Exercise on Maximum-Likelihood Fitting

Exercise 1: This exercise concerns maximum-likelihood fitting with the minimization program MINUIT using either its python implementation iminuit. The exercise is carried out by modifying and running the program mlFit.py (or the jupyter notebook mlFit.ipynb). These can be found on the web page

https://www.pp.rhul.ac.uk/~cowan/stat/exercises/fitting/

To use python on your own computer, you will need to install the package iminuit (should just work with "pip install iminuit"). See:

https://pypi.org/project/iminuit/

Alternatively, you can run the code in google colaboratory. Please see the school's website for further information on how to access and run the software.

The program provided generates a data sample of 200 values from a pdf that is a mixture of an exponential and a Gaussian:

$$f(x;\theta,\xi) = \theta \frac{1}{\sqrt{2\pi}\sigma} e^{-(x-\mu)^2/2\sigma^2} + (1-\theta)\frac{1}{\xi} e^{-x/\xi} , \qquad (1)$$

The pdf is modified so as to be truncated on the interval $0 \le x \le x_{\text{max}}$. The program Minuit is used to find the MLEs for the parameters θ and ξ , with the other parameters treated here as fixed. You can think of θ as representing the fraction of signal events in the sample (the Gaussian component), and the parameter ξ characterizes the shape of the background (exponential) component.

- **1(a)** By default the program mlFit.py fixes the parameters μ and σ , and treats only θ and ξ as free. By running the program, obtain the following plots:
 - the fitted pdf with the data;
 - a "scan" plot of $-\ln L$ versus θ ;
 - a contour of $\ln L = \ln L_{\text{max}} 1/2$ in the (θ, ξ) plane;
 - confidence regions in the (θ, ξ) plane with confidence levels 68.3% and 95%.

From the graph of $-\ln L$ versus θ , show that the standard deviation of $\hat{\theta}$ is the same as the value printed out by the program.

From the graph of $\ln L = \ln L_{\text{max}} - 1/2$, show that the distances from the MLEs to the tangent lines to the contour give the same standard deviations $\sigma_{\hat{\theta}}$ and $\sigma_{\hat{\xi}}$ as printed out by the program.

1(b) Recall that the inverse of the covariance matrix variance of the maximum-likelihood estimators $V_{ij} = \text{cov}[\hat{\theta}_i, \hat{\theta}_j]$ can be approximated in the large sample limit by

$$V_{ij}^{-1} = -E \left[\frac{\partial^2 \ln L}{\partial \theta_i \partial \theta_j} \right] = -\int \frac{\partial^2 \ln P(\mathbf{x}|\boldsymbol{\theta})}{\partial \theta_i \partial \theta_j} P(\mathbf{x}|\boldsymbol{\theta}) d\mathbf{x} , \qquad (2)$$

where here $\boldsymbol{\theta}$ represents the vector of all of the parameters. Show that V_{ij}^{-1} is proportional to the sample size n and thus show that the standard deviations of the MLEs of all of the parameters decrease as $1/\sqrt{n}$. (Hint: write down the general form of the likelihood for an i.i.d. sample: $L(\boldsymbol{\theta}) = \prod_{i=1}^{n} f(x_i; \boldsymbol{\theta})$. There is no need to use the specific $f(x; \boldsymbol{\theta})$ for this problem.)

1(c) By modifying the line

numVal = 200

rerun the program for a sample size of n=100,400 and 800 events, and find in each case the standard deviation of $\hat{\theta}$. Plot (or sketch) $\sigma_{\hat{\theta}}$ versus n for n=100,200,400,800 and comment on how this stands in relation to what you expect.

1(d) By modifying the line

find $\hat{\theta}$ and its standard deviation $\sigma_{\hat{\theta}}$ in the following four cases:

- θ free, μ , σ , ξ fixed;
- θ and ξ free, μ , σ fixed;
- θ , ξ and σ free, μ fixed;
- θ , ξ , μ and σ all free.

Comment on how the standard deviation $\sigma_{\hat{\theta}}$ depends on the number of adjustable parameters in the fit.

1(e) Consider the case where θ and ξ are adjustable and σ and μ are fixed. Suppose that one has an independent estimate u of the parameter ξ in addition to the n=200 values of x. Treat u as Gaussian distributed with a mean ξ and standard deviation $\sigma_u=0.5$ and take the observed value u=5. Find the log-likelihood function that includes both the primary measurements (x_1,\ldots,x_n) and the auxiliary measurement u and modify the fitting program accordingly. Investigate how the uncertainties of the MLEs for θ and ξ are affected by including u.