10707
Deep Learning: Spring 2020

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Lecture 9:
Common parametric distributions, Bayesian networks

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**)

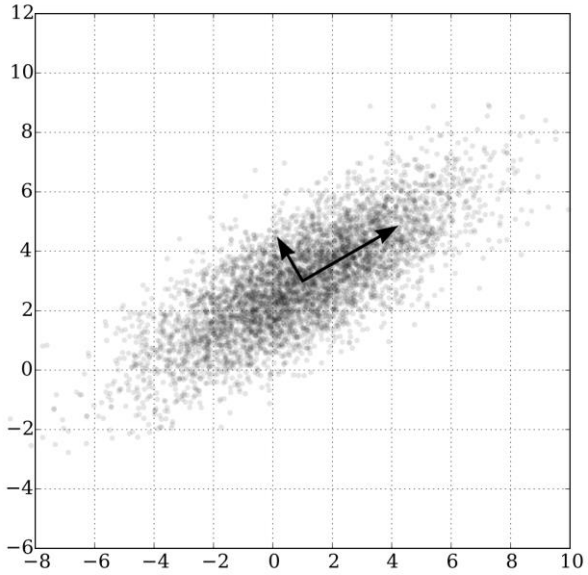
Task C: Learn a (parametrized) distribution that implicitly reveals an **"embedding"/"representation"** of data for downstream tasks. (**Representation/feature learning**)

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

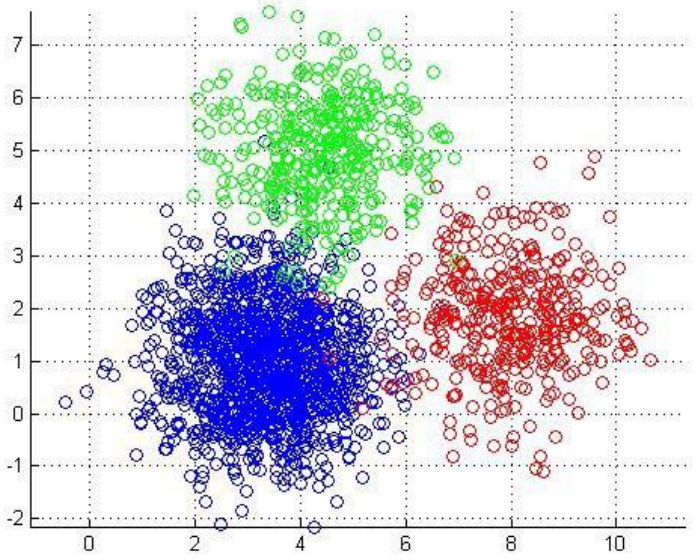
Structure learning

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



The classics: PCA

Figure 1: Population structure within Europe.

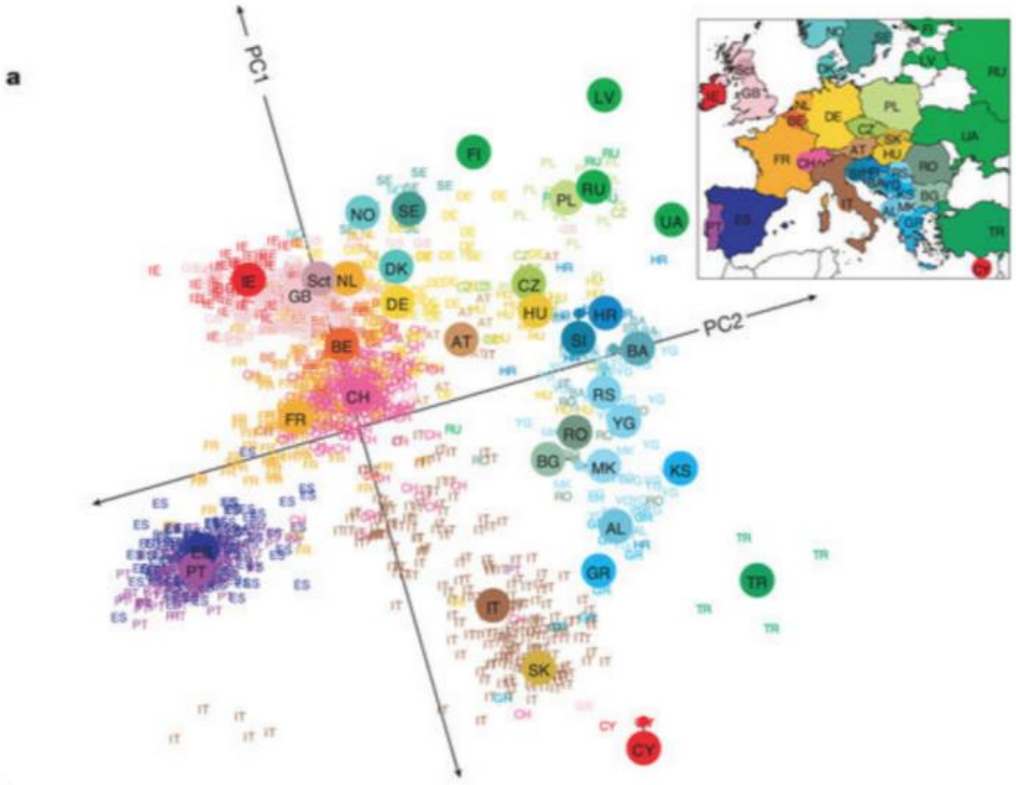


Figure 6: Plot from [1], depicting genomes for 1387 Europeans projected onto top 2 principal components. Colors/labels of datapoints correspond to geographic location of the individuals. Map of Europe (with same coloring) included in upper right for reference.

Novembre et al '08

The classics: PCA

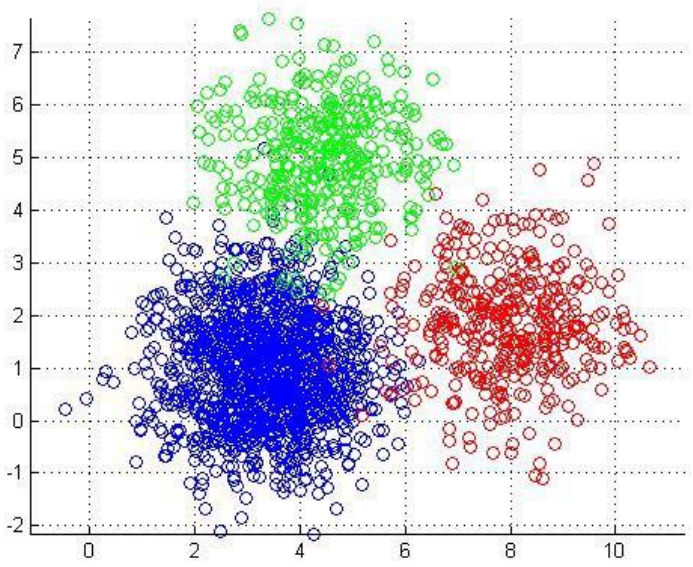
Goal: find a k-dimensional (linear) subspace explaining most of the variance in the data.

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

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

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

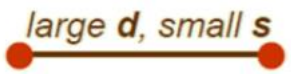
The classics: clustering

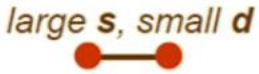


Goal: group the data into clusters of nearby points.

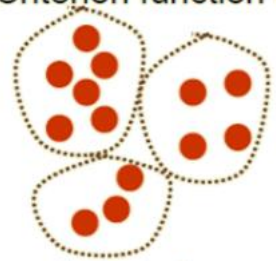
What's needed for clustering?

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

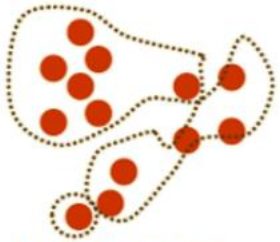




2. Criterion function to evaluate a clustering



good clustering



bad clustering

3. Algorithm to compute clustering

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

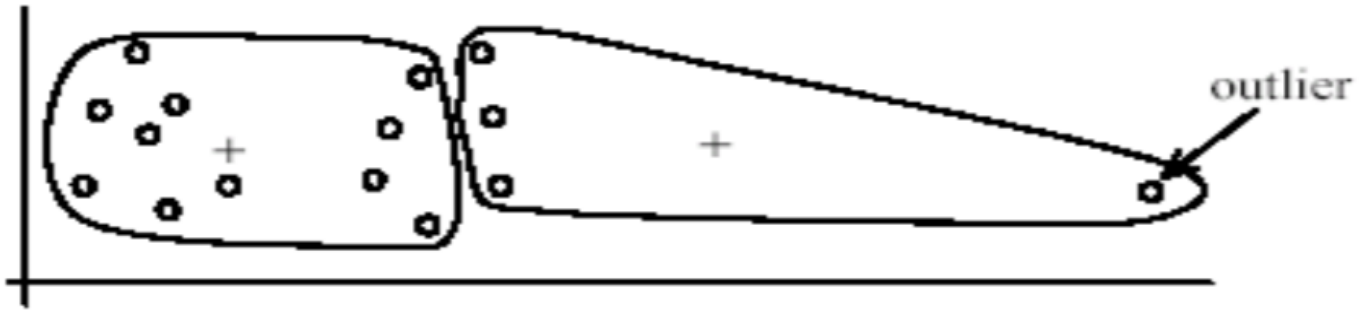
Output: Cluster centroids $\mu_{i=1,\cdots,k} \in \mathbb{R}^n$;Cluster assignments $c \in \mathbb{Z}$

