### Computational Statistics with Python

Topics 6-7: Monte Carlo integration and approximation - The EM algorithm

**Expected lecture time: 4 hours** 

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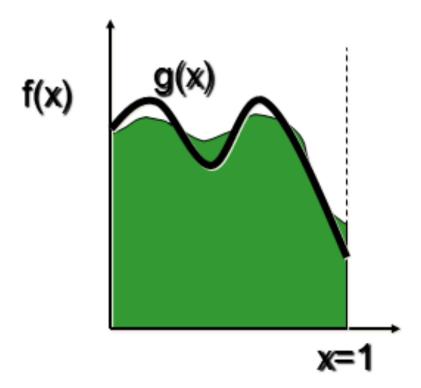
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### Other Monte Carlo numerical

### algorithms

### **Numerical integration**

- What is Monte Carlo integration?
- Monte Carlo integration is a technique for numerical integration using random numbers.
- It is a particular Monte Carlo method that computes definite integrals.
- One can use numerical approximation like the trapezium rule or the Simpson rule using quadratic polynomials g(x):  $\int_0^1 f(x)dx \approx \int_0^1 g(x)dx.$



• Python has many numerical integration

### functions:

- The scipy.integrate sub-package provides several integration techniques including an ordinary differential equation integrator. An overview of the module is provided by the help command
- quad -- General purpose integration.
- dblquad -- General purpose double integration.
- tplquad -- General purpose triple integration.
- fixed\_quad -- Integrate func(x) using Gaussian quadrature of order n.
- quadrature -- Integrate with given tolerance using Gaussian quadrature.
- romberg -- Integrate func using Romberg integration.
- trapz -- Use trapezoidal rule to compute integral from samples.
- cumtrapz -- Use trapezoidal rule to cumulatively compute integral.
- simps -- Use Simpson's rule to compute integral from samples.
- romb -- Use Romberg Integration to compute integral from

(2\*\*k + 1)
evenly-spaced samples

• See

https://docs.scipy.org/doc/scipy/reference/tutorial/integr

(https://docs.scipy.org/doc/scipy/reference/tutorial/integ for details.

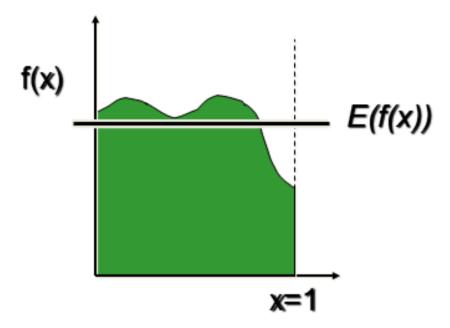
- These MC methods have some advantages:
  - They converges fast for smooth integrands.
  - Work well for low dimensions.
  - Are deterministic.
- ...But also have some disadvantages:
  - Not rapid convergence for discontinuities.
  - Sometimes they cannot deal with infinite bounds.
  - Can give untrustworthy results.

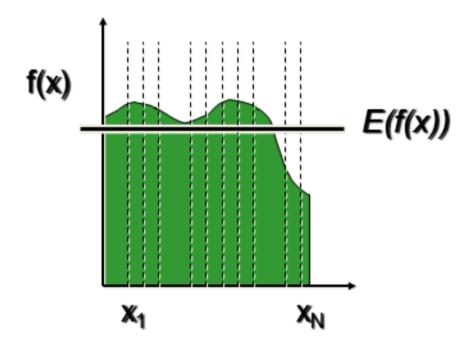
# Other Monte Carlo numerical algorithms

### **Numerical integration**

- Instead of using numerical approximation, one can average :  $\int_0^1 f(x)dx \approx E[f(x)](!!)$
- One can simply use the following approximation where n values from r.v.  $X_i$  are drawn independently from density f(x):

$$\int_0^1 f(x)dx \approx \frac{1}{n} \sum_{i=1}^n f(x_i).$$





- Consider the value  $\theta$  of the simple integral:  $\theta = \int_0^1 f(x)dx$ .
- The definition of the expectation of a function on a random variable X in the (0, 1) support is:  $E[f(X)] = \int_0^1 f(x)p(x)dx$ , where p(X) is the density of X.

