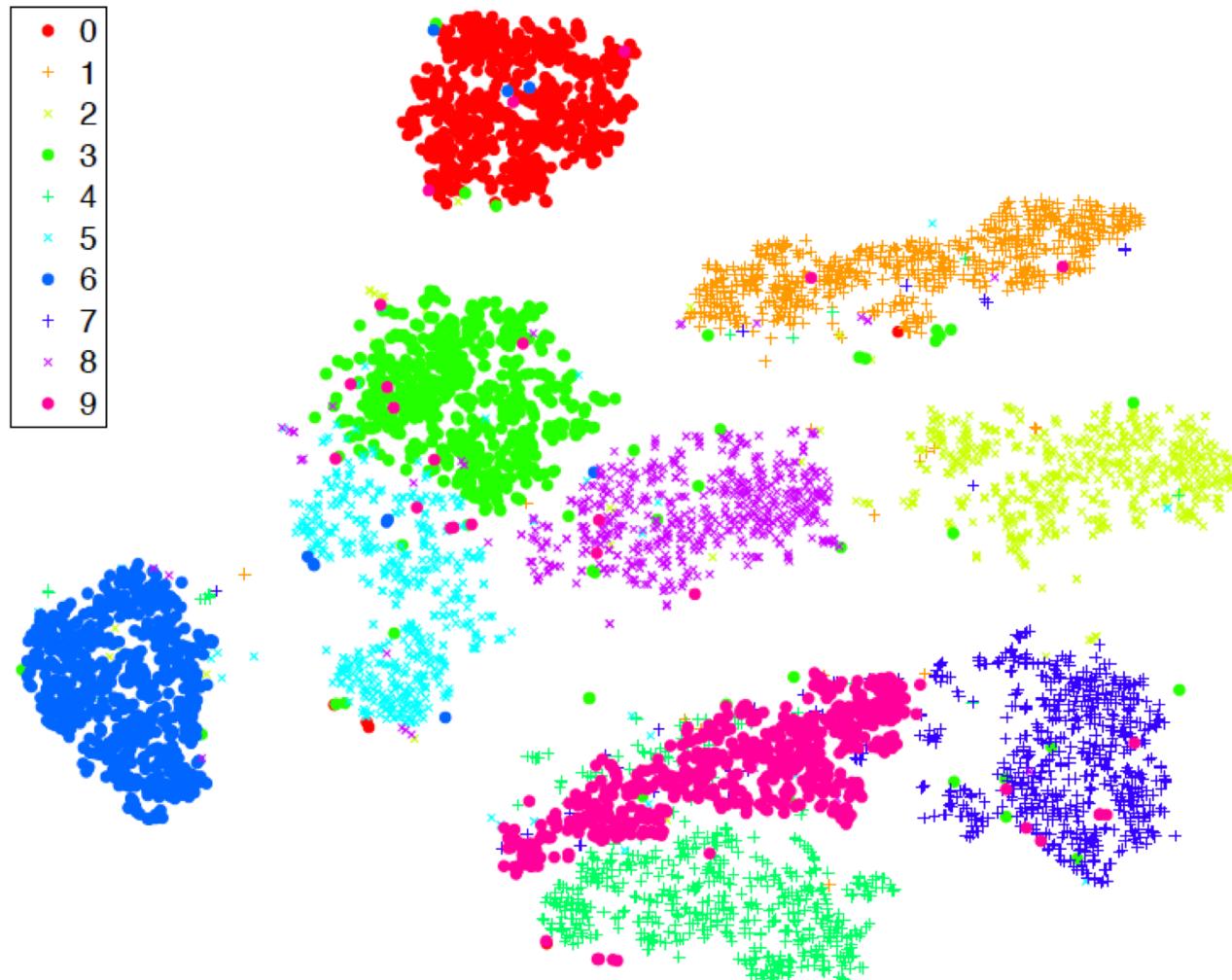
$$H(P_i) = - \sum_j p_{j|i} \log_2(p_{j|i})$$

- Perplexity is a smooth measure of the effective number of neighbors
- t-SNE is not sensitive to this value: set between 5 and 50

t-SNE (11): Sammon map of digit data



t-SNE (12): t-SNE map of digit data



MDS conclusions

- Experts or measurements give distances
- Optimise a *stress-function* (MDS) or KL distance (t-SNE)
- Important:
 - *the distance measure used*: is it representative?
 - *the weighting of distances (q)*: can influence outcome heavily.
 - t-SNE run with defaults is quite reliable
- Largest risk:
seeing structure in the data that is not really there
- Remaining problem: embedding new data points
- T-SNE (and now UMAP) are modern techniques to perform representation of data in high-D space in 2D

Feature selection

- For feature selection, we need:
 - A **criterion function**
e.g. error, class overlap, information loss
 - A **search algorithm**
e.g. pick the best single feature at each time

Criteria

1. Wrapper: exact performance measure

- base performance estimate on classifier;
- estimate performance using cross-validation:
- very expensive!

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2. Filter: approximate performance predictors:

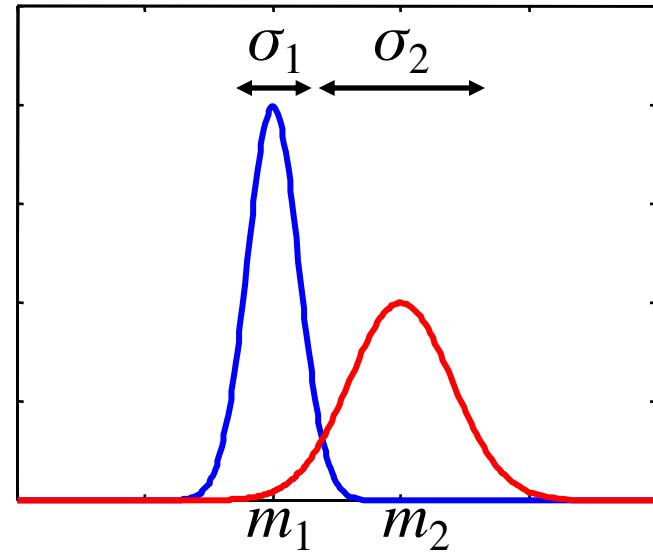
- calculate the performance of an easy-to-use model
- indication of how well a more powerful model may perform
- is much faster to compute.

Criteria (2)

- Example

- Simple measure of the ‘separability’ of classes given a feature
- 1D case: Signal-to-Noise Ratio (SNR) or Fisher criterion:

$$J_F = \frac{|m_1 - m_2|^2}{(\sigma_1^2 + \sigma_2^2)}$$



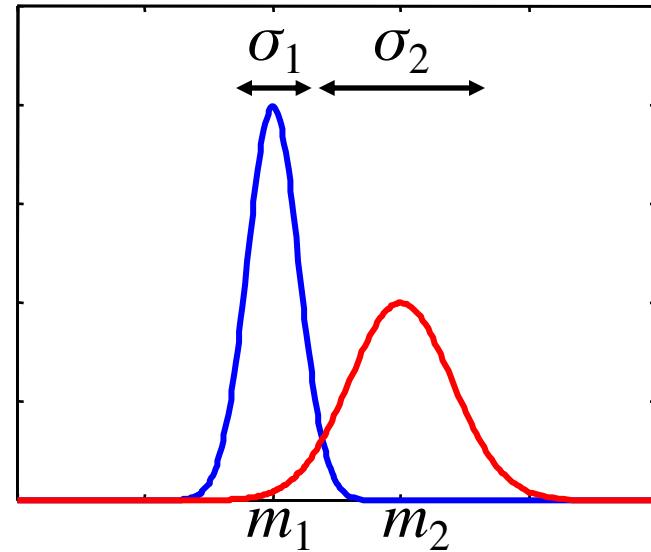
Criteria (3)

- Example

- Simple measure of the ‘separability’ of classes given a feature
- 1D case: Signal-to-Noise Ratio (SNR) or Fisher criterion:

$$J_F = \frac{|m_1 - m_2|^2}{(\sigma_1^2 + \sigma_2^2)}$$

- If J_F is large: good separability
- If J_F is small: poor separability

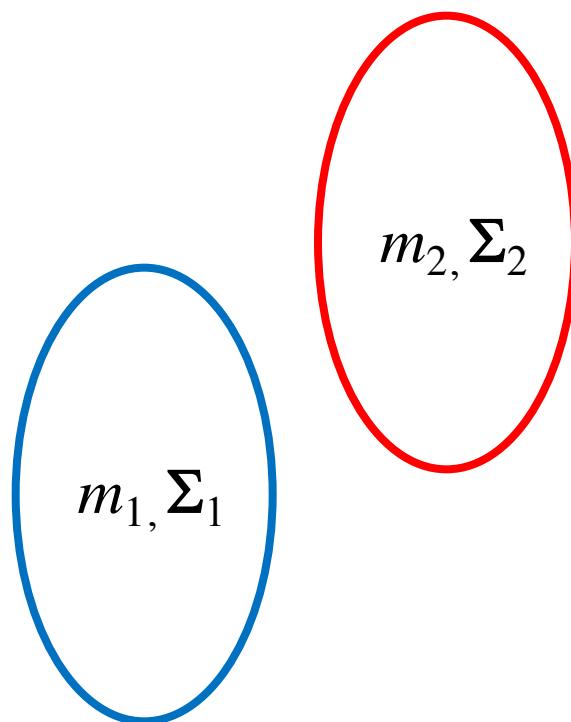


Criteria (4)

- The multi-variate equivalent of Fisher criterion is the
- Mahalanobis distance:
 - assumes
 - Gaussian distributions with
 - equal covariance matrix Σ :

$$D_M = (m_1 - m_2)^T \Sigma^{-1} (m_1 - m_2)$$

$$\Sigma = \sum_{i=1}^C \frac{n_i}{n} \Sigma_i$$



Criteria (5)

- Recall

$$\mathbf{S}_w = \sum_{i=1}^C \frac{n_i}{n} \Sigma_i \quad \mathbf{S}_B = \sum_{i=1}^C \frac{n_i}{n} (\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^T$$

- Scatter-based classification performance indicators:

$$J_1 = \text{trace}(\mathbf{S}_W + \mathbf{S}_B) = \text{trace}(\Sigma)$$

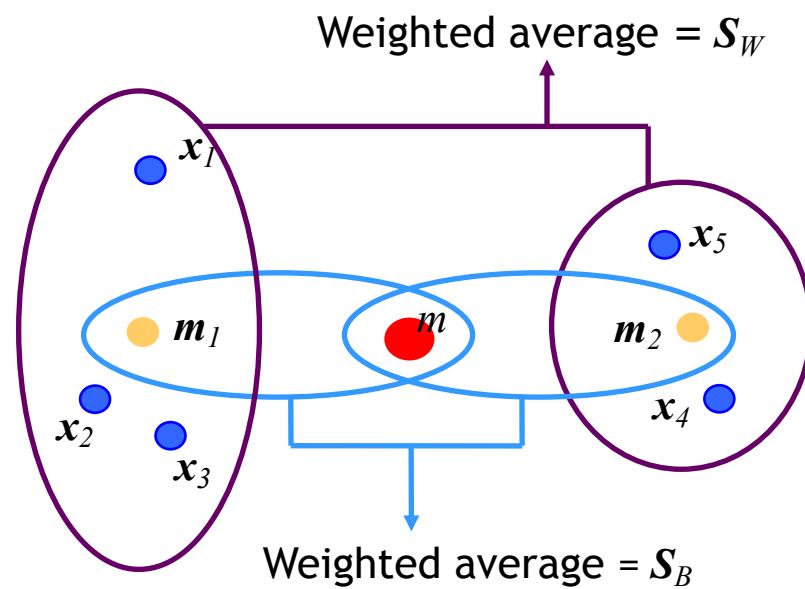
$$J_2 = \text{trace}(\mathbf{S}_B / \mathbf{S}_w)$$

$$J_3 = \det(\Sigma) / \det(\mathbf{S}_w)$$

$$J_4 = \text{trace}(\mathbf{S}_W) / \text{trace}(\mathbf{S}_B)$$

(trace = sum of diagonal elements)

- These are all just approximations!



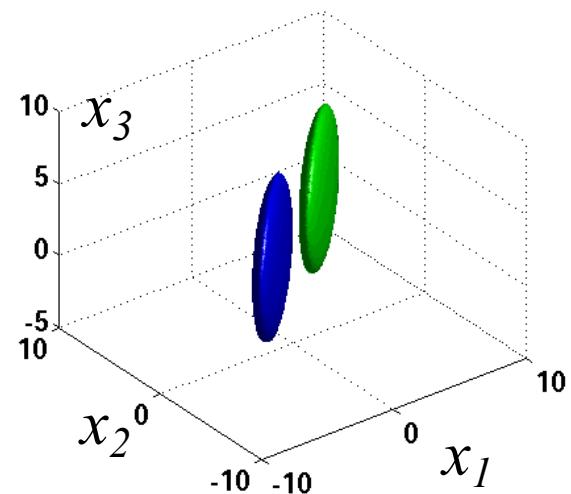
Search algorithms

- Feature selection: select a subset of d out of p features which optimises the criterion
- Simplest solution: look at all possible subsets
- Problem: there are $\binom{p}{d} = \frac{p!}{(p-d)!d!}$ subsets
 - e.g. $p = 50$ features,
 $d = 2$: 1225 subsets
 $d = 5$: 2.1×10^6 subsets
 $d = 25$: 1.3×10^{14} subsets

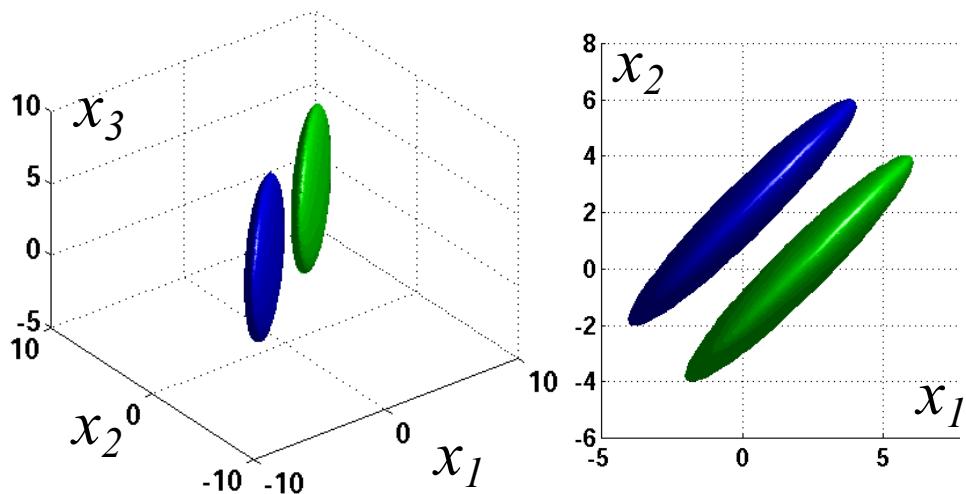
Search algorithms (2)

- Sub-optimal algorithms: select or deselect one feature (or a few features) at a time
- Simplest: best individual d
but these are not necessarily the best d !
- Demonstration: two Gaussians;
select 2 features out of 3 for classification

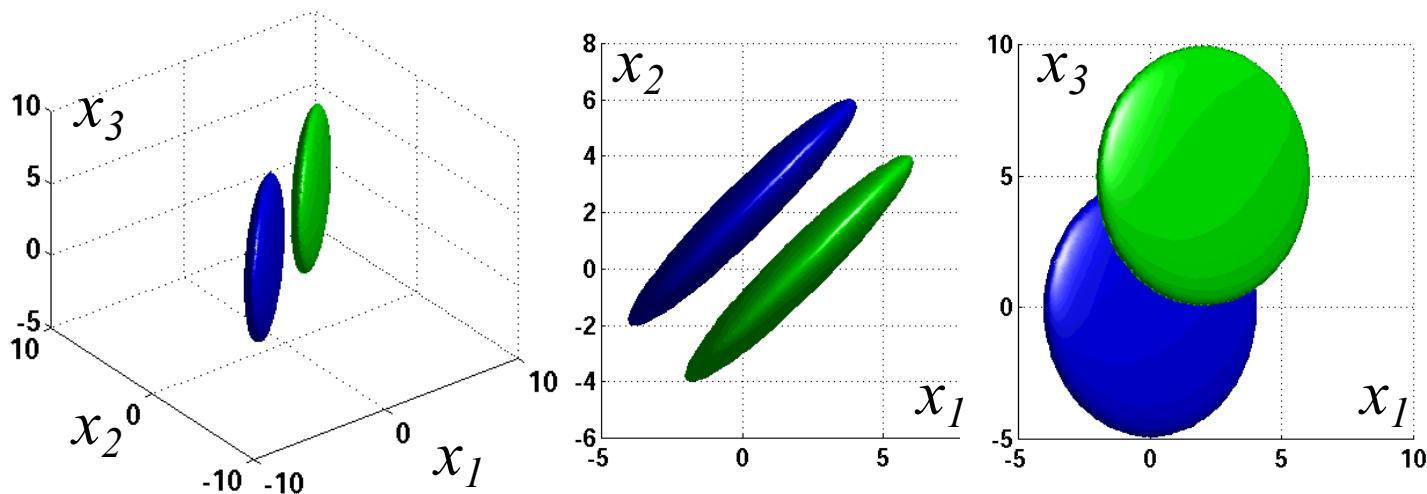
Search algorithms (3)



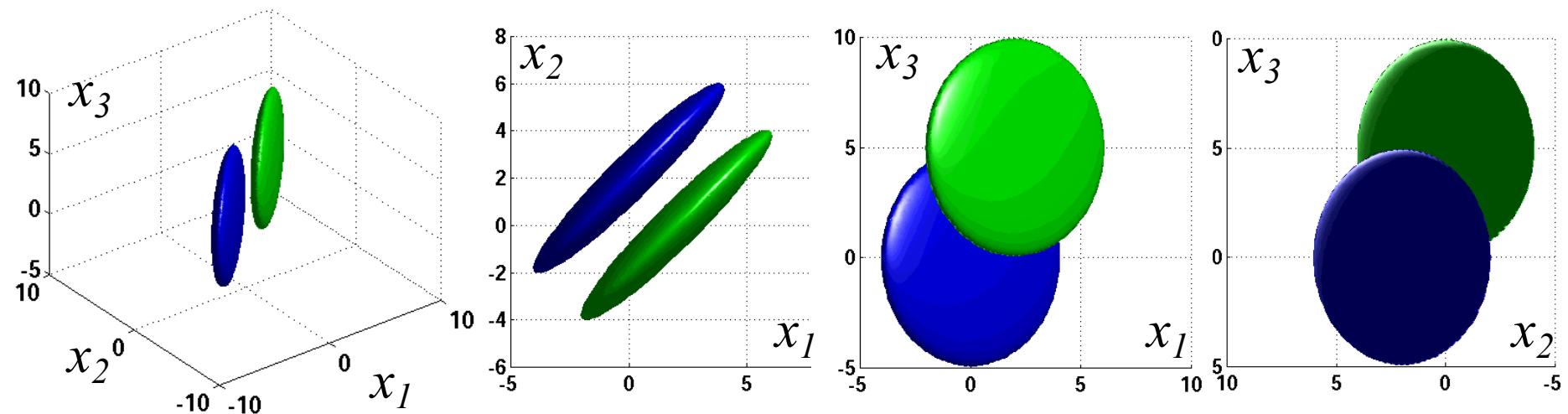
Search algorithms (3)



