Laboratory 4

In this laboratory we will focus on computing probability densities and ML estimates.

Multivariate Gaussian density

The Multivarite Gaussian (MVG) density is defined as

$$\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{\frac{M}{2}}|\boldsymbol{\Sigma}|^{\frac{1}{2}}} e^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})}$$

where M is the size of the feature vector $\boldsymbol{x}$, and $|\boldsymbol{\Sigma}|$ is the determinant of $\boldsymbol{\Sigma}$.
To avoid numerical issues due to exponentiation of large numbers, in many practical cases it's more convenient to work with the logarithm of the density

$$\log\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = -\frac{M}{2}\log 2\pi - \frac{1}{2}\log|\boldsymbol{\Sigma}| - \frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})$$

Write a function to compute the log-density `logpdf_GAU_ND(x, mu, C)` for a sample `x`. `mu` should be a numpy `array` of shape `(M, 1)`, whereas `C` is a numpy `array` of shape `(M, M)` representing the covariance matrix $\boldsymbol{\Sigma}$.

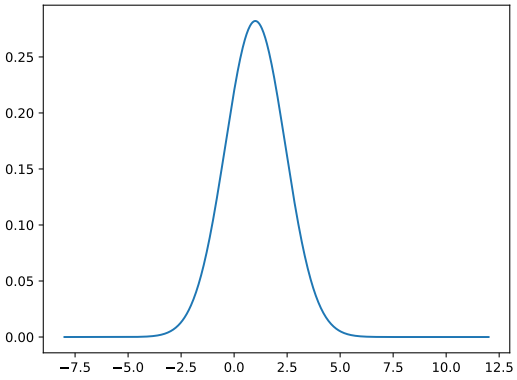
Suggestion 1: The inverse of a 2-D array `C` can be computed using `numpy.linalg.inv`. The log-determinant $\log|C|$ of `C` can be computed using `numpy.linalg.slogdet` — pay attention that the function returns **two** values, the absolute value of the log-determinant is the second one (the first is the sign of the determinant, which, for covariance matrices, is positive). Again, directly computing the logarithm of the determinant can cause numerical issues. `numpy.linalg.slogdet` performs the computations in a way that is robust also for very small values of $|C|$.

Suggestion 2: In some cases we will need to compute the log-density for a set of N samples $\boldsymbol{X} = [\boldsymbol{x}_1 \dots \boldsymbol{x}_N]$. It can be convenient to write the function `logpdf_GAU_ND` so that it takes as argument a $M \times N$ matrix `X` rather than a single sample `x`, and computes the vector of log-densities $Y = [\log\mathcal{N}(\boldsymbol{x}_1|\boldsymbol{\mu},\boldsymbol{\Sigma}) \dots \log\mathcal{N}(\boldsymbol{x}_N|\boldsymbol{\mu},\boldsymbol{\Sigma})]$. The term $\boldsymbol{x}_i$ here refers to the i-th sample, and corresponds to the i-th column of `X`.

Suggestion 3: Broadcasting and re-arranging of the computations can be used in this case to significantly speed up the computation of Y, and to avoid explicitly looping over the elements of $\boldsymbol{X}$. However, getting it right is non trivial. If you want to try you can ask for more insights. Otherwise, simply compute the array of log-densities using a loop over the columns of the data matrix `X`.

In the following we assume that `logpdf_GAU_ND(X, mu, C)` takes as input a data matrix `X` and returns a 1-D numpy array of log-densities Y. You can visualize your density — in the example we plot the density for $\mu = 1, \Sigma = 2$ (remember that these should be 1×1 numpy arrays):

```
import matplotlib.pyplot as plt
plt.figure()
XPlot = numpy.linspace(-8, 12, 1000)
m = numpy.ones((1,1)) * 1.0
C = numpy.ones((1,1)) * 2.0
plt.plot(XPlot.ravel(), numpy.exp(logpdf_GAU_ND(vrow(XPlot), m, C)))
plt.show()
```



