Statistical Data Analysis
Discussion notes – week 7

- Problem sheet 4
- Maximum Likelihood examples

Problem sheet 4

Exercise 1(a) [2 marks] Let $x_N = \sum_{i=1}^{N} r_i$, where the r_i are independent and uniformly distributed between 0 and 1. Find the mean μ_N and standard deviation σ_N of x_N as a function of N.

1(a) [2 marks] The variable x_N is defined as

$$x_N = \sum_{i=1}^{N} r_i ,$$

where the r_i are independent and uniformly distributed on [0,1]. From the lectures (or rederive) we have the mean and variance $E[r_i] = 1/2$ and $V[r_i] = 1/12$. The expectation value of x_N is therefore

$$E[x_N] \equiv \mu_N = E\left[\sum_{i=1}^{N} r_i\right] = \sum_{i=1}^{N} E[r_i] = \sum_{i=1}^{N} \frac{1}{2} = \frac{N}{2} .$$

The variance of x_N is

$$V[x_N] = V\left[\sum_{i=1}^{N} r_i\right] = \sum_{i=1}^{N} V[r_i] = \sum_{i=1}^{N} \frac{1}{12} = \frac{N}{12}$$

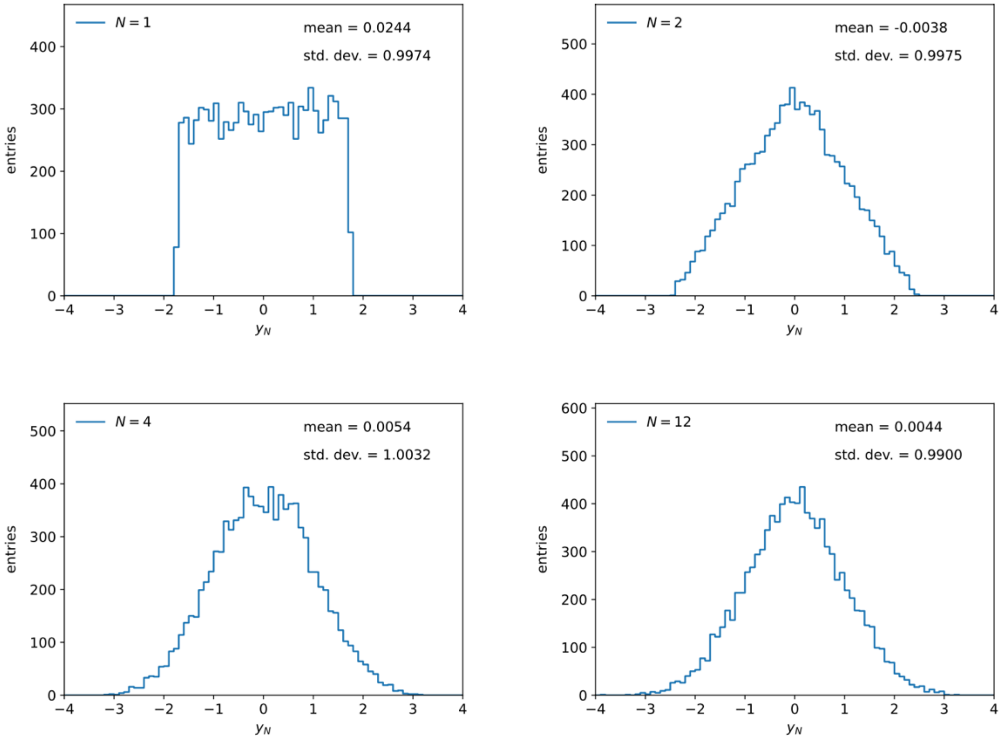
and so its standard deviation is

$$\sigma[x_N] = \sqrt{\frac{N}{12}} .$$

1(b) [5 marks] Using the results from (a), construct the standardized variable

$$y_N = \frac{x_N - \mu_N}{\sigma_N} = \sqrt{\frac{12}{N}} \left(\sum_{i=1}^{N} r_i - \frac{N}{2} \right) .$$

Using the `simpleMC` program (either C++ or Python) from problem sheet 3 as a starting point, write a computer program to make histograms of 10000 values of y_N as defined above for $N = 1, 2, 4, 12$. Make sure to set the limits of the histogram such that the entire distribution is plotted.



Histograms of y_N *for* N = 1, 2, 4, 12. The means and standard deviations are indicated on the plots. As shown, they are close to $\mu = 0$ and $\sigma = 1$, as must emerge by construction for the standardized variable y_N.

