# *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*

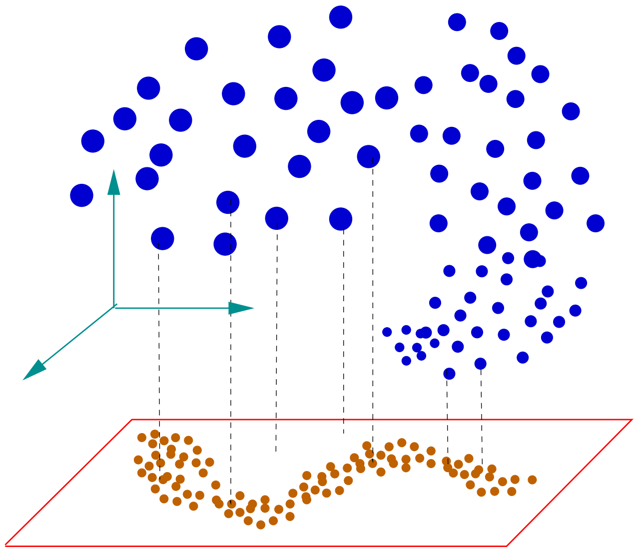
➤ Goal is not as much to reduce size (& cost) but to:

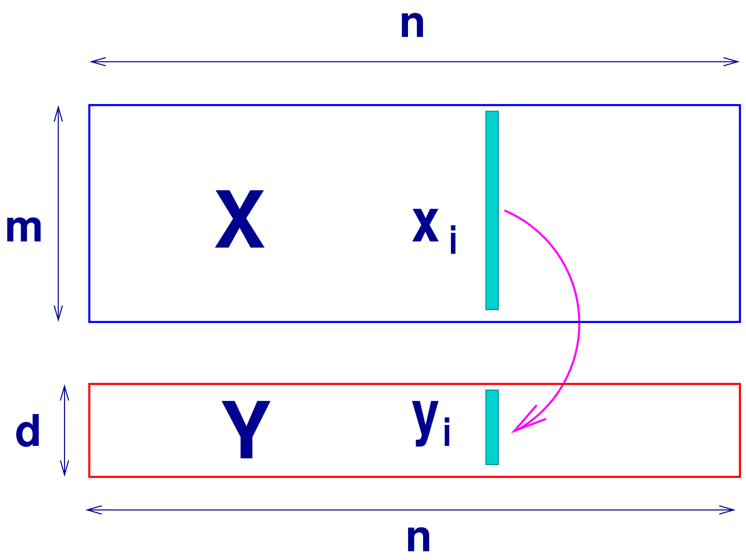
- Reduce noise and redundancy in data before performing a task [e.g., classification as in digit/face recognition]
- Discover important 'features' or 'paramaters'

**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:

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






- $\Phi$ may be linear : $y_j = W^\top x_j, \ \forall j$, or, $Y = W^\top X$
- ... or nonlinear (implicit).
- Mapping $\Phi$ required to: Preserve proximity? Maximize variance? Preserve a certain graph?

## *Basics: Principal Component Analysis (PCA)*

PCA: Compute $W$ to maximize variance of projected data:

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

- Leads to maximizing

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

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

## SVD:

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

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

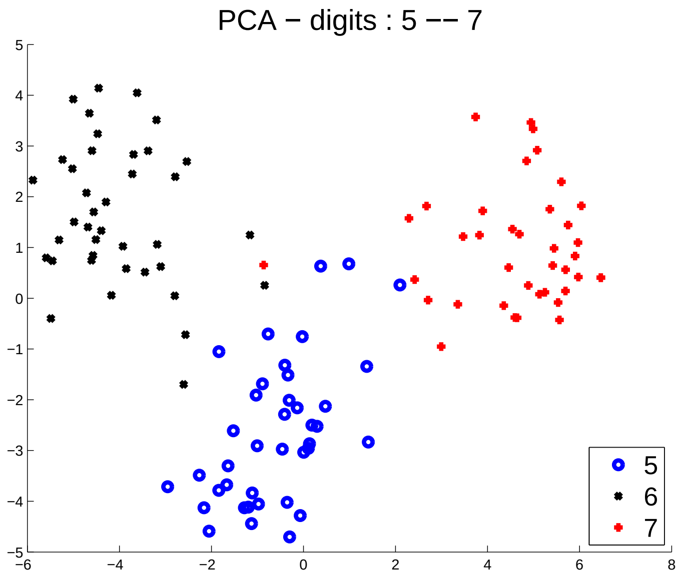
$$\sum_i \|\boldsymbol{x}_i - \boldsymbol{W}\boldsymbol{W}^T\boldsymbol{x}_i\|^2 = \sum_i \|\boldsymbol{x}_i - \boldsymbol{W}\boldsymbol{y}_i\|^2$$

