Classification of Data Sets

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Robotics and Intelligent Systems MAE 345,
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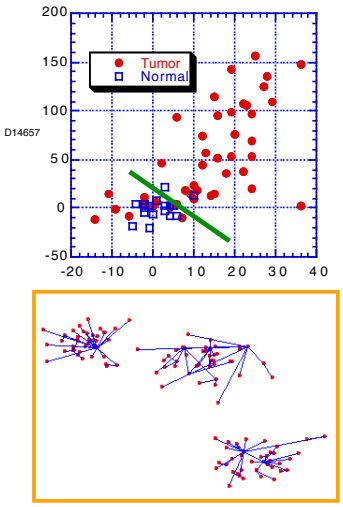
Learning Objectives

- **Unsupervised learning**
  - Cluster analysis
    - Patterns, Clumps, and Joining
- **Supervised learning**
  - Graph/tree search
  - Hypothesis testing
  - Linear discriminant
  - Nearest neighbor method
- **Estimating classification errors**



Classification Objectives

- **Class comparison**
  - Identify feature sets for predefined classes [Induction]

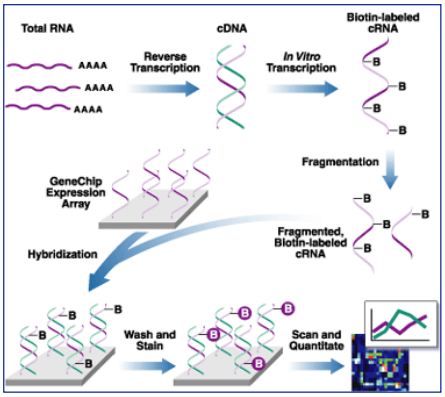
- **Class prediction**
  - Develop mathematical function/algorithm that predicts class membership for a novel feature set [Inference]

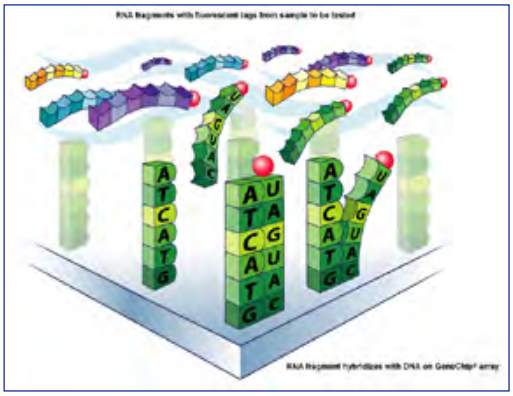
- **Class discovery**
  - Identify new classes, sub-classes, or features related to classification objectives [Inference]

Microarray Application

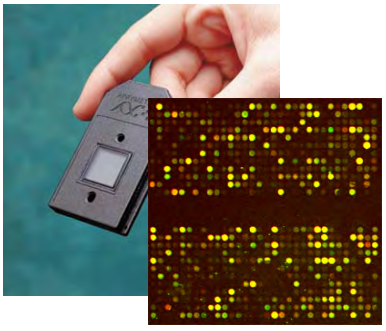
cDNA produced from sample RNA, labeled, and hybridized to the array

Array is washed, stained, scanned, and quantified

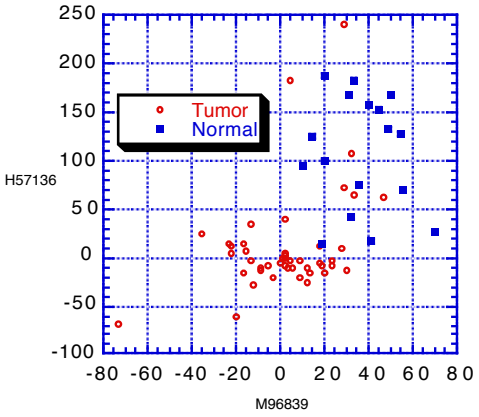


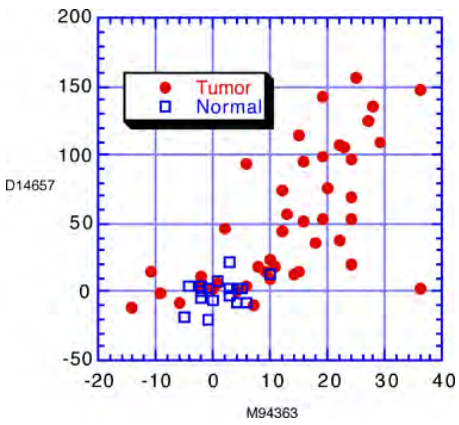


Comparison of Typical Gene Pairs in Microarray Data

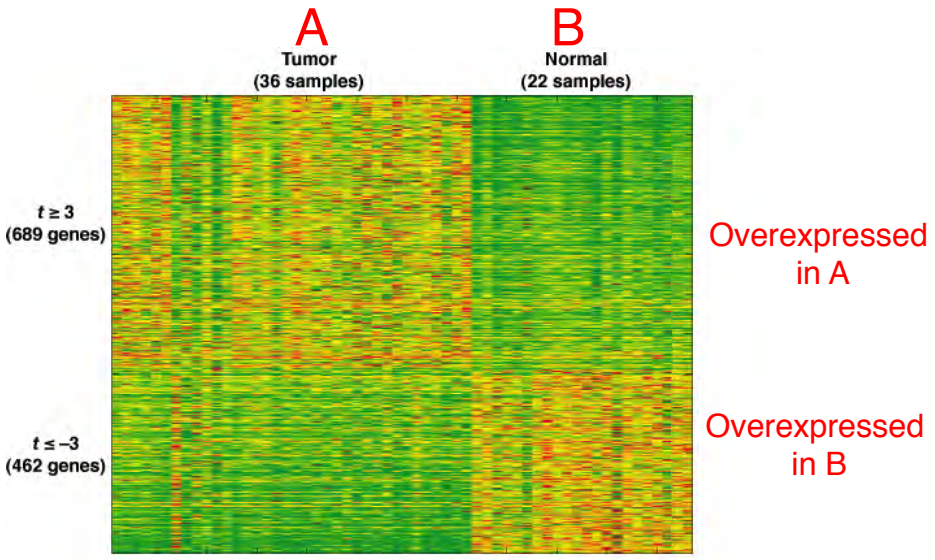


- **Each sample processed by a separate microarray**
- **Color of dot represents over- or under-expression of an RNA gene transcript in the sample**



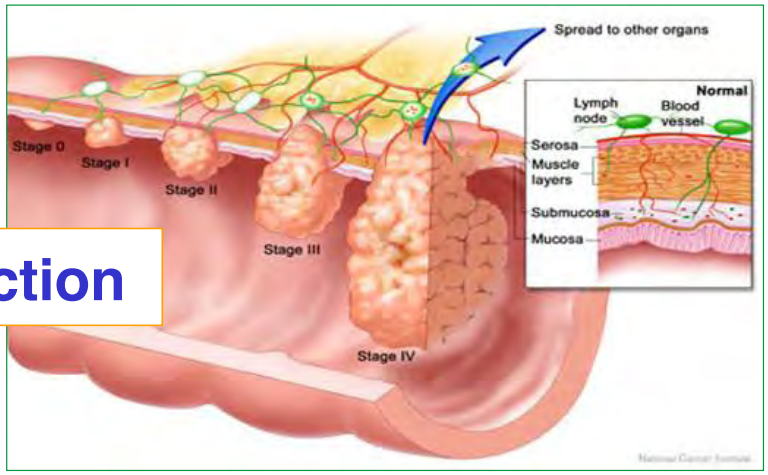


Class Comparison



- **Feature sets for predefined classes**
  - **Group A samples from tumor tissue**
  - **Group B samples from normal tissue**
    - **Genes overexpressed in Group A**
    - **Genes overexpressed in Group B**

