Statistical Data Analysis 2024/25
Lecture Week 9

London Postgraduate Lectures on Particle Physics

University of London MSc/MSci course PH4515

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Statistical Data Analysis
Lecture 9-1

- Least squares with histogram data

LS with histogram data

The fit function in an LS fit is not a pdf, but it could be proportional to one, e.g., when we fit the "envelope" of a histogram.

Suppose for example, we have an i.i.d. data sample of n values $x_1,\ldots, x_n$ sampled from a pdf $f(x;\boldsymbol{\theta})$. Goal is to estimate $\boldsymbol{\theta}$.

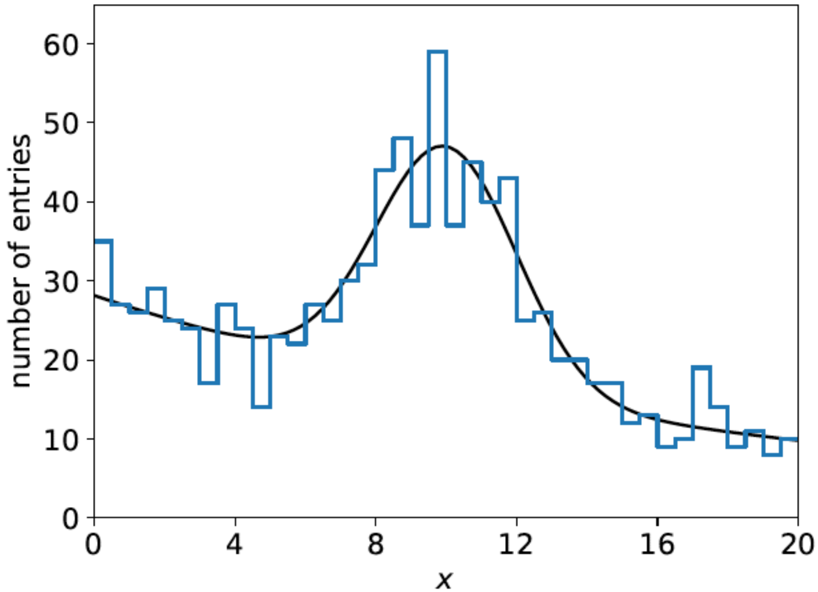
Instead of using all n values, put them in a histogram with N bins, i.e., y_i = number of entries in bin i: $\boldsymbol{y} = (y_1,\ldots, y_N)$.

The model predicts mean values:

$$
\begin{aligned}
E[y_i] &= \mu_i(\boldsymbol{\theta}) \\
&= n \int_{\mathrm{bin}\, i} f(x;\boldsymbol{\theta})\, dx \\
&\approx n f(x_i;\boldsymbol{\theta})\, \Delta x
\end{aligned}
$$

bin centre

bin width



LS with histogram data (2)

The usual models:

for fixed sample size n, take $\boldsymbol{y} \sim$ multinomial,
if n not fixed, $y_i \sim$ Poisson(μ_i)

Suppose that the expected number of entries in each μ_i are all $\gg 1$ and probability to be in any individual bin $p_i \ll 1$, one can show

$\rightarrow y_i$ indep. and ~ Gauss with $\sigma_i \approx \sqrt{\mu_i}$. ($\rightarrow \sigma_i$ depends on $\boldsymbol{\theta}$).

The (log-) likelihood functions are then

$$L(\boldsymbol{\theta}) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma_i(\boldsymbol{\theta})} e^{-(y_i - \mu_i(\boldsymbol{\theta}))^2/2\sigma_i^2(\boldsymbol{\theta})}$$

$$\ln L(\boldsymbol{\theta}) = -\frac{1}{2}\sum_{i=1}^{N} \frac{(y_i - \mu_i(\boldsymbol{\theta}))^2}{\sigma_i(\boldsymbol{\theta})^2} - \sum_{i=1}^{N} \ln \sigma_i(\boldsymbol{\theta}) + C$$

LS with histogram data (3)

Still define the least-squares estimators to minimize

$$\chi^2(\boldsymbol{\theta}) = \sum_{i=1}^{N} \frac{(y_i - \mu_i(\boldsymbol{\theta}))^2}{\sigma_i(\boldsymbol{\theta})^2}$$

No longer equivalent to maximum likelihood (equal for $\mu_i \gg 1$).

Two possibilities for σ_i:

$\sigma_i = \sqrt{\mu_i(\boldsymbol{\theta})}$ (LS method)

$\sigma_i = \sqrt{y_i}$ (Modified LS method)

Modified LS can be easier computationally but not defined if any $y_i = 0$.

For either method, $\chi^2_{\min}$ ~ chi-square pdf for $\mu_i \gg 1$, but this breaks down for when the μ_i are not large.

LS with histogram data — normalization

Do not "fit" the normalization, i.e., $n \to$ free parameter ν:

$$\mu_i(\boldsymbol{\theta}, \nu) = \nu \int_{\mathrm{bin}\, i} f(x; \boldsymbol{\theta})\, dx$$

If you do this, one finds the LS estimator for ν is not n, but rather

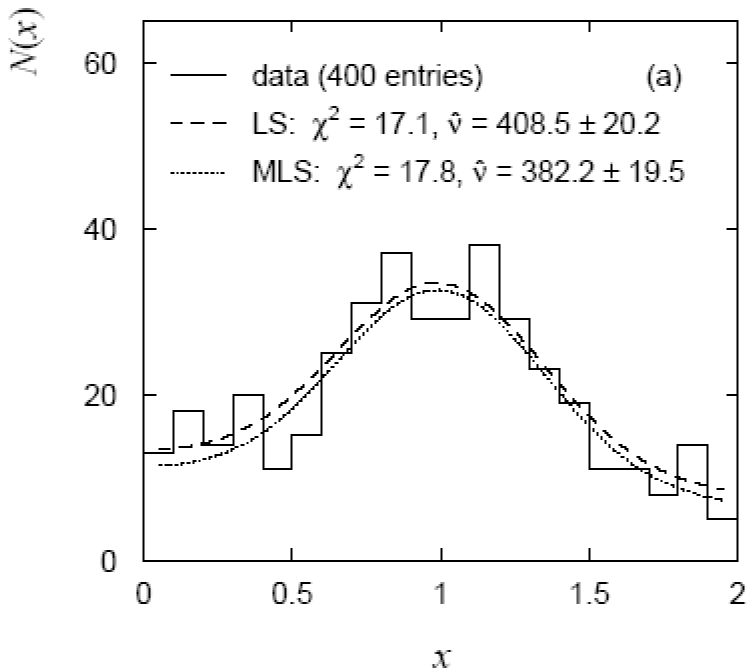
$$\hat{\nu}_{\mathrm{LS}} = n + \frac{\chi^2_{\mathrm{min}}}{2}$$

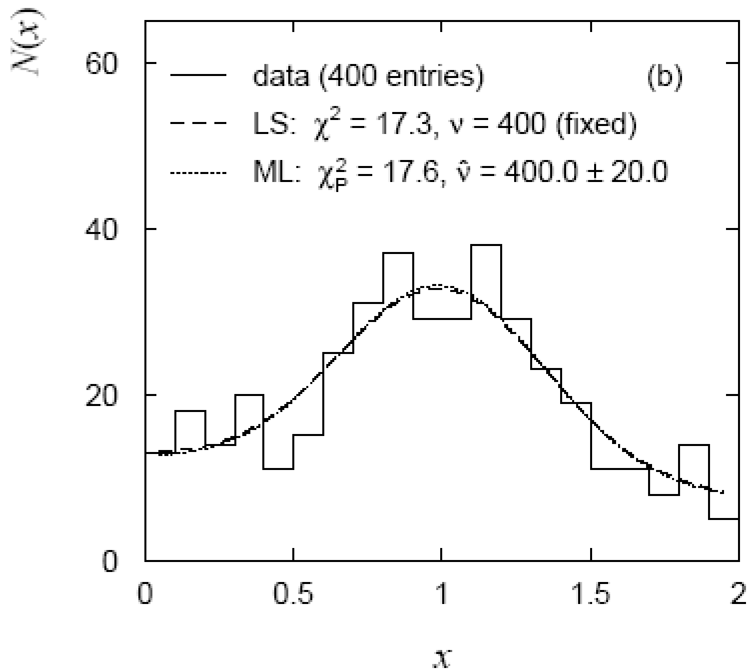
$$\hat{\nu}_{\mathrm{MLS}} = n - \chi^2_{\mathrm{min}}$$

Software may include adjustable normalization parameter as default; better to use known n.

LS normalization example

Example with $n = 400$ entries, $N = 20$ bins:





Expect $\chi^2_{\min}$ around $N - m$,

$\rightarrow$ relative error in $\hat{\nu}$ large when N large, n small

Either get n directly from data for LS (or better, use ML).

Statistical Data Analysis
Lecture 9-2

- Goodness-of-fit from the likelihood ratio
- Wilks' theorem
- MLE and goodness-of-fit all in one

Goodness of fit from the likelihood ratio

Suppose we model data using a likelihood $L(\boldsymbol{\mu})$ that depends on N parameters $\boldsymbol{\mu} = (\mu_1,\ldots, \mu_N)$. Define the statistic

$$t_{\boldsymbol{\mu}} = -2 \ln \frac{L(\boldsymbol{\mu})}{L(\hat{\boldsymbol{\mu}})}$$

where $\hat{\boldsymbol{\mu}}$ is the ML estimator for $\boldsymbol{\mu}$. Value of $t_{\boldsymbol{\mu}}$ reflects agreement between hypothesized $\boldsymbol{\mu}$ and the data.

Good agreement means $\boldsymbol{\mu} \approx \hat{\boldsymbol{\mu}}$, so $t_{\boldsymbol{\mu}}$ is small;

Larger $t_{\boldsymbol{\mu}}$ means less compatibility between data and $\boldsymbol{\mu}$.