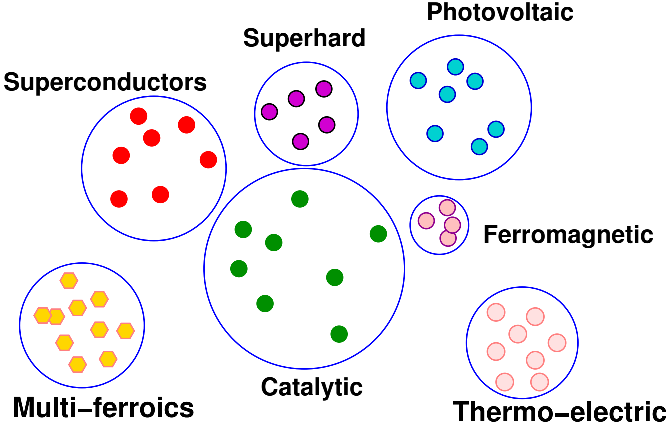
- In some methods recentering to zero is not done, i.e., $\bar{\boldsymbol{X}}$ replaced by $\boldsymbol{X}$.

# Unsupervised learning

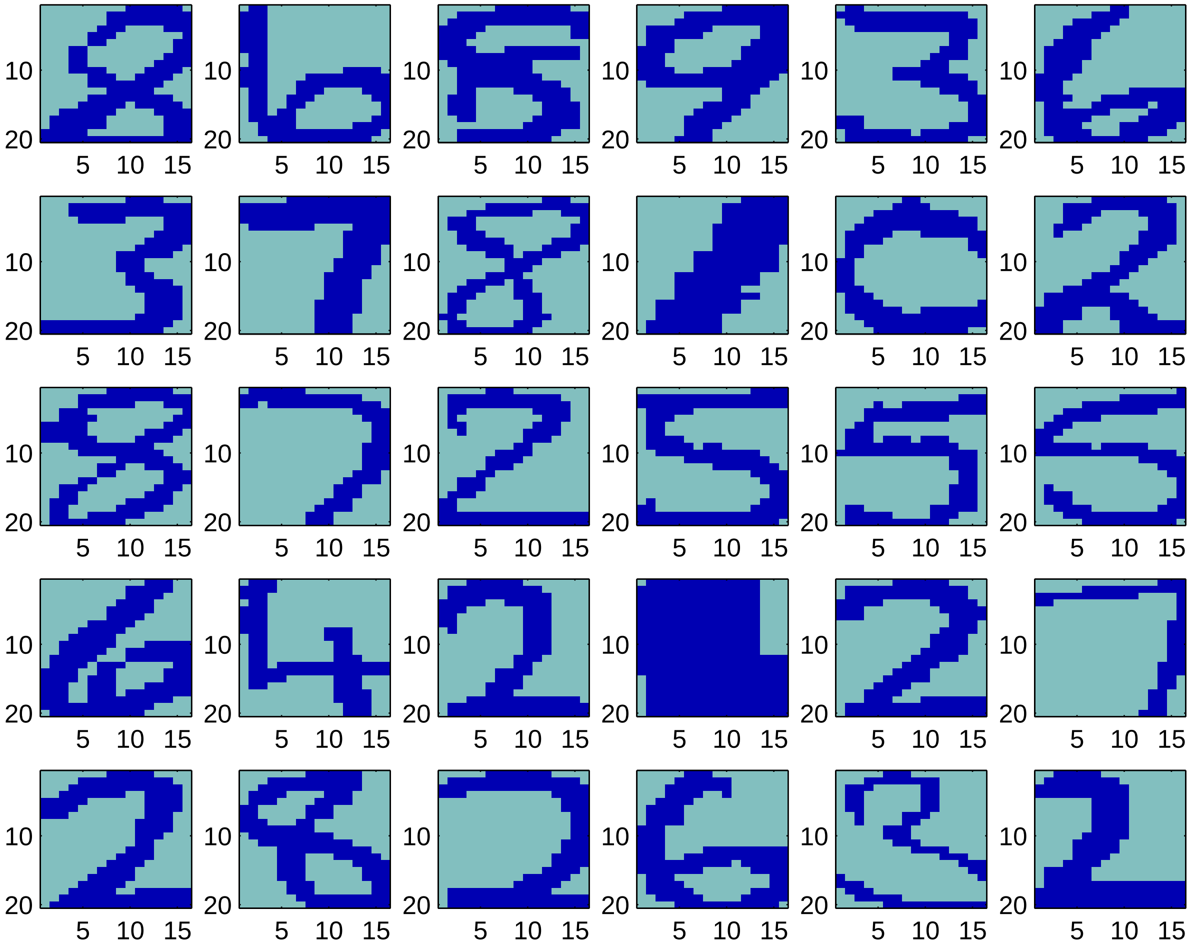
*"Unsupervised learning"* : methods do not exploit labeled data

