CSC2545 – Topics in Machine Learning:
Kernel Methods and Support Vector Machines

- A comprehensive introduction to SVMs and other kernel methods, including theory, algorithms and applications.
- Instructor: Anthony Bonner
- Prerequisites: linear algebra, vector calculus, basic probability, mathematical maturity, programming experience.
- Expected work: 3-4 assignments.
- Lectures: TF 2-3:30pm (sometimes 2-3pm)
- For more information see www.cs.toronto.edu/~bonner

Course Content

- Some things kernel methods and SVMs can do:
  - non-linear classification
  - non-linear regression
  - non-linear dimensionality reduction
- How and why they work:
  - Hilbert space
  - statistical learning theory
  - regularization
- Possible additional topics:
  - convex optimization
  - implementation issues
  - Bayesian kernel methods

Data

Vectors

- Collections of features
  e.g. height, weight, blood pressure, age, ...
- Can map categorical variables into vectors

Matrices

- Images, Movies
- Remote sensing and satellite data (multispectral)

Strings

- Documents
- Gene sequences

Structured Objects

- XML documents
- Graphs

Optical Character Recognition

Reuters Database

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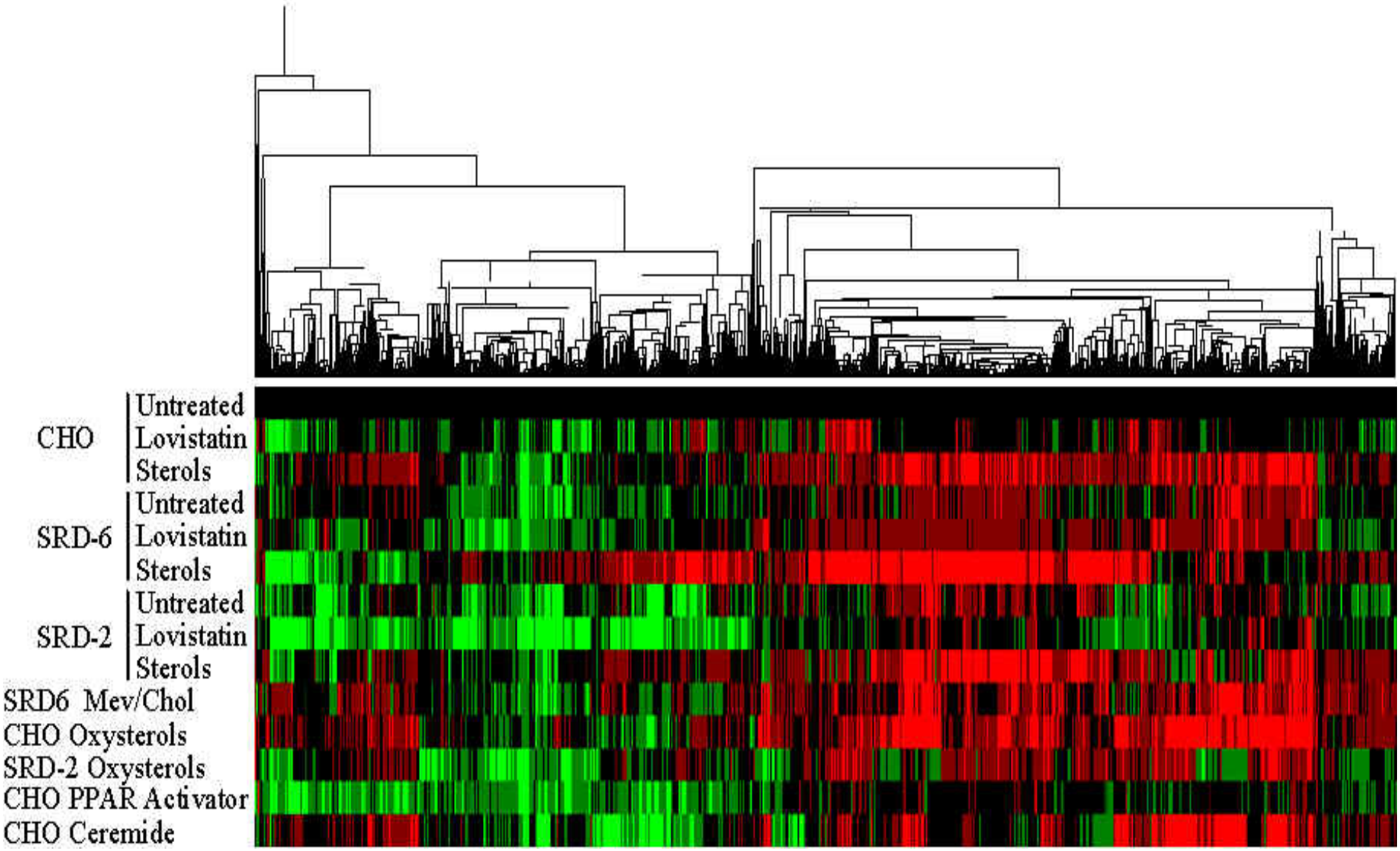
Faces

More Faces

Microarray Data



Biological Sequences

Goal

Estimate function of protein based on sequence information.