Quantify "goodness of fit" with p-value: $$p_{\boldsymbol{\mu}} = \int_{t_{\boldsymbol{\mu},\mathrm{obs}}}^{\infty} f(t_{\boldsymbol{\mu}}|\boldsymbol{\mu})\, dt_{\boldsymbol{\mu}}$$

need this pdf

Likelihood ratio (2)

Now suppose the parameters $\boldsymbol{\mu} = (\mu_1,\ldots, \mu_N)$ can be determined by another set of parameters $\boldsymbol{\theta} = (\theta_1,\ldots, \theta_M)$, with $M < N$.

E.g., curve fit with $\mu_i = E[y_i] = \mu(x_i; \boldsymbol{\theta})$, $i = 1,\ldots,N$, $\boldsymbol{\theta} = (\theta_1,\ldots, \theta_M)$.

Want to test hypothesis that the true model is somewhere in the subspace $\boldsymbol{\mu} = \boldsymbol{\mu}(\boldsymbol{\theta})$ versus the alternative of the full parameter space $\boldsymbol{\mu}$. Generalize the LR test statistic to be

fit M parameters

$$t_{\boldsymbol{\mu}} = -2 \ln \frac{L(\boldsymbol{\mu}(\hat{\boldsymbol{\theta}}))}{L(\hat{\boldsymbol{\mu}})}$$

fit N parameters

To get p-value, need pdf $f(t_{\mu}|\boldsymbol{\mu}(\boldsymbol{\theta}))$.

Wilks' Theorem

Wilks' Theorem: if the hypothesized $\mu_i(\boldsymbol{\theta})$, $i = 1,\ldots,N$, are true for some choice of the parameters $\boldsymbol{\theta} = (\theta_1,\ldots, \theta_M)$, then in the large sample limit (and provided regularity conditions are satisfied)

MLE of $(\theta_1,\ldots, \theta_M)$

$$t_{\boldsymbol{\mu}} = -2\ln\frac{L(\boldsymbol{\mu}(\hat{\boldsymbol{\theta}}))}{L(\hat{\boldsymbol{\mu}})}$$

follows a chi-square distribution for $N - M$ degrees of freedom.

MLE of $(\mu_1,\ldots, \mu_N)$

The regularity conditions include: the model in the numerator of the likelihood ratio is "nested" within the one in the denominator, i.e., $\boldsymbol{\mu}(\boldsymbol{\theta})$ is a special case of $\boldsymbol{\mu} = (\mu_1,\ldots, \mu_N)$.

Proof boils down to having all estimators ~ Gaussian.

S.S. Wilks, *The large-sample distribution of the likelihood ratio for testing composite hypotheses*, Ann. Math. Statist. **9** (1938) 60-2.

Wilks' Theorem (2)

To find $p_{\boldsymbol{\theta}} = \int_{t_{\boldsymbol{\mu}},\mathrm{obs}}^{\infty} f(t_{\boldsymbol{\mu}}|\boldsymbol{\mu}(\boldsymbol{\theta}))\,dt_{\boldsymbol{\mu}}$ e.g. with Monte Carlo we would need to choose a point in $\boldsymbol{\theta}$ space, then $p = \max_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}$

But if we can use Wilks', the chi-square dist. should hold for all $\boldsymbol{\theta}$.

The chi-square pdf for $-2\ln\lambda$ breaks down:

- if the sample size is too small;
- if the true value of a parameter is on the boundary of the allowed parameter space;
- if the model in the numerator is not a special case of the denominator (models must be "nested");
- if variance of estimators of any components of $\boldsymbol{\mu}$ too large (e.g., parameter refers to location of a feature not present in the null hypothesis, such as the position of a peak).

Goodness of fit with Gaussian data

Suppose the data are N independent Gaussian distributed values:

$$y_i \sim \mathrm{Gauss}(\mu_i, \sigma_i) \ , \qquad i = 1, \ldots, N$$

want to estimate — known

N measurements and N parameters (= "saturated model")

Likelihood: $$L(\mu) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma_i} e^{-(y_i - \mu_i)^2/2\sigma_i^2}$$

Log-likelihood: $$\ln L(\mu) = -\frac{1}{2} \sum_{i=1}^{N} \frac{(y_i - \mu_i)^2}{\sigma_i^2} + C$$

ML estimators: $$\hat{\mu}_i = y_i \qquad i = 1, \ldots, N$$

Likelihood ratio for Gaussian data

Now suppose $\boldsymbol{\mu} = \boldsymbol{\mu}(\boldsymbol{\theta})$, e.g., in an LS fit with $\mu_i(\boldsymbol{\theta}) = \mu(x_i; \boldsymbol{\theta})$.

The goodness-of-fit statistic for the test of the hypothesis $\boldsymbol{\mu}(\boldsymbol{\theta})$ becomes

$$t_{\boldsymbol{\mu}} = -2 \ln \frac{L(\boldsymbol{\mu}(\hat{\boldsymbol{\theta}}))}{L(\hat{\boldsymbol{\mu}})} = \sum_{i=1}^{N} \frac{(y_i - \mu_i(\hat{\boldsymbol{\theta}}))^2}{\sigma_i^2} \sim \chi^2_{N-M}$$

chi-square pdf for N-M degrees of freedom

Here $t_{\boldsymbol{\mu}}$ is the same as $\chi^2_{\min}$ from an LS fit.

So Wilks' theorem formally states the property that we claimed for the minimized chi-squared from an LS fit with N measurements and M fitted parameters.

Likelihood ratio for Poisson data

Suppose the data are a set of values $\boldsymbol{n} = (n_1,\ldots, n_N)$, e.g., the numbers of events in a histogram with N bins.

Assume $n_i \sim$ Poisson(ν_i), $i = 1,\ldots, N$, all independent.

First (for LR denominator) use saturated model, i.e., treat $\boldsymbol{\nu} = (\nu_1,\ldots, \nu_N)$ as all adjustable:

Likelihood: $$L(\boldsymbol{\nu}) = \prod_{i=1}^{N} \frac{\nu_i^{n_i}}{n_i!} e^{-\nu_i}$$

Log-likelihood: $$\ln L(\boldsymbol{\nu}) = \sum_{i=1}^{N} [n_i \ln \nu_i - \nu_i] + C$$

ML estimators: $$\hat{\nu}_i = n_i \ , \qquad i = 1, \ldots, N$$

Goodness of fit with Poisson data (2)

For LR numerator find $\boldsymbol{\nu}(\boldsymbol{\theta})$ with M fitted parameters $\boldsymbol{\theta} = (\theta_1,\ldots, \theta_M)$:

$$t_{\boldsymbol{\nu}} = -2 \ln \frac{L(\boldsymbol{\nu}(\hat{\boldsymbol{\theta}}))}{L(\hat{\boldsymbol{\nu}})} = -2 \sum_{i=1}^{N} \left[n_i \ln \frac{\nu_i(\hat{\boldsymbol{\theta}})}{n_i} - \nu_i(\hat{\boldsymbol{\theta}}) + n_i \right]$$

if $n_i = 0$, skip log term

Wilks' theorem: in large-sample limit $t_{\boldsymbol{\nu}} \sim \chi^2_{N-M}$

Exact in large sample limit; in practice good approximation for surprisingly small n_i (~several).

As before use t_ν to get p-value of $\boldsymbol{\nu}(\boldsymbol{\theta})$,

independent of $\boldsymbol{\theta}$

$$p_{\boldsymbol{\nu}} = \int_{t_{\boldsymbol{\nu},\mathrm{obs}}}^{\infty} f(t_{\boldsymbol{\nu}} | \boldsymbol{\nu}(\boldsymbol{\theta}))\, dt_{\boldsymbol{\nu}} = 1 - F_{\chi^2}(t_{\boldsymbol{\nu},\mathrm{obs}}; N - M)$$

Goodness of fit with multinomial data

Similar if data $\boldsymbol{n} = (n_1,\ldots, n_N)$ follow multinomial distribution:

$$P(\mathbf{n}|\mathbf{p}, n_{\mathrm{tot}}) = \frac{n_{\mathrm{tot}}!}{n_1! n_2! \ldots n_N!} p_1^{n_1} p_2^{n_2} \ldots p_N^{n_N}$$

E.g. histogram with N bins but fix: $\quad n_{\mathrm{tot}} = \sum_{i=1}^{N} n_i$

Log-likelihood: $\quad \ln L(\boldsymbol{\nu}) = \sum_{i=1}^{N} n_i \ln \frac{\nu_i}{n_{\mathrm{tot}}} + C \qquad (\nu_i = p_i n_{\mathrm{tot}})$

ML estimators: $\quad \hat{\nu}_i = n_i \qquad$ (Only N–1 independent; one is n_{tot} minus sum of rest.)

Goodness of fit with multinomial data (2)

The likelihood ratio statistics become:

$$t_{\boldsymbol{\nu}} = -2 \ln \frac{L(\boldsymbol{\nu}(\hat{\boldsymbol{\theta}}))}{L(\hat{\boldsymbol{\nu}})} = -2 \sum_{i=1}^{N} n_i \ln \frac{\nu_i(\hat{\boldsymbol{\theta}})}{n_i}$$

if $n_i = 0$, skip term

Wilks: in large sample limit $t_{\boldsymbol{\nu}} \sim \chi^2_{N-M-1}$

One less degree of freedom than in Poisson case because effectively only $N\!-\!1$ parameters fitted in denominator of LR.

Estimators and g.o.f. all at once

Evaluate numerators with $\boldsymbol{\theta}$ (not its estimator); if any $n_i = 0$, omit the corresponding log terms:

$$\chi_{\mathrm{P}}^2(\boldsymbol{\theta}) = -2\sum_{i=1}^{N}\left[n_i \ln \frac{\nu_i(\boldsymbol{\theta})}{n_i} - \nu_i(\boldsymbol{\theta}) + n_i\right]$$ (Poisson)

$$\chi_{\mathrm{M}}^2(\boldsymbol{\theta}) = -2\sum_{i=1}^{N} n_i \ln \frac{\nu_i(\boldsymbol{\theta})}{n_i}$$ (Multinomial)

These are equal to the corresponding $-2 \ln L(\boldsymbol{\theta})$ plus terms not depending on $\boldsymbol{\theta}$, so minimizing them gives the usual ML estimators for $\boldsymbol{\theta}$.