- 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 clustering technique: K-means

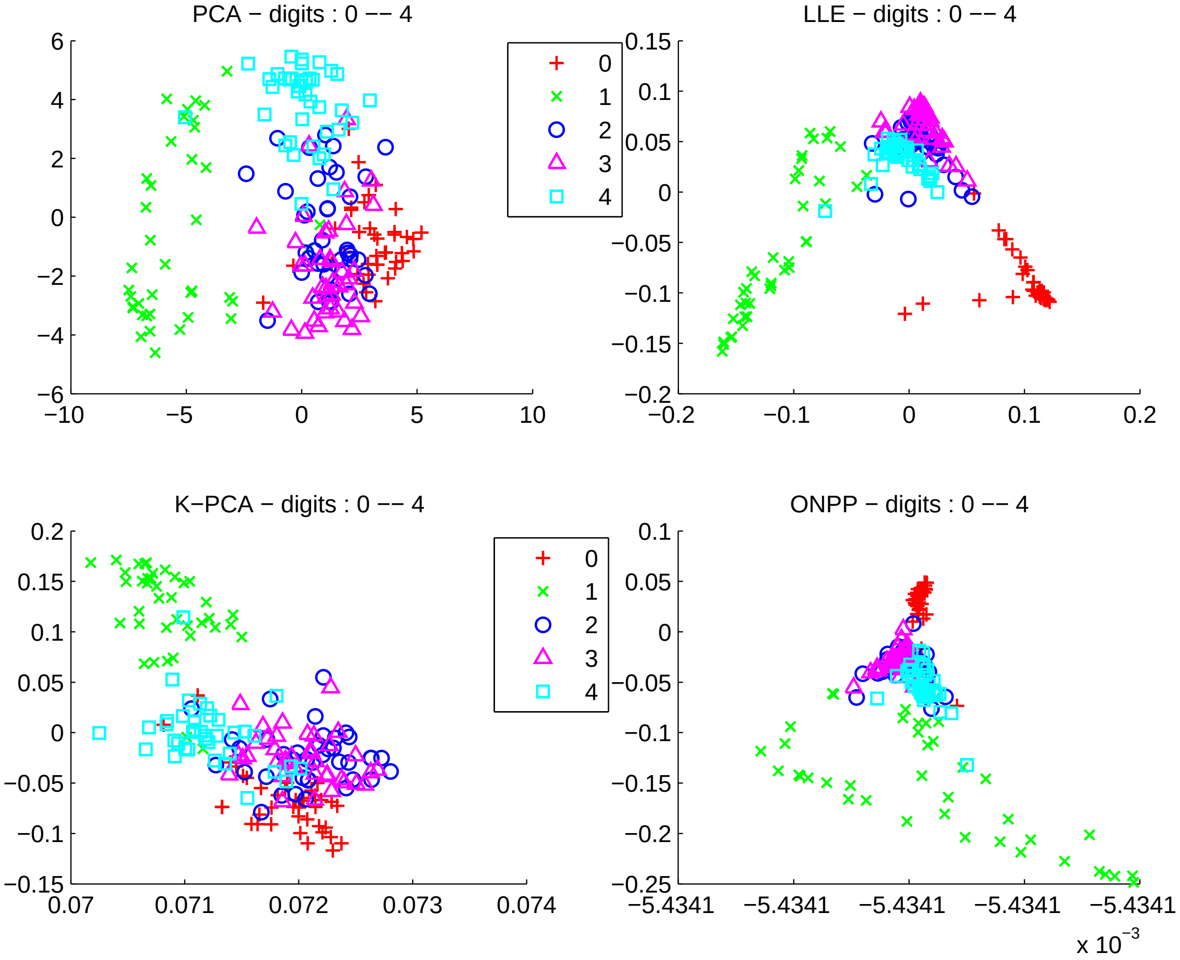


# *Example: Digit images (a random sample of 30)*



# 2-D 'reductions':

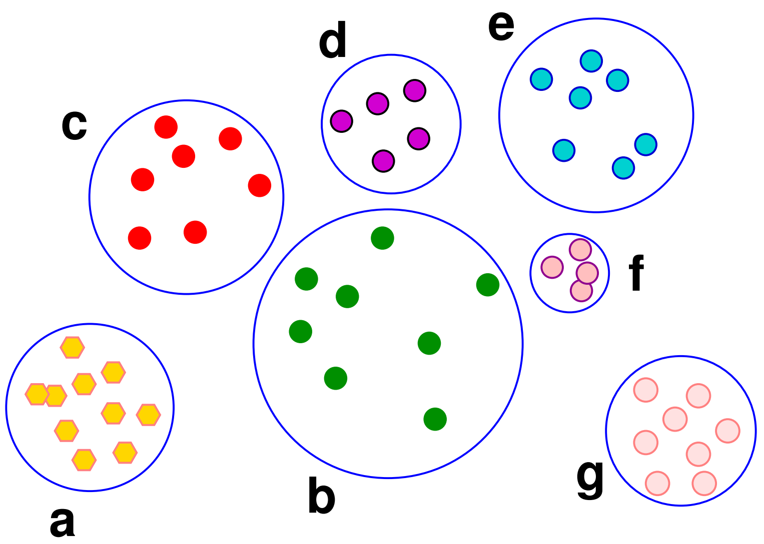


