IFT6390
Fondements de l'apprentissage machine

Probability distributions

The multivariate Gaussian

Professor: Ioannis Mitliagkas
Slides: Pascal Vincent

Distributions

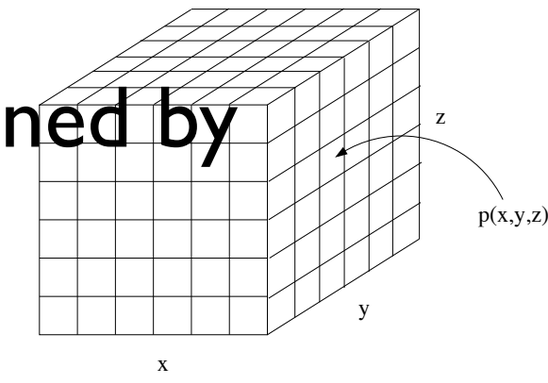
Reminder: https://en.wikipedia.org/wiki/Random_variable

- A probability distribution over a random variable is a function that provides the probabilities of occurrence of different possible values of the variable.

- A distribution over a random variable can be given by its cumulative distribution function (c.d.f.):

$$F_X(x) = P(X \leq x) = P(X_1 \leq x_1, \cdots, X_n \leq x_n)$$

- The distribution of a discrete variable is determined by the probability of each value it can take.



=> probability table (must sum to one...).

- The distribution of a continuous variable can be given by its probability density function (p.d.f.) which is the derivative of the c.d.f.** *The probability that a draw falls within some region is equal to the integral of the p.d.f. over this region.*

Operations on distributions

Given a distribution, we may want to

- Generate data, i.e. draw samples from this distribution.
- Compute the probability/likelihood of a configuration
  (e.g. knowing the value of some of the variables, after marginalizing the unknown variables).
- Inference: *infer* the most likely value or the expectation of some variables given the values of other variables.
- Learn the parameters of a distribution given a data set
  (such that the likelihood of the data being generated by this distribution with these parameters is maximized: *maximum likelihood estimation*).

Ex. Discrete variable X

Probability table:

x	$P(X=x)$
1	0.10
2	0.80
3	0.10

Generate

Learn

Data set:

2
2
2
1
2
2
2
3
2
2
...