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 μ and c;

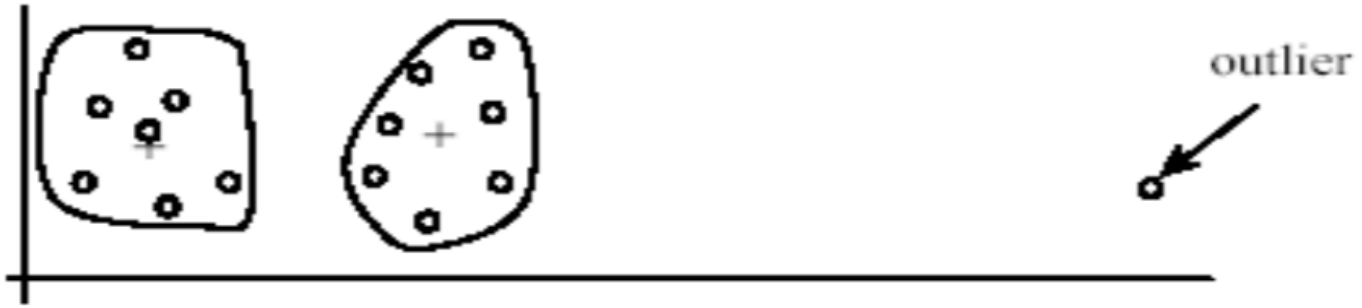
Algorithm 1: Algorithm of batch-version for K-means

Some weaknesses

Very sensitive to outliers:



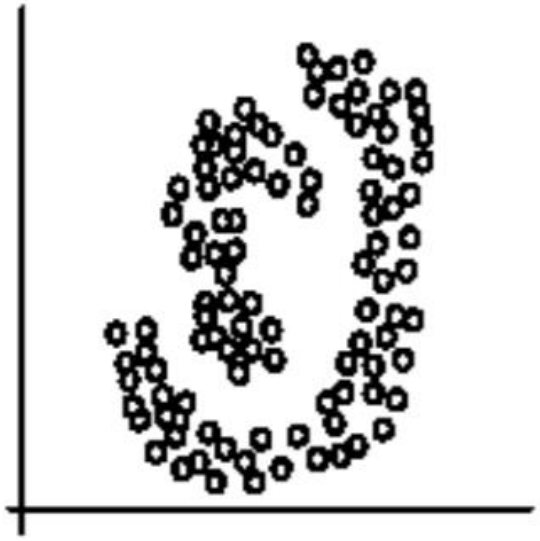
(A): Undesirable clusters



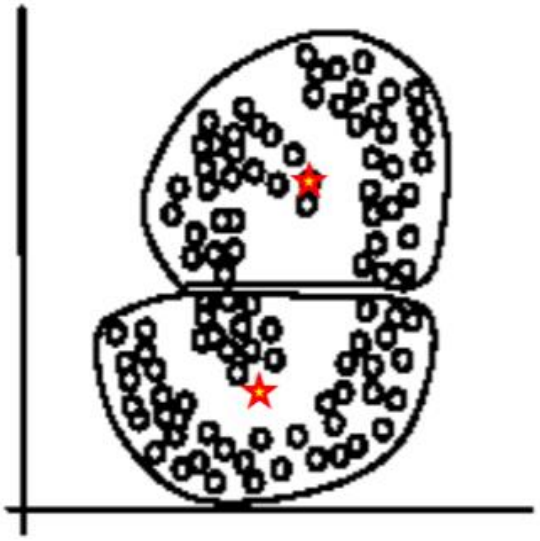
(B): Ideal clusters

Some weaknesses

Not suitable for non-spherical clusters:



(A): Two natural clusters

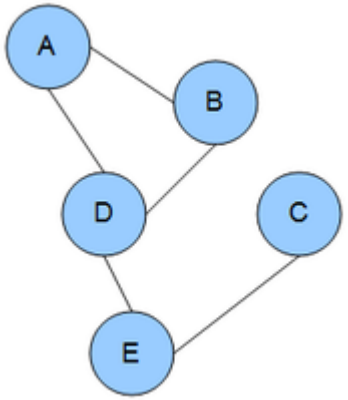


(B): *k*-means clusters

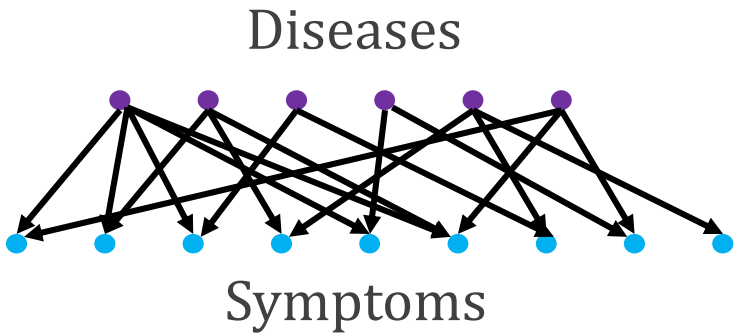
Distribution learning

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"



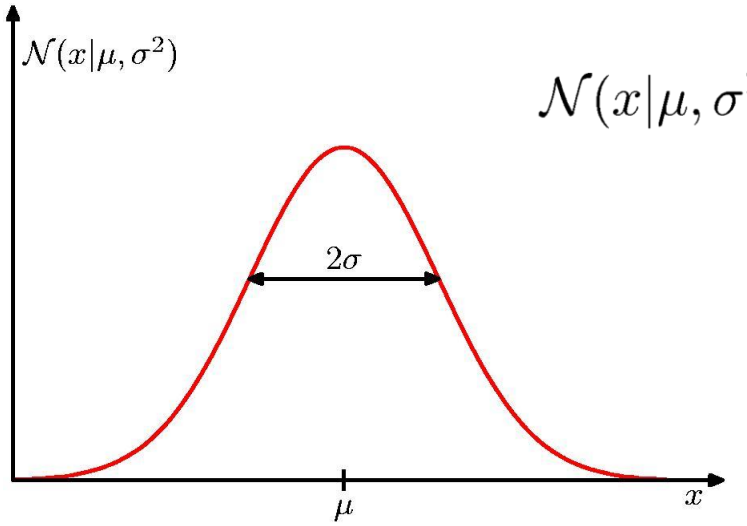
Latent variable models: data is "simple" conditioned on some unobserved (latent) variables

Distribution learning

Before getting to graphical models, let's recap some basic distributions we will use as building blocks.

Gaussian Univariate Distribution

In the case of a single variable x, the pdf of the Gaussian distribution is:



$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$

which is governed by two parameters:

μ (**mean**)
σ (**variance**)

(In that, given the values of the mean/variance, there is a unique Gaussian with those mean/variance.)

Why are mean and variance as claimed?

$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$

We wish to show that $\mathbb{E}[x] = \mu, \mathbb{E}[(x-\mu)^2] = \sigma^2$

By change of variables, suffices to show this for $\mu = 0, \sigma = 1$

$$\mathbb{E}[x] = \int_{-\infty}^{\infty} x \frac{1}{\sqrt{2\pi}} \exp(-x^2/2)\, dx = \frac{1}{2}\int_{-\infty}^{\infty} (x + (-x)) \frac{1}{\sqrt{2\pi}} \exp(-x^2/2)\, dx = 0$$

$$\mathbb{E}[(x-\mu)^2] = \int_{-\infty}^{\infty} x^2 \frac{1}{\sqrt{2\pi}} \exp(-x^2/2)\, dx = 2\int_{0}^{\infty} x^2 \frac{1}{\sqrt{2\pi}} \exp(-x^2/2)\, dx$$

$$= \frac{2}{\sqrt{2\pi}} \int_0^{\infty} x \underbrace{(x \exp(-x^2/2))}\, dx = \frac{2}{\sqrt{2\pi}} \int_0^{\infty} x\, dv = \frac{2}{\sqrt{2\pi}} \left(xv \Big|_0^{\infty} - \int_0^{\infty} v\, dx \right)$$

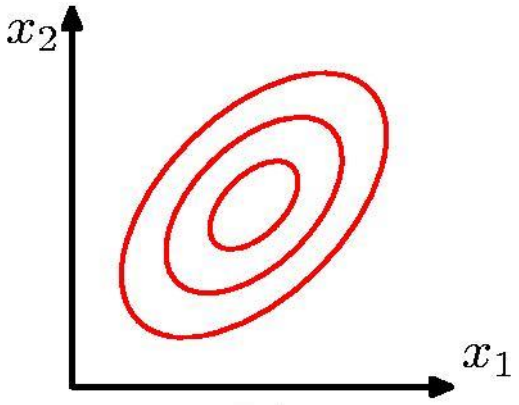
$$:= dv, v = -\left(\exp\left(-\frac{x^2}{2}\right)\right)$$

$$= \frac{2}{\sqrt{2\pi}} \left(\int_0^{\infty} \exp\left(-\frac{x^2}{2}\right) dx \right) = \frac{1}{\sqrt{2\pi}} \left(\int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{2}\right) dx \right) = 1$$

Multivariate Gaussian Distribution

For a D-dimensional vector **x**, the Gaussian distribution takes form:

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}}\frac{1}{|\boldsymbol{\Sigma}|^{1/2}}\exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$



which is governed by two parameters:

$\boldsymbol{\mu}$ (**mean**) is a D-dimensional mean vector.