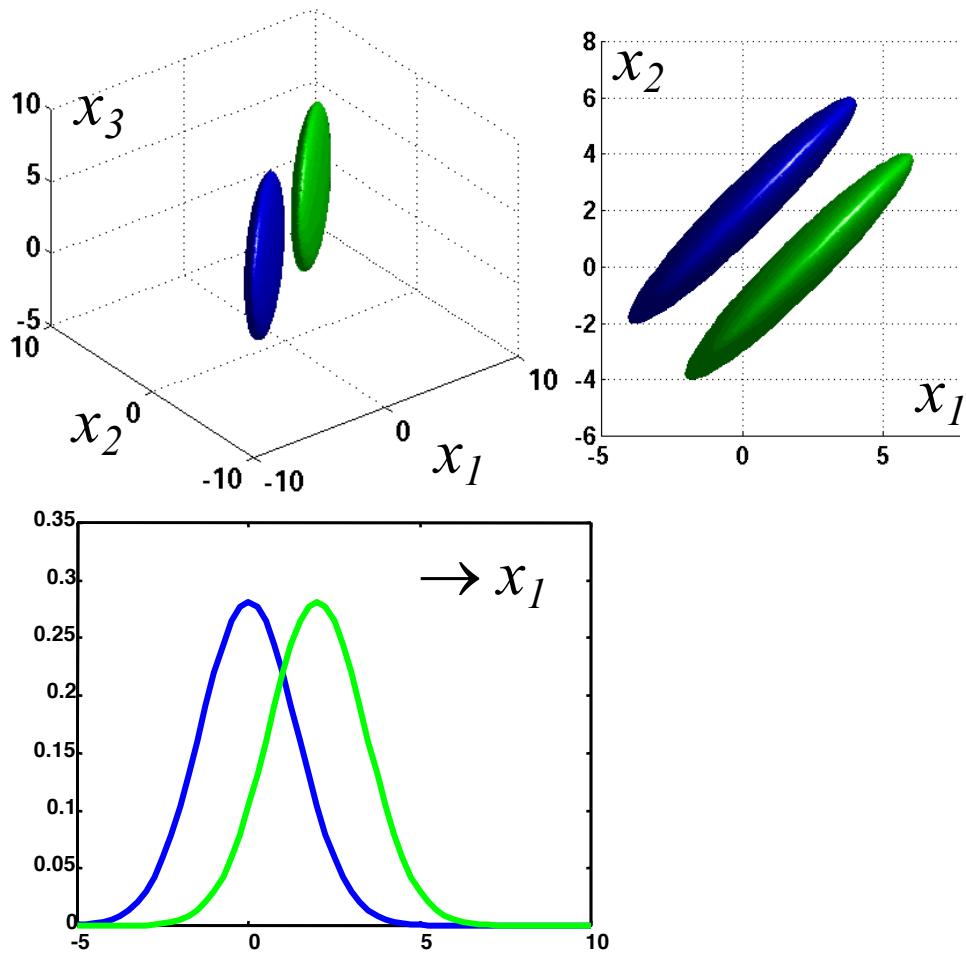
Search algorithms (3)



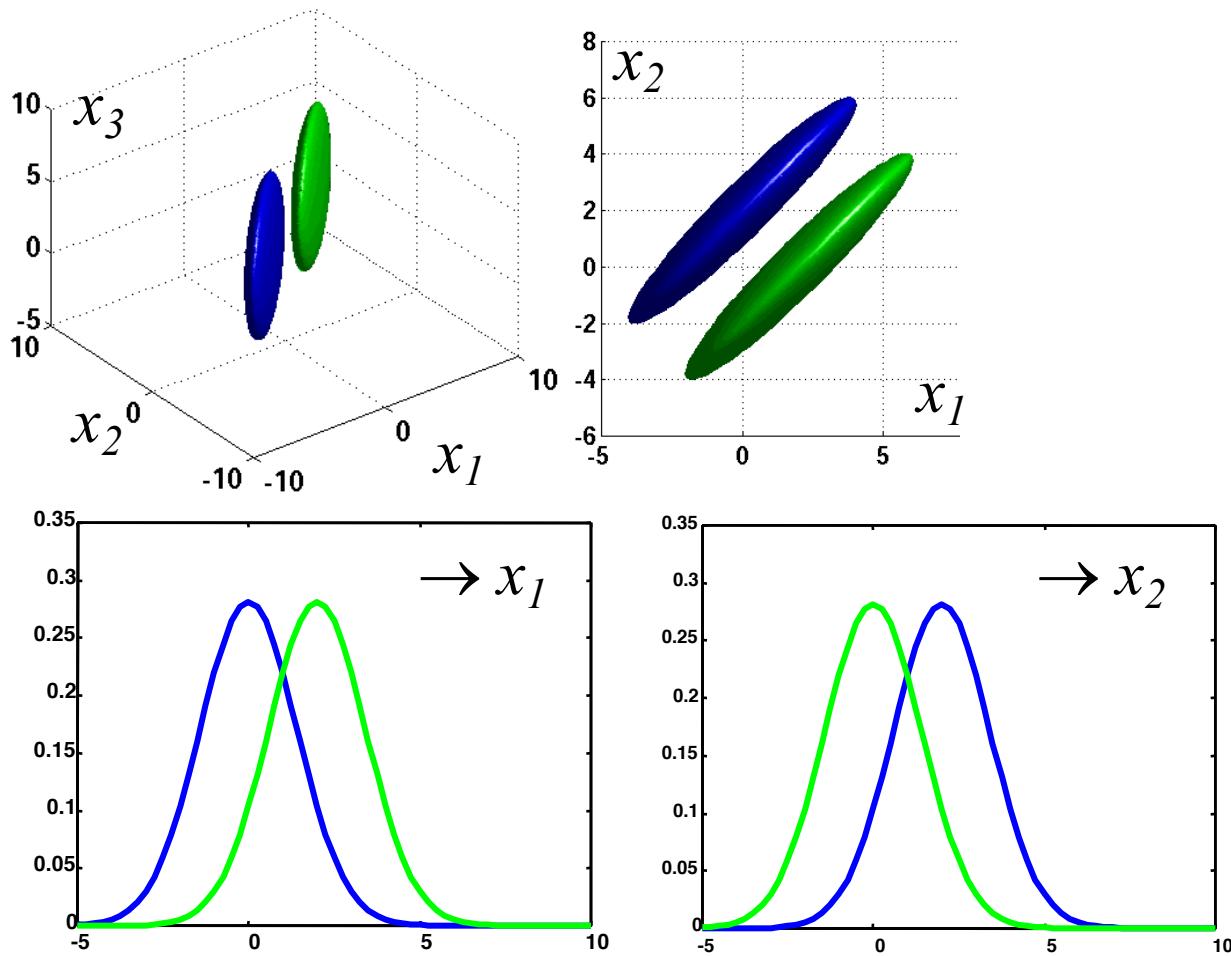
Search algorithms (3)



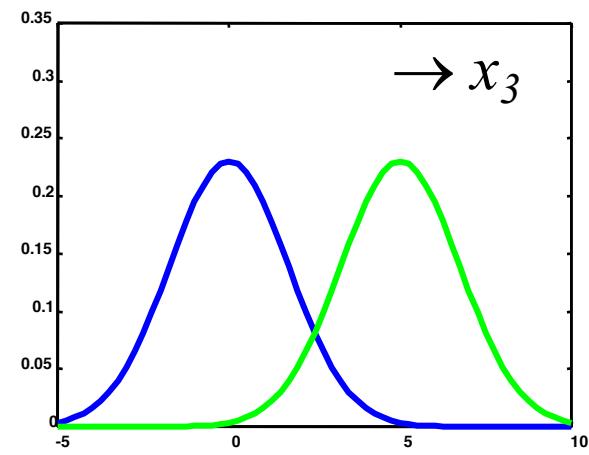
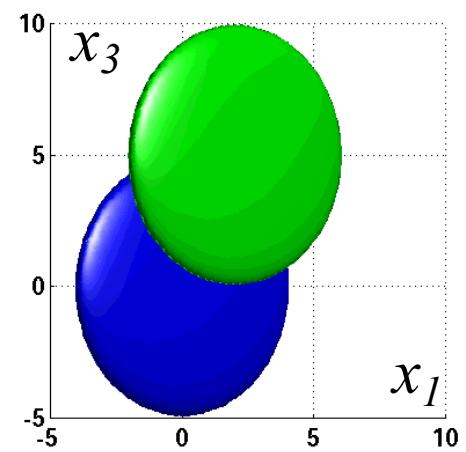
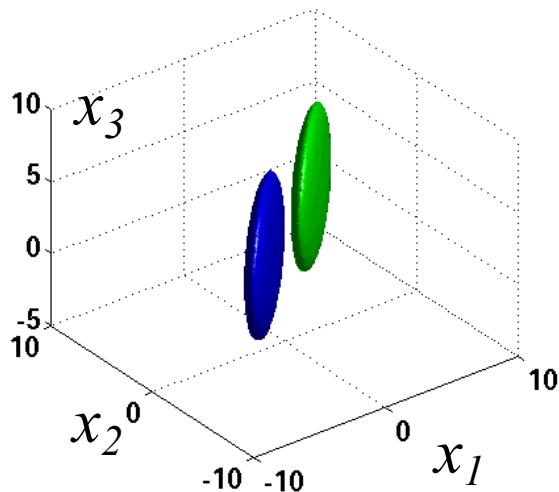
Search algorithms (3)



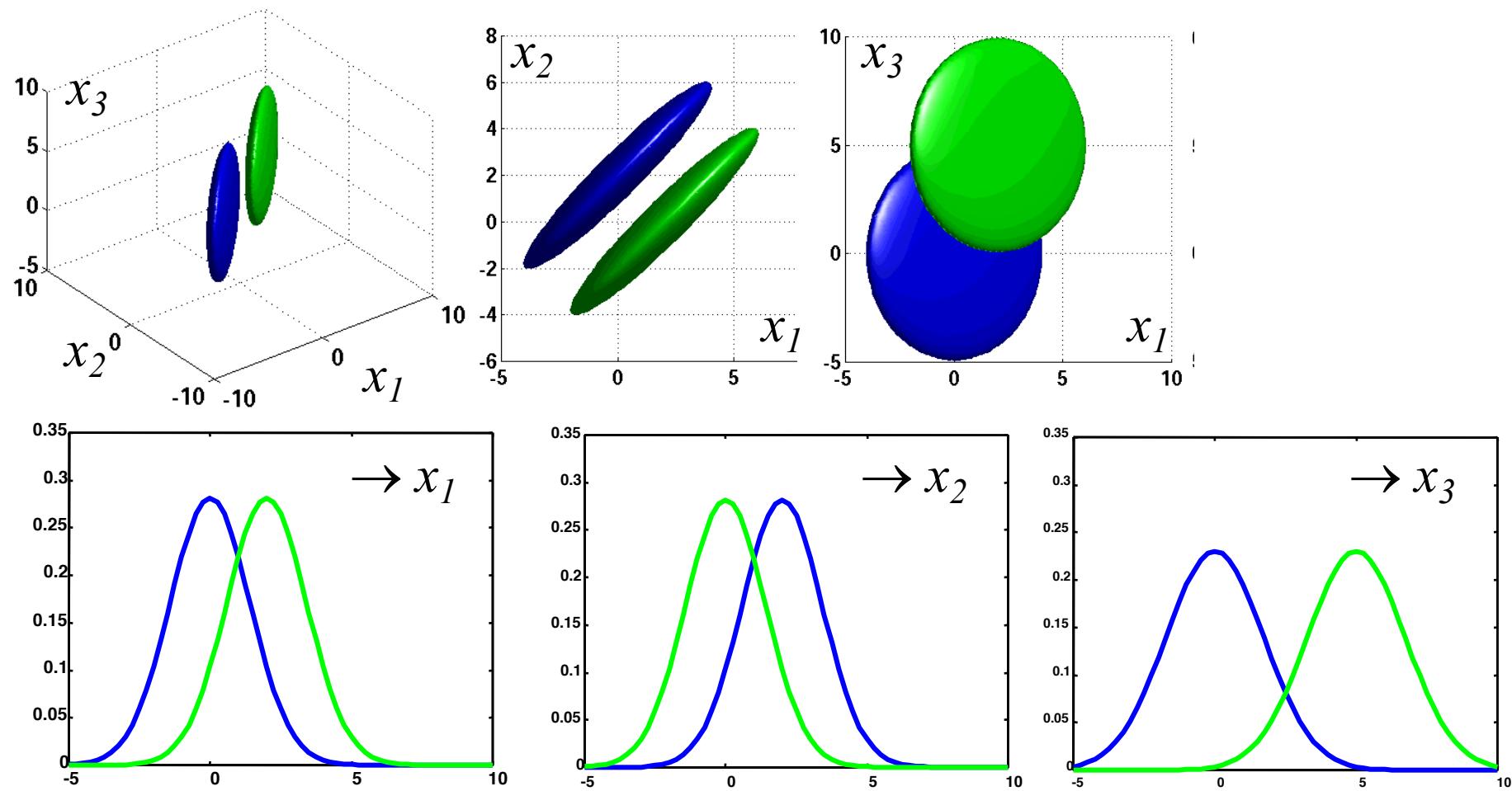
Search algorithms (3)



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Search algorithms (3)



Search algorithms (4)

- Other sub-optimal algorithms:
 - Forward selection (for when d is low)
 - start with empty set
 - keep adding one feature at a time so that the entire subset so far performs best

Search algorithms (4)

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 - Forward selection (for when d is low)
 - start with empty set
 - keep adding one feature at a time so that the entire subset so far performs best
 - Backward selection (for when d is high)
 - start with entire set
 - keep removing one feature at a time so that the entire subset so far performs best

Search algorithms (4)

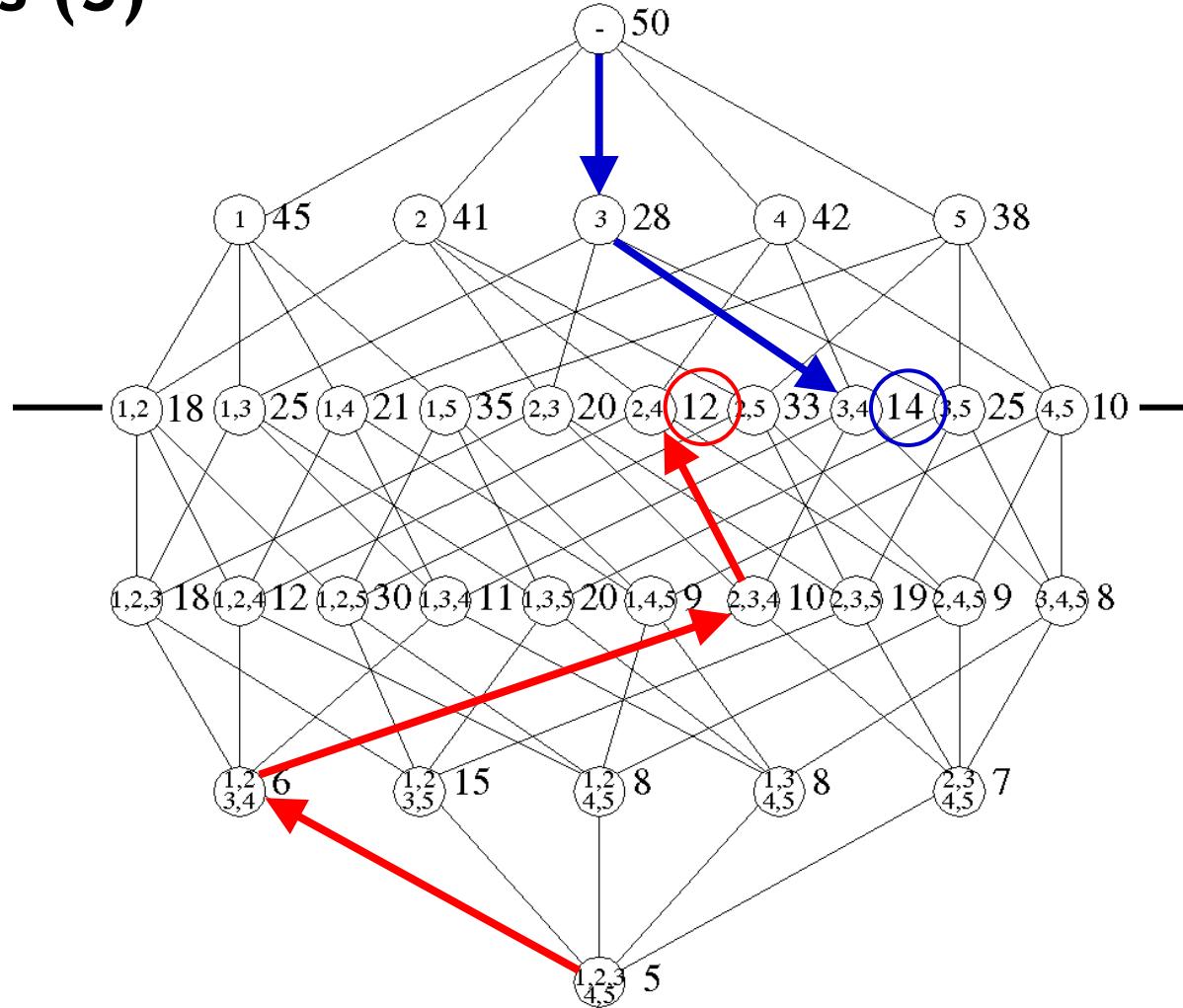
- Other sub-optimal algorithms:
 - Forward selection (for when d is low)
 - start with empty set
 - keep adding one feature at a time so that the entire subset so far performs best
 - Backward selection (for when d is high)
 - start with entire set
 - keep removing one feature at a time so that the entire subset so far performs best
 - Plus- l -takeaway- r (may be slightly better)
 - start with empty set (if $l > r$) or entire set (if $l < r$)
 - keep adding best l and removing worst r

Search algorithms (5)

- Select $d = 2$ out of $p = 5$ features
- Sub-optimality illustrated:
 - forward
 - backward

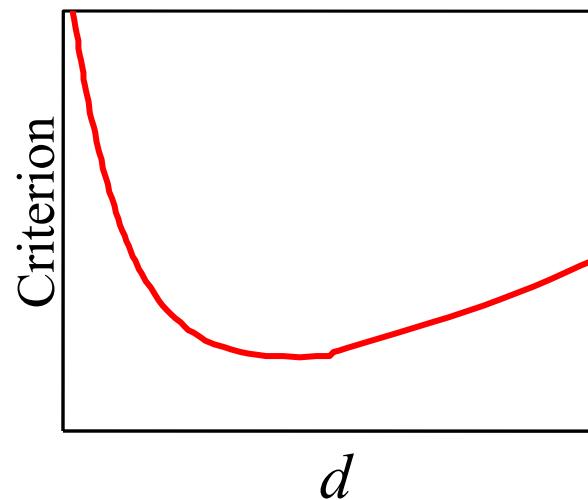
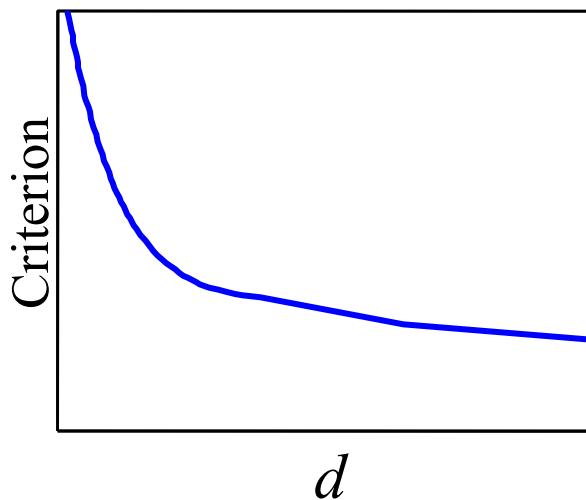
Feature subset