# SUPERVISED LEARNING

# *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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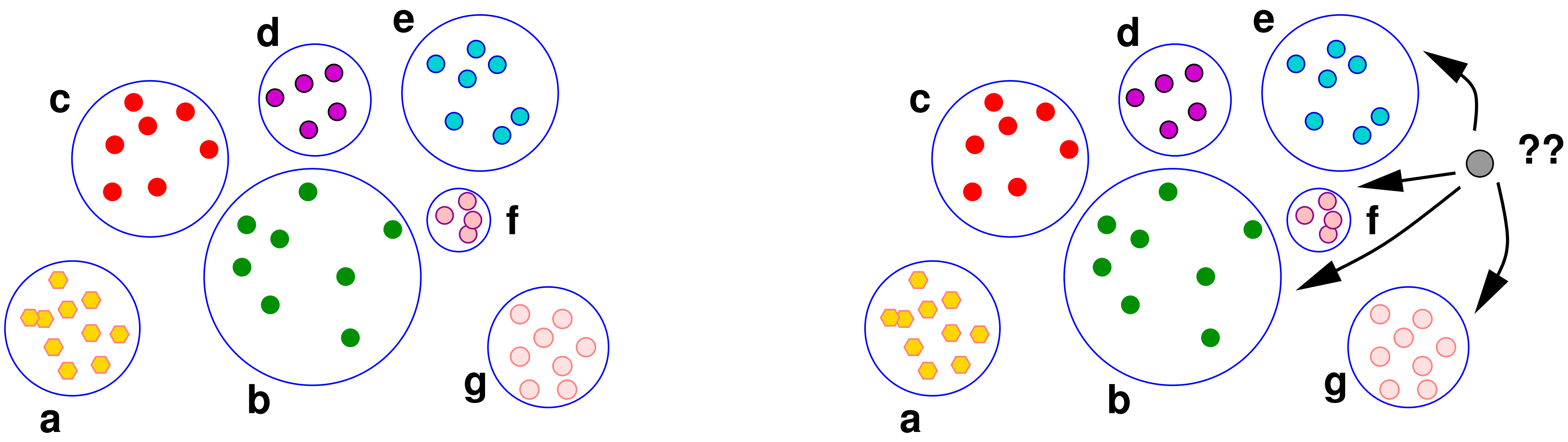
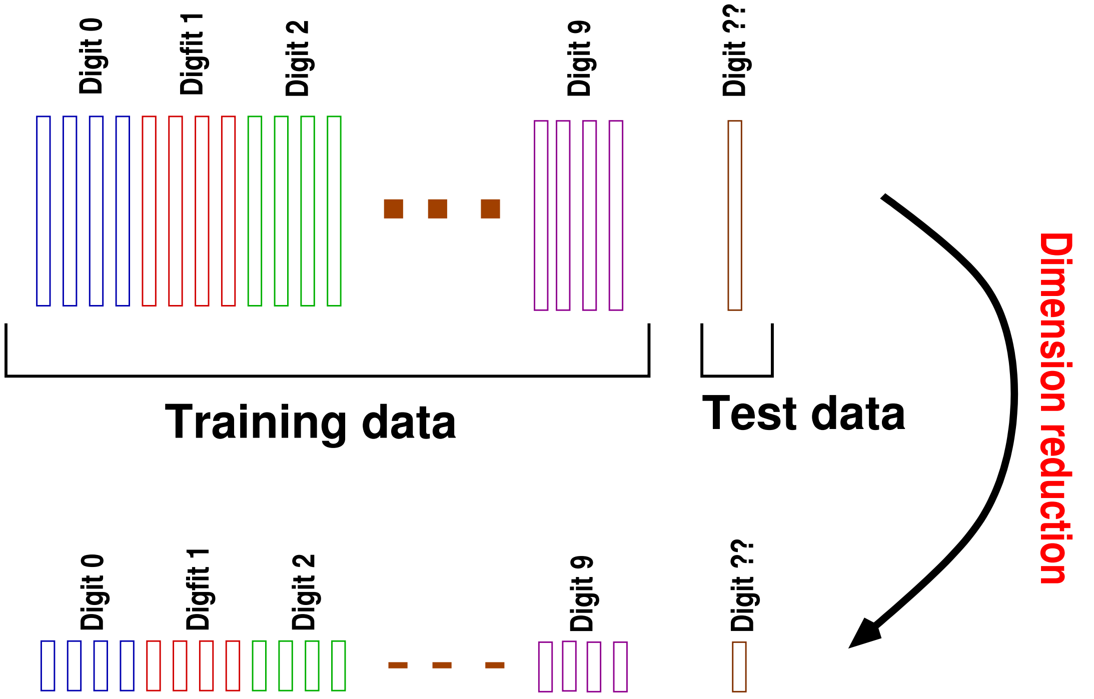