Exercise 2 Consider the pdf $f(x) = 4x^3$, $0 \leq x \leq 1$.

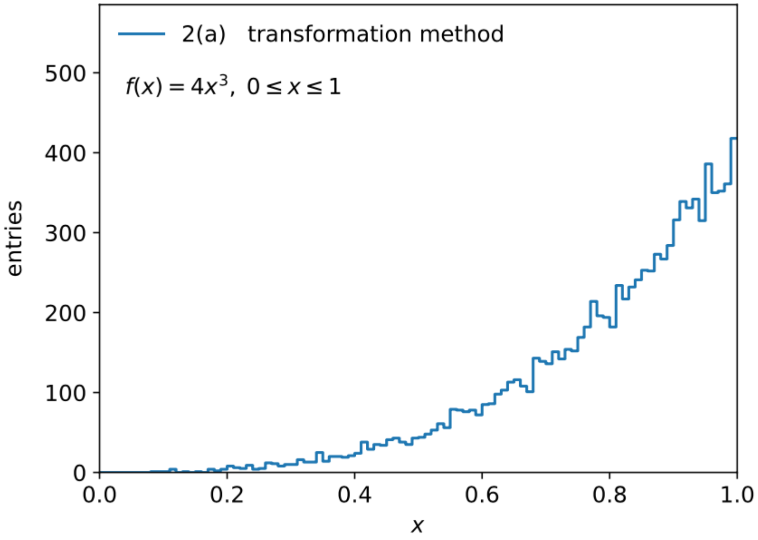
2(a) [**4 marks**] Use the transformation method to find the function $x(r)$ to generate random numbers according $f(x)$. Implement the method in a short computer program and make a histogram with 10000 values.

2(a) [4 marks] Find the transformation $x(r)$ to produce $x \sim f(x)$. First find the cumulative distribution

$$F(x) = \int_0^x 4x'^3 \, dx' = x^4 \; .$$

Set $F(x) = r$ and solving for x gives

$$x(r) = r^{1/4} \; .$$



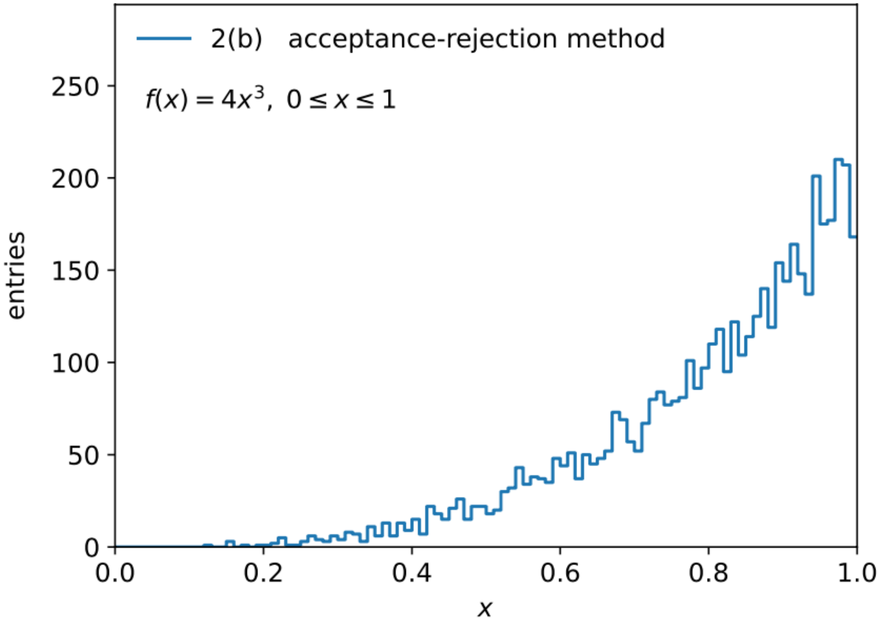
```
numVal = 10000
nBins = 100
rData = np.random.uniform(0., 1., numVal)
xMin=0.
xMax=1.
xData = pow(rData, 0.25)
xHist, bin_edges = np.histogram(xData, bins=nBins, range=(xMin, xMax))
plotHist(xHist, bin_edges, r'$x$', r'entries', r'2(a)   transformation method')
plt.figtext(0.18, 0.74, r'$f(x) = 4x^{3}, \; 0 \leq x \leq 1$')
```

