# 10707
# Deep Learning: Spring 2020

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## Lecture 7:
Intro to unsupervised learning

# Unsupervised learning

Learning from data **without** labels.

What can we hope to do:

**Task A**: Fit a parametrized **structure** (e.g. clustering, low-dimensional subspace, manifold) to data to reveal something meaningful about data. (**Structure learning**)

**Task B:** Learn a (parametrized) **distribution** *close* to data generating distribution. (**Distribution learning**)

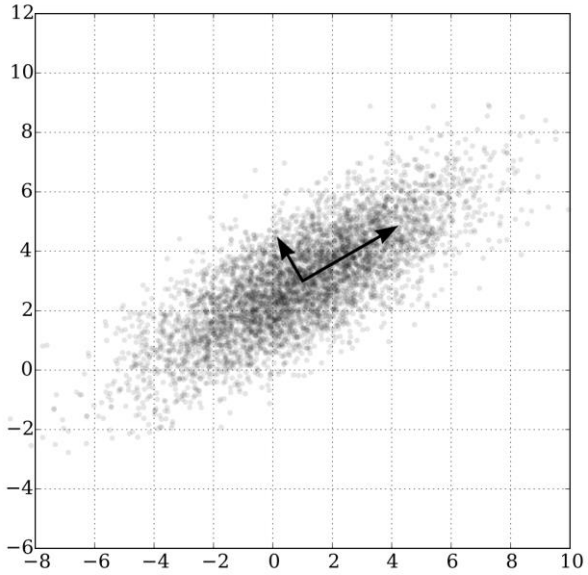
**Task C:** Learn a (parametrized) distribution that implicitly reveals an **"embedding"/"representation"** of data for downstream tasks. (**Representation/feature learning**)

*Entangled*! The "structure" and "distribution" often reveals an embedding.

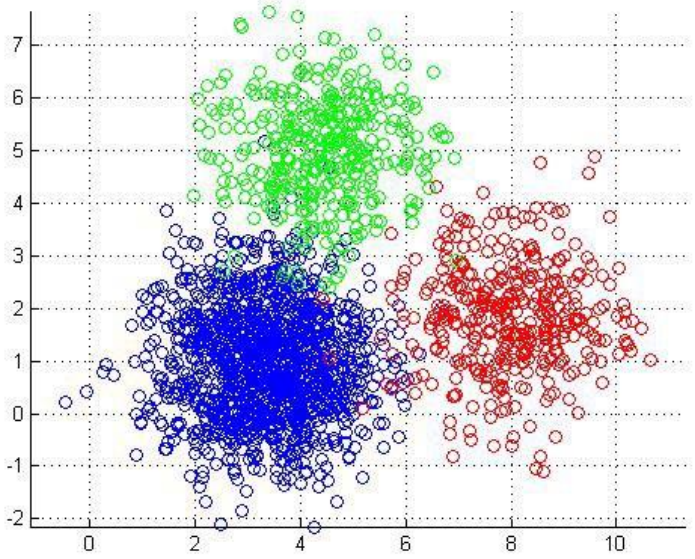
# Structure learning

Fit a parametrized **structure** (e.g. clustering, low-dimensional subspace) to data to reveal something meaningful about data.

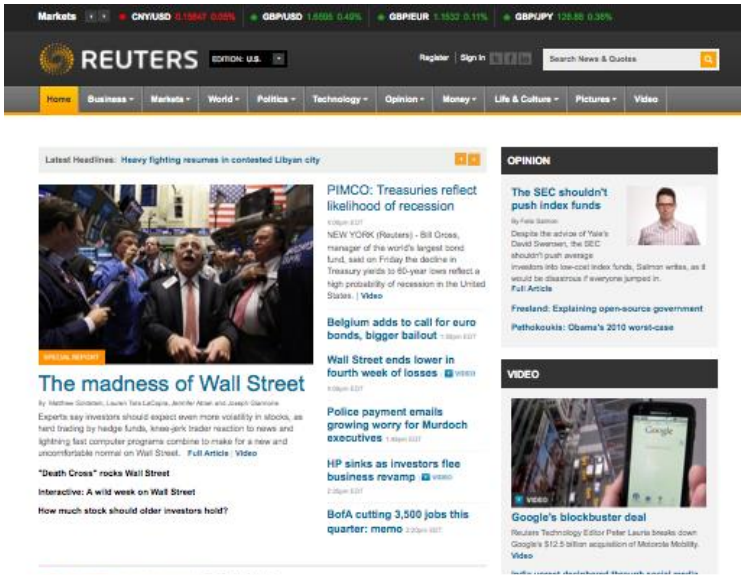
**PCA**(principal component analysis), direction of highest variance