# *Supervised learning: classification*

➤ Best illustration: written digits recognition example

**Given:** set of labeled samples (training set), and an (unlabeled) test image $x$.

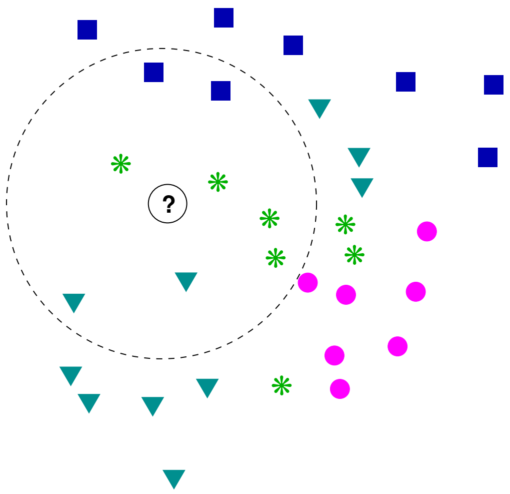
**Problem:** label of $x$ =?




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

# *Basic method: K-nearest neighbors (KNN) classification*

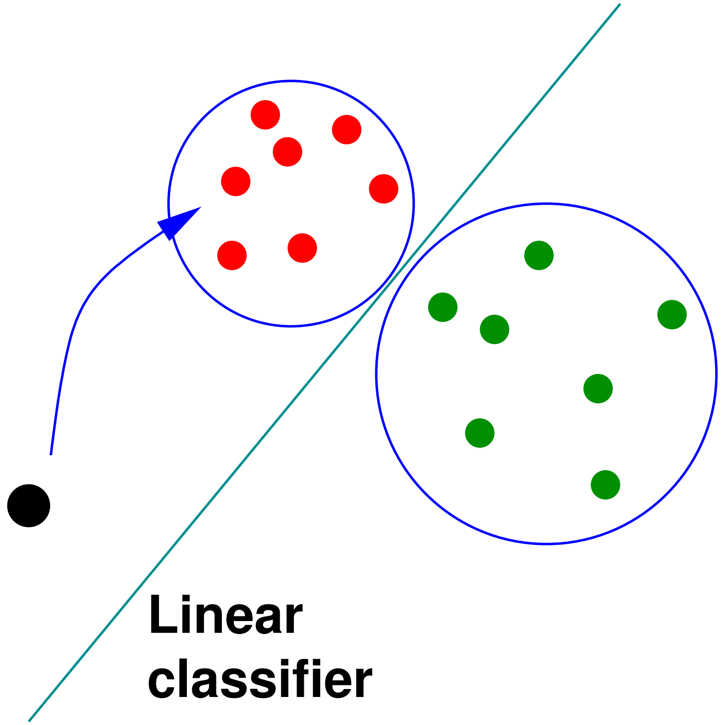
- Idea of a voting system: get distances between test sample and training samples
- Get the $k$ nearest neighbors (here $k = 8$)
- Predominant class among these $k$ items is assigned to the test sample ("$*$" here)



# *Supervised learning: Linear classification*

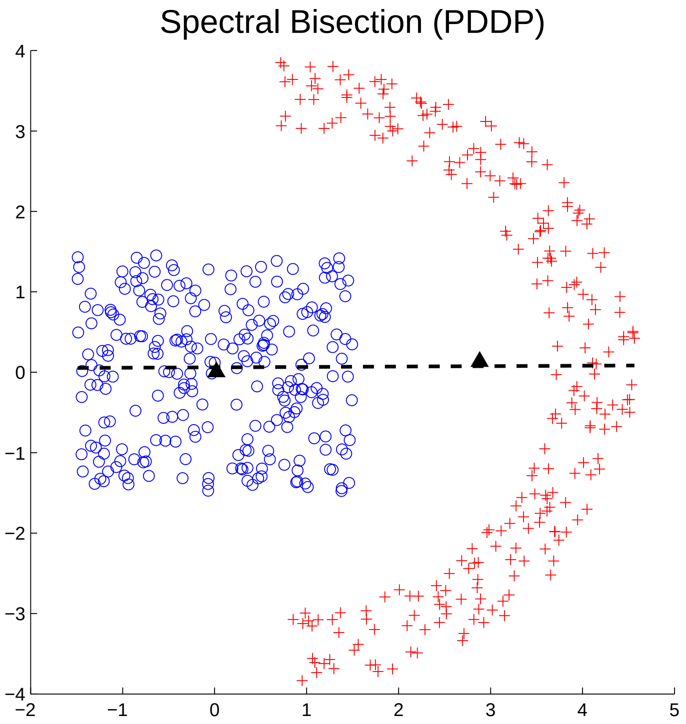
*Linear classifiers:* Find a hyperplane which best separates the data in classes A and B.