Criterion value



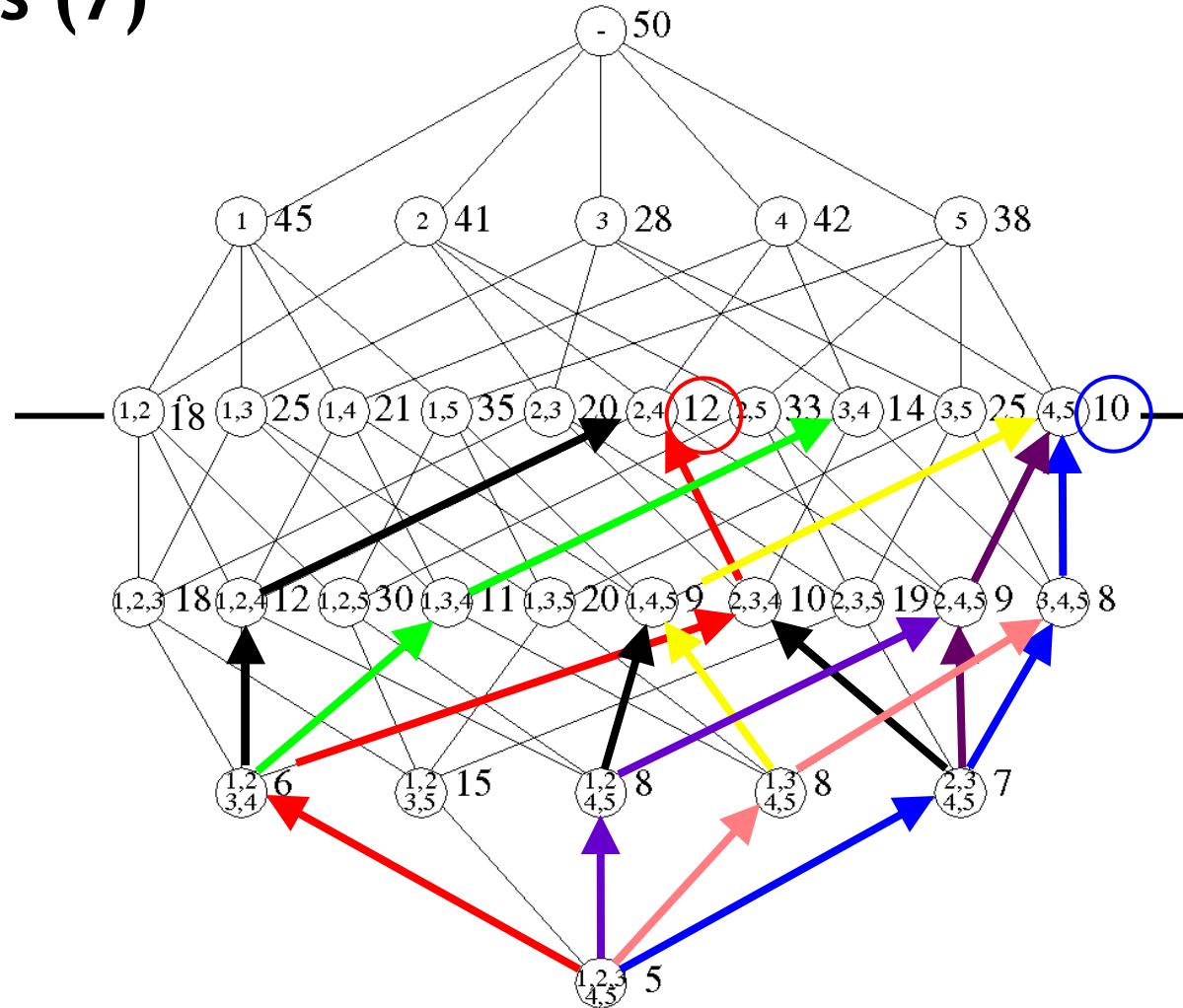
Search algorithms (6)

- Branch & bound: backtracking
- Optimal when criterion is monotonic in the number of features d



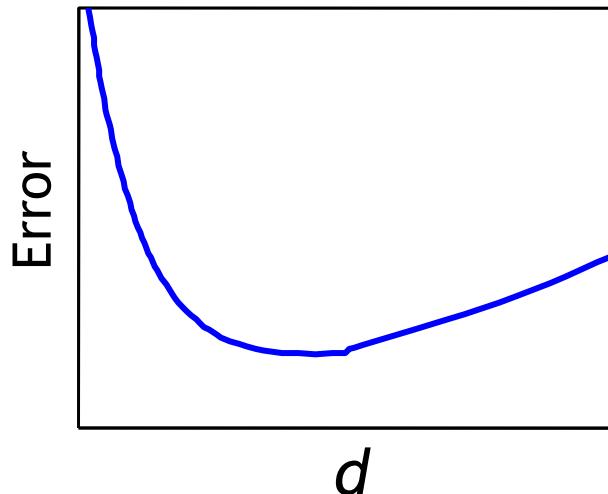
Search algorithms (7)

- Branch & bound
 - Use backward search to find preset number of features
 - Set *bound*, backtrack (*branch*) and use backward search again, considering just sets with criterion values better than the bound



Search algorithms (8)

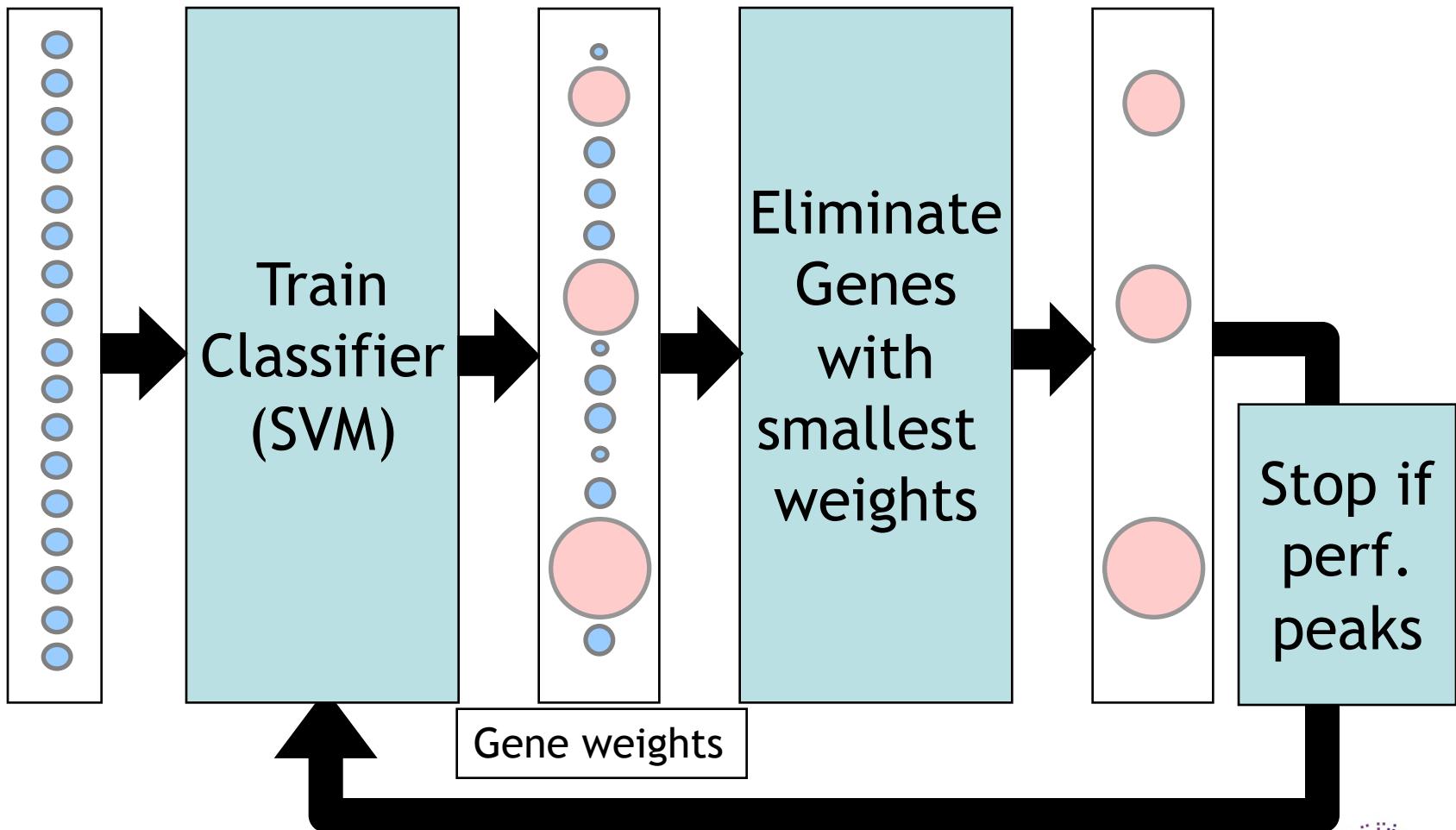
- When should we stop?
 - Due to estimation problems (e.g. covariance matrix), we may be overtraining on training set (in cross validation)
 - This is revealed by increasing error on the test set



- Otherwise (with very large sample sizes), we will have to specify a desired number of measurements

Example: Recursive feature elimination (RFE)

Wrapper, Backward search

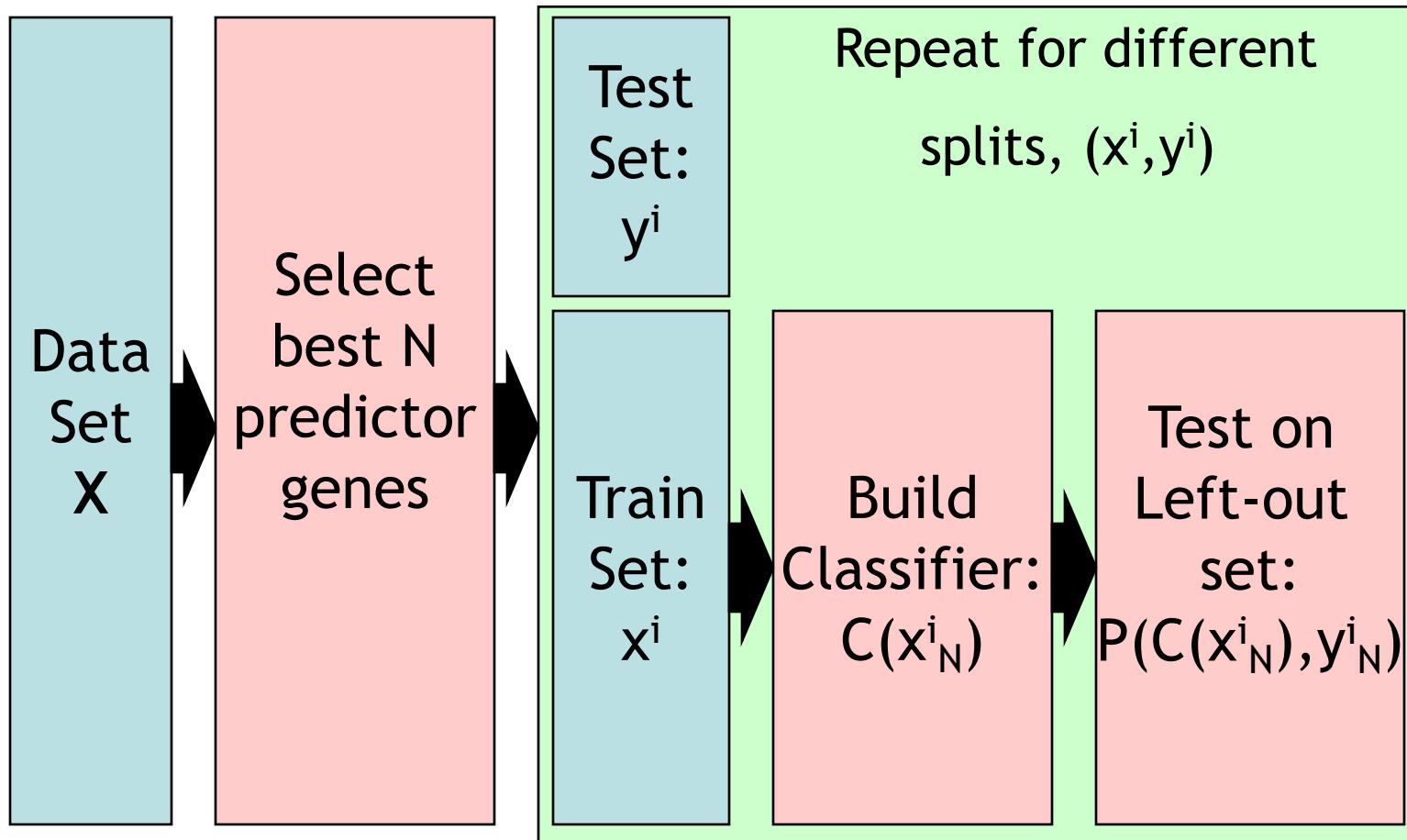


What can go wrong?

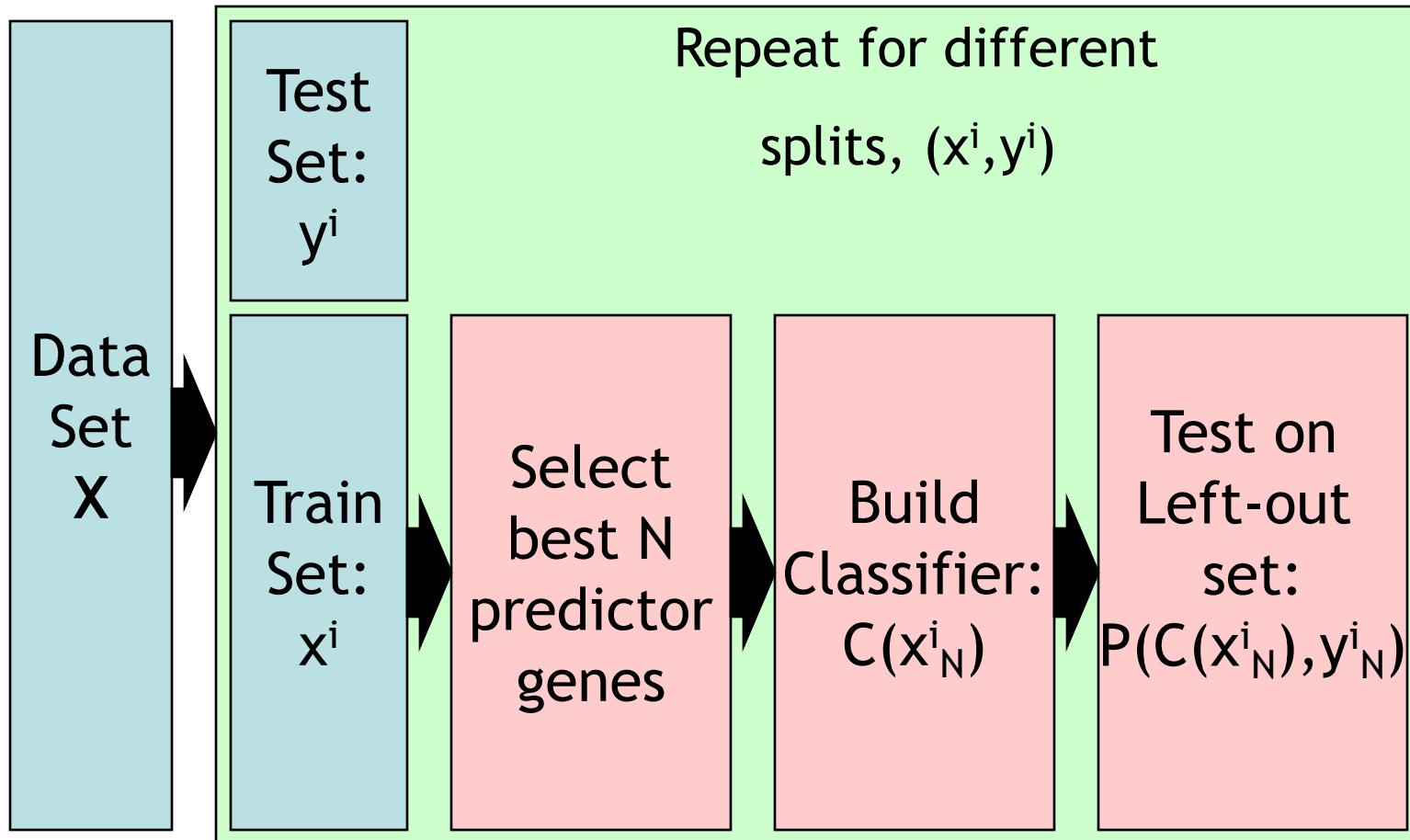
Selection bias...

- Guyon et al. (2002). Machine Learning **46**, 389 - 422.
- Ambroise and McLachlan (2002). PNAS **99**, 6562-6566.