• In particular, if *X* is uniformly distributed in (0, 1), then we can write:

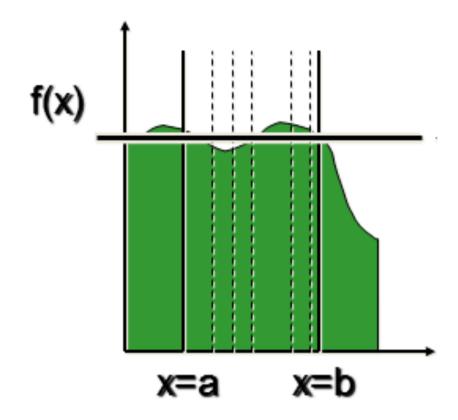
$$E[f(X)] = \int_0^1 f(x)dx = \theta.$$

# Other Monte Carlo numerical algorithms

### **Numerical integration**

• In domains other than (0, 1) we have, for example in (a, b):

$$\int_a^b f(x)dx \approx \frac{b-a}{n} \sum_{i=1}^n f(x_i).$$



- We can also use the *classical (crude) Monte Carlo integration*. How?
- Suppose  $(\xi_1, \xi_2, \dots, \xi_n)$  are independent random variables uniformly distributed.
- Then  $f_i = f(\xi_i)$  are random variates with expected values  $\theta$ , and:

$$\bar{f} = \frac{1}{n} \sum_{i=1}^{n} f_i$$

can be considered an "unbiased estimator" of  $\theta$  with variance:

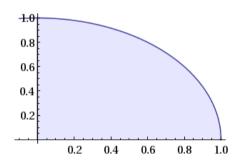
$$E[\bar{f} - \theta]^2 = \frac{1}{n-1} \int_0^1 [f(x) - \theta]^2 dx.$$

**Numerical integration**: silly example

• Suppose we want to solve (answer:  $\frac{\pi}{4}$ ):

$$\int_0^1 \sqrt{1-x^2} dx$$

which is the area of a unit-radius quarter-circle):



• This is equivalent to

$$\int_0^1 \sqrt{1 - x^2} dx = \int_0^1 \sqrt{1 - x^2} \cdot 1 dx = \int_0^1 \sqrt{1 - x^2} p(x) dx$$

$$= \int_0^1 \sqrt{1 - x^2} dx = \int_0^1 \sqrt{1$$

=  $E[\sqrt{1-X^2}]$  [where X has density  $p(\cdot) \sim U(0,1)$ ] = I

where  $f(x) = \sqrt{1 - x^2}$ . The problem is equivalent to evaluating:

$$\theta = E[f(X), X \sim U(0, 1), f(x) = \sqrt{1 - x^2}.$$

• We can generate  $(X_1, X_2, \dots, X_n) \sim U(0, 1)$ ,

then estimate  $\theta$  by:

$$\hat{\theta} = \frac{1}{n} \sum_{i=1}^{n} f(X_i).$$

- 0.7837464705688125
- 0.7853981633974483

# Other Monte Carlo numerical algorithms

MC integration: generalization

• The example before can be generalized when:

$$\theta = E[f(X)],$$

where X has a density p not necessarily uniform.

• For example, let's take a r.v. X distributed as a standard Cauchy with pdf  $p(x; 0, 1) = \frac{1}{\pi(1+x^2)}$  and parameters 0 and 1.

• We can write, with  $f(X) = I_{X>2}(X)$ :

$$E[f(X)] = E[I_{X>2}(X)] = \int_{-\infty}^{\infty} I_{X>2}(X) \frac{1}{\pi(1+x^2)} dx$$
$$= \int_{2}^{\infty} \frac{1}{\pi(1+x^2)} dx = \theta,$$

where *X* is Cauchy.

• Note that the method can be generalized to higher dimension:

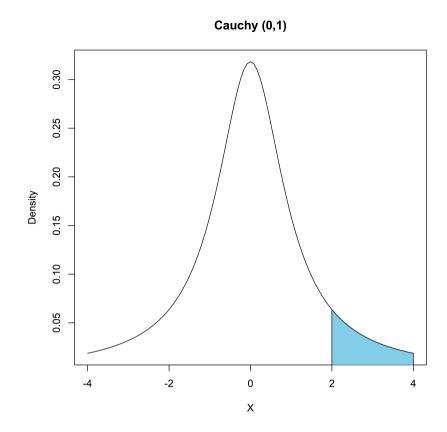
$$\int_0^1 \int_0^1 f(x_1, x_2) dx_1 dx_2 = E[f(X_1, X_2)],$$

with  $X_1, X_2 \stackrel{\text{i.i.d}}{\sim} U(0, 1)$ .