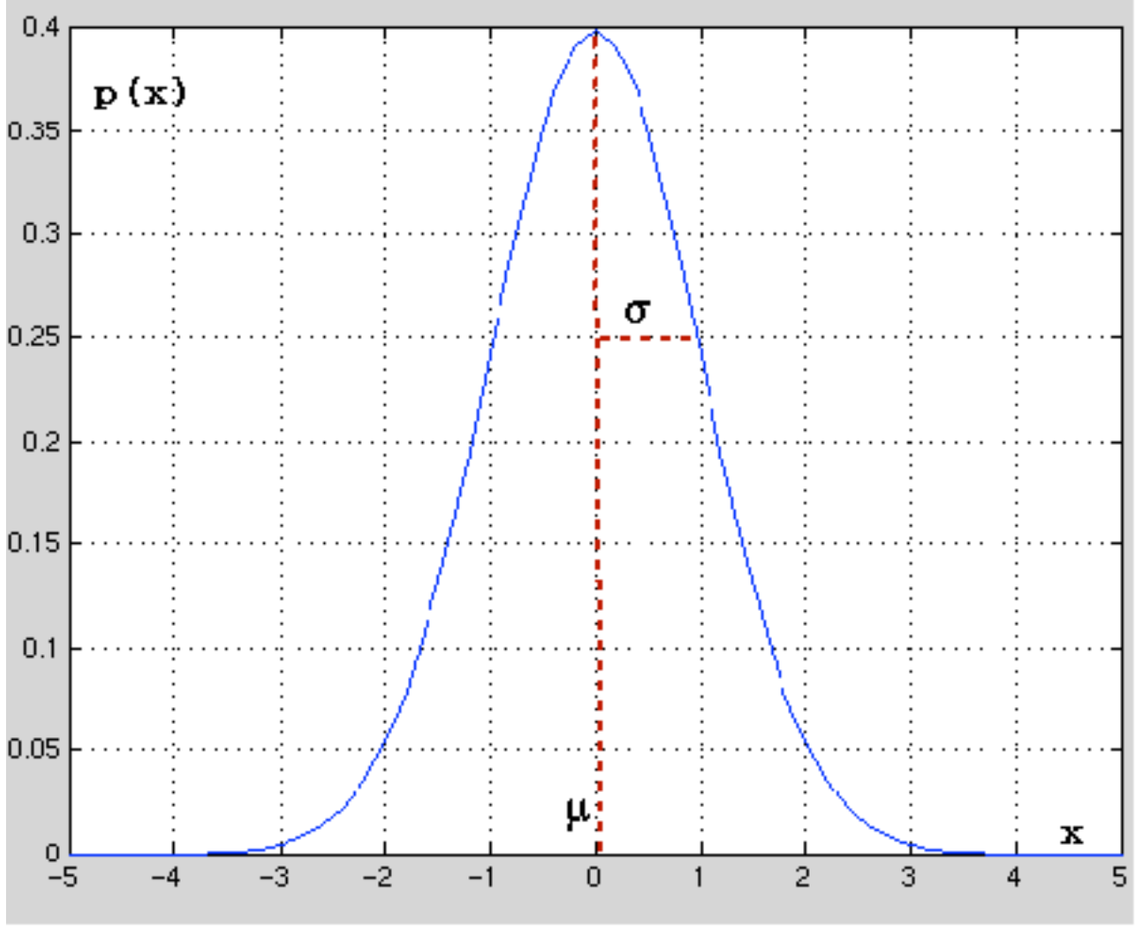
Ex. continuous (scalar) variable x

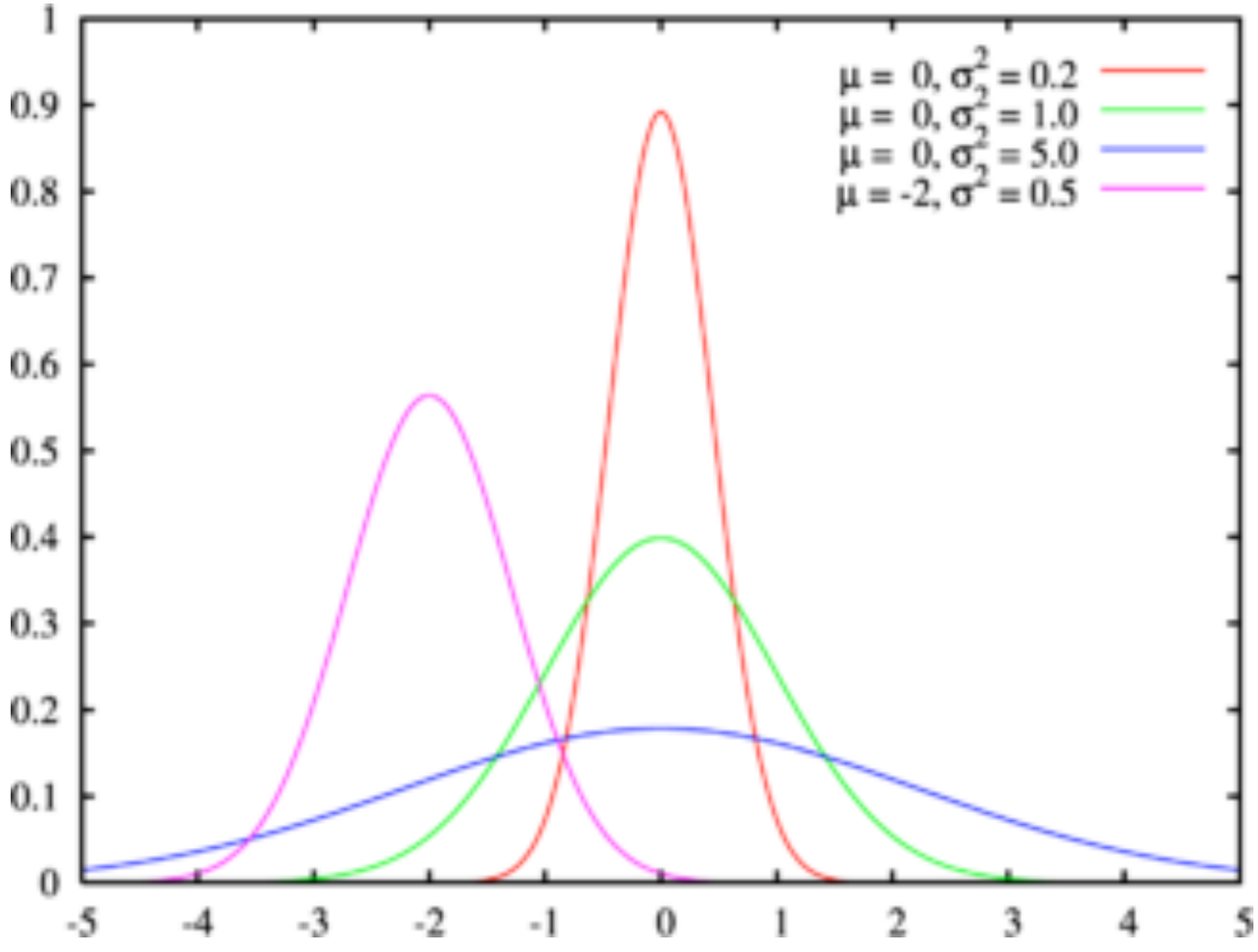
Univariate Gaussian/ Normal distribution