Example Data

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CSGKQESMNSNVSVYQ
>0_d1tlk__ 2.1.1.4.3 Telokin [turkey (Meleagris gallopavo)]
VAEEKPHVKPYFTKTILDMDVVEGSAARFDCKVEGYPDPEVMWFKDDNPVKESRHFQIDYDEEGNCSLTI
SEVCGDDDAKYTCKAVNSLGEATCTAELLVETM
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RVLQVDIVPSQGEISVGESKFFLCQVAGDAKDKDISWFSPNGEKLSPNQQRISVVWNDDDSSTLTIYNAN
IDDAGIYKCVVTAEDGTQSEATVNVKIFQ
>0_d1tnm__ 2.1.1.4.5 Titin [Human (Homo sapiens), module M5]
RILTKPRSMTVYEGESARFSCDTDGEPVPTVTWLRKGQVLSTSARHQVTTTKYKSTFEISSVQASDEGNY
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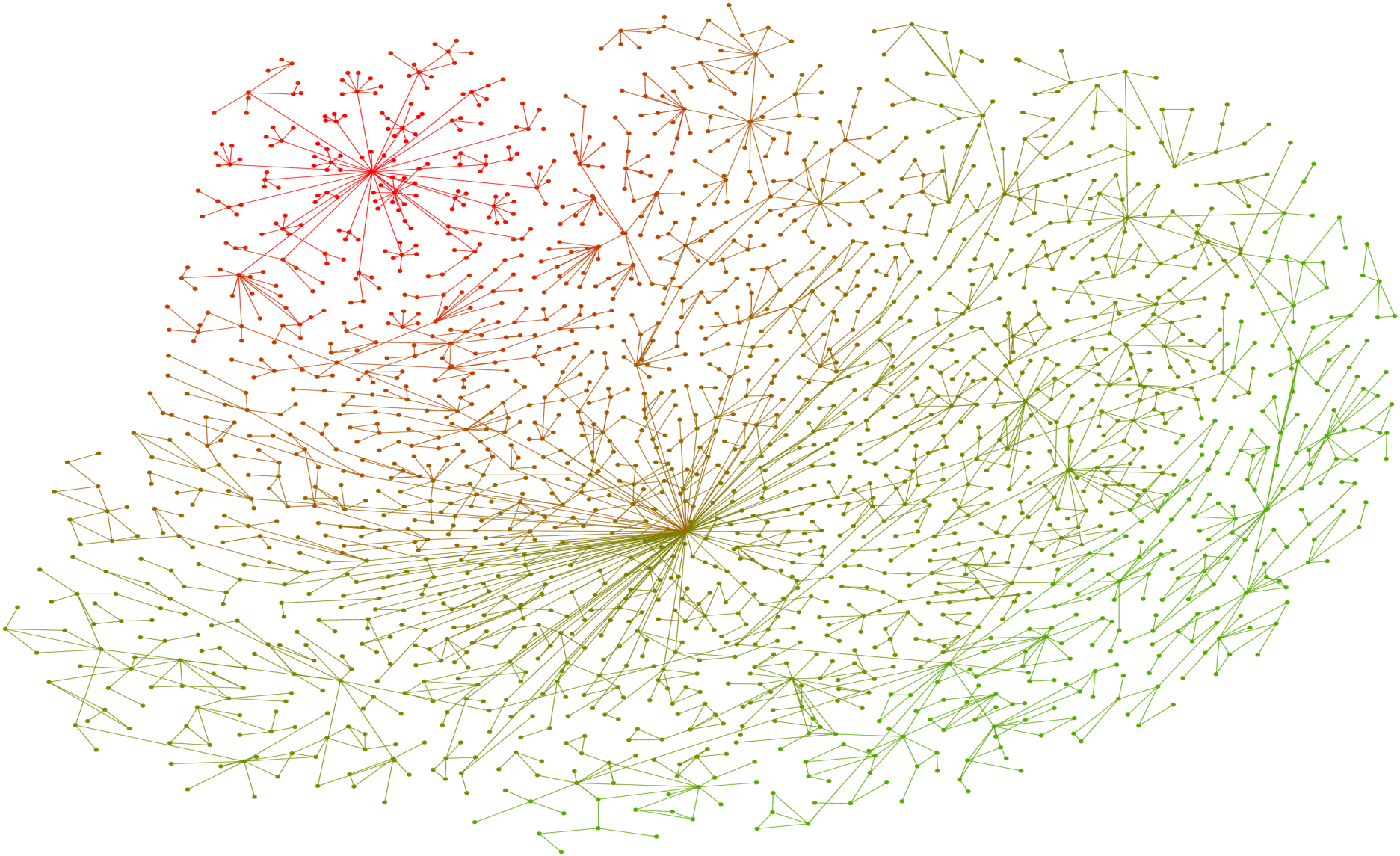
Graphs



What to do with data

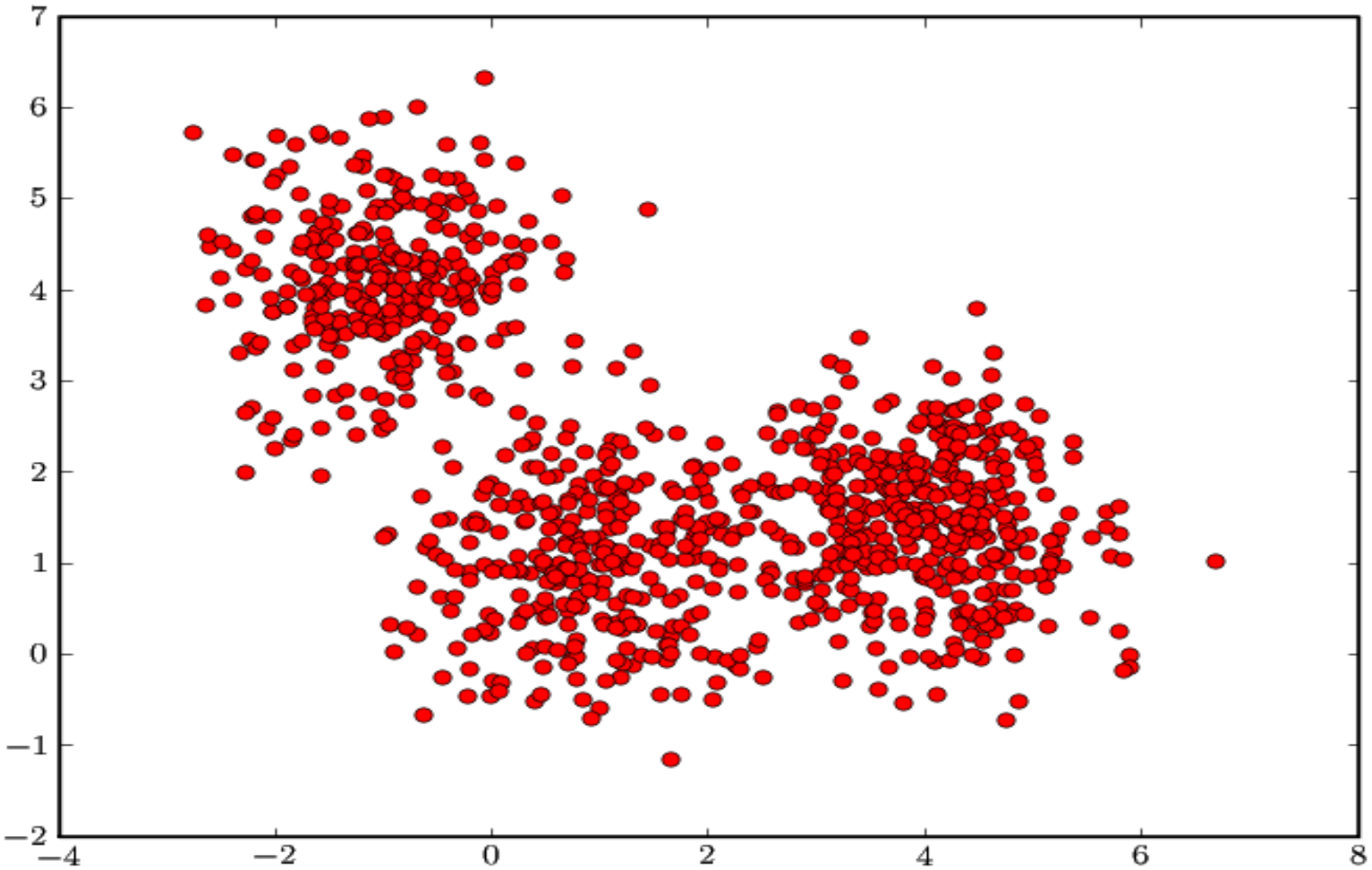
Unsupervised Learning

- Find clusters of the data
- Find low-dimensional representation of the data (e.g. unroll a swiss roll, find structure)
- Find interesting directions in data
- Interesting coordinates and correlations
- Find novel observations / database cleaning

