IFT6390
Fondements de l'apprentissage machine

Density estimation
Maximum Likelihood Estimation

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Probabilistic approach to learning

- We assumed that the data is generated by an unknown process.
- X, Y is seen as a pair of random variables, distributed according to an unknown probability law P (X,Y).
- X (a vector variable) is itself seen as a set of scalar random variables.

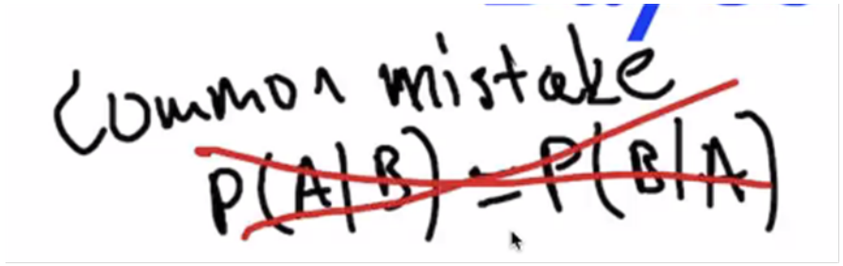
$$P(X,Y) = P(X_{[1]}, \ldots, X_{[d]}, Y)$$

Probability

(what you should be familiar with)

- Discrete and continuous random variables
- Joint probability distribution
- Marginal distribution, marginalization
- Conditionnal probability
- Bayes Rule
- Independence

Bayes Rule



$$P(A|B) = \frac{P(B|A)\,P(A)}{P(B)}$$

Thomas Bayes
1702 - 1761

Homework 1

Operation on distribution

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.

To handle the missing value. ie To get the most likely value

- 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*).

Parametric methods

Objective:

It is density estimation, so no Y

- Estimate the density $p(x)$ given an iid dataset $D_n = (X_1, X_2, \ldots, X_n)$ drawn from p (p is either a discrete probability or a pdf)

We use a parametric density $p(\mathbf{x}) = p(\mathbf{x}|\theta)$

- θ: vector of parameters (ex: probability of landing on heads for a biased coin, mean and variance for a Gaussian distribution, ...)

Maximum likelihood estimation

- To find the *unknown* parameters, we find the value of θ which maximizes the probability of the data

Maximum Likelihood Principle

Likelihood of θ with respect to the dataset D_n :

$$p(D_n|\theta) = p(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n|\theta) = \prod_{i=1}^{n} p(\mathbf{x}_i|\theta)$$

Joint distribution over the $\mathbf{x}_i$

The $\mathbf{x}_i$ are independent (i.i.d. assumption)

Log-likelihood of θ with respect to the dataset D_n :

$$\mathcal{L}(\theta) = \log p(D_n|\theta) = \sum_{i=1}^{n} \log p(\mathbf{x}_i|\theta)$$

Sums are often easier to deal with than products (e.g., derivatives)

Maximum Likelihood Estimation

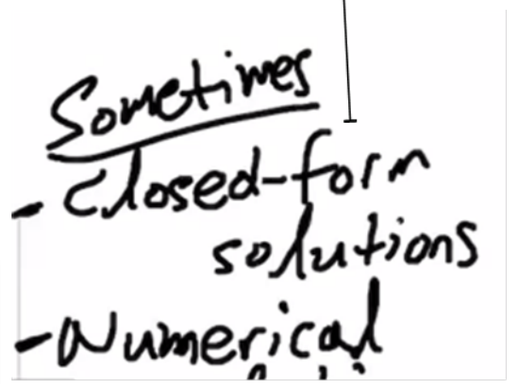
- We look for the value of θ (parameters) which maximizes the likelihood:

$$\widehat{\theta} = \arg\max_{\theta} p(D_n|\theta) = \arg\max_{\theta} \prod_{i=1}^{n} p(\mathbf{x}_i|\theta)$$

$$= \arg\max_{\theta} \sum_{i=1}^{n} \log p(\mathbf{x}_i|\theta) = \arg\max_{\theta} \mathcal{L}(\theta)$$