Class Prediction

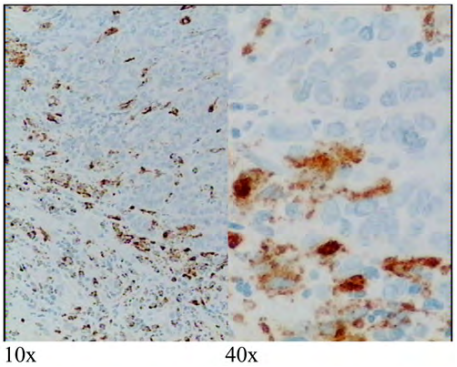


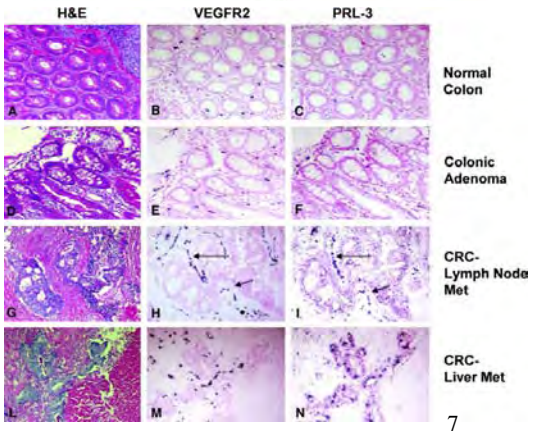
- **Algorithm that predicts class membership for a novel feature set**
  - **Genes of a new sample are analyzed**
    - **New sample in Group A or Group B?**

Class Discovery

- **New features revealed in classification**
  - **New class in universal set?**
  - **Novel sample type (e.g., antibody) correlates with group?**
  - **Novel characteristic (e.g., gender, age, or metastasis) correlates with group?**

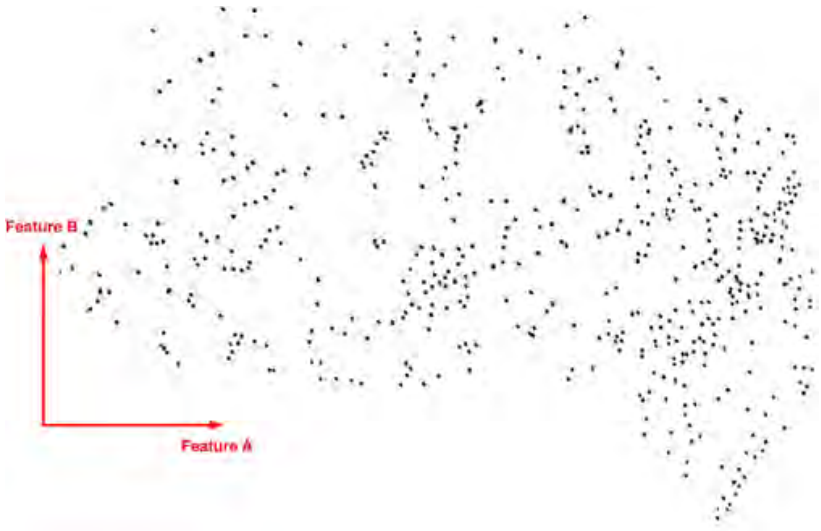
Example: Different stains used in histology





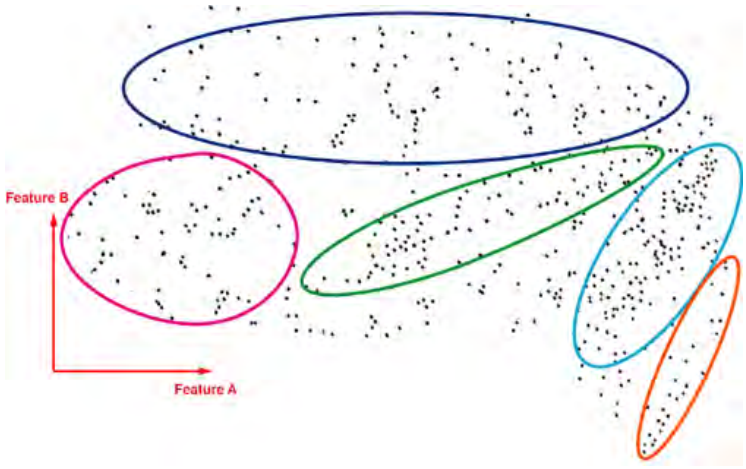
Example for Data Classification

- **Data set characterized by two features**



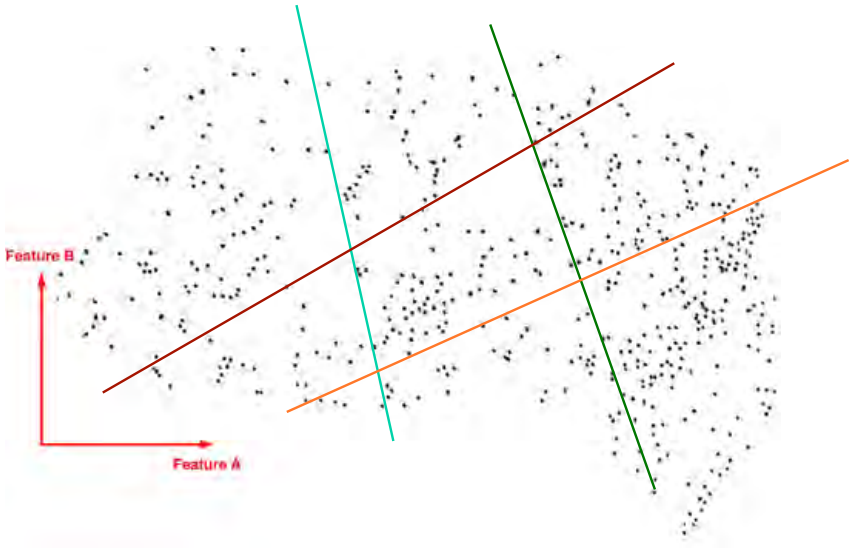
Clustering of Data

- What characterizes a cluster?
- How many clusters are there?