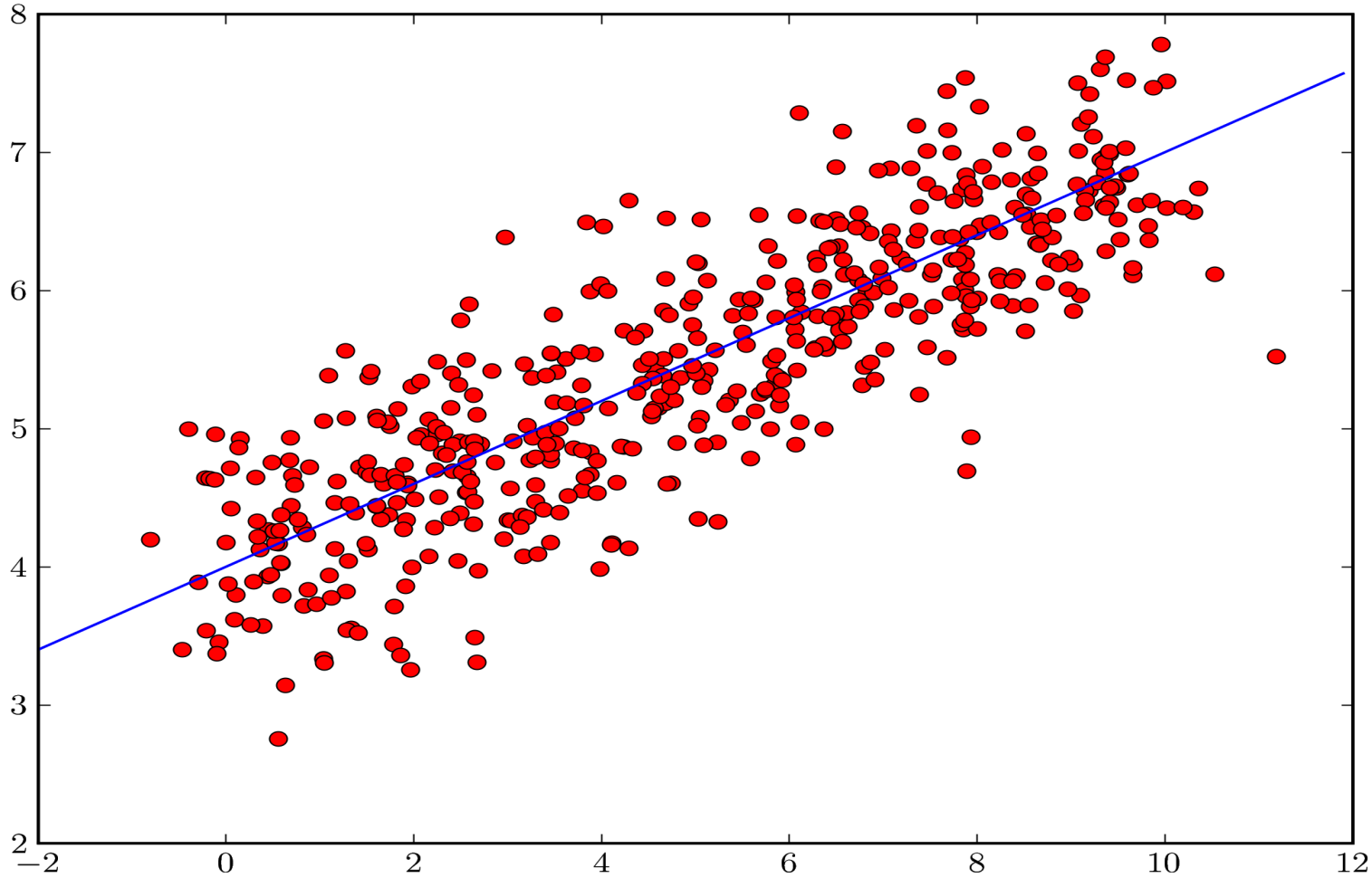
Supervised Learning

- Classification (distinguish apples from oranges)
- Speech recognition
- Regression (tomorrow's stock value)
- Predict time series
- Annotate strings