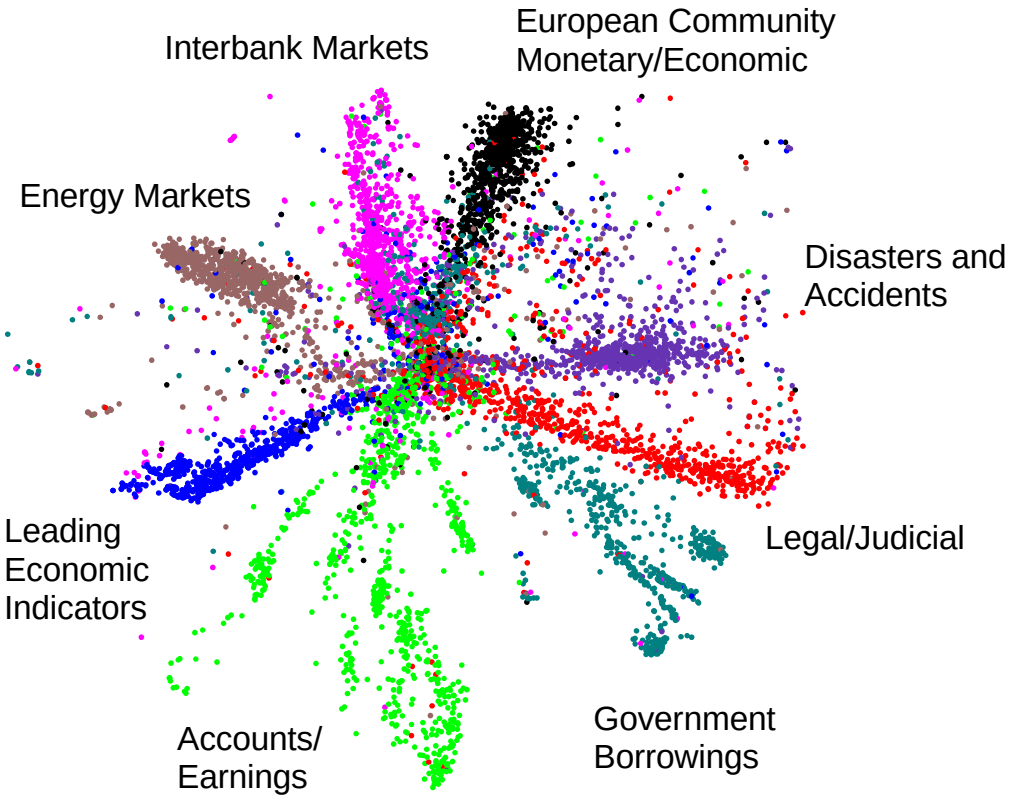

**Clustering**



# Structure learning



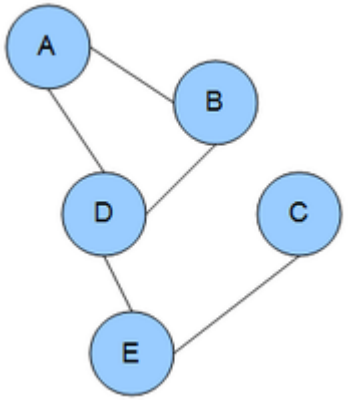

804,414 newswire stories



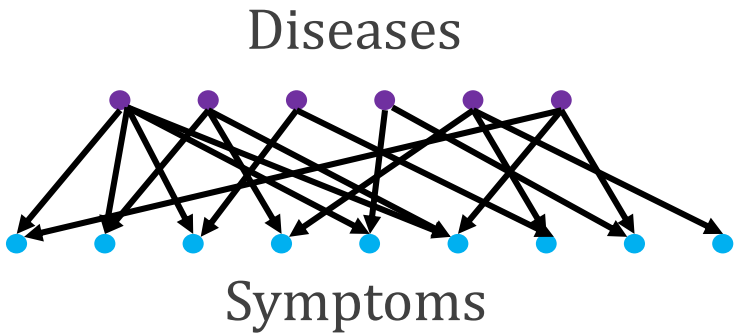
# Distribution learning

Some typical choices of parametrized distributions:

**Classical choices**: fully-observed graphical models (undirected and directed), latent-variable graphical models (mixture models, sparse coding, topic models).




**Markov Random Fields**: sparse independence structure: "A is independent of other vars, given B, D"

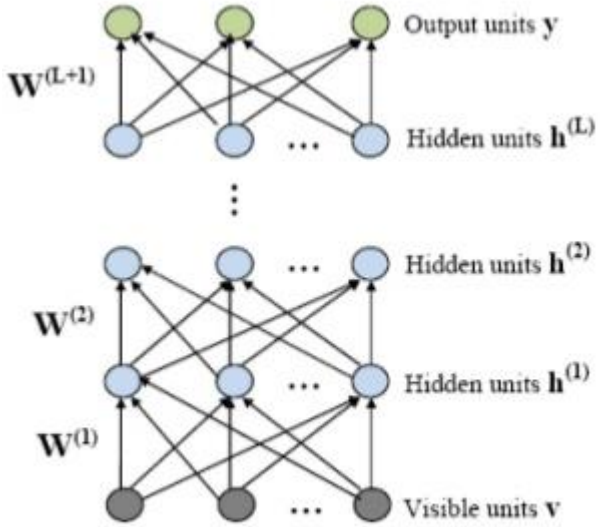



**Latent variable models**: data is "simple" conditioned on some unobserved (latent) variables

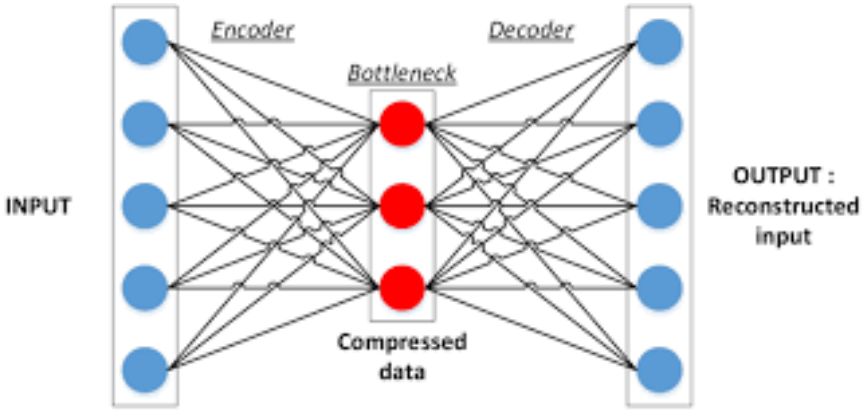
# Distribution learning

Some typical choices of parametrized distributions:

**Semi-modern choices**: deep Boltzmann machines, deep belief networks, (variational) auto-encoders, energy models.




**Deep Boltzmann machines, belief networks**: graphical model analogues of deep neural networks.

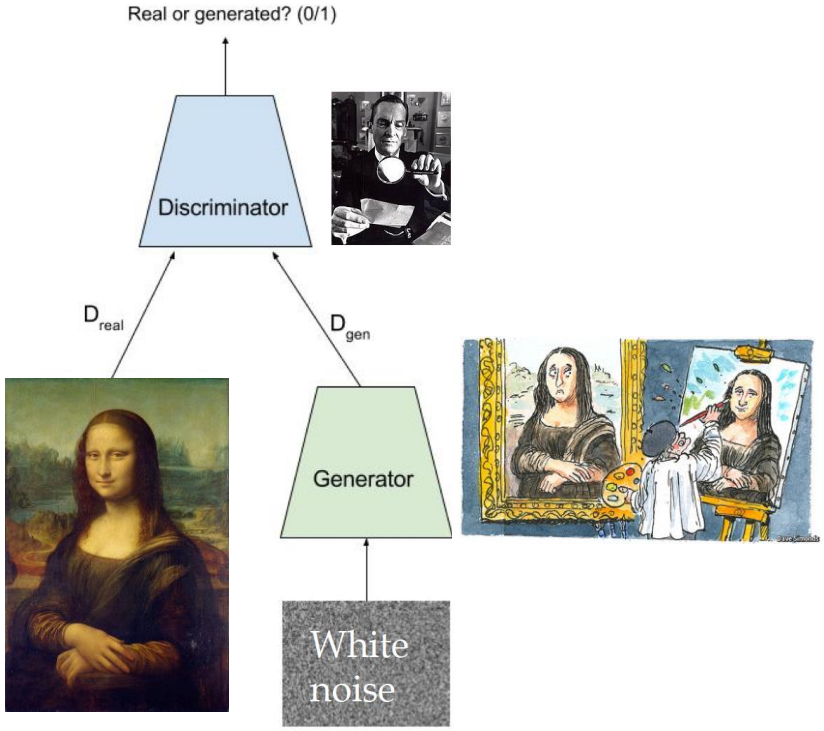


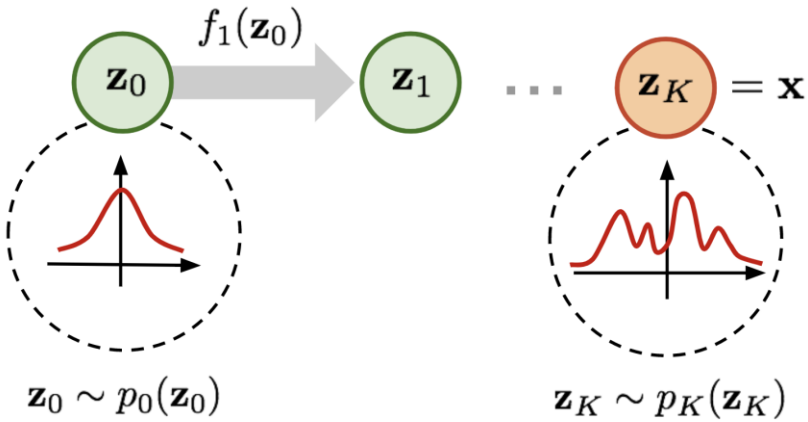

**(Variational) autoencoders**: model data by enforcing a latent space "bottleneck:

# Distribution learning

Some typical choices of parametrized distributions:

**Modern choices**: generative adversarial networks, autoregressive models (pixelRNN, pixelCNN), flow models, etc.



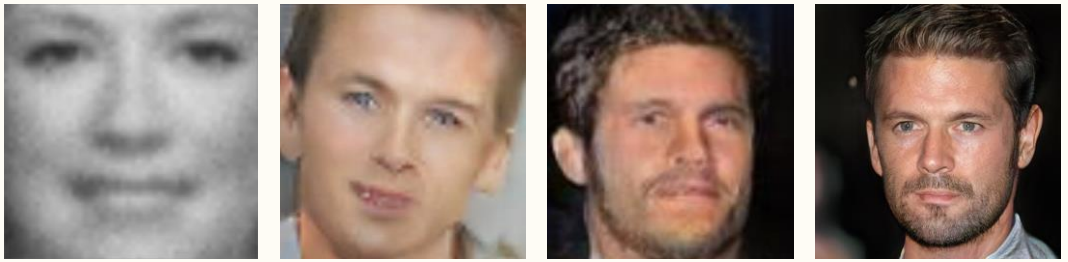



# Distribution learning

Training Data(CelebA)

Model Samples (Karras et.al., 2018)

4 years of progression on Faces




Brundage et al., 2017

# Distribution learning

Conditional generative model P(zebra images| horse images)

Style Transfer

Input Image

Monet

Van Gogh

Zhou el al., Cycle GAN 2017

# Distribution learning

Source actor


Target actor

Real-time reenactment

[Face2Face, Thies et al, CVPR 2016]

# Representation learning and self-supervised learning

Given unlabeled data, design supervised tasks that induce a good representation for downstream tasks.