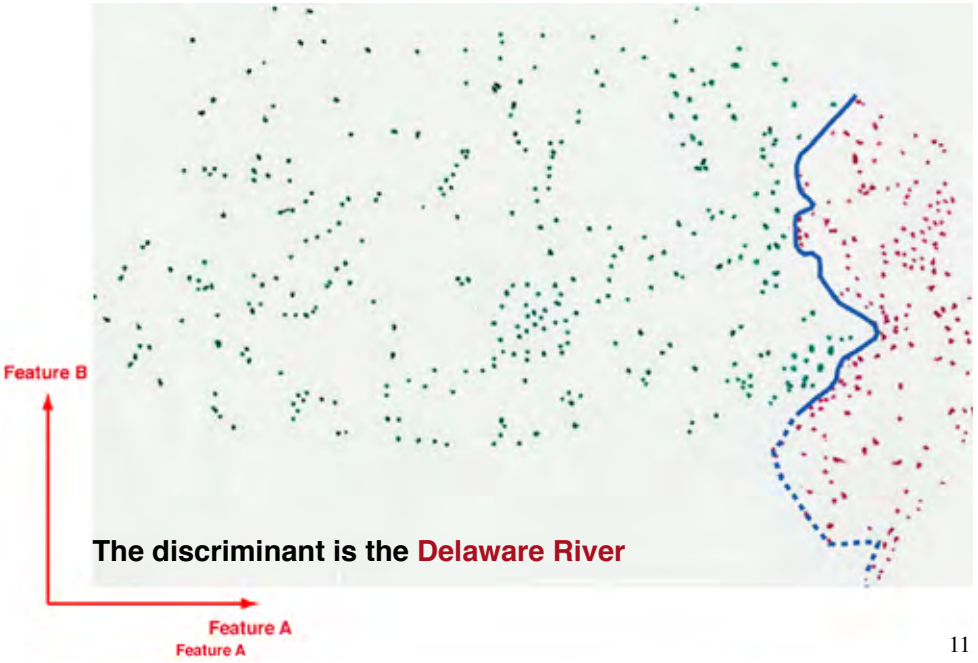


Discriminants of Data

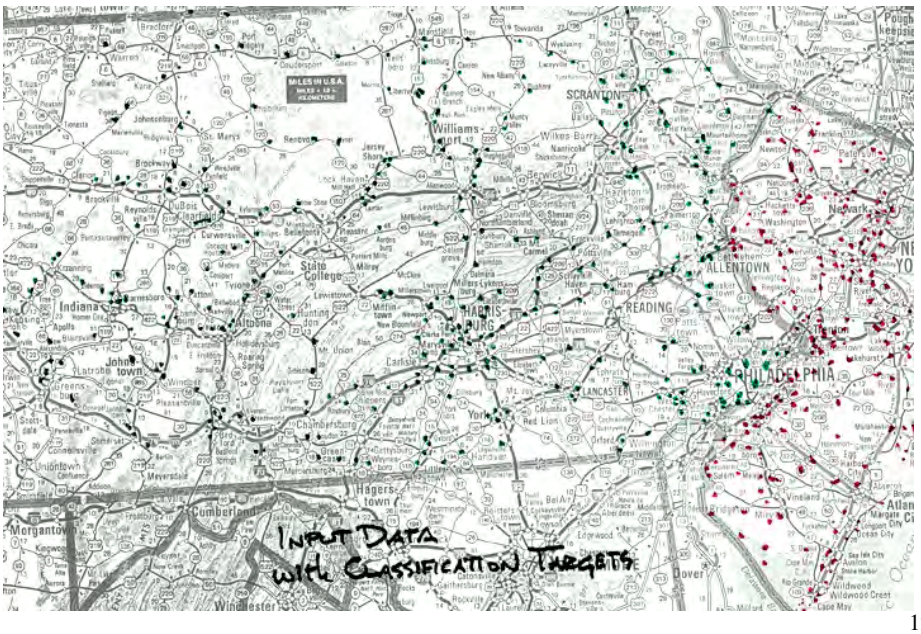
Where are the boundaries between sets?



The Data Set Revealed



Towns and Crossroads of Pennsylvania and New Jersey



Choosing Features for Classification

- How many?
- How "strong"?
- Correlation between strong and weak features
- Degree of overlap
- Use of exogenous information for selection
- Statistical significance
- Closeness to boundaries

- To distinguish New Jersey from Pennsylvania, we could consider
  - Longitude
  - Latitude
  - Altitude
  - Temperature
  - Population
  - # of fast-food stores
  - Cultural factors
  - Zip Code

Recall: Membership in a Set

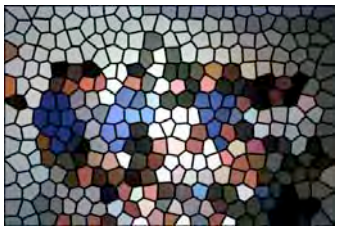
- *A* = a particular set in *U*
  - defined in a list or rule, or a membership function
- Universal set = all guests at a party
- Particular sets = distinguishing features of guests

Distorted Membership Functions*: Photo

Ambiguity and uncertainty in data sets to be classified





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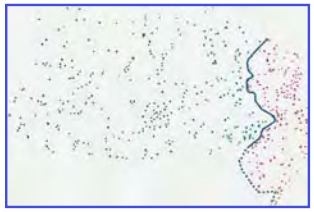
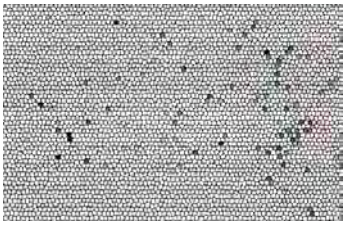
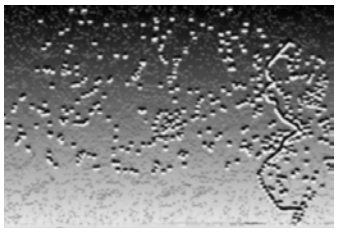
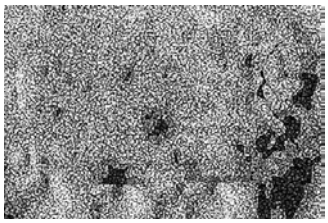


Distorted Membership Functions*: Map



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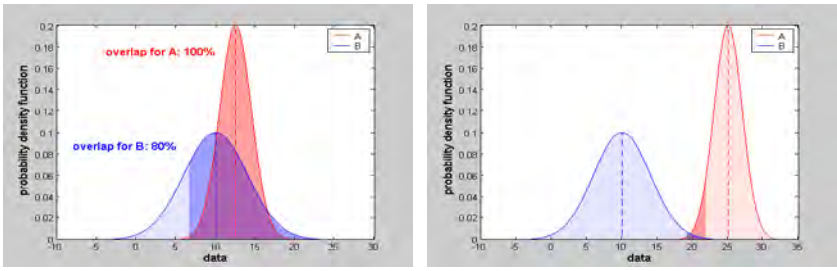
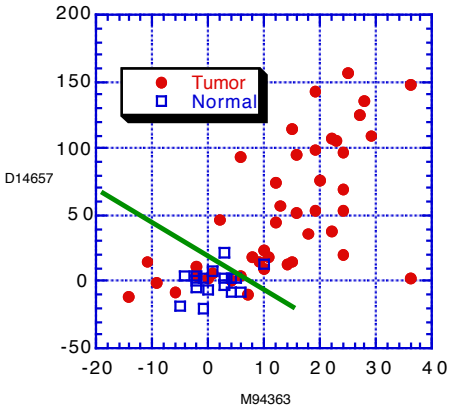
Characteristics of Classification Features



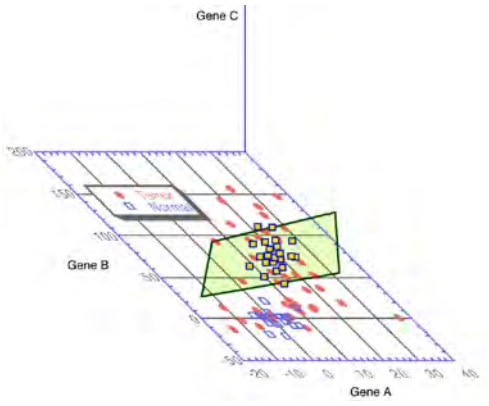
- **Strong feature**
  - Individual feature provides good classification
  - Minimal overlap of feature values in each class
  - Significant difference in class mean values
  - Low variance in class
- **Additional features**
  - Orthogonal feature (low correlation) adds new information to the set
  - Co-expressed feature (high correlation) is redundant; averaging reduces error

