1 Upper Limits

Consider an experiment designed to measure an unknown physical quantity $x$, which returns a value $y$ whose pdf is defined by the likelihood function

$$f(y|x) = \frac{e^{-(y-x)^2/2\sigma^2}}{\sigma \sqrt{2\pi}} \, \sigma \sqrt{2\pi} (1.1)$$

a) Suppose the experiment has been performed and the result $\hat{y}$ has been found. Calculate the frequentist upper limit $x_{UL}^{freq}$ at confidence level $\alpha$, defined by

$$\int_{\hat{y}}^{\infty} f(y|x_{UL}^{freq}) \, dy = \alpha \, . \quad (1.2)$$

You should be able to write this with the help of the inverse complementary error function $\text{erfc}^{-1}(\xi)$. Note that $\text{erfc}^{-1}(\xi)$ is positive if $0 < \xi < 1$ and negative if $1 < \xi < 2$, and that $\text{erfc}^{-1}(2-\xi) = -\text{erfc}^{-1}(\xi)$

b) Consider a Bayesian analysis with a uniform prior on $x$, so that by Bayes’s theorem, the posterior is

$$f(x|y) = \frac{f(x)}{f(y)} f(y|x) = \mathcal{A} f(y|x) \, . \quad (1.3)$$

Using the explicit form of the likelihood (1.1) and the normalization requirement

$$\int_{-\infty}^{\infty} f(x|y) \, dx = 1 \quad (1.4)$$

find the value of $\mathcal{A}$ and therefore the explicit form of the posterior $f(x|y)$.

c) Supposing again that we’ve performed the experiment and found a result $\hat{y}$, find the Bayesian upper limit $x_{UL}^{Bayes}$ at confidence level $\alpha$, defined by

$$\int_{-\infty}^{x_{UL}^{Bayes}} f(x|\hat{y}) \, dx = \alpha \quad (1.5)$$
d) For the case where \( \alpha = 0.9 \), write \( x_{\text{UL}}^{\text{freq}} \) and \( x_{\text{UL}}^{\text{Bayes}} \) explicitly in terms of \( \hat{y} \) and \( \sigma \), with any constants evaluated to three significant figures. (You’ll need to refer to the explicit value of \( \text{erfc}^{-1}(\xi) \) for a particular \( \xi \); in matplotlib you can get access to the inverse complementary error function via \texttt{from scipy.special import erfcinv}.)

e) Suppose now that \( x \) is physically constrained to be positive and let the prior be uniform for positive \( x \), so that the posterior can be written in terms of the Heaviside step function

\[
\Theta(x) = \begin{cases} 
0 & x < 0 \\
1 & x > 0 
\end{cases}
\]  

(1.6)

as

\[
f(x|y) = \frac{f(x)}{f(y)} f(y|x) = \mathcal{B} \Theta(x) f(y|x).
\]  

(1.7)

Use the normalization condition

\[
1 = \int_{0}^{\infty} f(x|y) \, dx = \mathcal{B} \int_{0}^{\infty} f(y|x) \, dx
\]  

(1.8)

to find the value of \( \mathcal{B} \) and therefore the explicit form of \( f(x|y) \).

f) Supposing again that we’ve performed the experiment and found a result \( \hat{y} \), calculate the Bayesian upper limit \( x_{\text{UL}}^{\text{Bayes}+} \) associated with the posterior (1.7), defined by

\[
\int_{0}^{x_{\text{UL}}^{\text{Bayes}+}} f(x|\hat{y}) \, dx = \alpha
\]  

(1.9)

2 Marginalization and the Inverse Fisher Matrix

Consider two variables \( X_1 \) and \( X_2 \) whose joint pdf is a Gaussian with zero mean:

\[
f(x) = \frac{\sqrt{\det F}}{2\pi} \exp \left[ -\frac{1}{2} x^T F x \right] = \frac{\sqrt{F_{11}F_{22} - F_{12}^2}}{2\pi} \exp \left[ -\frac{1}{2} \frac{F_{11}}{2} (x_1)^2 - F_{12} x_1 x_2 - \frac{F_{22}}{2} (x_2)^2 \right]
\]  

(2.1)

where \( F \) is some symmetric, positive definite matrix.

a) Show that \( F \) is indeed the Fisher matrix.

b) Marginalize over \( x_2 \) and show that the resulting pdf for \( x_1 \) is a Gaussian whose variance is the \( 1,1 \) component of the inverse Fisher matrix \( F^{-1} \):

\[
f_{X_1}(x_1) = \int_{-\infty}^{\infty} f(x_1, x_2) \, dx_2 = \frac{1}{\sqrt{2\pi (F^{-1})_{11}}} \exp \left( -\frac{x_1^2}{2(F^{-1})_{11}} \right)
\]  

(2.2)
Consider measurements \( \{y_i\} \) taken at times \( \{t_i\} = \{-1, 0, 1, 2\} \). We wish to fit these measurements with a straight-line model with predicted expectation values \( \mu_i = \lambda_1 + \lambda_2 t_i \). The model predicts measurements which differ from \( \mu_i \) by uncorrelated Gaussian errors with standard deviations \( \{\sigma_i\} = \{\sqrt{2}, 1, \sqrt{2}, \sqrt{3}\} \).

a) Find the matrix \( A \) describing the linear relationship \( \mu = A\lambda \), i.e.,

\[
\begin{pmatrix}
\mu_1 \\
\mu_2 \\
\mu_3 \\
\mu_4
\end{pmatrix} = A \begin{pmatrix}
\lambda_1 \\
\lambda_2
\end{pmatrix}
\]  

b) Since the errors are uncorrelated, the standard deviations are described by a matrix

\[
\sigma = \begin{pmatrix}
\sigma_1 & 0 & 0 & 0 \\
0 & \sigma_2 & 0 & 0 \\
0 & 0 & \sigma_3 & 0 \\
0 & 0 & 0 & \sigma_4
\end{pmatrix}
\]  

Construct the matrix \( A^T \sigma^{-2} A \) and find its inverse \( [A^T \sigma^{-2} A]^{-1} \). (Since it is a \( 2 \times 2 \) matrix, you should actually be able to invert it by hand.)

c) In class we showed that if the measured values are \( y \), the maximum likelihood estimates of the parameters will be \( \hat{\lambda}(y) = [A^T \sigma^{-2} A]^{-1} A^T \sigma^{-2} y \). Work out the elements of the matrix appearing for this problem in

\[
\begin{pmatrix}
\hat{\lambda}_1 \\
\hat{\lambda}_2
\end{pmatrix} = [A^T \sigma^{-2} A]^{-1} A^T \sigma^{-2} \begin{pmatrix}
y_1 \\
y_2 \\
y_3 \\
y_4
\end{pmatrix}
\]

d) Suppose we measure \( \{y_i\} = \{1.07241020, 0.40438919, 2.89906726, 8.98526374\} \). Calculate, to three significant figures,

i) The best-fit parameters \( \hat{\lambda}_1 \) and \( \hat{\lambda}_2 \)

ii) The \( \chi^2 \) value relating the data to the best-fit model,

\[
\chi^2 = (y - A\hat{\lambda})^T \sigma^{-2} (y - A\hat{\lambda})
\]

iii) The \( p \) value, i.e., probability that data generated according to the model would have a \( \chi^2 \) equal to or higher than the one observed.