Gaussian density

Univariate (i.e. one dimensional) Gaussian density with mean μ and variance σ (standard deviation σ^2).

$$p(x) = \mathcal{N}_{\mu,\sigma^2}(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

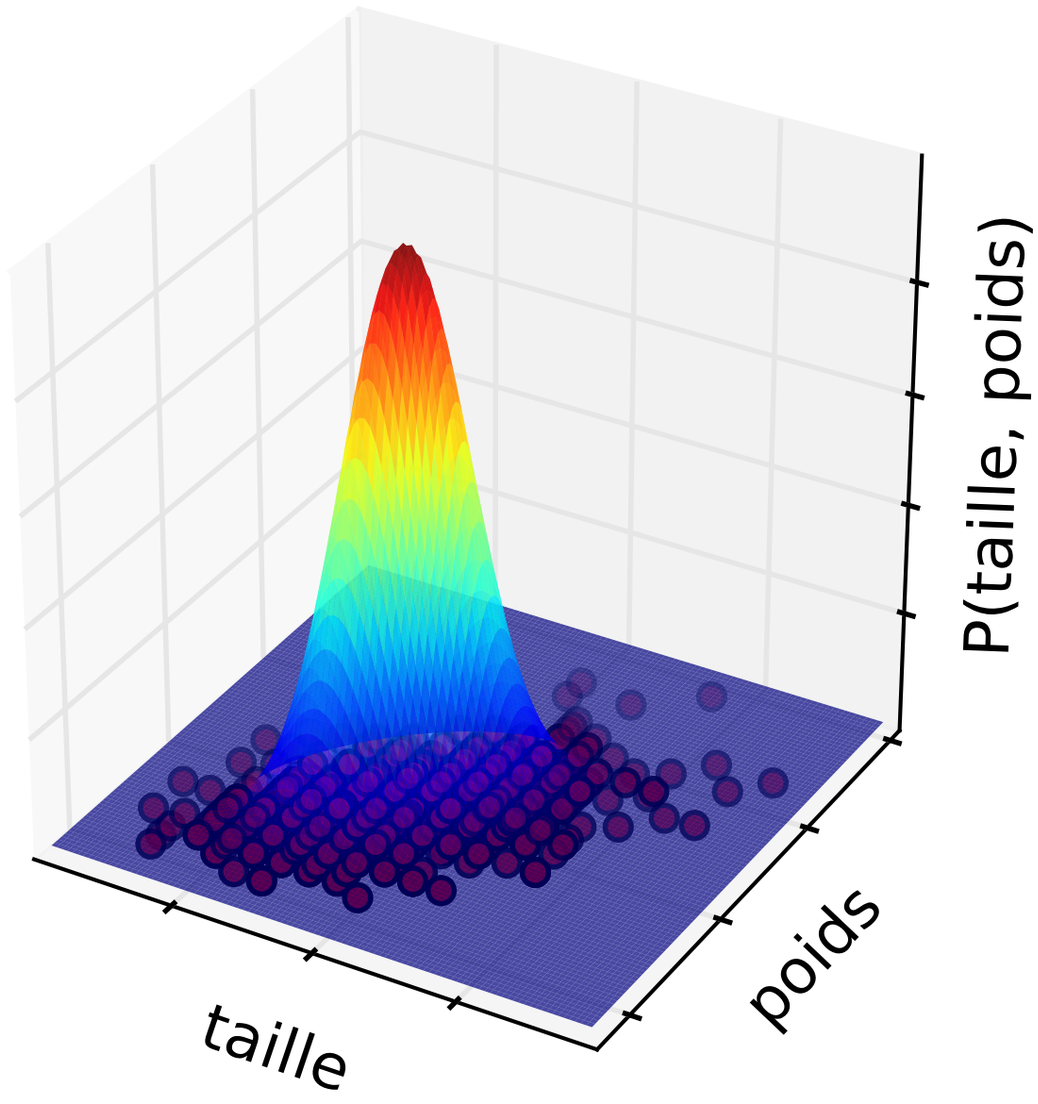




La plupart des graphiques de cette partie proviennent de la page http://www.cs.mcgill.ca/~mcleish/644/normal.html par **Erin Mcleish**