Feature Sets

Best line or curve may classify with significant error

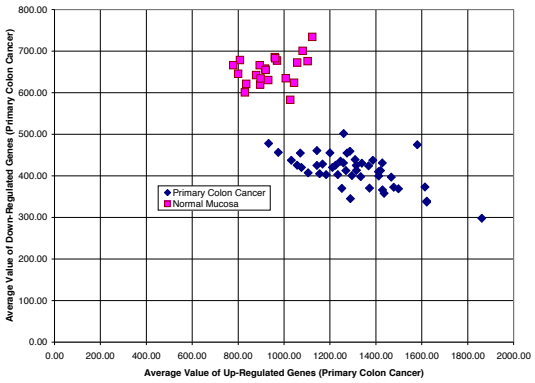


Best plane or surface classifies with equal or less error

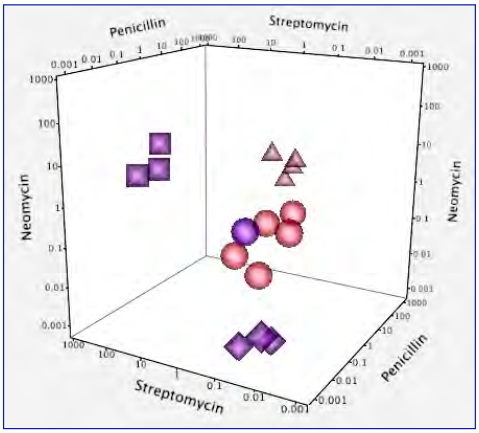


Separable Sets

Gene Analysis (2-D)

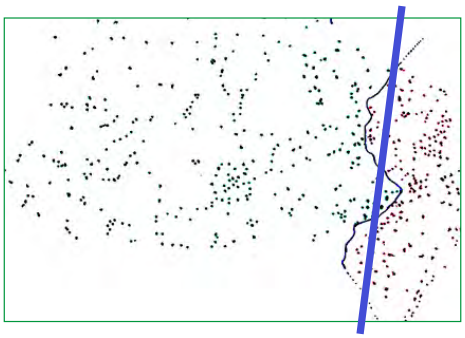


Bacterial Response to Antibiotics (3-D)



Errors in Classification

- **Expected error in classifier**
  - **Minimum possible error with statistically optimal discriminant (e.g., Delaware River) plus**
  - **Error due to constraint imposed by sub-optimal discriminant (e.g., straight vs. curved line) plus**
  - **Error due to sampling (i.e., number and distribution of points)**

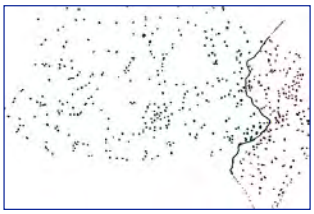


Errors in Classification

- **Over-/under-fitting**
  - **Excessive/inadequate sensitivity to details** in training data set
  - **Lack of generalization** to novel data

- **Validation**
  - **Train with less** than all available data
  - **Reserve some data** for evaluation of trained classifier
  - **Vary sets** used for training and validation

Validation of Classifier



- **Reserve some data for evaluation of trained classifier**
- **Train with A, test with B**
  - **A: Training set (or sample)**
  - **B: Novel set (or sample)**
  - **Vary sets used for training and validation**

- **Leave-one-out validation**
  - **Remove a single sample**
  - **Train on remaining samples**
  - **Does the trained classifier identify the single sample?**
  - **Repeat with all sets, removing all samples, one-by-one**

3 x 3 Confusion Matrix

Number of cases predicted to be in each class vs. actual numbers

	True Class		
Predicted Class	Cats	Dogs	Rabbits
Cats	5	2	0
Dogs	3	3	2
Rabbits	0	1	11

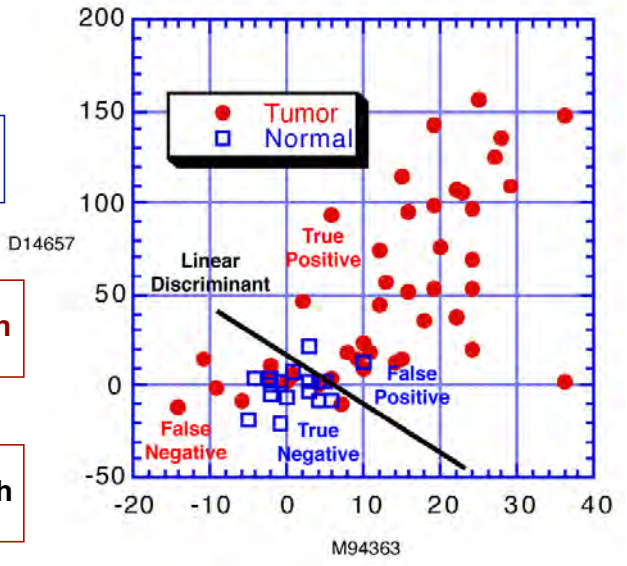
- **Interpretation: Actually, there are**
  - **8 cats:** 5 predicted to be cats, 3 to be dogs, and none to be rabbits
  - **6 dogs:** 2 predicted to be cats, 3 to be dogs, and 1 to be rabbit
  - **13 rabbits:** None predicted to be cats, 2 to be dogs, and 11 to be rabbits

Classification of Overlapping Sets

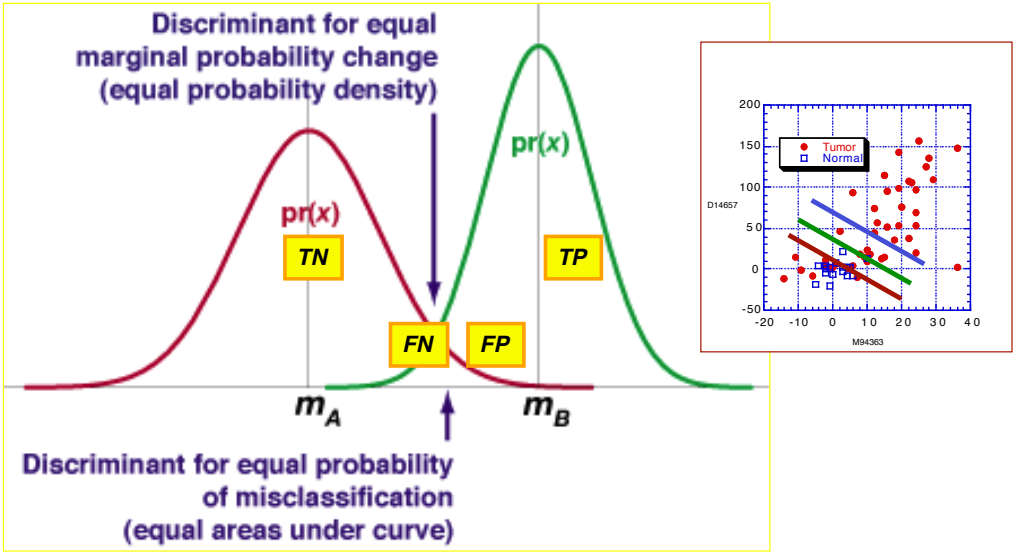
- **Tumor = Positive**
- **Normal = Negative**