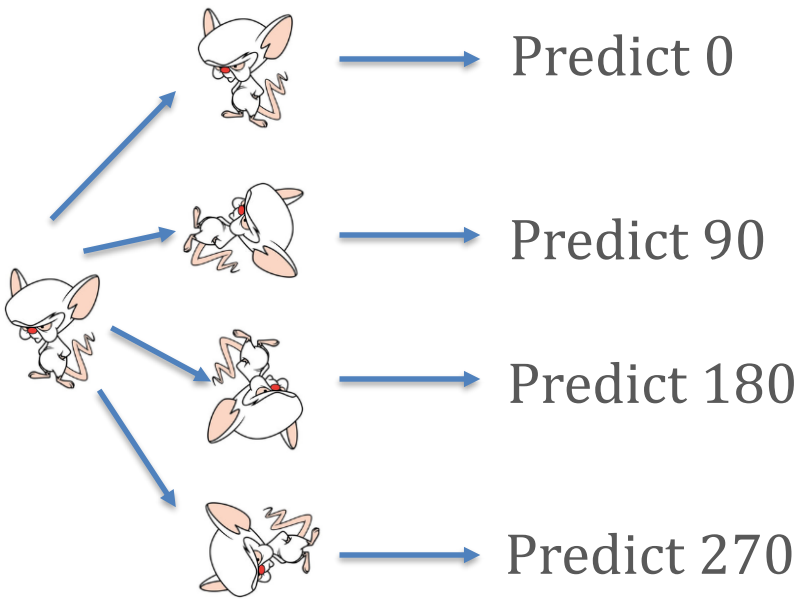
No good mathematical formalization, but the intuition is to "force" the predictor used in the task to learn something "semantically meaningful" about the data.

**Examples in NLP**: predict next word, given previous 5 words; predict middle word, given surrounding 5 words; etc.

# Representation learning and self-supervised learning

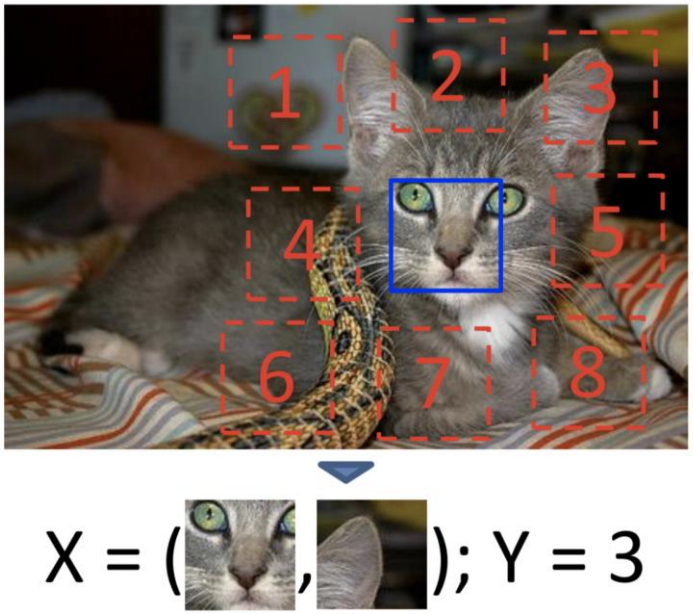
**Examples in vision**: a lot, and quite different in nature.

**Rotation prediction**




Predict one of four angles an image is rotated by

**Jigsaw puzzles**




Predict position of second piece wrt to first

# Desiderata for a good representation

**Semantically meaningful**: if we train a linear classifier on top of these features, should work well for (many, most?) reasonable tasks.

**"Disentangled"**: in generative setting, can "vary" features independently, and generate an output that is reasonable.

(Contraversial and not well understood: are the features disentangled in priors, posteriors? Models can be reparametrized to produce arbitrarily bad entangling:
*Locatello et al*, *Best paper award at ICML'19*)

**Improve sample complexity**: if we wish to use feature to train a supervised model on top of, good representation could save us on sample complexity.
(See e.g. Arora-Risteski https://arxiv.org/pdf/1706.04601.pdf)

# Relationships between the tasks

**Structure learning and feature learning often blend**
E.g. low dimensional features in PCA or cluster a point belongs to in clustering can be viewed as features.

**Structure learning/feature learning is in general weaker than distribution learning:**
E.g. methods like PCA/clustering can't be used to generate new samples.

*Feature, not a bug*: it has been argued that self-supervised learning works because the task we are solving is easier (both computationally and statistically)

# Relationships between the tasks

**Distribution learning often implies representation learning**:
Many distributions we fit are **latent-variable** models (i.e. model the joint distribution between some latent variables **h** and the observed data **x**)

$$P_\theta(x, h) = P_\theta(h)P_\theta(x|h)$$

The latent variables are often viewed as a "***representation***".

The **posterior** distribution $P_\theta(h|x)$ captures a distribution over representations, given some values of the observed data.

