SUPERVISED LEARNING - (Brief)

- *Supervised learning; basics; labeled data*
- *Classification problems; KNN classification*
- *Linear Classifiers; Fisher Lin. Discrimants*
- *Support Vector Machines; Deep Neural Networks*

Major tool of Data Mining: Dimension reduction

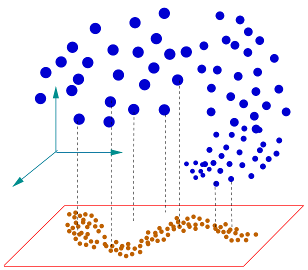
➤ Goal is not as much to reduce size (& cost) but to:

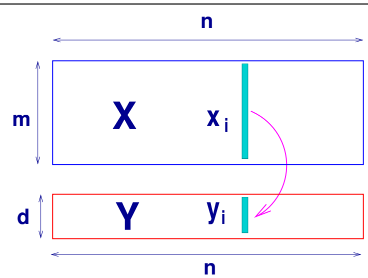
- Reduce noise and redundancy in data before performing a task [e.g., classification as in digit/face recognition]
- Discover important 'features' or 'paramaters'

The problem: Given: $X = [x_1, \cdots, x_n] \in \mathbb{R}^{m\times n}$, find a low-dimens. representation $Y = [y_1, \cdots, y_n] \in \mathbb{R}^{d\times n}$ of X

➤ Achieved by a mapping $\Phi : x \in \mathbb{R}^m \longrightarrow y \in \mathbb{R}^d$ so:

$$\phi(x_i) = y_i, \quad i = 1, \cdots, n$$





➤ Φ may be linear : $y_j = W^\top x_j, \forall j$, or, $Y = W^\top X$

➤ ... or nonlinear (implicit).

➤ Mapping Φ required to: Preserve proximity? Maximize variance? Preserve a certain graph?

Basics: Principal Component Analysis (PCA)

PCA: Compute W to maximize variance of projected data:

$$\max_{W\in\mathbb{R}^{m\times d}; W^\top W = I} \sum_{i=1}^{n} \left\| y_i - \frac{1}{n}\sum_{j=1}^{n} y_j \right\|_2^2, \quad y_i = W^\top x_i.$$

➤ Leads to maximizing

$$\text{Tr}\left[W^\top (X - \mu e^\top)(X - \mu e^\top)^\top W\right], \quad \mu = \tfrac{1}{n}\Sigma_{i=1}^n x_i$$

➤ Solution W = { dominant eigenvectors } of the covariance matrix ≡ Set of left singular vectors of $\bar{X} = X - \mu e^\top$

SVD:

$$\bar{X} = U\Sigma V^\top, \quad U^\top U = I, \quad V^\top V = I, \quad \Sigma = \text{Diag}$$

- Optimal $W = U_d \equiv$ matrix of first d columns of U
- Solution W also minimizes 'reconstruction error' ..

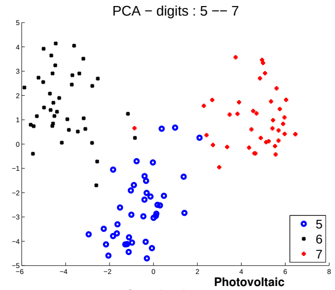
$$\sum_i \|x_i - WW^T x_i\|^2 = \sum_i \|x_i - W y_i\|^2$$

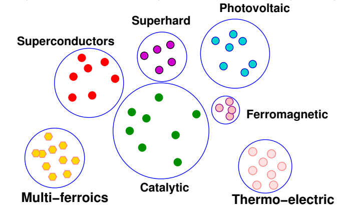
- In some methods recentering to zero is not done, i.e., $\bar{X}$ replaced by X.

Unsupervised learning

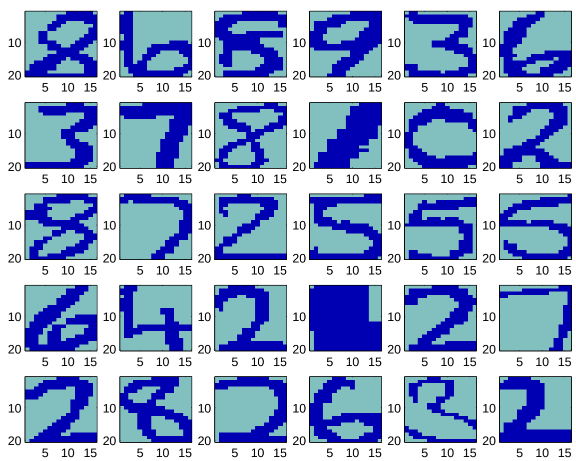
"Unsupervised learning" : methods do not exploit labeled data

- Example of digits: perform a 2-D projection
- Images of same digit tend to cluster (more or less)
- Such 2-D representations are popular for visualization
- Can also try to find natural clusters in data, e.g., in materials
- Basic clusterning technique: K-means

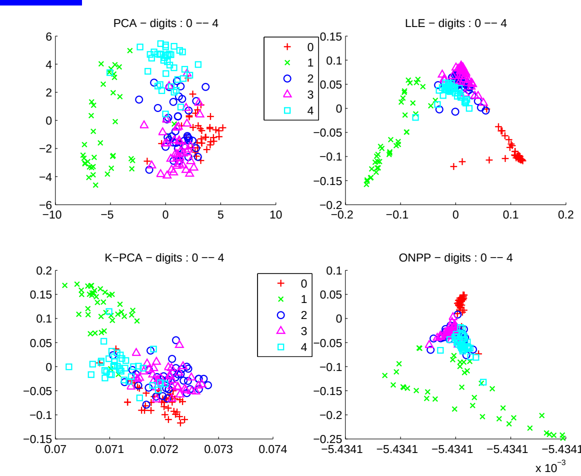




Example: Digit images (a random sample of 30)



2-D 'reductions':

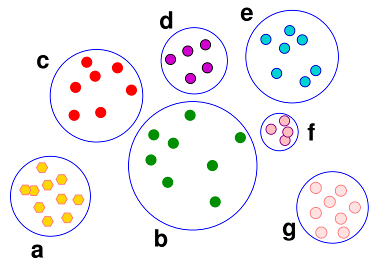


SUPERVISED LEARNING

Supervised learning

- We now have data that is 'labeled'

Examples: Health Sciences ('malignant'- 'non malignant') ; Materials ('photovoltaic', 'hard', 'conductor', ...) ; Digit Recognition ('0', '1', ..., '9')



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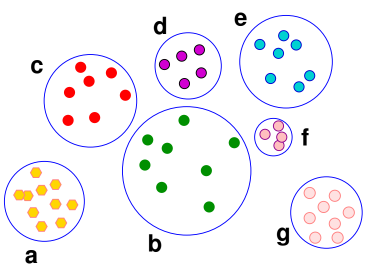
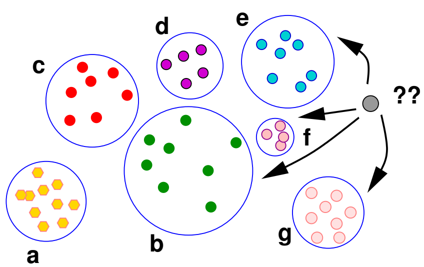
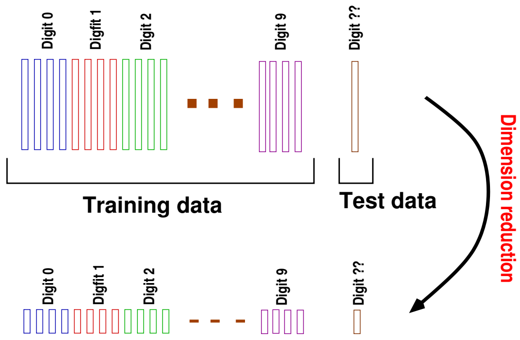




Supervised learning: classification

- Best illustration: written digits recognition example

Given: set of labeled samples (training set), and an (unlabeled) test image x.
Problem: label of x =?



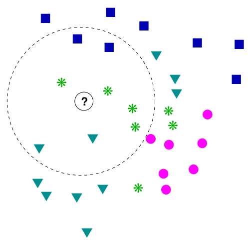
- Roughly speaking: we seek dimension reduction so that recognition is 'more effective' in low-dim. space

Basic method: K-nearest neighbors (KNN) classification

➤ Idea of a voting system: get distances between test sample and training samples

➤ Get the k nearest neighbors (here $k = 8$)

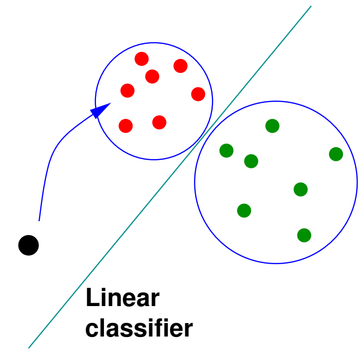
➤ Predominant class among these k items is assigned to the test sample ("$*$" here)



Supervised learning: Linear classification

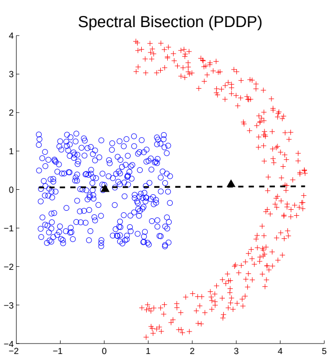
Linear classifiers: Find a hyperplane which best separates the data in classes A and B.

➤ Example of application: Distinguish between SPAM and non-SPAM e-mails

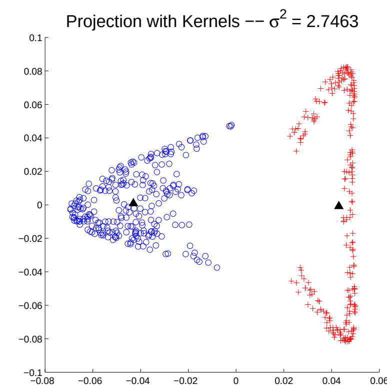


➤ Note: The world in non-linear. Often this is combined with Kernels – amounts to changing the inner product

A harder case:



➤ Use kernels to transform

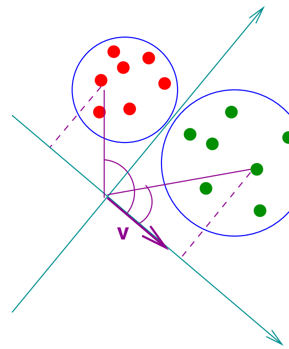


Transformed data with a Gaussian Kernel

Simple linear classifiers

- Let $X = [x_1, \cdots, x_n]$ be the data matrix.
- and $L = [l_1, \cdots, l_n]$== labels. $l_i = \pm 1$
- 1st Solution: Find a vector u such that $u^T x_i$ close to l_i, $\forall i$
- Common solution: SVD to reduce dimension of data [e.g. 2-D] then do comparison in this space. e.g.

A: $u^T x_i \geq 0$, B: $u^T x_i < 0$



[For clarity: principal axis u drawn below where it should be]

Fisher's Linear Discriminant Analysis (LDA)

Principle: Use label information to build a good projector, i.e., one that can 'discriminate' well between classes

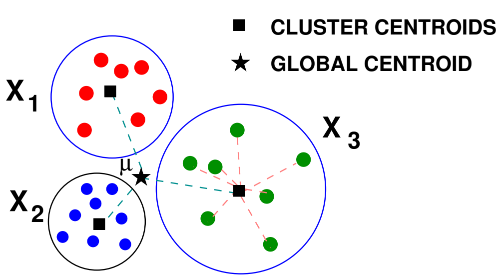
- Define "between scatter": a measure of how well separated two distinct classes are.
- Define "within scatter": a measure of how well clustered items of the same class are.
- Objective: make "between scatter" measure large and "within scatter" small.

Idea: Find projector that maximizes the ratio of the "between scatter" measure over "within scatter" measure

$$S_B = \sum_{k=1}^{c} n_k (\mu^{(k)} - \mu)(\mu^{(k)} - \mu)^T,$$
$$S_W = \sum_{k=1}^{c} \sum_{x_i \in X_k} (x_i - \mu^{(k)})(x_i - \mu^{(k)})^T$$

where:

- $\mu =$ mean (X)
- $\mu^{(k)}$ = mean (X_k)
- $X_k = k$-th class
- $n_k = |X_k|$



- Consider 2nd moments for a vector a:

$$a^T S_B a = \sum_{i=1}^{c} n_k \, |a^T (\mu^{(k)} - \mu)|^2,$$
$$a^T S_W a = \sum_{k=1}^{c} \sum_{x_i \in X_k} |a^T (x_i - \mu^{(k)})|^2$$

- $a^T S_B a \equiv$ weighted variance of projected μ_j's
- $a^T S_W a \equiv$ w. sum of variances of projected classes X_j's
- LDA projects the data so as to maximize the ratio of these two numbers:

$$\boxed{\max_a \frac{a^T S_B a}{a^T S_W a}}$$

- Optimal a = eigenvector associated with top eigenvalue of:

$$S_B u_i = \lambda_i S_W u_i \, .$$

LDA – Extension to arbitrary dimensions

- Criterion: maximize the ratio of two traces: $\frac{\text{Tr }[U^T S_B U]}{\text{Tr }[U^T S_W U]}$
- Constraint: $U^T U = I$ (orthogonal projector).
- Reduced dimension data: $Y = U^T X$.