You can also check whether your density is correct by comparing your values with those contained in `Solution/CheckGAUPdf.npy`

```
pdfSol = numpy.load('Solution/llGAU.npy')
pdfGau = logpdf_GAU_ND(vrow(XPlot), m, C)
print(numpy.abs(pdfSol - pdfGau).max())
```

The result should be zero or very close to zero (it may not be exactly zero due to numerical errors, however it should be a very small number, e.g. $\approx 10^{-17}$)

You can also check the density for the multi-dimensional case using the samples contained in `Solution/XND.npy`:

```
XND = numpy.load('Solution/XND.npy')
mu = numpy.load('Solution/muND.npy')
C = numpy.load('Solution/CND.npy')
pdfSol = numpy.load('Solution/llND.npy')
pdfGau = logpdf_GAU_ND(XND, mu, C)
print(numpy.abs(pdfSol - pdfGau).max())
```

Again, the result should be zero or close to zero.

Maximum Likelihood Estimate

The ML estimate for the parameters of a Multivariate Gaussian distribution correspond to the empirical dataset mean and the empirical dataset covariance

$$\boldsymbol{\mu}_{ML} = \frac{1}{N}\sum_{i=1}^{N} \boldsymbol{x}_i \ , \quad \boldsymbol{\Sigma}_{ML} = \frac{1}{N}\sum_{i=1}^{N} (\boldsymbol{x}_i - \boldsymbol{\mu})(\boldsymbol{x}_i - \boldsymbol{\mu})^T$$

These can be computed as in Laboratory 3. For the samples contained in `'Solution/XND.npy'` you should obtain

$$\boldsymbol{\mu}_{ML} = \begin{bmatrix} -0.07187197 \\ 0.05979594 \end{bmatrix} \ , \quad \boldsymbol{\Sigma}_{ML} = \begin{bmatrix} 0.94590166 & 0.09313534 \\ 0.09313534 & 0.8229693 \end{bmatrix}$$

We can also compute the log-likelihood for our estimates. The log-likelihood corresponds to the sum of the log-density computed over all the samples

$$\ell(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{i=1}^{n} \log \mathcal{N}(x_i | \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

Write a function to compute the log-likelihood. Using the ML estimates (`m_ML` and `C_ML` in the following code) the log-likelihood should be

```
ll = loglikelihood(XND, m_ML, C_ML)
print(ll)
```

```
-270.70478023795044
```

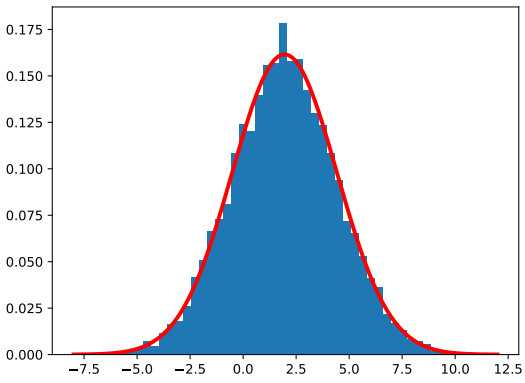
A second dataset corresponding to the file `'Solution/X1D.npy'` contains one-dimensional samples. It can be loaded with `numpy.load`. For this dataset you should obtain

$$\boldsymbol{\mu}_{ML} = \begin{bmatrix} 1.9539157 \end{bmatrix} \ , \quad \boldsymbol{\Sigma}_{ML} = \begin{bmatrix} 6.09542485 \end{bmatrix}$$

We can visualize how well the estimated density fits the samples plotting both the histogram of the samples and the density (again, `m_ML` and `C_ML` are the ML estimates):

```
plt.figure()
plt.hist(X1D.ravel(), bins=50, density=True)
XPlot = numpy.linspace(-8, 12, 1000)
plt.plot(XPlot.ravel(), numpy.exp(logpdf_GAU_ND(vrow(XPlot), m_ML, C_ML)))
```

where `m` and `C` are the ML estimates for the dataset



In this case, the log-likelihood for the ML estimates is

```
ll = loglikelihood(X1D, m_ML, C_ML)
print(ll)
```

```
-23227.07765460272
```

You can verify that computing the log-likelihood for other values of $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ would results in a lower value of the log-likelihood.