Maximum likelihood estimate of θ

We solve and find the perfect solution in one shot - Matrix solving

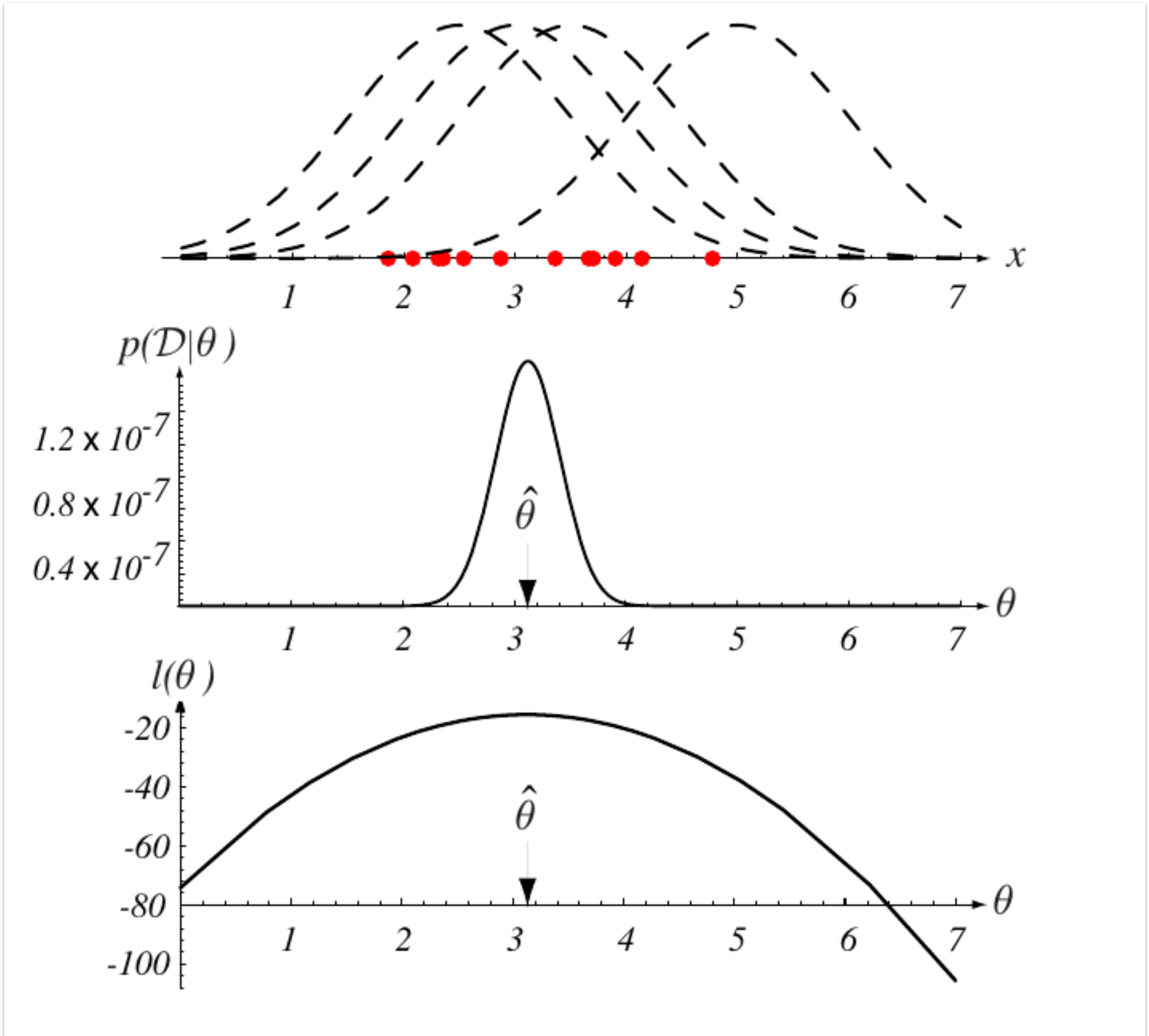


Numerical --> Gradient Descent

- Necessary condition: $\nabla_\theta \mathcal{L}(\theta) = \sum_{i=1}^{n} \nabla_\theta \log p(\mathbf{x}_i|\theta) = \mathbf{0}$

(more on this next week)

Maximum Likelihood Estimation



Exercise: Multivariate Gaussian

- We can easily learn the parameters of a Gaussian distribution from a data set:
  - The maximum likelihood estimate of μ is the empirical mean ("centroid" of the training points).

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

  - The maximum likelihood estimate of Σ is the empirical covariance matrix:

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

=> Try to show these formulas by yourself!