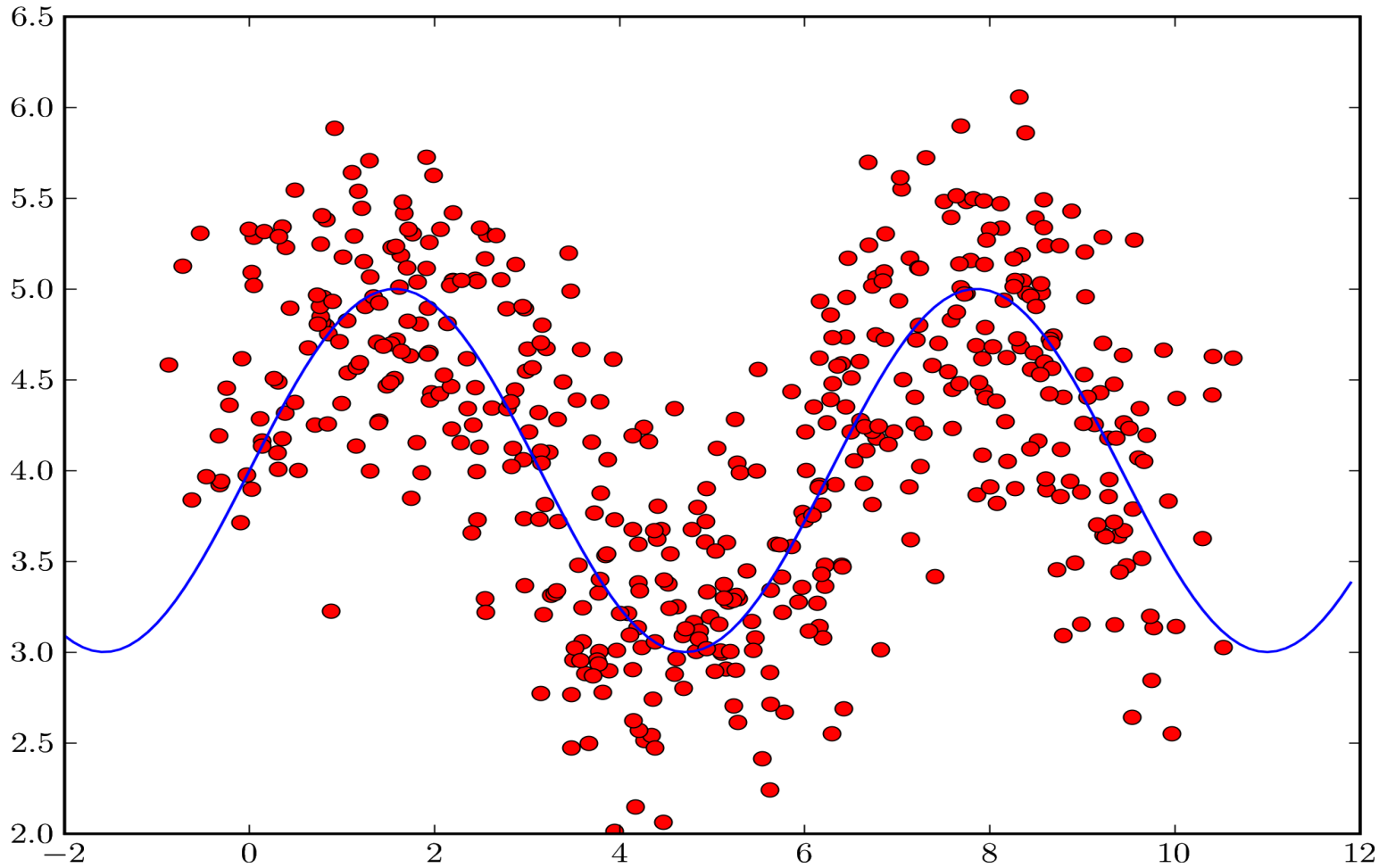
Clustering



Principal Components



Linear Subspace



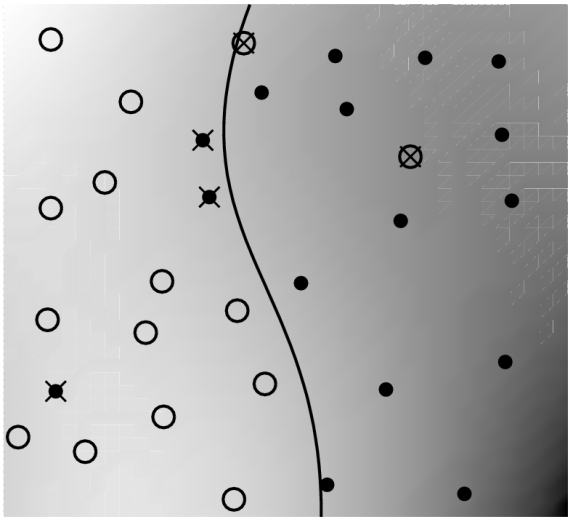
Classification

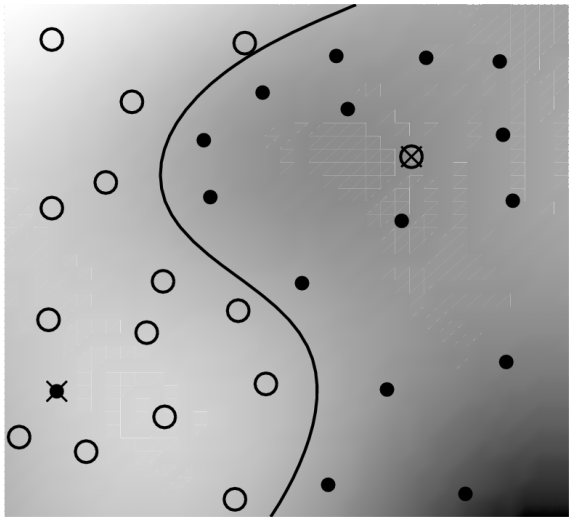
Data

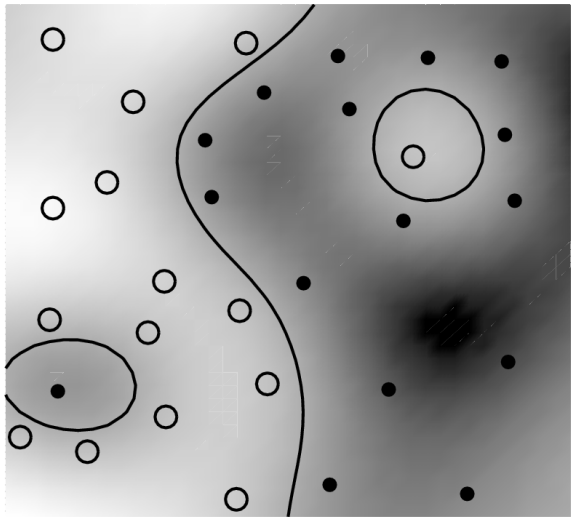
Pairs of observations (x_i, y_i) drawn from distribution
e.g., (blood status, cancer), (credit transactions, fraud), (sound profile of jet engine, defect)

Goal

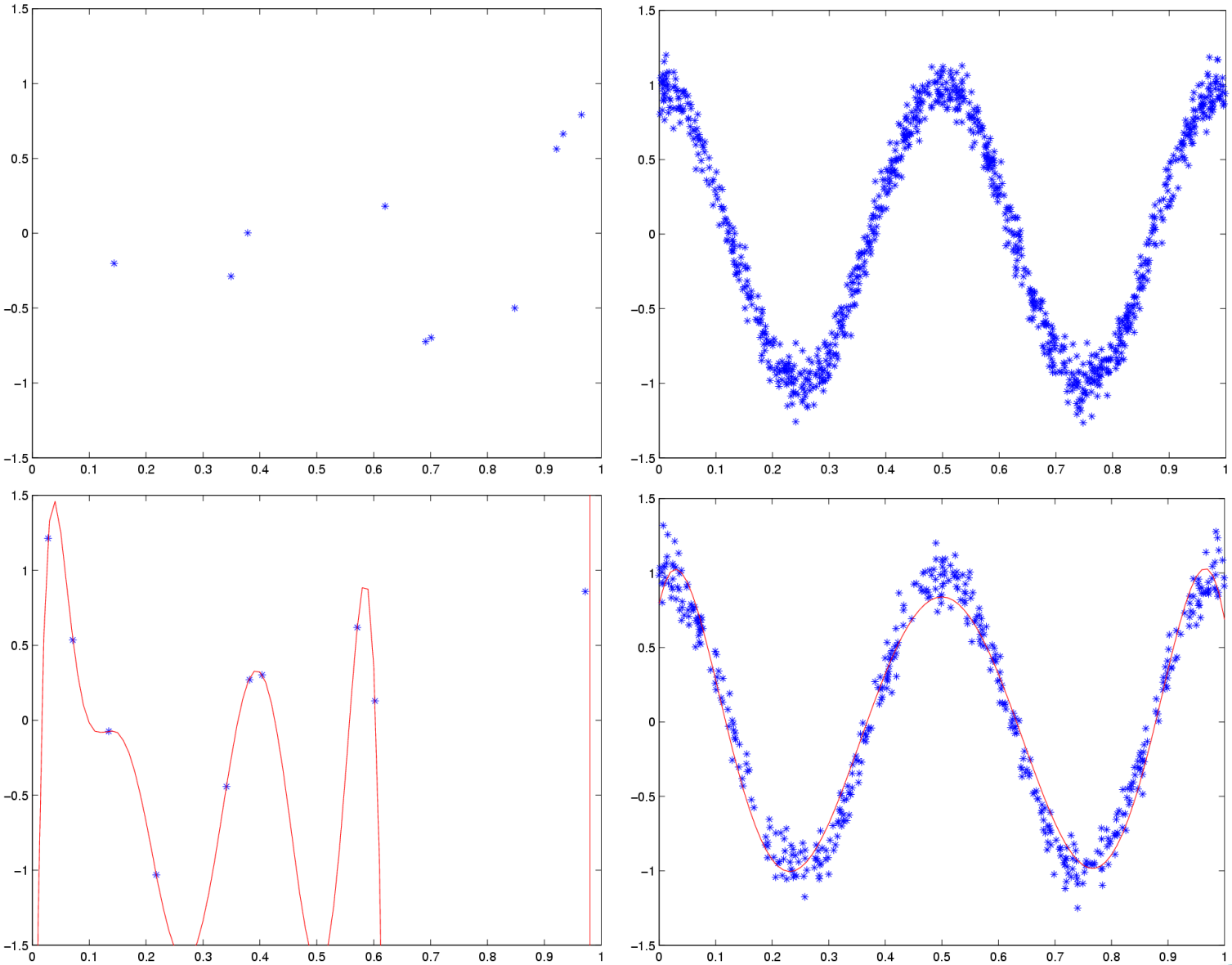
Estimate $y \in \{\pm 1\}$ **given** x at a new location. Or find a function $f(x)$ that does the trick.







Regression



Regression

Data

Pairs of observations (x_i, y_i) generated from some joint distribution $\Pr(x, y)$, e.g.,

- market index, SP100
- fab parfameters, yield
- user profile, price

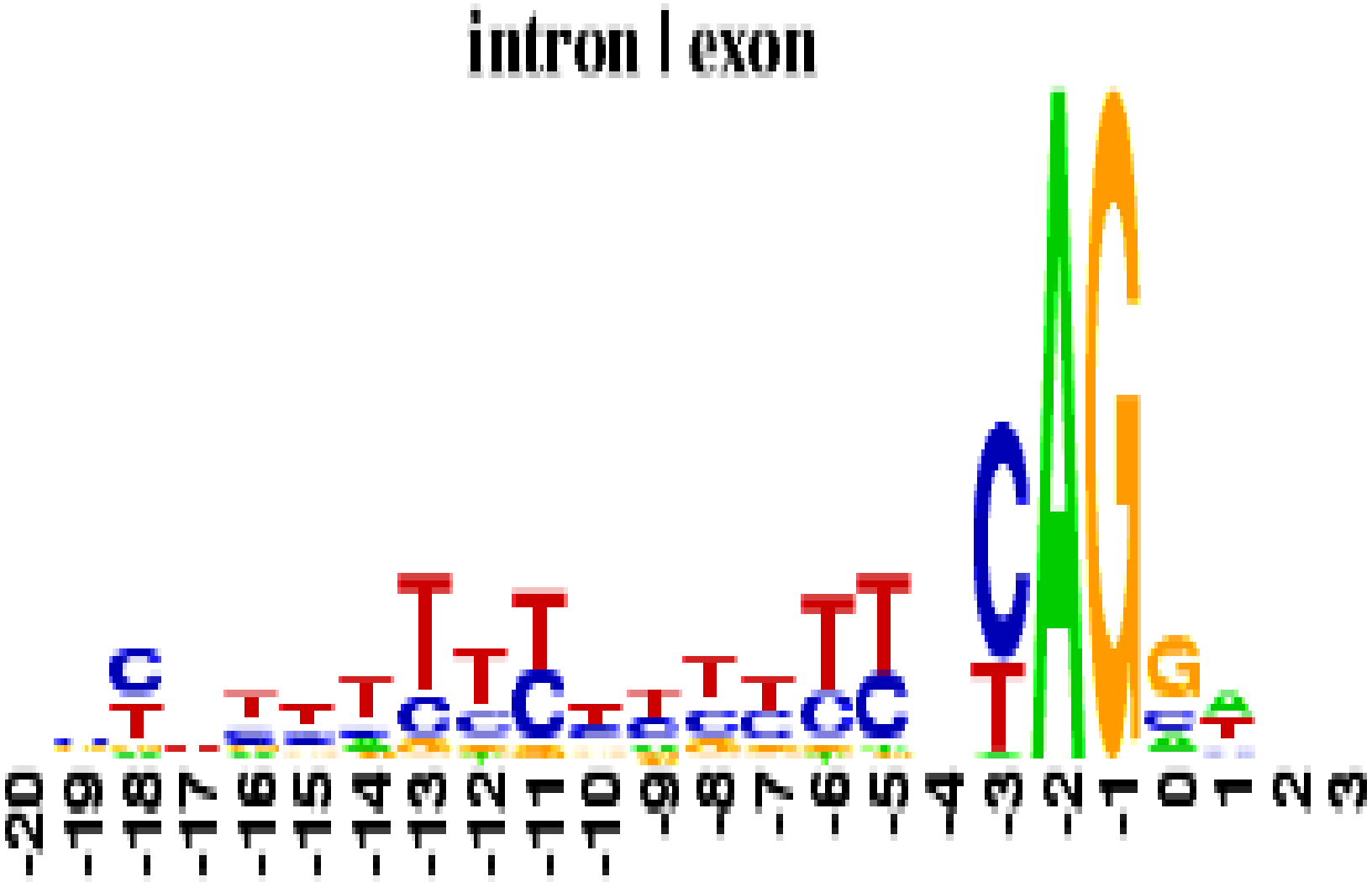
Task

Estimate y, given x, such that some loss $c(x, y, f(x))$ is minimized.

Examples

- Quadratic error between y and $f(x)$, i.e. $c(x, y, f(x)) = \frac{1}{2}(y - f(x))^2$.
- Absolute value, i.e., $c(x, y, f(x)) = |y - f(x))|$.

Annotating Strings



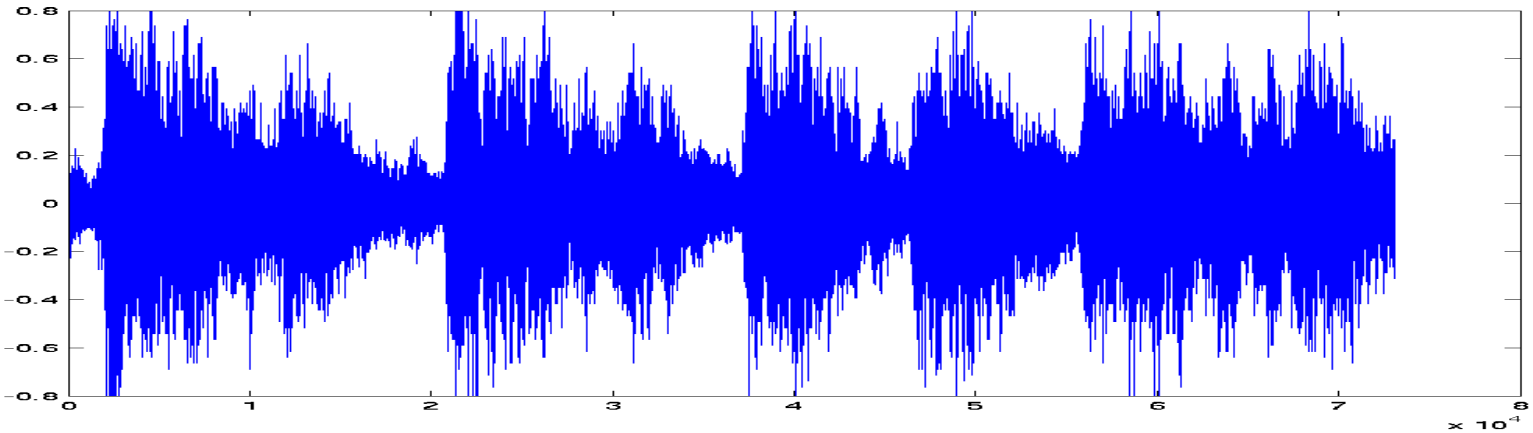
Annotating Audio

Goal

- Possible meaning of an audio sequence
- Give confidence measure

Example (from Australian Prime Minister's speech)

- a stray alien
- Australian



Novelty Detection

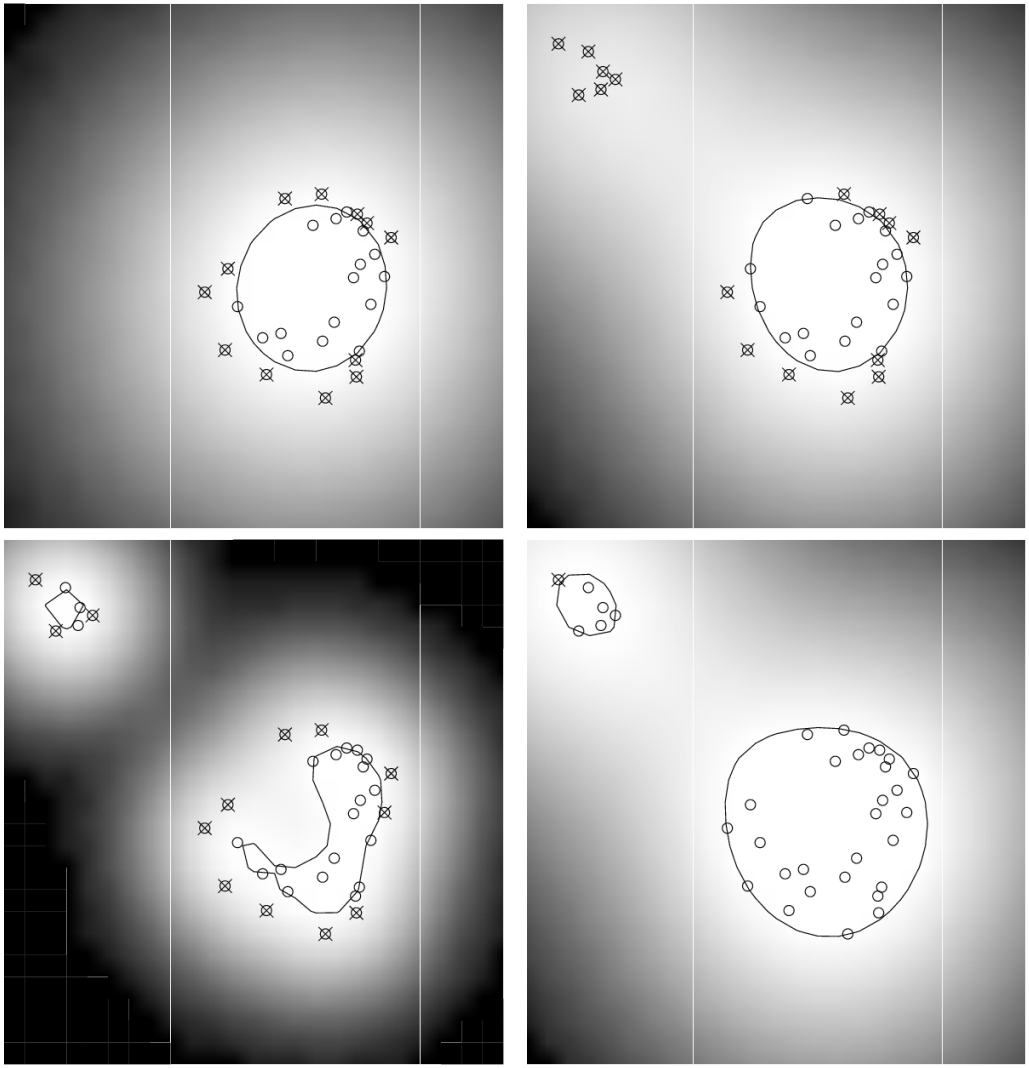
Data

Observations x_i from some $\mathrm{P}(x)$, e.g.,

- network usage patterns
- handwritten digits
- alarm sensors
- factory status

Task

Find unusual events, clean database, distinguish typical examples.



Learning and Similarity: some Informal Thoughts

- input/output sets $\mathcal{X}, \mathcal{Y}$
- training set $(x_1, y_1), \ldots, (x_m, y_m) \in \mathcal{X} \times \mathcal{Y}$
- "generalization": given a previously unseen $x \in \mathcal{X}$, find a suitable $y \in \mathcal{Y}$
- (x, y) should be "similar" to $(x_1, y_1), \ldots, (x_m, y_m)$
- how to measure similarity?
  - for outputs: *loss function* (e.g., for $\mathcal{Y} = \{\pm 1\}$, zero-one loss)
  - for inputs: *kernel*

Similarity of Inputs

- symmetric function

$$k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$$
$$(x, x') \mapsto k(x, x')$$

- for example, if $\mathcal{X} = \mathbb{R}^N$: canonical dot product

$$k(x, x') = \sum_{i=1}^{N} [x]_i [x']_i$$

- if $\mathcal{X}$ is not a dot product space: assume that k has a representation as a dot product in a linear space $\mathcal{H}$, i.e., there exists a map $\Phi : \mathcal{X} \to \mathcal{H}$ such that

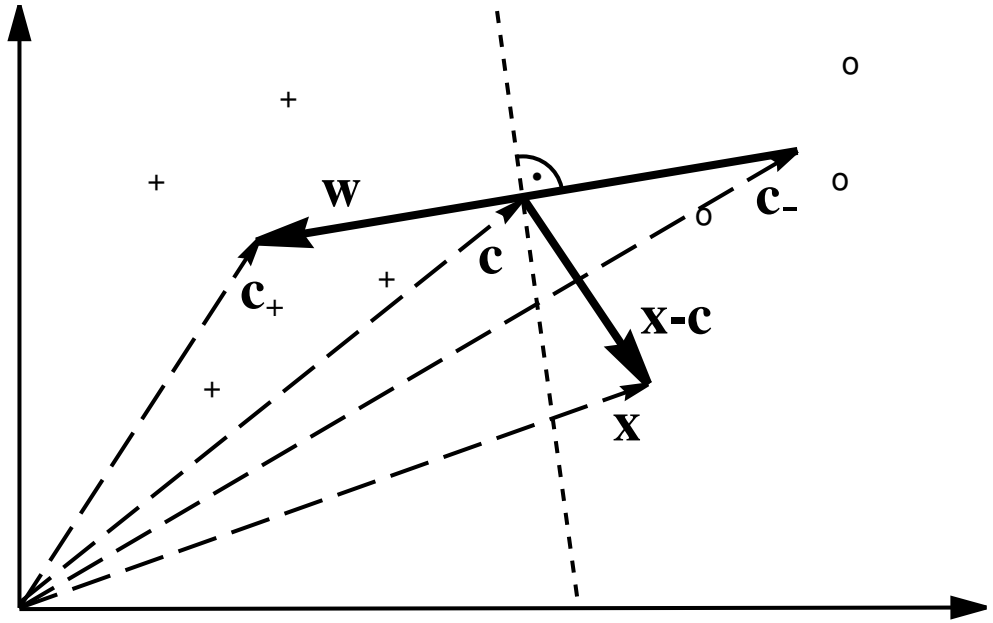
$$k(x, x') = \left\langle \Phi(x), \Phi(x') \right\rangle .$$

- in that case, we can think of the patterns as $\Phi(x), \Phi(x')$, and carry out geometric algorithms in the dot product space ("feature space") $\mathcal{H}$.

An Example of a Kernel Algorithm

Idea: classify points $\mathbf{x} := \Phi(x)$ in feature space according to which of the two class means is closer.

$$\mathbf{c}_+ := \frac{1}{m_+} \sum_{y_i=1} \Phi(x_i), \quad \mathbf{c}_- := \frac{1}{m_-} \sum_{y_i=-1} \Phi(x_i)$$



Compute the sign of the dot product between $\mathbf{w} := \mathbf{c}_+ - \mathbf{c}_-$ and $\mathbf{x} - \mathbf{c}$.

An Example of a Kernel Algorithm, ctd. [25]

$$f(x) = \operatorname{sgn}\left(\frac{1}{m_+}\sum_{\{i:y_i=+1\}}\langle\Phi(x),\Phi(x_i)\rangle - \frac{1}{m_-}\sum_{\{i:y_i=-1\}}\langle\Phi(x),\Phi(x_i)\rangle + b\right)$$

$$= \operatorname{sgn}\left(\frac{1}{m_+}\sum_{\{i:y_i=+1\}}k(x,x_i) - \frac{1}{m_-}\sum_{\{i:y_i=-1\}}k(x,x_i) + b\right)$$

where

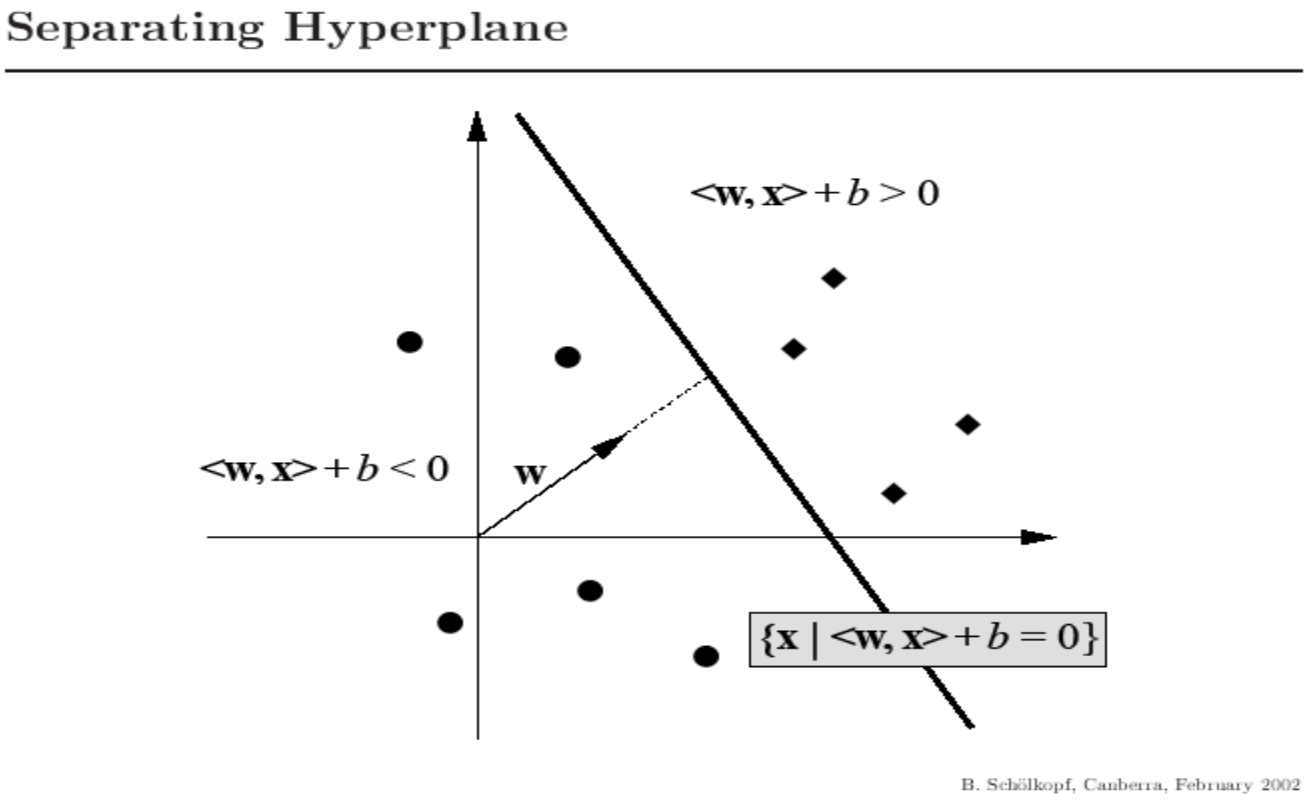
$$b = \frac{1}{2}\left(\frac{1}{m_-^2}\sum_{\{(i,j):y_i=y_j=-1\}}k(x_i,x_j) - \frac{1}{m_+^2}\sum_{\{(i,j):y_i=y_j=+1\}}k(x_i,x_j)\right).$$

- provides a geometric interpretation of Parzen windows

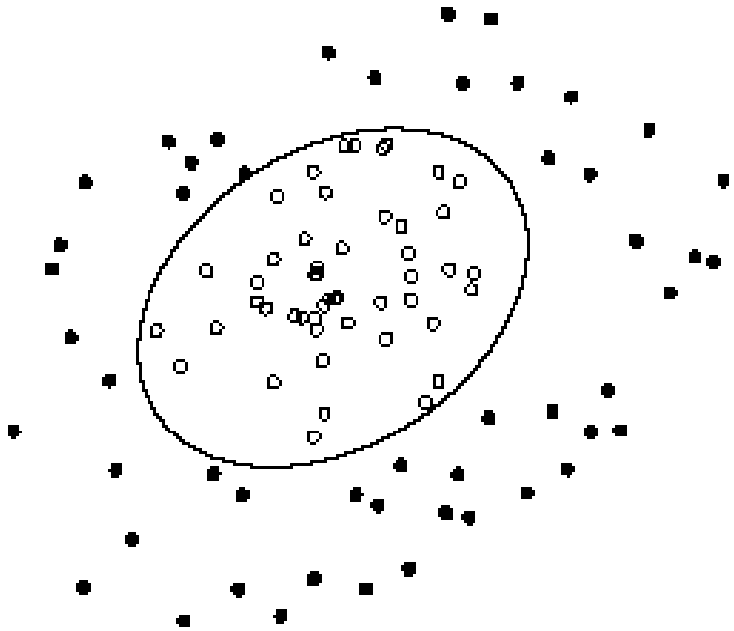
Non-linear Classification via Support Vector Machines

- Based on several ideas:
  - linear classification
  - *increasing* the dimensionality
  - the kernel trick
  - maximizing the margin
  - duality

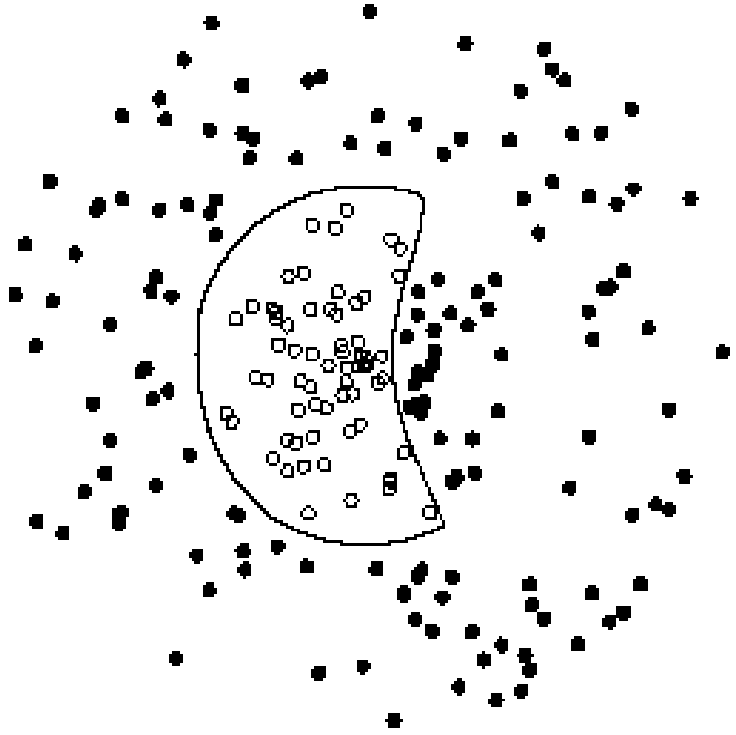
Linear Classification



Non-linear Classification



separation by ellipsoid



separation by 4th degree polynomial

Kernel trick

kernel trick: dot-products in feature space can be computed as a kernel function $K(\mathbf{x}_i, \mathbf{x}_j) = \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j)$

idea: work directly on $\mathbf{x}$, avoid having to compute $\Phi(\mathbf{x})$ at all

example:

$$\begin{aligned} K(\mathbf{a}, \mathbf{b}) &= (\mathbf{a} \cdot \mathbf{b})^3 = ((a_1, a_2) \cdot (b_1, b_2))^3 \\ &= (a_1 b_1 + a_2 b_2)^3 \\ &= a_1^3 b_1^3 + 3 a_1^2 b_1^2 a_2 b_2 + 3 a_1 b_1 a_2^2 b_2^2 + a_2^3 b_2^3 \\ &= ((a_1^3, \sqrt{3} a_1^2 a_2, \sqrt{3} a_1 a_2^2, a_2^3) \cdot (b_1^3, \sqrt{3} b_1^2 b_2, \sqrt{3} b_1 b_2^2, b_2^3)) \\ &= \Phi(\mathbf{a}) \cdot \Phi(\mathbf{b}) \end{aligned}$$

Kernels

examples:

1. polynomial kernel: $K(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i \cdot \mathbf{x}_j + 1)^z$
2. Gaussian kernel: $K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-||\mathbf{x}_i - \mathbf{x}_j||^2/2\sigma^2)$
3. sigmoid kernel: $K(\mathbf{x}_i, \mathbf{x}_j) = \tanh(\kappa(\mathbf{x}_i \cdot \mathbf{x}_j) + a)$

each kernel computation corresponds to dot product calculation for particular mapping $\Phi(\mathbf{x})$ – implicitly maps to high-dim space

why useful?

- rewrite training examples using more complex features
- dataset not linearly separable in original space may be linearly separable in higher-dimensional space