- **Altering discriminant changes classification errors**

- **Classification error can never be zero with simple discriminant**



False Classification May Be Inevitable



Categories of Classification Performance

(2 x 2 Confusion Matrix)

	Actual Class		
Predicted Class	Positive	Negative	Number in Predicted Class
Positive	True Positive (TP)	False Positive (FP)	# Predicted(+) = (# TP + # FP)
Negative	False Negative (FN)	True Negative (TN)	# Predicted(–) = (# FN + # TN)
Number in Actual Class	# Actual(+) = (# TP + # FN)	# Actual(–) = (# FP + # TN)	

	Actual Class		
Predicted Class	Positive	Negative	Number in Predicted Class
Positive	True Positive (TP)	False Positive (FP)	# Predicted(+) = (# TP + # FP)
Negative	False Negative (FN)	True Negative (TN)	# Predicted(–) = (# FN + # TN)
Number in Actual Class	# Actual(+) = (# TP + # FN)	# Actual(–) = (# FP + # TN)	

Measures of Classification Performance

$$\textbf{Sensitivity}\ (\%/100) = \frac{\#\ True\ Positive}{\#\ Actual\ Positive}$$

$$\textbf{Specificity}\ (\%/100) = \frac{\#\ True\ Negative}{\#\ Actual\ Negative}$$

Measures of Classification Performance

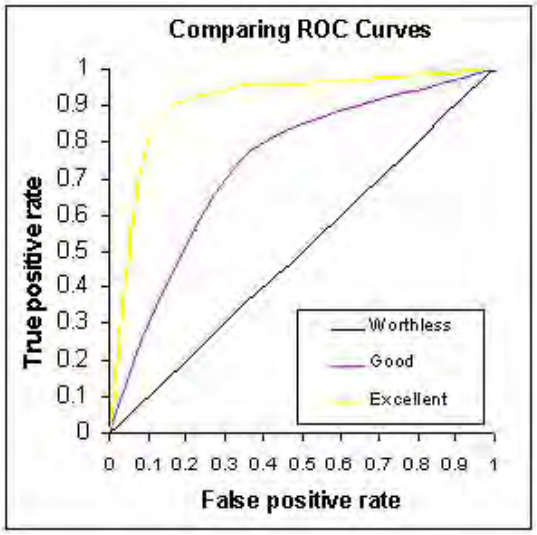
$$\textbf{Accuracy}\ (\%/100) = \frac{\#\ True\ Positive + \#\ True\ Negative}{\#\ Actual\ Positive + \#\ Actual\ Negative}$$

$$\textbf{Positive Predictive Value}\ (\%/100) = \frac{\#\ True\ Positive}{\#\ Predicted\ Positive}$$

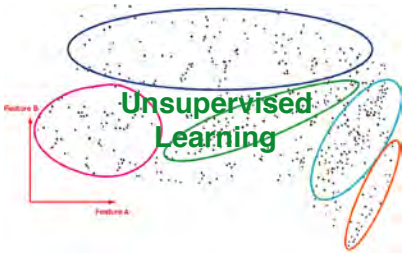
$$\textbf{Negative Predictive Value}\ (\%/100) = \frac{\#\ True\ Negative}{\#\ Predicted\ Negative}$$

Receiver Operating Characteristic* (ROC) Curve

- Comparison of 3 discriminants
- True positive rate (Sensitivity) vs. False positive rate (1 – Specificity) for a varying parameter (e.g., discriminant location)
- Choose discriminant to maximize the area under the ROC curve



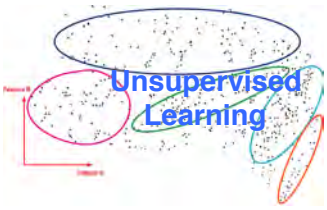
** Devised during WWII to evaluate radar target detection*



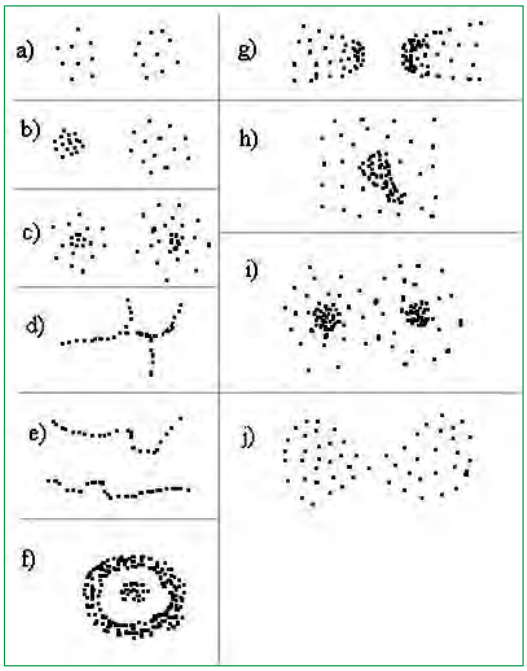
Unsupervised Learning

- Learning depends on "closeness" of related features
- Previously unknown correlations or features may be detected
- Meaning of classification occurs after learning via exogenous knowledge
- Same answer given for all questions

Cluster Analysis

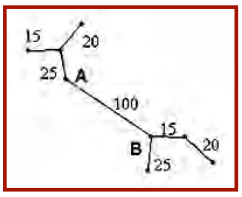


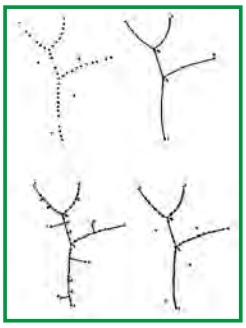
- Recognize patterns within data sets
- Group data points that are close to each other
  - Hierarchical trees
  - Two-way clustering
  - *k*-means clustering

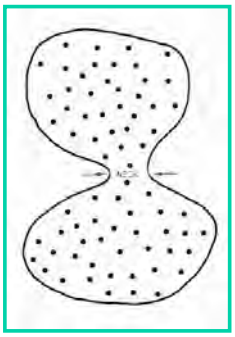


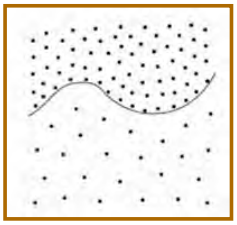
Pattern Recognition

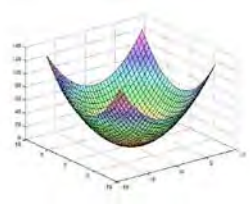
- **Minimum spanning tree**
  - Find smallest total edge length
  - Eliminate inconsistent edges
  - (e.g., A-B much longer than others)
  - Delete noisy points (e.g., bubble chamber track at right)
  - Recognize and span gaps
  - Delete necks by diameter comparison
  - Group by similar density
- **... plus other methods of digital image analysis** (shapes, edges, ...)