2(b) [4 marks] Write a program to generate random numbers according to $f(x)$ using the acceptance-rejection technique. Plot a histogram of the results.

```
numVal = 20000
nBins = 100

def f(x):
    return 4. * x**3

xMin = 0.
xMax = 1.
fMax = 4.
r1 = np.random.uniform(0., 1., numVal)
x = xMin + r1*(xMax - xMin)
r2 = np.random.uniform(0., 1., numVal)
u = fMax*r2
xData = x[u<f(x)]
nBins = 100
xHist, bin_edges = np.histogram(xData, bins=nBins, range=(xMin, xMax))
plotHist(xHist, bin_edges, r'$x$', r'entries', r'2(b)   acceptance-rejection
method')
plt.figtext(0.18, 0.74, r'$f(x) = 4x^{3}, \; 0 \leq x \leq 1$')
```



Exercise 3 [5 marks] Suppose $\vec{x} = (x_1, \ldots, x_n)$ follows an n-dimensional Gaussian distribution $f(\vec{x}; \vec{\mu}, V)$ with $\vec{\mu} = (\mu_1, \ldots, \mu_n)$ and covariance matrix $V_{ij} = \mathrm{cov}[x_i, x_j]$. (In the formulas below regard $\vec{x}$ and $\vec{\mu}$ to be column vectors.) Suppose we have two hypotheses for the vector of means, $\vec{\mu}_0$ and $\vec{\mu}_1$, where for both one uses the same covariance matrix V, and consider the test statistic

$$t(\vec{x}) = \ln \frac{f(\vec{x}|\vec{\mu}_1)}{f(\vec{x}|\vec{\mu}_0)} \, .$$

Show that this $t(\vec{x})$ can be written in the form

$$t(\vec{x}) = w_0 + \sum_{i=1}^{n} w_i x_i \, ,$$

or equivalently $t(\vec{x}) = w_0 + \vec{w}^T \vec{x}$, where $\vec{w}$ is a column vector of coefficients w_i, $i = 1, \ldots, n$.

i.e. $f(\vec{x}|\vec{\mu}_k) = \frac{1}{(2\pi)^{n/2} |V|^{1/2}} \exp\left[-\frac{1}{2} (\vec{x} - \vec{\mu}_k)^T V^{-1} (\vec{x} - \vec{\mu}_k) \right]$

Test statistic $t(x) = \ln \frac{f(\vec{x}|\vec{\mu}_1)}{f(\vec{x}|\vec{\mu}_0)}$

Ex. 3 (cont.)

$$\ln \frac{f(\vec{x}|\vec{\mu}_1)}{f(\vec{x}|\vec{\mu}_0)} = -\frac{1}{2}\left[(\vec{x}-\vec{\mu}_1)^T V^{-1} (\vec{x}-\vec{\mu}_1) - (\vec{x}-\vec{\mu}_0)^T V^{-1} (\vec{x}-\vec{\mu}_0) \right]$$

$$= -\frac{1}{2}\Big[\vec{x}^T V^{-1} \vec{x} - \vec{\mu}_1^T V^{-1} \vec{x} - \vec{x}^T V^{-1} \vec{\mu}_1 + \vec{\mu}_1^T V^{-1} \vec{\mu}_1$$

$$- \vec{x}^T V^{-1} \vec{x} + \vec{\mu}_0^T V^{-1} \vec{x} + \underbrace{\vec{x}^T V^{-1} \mu_0}_{= \vec{\mu}_0^T V^{-1} \vec{x}} - \vec{\mu}_0^T V^{-1} \mu_0 \Big]$$

since scalar $( ) = ( )^T$

and $V^{-1} = (V^{-1})^T$

Ex. 3 (cont.)

$$= -\frac{1}{2}\underbrace{\left[\vec{\mu}_1 V^{-1}\vec{\mu}_1 - \vec{\mu}_0^T V^{-1}\vec{\mu}_0\right]}_{w_0} + \underbrace{(\vec{\mu}_1 - \vec{\mu}_0)^T V^{-1}}_{\vec{w}^T}\vec{x}$$