$\boldsymbol{\Sigma}$ (**covariance**) is a D by D positive definite matrix, $|\boldsymbol{\Sigma}|$ denotes the determinant of $\boldsymbol{\Sigma}$.

(In that, given the values of the mean/variance, there is a unique Gaussian with those mean/variance.)

Why are mean and covariance as claimed?

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}}\frac{1}{|\boldsymbol{\Sigma}|^{1/2}}\exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

We wish to show that $\mathbb{E}[\boldsymbol{x}] = \boldsymbol{\mu}, \mathbb{E}[(\boldsymbol{x}-\boldsymbol{\mu})(\boldsymbol{x}-\boldsymbol{\mu})^{T}] = \boldsymbol{\Sigma}$

By change of variables, suffices to show this for $\mu = 0$

Expectation is easy:

$$\mathbb{E}[\boldsymbol{x}] = \int \boldsymbol{x}\frac{1}{\sqrt{2\pi^{\frac{D}{2}}|\Sigma|}}\exp\left(-\frac{1}{2}\boldsymbol{x}^{\boldsymbol{T}}\boldsymbol{\Sigma}^{-\mathbf{1}}\boldsymbol{x}\right)dx = \frac{1}{2}\int(\boldsymbol{x}+(-\boldsymbol{x}))\frac{1}{\sqrt{2\pi^{\frac{D}{2}}|\Sigma|}}\exp\left(-\frac{1}{2}\boldsymbol{x}^{\boldsymbol{T}}\boldsymbol{\Sigma}^{-\mathbf{1}}\boldsymbol{x}\right) = 0$$

Covariance can be reduced to $\boldsymbol{\Sigma}$=I:

One can produce a sample from a Gaussian w/ covariance $\boldsymbol{\Sigma}$ as $\boldsymbol{x} = \boldsymbol{\Sigma}^{1/2}\boldsymbol{y}$, y is sampled from a Gaussian w/ covariance I.
(Very useful, check it!)

Since the covariance of $\boldsymbol{x}$ is $\mathbb{E}[\boldsymbol{x}\boldsymbol{x}^{\boldsymbol{T}}] = \boldsymbol{\Sigma}^{\frac{1}{2}}\mathbb{E}[\boldsymbol{y}\boldsymbol{y}^{\boldsymbol{T}}]\boldsymbol{\Sigma}^{\frac{1}{2}}$, it suffices to show the covariance of $\boldsymbol{y}$ is I.

Why are mean and covariance as claimed?

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}}\frac{1}{|\boldsymbol{\Sigma}|^{1/2}}\exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

We wish to show that $\mathbb{E}[\boldsymbol{x}] = \boldsymbol{\mu}, \mathbb{E}[(\boldsymbol{x}-\boldsymbol{\mu})(\boldsymbol{x}-\boldsymbol{\mu})^{T}] = \boldsymbol{\Sigma}$

By change of variables, suffices to show this for $\mu = 0$

Expectation is easy:

$$\mathbb{E}[\boldsymbol{x}] = \int \boldsymbol{x}\frac{1}{\sqrt{2\pi^{\frac{D}{2}}|\Sigma|}}\exp\left(-\frac{1}{2}\boldsymbol{x^T\Sigma^{-1}x}\right)dx = \frac{1}{2}\int(\boldsymbol{x}+(-\boldsymbol{x}))\frac{1}{\sqrt{2\pi^{\frac{D}{2}}|\Sigma|}}\exp\left(-\frac{1}{2}\boldsymbol{x^T\Sigma^{-1}x}\right) = 0$$

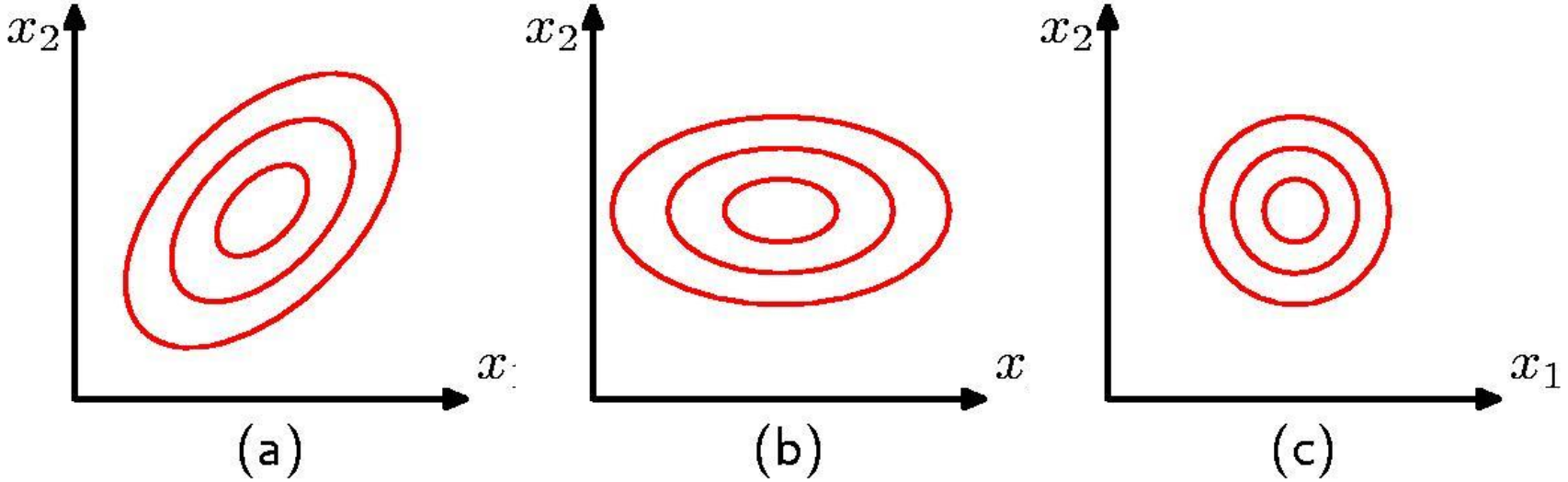
Covariance can be reduced to $\boldsymbol{\Sigma}$=I:

A Gaussian with $\boldsymbol{\Sigma}$=I is just a product distribution of standard Gaussians (check this!)

Hence, the covariance matrix has diagonals 1 (we showed this already), and off-diagonals 0 (since the off-diagonals are $\mathbb{E}[\boldsymbol{x_i x_j}] = \mathbb{E}[\boldsymbol{x_i}]\mathbb{E}[\boldsymbol{x_j}] = \boldsymbol{0}$)

Multivariate Gaussian Distribution

Contours of constant probability density:



Covariance matrix is of general form.

Diagonal, axis-aligned covariance matrix.

Spherical (proportional to identity) covariance matrix.

Central Limit Theorem

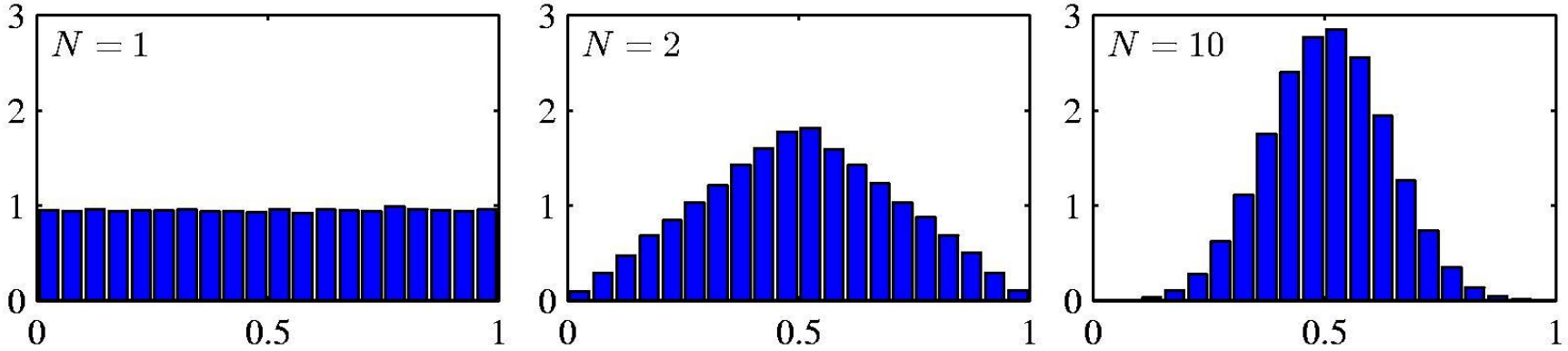
The distribution of the sum of N i.i.d. random variables becomes "increasingly Gaussian" as N grows. (Can be formalized.)

Consider N variables, each of which has a uniform distribution over the interval [0,1].

Let us look at the distribution over the mean:

$$\frac{x_1 + x_2 + ... + x_N}{N}.$$

As N increases, the distribution tends towards a Gaussian distribution. (Can be made quantative.)