Distance Measures Between Data Points

- **Distance between real vectors, x_1 and x_2:**
  - **Euclidean distance**
  - **Weighted Euclidean distance**
  - **Squared Euclidean distance**
  - **Manhattan distance**
  - **Chebychev distance**
- **"Distance" between different categories, x_1 and x_2:**
  - **Categorical disagreement distance**

$$\sqrt{(\mathbf{x}_1-\mathbf{x}_2)^T(\mathbf{x}_1-\mathbf{x}_2)}$$

$$\sqrt{(\mathbf{x}_1-\mathbf{x}_2)^T\mathbf{Q}(\mathbf{x}_1-\mathbf{x}_2)}$$

$$(\mathbf{x}_1-\mathbf{x}_2)^T(\mathbf{x}_1-\mathbf{x}_2)$$

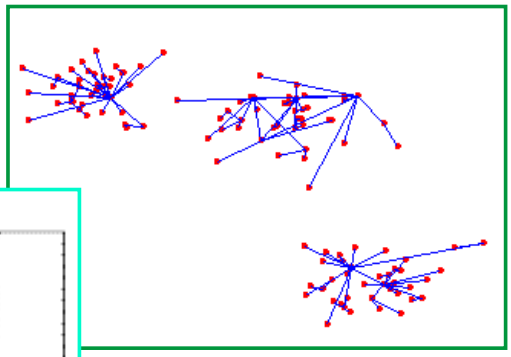
$$\sum_i \left|\mathbf{x}_{1_i}-\mathbf{x}_{2_i}\right|$$

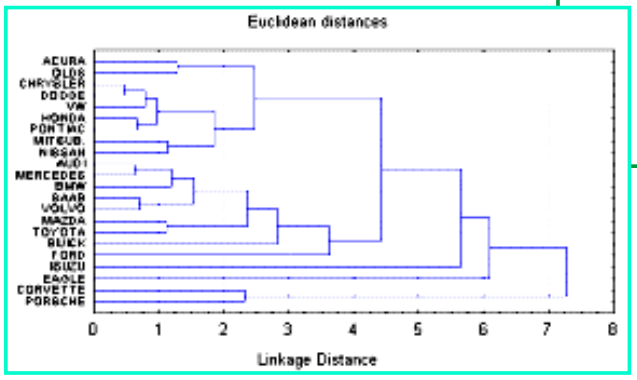
$$\max_i \left|\mathbf{x}_{1_i}-\mathbf{x}_{2_i}\right|$$

$$\left(Number\ of\ \mathbf{x}_{1_i} \neq \mathbf{x}_{2_i}\right)/i$$

Hierarchical Trees
(Dendrograms)

- **Top-down evolution**
  - **Begin with 2 best clusters**
  - **Increase number of clusters**
    - ***k*-means clustering**
    - **Self-organizing map**

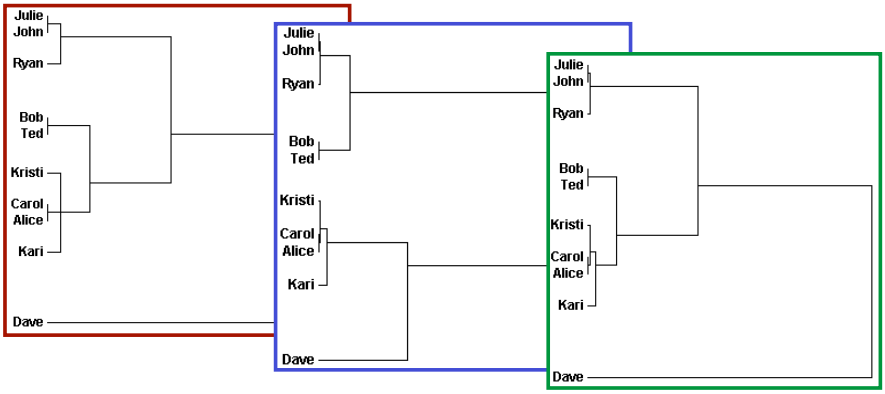




$$Centroid: \quad \bar{\mathbf{x}} = \frac{\sum_{i=1}^{N} \mathbf{x}_i}{N}$$

Hierarchical Trees
(Dendrograms)

- **Bottom-up evolution**
  - **Find nearest neighbor to each point in data set**
  - **Link pairs to closest pairs**
    - **Single linkage: distance between nearest neighbors in clusters**
    - **Complete linkage: distance between farthest neighbors in clusters**
    - **Pair-group average/centroid**



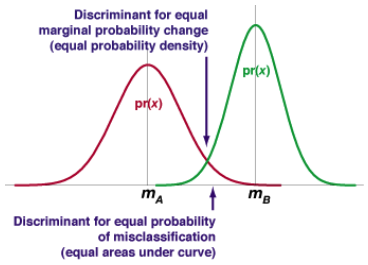
Supervised Learning

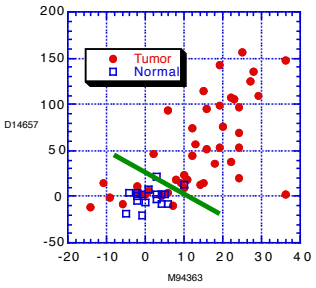
- **Learning depends on prior definition and knowledge of class**
- **Complex correlation between features is revealed**
- **Classification is inherent in learning**
- **Different answers given for different questions**

Discriminant Analysis

- **Hypothesis test**
  - Are 2 given populations different?
- **Linear discriminant**
  - What is(are) the best line(s)/plane(s)/ hyperplane(s) for separating 2 (or *k*) populations?

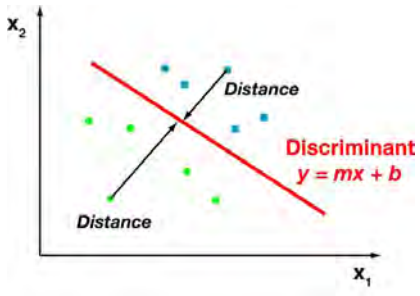
$$y = mx + b$$





Linear Discriminant

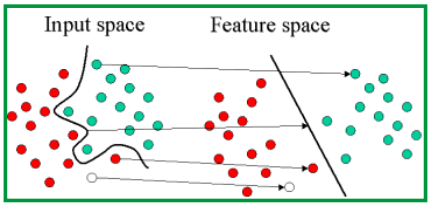
- What is(are) the best line(s)/plane(s)/ hyperplane(s) for separating 2 (or *k*) populations?
  - Fisher's linear discriminant
  - Gradient descent
  - Perceptron
- Nonseparable sets
  - Minimum square error

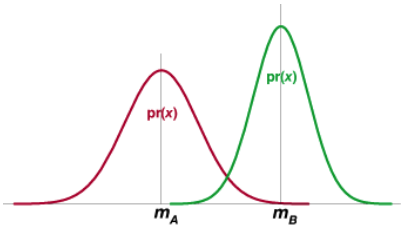


http://en.wikipedia.org/wiki/Linear_discriminant_analysis

Discriminant Analysis

- **Nearest neighbor method**
  - Ignore all points except those closest to evolving discriminant
    - Support vector machine
  - Reshape the space by transformation





Simple Hypothesis Test: *t* Test

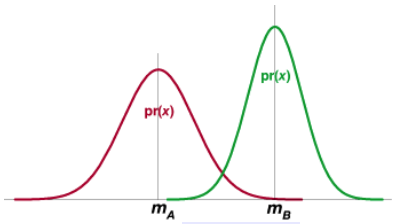
Is *A* greater than *B*?