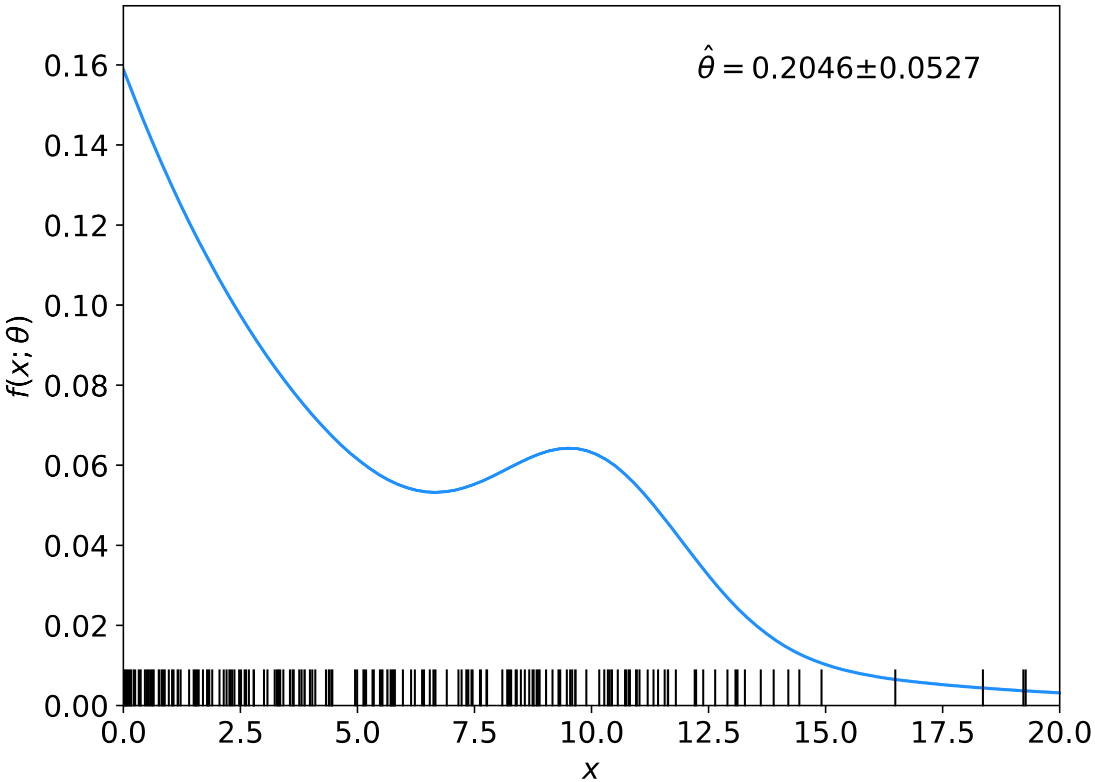
The minimized value gives the statistic t_μ, so we get goodness-of-fit for free.

Steve Baker and Robert D. Cousins, *Clarification of the use of the chi-square and likelihood functions in fits to histograms*, NIM **221** (1984) 437.

Examples of ML/LS fits

Unbinned maximum likelihood (mlFit.py, minimize negLogL)

$$\ln L(\boldsymbol{\theta}) = \sum_{i=1}^{n} \ln f(x_i;\boldsymbol{\theta})$$

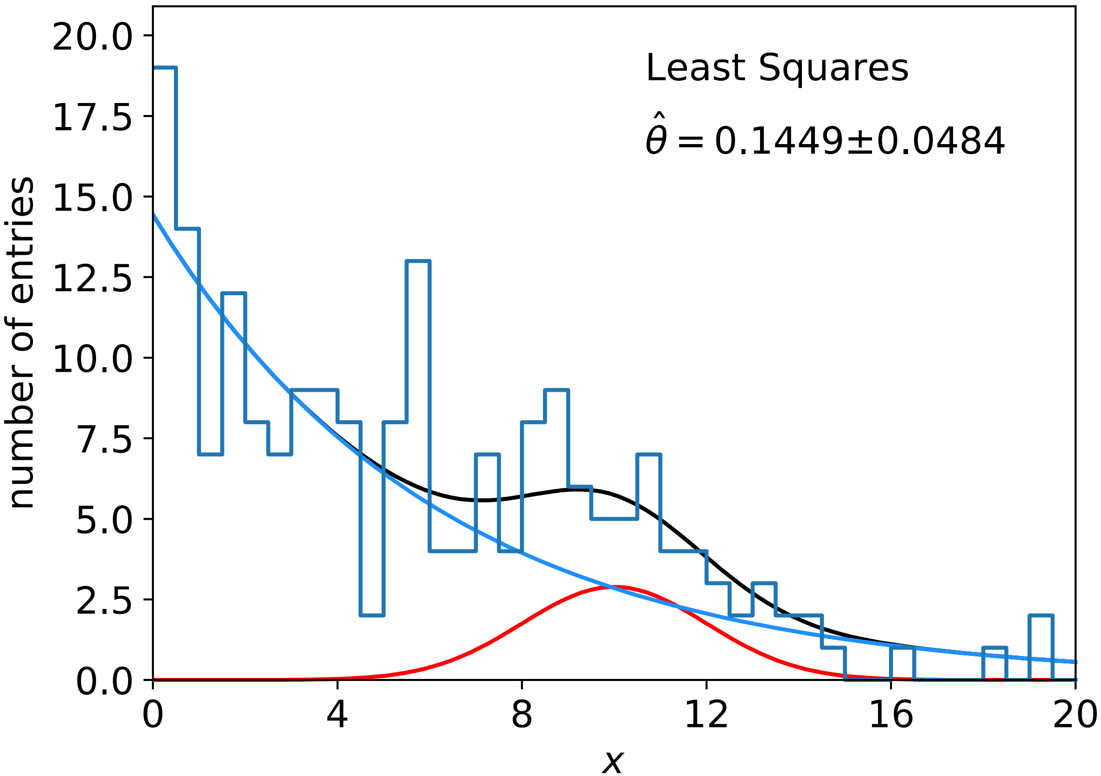


No useful measure of goodness-of-fit from unbinned ML.

Examples of ML/LS fits

Least Squares fit (histFit.py, minimize chi2LS)

$$\chi^2(\boldsymbol{\theta}) = \sum_{i=1}^{N} \frac{(y_i - \mu_i(\boldsymbol{\theta}))^2}{\mu_i(\boldsymbol{\theta})}$$



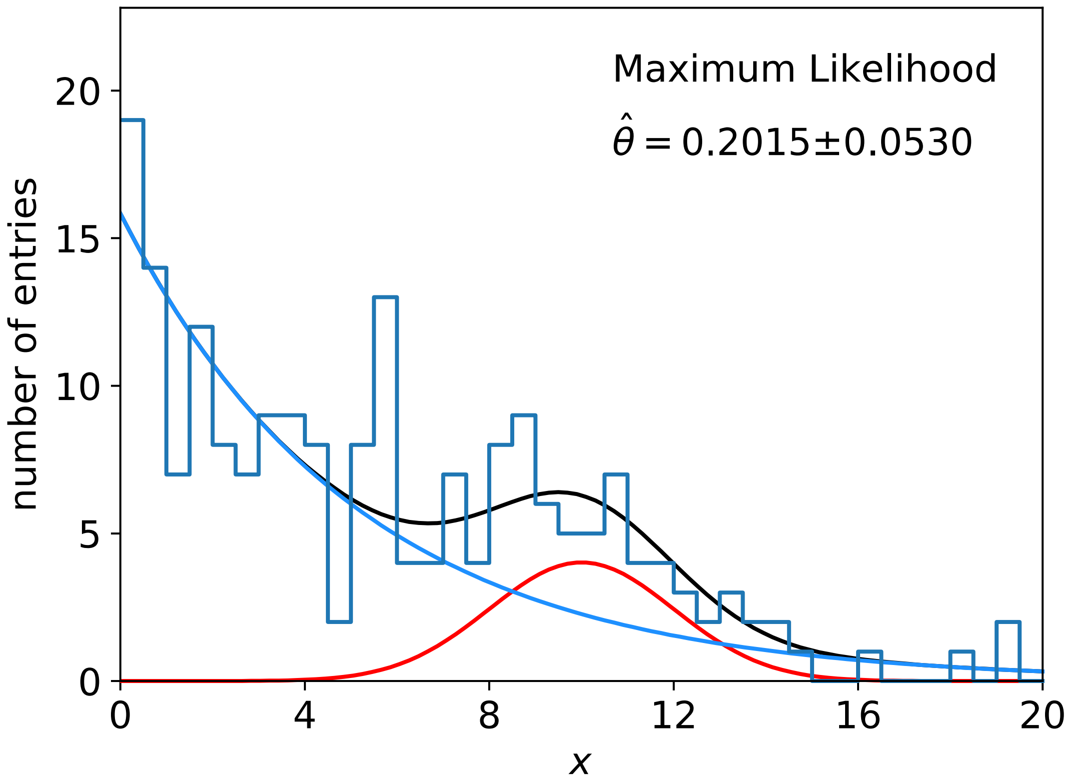
$\chi^2_{\min} = 32.7$
$n_{\mathrm{dof}} = 38$
$p = 0.71$

Many bins with few entries, LS not expected to be reliable.

Examples of ML/LS fits

Multinomial maximum likelihood fit (histFit.py, minimize chi2M)

$$\chi^2_{\rm M}(\boldsymbol{\theta}) = -2\sum_{i=1}^{N} n_i \ln \frac{\nu_i(\boldsymbol{\theta})}{n_i}$$



$\chi^2_{\rm min} = 35.3$
$n_{\rm dof} = 37$
$p = 0.55$

Essentially same result as unbinned ML.