Ex. continuous vector variable x

Multivariate Gaussian/normal distribution



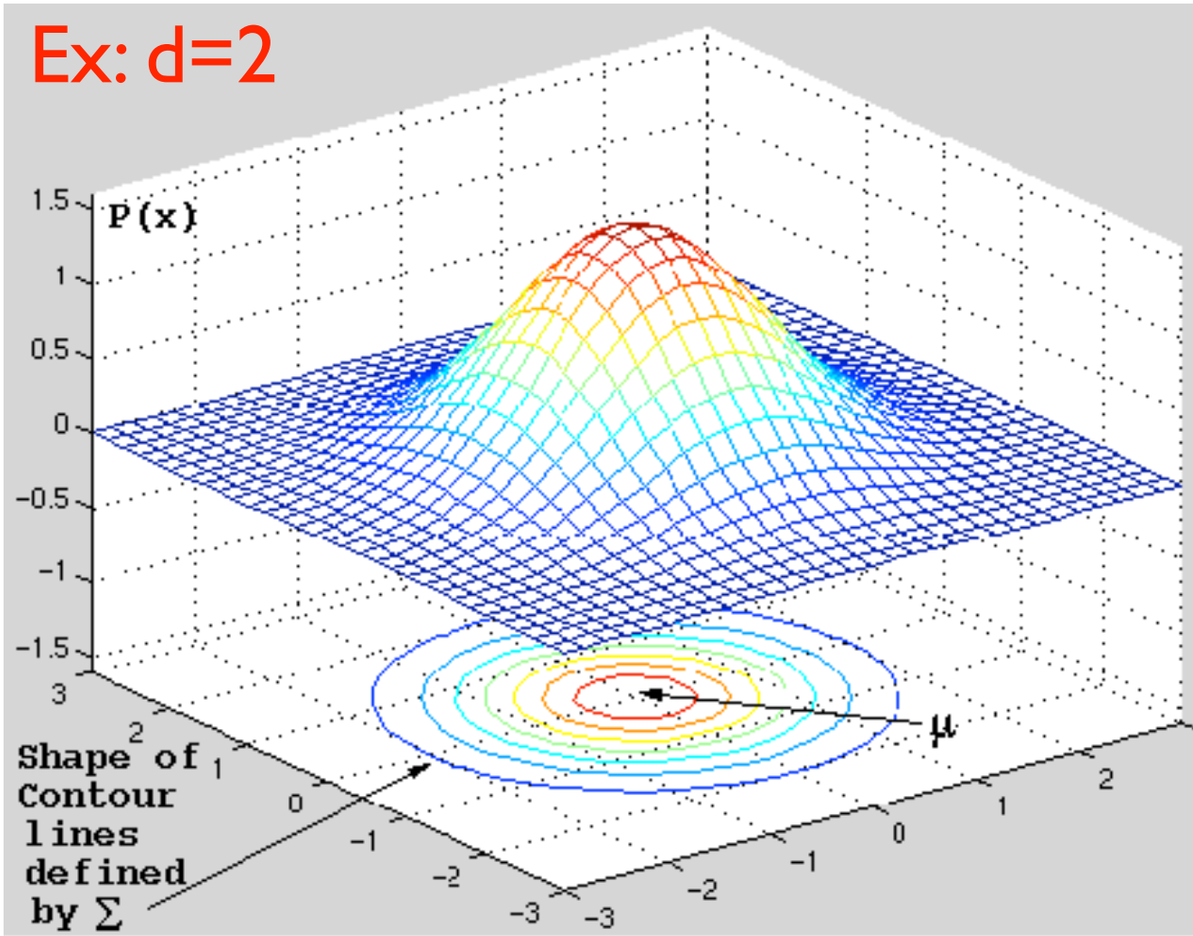
Multivariate Gaussian

Isotropic ("spherical") Gaussian in *d* dimensions:

$$p(x) = \mathcal{N}_{\mu,\sigma^2}(x) = \frac{1}{(2\pi)^{\frac{d}{2}}\sigma^d} e^{-\frac{1}{2}\frac{\|x-\mu\|^2}{\sigma^2}}$$