- ***Welch's t test*** **compares mean values of two data sets**
  - **Unequal numbers and variances**
  - **|*t*| is reduced by uncertainty in the data sets (*s*)**
  - **|*t*| is increased by number of points in the data sets (*n*)**

$$t = \frac{(m_A - m_B)}{\sqrt{\frac{\sigma_A^{\,2}}{n_A} + \frac{\sigma_B^{\,2}}{n_B}}}$$

- ***m*** **= mean value of data set**
- **σ = standard deviation of data set**
- ***n*** **= number of points in data set**

- **If |*t*| > 3, $m_A \neq m_B$ with ≥ 99.7% confidence** (error probability ≤ 0.003 for Gaussian distributions) [$n > 25$]



Analysis of Variance

Variance

$$\sigma_x^2 = \frac{\sum_{i=1}^{N}(x_i - \bar{x})^2}{(N-1)}$$

F Statistic

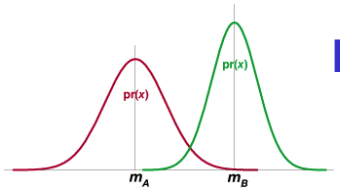
$$F_{AB} = \frac{\sigma_{x_1}^2}{\sigma_{x_2}^2} = \frac{\sigma_A^2}{\sigma_B^2}$$

- ***F* test of two populations**
  - **Populations are equivalent if**

$$F_{\min} < F_{AB} < F_{\max} \quad \text{or} \quad F_{AB} \approx 1$$

  - **Populations are strongly equivalent if**

$$F_{AB} \approx 1 \text{ and } t_{AB} \approx 0$$



Example of Gene-by-Gene Tumor/ Normal Classification by *t* Test

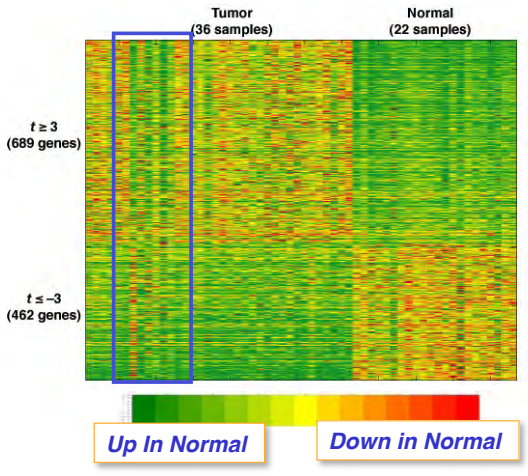
(Data from Alon *et al*, 1999)

$$t = (m_T - m_N) / \sqrt{\frac{\sigma_T^{\,2}}{36} + \frac{\sigma_N^{\,2}}{22}}$$

- **1,151 genes are over/under-expressed in tumor/normal comparison, $p \le 0.003$**
- **Genetically dissimilar samples are apparent**

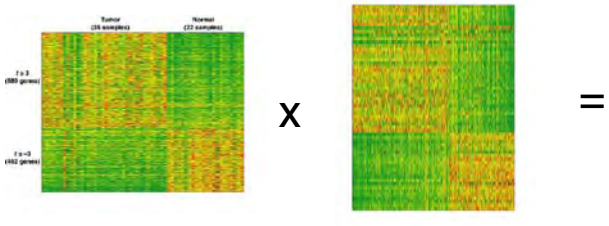
"Cancer-positive gene sets"

"Cancer-negative gene sets"

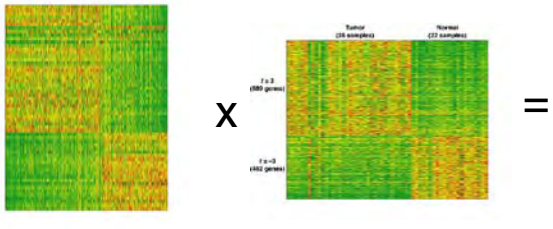


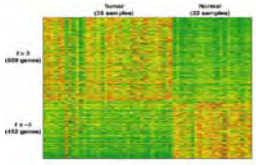
Different Correlation Matrices from Same Data Set

- Gene correlation ($D = B\,B^T$)



- Sample correlation ($E = C^T\,C$)





Ensemble Mean Values

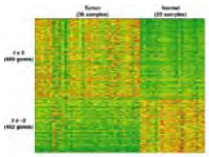
- Treat each probe set (row) as a redundant, corrupted measurement of the same tumor/normal indicator

$$z_{ij} = k_i y + \varepsilon_{ij}\ , \quad i = 1, m, \quad j = 1, n$$

- Compute column averages for each sample sub-group (i.e., sum each column and divide by *n*)

$$\hat{z}_j = \frac{1}{n}\sum_{i=1}^{n} z_{ij}$$

- Feature space is reduced from (# samples x # genes) to (# samples)
- Statistics of random variable sums are normal by central limit theorem



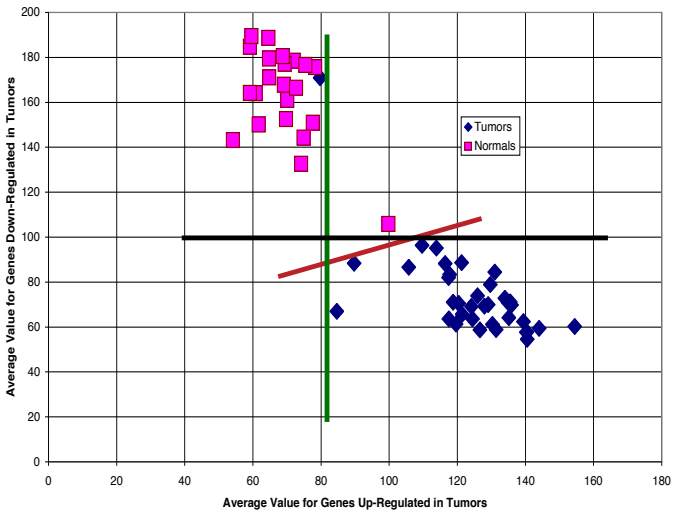
Two-Feature Discriminants for Class Prediction and Evaluation

(Alon, Notterman, 1999, data)

- Scatter plot presents average value of up genes vs. average value of down genes for each sample

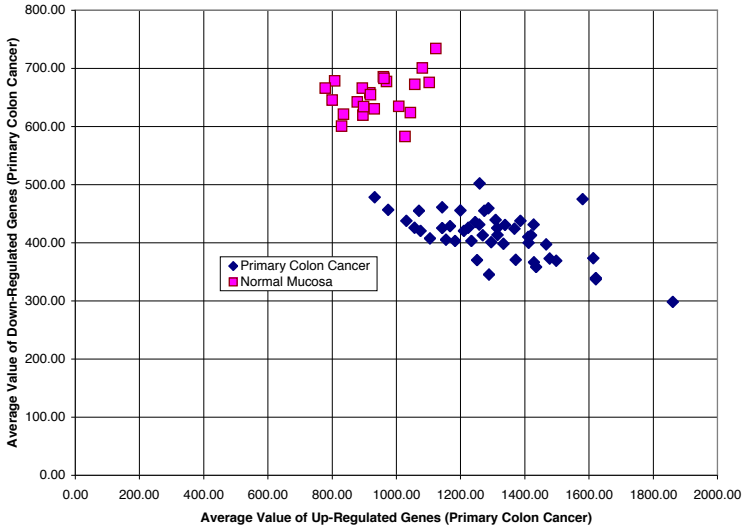
$$\left[\hat{\bar{z}}_{up_j}, \hat{\bar{z}}_{down_j}\right]$$

- Classification based on ensemble averages
- Mislabeled samples are identifiable