# Other Monte Carlo numerical algorithms

MC integration: Cauchy integral

• Suppose we want to compute the integral of a Cauchy(0,1) for  $X \ge 2$ :



i.e. the following integral:

$$\theta = \int_2^\infty \frac{1}{\pi (1 + x^2)} dx.$$

•  $\theta$  can be computed analytically and is equal to 0.14758.

Here are other possibilities you can use to compute it in a Monte Carlo fashion.

• Solution 1.  $p \sim \text{Cauchy}, f(x) = I_{X>2}(x)$ .

$$\hat{\theta}_1 = \frac{\#\{x_i > 2, 1 \le i \le n\}}{n} = \text{(proportion of } x_i > 2\text{)}.$$

$$var(\hat{\theta}_1) = \frac{\theta(1 - \theta)}{n} \approx \frac{0.14758 \times (1 - 0.14758)}{n} = \frac{0.126}{n}$$

since  $n\hat{\theta}_1 \sim \text{Bin}(n, \theta)$ .

• Solution 2.  

$$\theta = P(X > 2) = \frac{1}{2}P(|X| > 2) = \frac{1}{2}E[I_{|X| > 2}(x)].$$

$$\hat{\theta}_{2} = \frac{1}{2}\frac{\#\{|x_{i}| > 2, 1 \le i \le n\}}{n} = \frac{1}{2}(\text{proportion of }|x_{i}| > var(\hat{\theta}_{2})) = \frac{n(2\theta)(1 - 2\theta)}{(2n)^{2}} = \frac{\theta(1 - \theta)}{2n} \approx \frac{0.052}{n}$$

(since  $2n\hat{\theta}_2 \sim \text{Bin}(n, 2\theta)$ ), an improvement with respect to the previous result.

# Other Monte Carlo numerical algorithms

MC integration: Cauchy integral (cont'd)

• Solution 3. Another option is:

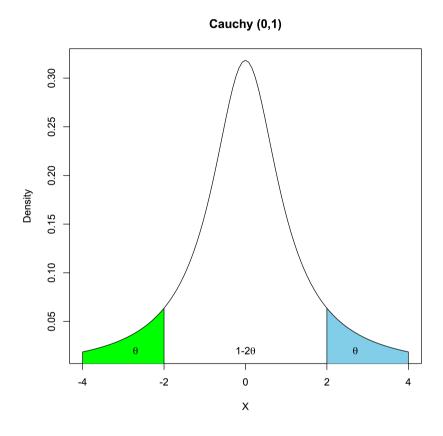
$$1 - 2\theta = \int_{-2}^{2} p(x)dx = 4 \int_{0}^{2} p(x) \cdot \frac{1}{2} dx$$
$$= 4 \int_{0}^{2} \frac{1}{2} \frac{1}{\pi(1+y^{2})} dy = 4E[f(Y)]$$

where  $Y \sim U(0, 2)$ . So,  $\theta = \frac{1}{2} - 2E[f(Y)]$ .

• Then:

$$\hat{\theta}_3 = \frac{1}{2} - 2 \cdot \frac{1}{n} \sum_{i=1}^n f(Y_i), \ Y_1, \dots, Y_n \overset{\text{i.i.d.}}{\sim} U(0, 2)$$
$$var(\hat{\theta}_3) = \frac{4}{n} var(f(Y_1)) \approx \frac{0.028}{n},$$

a further improvement.



• Solution 4. Let  $y = \frac{2}{x} (dx = -(2/y)^2 dy)$ , then:

$$\theta_4 = \int_2^\infty \frac{1}{\pi(1+x^2)} dx = \int_0^1 \frac{2}{\pi(4+y^2)} dy.$$

• This particular integral is in a form where it can be evaluated using crude Monte Carlo by sampling from the uniform distribution U(0, 1).