Marginals and conditional of Gaussians

Consider a D-dimensional Gaussian distribution: $p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$

Let us partition $\mathbf{x}$ into two disjoint subsets x_a and x_b:

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix} \qquad \boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{pmatrix} \qquad \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{pmatrix}$$

In many situations, it will be more convenient to work with the *precision matrix* (inverse of the covariance matrix):

$$\boldsymbol{\Lambda} \equiv \boldsymbol{\Sigma}^{-1} \qquad \boldsymbol{\Lambda} = \begin{pmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{pmatrix}$$

(Note that Λ_{aa} is not given by the inverse of Σ_{aa})

Helpful result: inverting block matrices

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix} \qquad \boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{pmatrix} \qquad \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{pmatrix}$$

$$\boldsymbol{\Lambda} \equiv \boldsymbol{\Sigma}^{-1} \qquad \boldsymbol{\Lambda} = \begin{pmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{pmatrix}$$

Block matrix inversion lemma:

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}^{-1} = \begin{bmatrix} (\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1} & -(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1}\mathbf{B}\mathbf{D}^{-1} \\ -\mathbf{D}^{-1}\mathbf{C}(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1} & \mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{C}(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1}\mathbf{B}\mathbf{D}^{-1} \end{bmatrix}.$$

Here, **D** and $\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}$ must be invertible.

So, for instance, $\boldsymbol{\Lambda}_{aa}^{-1} = \boldsymbol{\Sigma}_{aa} - \boldsymbol{\Sigma}_{ab}\boldsymbol{\Sigma}_{bb}^{-1}\boldsymbol{\Sigma}_{ba}$ etc.

Conditionals of Gaussian

It turns out that the conditional distribution is also a Gaussian distribution:

$$p(\boldsymbol{x}_B|\boldsymbol{x}_A) = \mathcal{N}(\boldsymbol{x}_B|\boldsymbol{\mu}_{B|A}, \boldsymbol{\Sigma}_{B|A})$$

Covariance does not depend on x_A.

$$\boldsymbol{\Sigma}_{B|A} = \boldsymbol{\Lambda}_{BB}^{-1} = \boldsymbol{\Sigma}_{BB} - \boldsymbol{\Sigma}_{BA}\boldsymbol{\Sigma}_{AA}^{-1}\boldsymbol{\Sigma}_{AB}$$

$$\boldsymbol{\mu}_{B|A} = \boldsymbol{\mu}_B - \boldsymbol{\Lambda}_{BB}^{-1}\boldsymbol{\Lambda}_{BA}(\boldsymbol{x}_A - \boldsymbol{\mu}_A)$$

$$= \boldsymbol{\mu}_B - \boldsymbol{\Sigma}_{BA}\boldsymbol{\Sigma}_{AA}^{-1}(\boldsymbol{x}_A - \boldsymbol{\mu}_A)$$

Linear function of x_A.

Why is this true?

First, write out the conditional explicitly:

$$p(x_B \mid x_A) = \frac{p(x_A, x_B; \mu, \Sigma)}{\int_{x_B \in \mathbf{R}^m} p(x_A, x_B; \mu, \Sigma) dx_A}$$
$$= \frac{1}{Z'} \exp\left(-\frac{1}{2} \begin{bmatrix} x_A - \mu_A \\ x_B - \mu_B \end{bmatrix}^T \begin{bmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{bmatrix}^{-1} \begin{bmatrix} x_A - \mu_A \\ x_B - \mu_B \end{bmatrix} \right)$$

where Z' is a normalizing constant.

The expression inside the exponential is a quadratic in x_A : so the conditional is a Gaussian!

We will massage the expression to get it into a nicer form to extract the covariance and mean. (We will do the matrix analogue of "**completing the square**".)

Why is this true?

First, write out the conditional explicitly:

$$p(x_B \mid x_A) = \frac{p(x_A, x_B; \mu, \Sigma)}{\int_{x_B \in \mathbf{R}^m} p(x_A, x_B; \mu, \Sigma) dx_A}$$

$$= \frac{1}{Z'} \exp\left(-\frac{1}{2} \begin{bmatrix} x_A - \mu_A \\ x_B - \mu_B \end{bmatrix}^T \begin{bmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{bmatrix}^{-1} \begin{bmatrix} x_A - \mu_A \\ x_B - \mu_B \end{bmatrix} \right)$$

where Z' is a normalizing constant.

Using the notation we introduced, we have:

$$p(x_B \mid x_A) = \frac{1}{Z'} \exp\left(-\frac{1}{2} \begin{bmatrix} x_A - \mu_A \\ x_B - \mu_B \end{bmatrix}^T \begin{bmatrix} \Lambda_{AA} & \Lambda_{AB} \\ \Lambda_{BA} & \Lambda_{BB} \end{bmatrix} \begin{bmatrix} x_A - \mu_A \\ x_B - \mu_B \end{bmatrix} \right)$$

$$= \frac{1}{Z'} \exp\Big(-\Big[\frac{1}{2}(x_A - \mu_A)^T \Lambda_{AA}(x_A - \mu_A) + \frac{1}{2}(x_A - \mu_A)^T \Lambda_{AB}(x_B - \mu_B)$$

$$\frac{1}{2}(x_B - \mu_B)^T \Lambda_{BA}(x_A - \mu_A) + \frac{1}{2}(x_B - \mu_B)^T \Lambda_{BB}(x_B - \mu_B) \Big] \Big).$$

Expanding block form

Why is this true?

Using the notation we introduced, we have:

$$p(x_B \mid x_A) = \frac{1}{Z'}\exp\Big(-\Big[\ \overbrace{\frac{1}{2}(x_A-\mu_A)^T\Lambda_{AA}(x_A-\mu_A)}^{c} + \overbrace{\frac{1}{2}(x_A-\mu_A)^T\Lambda_{AB}(x_B-\mu_B)}^{\frac{1}{2}b^Tz}$$
$$\underbrace{\frac{1}{2}(x_B-\mu_B)^T\Lambda_{BA}(x_A-\mu_A)}_{\frac{1}{2}b^Tz} + \underbrace{\frac{1}{2}(x_B-\mu_B)^T\Lambda_{BB}(x_B-\mu_B)}_{z^TA\,z}\ \Big]\Big).$$

The "completion of squares" trick:

$$\frac{1}{2}z^TAz + b^Tz + c = \frac{1}{2}(z+A^{-1}b)^TA(z+A^{-1}b) + c - \frac{1}{2}b^TA^{-1}b$$

Apply above: $z = x_B - \mu_B, A = \Lambda_{BB}, b = \Lambda_{BA}(x_A-\mu_A), c = 1/2(x_A-\mu_A)^T\Lambda_{AA}(x_A-\mu_A)$

$$p(x_B \mid x_A) = \frac{1}{Z'}\exp\Big(-\Big[\ \frac{1}{2}\Big(x_B-\mu_B+\Lambda_{BB}^{-1}\Lambda_{BA}(x_A-\mu_A)\Big)^T\Lambda_{BB}\Big(x_B-\mu_B+\Lambda_{BB}^{-1}\Lambda_{BA}(x_A-\mu_A)\Big)$$
$$+\frac{1}{2}(x_A-\mu_A)^T\Lambda_{AA}(x_A-\mu_A) - \frac{1}{2}(x_A-\mu_A)^T\Lambda_{AA}\Lambda_{BB}^{-1}\Lambda_{BA}(x_A-\mu_A)\ \Big]\Big)$$

Marginal Distribution

It turns out that the marginal distribution is also a Gaussian distribution:

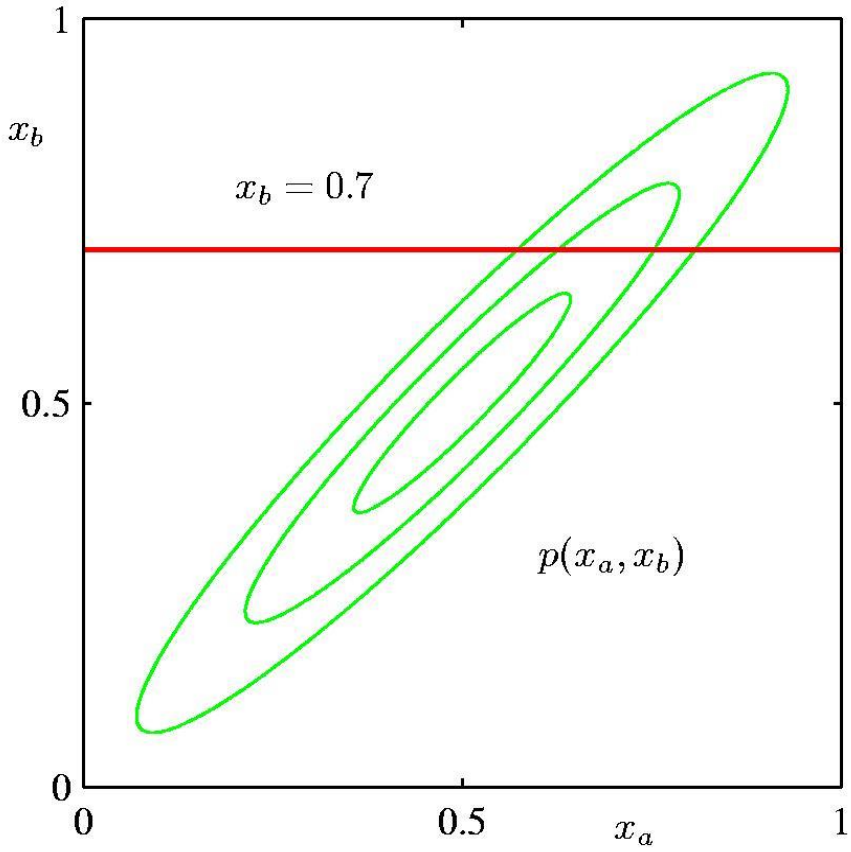
$$p(\mathbf{x}_a) = \int p(\mathbf{x}_a, \mathbf{x}_b)\, \mathrm{d}\mathbf{x}_b$$