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

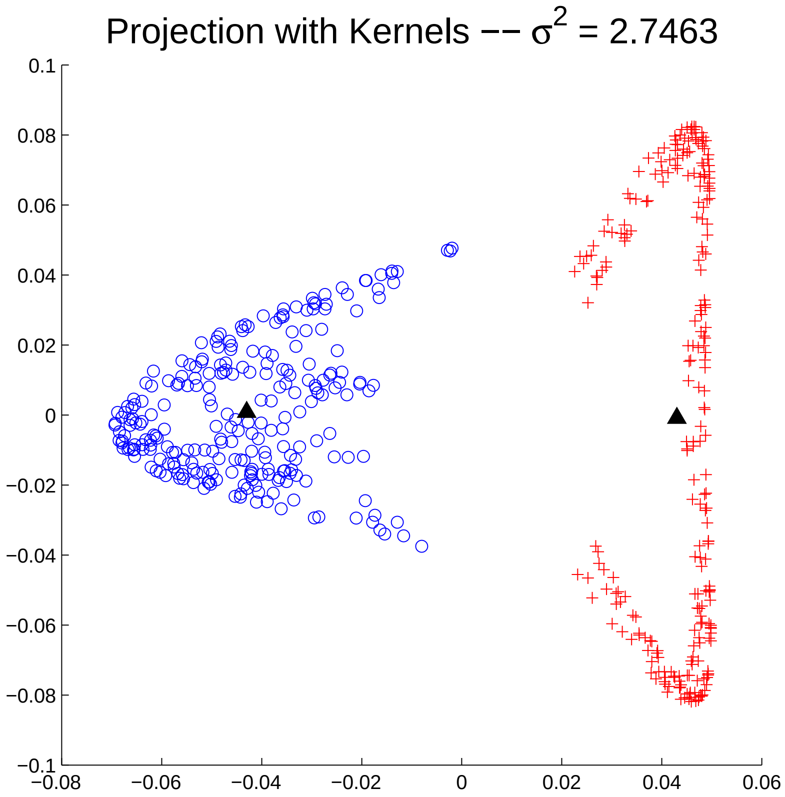



➤ Note: The world in non-linear. Often this is combined with Kernels – amounts to changing the inner product

# A harder case:




➤ Use kernels to transform

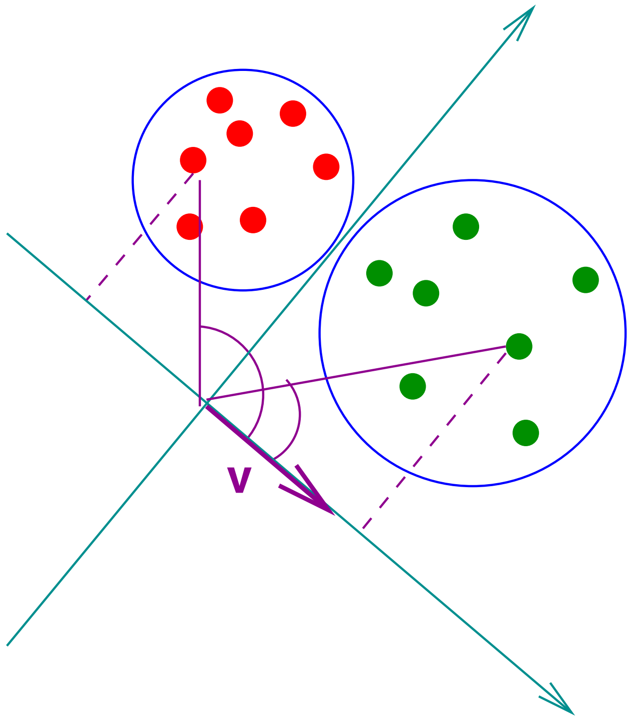



# Transformed data with a Gaussian Kernel

# *Simple linear classifiers*

- Let $\boldsymbol{X} = [\boldsymbol{x}_1, \cdots, \boldsymbol{x}_n]$ be the data matrix.
- and $\boldsymbol{L} = [\boldsymbol{l}_1, \cdots, \boldsymbol{l}_n]$== labels. $\boldsymbol{l}_i = \pm 1$
- 1st Solution: Find a vector $\boldsymbol{u}$ such that $\boldsymbol{u}^T \boldsymbol{x}_i$ close to $\boldsymbol{l}_i$, $\forall \boldsymbol{i}$
- Common solution: SVD to reduce dimension of data [e.g. 2-D] then do comparison in this space. e.g.