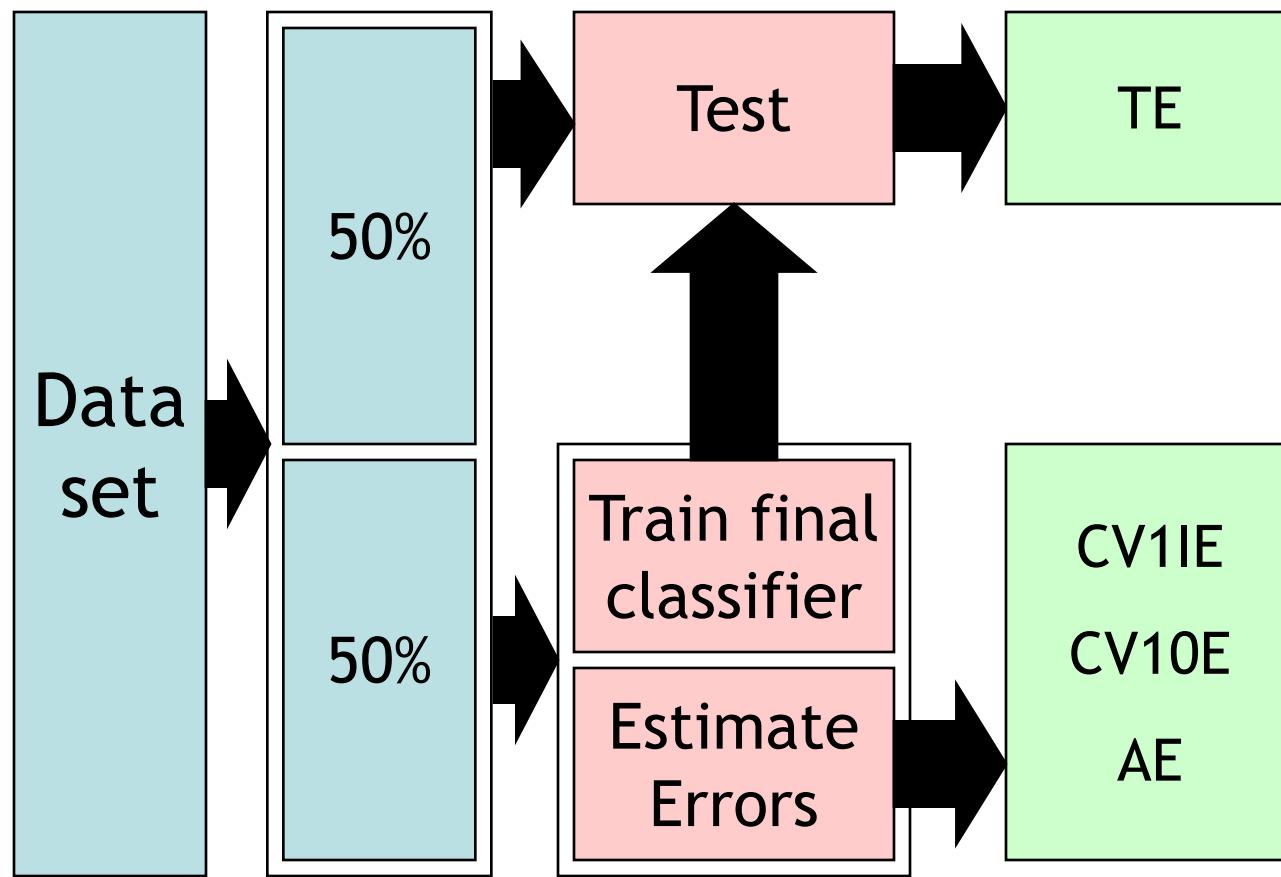
Biased selection



Unbiased selection

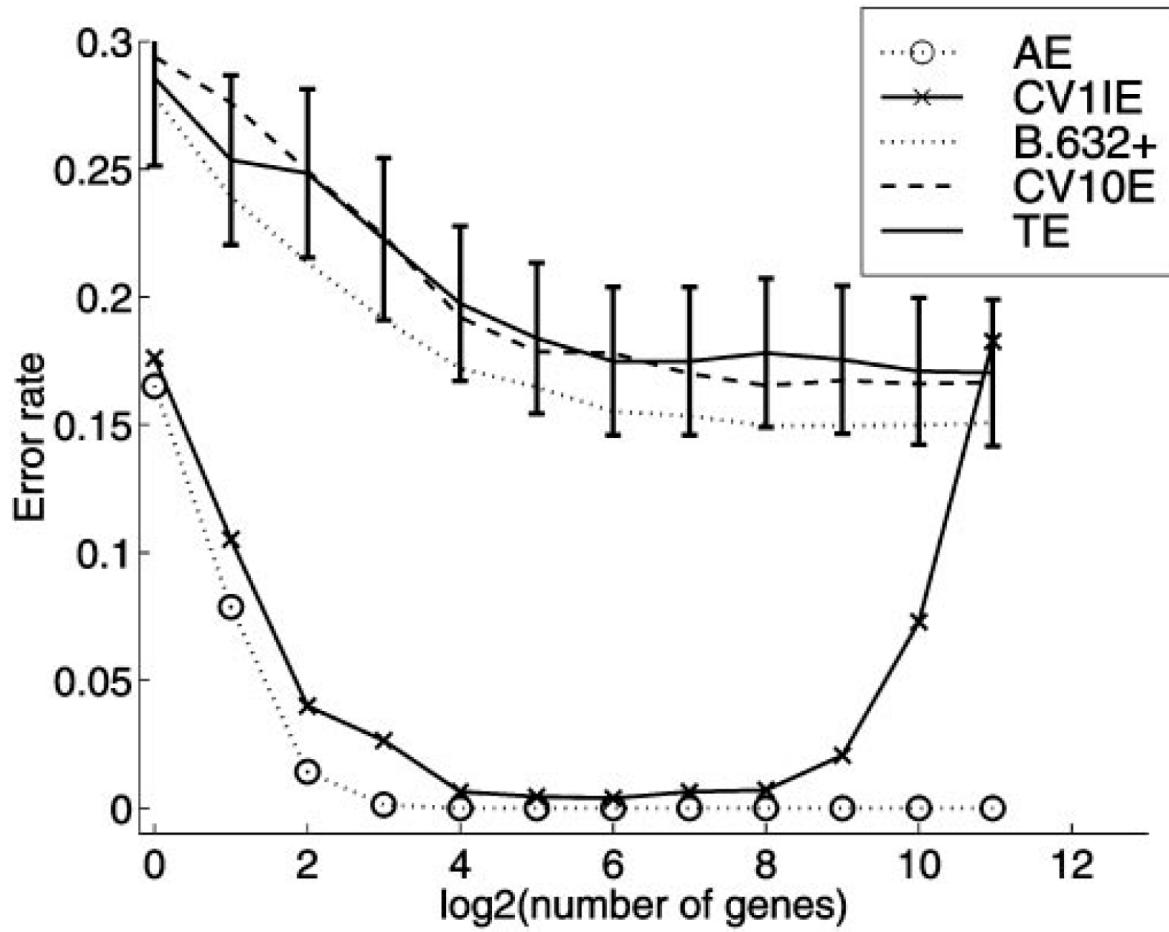


Ambroise & McLachlan experiments



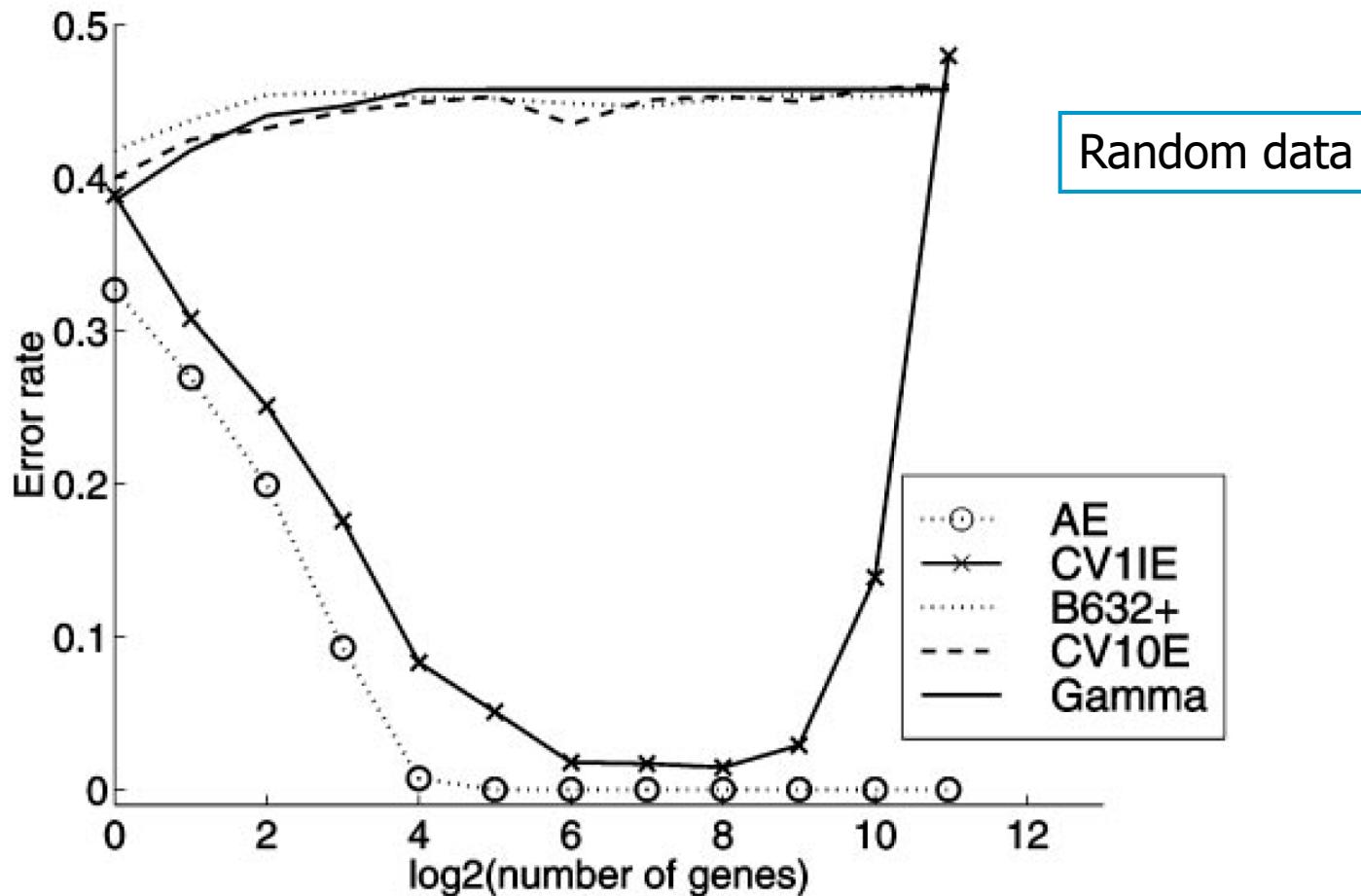
Ambroise & McLachlan experiments

Colon vs. normal data



Ambroise & McLachlan experiments

Random data



Cross-validation

- Remember:

Note:

we should never use the training set to calculate performance; this will give a biased estimate!

- for small sample size: use cross-validation
- Cross-validation should be applied to *every choice* made, including:
 - the number of features to use
 - the features to use
 - the type of classifier to use
 - ...

Feature selection: summary

- Feature selection can improve performance and help interpretation
- Requirements: a criterion and a search algorithm
- Methodology (cross-validation) is very important, especially for RNAseq data (' $p \gg n$ ')
- There seems to be some evidence that the simplest methods (individual selection) work best

Shrinkage

- Feature selection: selects a subset of features (1/0)
- Feature extraction: combinations of features are constructed based on variance and accuracy arguments
- Regularization 1: ‘shave off’ genes based on individual quality and control degree of ‘shaving’ with error
- Regularization 2: combines accuracy (error) and penalty on large weights (= simple models) in one criterion.

Shrunken centroids

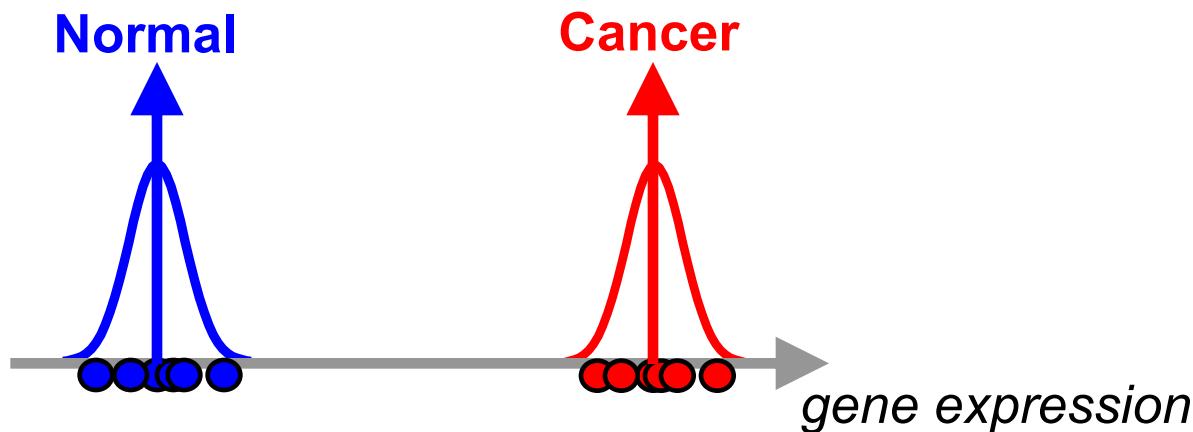
- Same principle as forward filtering
- Genes are evaluated *individually*
- BUT, do not start with the best and keep adding;
- RATHER, start removing worst genes from the back
- In PAM* genes can participate ‘partially’, in forward filtering a gene is either 100% in or out.

* PAM: Prediction analysis of micro-arrays

R. Tibshirani, T. Hastie, B. Narasimhan and G. Chu. Diagnosis of multiple cancer types by shrunken centroids of gene expression. PNAS 99(10):6567-6572, 2002.

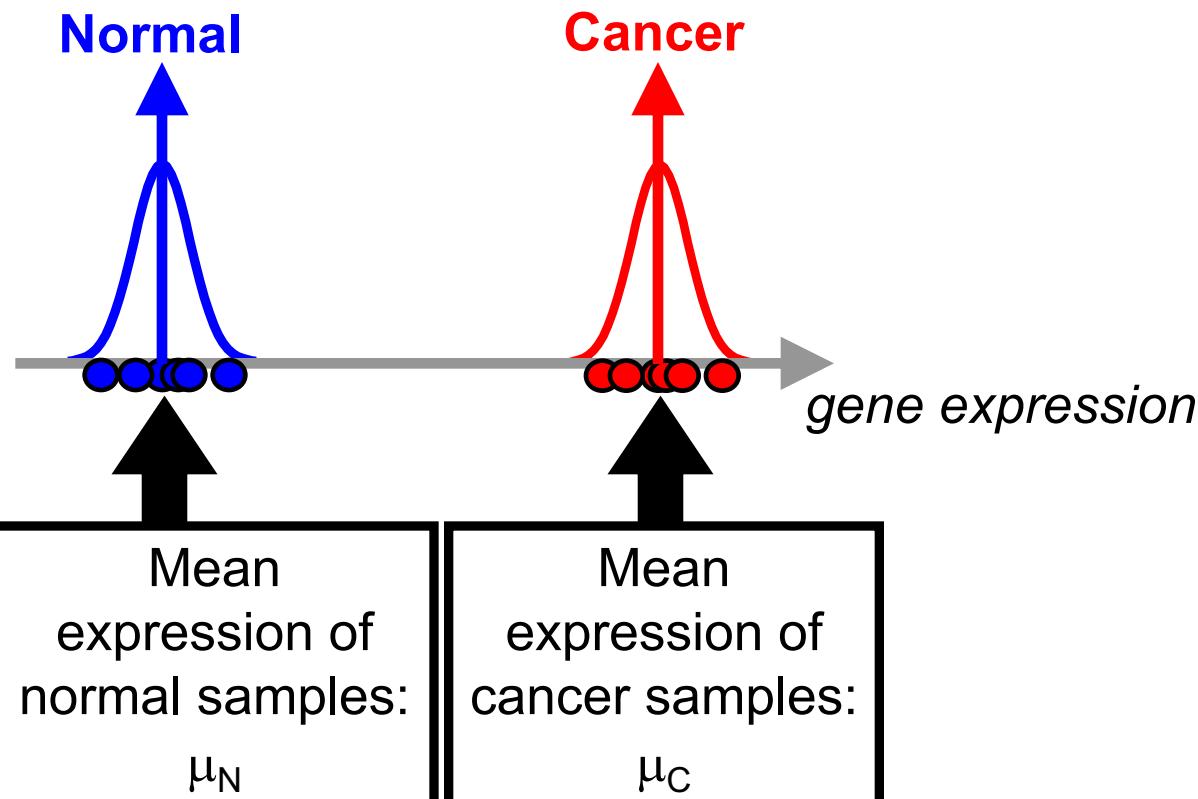
Shrunken centroids (1)

Step 1: Compute class centroids per gene



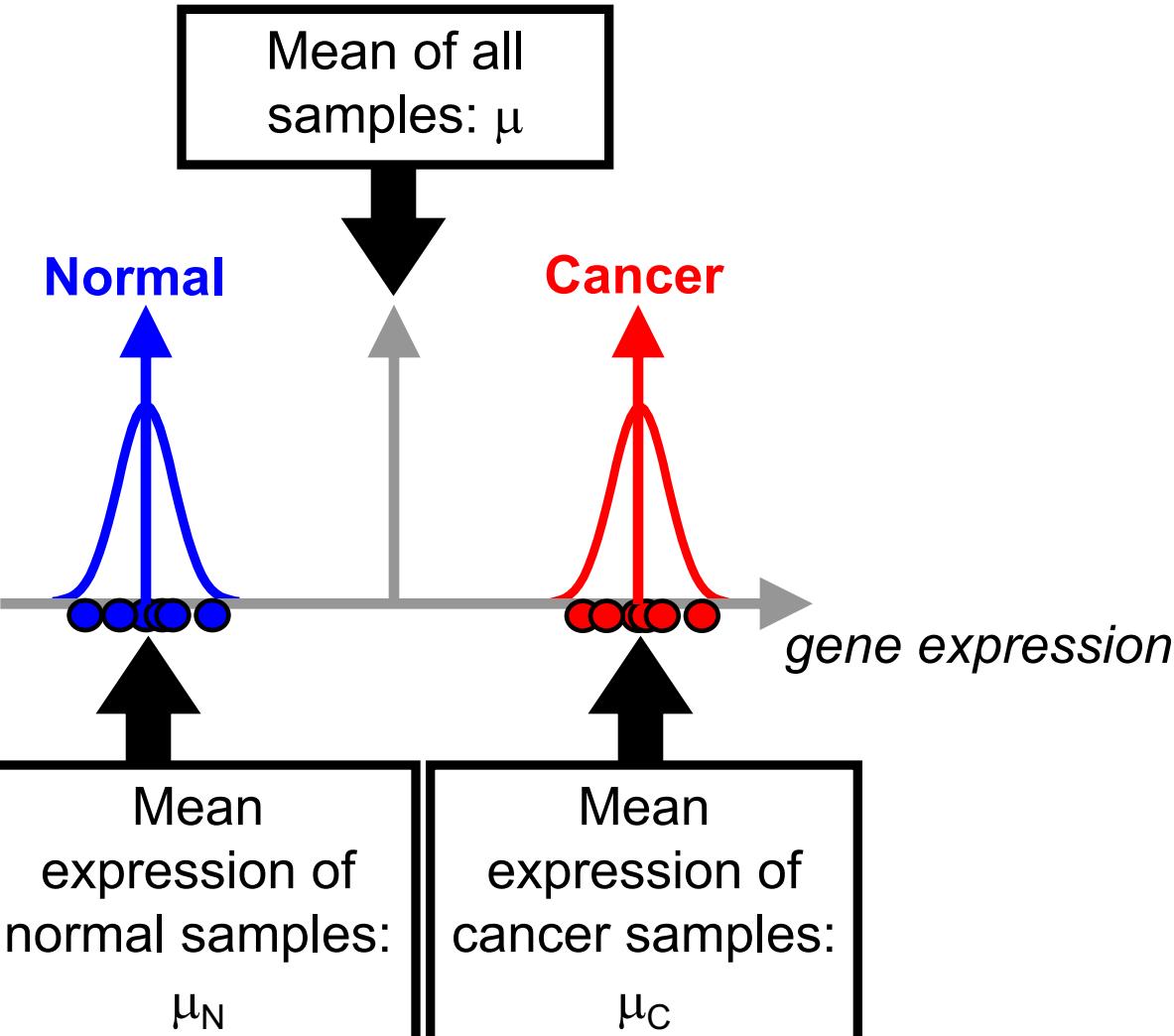
Shrunken centroids (2)

Step 1: Compute class centroids per gene



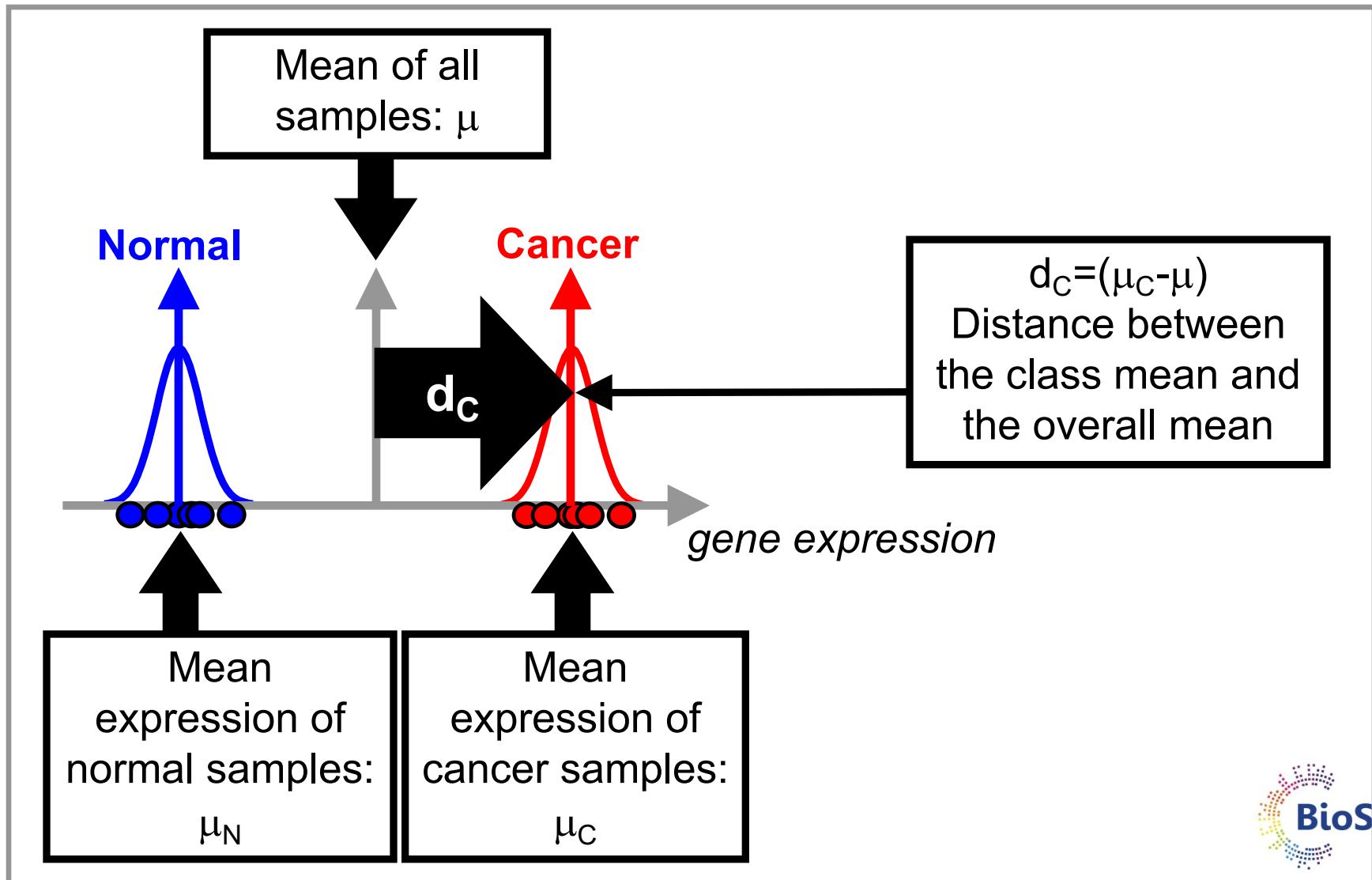
Shrunken centroids (3)