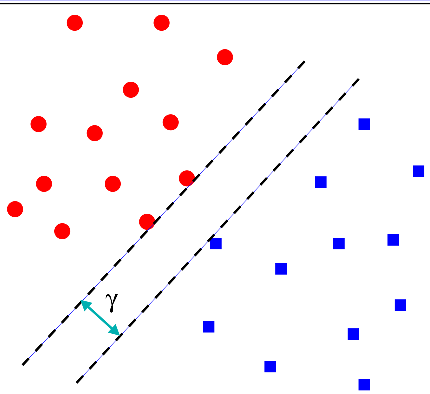
Common viewpoint: hard to maximize, therefore ...

- ... alternative: Solve instead the ('easier') problem: $\max_{U^T S_W U = I} \text{Tr }[U^T S_B U]$
- Solution: largest eigenvectors of $S_B u_i = \lambda_i S_W u_i$.

In Brief: Support Vector Machines (SVM)

- Similar in spirit to LDA. Formally, SVM finds a hyperplane that best separates two training sets belonging to two classes.
- If the hyperplane is: $\boxed{w^T x + b = 0}$
- Then the classifier is $f(x) = sign(w^T x + b)$: assigns $y = +1$ to one class and $y = -1$ to other
- Normalize parameters w, b by looking for hyperplanes of the form $w^T x + b \geq 1$ to include one set and $w^T x + b \leq -1$ to include the other.
- With $y_i = +1$ for one class and $y_i = -1$ for the other, we can write the constraints as $y_i(w^T x_i + b) \geq 1$.

- The margin is the maximum distance between two such planes: goal find w, b to maximize margin.
- Maximize margin subject to the constraint $y_i(w^T x_i + b) \geq 1$.



- As it turns out the margin is equal to: $\gamma = \frac{2}{\|w\|_2}$

✍1 Prove it.

- Need to solve the constrained quadratic programming problem:

$$\boxed{\begin{array}{ll} \min_{w.b} & \frac{1}{2}\|w\|_2^2 \\ \text{s.t.} & y_i(w^T x_i + b) \geq 1, \ \forall x_i. \end{array}}$$

Modification 1: Soft margin. Consider hinge loss: $\max\{0, 1 - y_i[w^T x_i + b]\}$

- Zero if constraint satisfied for pair x_i, y_i. Otherwise proportional to distance from corresponding hyperplane. Hence we can minimize

$$\lambda\|w\|^2 + \frac{1}{n}\sum_{i=1}^{n} \max\{0, 1 - y_i[w^T x_i + b]\}$$

✍2 Suppose $y_i = +1$ and let $d_i = 1 - y_i[w^T x_i + b]$. Show that the distance between x_i and hyperplane $\boxed{w^T x_i + b = +1}$ is $d_i/\|w\|$.

Modification 2 : Use in combination with a Kernel to improve separability

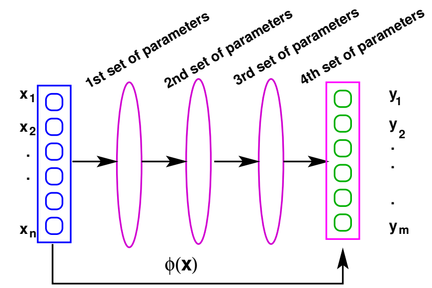
A few words on Deep Neural Networks (DNNs)

➤ Ideas of neural networks goes back to the 1960s - were popularized in early 1990s – then laid dormant until recently.

➤ Two reasons for the come-back:

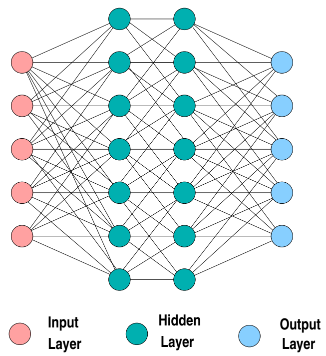
- DNN are remarkably effective in some applications
- big progress made in hardware [→ affordable 'training cost']

➤ Training a neural network can be viewed as a problem of approximating a function ϕ which is defined via sets of parameters:



Problem: find sets of parameters such that $\phi(x) \approx y$

Input: x, **Output:** y
Set: $z_0 = x$
For $l = 1 :$ L+1 **Do:**
$z_l = \sigma(W_l^T z_{l-1} + b_l)$
End
Set: $y = \phi(x) := z_{L+1}$



- layer # 0 = input layer
- layer # $(L + 1)$ = output layer

➤ A matrix W_l is associated with layers 1,2, $L + 1$.

➤ Problem: Find ϕ (i.e., matrices W_l) s.t. $\phi(x) \approx y$

DNN (continued)

➤ Problem is not convex, highly parameterized, ...,

➤ .. Main method used: Stochastic gradient descent [basic]

➤ It all looks like alchemy... but it works well for certain applications

➤ Training is still quite expensive – GPUs can help

➤ *Very* active area of research