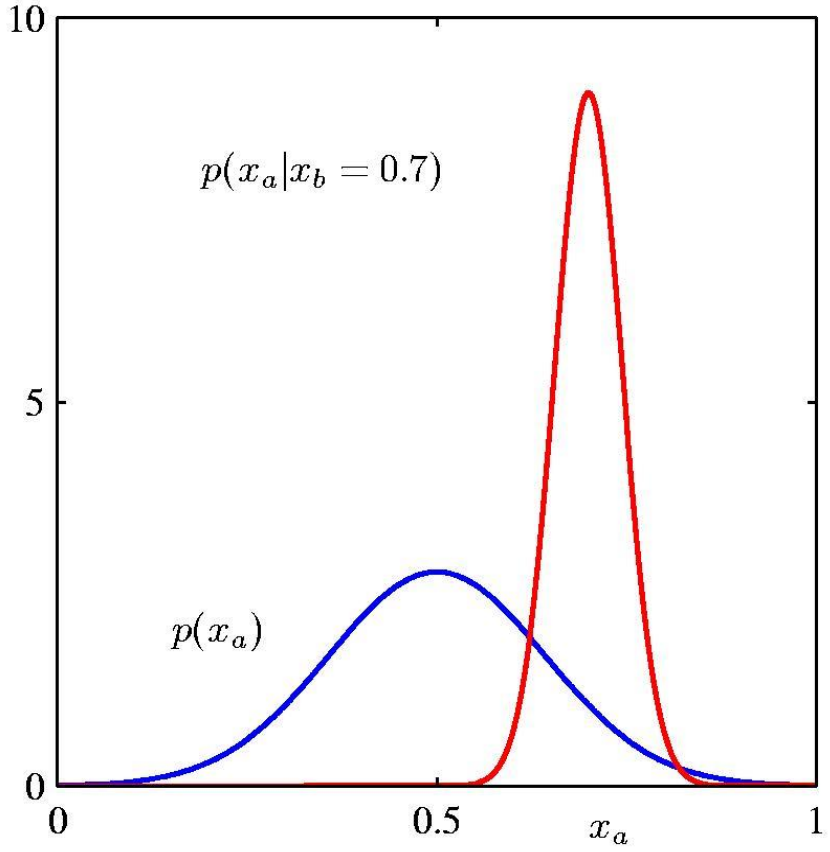
Similarly as before, one can show that the corresponding covariance and mean are:

Covariance: $(\boldsymbol{\Lambda}_{AA} - \boldsymbol{\Lambda}_{BA}\boldsymbol{\Lambda}_{BB}^{-1}\boldsymbol{\Lambda}_{AB})^{-1}$

Mean: $\boldsymbol{\mu}_A$

Conditional and Marginal Distributions

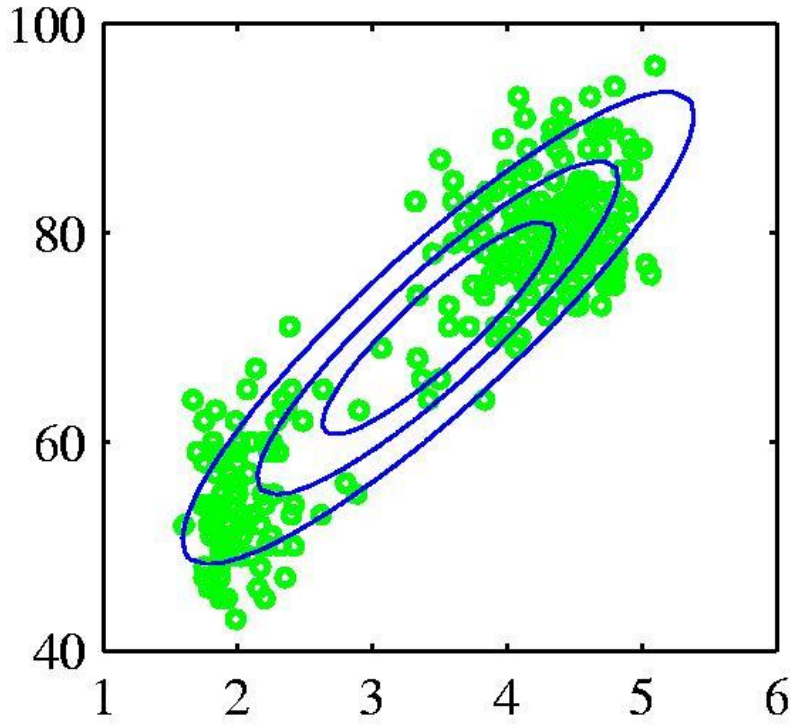




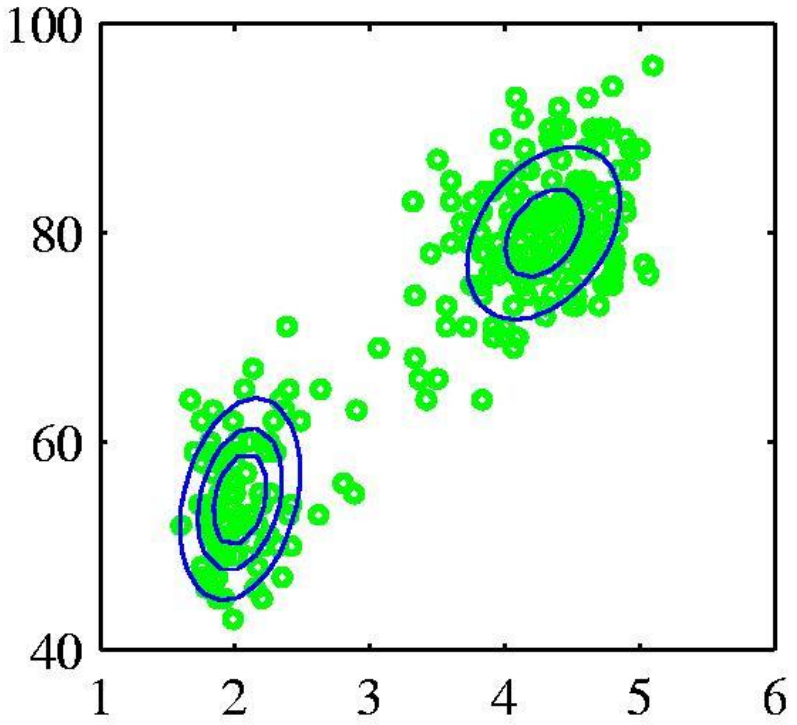
Mixture of Gaussians

When modeling real-world data, Gaussian assumption may not be appropriate.

Consider the following example: Old Faithful Dataset



Single Gaussian

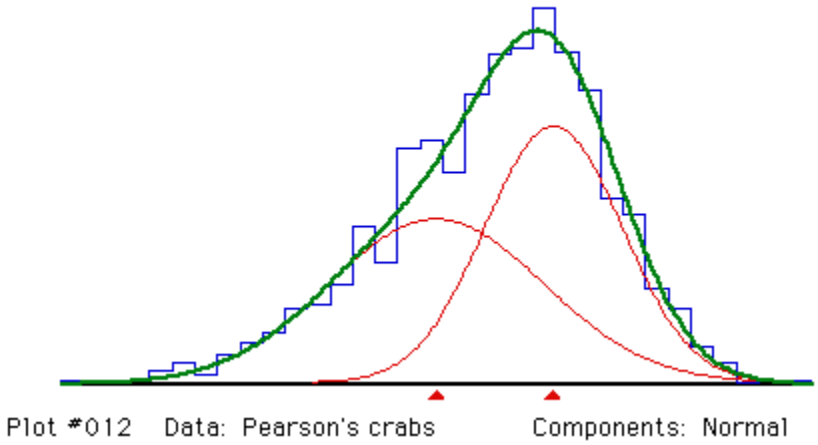


Mixture of two Gaussians

Mixture of Gaussians

When modeling real-world data, Gaussian assumption may not be appropriate.

Historical aside: Karl Pearson's crabs (1894)



Pearson had access to ~1000 collected width/length crab measurements from an island on Malta.

He (ahead of his time) argued that there is a mixture that matches the measurements much better than a Gaussian (fitted the mixture by hand a novel procedure!).

Thus, he argued that there are two separate species of crabs.