Step 2: Compute overall centroids per gene



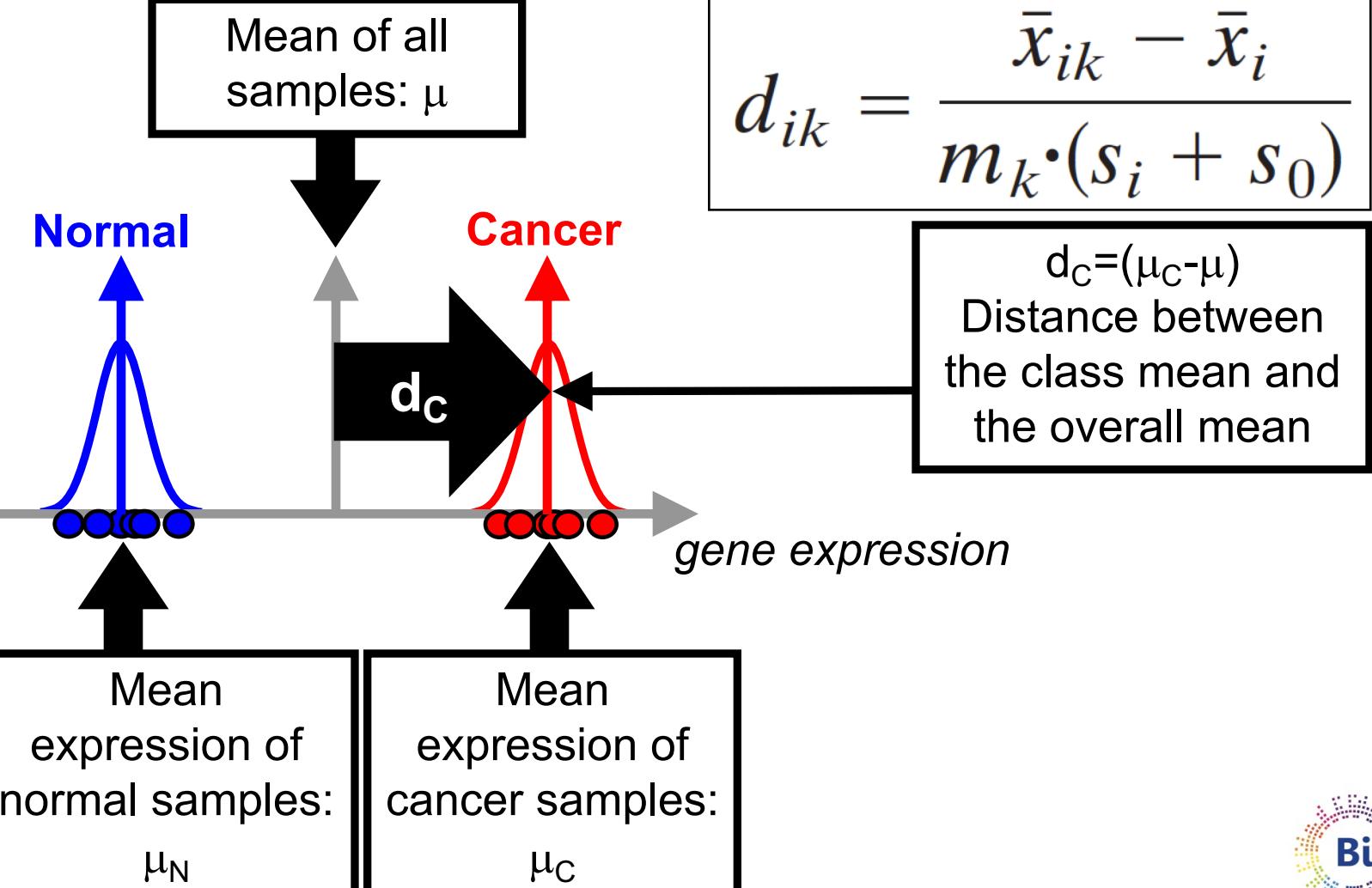
Shrunken centroids (4)

Step 3: Compute d per gene



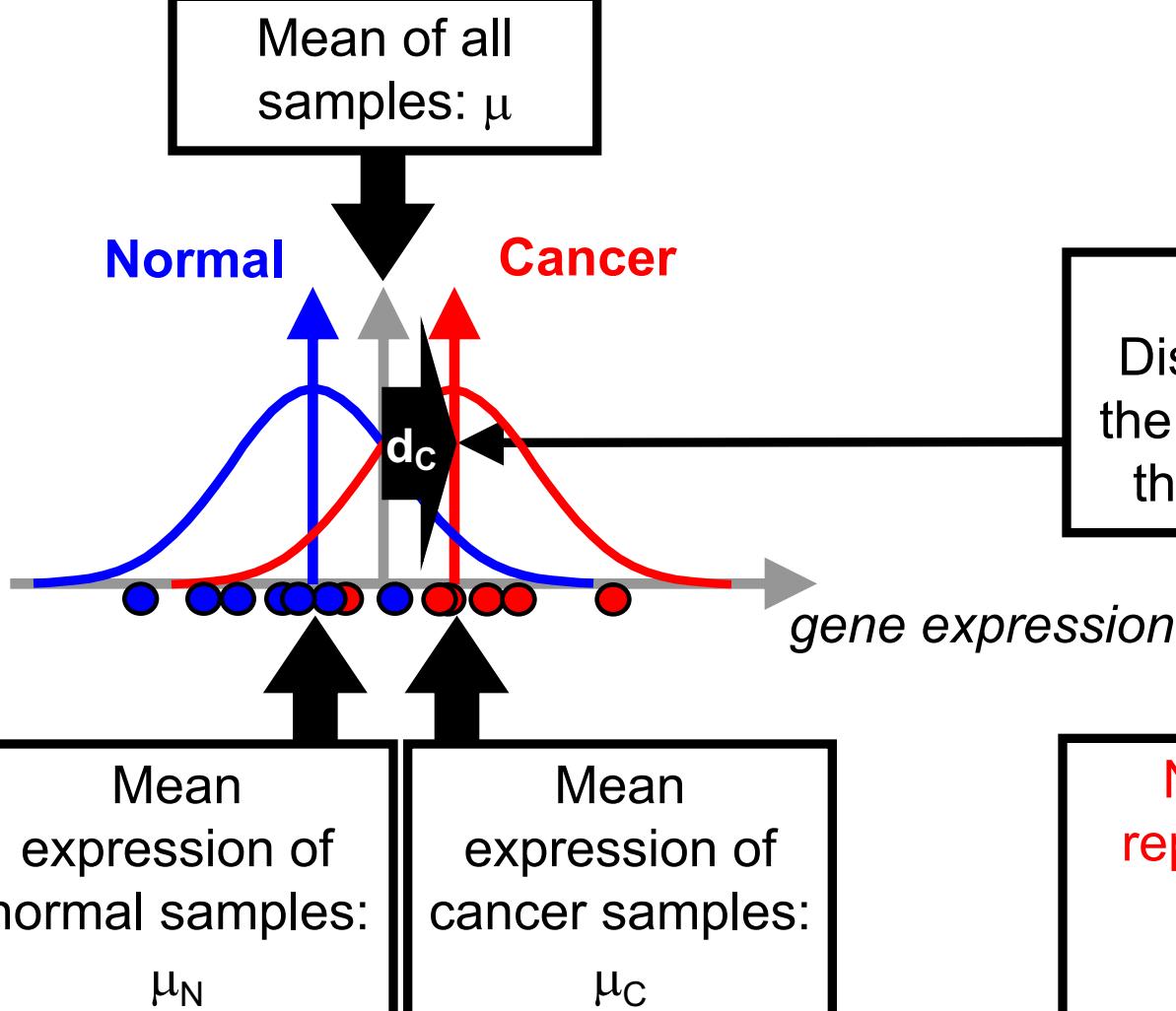
Shrunken centroids (4)

Step 3: Compute d per gene



Shrunken centroids (5)

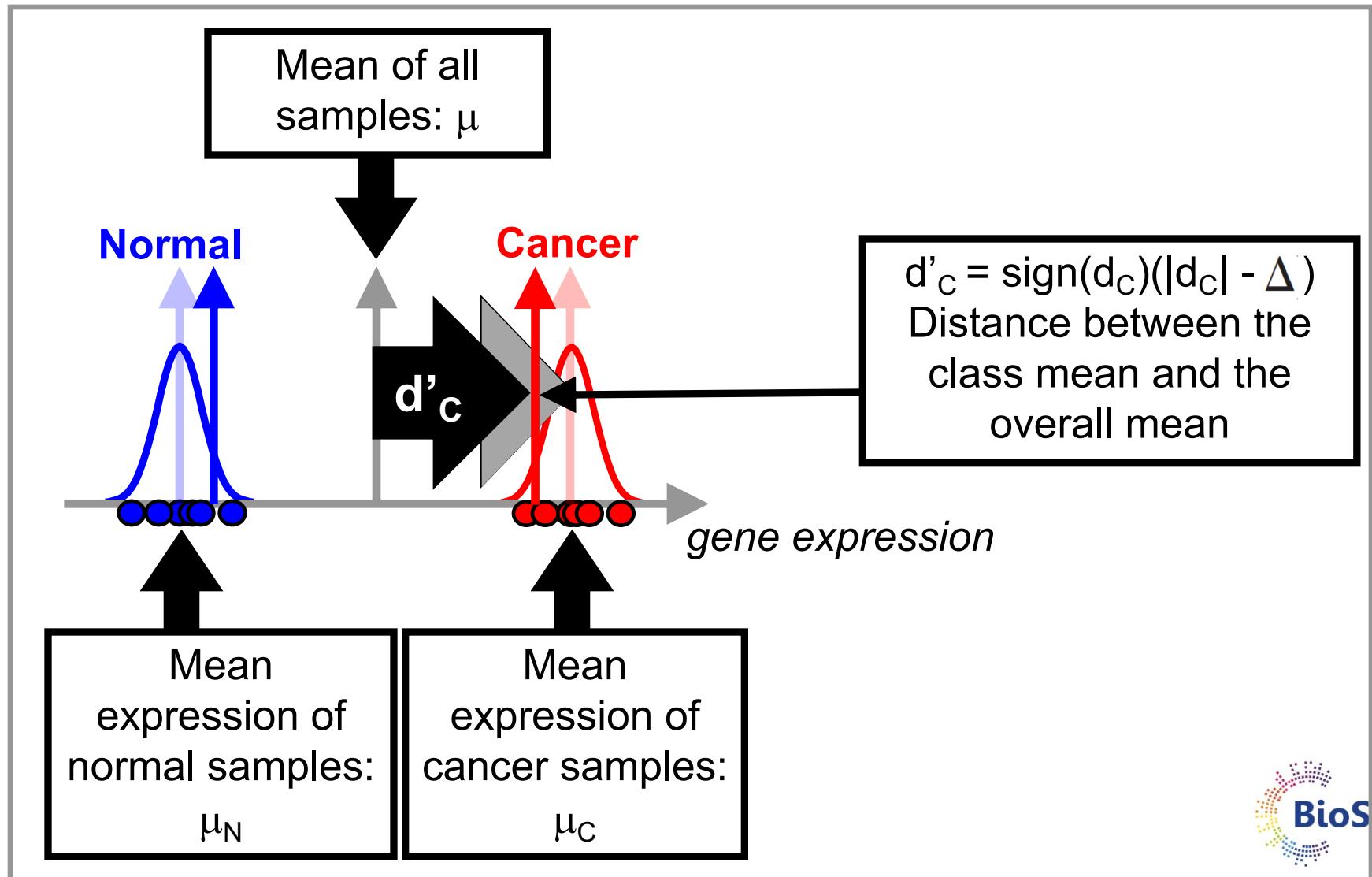
Step 3: Compute d per gene



Note: for poor reporters, SNR is small AND D is small

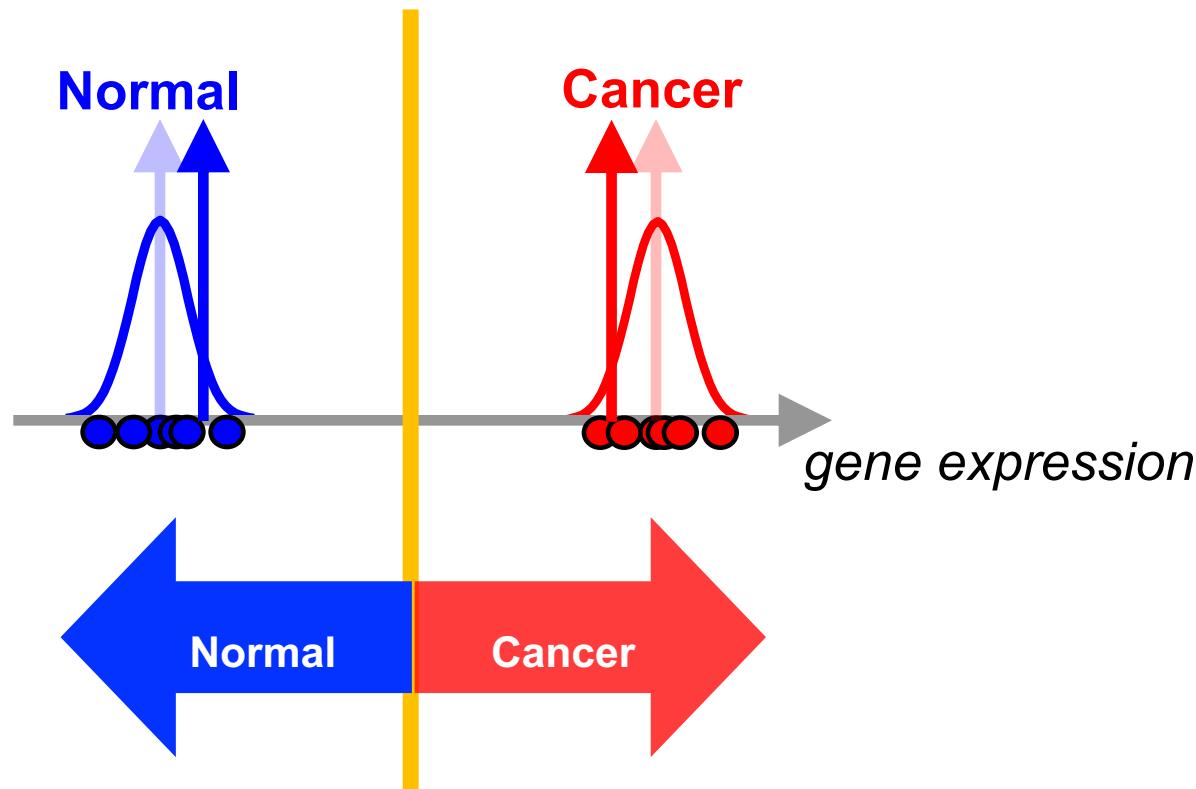
Shrunken centroids (6)

Step 4: Shrink the centroids



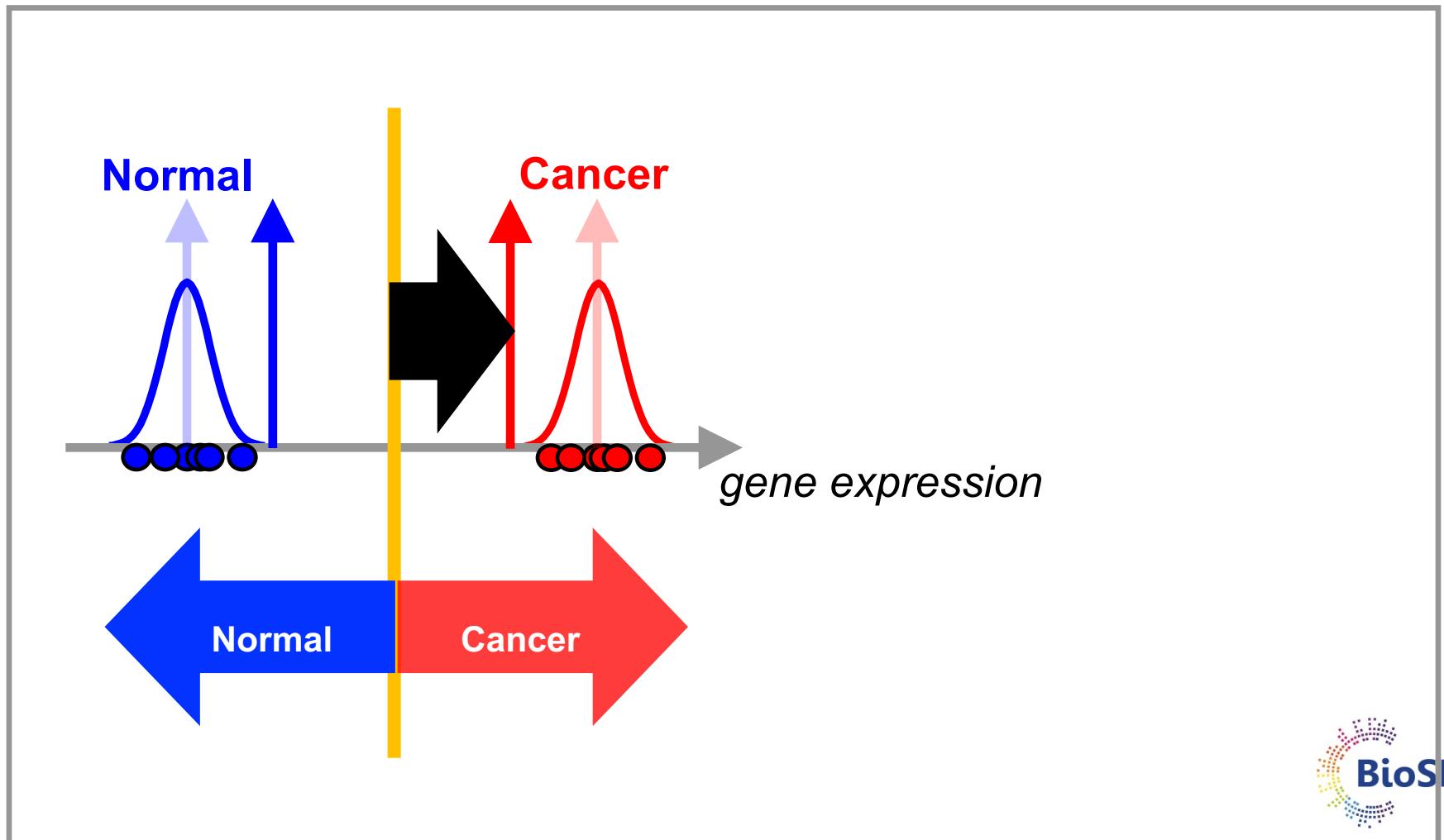
Shrunken centroids (7)

Step 5: Classify with shrunken centroids / perf.