### • Another improvement.

```
In [2]: #Using quad:
    from scipy import integrate
    import numpy as np
    import math
    x2 = lambda x: 1/(math.pi *(1+ x**2))
    print(integrate.quad(x2, 2, np.inf))
    #########
    #Compare with empirical result (next slide)
```

(0.1475836176504333, 1.3085563320472785e-10)

0.14549

0.14729

```
In [5]: #Solution 3:
import numpy as np
import math
n = 100000
unif_values = np.random.uniform(0, 2, n)
f_y = (1/(math.pi*(1+unif_values**2)))
theta3 = 0.5 - 2 * (np.sum(f_y)/n)
print(theta3)
```

### 0.1473974839682871

```
In [6]: #Solution 4:
    import numpy as np
    import math
    n = 100000
    unif_values = np.random.uniform(0, 1, n)
    f_y = (2/(math.pi*(4+unif_values**2)))
    theta4 = (np.sum(f_y)/n)
    print(theta4)
```

### 0.14758846136239862

### **Importance Sampling (IS)**

- With IS we want to estimate  $\theta = \int f(x)p(x)dx = E_p[f(X)]$  (with X having pdf p) through  $\hat{\theta}_p = \frac{1}{n} \sum_{i=1}^n f(X_i)$  (with  $(X_1, \dots, X_n) \stackrel{\text{i.i.d.}}{\sim} p$ .
- The idea here is that instead of sampling directly from p, we sample from another pdf g. i.e.,  $(X_1, \ldots, X_n) \stackrel{\text{i.i.d.}}{\sim} g$ .
- Our new estimate based on this g will be:  $\hat{\theta}_g = \frac{1}{n} \sum_{i=1}^n f(X_i) \frac{p(X_i)}{g(X_i)} = \frac{1}{n} \sum_{i=1}^n \psi(X_i).$
- Note that, by setting  $\psi(x) = f(x) \frac{p(x)}{g(x)}$ :  $\theta = \int f(x)p(x)dx = \int \left[ f(x) \frac{p(x)}{g(x)} \right] g(x)dx$   $= \int \psi(x)g(x)dx$   $= E[\psi(X)], \quad X \sim g.$

### Importance Sampling (IS). Example

• Suppose we want to simulate the value of the integral:

$$\int_{4.5}^{\infty} p(u)du,$$

where  $p(\cdot)$  is the density of a r.v.  $Z \sim N(0, 1)$ .

- We know from elementary statistics that this is rather a low value (you even cannot find the value in standardized normal tables!).
- And in fact Python gives us:
- In []: from scipy.stats import norm

1-norm.cdf(4.5, loc=0, scale=1)

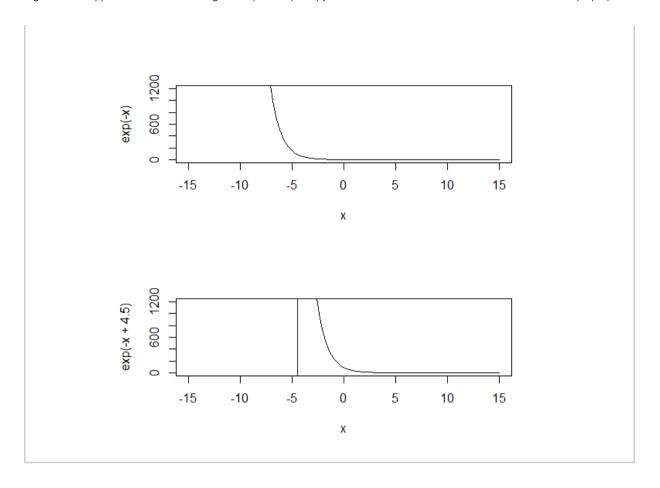
- Out []: 3.3976731247387093e-06
- This means that with crude Monte Carlo simulation we have to wait a lot before we get a hit, i.e. a simulated value greater than 4.5.

Importance Sampling (IS). Example from Robert & Casella.

- We can use importance sampling in this case, simulating r.v. values from another density g.
- Our *g* will be an exponential truncated at 4.5 which has density:

$$g(y) = e^{-(y-4.5)}$$
.