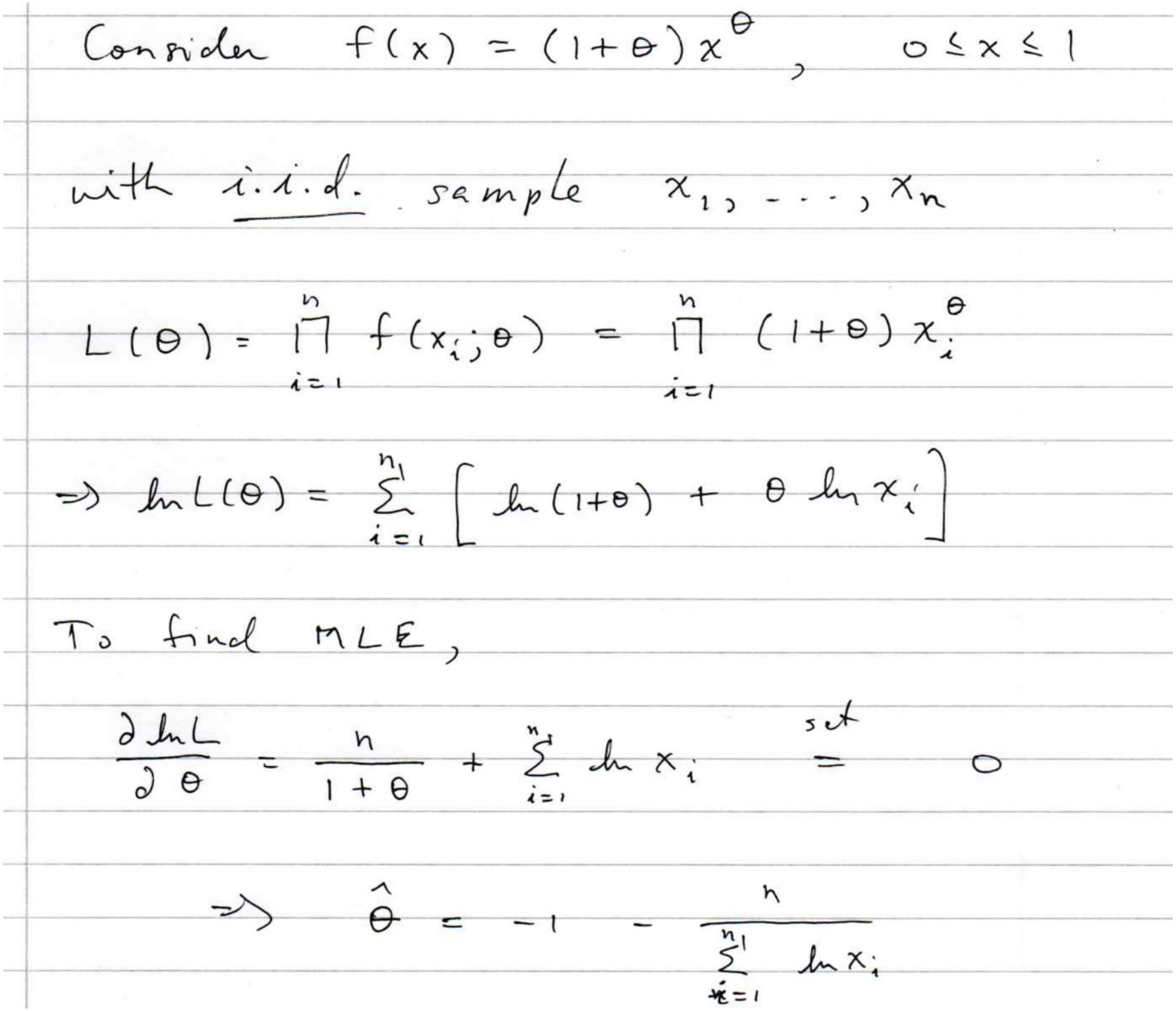
$$= w_0 + \vec{w}^T\vec{x}$$

$$\vec{w} = \left[(\vec{\mu}_1 - \vec{\mu}_0)^T V^{-1}\right]^T = \overbrace{(V^{-1})^T}^{= V^{-1}}(\vec{\mu}_1 - \vec{\mu}_0)$$

If $W = V + V$, $W^{-1} = \frac{1}{2}V^{-1}$

$$\Rightarrow \vec{w} = 2W^{-1}(\vec{\mu}_1 - \vec{\mu}_0)$$

Example of Maximum Likelihood



Consider $f(x) = (1+\theta)x^{\theta}$, $0 \leq x \leq 1$

with i.i.d. sample $x_1, \ldots, x_n$

$$L(\theta) = \prod_{i=1}^{n} f(x_i;\theta) = \prod_{i=1}^{n} (1+\theta)x_i^{\theta}$$

$$\Rightarrow \ln L(\theta) = \sum_{i=1}^{n} \left[\ln(1+\theta) + \theta \ln x_i \right]$$