Mixture of Gaussians

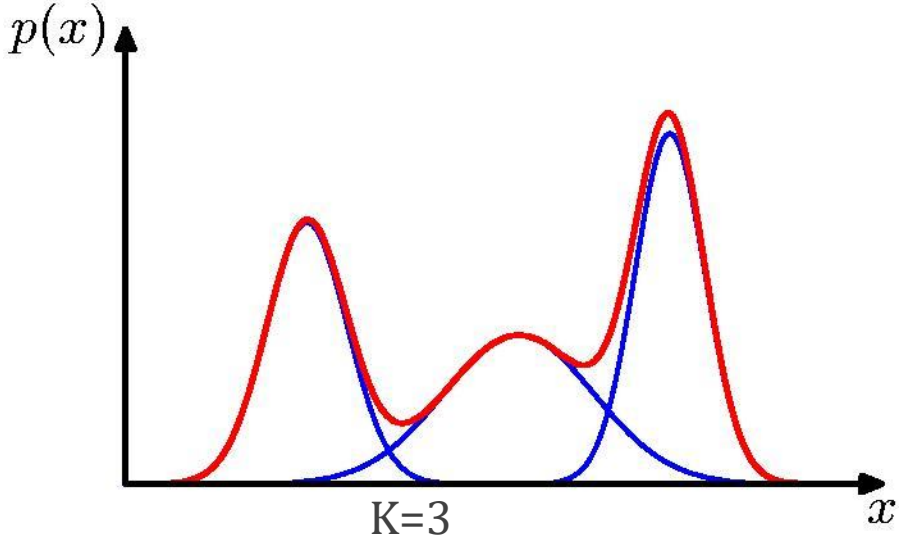
We can combine simple models into a complex model by defining a superposition of K Gaussian densities of the form:

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

Component

Mixing coefficient

$$\forall k : \pi_k \geqslant 0 \qquad \sum_{k=1}^{K} \pi_k = 1$$

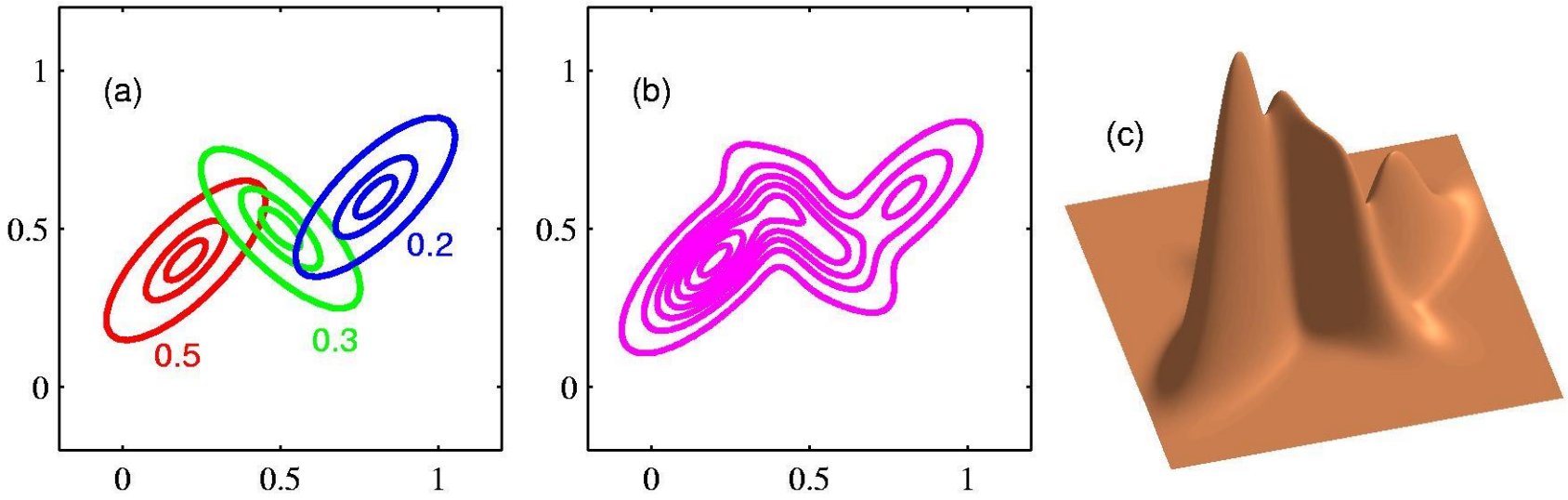


Note that each Gaussian component has its own mean $\boldsymbol{\mu_k}$ and covariance $\boldsymbol{\Sigma_k}$. The parameters $\boldsymbol{\pi_k}$ are called mixing coefficients.

Mote generally, mixture models can comprise linear combinations of other distributions.

Mixture of Gaussians

Illustration of a mixture of 3 Gaussians in a 2-dimensional space:



(a) Contours of constant density of each of the mixture components, along with the mixing coefficients

(b) Contours of marginal probability density $p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$

(c) A surface plot of the distribution p(x).

Bernoulli Distribution

Consider a single *binary* random variable $x \in \{0, 1\}$. For example, x can describe the outcome of flipping a coin:

Coin flipping: heads = 1, tails = 0.

The probability of x=1 will be denoted by the parameter μ, so that:

$$p(x = 1|\mu) = \mu \qquad 0 \leq \mu \leq 1.$$

The resulting Bernoulli distribution can be written as:

$$\begin{aligned} \text{Bern}(x|\mu) &= \mu^x(1-\mu)^{1-x} \\ \mathbb{E}[x] &= \mu \\ \text{var}[x] &= \mu(1-\mu) \end{aligned}$$

Binomial Distribution

We can also work out the distribution of the number m of observations of x=1 (e.g. the number of heads), i.e.

$$\sum_{i=1}^{N} X_i \, , X_i \text{ is Bernoulli with parameter } \mu$$

The probability of observing m heads given N coin flips and a parameter μ is given by:

$$p(m \text{ heads} | N, \mu) = \text{Bin}(m|N, \mu) = \binom{N}{m} \mu^m (1-\mu)^{N-m}$$

The mean and variance can be easily derived as:

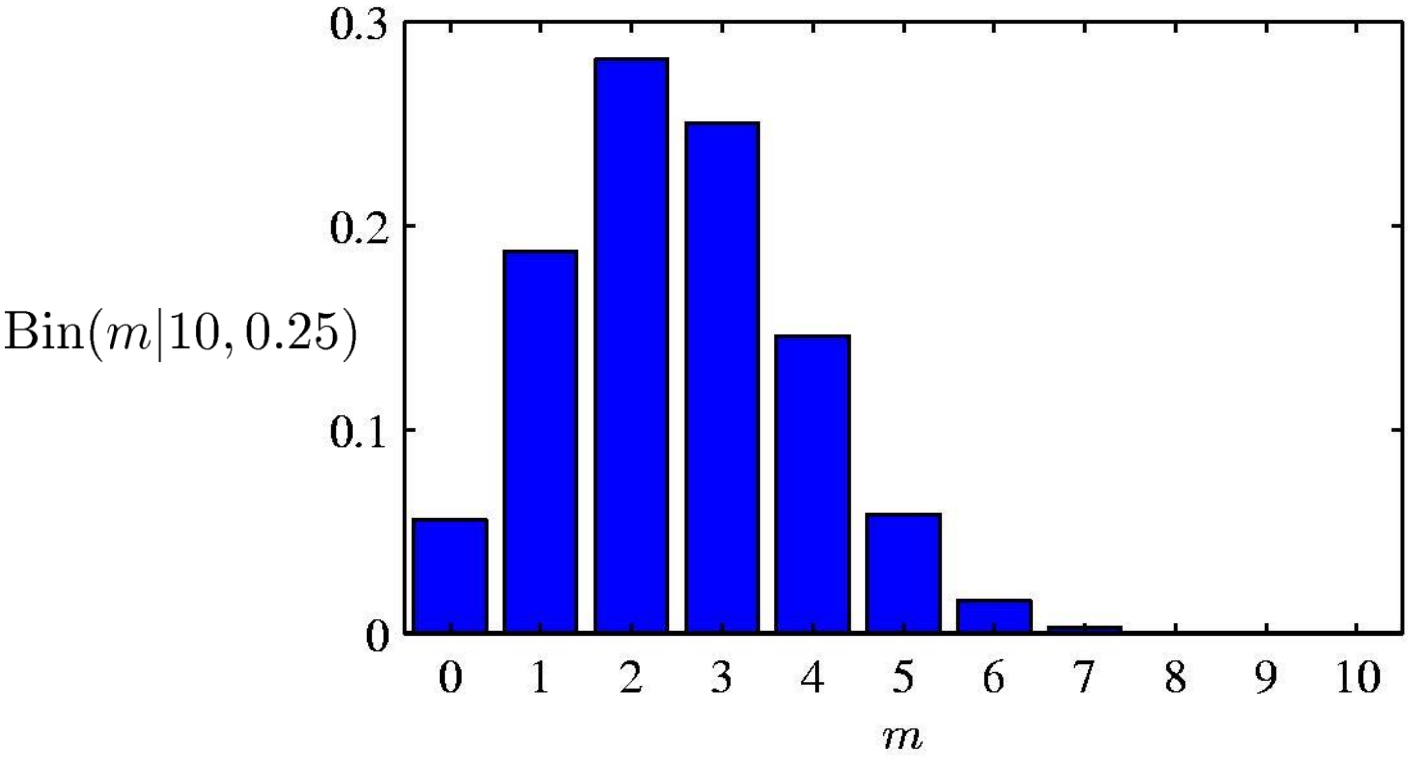
$$\mathbb{E}[m] = N \, \mu$$

$$\text{var}[m] = N \, \mu(1-\mu)$$

By law of large number, for large N, close to $\mathcal{N}\big(N \, \mu, N \, \mu(1-\mu)\big)$

Example

Histogram plot of the Binomial distribution as a function of m for N=10 and μ = 0.25.