However, a-priori, distribution $P_\theta(h|x)$ is a-priori not an easy distribution to **approximate/sample** from!

$$P_\theta(h|x) = \frac{P_\theta(x|h)p(h)}{\int_{h'} p(h')p(x|h')}$$

*Hard high-dimensional sum/integral*

# Representation learning and distribution learning

Common ways to get a handle of $P_\theta(h|x)$: variational methods and MCMC methods.

**Question**: how accurately do we need to approximate $P_\theta(h|x)$ if we want a good representation?

(Arora-Risteski blogpost: http://www.offconvex.org/2017/06/26/unsupervised1/)

**Answer**: Let $Q_\theta(h|x)$ be an approximation of $P_\theta(h|x)$ s.t.

$$KL(Q_\theta(h|x) \,||\, P_\theta(h|x)) \leq \epsilon$$

(KL is a natural metric, as a lot of the variational methods operate in this metric. Stay tuned! )

(Recall the definition of KL divergence: $KL(q \,||\, p) = \mathbb{E}_q \log\left(\frac{q}{p}\right)$ )

# Representation learning and distribution learning

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Suppose the way we will use the representation h is to solve **classification tasks.** Namely, let's say the labels for task are:

$(x_t, c(h_t))$, where $(h_t, x_t) \sim P_\theta(h, x)$ and $c(h_t) = \{\pm 1\}$

*In other words, the labels are a function of the **latent** variables, and the observables are the data.*

# Representation learning and distribution learning

Let $Q_\theta(h|x)$ be an approximation of $P_\theta(h|x)$ s.t.

$KL(Q_\theta(h|x) \,||\, P_\theta(h|x)) \leq \epsilon$

Suppose the way we will use the representation h is to solve classification tasks. Namely, let's say the binary classification task is:

$(x_t, c(h_t))$, where $(h_t, x_t) \sim P_\theta(h, x)$ and $c(h_t) = \{\pm 1\}$

The natural way to measure the distance with an eye towards classification tasks is total variation distance:

$TV(Q_\theta(\cdot\,|x) \,||\, P_\theta(\cdot\,|x)) = \sup_\Omega \left| \Pr_{h\sim Q_\theta(\cdot|x)}[\Omega] - \Pr_{h\sim P_\theta(\cdot|x)}[\Omega] \right|$

Why is this useful? Take $\Omega = \{$"C(h) is the correct label"$\}$

$\Pr_{h\sim Q_\theta(\cdot|x)}[\Omega]$ is the probability of having the correct answer using $Q_\theta(\cdot|x)$

$\left| \Pr_{h\sim Q_\theta(\cdot|x)}[\Omega] - \Pr_{h\sim P_\theta(\cdot|x)}[\Omega] \right|$ is the *difference in probability* of having the correct answer between $Q_\theta(\cdot|x)$!

# Representation learning and distribution learning

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Hence, $TV(Q_\theta(\cdot\,|x) \,||\, P_\theta(\cdot\,|x)) \leq \epsilon'$ implies that the difference in performance b/w using $P_\theta(\cdot\,|x)$ and $Q_\theta(\cdot\,|x)$ is at most $\epsilon'$ (on the input sample $x$)

Hence, $\mathbb{E}_x[TV(Q_\theta(\cdot\,|x) \,||\, P_\theta(\cdot\,|x))] \leq \epsilon'$ implies that the difference in performance on the classification task is at most $\epsilon'$.

# Representation learning and distribution learning

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To conclude, by Pinsker's inequality, we have

$$TV(Q_\theta(\cdot\,|x) \,||\, P_\theta(\cdot\,|x)) \leq \sqrt{\frac{1}{2} KL(Q_\theta(\cdot\,|x) \,||\, P_\theta(\cdot\,|x))} \leq \sqrt{\frac{1}{2}\epsilon}$$

*So, if we want a good performance on classification task, we need an extremely close approximation to the posterior!*

# Representation learning and distribution learning

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# Training techniques: Likelihood-based vs likelihood-free

**Two typical** families of training algorithms:

**Likelihood-based**: maximize the likelihood of the data under the model (possibly with some approximations)

*Typical approximations used*: variational inference (optimize tractable deterministic approximation of posteriors), MCMC methods (idea: approximate difficult quantities like posteriors with sampling)

**Likelihood-free**: use a surrogate loss – e.g. in GANs, train a discriminator to tell real and generated samples apart; noise-contrastive training: encourage model to put probability mass away from "fake" samples.