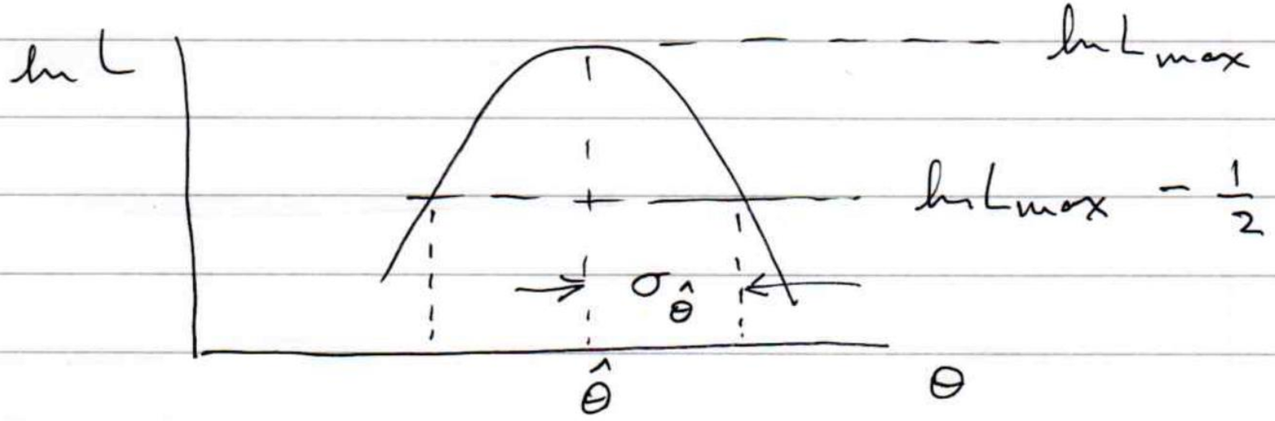
To find MLE,

$$\frac{\partial \ln L}{\partial \theta} = \frac{n}{1+\theta} + \sum_{i=1}^{n} \ln x_i \overset{\text{set}}{=} 0$$

$$\Rightarrow \hat{\theta} = -1 - \frac{n}{\sum_{i=1}^{n} \ln x_i}$$

MLE example (cont.)

For variance (graphical method)



$\sigma_{\hat{\theta}}$ found by moving θ away from $\hat{\theta}$ until $\ln L$ decreases by ½ from $\ln L_{max}$

Variance from asymptotic properties

Assume large n,

$$V[\hat{\theta}] \approx \text{MVB} = -\frac{\left(1 + \overbrace{\frac{\partial b}{\partial \theta}}^{\longrightarrow\, \approx 0}\right)^2}{E\left[\frac{\partial^2 \ln L}{\partial \theta^2}\right]}$$

$$\frac{\partial^2 \ln L}{\partial \theta^2} = -\frac{n}{(1+\theta)^2}$$ so indep. of data x_i

$$-E\left[\frac{\partial^2 \ln L}{\partial \theta^2}\right] = \frac{n}{(1+\theta)^2}$$

$$\Rightarrow \quad V[\hat{\theta}] \approx \frac{(1+\theta)^2}{n} \quad \Rightarrow \quad \sigma_{\hat{\theta}} \approx \frac{1+\theta}{\sqrt{n}}$$

Now suppose problem is parametrized using $\lambda = \exp\left[\frac{-1}{1+\theta}\right]$ → find MLE of λ.

Use $\hat{\lambda} = \lambda(\hat{\theta})$

$$\Rightarrow \hat{\lambda} = \exp\left[- \frac{1}{1 + \left(-1 - \frac{n}{\sum_{i=1}^{n} \ln x_i} \right)} \right]$$

$$= \exp\left[\frac{1}{n} \sum_{i=1}^{n} \ln x_i \right] = \exp\left[\sum_i \ln x_i^{1/n} \right]$$

$$= \prod_{i=1}^{n} x_i^{1/n}$$

Or the hard way: $\theta = -1 - \frac{1}{\ln \lambda}$

$$f(x;\lambda) = -\frac{1}{\ln \lambda} \, x^{\left(-1 - \frac{1}{\ln \lambda}\right)}$$

$$L(\lambda) = \prod_{i=1}^{n} f(x_i;\lambda)$$

$\to \ln \lambda \longrightarrow \frac{\partial \ln L}{\partial \lambda} = 0 \longrightarrow$ same $\hat{\lambda}$ as above.

Example of MLEs for two parameters

Consider two independent i.i.d. samples:

$$f(x|\theta) = \frac{1}{\theta} e^{-x/\theta} \qquad \rightarrow \qquad x_1, \ldots, x_n$$

$$g(y|\theta, \lambda) = \frac{1}{\theta\lambda} e^{-y/\theta\lambda} \qquad \rightarrow \qquad y_1, \ldots, y_m.$$

The likelihood function and its log are:

$$p(\boldsymbol{x}, \boldsymbol{y}|\theta, \lambda) = L(\theta, \lambda) = \prod_{i=1}^{n} \frac{1}{\theta} e^{-x_i/\theta} \prod_{j=1}^{m} \frac{1}{\theta\lambda} e^{-y_j/\theta\lambda}$$

$$\begin{aligned} \ln L(\theta, \lambda) &= -n \ln \theta - \sum_{i=1}^{n} \frac{x_i}{\theta} - m \ln(\theta\lambda) - \sum_{j=1}^{m} \frac{y_j}{\theta\lambda} \\ &= -(n+m) \ln \theta - m \ln \lambda - \frac{n\bar{x}}{\theta} - \frac{m\bar{y}}{\theta\lambda} \end{aligned}$$

Example of MLEs for two parameters (2)

Set the derivatives of the log-likelihood function to zero:

$$\frac{\partial \ln L}{\partial \theta} = -\frac{n+m}{\theta} + \frac{n\overline{x}}{\theta^2} + \frac{m\overline{y}}{\lambda\theta^2} = 0$$ Eq. (1)

$$\frac{\partial \ln L}{\partial \lambda} = -\frac{m}{\lambda} + \frac{m\overline{y}}{\theta\lambda^2} = 0$$ Eq. (2)

From Eq. (2), find $\lambda = \frac{\overline{y}}{\theta}$ $\longrightarrow$ use in Eq. (1)

$$-\frac{n+m}{\theta} + \frac{n\overline{x}}{\theta^2} + \frac{m}{\theta} = 0$$

Solve for the MLEs: $\hat{\theta} = \overline{x}$, $\hat{\lambda} = \frac{\overline{y}}{\overline{x}}$

Not defined if $n = 0$.

Bias of MLEs

For bias of $\hat{\theta}$ $$E[\hat{\theta}] = E\left[\frac{1}{n}\sum_{i=1}^{n} x_i\right] = \frac{1}{n}\sum_{i=1}^{n} E[x_i] = \frac{n\theta}{n} = \theta$$

so $b = E[\hat{\theta}] - \theta = 0$

Expectation of $\hat{\lambda}$ not calculable in closed form, could investigate bias with Monte Carlo study:

Find cdf $$F(x) = \int_0^x \frac{1}{\theta} e^{-x'/\theta}\, dx' = 1 - e^{-x/\theta}$$

or use $-\theta \ln r$

Set $F(x) = r\,, \quad r \sim \mathrm{U}[0,1] \quad \longrightarrow \quad x(r) = -\theta \ln(1 - r)$

Generate a data set: $$x_i = -\theta \ln r_i\ , i = 1, \ldots, n$$ $$y_j = -\theta\lambda \ln r_j\ , j = 1, \ldots, m$$ $$\longrightarrow \quad \hat{\lambda} = \frac{\overline{y}}{\overline{x}}$$

Repeat N times, estimate bias : $$b_{\hat{\lambda}} = \frac{1}{N}\sum_{i=1}^{N} \hat{\lambda}_i - \lambda$$

Depends in general on n, m, λ, θ

Covariance of MLEs from Fisher information

Find the 2nd derivatives of ln *L*

$$\frac{\partial^2 \ln L}{\partial \theta^2} = \frac{n}{\theta^2} - \frac{2n\overline{x}}{\theta^3} + \frac{m}{\theta^2} - \frac{2m\overline{y}}{\theta^3 \lambda}$$

$$\frac{\partial^2 \ln L}{\partial \theta \, \partial \lambda} = - \frac{m\overline{y}}{\theta^2 \lambda^2}$$

$$\frac{\partial^2 \ln L}{\partial \lambda^2} = \frac{m}{\lambda^2} - \frac{2m\overline{y}}{\theta \lambda^3}$$

Using

$$E[\overline{x}] = E[x] = \theta$$

$$E[\overline{y}] = E[y] = \theta \lambda$$

find expectations:

$$E\left[\frac{\partial^2 \ln L}{\partial \theta^2}\right] = \frac{n+m}{\theta^2} - \frac{2n}{\theta^2} - \frac{2m}{\theta^2} = - \frac{n+m}{\theta^2}$$

$$E\left[\frac{\partial^2 \ln L}{\partial \theta \, \partial \lambda}\right] = \frac{n+m}{\theta^2} - \frac{2n}{\theta^2} - \frac{2m}{\theta^2} = - \frac{m}{\theta \lambda}$$

$$E\left[\frac{\partial^2 \ln L}{\partial \lambda^2}\right] = \frac{m}{\lambda^2} - \frac{2m}{\lambda^2} = - \frac{m}{\lambda^2}$$

Covariance of MLEs from Fisher information (2)

$$I = \begin{pmatrix} \frac{n+m}{\theta^2} & \frac{m}{\theta\lambda} \\ \frac{m}{\theta\lambda} & \frac{m}{\lambda^2} \end{pmatrix} \qquad \det I = \frac{nm}{\theta^2 \lambda^2}$$

$$V[\hat{\theta}] \qquad \mathrm{cov}[\hat{\theta}, \hat{\lambda}]$$

$$V \approx I^{-1} = \frac{\theta^2 \lambda^2}{nm} \begin{pmatrix} \frac{m}{\lambda^2} & -\frac{m}{\theta\lambda} \\ -\frac{m}{\theta\lambda} & \frac{n+m}{\lambda^2} \end{pmatrix} = \begin{pmatrix} \frac{\theta^2}{n} & -\frac{\theta\lambda}{m} \\ -\frac{\theta\lambda}{m} & \lambda^2 \left(\frac{n+m}{nm} \right) \end{pmatrix}$$

$$V[\hat{\lambda}]$$

For *estimates* of the covariances, evaluate with the MLEs.

MLE for number of taxis

The number plate of taxis in every canton in Switzerland ends with a number N from 1 to N_{tot}, where N_{tot} is the total number of taxis.

Model the probability for observing plate number N with

$$P(N|N_{\text{tot}}) = \frac{1}{N_{\text{tot}}}, \quad 1 \leq N \leq N_{\text{tot}}$$

MLE for N_{tot}

Suppose you observe one taxi at random with plate number N.

The likelihood function is $L(N_{\mathrm{tot}}) = \dfrac{1}{N_{\mathrm{tot}}}\,, \quad N_{\mathrm{tot}} \geq N$

which is maximized for $\widehat{N}_{\mathrm{tot}} = N$

The expectation value and bias of the MLE are

$$E[\widehat{N}_{\mathrm{tot}}] = E[N] = \sum_{N=1}^{N_{\mathrm{tot}}} \frac{N}{N_{\mathrm{tot}}} = \frac{N_{\mathrm{tot}}+1}{2} \qquad b = \frac{1-N_{\mathrm{tot}}}{2}$$

For better estimators, see similar problem with tanks in WW2:
https://en.wikipedia.org/wiki/German_tank_problem

E.g. the minimum-variance unbiased estimator is: $\widehat{N}_{\mathrm{tot}} = 2N - 1$

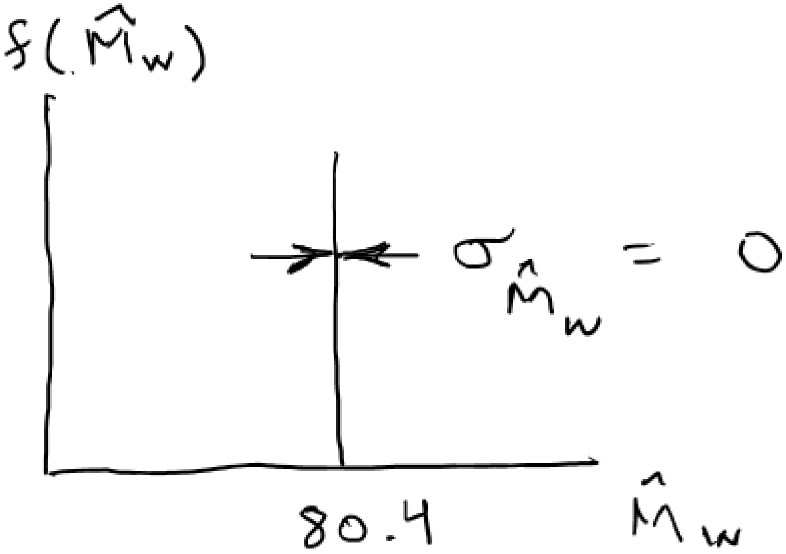
Cheap estimator for mass of W boson

The Particle Physics community has spent huge sums trying to estimate the mass of the W boson with the smallest possible statistical and systematic uncertainty.

Here is an estimator with zero statistical uncertainty. And it's free!

$$\widehat{M}_W = 80.4\,\mathrm{GeV}$$

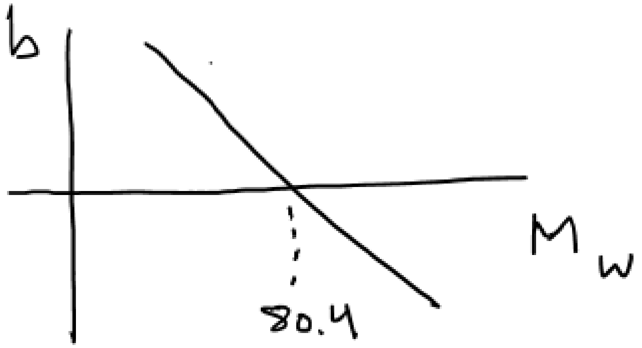
Here is its sampling distribution:



Does this violate the information inequality?

Cheap estimator for mass of W boson (2)

This estimator's bias is $b = E[\widehat{M_W}] - M_W = 80.4\,\mathrm{GeV} - M_W$



Note best estimate of M_W is (in 2020) 80.379±0.012 GeV, so the numerical value of the bias may be fairly small.

But we have $\frac{\partial b}{\partial M_W} = -1$ and so

$$\mathrm{MVB} = -\left(1 + \frac{\partial b}{\partial M_W}\right)^2 \Bigg/ E\left[\frac{\partial^2 \ln L}{\partial M_W^2}\right] = 0$$

So the information inequality is still satisfied.

Extended ML example

Consider two types of events (e.g., signal and background) each of which predict a given pdf for the variable x: $f_s(x)$ and $f_b(x)$.

We observe a mixture of the two event types, signal fraction $= \theta$, expected total number $= \nu$, observed total number $= n$.

Let $\mu_{\rm s} = \theta\nu\,,\ \mu_{\rm b} = (1-\theta)\nu\,,$ goal is to estimate μ_s, μ_b.

$$f(x; \mu_{\rm s}, \mu_{\rm b}) = \frac{\mu_{\rm s}}{\mu_{\rm s} + \mu_{\rm b}} f_{\rm s}(x) + \frac{\mu_{\rm b}}{\mu_{\rm s} + \mu_{\rm b}} f_{\rm b}(x)$$

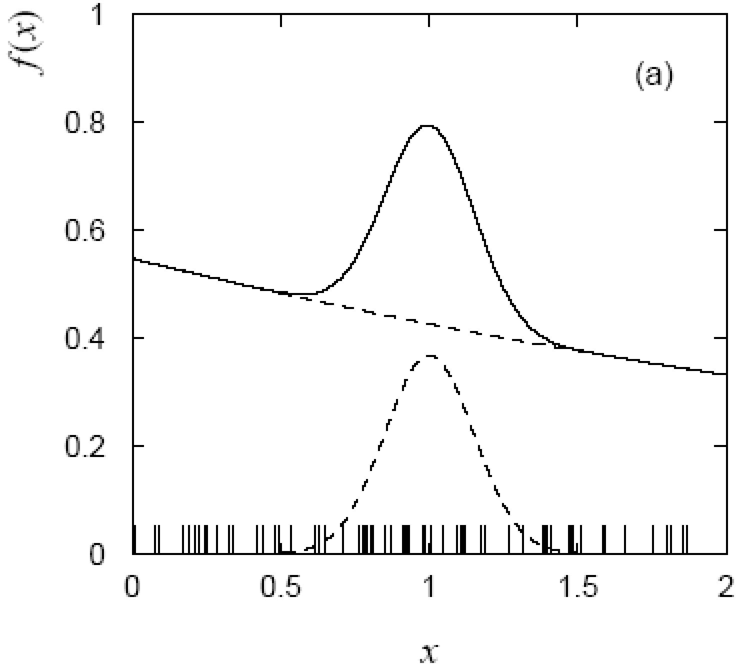
$$P(n; \mu_{\rm s}, \mu_{\rm b}) = \frac{(\mu_{\rm s} + \mu_{\rm b})^n}{n!} e^{-(\mu_{\rm s} + \mu_{\rm b})}$$

$$\rightarrow \quad \ln L(\mu_{\rm s}, \mu_{\rm b}) = -(\mu_{\rm s} + \mu_{\rm b}) + \sum_{i=1}^{n} \ln\left[(\mu_{\rm s} + \mu_{\rm b}) f(x_i; \mu_{\rm s}, \mu_{\rm b})\right]$$

Extended ML example (2)

Monte Carlo example with combination of exponential and Gaussian:

$$\mu_s = 6$$
$$\mu_b = 60$$



Maximize log-likelihood in terms of μ_s and μ_b:

$$\hat{\mu}_s = 8.7 \pm 5.5$$
$$\hat{\mu}_b = 54.3 \pm 8.8$$

Here errors reflect total Poisson fluctuation as well as that in proportion of signal/background.