• Its graph compared with the  $\mathcal{E}xp(1)$  is the following:



Importance Sampling (IS). Example from Robert & Casella

• We draw n values  $y_i$  from g, then we calculate the ratios of the densities  $\frac{p}{g}$ , obtaining the corresponding importance sampling estimator of the tail probability:

$$\frac{1}{n} \sum_{i=1}^{n} \frac{p(Y^{(i)})}{g(Y^{(i)})} = \frac{1}{n} \sum_{i=1}^{n} \frac{\frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}Y_{i}^{2}}}{e^{(-Y_{i}+4.5)}} = \frac{1}{n} \sum_{i=1}^{n} \frac{e^{-(\frac{Y_{i}^{2}}{2}+Y_{i}-4.5)}}{\sqrt{2\pi}}$$

where the  $Y_i$ 's are iid generations from g.

• The corresponding Python code is the following producing a value remarkably close to the true value of  $3.398 \times 10^{-6}$ :

Out[7]: 3.39623384392559e-06

The Expectation-Maximization (EM) algorithm (Dempster et al., 1977; see Robert & Casella, pp. 152-163)

- An important algorithm for detecting parameter estimation of *latent* variables.
- Therefore, useful in missing data contexts, Bayesian networks, mixtures of distributions, even cluster detection.
- Quite a heavy mathematical burden, so we will use a quick definition and a toy example.
- Based on the concept of ML estimation (please revise it!).

### Other Monte Carlo numerical algorithms

### (cont'd)

### The Expectation-Maximization (EM) algorithm (cont'd)

- (EM) method is an iterative method for maximizing difficult likelihood functions in order to find MLE estimators.
- Suppose we have a random sample  $X = (X_1, \dots, X_n)$  iid from  $f(x|\theta)$ .
- We wish to find the ML estimator

$$\hat{\theta} = \arg \max_{\theta} \prod_{i=1}^{n} f(x_i | \theta) = \arg \max_{\theta} \sum_{i=1}^{n} \log f(x_i | \theta).$$

- Suppose we are in a situation where this optimization problem is difficult to solve.
- We *augment* the data, i.e. we guess that an unobservable variable is governing this likelihood problem.
- (That's why EM is suitable for missing data problems).
- We denote these unobserved or missing data with  $X^m$ , such that we get the *complete data*  $X^c = (X, X^m)$ .

The Expectation-Maximization (EM) algorithm (cont'd)

• The joint density of the complete data  $X^c$  is:

$$X^{c} = (X, X^{m}) \sim f(x^{c}) = f(x, x^{m}).$$

• The conditional density for the missing data  $X^m$  with respect to the observed data is:

$$f(x^m|x,\theta) = \frac{f(x,x^m|\theta)}{f(x|\theta)}.$$

• Rearranging terms:

$$f(x|\theta) = \frac{f(x, x^m | \theta)}{f(x^m | x, \theta)}.$$

• Taking logarithm, we get the log-likelihood:

$$\log f(X|\theta) = \log f(X^c|\theta) - \log f(X^m|X,\theta).$$

The Expectation-Maximization (EM) algorithm (cont'd)

• Finally, taking expectation with respect to  $f(x^m|x, \theta_0)$  (considering a given value for  $\theta$ ,  $\theta_0$ ) so that X can be considered constant:

$$\mathbb{E}[\log f(X|\theta)] = \mathbb{E}[\log f(X^c|\theta)|X, \theta_0] - \mathbb{E}[\log f(X^m|X,\theta)|X, \theta_0].$$

• Let's denote the log-likelihood of the complete data (which is the focus of our algorithm) with the following expression:

$$Q(\theta|\theta_0, x) = \mathbb{E}[\log f(X^c|\theta)|X, \theta_0].$$

- The EM algorithm works going across these two steps until convergence is reached:
  - 1. Expectation-step: compute  $Q(\theta|\hat{\theta}_{j-1}, x)$ ;
  - 2. Maximization-step: maximize  $Q(\theta|\hat{\theta}_{j-1}, x)$  and take  $\hat{\theta}_j = \arg\max_{\alpha} Q(\theta|\hat{\theta}_{j-1}, x)$ .

The Expectation-Maximization (EM) algorithm (cont'd)

A toy example (or, an example with toys - presented in the original paper by Dempster et al., 1977).