Gaussian "hill" ***"centered"*** *in* μ *with* ***"width"*** σ*, (same width in all directions)*

Ex: d=2



General Gaussian distribution in *d* dimensions, with mean μ and covariance matrix Σ.

$$p(x) = \mathcal{N}_{\mu,\Sigma}(x) = \frac{1}{(2\pi)^{\frac{d}{2}}\sqrt{|\Sigma|}} e^{-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)}$$

determinant of Σ

$$\mu = \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_d \end{bmatrix} \qquad \Sigma = \begin{bmatrix} \sigma_{11} & \cdots & \sigma_{1d} \\ \vdots & & \vdots \\ \sigma_{d1} & \cdots & \sigma_{dd} \end{bmatrix}$$

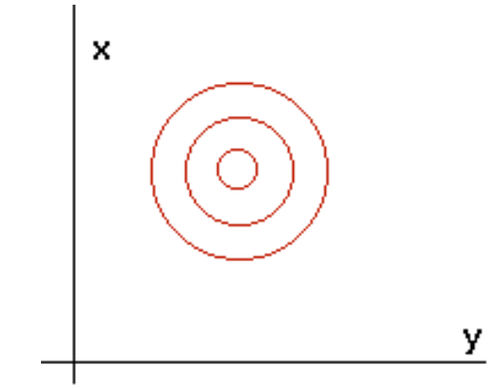
Note: this denominator is only the normalization constant (assuring that the density integrates to 1).

Multivariate Gaussian

example of covariance matrices

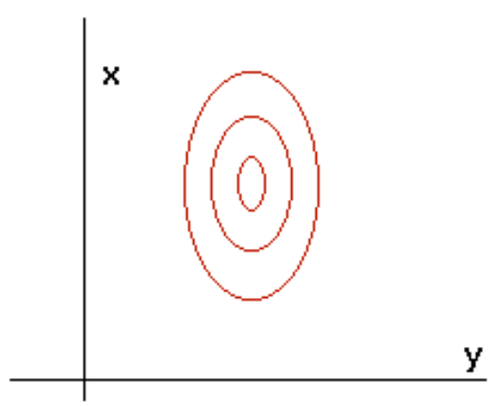
- Isotropic/spherical Gaussian: $\Sigma = \sigma^2 I$

  (I is the identity matrix)



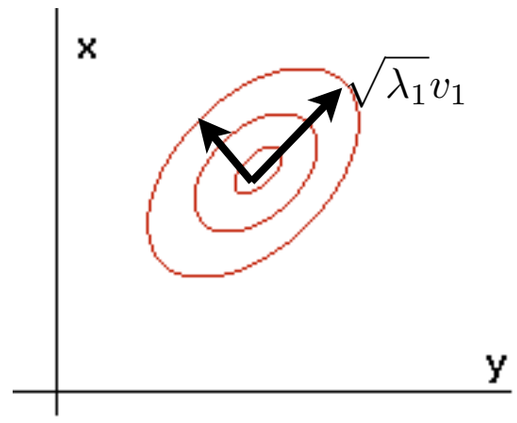
- Diagonal Gaussian:

$$\Sigma = \begin{pmatrix} \sigma_1^2 & & 0 \\ & \sigma_2^2 & \\ 0 & & \ddots \\ & & & \sigma_d^2 \end{pmatrix}$$



- Eigendecomposition:

$$\Sigma = \sum_{i=1}^{d} \lambda_i v_i v_i^T$$



The eigenvectors correspond to the ellipsoid axes, and the eigenvalues to the corresponding widths…

The determinant $|\Sigma| = \lambda_1 \lambda_2 \ldots \lambda_d$ *gives the "size" of the ellipsoid…*

Multivariate Gaussian

Learning the parameters

- We can easily learn the parameters of a Gaussian distribution from a data set:

- μ is estimated by the empirical mean ("centroid" of the training points).

$$\mu = \frac{1}{n}\sum_{t=1}^{n} \mathbf{x}_t$$

- Σ is estimated by the empirical covariance matrix:

$$\Sigma_{ij} = \frac{1}{n}\sum_{t=1}^{n}(\mathbf{x}_{ti} - \mu_i)(\mathbf{x}_{tj} - \mu_j) \quad \text{or} \quad \Sigma = \frac{1}{n}\sum_{t=1}^{n}(\mathbf{x}_t - \mu)(\mathbf{x}_t - \mu)'$$

- We will see later in the course how to derive these formulas *(maximum likelihood principle)*.