Categorical distribution

Consider a random variable that can take on one of K possible mutually exclusive states (e.g. roll of a dice).

We will use so-called 1-of-K encoding scheme.

If a random variable can take on K=6 states, and a particular observation of the variable corresponds to the state x_3=1, then $\mathbf{x}$ will be represented as:

$$\mathbf{x} = (0, 0, 1, 0, 0, 0)^{\mathrm{T}}$$

If we denote the probability of x_k=1 by the parameter μ_k, then the categorical distribution over $\mathbf{x}$ is defined as:

$$p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{k=1}^{K} \mu_k^{x_k} \qquad \forall k : \mu_k \geqslant 0 \quad \text{and} \quad \sum_{k=1}^{K} \mu_k = 1$$

Categorical distribution

Categorical distribution can be viewed as a generalization of Bernoulli distribution to more than two outcomes.

$$p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{k=1}^{K} \mu_k^{x_k}$$

It is easy to see that the distribution is normalized:

$$\sum_{\mathbf{x}} p(\mathbf{x}|\boldsymbol{\mu}) = \sum_{k=1}^{K} \mu_k = 1$$

and

$$\mathbb{E}[\mathbf{x}|\boldsymbol{\mu}] = \sum_{\mathbf{x}} p(\mathbf{x}|\boldsymbol{\mu})\mathbf{x} = (\mu_1, \ldots, \mu_K)^{\mathrm{T}} = \boldsymbol{\mu}$$

Multinomial Distribution

We can construct the joint distribution of the quantities $\{m_i\}$ given the parameters $\{\mu_i\}$ and the total number N of observations:

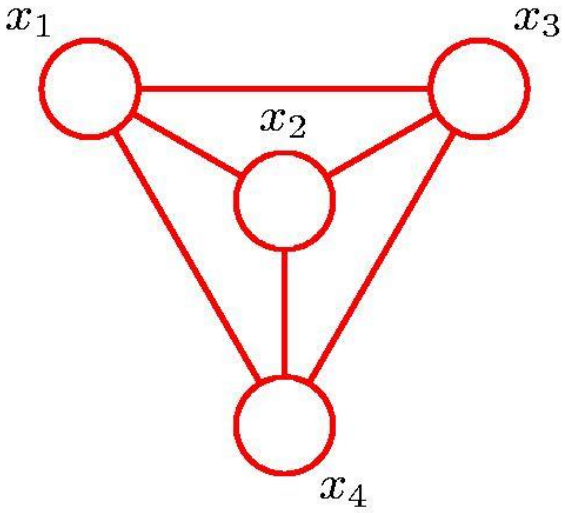
$$\begin{aligned}
\mathrm{Mult}(m_1, m_2, \ldots, m_K | \boldsymbol{\mu}, N) &= \binom{N}{m_1 m_2 \ldots m_K} \prod_{k=1}^{K} \mu_k^{m_k} \\
\mathbb{E}[m_k] &= N\mu_k \\
\mathrm{var}[m_k] &= N\mu_k(1-\mu_k) \\
\mathrm{cov}[m_j m_k] &= -N\mu_j\mu_k
\end{aligned}$$

The normalization coefficient is the number of ways of partitioning N objects into K groups of size $m_1, m_2, \ldots, m_K$.

Note that $\sum_k m_k = N.$

Graphical Models

Recall: graph contains a set of nodes connected by edges.



In a probabilistic graphical model, each node represents a random variable, links represent "probabilistic dependencies" between random variables.

Graph specifies how joint distribution over all random variables decomposes into a **product** of factors, each factor depending on a subset of the variables.

Two types of graphical models:

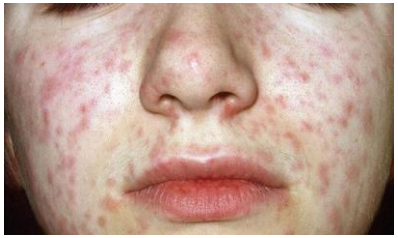
- **Bayesian networks**, also known as Directed Graphical Models (the links have a particular directionality indicated by the arrows)
- **Markov Random Fields**, also known as Undirected Graphical Models (the links do not carry arrows and have no directional significance).

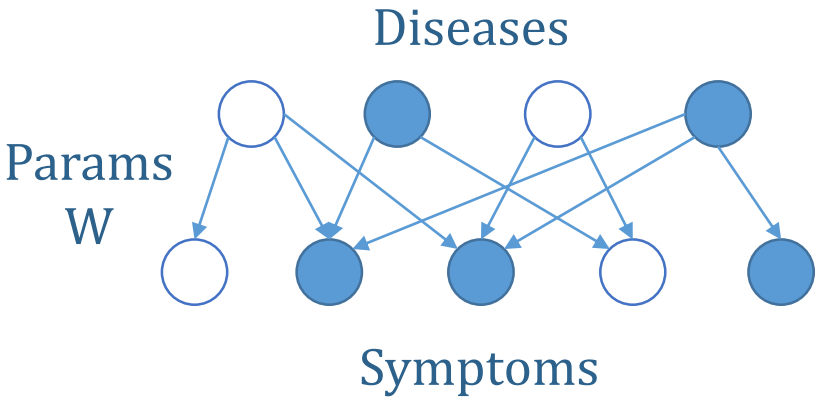
Bayesian Networks

Directed Graphs are useful for expressing causal relationships between random variables.

Your symptoms: fever + red spots.

Probability that you have measles?

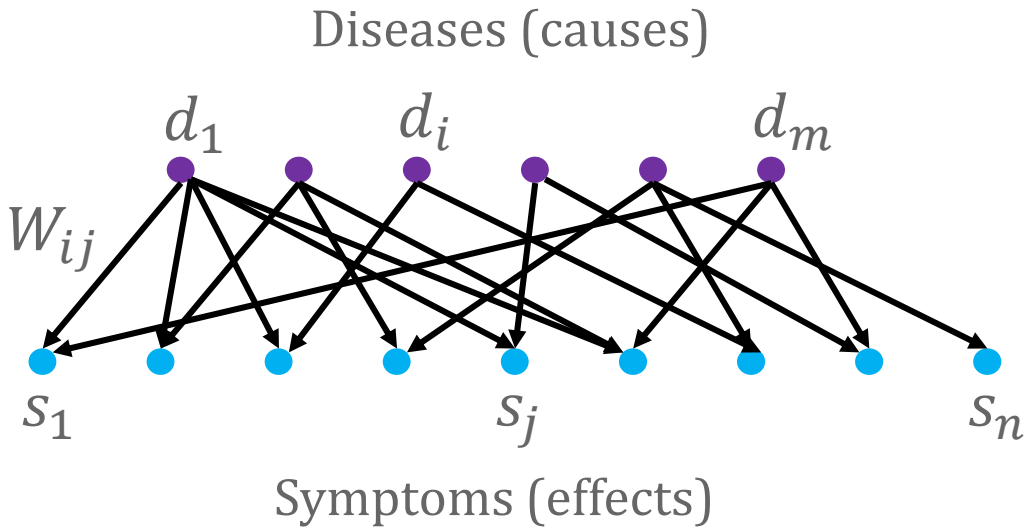




Bayesian network succinctly describes Pr[symptom| diseases]

Noisy-OR networks

$d_i, s_j \in \{0,1\}$
$W_{ij} \geq 0$



- Each d_i is on **independently** with prob. ρ
- When d_i is on, it **activates** s_j with probability $1 - \exp(-W_{ij})$.
- s_j is **on** if one of d_i's **activates** s_j

Bayesian Networks

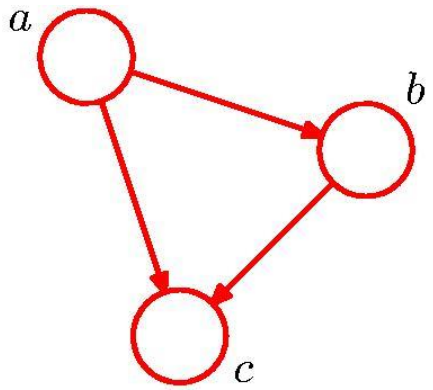
Directed Graphs are useful for expressing causal relationships between random variables.

"Deriving" Bayesian Networks as restrictions of arbitrary distributions:

An **arbitrary** joint distribution $p(a, b, c)$ over three random variables a,b, and c can be written as

$$p(a, b, c) = p(c|a, b)p(a, b) = p(c|a, b)p(b|a)p(a)$$

Associate a graph with the decomposition:



- Node for each of the random variables.
- Add **directed** links to the graph from the nodes corresponding to the vars on which the distribution is conditioned.

Bayesian Networks

Directed Graphs are useful for expressing causal relationships between random variables.

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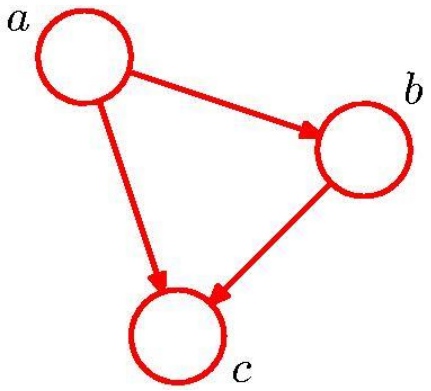


Different ordering => different graphical representation.

Joint distribution over K variables factorizes:

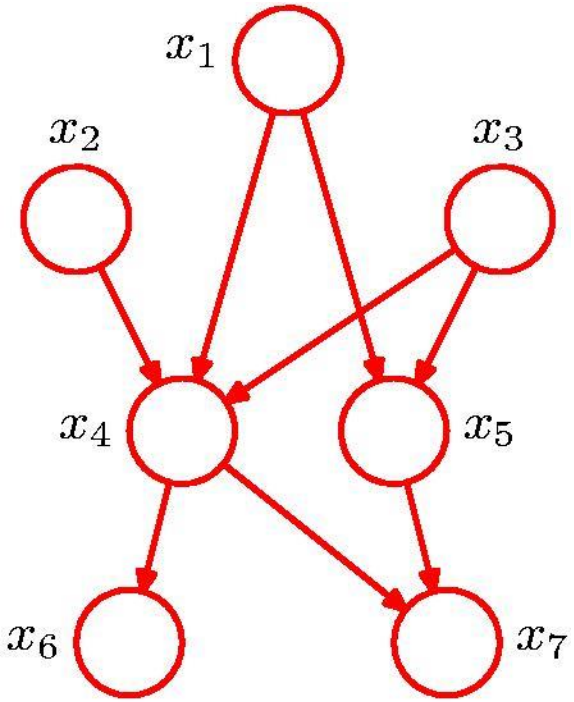
$$p(x_1, \ldots, x_K) = p(x_K|x_1, \ldots, x_{K-1}) \ldots p(x_2|x_1)p(x_1)$$

Corresponding undirected graph is fully connected:

(as each lower-numbered node points to each higher-numbered node)

Bayesian Networks

A graph that is **not** fully connected conveys information about the conditional independence structure of the distribution it encodes.



E.g. consider the graph on the left.

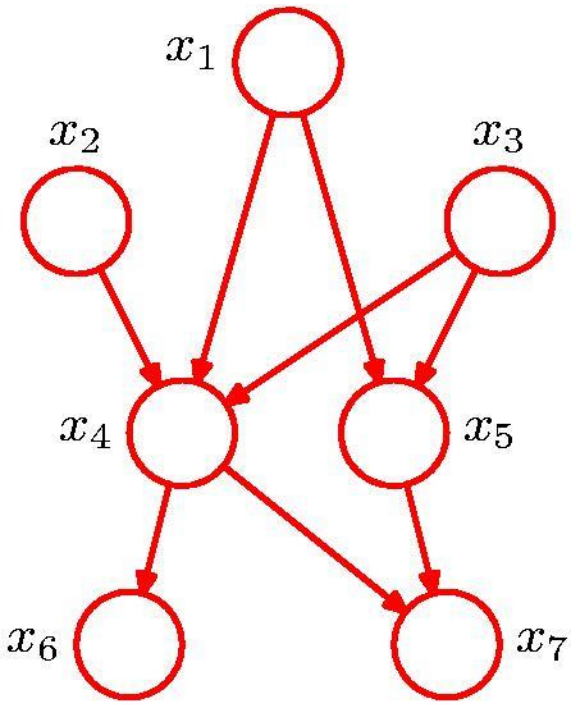
It encodes distributions over $x_1,\ldots,x_7$ that can be written as the product:

$$p(x_1,\ldots,x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1,x_2,x_3)\, p(x_5|x_1,x_3)p(x_6|x_4)p(x_7|x_4,x_5)$$

Note the change from the previous slide: e.g. x_5 is **not** conditioned on all of x_1, x_2, x_3, x_4 but only on x_1, x_3.

The general case: factorization

The joint distribution defined by the graph is given by the product of a conditional distribution for each node conditioned on its parents:



$$p(\mathbf{x}) = \prod_{k=1}^{K} p(x_k|\mathrm{pa}_k)$$

where pa_k denotes a set of parents for the node x_k.

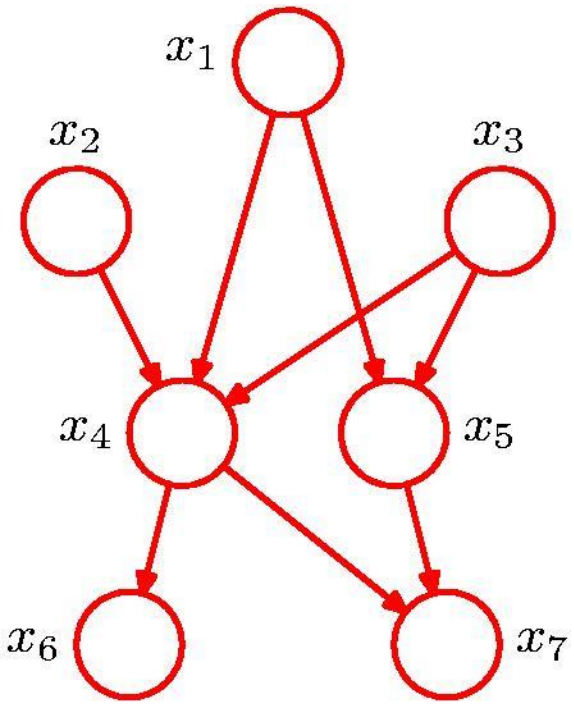
Each of the conditional distributions will typically have some parametric form. (e.g. product of Bernoullis in the noisy-OR case)

Important restriction: There must be **no directed cycles!** (i.e. graph is a DAG)

Crucial property: easy sampling

Consider a joint distribution over K random variables $p(x_1, x_2, ..., x_K)$t factorizes as:

$$p(\mathbf{x}) = \prod_{k=1}^{K} p(x_k|\mathrm{pa}_k)$$



Suppose each of the conditional distributions are easy to sample from. How do we sample from the joint?

Start at the top and sample in order.

$$\hat{x}_1 \sim p(x_1)$$
$$\hat{x}_2 \sim p(x_2)$$
$$\hat{x}_3 \sim p(x_3)$$
$$\hat{x}_4 \sim p(x_4|\hat{x}_1, \hat{x}_2, \hat{x}_3)$$
$$\hat{x}_5 \sim p(x_5|\hat{x}_1, \hat{x}_3)$$

The parent variables are set to their sampled values

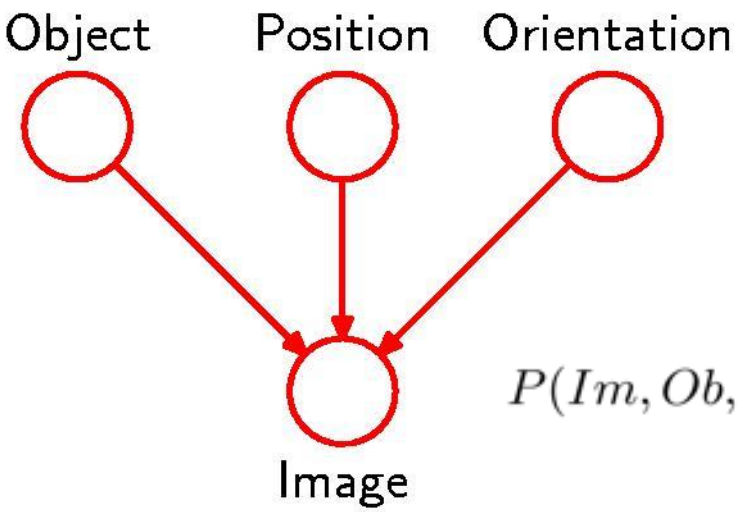
To obtain a sample from the marginal distribution, e.g. $p(x_2, x_5)$, sample from the full joint distribution, retain $\hat{x}_2, \hat{x}_5$, discard the remaining values.

Typical deep learning application

Higher-up nodes will typically represent **latent** (hidden) random variables.

The role of latent variables is to allow modeling a **complicated** distribution over observed variables **constructed** from **simpler** conditional distributions.

Latent-variable model of image



Object identity, position, and orientation have independent *prior probabilities*.

Image has probability distr that depends on object identity, position, and orientation (*conditional distribution/likelihood*).

$$P(Im, Ob, Po, Or) = \underbrace{P(Im|Ob, Po, Or)}_{\text{Likelihood}} \underbrace{P(Ob)P(Po)P(Or)}_{\text{Prior}}$$

Likelihood and prior are modeled by parametric distribution whose parameters are fitted throughout training.

Why restrict connectivity?

Why would we not want fully connected graphs?

Restricts the richness of the class!!

Consider discrete joint distribution over $\boldsymbol{n}$ variables, where each variable takes one of $\boldsymbol{k}$ values.

To **fully** specify it in general, we need the values of probabilities of every possibly outcome – so we need to specify $\boldsymbol{k^n}$ values.

To specify the conditionals $p(x_1|x_2, x_3, \dots x_d)$ we need to specify k^{d} values. Hence, in a graph of in-degree at most d, we need to specify at most n $\mathrm{k}^{\mathrm{d}} \ll k^n$ values!!