Clustering of Sample Averages for Primary Colon Cancer vs. Normal Mucosa

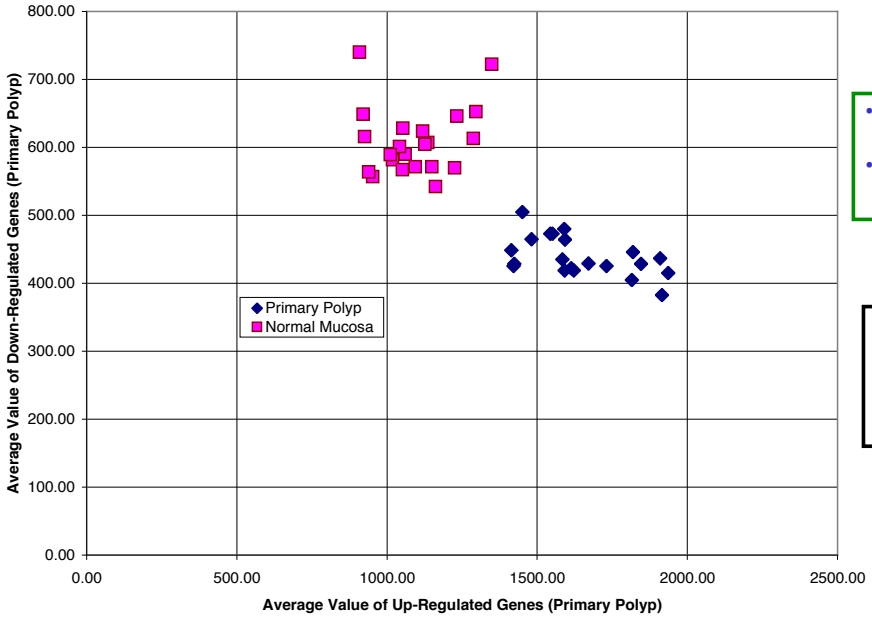
(PPG data, 2004)



- 144 samples, 3,437 probe sets analyzed
- 47 primary colon cancer
- 22 normal mucosa
- *Affymetrix HGU-133A GeneChip*
- All transcripts "Present" in all samples

# Probe sets	
Up:	1067
Down:	290
Constant:	19

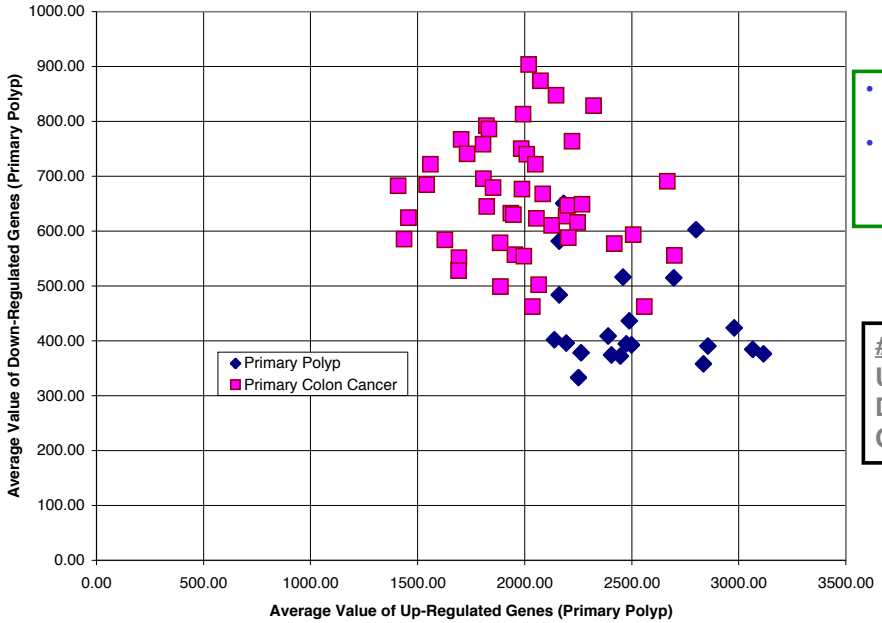
Clustering of Sample Averages for Primary Polyp vs. Normal Mucosa



- 21 primary polyp
- 22 normal mucosa

# Probe sets	
Up:	1014
Down:	219
Constant:	40

Clustering of Sample Averages for Primary Polyp vs. Primary Colon Cancer



- 21 primary polyp
- 47 primary colon cancer

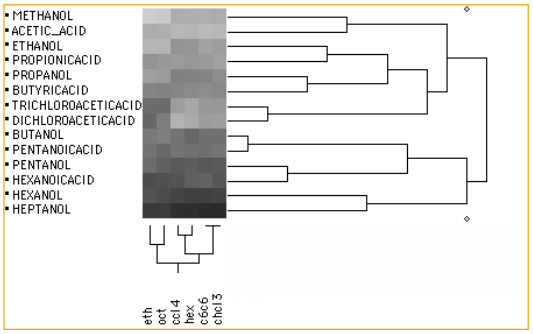
# Probe sets	
Up:	273
Down:	126
Constant:	172

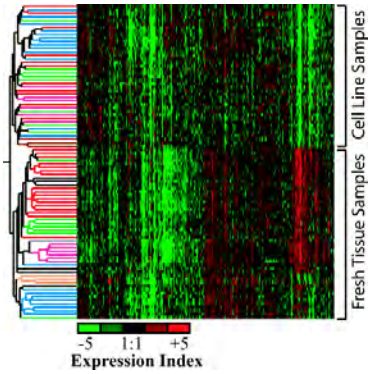
Next Time: Introduction to Neural Networks

Supplemental Material

Dual Hierarchical Trees

- **Two-way joining**
  - –**Trees derived from two independent variables**
    - **Cluster by feature and by sample**
    - **Cluster by different components of measurement**



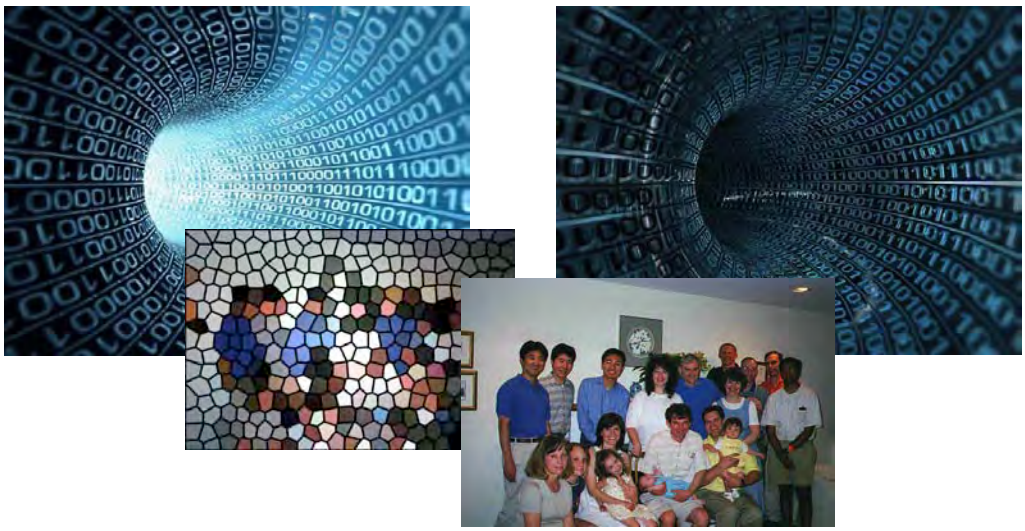


"Big Data" and Data Mining

Multi-dimensional classification

Ray of hope …?

… or infinite harm?



http://en.wikipedia.org/wiki/Big_data