A: $\boldsymbol{u}^T \boldsymbol{x}_i \geq 0$ , B: $\boldsymbol{u}^T \boldsymbol{x}_i < 0$




[For clarity: principal axis $\boldsymbol{u}$ 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.

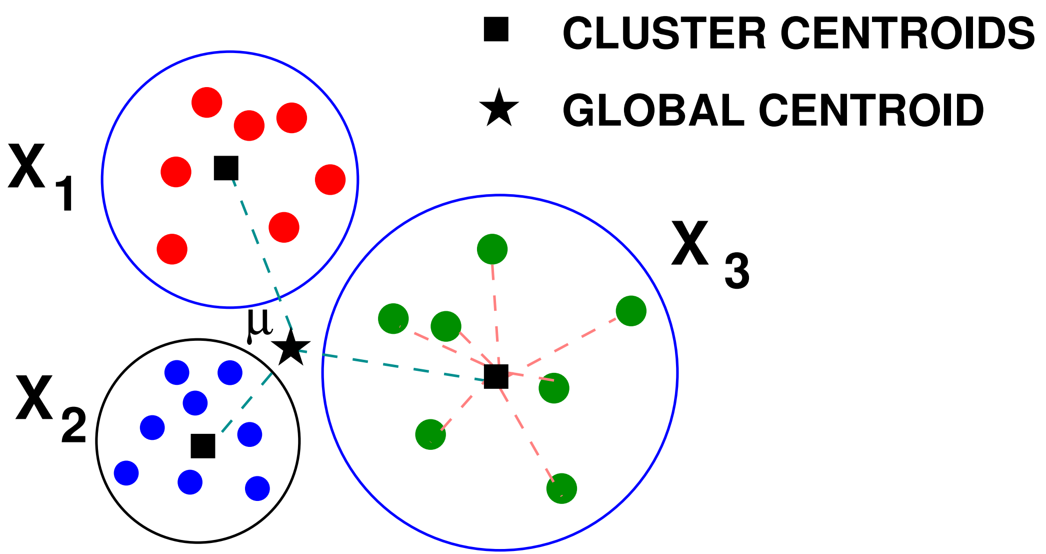
*Idea:* Find projector that maximizes the ratio of the "between scatter" measure over "within scatter" measure

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

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

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 $\mu_j$'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: $\dfrac{\text{Tr}\,[U^T S_B U]}{\text{Tr}\,[U^T S_W U]}$

➤ 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.

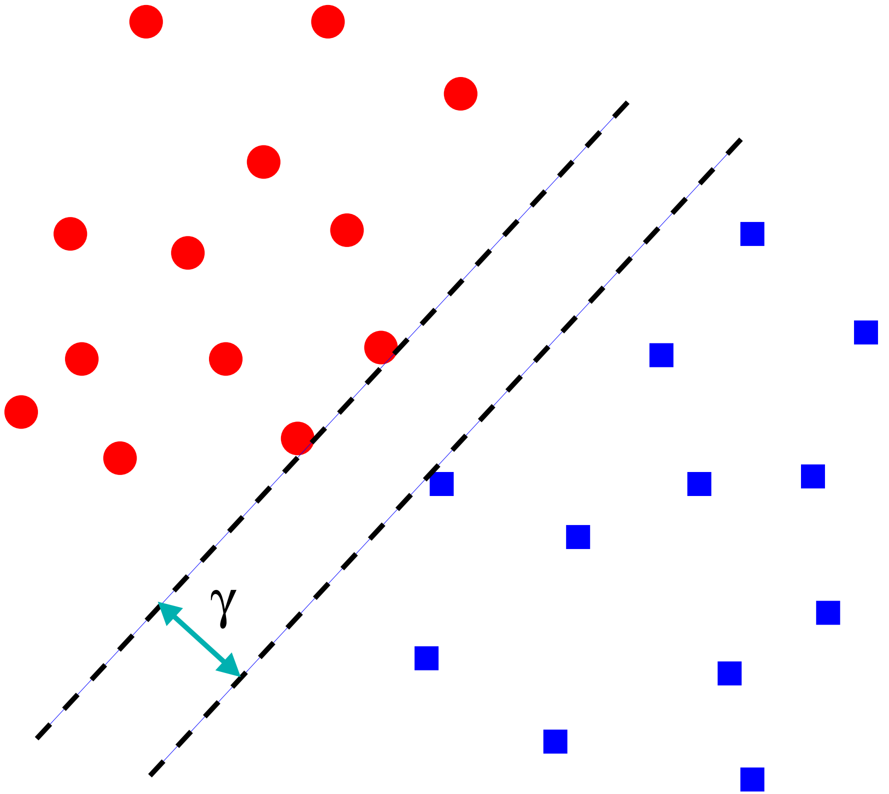
- If the hyperplane is: $\boxed{w^Tx + b = 0}$