# The classics: PCA

**Figure 1: Population structure within Europe.**

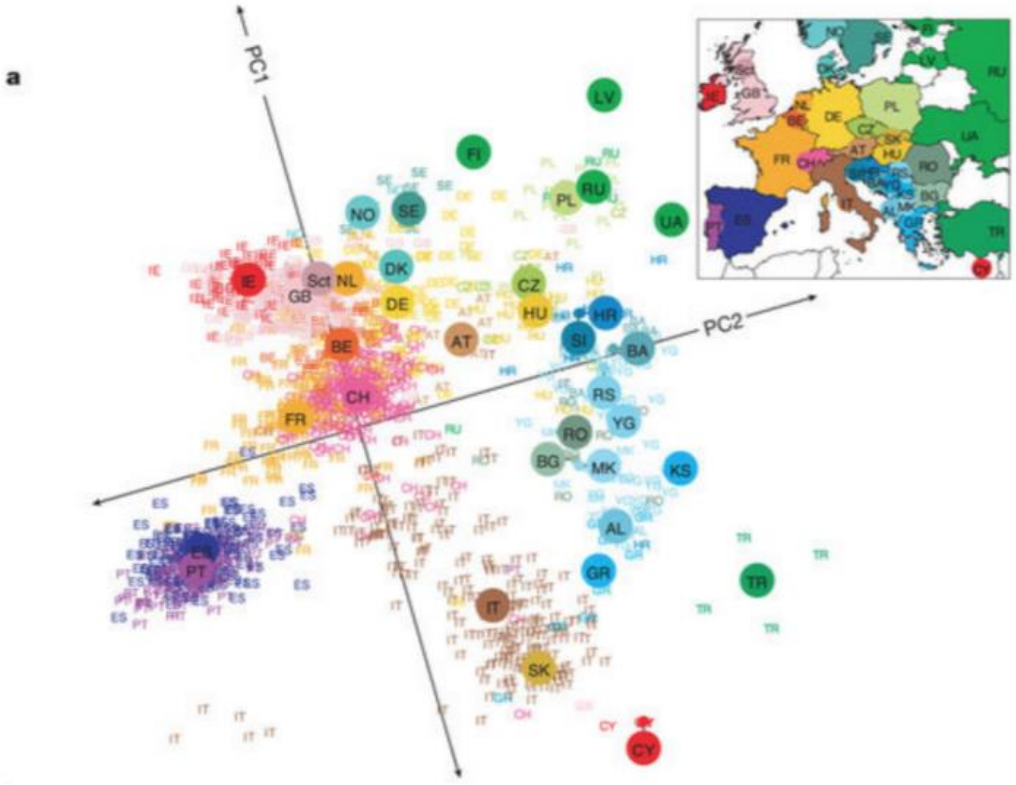



Figure 6: Plot from [1], depicting genomes for 1387 Europeans projected onto top 2 principal components. Colors/labels of datapoints correspond to geographic location of the individuals. Map of Europe (with same coloring) included in upper right for reference.

*Novembre et al '08*

# The classics: PCA

**Goal:** find a k-dimensional (linear) subspace explaining most of the variance in the data.

Assume the data is whitened, that is $\mathbb{E}[x] = 0$

*Warmup*: let k=1.

$$\max_{\{v:\,||v||=1\}} \frac{1}{m} \sum_{\text{samples } x_i} \langle v, x_i \rangle^2$$

*Variance:* $\mathbb{E}[\langle v, x \rangle^2]$

# The classics: PCA

**Goal:** find a k-dimensional (linear) subspace explaining most of the variance in the data.

$$\max_{\{v_1,v_2,\dots,v_k\}} \frac{1}{m} \sum_{\text{samples } x_i} \left(\text{length of } x_i \text{ on } \text{span}(v_1, v_2, \dots, v_k)\right)^2$$

$$= \max_{\text{orthonormal } \{v_1,v_2,\dots,v_k\}} \frac{1}{m} \sum_{\text{samples } x_i} \sum_{j=1}^{k} \langle x_i, v_j \rangle^2$$

*Variance:* $\mathbb{E}[\sum_j \langle v_j, x \rangle^2]$

# The classics: PCA

*How to do this efficiently?*

$$\max_{\text{orthonormal } \{v_1, v_2, \ldots, v_k\}} \frac{1}{m} \sum_{\text{samples } x_i} \sum_{j=1}^{k} \langle x_i, v_j \rangle^2$$

A convenient rewrite:

$$= \max_{\text{orthonormal } \{v_1, v_2, \ldots, v_k\}} \frac{1}{m} \sum_{\text{samples } x_i} \sum_{j=1}^{k} (v_j^T x_i)(x_i^T v_j)$$

$$= \max_{\text{orthonormal } \{v_1, v_2, \ldots, v_k\}} \frac{1}{m} \sum_{\text{samples } x_i} \sum_{j=1}^{k} v_j^T (x_i x_i^T) v_j$$

$$= \max_{\text{orthonormal } \{v_1, v_2, \ldots, v_k\}} \sum_{j=1}^{k} v_j^T \left( \frac{1}{m} \sum_{\text{samples } x_i} \left( x_i x_i^T \right) \right) v_j$$

# The classics: PCA

*How to do this efficiently? –* ***Singular Value Decomposition****!!*

$$\max_{\text{orthonormal } \{v_1, v_2, \ldots, v_k\}} \frac{1}{m} \sum_{\text{samples } x_i} \sum_{j=1}^{k} \langle x_i, v_j \rangle^2$$

A convenient rewrite:

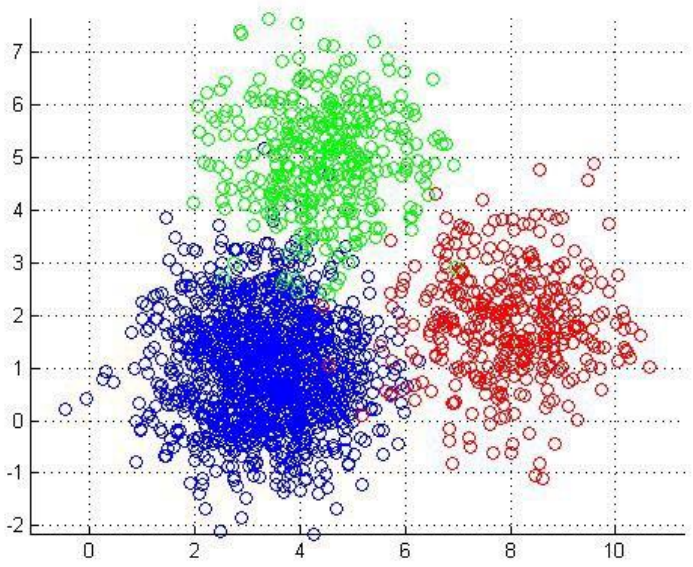
$$= \max_{\text{orthonormal } \{v_1, v_2, \ldots, v_k\}} \sum_{j=1}^{k} v_j^T \underbrace{\left( \frac{1}{m} \sum_{\text{samples } x_i} \left( x_i x_i^T \right) \right)}_{\mathrm{D}} v_j$$

$$= \max_{\text{orthonormal } \{v_1, v_2, \ldots, v_k\}} \sum_{j=1}^{k} v_j^T \mathrm{D} v_j$$

If D is **diagonal** (w/ positive entries): easy to see max is $\sum_{i=1}^{k} D_{ii}$

O/w: reduce to diagonal case by taking SVD of $\mathrm{D} = \mathrm{U}\, \widetilde{D} U^T$ and reducing to diagonal case: easy to see max is $\sum_{i=1}^{k} \lambda_i(D)$

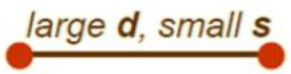
# The classics: clustering

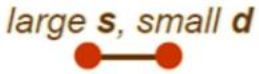



**Goal**: group the data into clusters of nearby points.

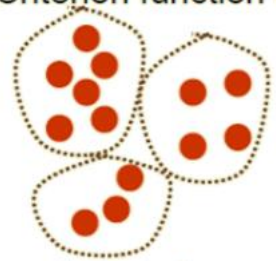
## What's needed for clustering?

1. Proximity measure, *either*
   - similarity measure $s(x_i,x_k)$: large if $x_i,x_k$ are similar
   - dissimilarity(or distance) measure $d(x_i,x_k)$: small if $x_i,x_k$ are similar

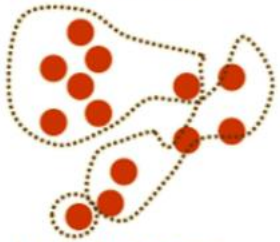



2. Criterion function to evaluate a clustering



*good clustering*



*bad clustering*

3. Algorithm to compute clustering

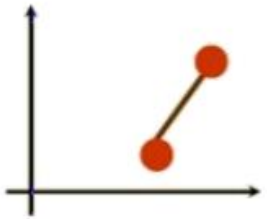
# The classics: clustering

**Popular distance metrics:**

- Euclidean distance

$$d(x_i, x_j) = \sqrt{\sum_{k=1}^{d} (x_i^{(k)} - x_j^{(k)})^2}$$

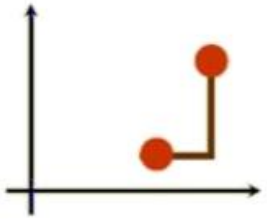
  - translation invariant



- Manhattan (city block) distance

$$d(x_i, x_j) = \sum_{k=1}^{d} |x_i^{(k)} - x_j^{(k)}|$$

  - approximation to Euclidean distance, cheaper to compute



- They are special cases of **Minkowski distance**:

$$d_p(\mathbf{x}_i, \mathbf{x}_j) = \left( \sum_{k=1}^{m} |x_{ik} - x_{jk}|^p \right)^{\frac{1}{p}}$$

(p is a positive integer)

# The classics: clustering

**Criterion functions:**

Intra-cluster cohesion
– Cohesion measures how near the data points in a cluster are to the cluster “center”.

Inter-cluster separation
– Separation means that different cluster centroids should be far away from one another.

In most applications, expert judgments are still the key

# The classics: clustering

**How many clusters?**

*3 clusters or 2 clusters?*

- Possible approaches
  1. fix the number of clusters to ***k***
  2. find the best clustering according to the criterion function (number of clusters may vary)

# K-means clustering

If the distance metric is the Euclidean distance, and the measure of cohesion is the average distance from the centroid: we get the **k-means objective.**

$$argmin_{\{r_{nk},\boldsymbol{\mu_k}\}} \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x_n} - \boldsymbol{\mu_k}\|^2$$

*Is point n in cluster k?*

*Centroid of k-th cluster*

# K-means clustering

A natural iterative algorithm, which as we will see later is a variant of the **EM (expectation-maximization)** algorithm:

**Input**: Data set $X = \{x^{(1)}, x^{(2)}, \cdots, x^{(m)} | x^{(i)} \in \mathbb{R}^n\}$

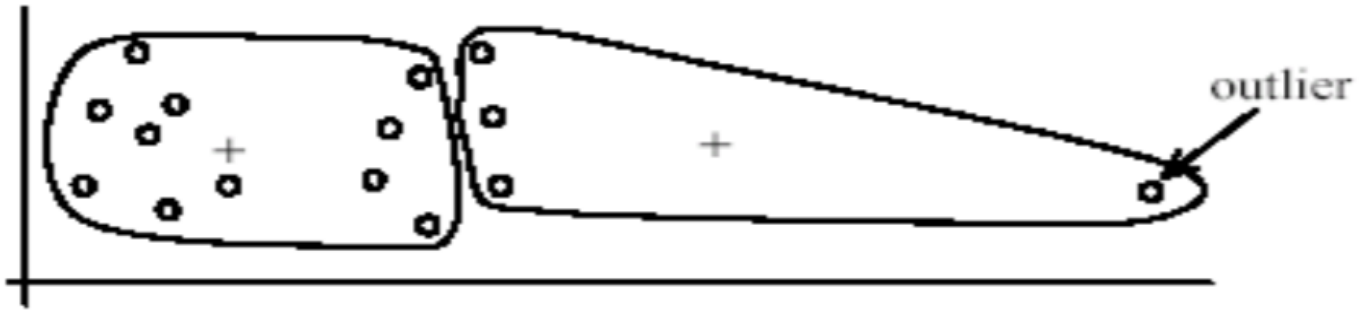
**Output**: Cluster centroids $\mu_{i=1,\cdots,k} \in \mathbb{R}^n$;Cluster assignments $c \in \mathbb{Z}$

Initialize $k$ cluster centroids $\mu_1, \cdots, \mu_k \in \mathbb{R}^n$ randomly from $X$;
**repeat**
  **for** $i = 1, \cdots, m$ **do** // Update cluster assignments
    set $c^{(i)} = arg\ \min_j \|x^{(i)} - \mu_j\|^2$;
  **end**
  **for** $j = 1, \cdots, k$ **do** // Update cluster centroids
    set $\mu_j = \frac{\sum_{i=1}^{m} 1\{c^{(i)}=j\} x^{(i)}}{\sum_{i=1}^{m} 1\{c^{(i)}=j\}}$;
  **end**
**until** *Convergence*;
**return** $\mu$ and $c$;

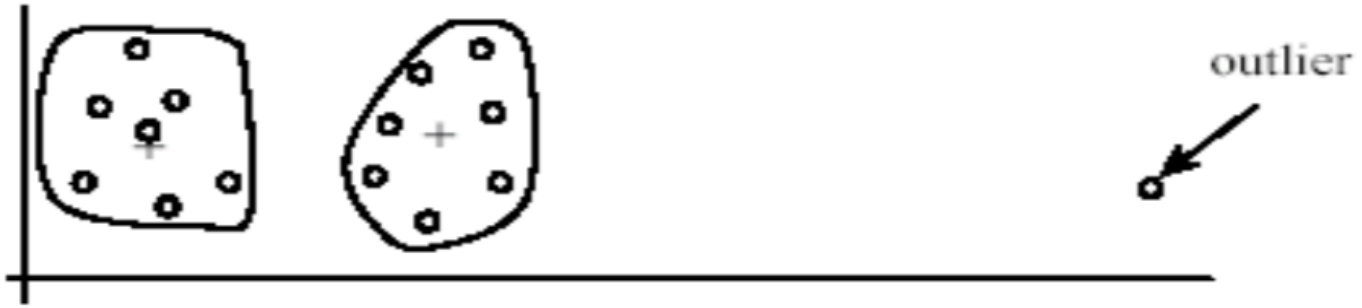
**Algorithm 1:** Algorithm of batch-version for K-means

# Some weaknesses

Very sensitive to outliers:



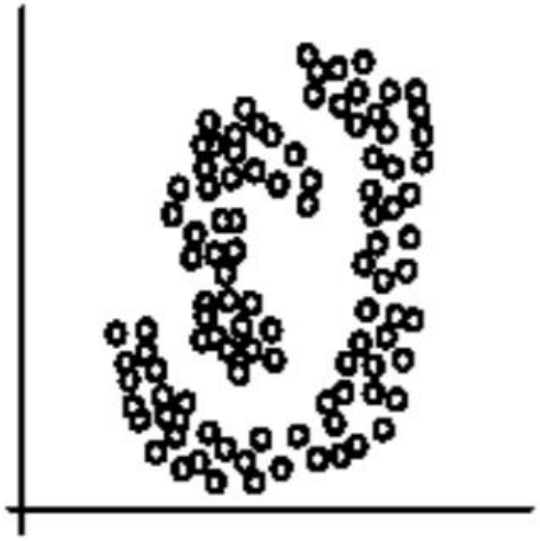

(A): Undesirable clusters



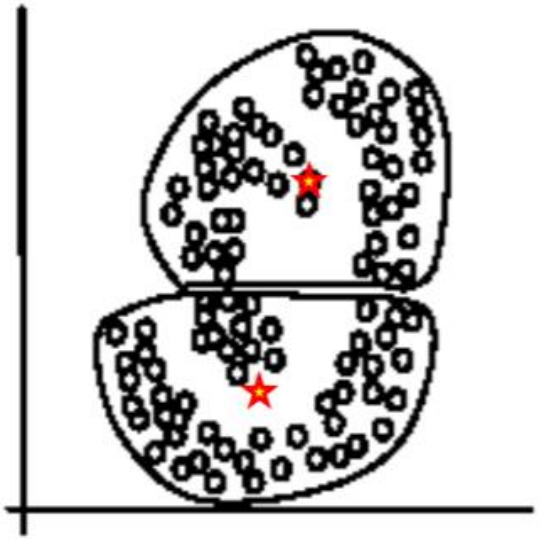

(B): Ideal clusters

# Some weaknesses

Not suitable for non-spherical clusters:



(A): Two natural clusters



(B): *k*-means clusters