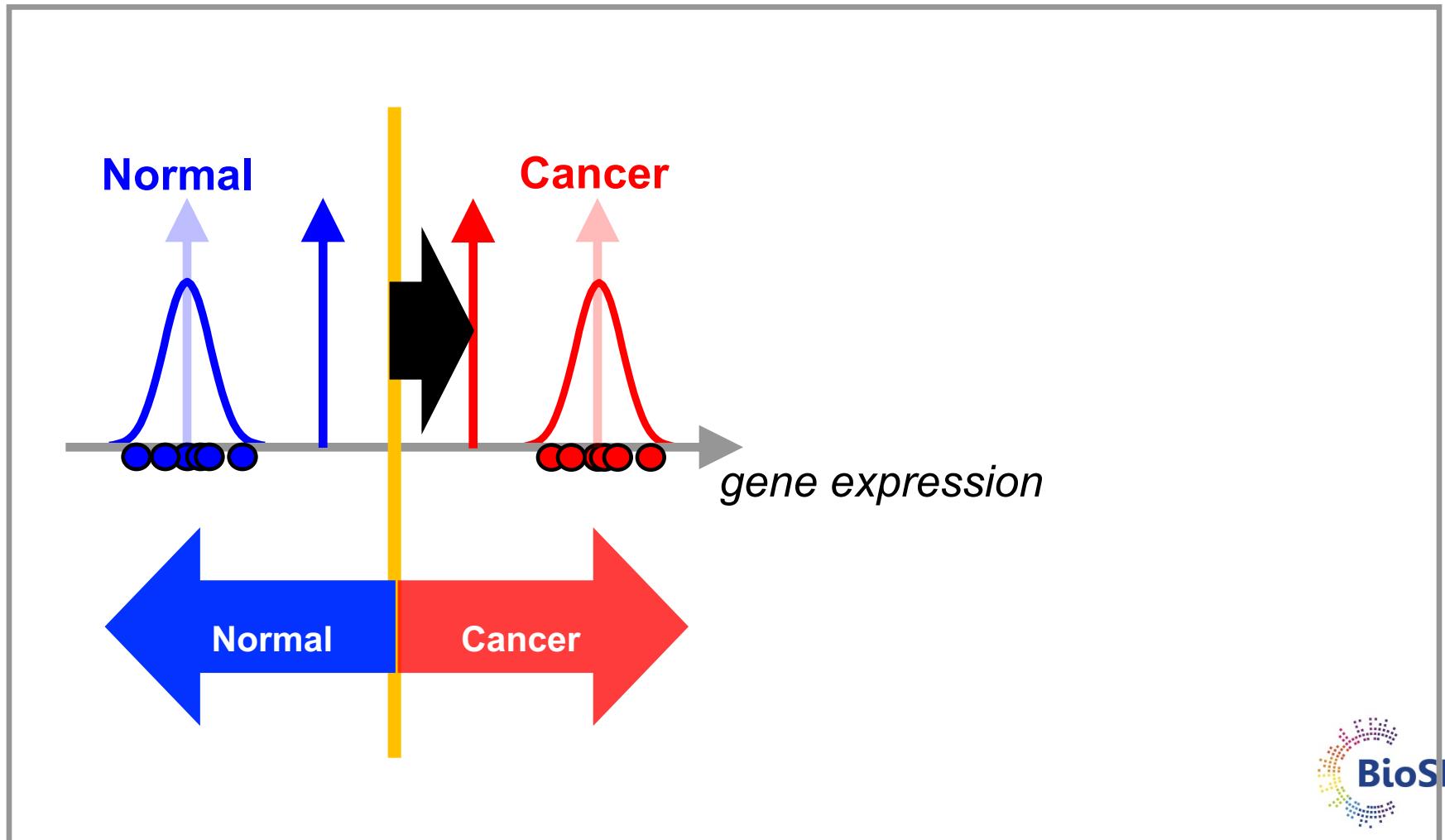
Shrunken centroids (8)

Repeat shrinking and evaluation of classifier till all genes shrunk away



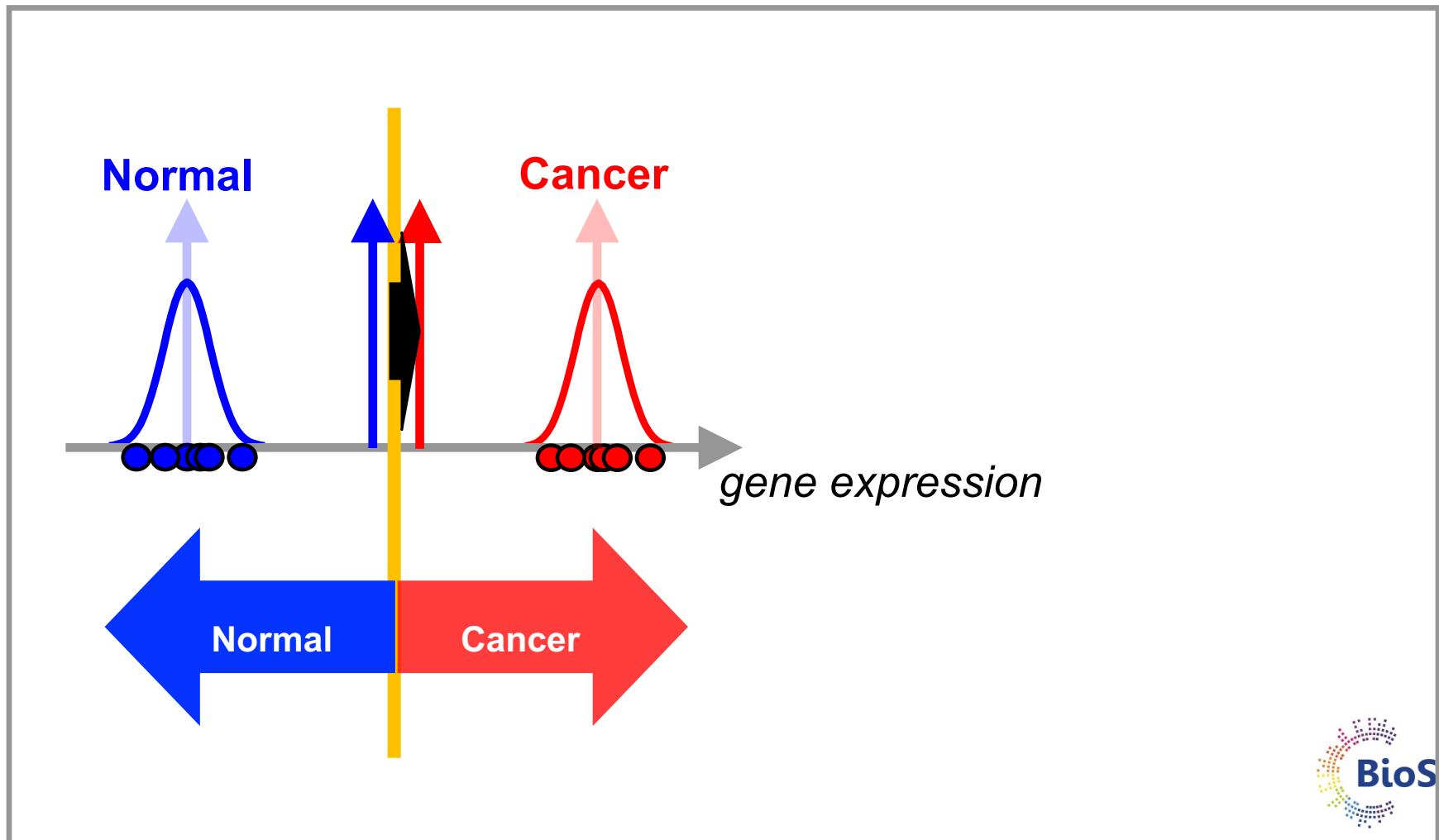
Shrunken centroids (8)

Repeat shrinking and evaluation of classifier till all genes shrunk away



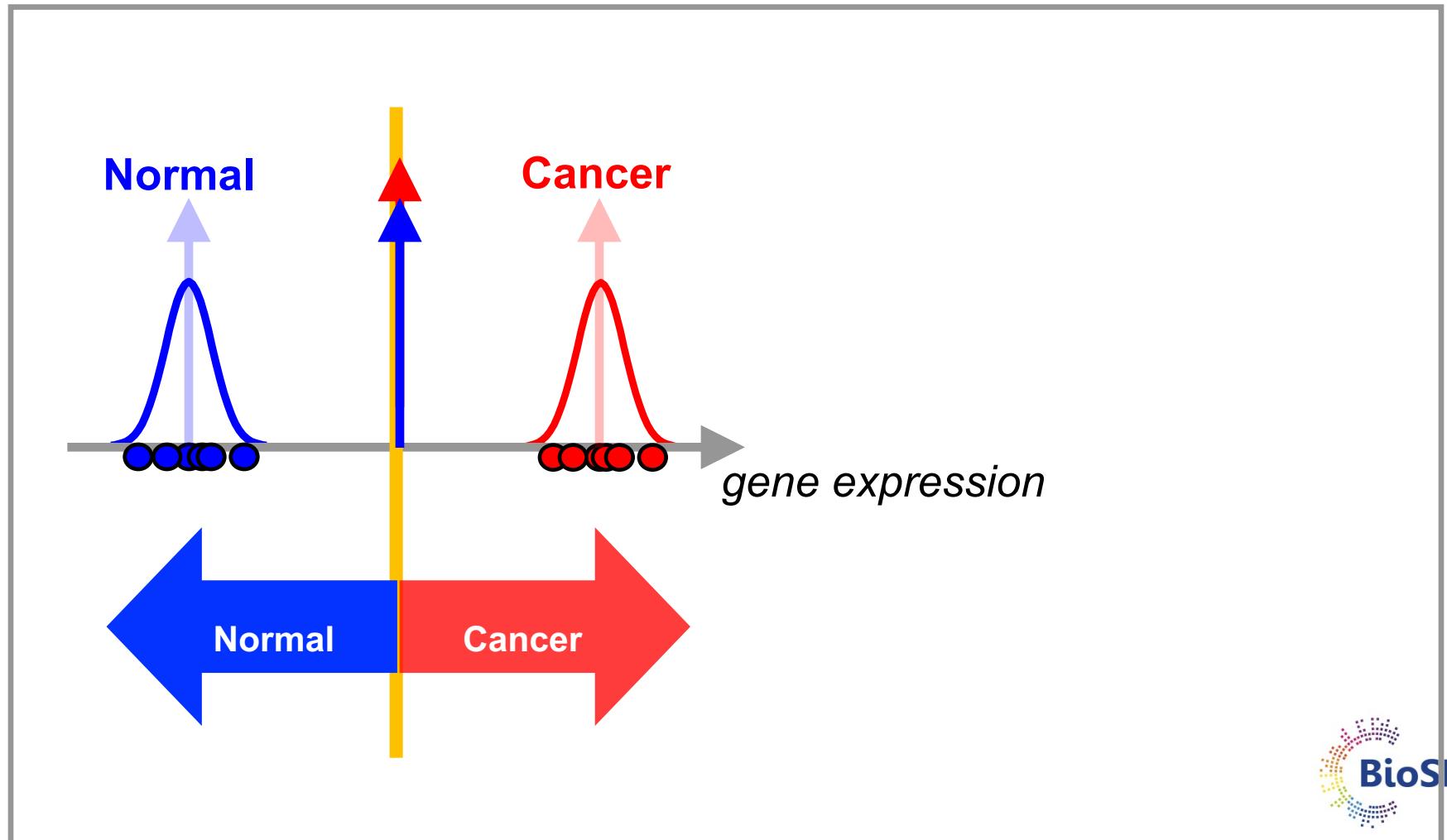
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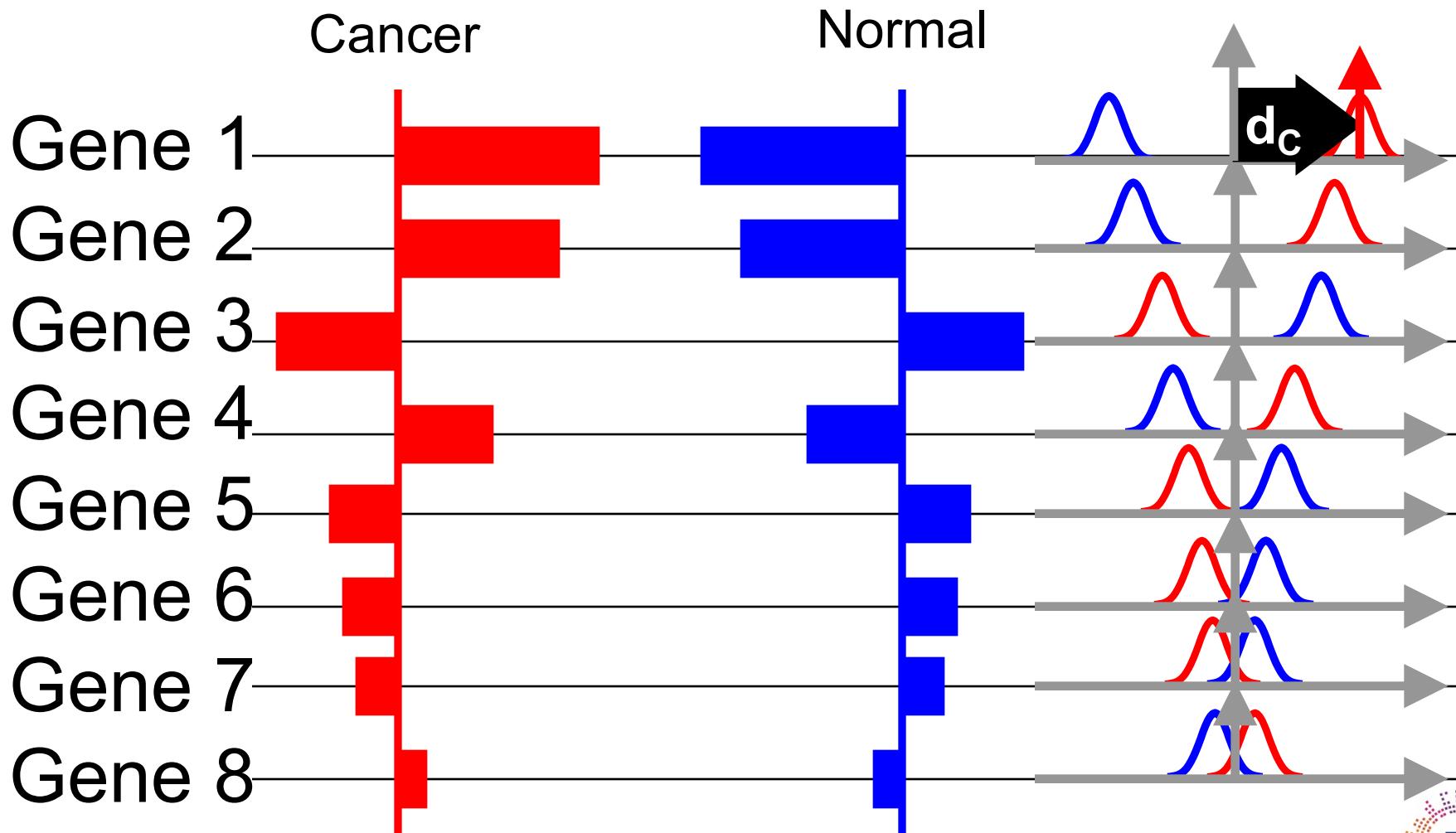


Shrunken centroids (8)

Repeat shrinking and evaluation of classifier till all genes shrunk away

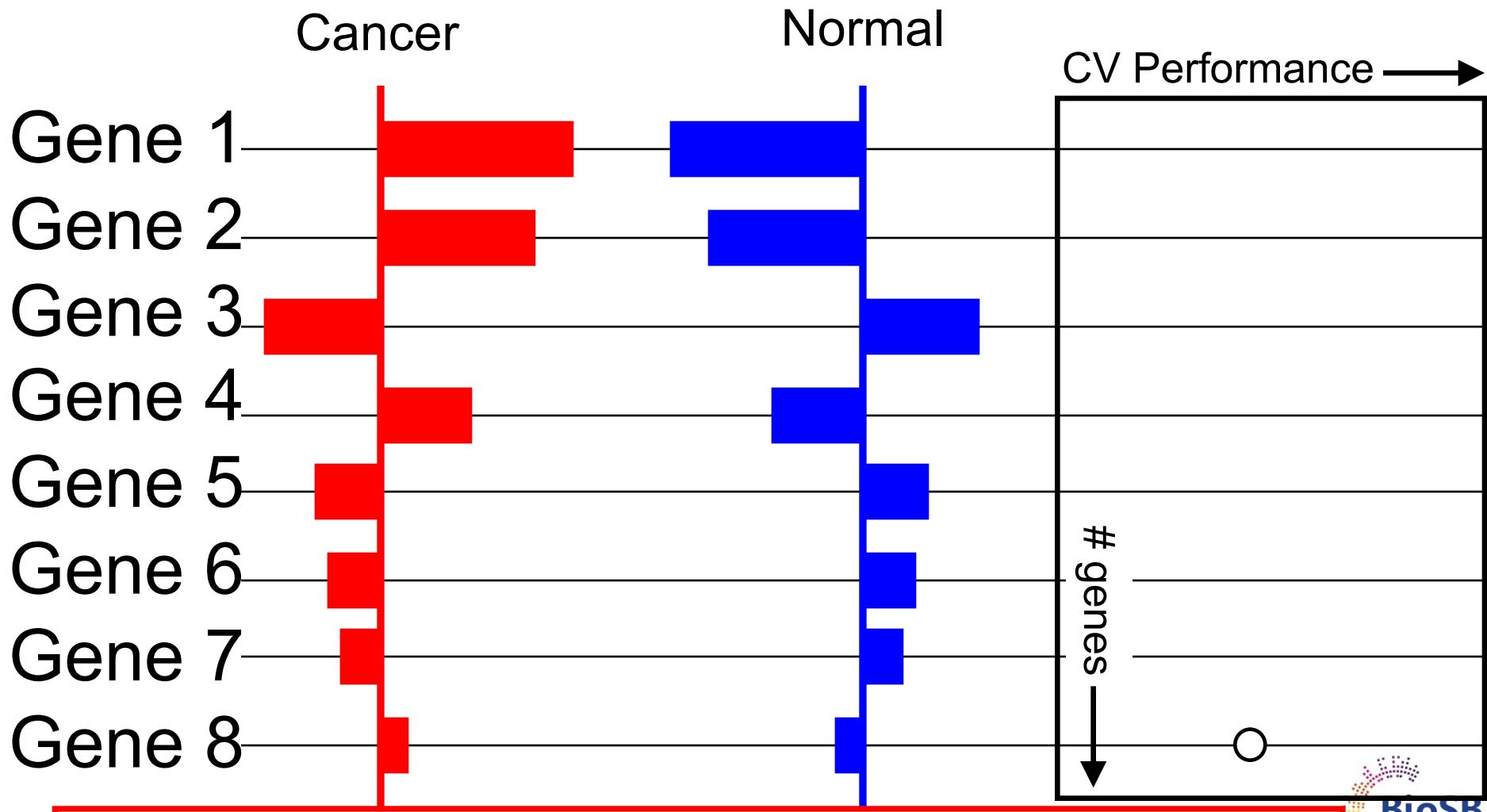


Shrunken centroids: selecting the genes



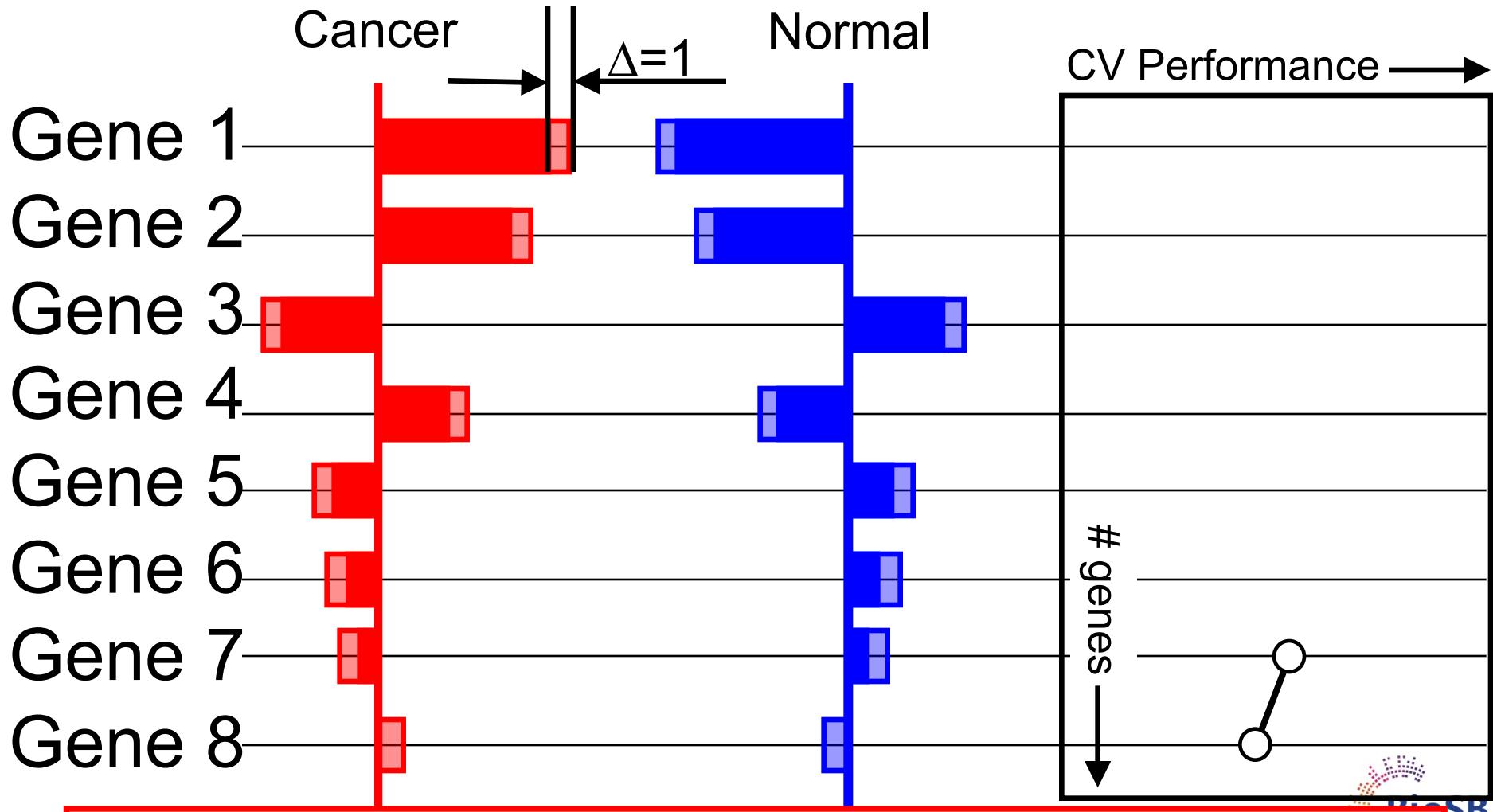
Genes sorted based on D-measure: best to worse

Shrunken centroids: selecting the genes



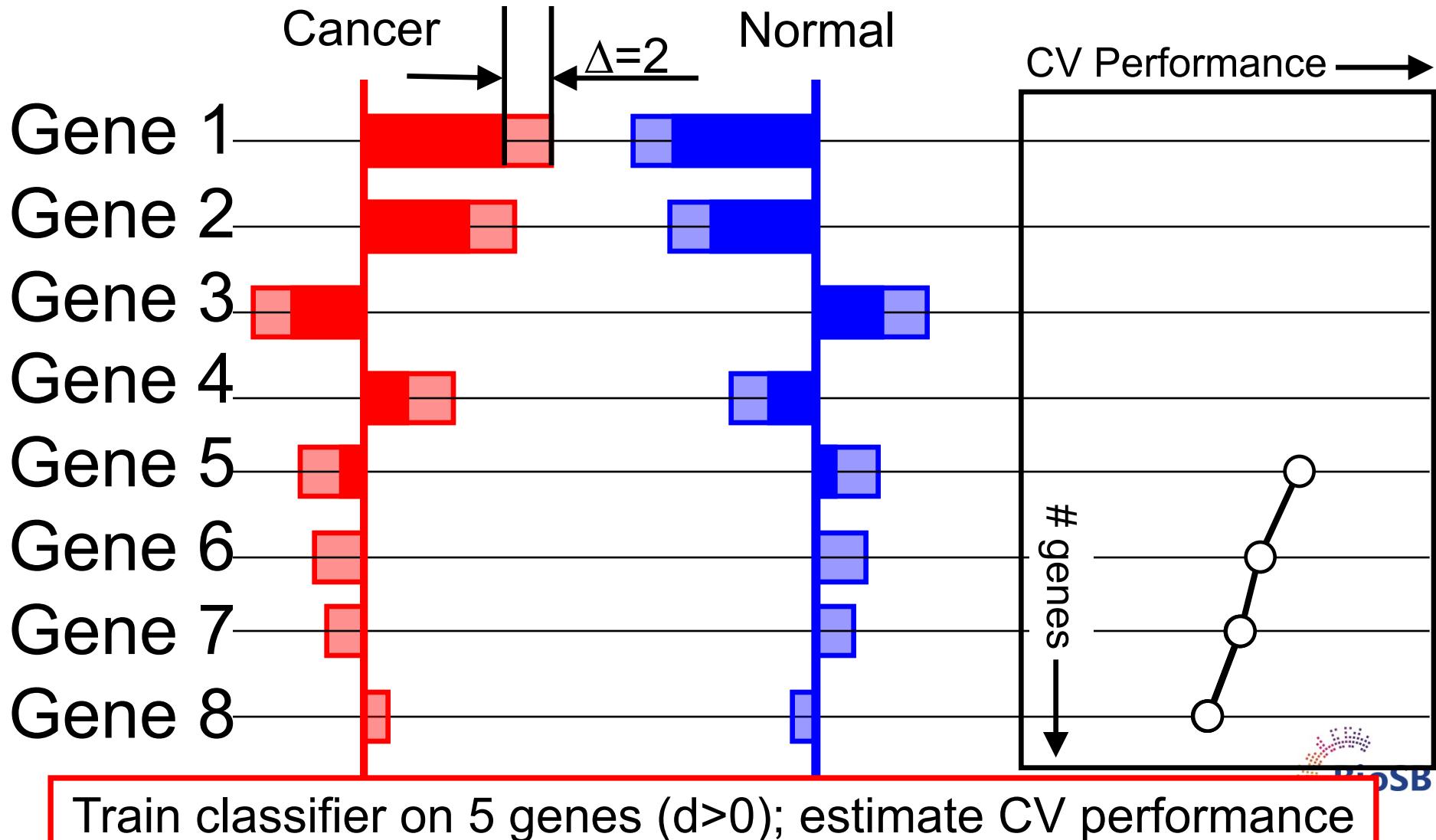
Train classifier on all 8 genes; estimate CV performance

Shrink all d by $\Delta=1$: reduce length by 1

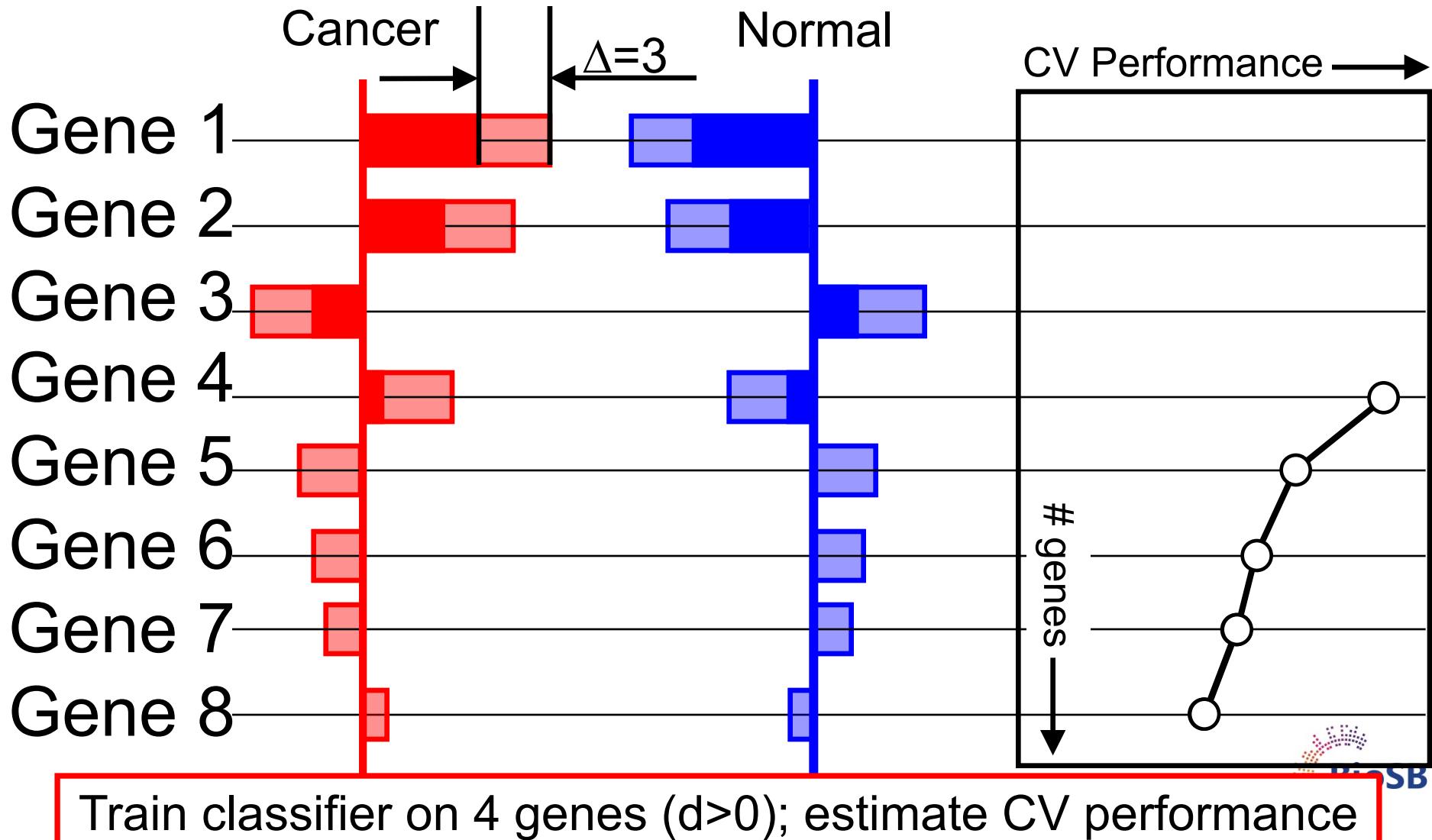


Train classifier on 7 genes ($d>0$); estimate CV performance

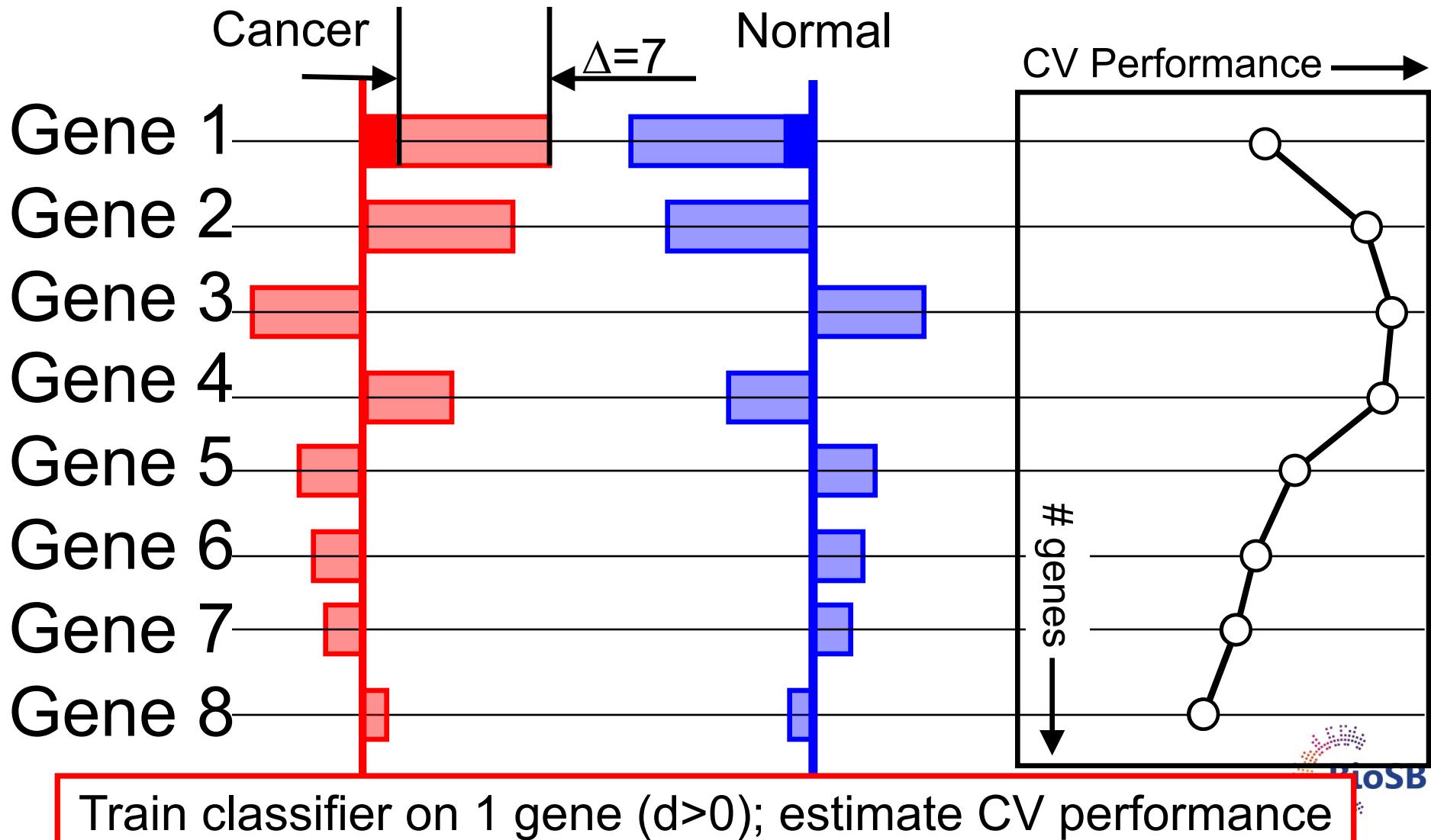
Shrink all d by $\Delta=2$: reduce length by 2



Shrink all d by $\Delta=3$: reduce length by 3



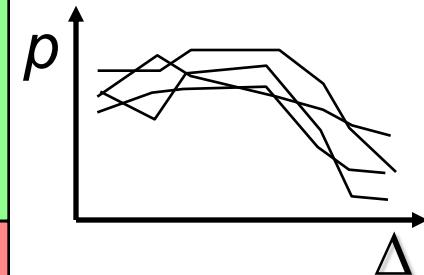
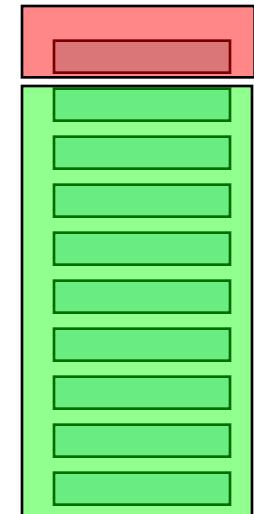
Shrink all d by $\Delta=7$: reduce length by 7



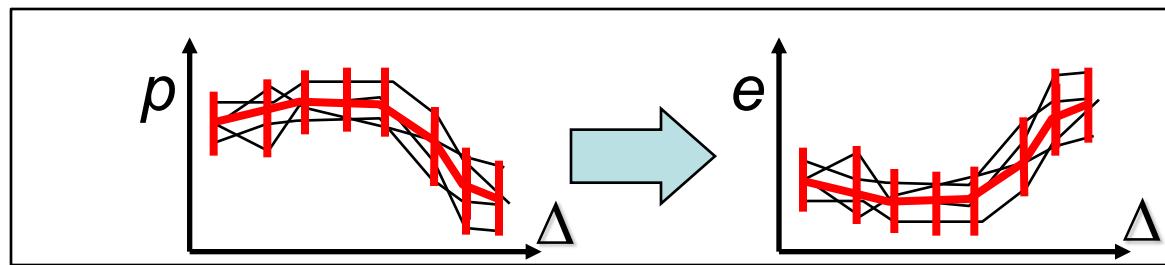
Determining the optimal Δ

1. Split the data (X) in 10 equal parts (x_1, \dots, x_{10})
2. For each of the 10 folds ($i=1, 2, \dots, 10$)
3. On the training set ($X \setminus x_i$)

1. Compute the class and overall centroids
2. For a range of Δ ($\Delta = [0, 0.5, \dots, 7]$)
 - i. Shrink d for all genes
 - ii. Compute 'shrunken centroids' on training set
 - iii. Test the resulting classifier on the test set (x_i)
3. Result: 10 Curves of performance vs. Δ

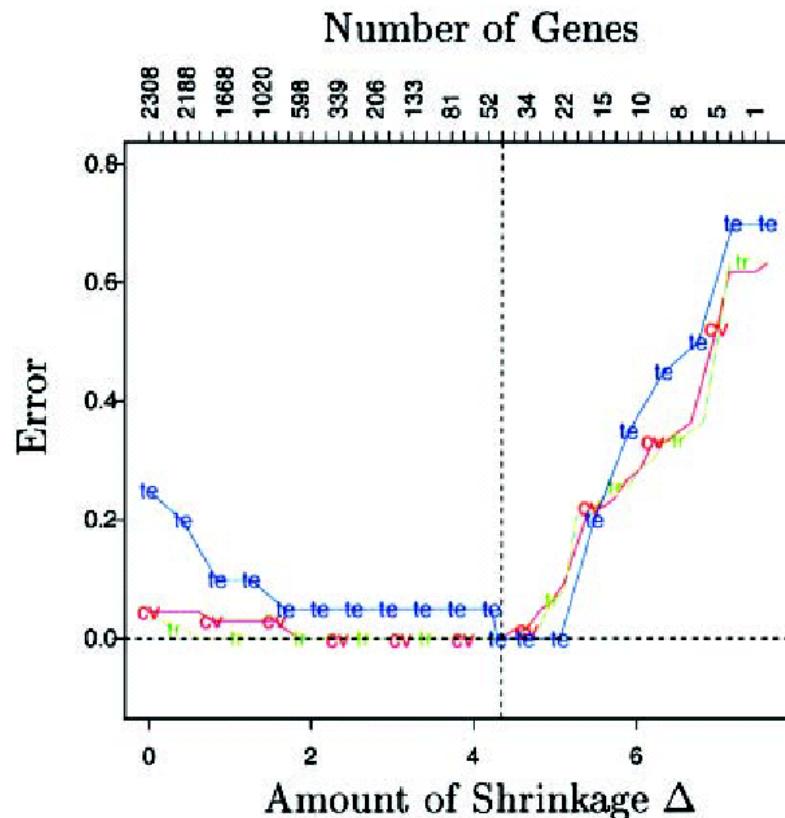


4. Average all 10 curves and compute std. dev. at each Δ
5. Pick the Δ where the performance is maximal (error min.)



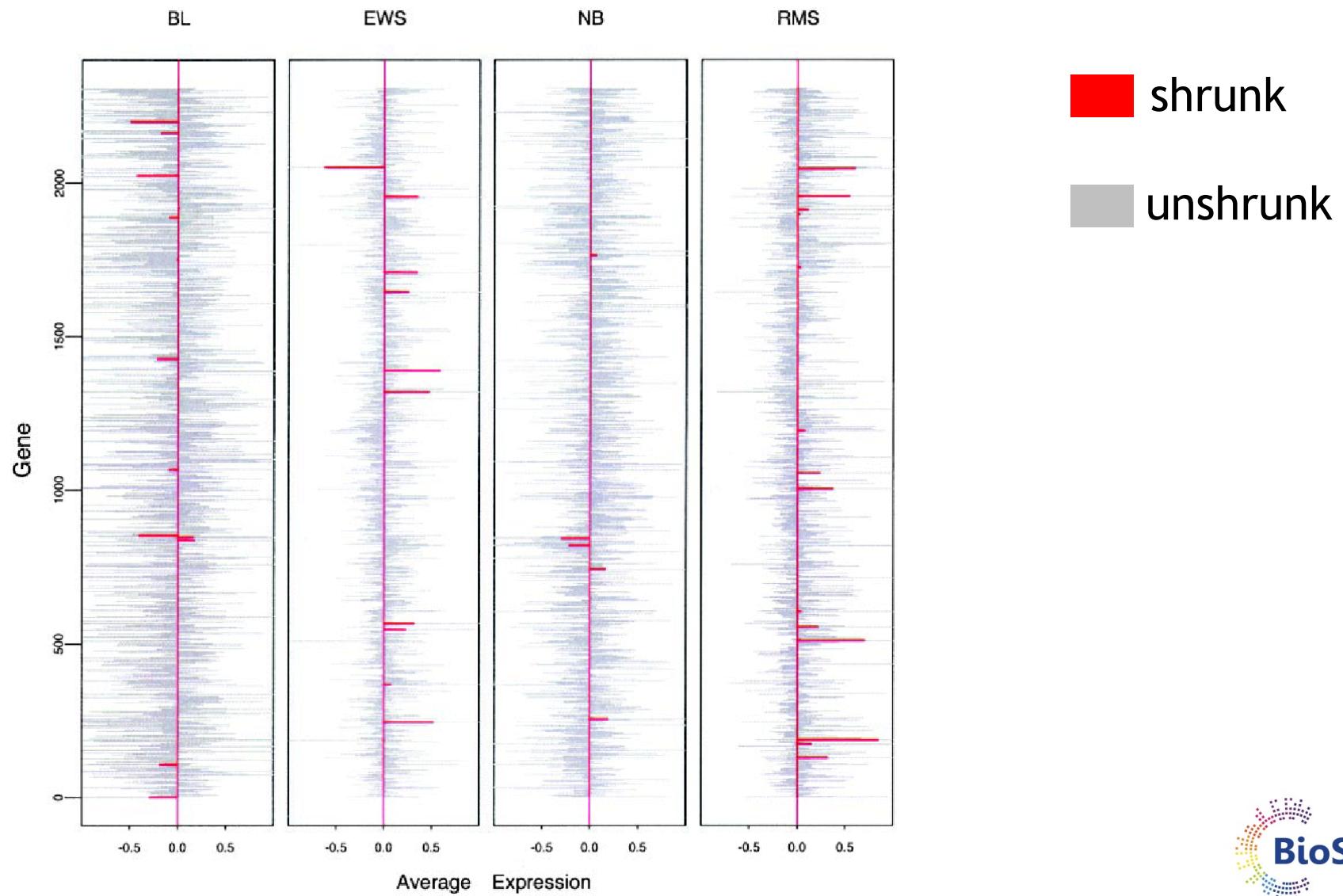
PAM

- For the Khan dataset; 4 classes: BL, EWS, NB, RMS
- At optimal Δ : 43 genes *not* shrunk away