- We use a toy example (literally!) to explain how the EM algorithm works.
- Imagine you ask *n* kids to choose a toy out of 4 possible choices.
- Let  $Y = [Y_1, ..., Y_4]^T$  be the histogram of their n choices, i.e.  $Y_1$  is the number of kids that chose toy  $1, ..., Y_4$  is the number of kids that chose toy 4.
- What is the r.v. that models this data? A multinomial r.v.
- Therefore, the histogram is "distributed" according to a multinomial distribution.
- The multinomial has two sets of parameters: the number of trials *n* and the probabilities

 $p_1, p_2, p_3, p_4$  of choosing toys 1, 2, 3, 4, respectively.

# Other Monte Carlo numerical algorithms (cont'd)

The Expectation-Maximization (EM) algorithm (cont'd)

A toy example (or, an example with toys - cont'd).

• Therefore, the probability of seeing some particular histogram *y* is:

$$P(y|\theta) = \frac{n!}{y_1!y_2!y_3!y_4!} p_1^{y_1} p_2^{y_2} p_3^{y_3} p_4^{y_4}. (3)$$

• For this example it is assumed that the vector of probabilities p is parameterized by some hidden parameter  $\theta \in (0, 1)$  such that it can be written as:

$$[p_1 = \frac{1}{2} + \frac{1}{4}\theta, p_2 = \frac{1}{4}(1 - \theta), p_3 = \frac{1}{4}(1 - \theta), p_4 = \frac{1}{4}(\theta)]$$
  
so that  $\sum p_i = 1$ .

• The estimation problem is to guess the value of

- $\theta$  that maximizes the probability of the observed histogram.
- For this simple example, one could directly maximize the log-likelihood log  $P(y|\theta)$ , but here we will instead illustrate how to use the EM algorithm to find the MLE of  $\theta$ .

The Expectation-Maximization (EM) algorithm (cont'd)

A toy example (or, an example with toys - cont'd).

• With the parameterization above, we can write the probability in (3) as follows:

$$P(y|\theta) = \frac{n!}{y_1!y_2!y_3!y_4!} \left[\frac{1}{2} + \frac{1}{4}\theta\right]^{y_1} \left[\frac{1}{4}(1-\theta)\right]^{y_2} \left[\frac{1}{4}(1-\theta)\right]^{y_3} \left[\frac{1}{4}(1-\theta)\right]^{y_4} \left[\frac{1}{4}(1-\theta)\right]^{y_5} \left[\frac{1}{4}(1-\theta)\right]^{y_6} \left[\frac{$$

- Now, in order to properly apply EM, we need to specify what the complete data *X* is.
- To that purpose, we define the complete data as  $X = [X_1, ..., X_5]$ , with X multinomial with number of trials n and probability of each event:

$$[p_1 = \frac{1}{2}, p_2 = \frac{1}{4}\theta, p_3 = \frac{1}{4}(1-\theta), p_4 = \frac{1}{4}(1-\theta), p_5 =$$

The Expectation-Maximization (EM) algorithm (cont'd)

A toy example (or, an example with toys - cont'd).

• By defining *X* in this way, we can write the observed data *Y* as:

$$Y = T(X) = [X_1 + X_2, X_3, X_4, X_5].$$

• Therefore, the likelihood of a realization *x* of the complete data is:

$$P(x|\theta) = \frac{n!}{\prod_{i=1}^{5} x_i!} (\frac{1}{2})^{x_1} (\frac{\theta}{4})^{x_2 + x_5} (\frac{1 - \theta}{4})^{x_3 + x_4}.$$

• For the EM algorithm, we should maximize the *Q* function:

$$\theta^{(m+1)} = \underset{\theta \in (0,1)}{\operatorname{arg\,max}} Q(\theta | \theta^{(m)}) = \underset{\theta \in (0,1)}{\operatorname{arg\,max}} E_{X|y,\theta^{(m)}} [\log p(X|\theta)]$$

### Other Monte Carlo

### numerical algorithms (cont'd)

The Expectation-Maximization (EM) algorithm (cont'd)

A toy example (or, an example with toys - cont'd).