- Then the classifier is $f(x) = \text{sign}(w^Tx + b)$: assigns $y = +1$ to one class and $y = -1$ to other

- Normalize parameters $w, b$ by looking for hyperplanes of the form $w^Tx + b \geq 1$ to include one set and $w^Tx + b \leq -1$ to include the other.

- With $y_i = +1$ for one class and $y_i = -1$ for the other, we can write the constraints as $y_i(w^Tx_i + b) \geq 1$.

➤ 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:

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

*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

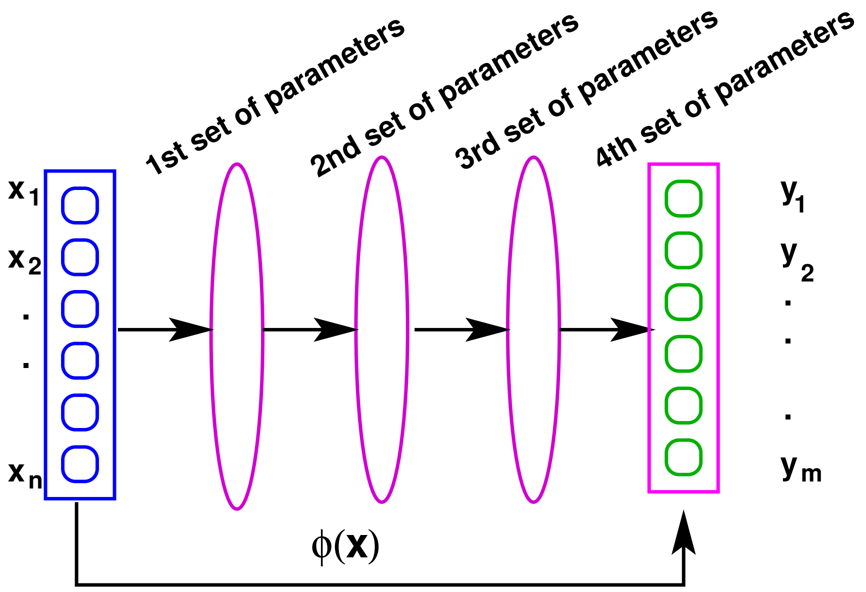
# A few words on Deep Neural Networks (DNNs)

➤ 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 [$\rightarrow$ affordable 'training cost']

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




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

**Input:** $x$, **Output:** $y$

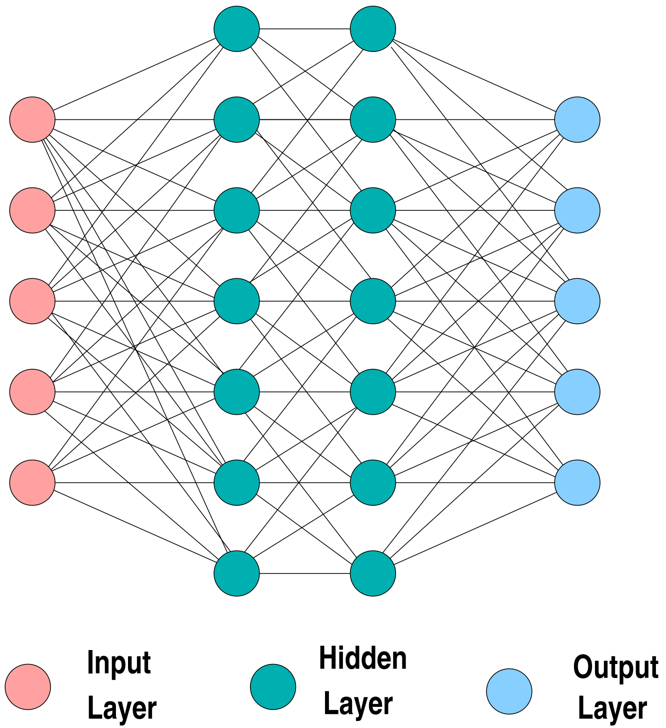
**Set:** $z_0 = x$

**For** $l = 1 : \texttt{L+1}$ **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 $\phi$ (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