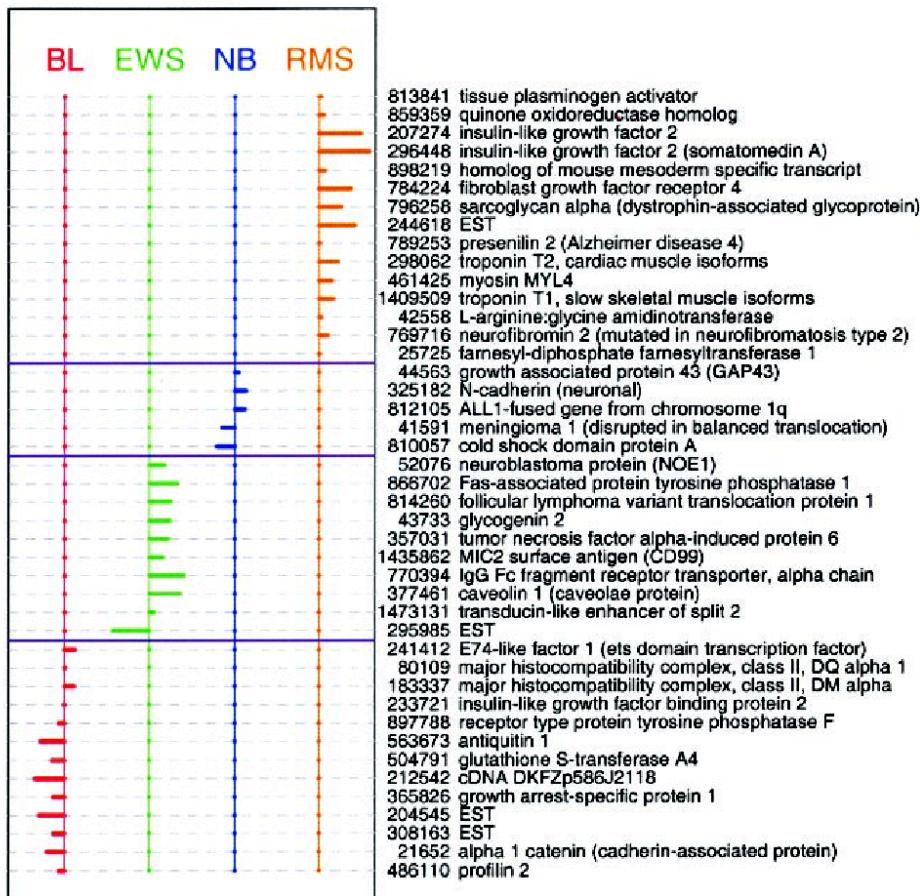
Neuroblastoma (NB)
Rhabdomyosarcoma (RMS)
Burkitt lymphoma (BL)
Ewing family of tumors (EWS),

PAM (2)



PAM (3)

At optimal Δ : 43 genes *not* shrunk away

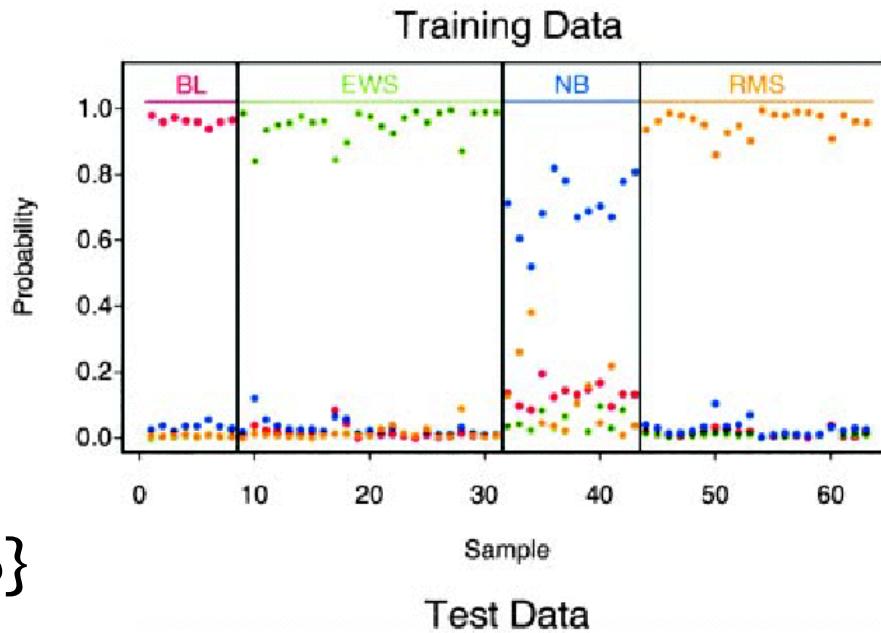


- Neuroblastoma (NB)
- Rhabdomyosarcoma (RMS)
- Burkitt lymphoma (BL)
- Ewing family of tumors (EWS),

R. Tibshirani *et al.* (2002) PNAS 99(10):6567-6572, 2002.

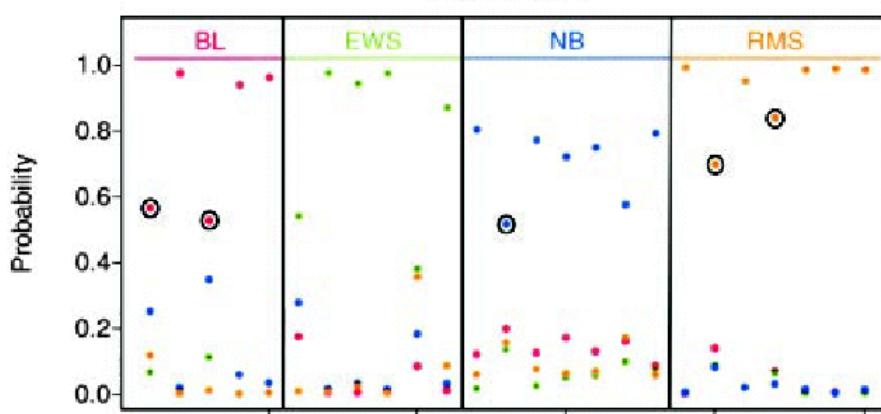
Scoring samples by posterior prob's

$$\hat{p}(k|x^*)$$



$$k = \{\text{BL}, \text{EWS}, \text{NB}, \text{RMS}\}$$

$$\hat{p}(k|x^*)$$



Shrinkage

- PAM determines a weight for every gene based on the predictive capacity of the gene (type of t-statistic)
- This weight determines role of the gene in a DLDA classifier (weights can be zero, i.e. no participation)
- Weights of all genes are shrunk by the same amount (Δ)
- PAM computes effect of shrinkage on error rate, and chooses shrinkage (=number of genes) with lowest error
- PAM: implicit simultaneous error and complexity minimisation
- Other approach: regularisation, combine error and penalty for number of genes explicitly

Shrinkage (2)

- Model: $y = \beta_0 + \sum_{i=1}^p \beta_i x_i + \varepsilon$
- Penalised (*aka* regularised) least squares:
 - Ridge regression:

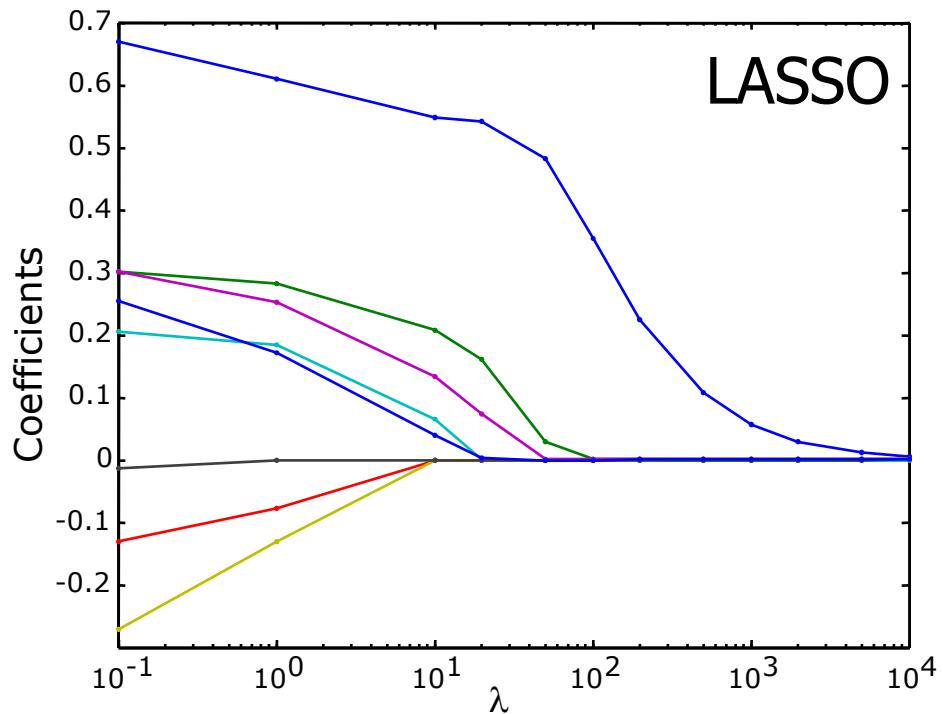
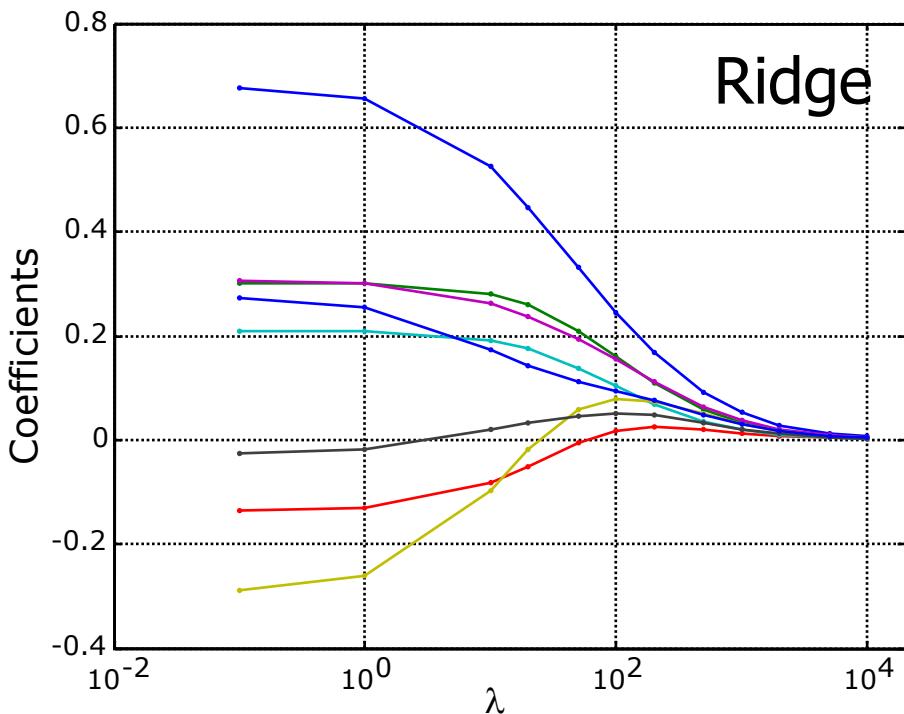
$$\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta}} \left[\sum_{j=1}^n \left(y_j - \beta_0 - \sum_{i=1}^p \beta_i x_{j,i} \right)^2 + \lambda \sum_{i=1}^p \beta_i^2 \right]$$

- LASSO: minimise

$$\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta}} \left[\sum_{j=1}^n \left(y_j - \beta_0 - \sum_{i=1}^p \beta_i x_{j,i} \right)^2 + \lambda \sum_{i=1}^p |\beta_i| \right]$$

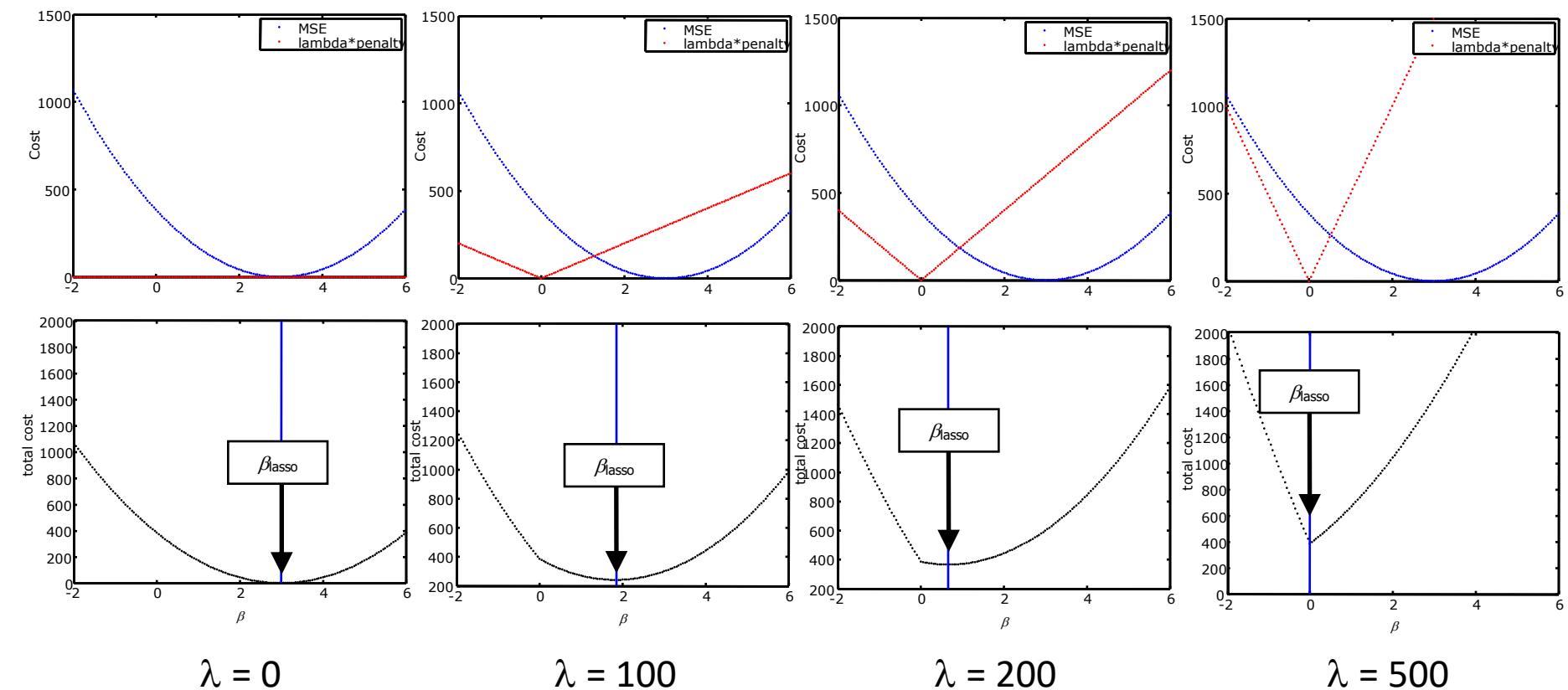
LASSO

- Difference seems small, but effect of LASSO is that genes are no longer used (like in PAM!)



LASSO (2)

- Example: true function $y = 3x$

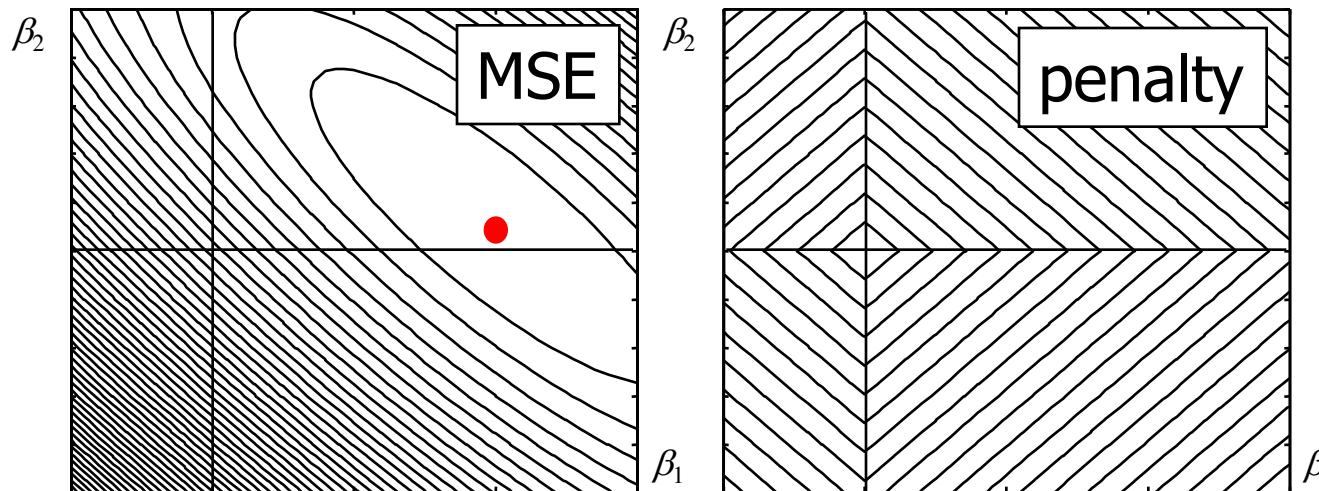


LASSO (3)

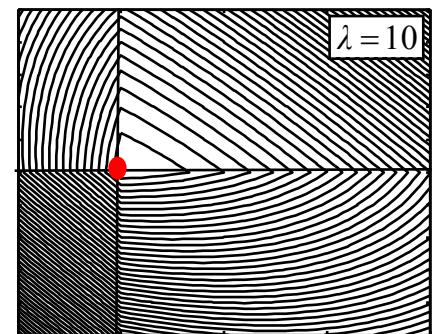
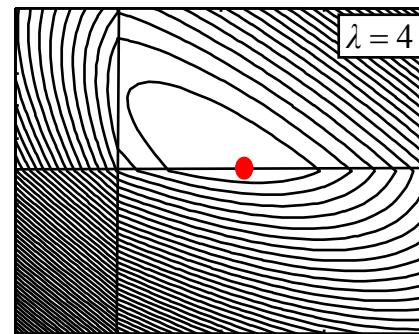
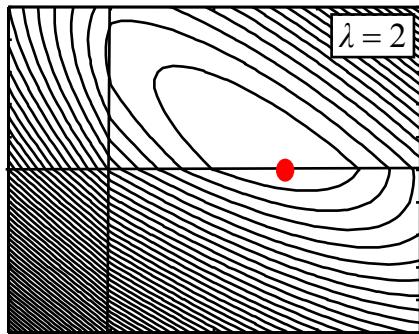
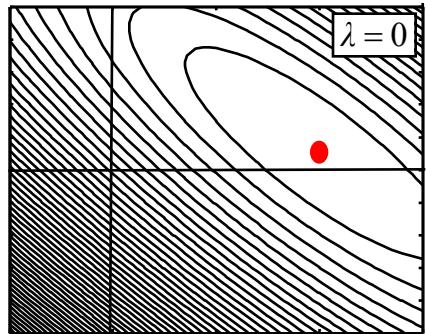
Example:

$$y = 0.1x_1 + 0.01x_2$$

● Optimum



↑
 β_2



β_1 →

Final summary

- Feature extraction:
 - Linear:
 - PCA,
 - Fisher
 - Non-linear
 - MDS
- Feature selection:
 - Criteria
 - search algorithms
 - forward,
 - backward,
 - branch & bound.
- Sparse classifiers:
 - Ridge,
 - LASSO