Statistical Data Analysis
Lecture 9-3

- Interval estimation
- Confidence interval from inverting a test
- Example: limits on mean of Gaussian

Confidence intervals by inverting a test

In addition to a 'point estimate' of a parameter we should report an interval reflecting its statistical uncertainty.

Confidence intervals for a parameter θ can be found by defining a test of the hypothesized value θ (do this for all θ):

Specify values of the data that are 'disfavoured' by θ (critical region) such that $P(\text{data in critical region} \mid \theta) \leq \alpha$ for a prespecified α, e.g., 0.05 or 0.1.

If data observed in the critical region, reject the value θ.

Now invert the test to define a confidence interval as:

set of θ values that are not rejected in a test of size α (confidence level CL is $1-\alpha$).

Relation between confidence interval and p-value

Equivalently we can consider a significance test for each hypothesized value of θ, resulting in a p-value, p_θ.

If $p_\theta \leq \alpha$, then we reject θ.

The confidence interval at CL $= 1 - \alpha$ consists of those values of θ that are not rejected.

E.g. an upper limit on θ is the greatest value for which $p_\theta > \alpha$.

In practice find by setting $p_\theta = \alpha$ and solve for θ.

For a multidimensional parameter space $\boldsymbol{\theta} = (\theta_1, \ldots \theta_M)$ *use* same idea – result is a confidence "region" with boundary determined by $p_{\boldsymbol{\theta}} = \alpha$.

Coverage probability of confidence interval

If the true value of θ is rejected, then it's not in the confidence interval. The probability for this is by construction (equality for continuous data):

$$P(\text{reject } \theta | \theta) \leq \alpha = \text{type-I error rate}$$

Therefore, the probability for the interval to contain or "cover" θ is

$$P(\text{conf. interval “covers” } \theta | \theta) \geq 1 - \alpha$$

This assumes that the set of θ values considered includes the true value, i.e., it assumes the composite hypothesis $P(\boldsymbol{x}|H,\theta)$.

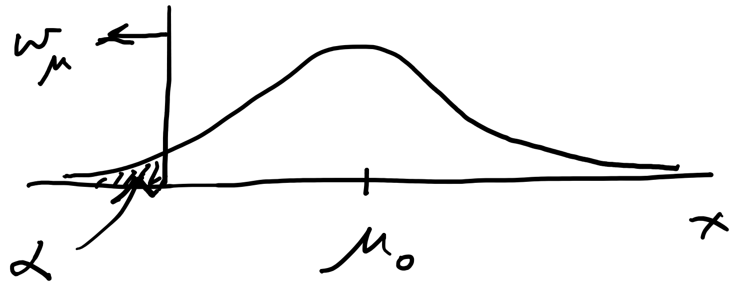
Example: upper limit on mean of Gaussian

When we test the parameter, we should take the critical region to maximize the power with respect to the relevant alternative(s).

Example: $x \sim \text{Gauss}(\mu, \sigma)$ (take σ known)

Test $H_0 : \mu = \mu_0$ versus the alternative $H_1 : \mu < \mu_0$

→ Put w_μ at region of x-space characteristic of low μ (i.e. at low x)

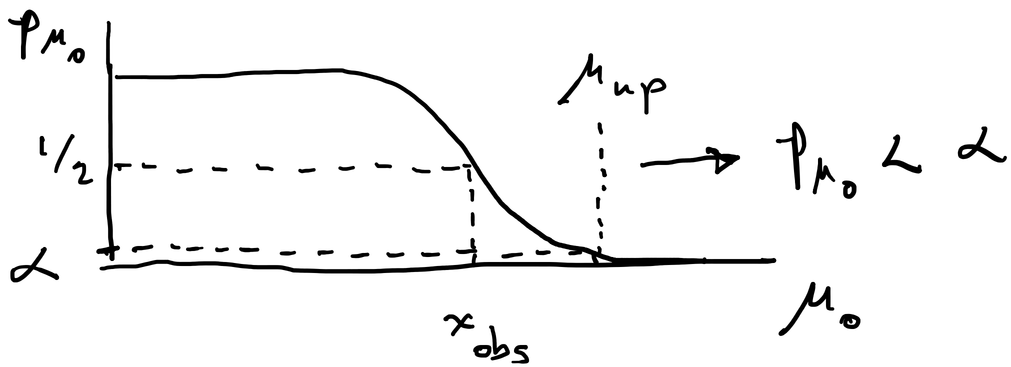


Equivalently, take the p-value to be

$$p_{\mu_0} = P(x \leq x_{\text{obs}} | \mu_0) = \int_{-\infty}^{x_{\text{obs}}} \frac{1}{\sqrt{2\pi}\sigma} e^{-(x-\mu_0)^2/2\sigma^2} \, dx = \Phi\left(\frac{x_{\text{obs}} - \mu_0}{\sigma}\right)$$

Upper limit on Gaussian mean (2)

To find confidence interval, repeat for all μ_0, i.e., set $p_{\mu 0} = \alpha$ and solve for μ_0 to find the interval's boundary



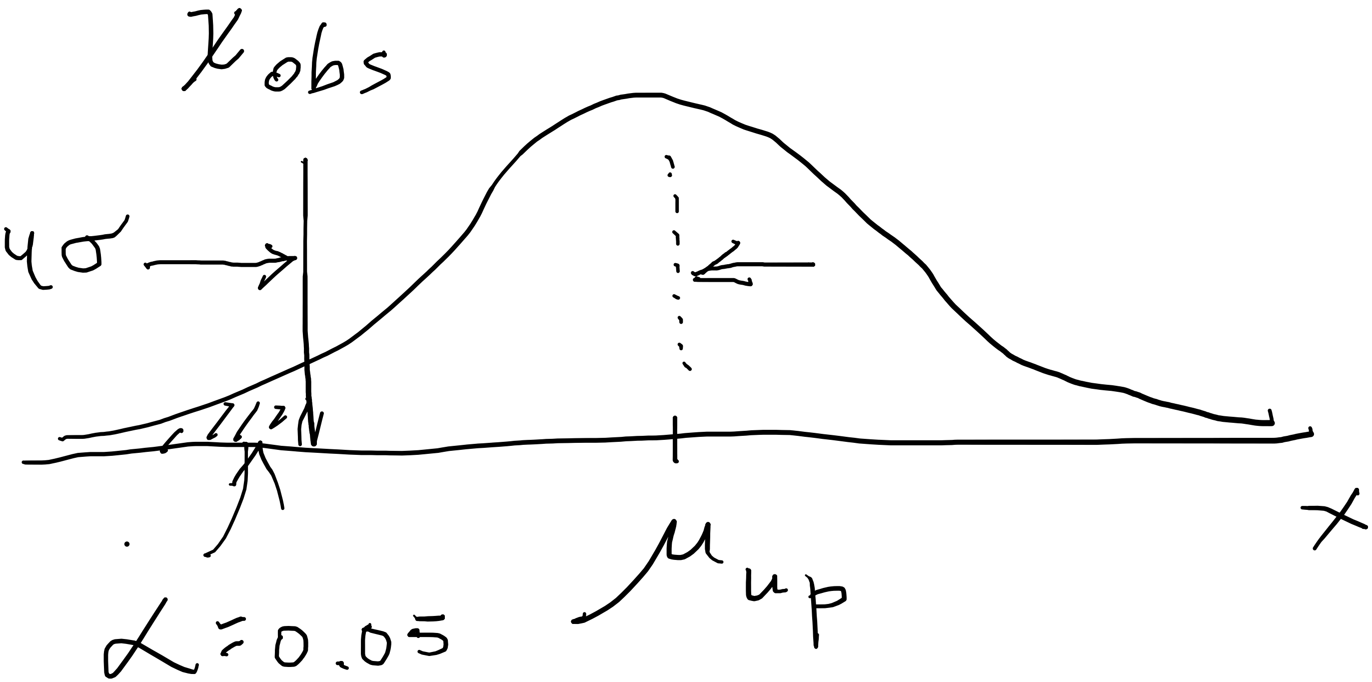
$$\mu_0 \to \mu_{\rm up} = x_{\rm obs} - \sigma\Phi^{-1}(\alpha) = x_{\rm obs} + \sigma\Phi^{-1}(1-\alpha)$$

This is an upper limit on μ, i.e., higher μ have even lower p-value and are in even worse agreement with the data.

Usually use $\Phi^{-1}(\alpha) = -\Phi^{-1}(1-\alpha)$ so as to express the upper limit as $x_{\rm obs}$ plus a positive quantity. E.g. for $\alpha = 0.05$, $\Phi^{-1}(1-0.05) = 1.64$.

Upper limit on Gaussian mean (3)

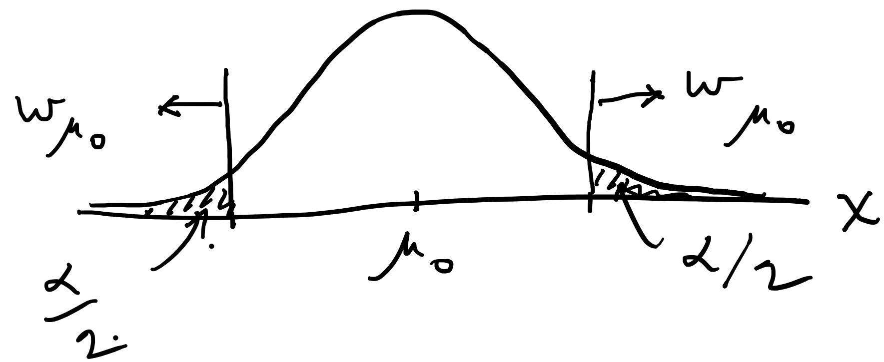
μ_{up} = the hypothetical value of μ such that there is only a probability α to find $x < x_{\text{obs}}$.



1- vs. 2-sided intervals

Now test: $H_0 : \mu = \mu_0$ versus the alternative $H_1 : \mu \neq \mu_0$

I.e. we consider the alternative to μ_0 to include higher and lower values, so take critical region on both sides:



Result is a "central" confidence interval $[\mu_{\rm lo}, \mu_{\rm up}]$:

$$\mu_{\rm lo} = x_{\rm obs} - \sigma \Phi^{-1}\left(1 - \frac{\alpha}{2}\right)$$

$$\mu_{\rm up} = x_{\rm obs} + \sigma \Phi^{-1}\left(1 - \frac{\alpha}{2}\right)$$

E.g. for $\alpha = 0.05$

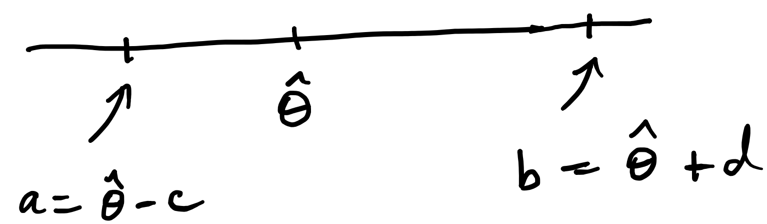
$$\Phi^{-1}\left(1 - \frac{\alpha}{2}\right) = 1.96 \approx 2$$

Note upper edge of two-sided interval is higher (i.e. not as tight of a limit) than obtained from the one-sided test.

On the meaning of a confidence interval

Often we report the confidence interval $[a,b]$ together with the point estimate as an "asymmetric error bar", e.g.,

$$\hat{\theta}^{+d}_{-c}$$



E.g. (at CL $= 1 - \alpha = 68.3\%$):

$$\hat{\theta} = 80.25^{+0.31}_{-0.25}$$

Does this mean $P(80.00 < \theta < 80.56) = 68.3\%$? No, not for a frequentist confidence interval. The parameter θ does not fluctuate upon repetition of the measurement; the endpoints of the interval do, i.e., the endpoints of the interval fluctuate (they are functions of data):

$$P(a(x) < \theta < b(x)) = 1 - \alpha$$

Example with binomial parameter

Suppose $m \sim \mathrm{Binomial}(N,\theta)$ with N trials (known)and success probability per trial θ (unknown). We observe a single value m.

The likelihood function is

$$L(\theta) = P(m|N,\theta) = \frac{N!}{m!(N-m)!}\theta^m (1-\theta)^{N-m}$$

so the log-likelihood is $\ln L(\theta) = m \ln \theta + (N-m)\ln(1-\theta) + C$

Set its derivative to zero $\dfrac{\partial \ln L}{\partial \theta} = \dfrac{m}{\theta} - \dfrac{N-m}{\theta} = 0$

to find the MLE $\hat{\theta} = \dfrac{m}{N}$.

Since $V[m] = N\theta(1-\theta) \;\longrightarrow\; \sigma_{\hat{\theta}} = \dfrac{1}{N}\sqrt{\theta\,(1-\theta)} \;\longrightarrow\; \hat{\sigma}_{\hat{\theta}} = \dfrac{1}{N}\sqrt{\dfrac{m}{N}\left(1-\dfrac{m}{N}\right)}$

Limits on binomial parameter

To give the MLE and a 68.3% central confidence interval, it is often sufficient to report $\hat{\theta} \pm \sigma_{\hat{\theta}}$.

Suppose we find $m_{\rm obs}$ and we want to know an upper limit on θ.

To quantify how big θ could be, find upper limit at CL = 1−α = 95%.

$$p_\theta = P(m \leq m_{\rm obs}|\theta) = \sum_{m=0}^{m_{\rm obs}} \frac{N!}{m!(N-m)!} \theta^m (1-\theta)^{N-m}$$

Set $p_\theta = \alpha$ and solve for $\theta \longrightarrow \theta_{\rm up}$.

Can be done in closed form; see PDG Eq. (40.83):

$$\theta_{\rm up} = \frac{(m+1)F_F^{-1}[1-\alpha; 2(m+1), 2(N-m)]}{(N-m) \; + \; (m+1)F_F^{-1}[1-\alpha; 2(m+1), 2(N-m)]}$$

usually just solve with computer

where F is the Fisher-Snedecor distribution .

Upper limit for θ for $m_{\mathrm{obs}} = 0$

Suppose we find $m_{\mathrm{obs}} = 0$.

$\hat{\theta} = 0$ makes sense

$\hat{\sigma}_{\hat{\theta}} = 0$ not incorrect but does not provide a useful interval

For the *p*-value (for upper limit) we find

$$p_\theta = \sum_{m=0}^{0} \frac{N!}{0!(N-0)!} \theta^0 (1-\theta)^{N-0} = (1-\theta)^N$$

Set $p_\theta = \alpha$ and solving for θ gives the upper limit $\theta_{\mathrm{up}} = 1 - \alpha^{1/N}$

For example, $N = 20, \alpha = 0.05, \to \theta_{\mathrm{up}} = 0.14$ at 95% CL.

Statistical Data Analysis
Lecture 9-4

- Confidence intervals from the likelihood function

Approximate confidence intervals/regions from the likelihood function

Suppose we test parameter value(s) $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_N)$ using the ratio

$$\lambda(\boldsymbol{\theta}) = \frac{L(\boldsymbol{\theta})}{L(\hat{\boldsymbol{\theta}})} \qquad\qquad 0 \leq \lambda(\boldsymbol{\theta}) \leq 1$$

Lower $\lambda(\boldsymbol{\theta})$ means worse agreement between data and hypothesized $\boldsymbol{\theta}$. Equivalently, usually define

$$t_{\boldsymbol{\theta}} = -2 \ln \lambda(\boldsymbol{\theta})$$

so higher $t_{\boldsymbol{\theta}}$ means worse agreement between $\boldsymbol{\theta}$ and the data.

p-value of $\boldsymbol{\theta}$ therefore

$$p_{\boldsymbol{\theta}} = \int_{t_{\boldsymbol{\theta},\mathrm{obs}}}^{\infty} f(t_{\boldsymbol{\theta}}|\boldsymbol{\theta})\, dt_{\boldsymbol{\theta}}$$

need pdf

Confidence region from Wilks' theorem

Wilks' theorem says (in large-sample limit and provided certain conditions hold...)

$$f(t_{\boldsymbol{\theta}}|\boldsymbol{\theta}) \sim \chi^2_N$$

chi-square dist. with # d.o.f. = # of components in $\boldsymbol{\theta} = (\theta_1, ..., \theta_N)$.

Assuming this holds, the p-value is

$$p_{\boldsymbol{\theta}} = 1 - F_{\chi^2_N}(t_{\boldsymbol{\theta}}|\boldsymbol{\theta})$$ ← set equal to α

To find boundary of confidence region set $p_\theta = \alpha$ and solve for t_θ:

$$t_{\boldsymbol{\theta}} = F^{-1}_{\chi^2_N}(1-\alpha)$$

Recall also

$$t_\theta = -2\ln\frac{L(\theta)}{L(\hat{\theta})}$$

Confidence region from Wilks' theorem (cont.)

i.e., boundary of confidence region in $\boldsymbol{\theta}$ space is where

$$\ln L(\boldsymbol{\theta}) = \ln L(\hat{\boldsymbol{\theta}}) - \tfrac{1}{2} F^{-1}_{\chi^2_N}(1-\alpha)$$

For example, for $1 - \alpha = 68.3\%$ and $n = 1$ parameter,

$$F^{-1}_{\chi^2_1}(0.683) = 1$$

and so the 68.3% confidence level interval is determined by

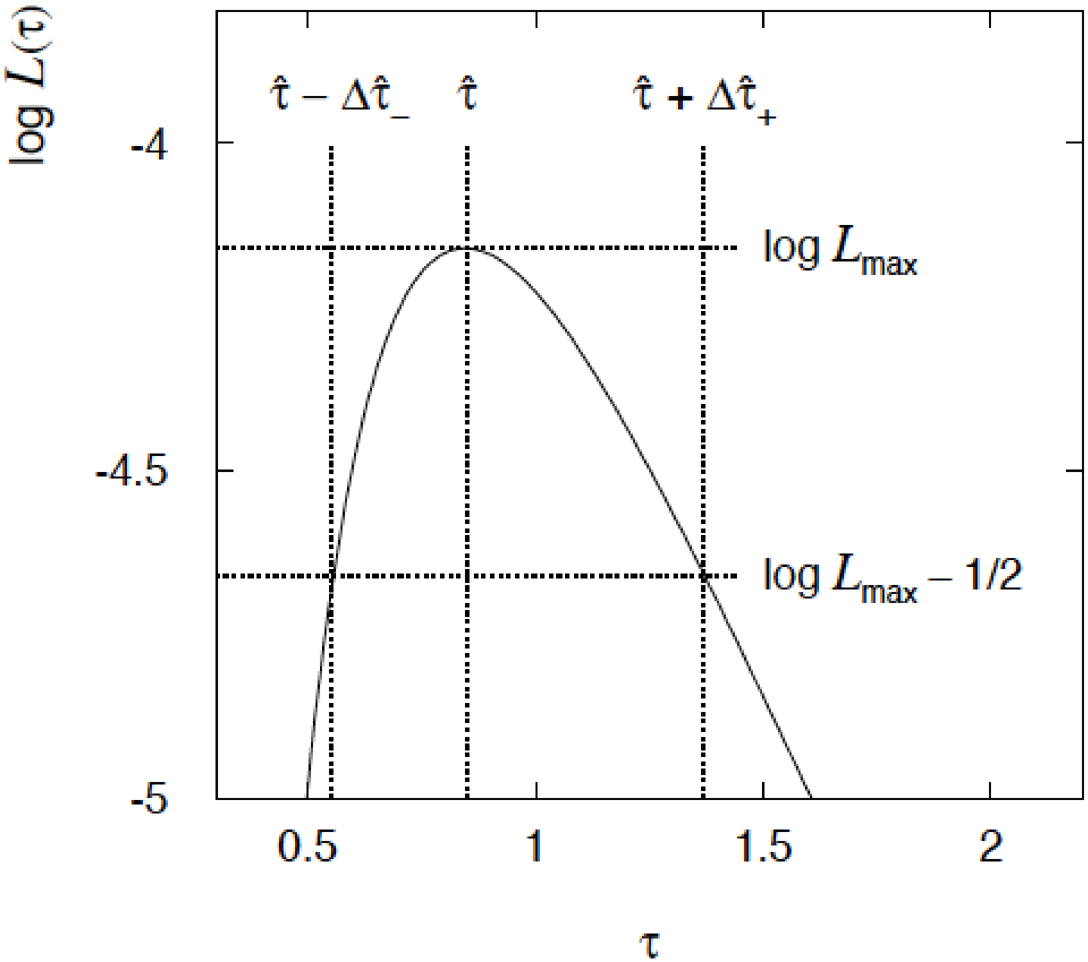
$$\ln L(\theta) = \ln L(\hat{\theta}) - \frac{1}{2}$$

Same as recipe for finding the estimator's standard deviation, i.e.,

$[\hat{\theta} - \sigma_{\hat{\theta}}, \hat{\theta} + \sigma_{\hat{\theta}}]$ is a 68.3% CL conf. interval (in large sample limit).

Example of interval from $\ln L(\theta)$

For N =1 parameter, CL = 0.683, $Q_\alpha = 1$.



Our exponential example, now with only $n = 5$ events.

Can report ML estimate with approx. confidence interval from $\ln L_{\max} - 1/2$ as “asymmetric error bar”:

$$\hat{\tau} = 0.85^{+0.52}_{-0.30}$$

Multiparameter case

For increasing number of parameters, CL $= 1 - \alpha$ decreases for confidence region determined by a given

$$Q_\alpha = F^{-1}_{\chi^2_n}(1-\alpha)$$

Q_α	$1-\alpha$				
	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$ ← # of par.
1.0	0.683	0.393	0.199	0.090	0.037
2.0	0.843	0.632	0.428	0.264	0.151
4.0	0.954	0.865	0.739	0.594	0.451
9.0	0.997	0.989	0.971	0.939	0.891

Multiparameter case (cont.)

Equivalently, Q_α increases with n for a given CL = $1 - \alpha$.

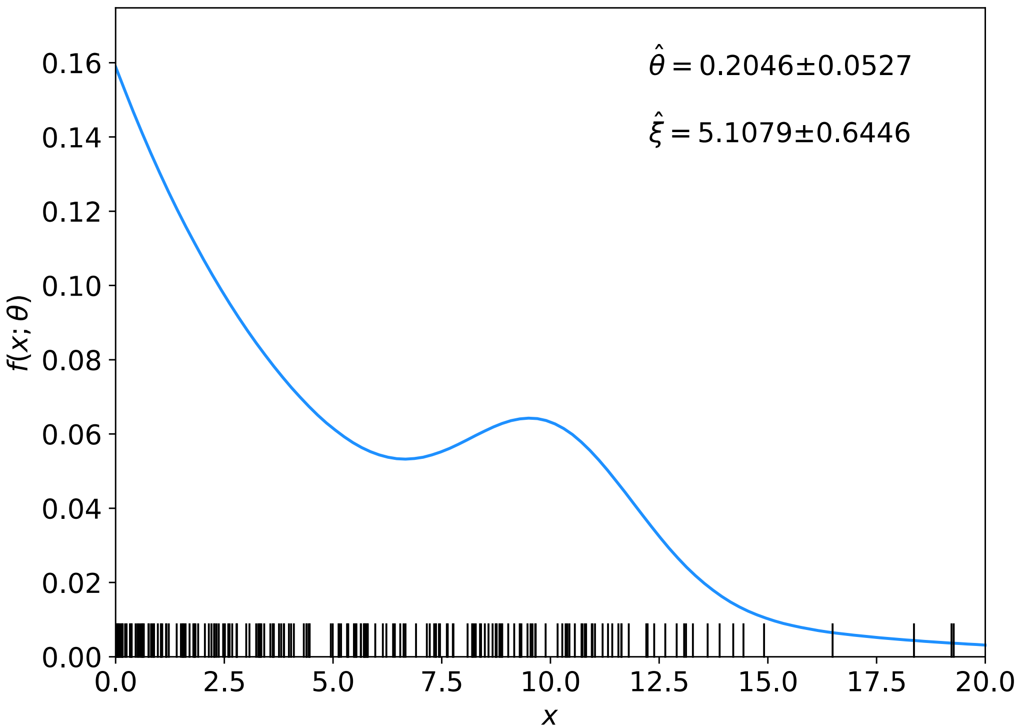
$1-\alpha$	$\tilde{Q}_\alpha$				
	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$
0.683	1.00	2.30	3.53	4.72	5.89
0.90	2.71	4.61	6.25	7.78	9.24
0.95	3.84	5.99	7.82	9.49	11.1
0.99	6.63	9.21	11.3	13.3	15.1

← # of par.

Example: 2 parameter fit:

Example from problem sheet 8, i.i.d. sample of size 200

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

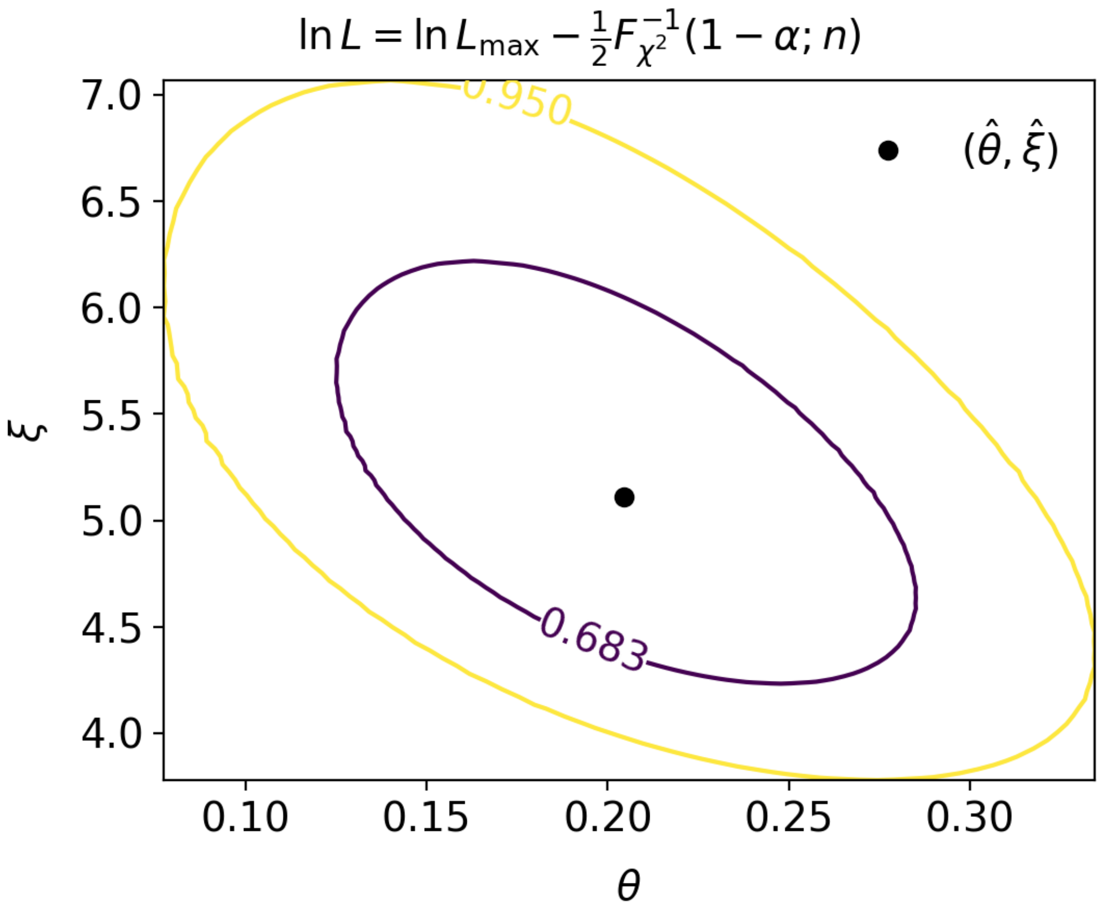


Here fit two parameters: θ and ξ.

Example: 2 parameter fit:

In iminuit v2, user can set $\mathrm{CL} = 1 - \alpha$

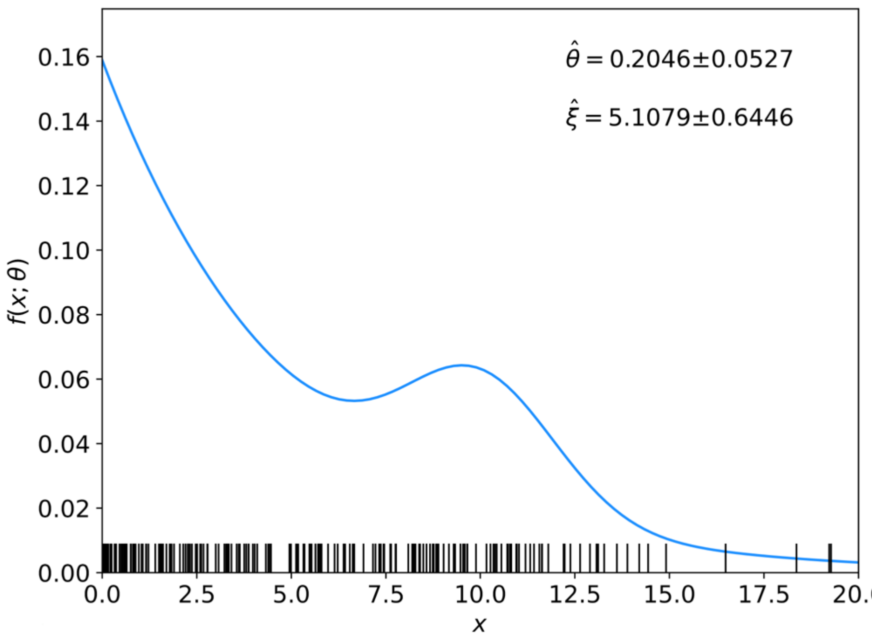
```
m.draw_mncontour('theta', 'xi', cl=[0.683, 0.95], size=200)
```



Extra slides

Comments on using iminuit

In our earlier iminuit example mlFit.py, the only argument of the log-likelihood function was the parameter array, and the data array xData entered as global (usually not a good idea):



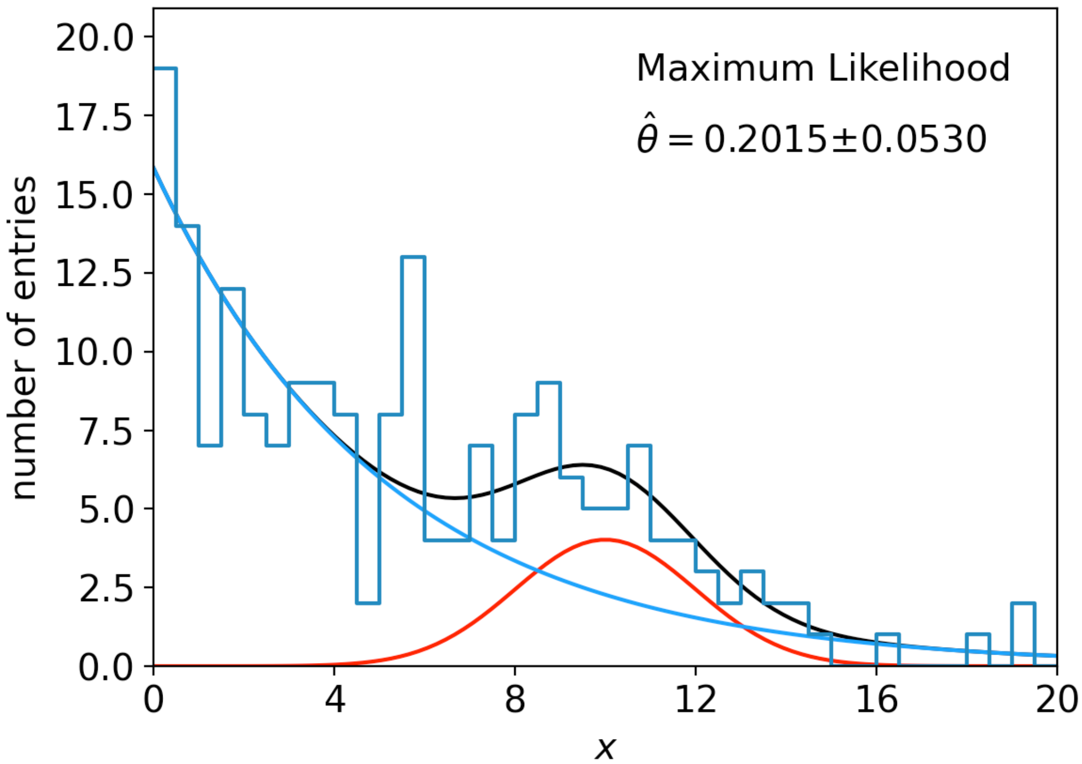

```
def negLogL(par):
    pdf = f(xData, par)
    return -np.sum(np.log(pdf))

        ⋮

m = Minuit(negLogL, par, name=parname)
```

ln*L* in a class, binned data,...

Sometimes it is convenient to have the function being minimized as a method of a class. An example of this is shown in the program histFit.py, which does the same fit as in mlFit.py but with a histogram of the data:



Commentary on histFit.py

The global data can be avoided if we make the objective function a method of a class:

```
class ChiSquared:                          # function to be minimized

    def __init__(self, xHist, bin_edges, fitType):
        self.setData(xHist, bin_edges)
        self.fitType = fitType

    def setData(self, xHist, bin_edges):
        numVal = np.sum(xHist)
        numBins = len(xHist)
        binSize = bin_edges[1] - bin_edges[0]
        self.data = xHist, bin_edges, numVal, numBins, binSize

    def chi2LS(self, par):                 # least squares
        xHist, bin_edges, numVal, numBins, binSize = self.data
        xMid = bin_edges[:numBins] + 0.5*binSize
        binProb = f(xMid, par)*binSize
        nu = numVal*binProb
        sigma = np.sqrt(nu)
        z = (xHist - nu)/sigma
        return np.sum(z**2)
```

class ChiSquared (continued)

```
def chi2M(self, par):               # multinomial maximum likelihood
    xHist, bin_edges, numVal, numBins, binSize = self.data
    xMid = bin_edges[:numBins] + 0.5*binSize
    binProb = f(xMid, par)*binSize
    nu = numVal*binProb
    lnL = 0.
    for i in range(len(xHist)):
        if xHist[i] > 0.:
            lnL += xHist[i]*np.log(nu[i]/xHist[i])
    return -2.*lnL

def __call__(self, par):
    if self.fitType == 'LS':
        return self.chi2LS(par)
    elif self.fitType == 'M':
        return self.chi2M(par)
    else:
        print("fitType not defined")
        return -1
```

Using the ChiSquared class

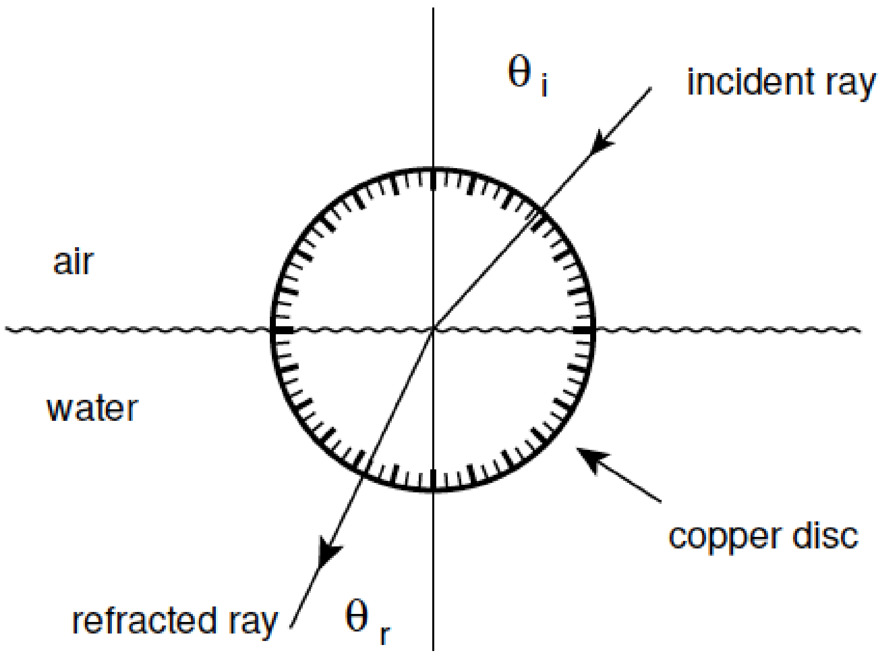
```
# Put data values into a histogram
numBins=40
xHist, bin_edges = np.histogram(xData, bins=numBins, range=(xMin, xMax))
binSize = bin_edges[1] - bin_edges[0]

# Initialize Minuit and set up fit:
parin   = np.array([theta, mu, sigma, xi])      # initial values (here = true)
parname = ['theta', 'mu', 'sigma', 'xi']
parstep = np.array([0.1, 1., 1., 1.])           # initial setp sizes
parfix  = [False, True, True, False]            # change to fix/free param.
parlim  = [(0.,1), (None, None), (0., None), (0., None)]
chisq = ChiSquared(xHist, bin_edges, fitType)
m = Minuit(chisq, parin, name=parname)
m.errors = parstep
m.fixed = parfix
m.limits = parlim
m.errordef = 1.0                      # errors from chi2 = chi2min + 1
```

For full program see
https://www.pp.rhul.ac.uk/~cowan/stat/exercises/fitting/python/

LS example: refraction data from Ptolemy

Astronomer Claudius Ptolemy obtained data on refraction of light by water in around 140 A.D.:



Angles of incidence and refraction (degrees)

θ_i	θ_r
10	8
20	$15\frac{1}{2}$
30	$22\frac{1}{2}$
40	29
50	35
60	$40\frac{1}{2}$
70	$45\frac{1}{2}$
80	50

Suppose the angle of incidence is set with negligible error, and the measured angle of refraction has a standard deviation of ½° .

Laws of refraction

A commonly used law of refraction was

$$\theta_{\rm r} = \alpha \theta_{\rm i} \ ,$$

although it is reported that Ptolemy preferred

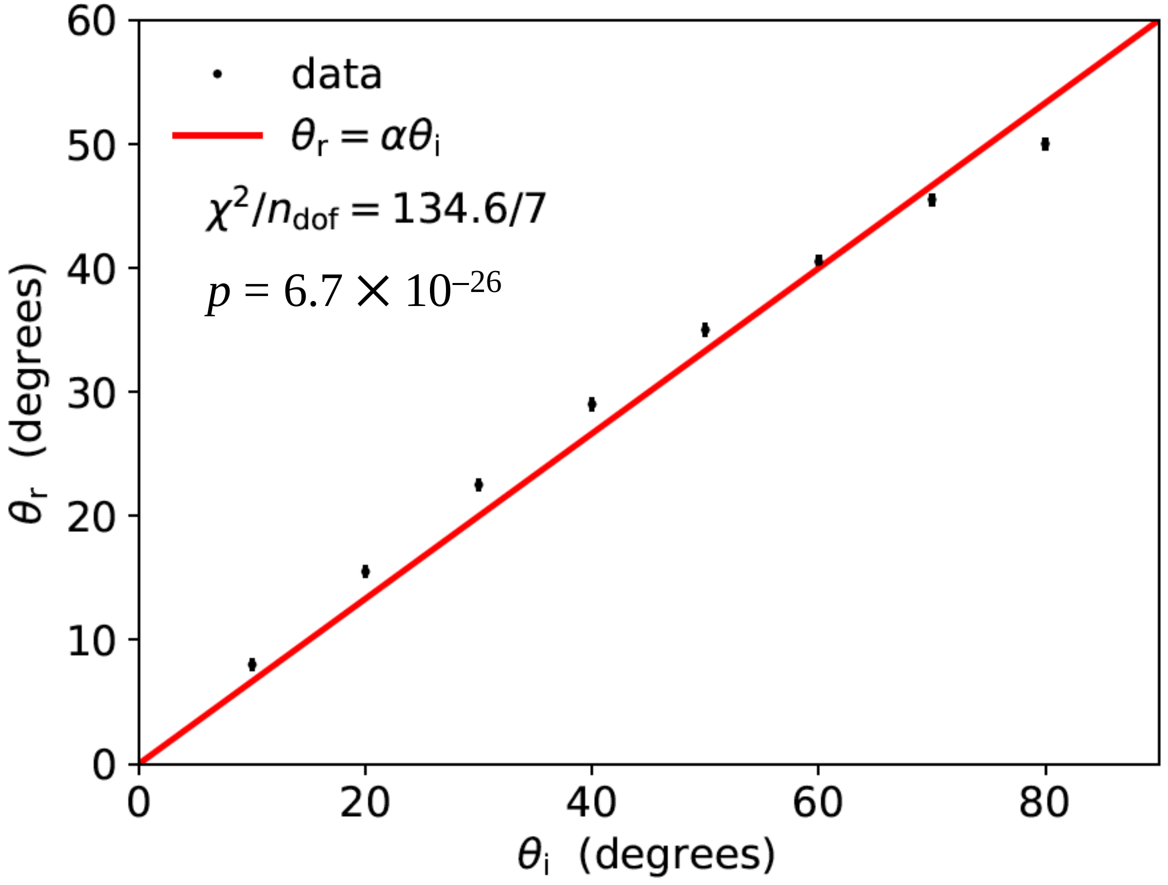
$$\theta_{\rm r} = \alpha \theta_{\rm i} - \beta \theta_{\rm i}^2 \ .$$

The law of refraction discovered by Ibn Sahl in 984 (and rediscovered by Snell in 1621) is

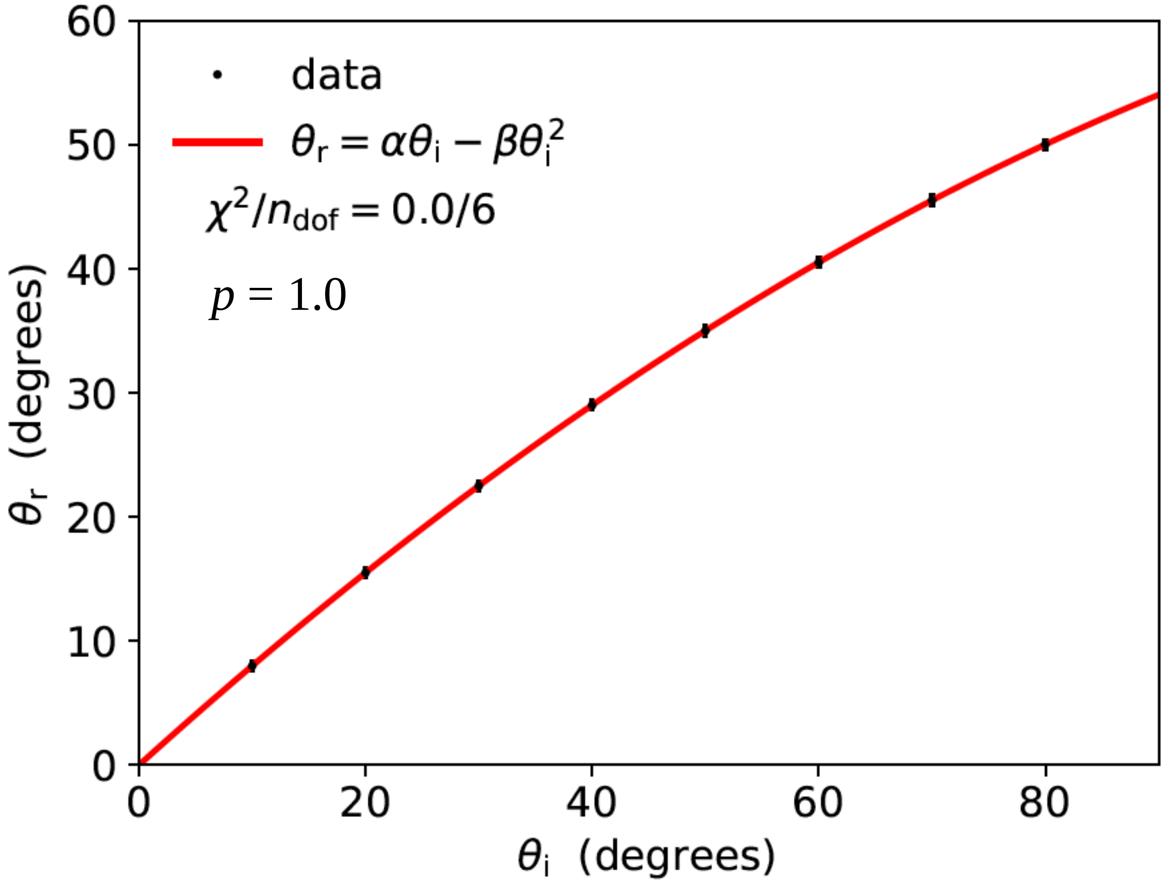
$$\theta_{\rm r} = \sin^{-1} \left(\frac{\sin \theta_{\rm i}}{r} \right) .$$

where $r = n_{\rm r}/n_{\rm i}$ is the ratio of indices of refraction of the two media.

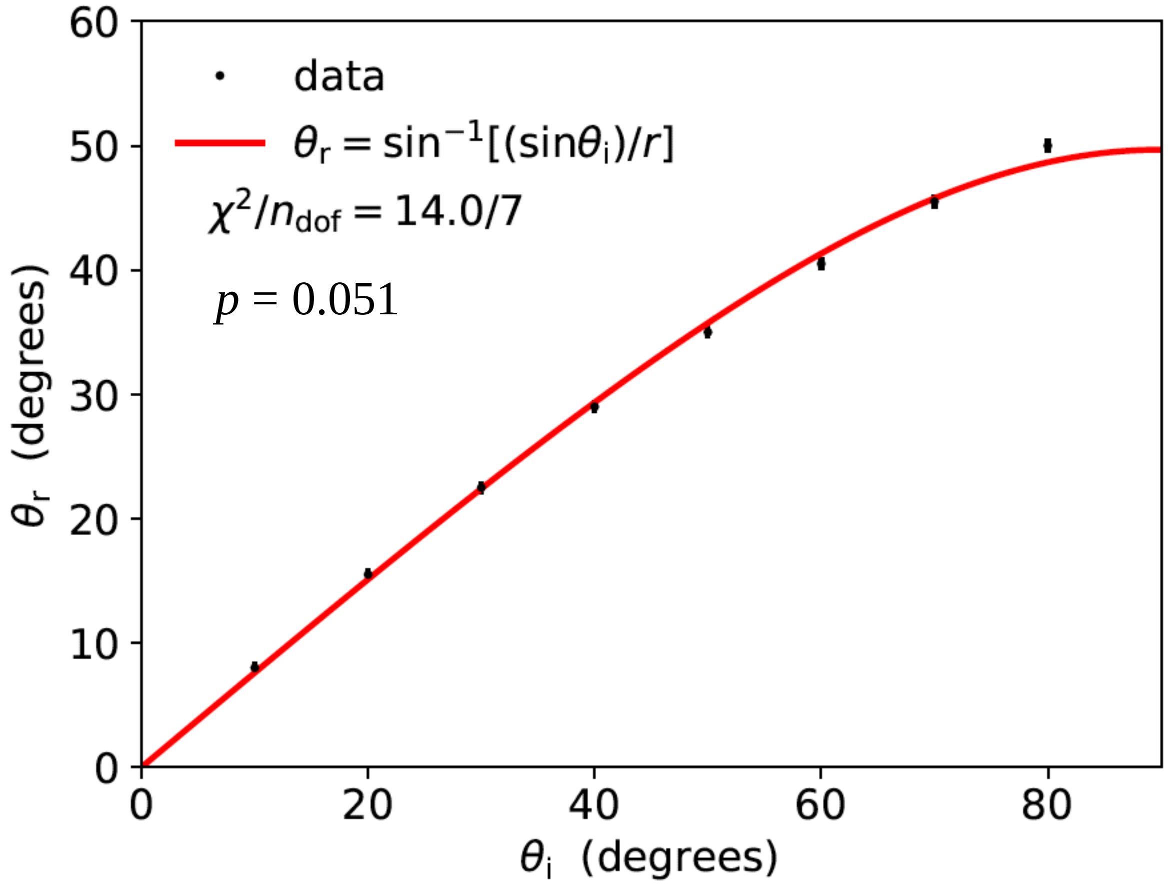
LS fit: $\theta_\mathrm{r} = \alpha\theta_\mathrm{i}$



LS fit: $\theta_{\rm r} = \alpha\theta_{\rm i} - \beta\theta_{\rm i}^2$



LS fit: Snell's Law



Fitted index of refraction of water r = 1.3116 ± 0.0056 found not quite compatible with currently known value 1.330.