• To solve (4) for  $\theta$ , we need the terms of  $\log p(X|\theta)$  that depend on  $\theta$ , because the other terms are irrelevant for maximizing the function over  $\theta$ :

$$\theta^{(m+1)} = \underset{\theta \in (0,1)}{\arg \max} E_{X|y,\theta^{(m)}} [(X_2 + X_5) \log \theta + (X_3 + X_4) \log \theta]$$

$$= \underset{\theta \in (0,1)}{\arg \max} \left\{ \log \theta (E_{X|y,\theta^{(m)}} [X_2] + E_{X|y,\theta^{(m)}} [X_5]) + 1 \right\}$$

$$(1 - \theta)(E_{X|y,\theta^{(m)}} [X_3] + E_{X|y,\theta^{(m)}} [X_4]) \right\} (5)$$

where we have considered only terms that depend on  $\theta$ .

- To solve (5) we need the conditional expectation of the complete data X conditioned on already knowing the incomplete data y, which only leaves the uncertainty about  $X_1$  and  $X_2$ .
- But we know that  $X_1 + X_2 = y_1$ , and therefore we can say that given  $y_1$ , the pair  $X_1$ ,  $X_2$  is binomially distributed.

The Expectation-Maximization (EM) algorithm (cont'd)

A toy example (or, an example with toys - cont'd).

• Exploiting the last point in the previous slide, we end up with this conditional distribution to be plugged in (5) to solve the problem:

$$E_{X|y,\theta[X]} = \left[\frac{2}{2+\theta}y_1, \frac{\theta}{2+\theta}y_1, y_2, y_3, y_4\right].$$

• Therefore (4) becomes:

$$\theta^{(m+1)} =$$

$$= \underset{\theta \in (0,1)}{\arg \max} (\log \theta (\frac{\theta^{(m)} y_1}{2 + \theta^{(m)}} + y_4) + \log(1 - \theta)(y_2 + y_4)$$

$$= \frac{\frac{\theta^{(m)}}{2 + \theta^{(m)}} y_1 + y_4}{\frac{\theta^{(m)}}{2 + \theta^{(m)}} y_1 + y_2 + y_3 + y_4}.$$

### Suggested references and reading

- Brewer, B.J., Introduction to Bayesian Statistics. Course notes. University of Auckland.
- De Finetti, B (1931). Funzione caratteristica di un fenomeno aleatorio. Accademia dei Lincei, Roma.
- Dempster, A.P., Laird, N. M., Rubin, D. B. (1977). Maximum Likelihood from Incomplete Data via the EM Algorithm. Journal of the Royal Statistical Society, Series B. 39(1): 1-38.

Example with a mixture of Normals using the *sklearn* Gaussian Mixture class which implements the EM algorithm for fitting a mixture of normal distribution

In [2]:

from sklearn.mixture import GaussianMixture

2 **import** numpy **as** np

import matplotlib.pyplot as plt

```
X = np.array([[1, 2], [1, 4], [1, 0], [10, 2], [10, 4], [10, 0])
In [19]:
             #Each row corresponds to a single data point.
Out[19]: array([[ 1,
                       2],
                       4],
                 [ 1,
                       0],
                       2],
                 [10,
                 [10,
                       4],
                       0]])
                 [10,
In [22]:
             gm = GaussianMixture(n_components=2, random_state=0).fit(X)
             print(gm.means )
             #two 2-sized means, centres of the components
             # Predict the labels for the data samples in X using trained mo
             print(gm.predict([[0, 0], [12, 3]]))
          [[10.
                2.]
                2.]]
          [ 1.
          [1 0]
```

```
In [1]:
```

```
# To run slideshow type jupyter nbconvert /Users/giancarlomanzi
# from terminal
#/Users/giancarlomanzi/Documents/Box Sync BackUp PC Lavoro 2406
#This is to let you have larger fonts...
from IPvthon.core.display import HTML
HTML("""
<style>
div.cell { /* Tunes the space between cells */
margin-top:1em;
margin-bottom:1em;
div.text_cell_render h1 { /* Main titles bigger, centered */
font-size: 2.2em;
line-height:1.4em;
text-align:center;
div.text_cell_render h2 { /* Parts names nearer from text */
margin-bottom: -0.4em;
div.text_cell_render { /* Customize text cells */
font-family: 'Times New Roman';
font-size:1.5em;
line-height: 1.4em;
padding-left:3em;
padding-right:3em;
</style>
""")
```

### Out[1]: