Statistics for Particle Physicists
Lecture 2: Parameter Estimation

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Outline

Lecture 1: Introduction, probability,

Lecture 2: Parameter estimation

(see exercise on fitting with iminuit here)

Lecture 3: Hypothesis tests

Lecture 4: Introduction to Machine Learning

Hypothesis, likelihood

Suppose the entire result of an experiment (set of measurements) is a collection of numbers $\boldsymbol{x}$.

A (simple) hypothesis is a rule that assigns a probability to each possible data outcome:

$$P(\mathbf{x}|H) \quad = \quad \text{the likelihood of } H$$

Often we deal with a family of hypotheses labeled by one or more undetermined parameters (a composite hypothesis):

$$P(\mathbf{x}|\boldsymbol{\theta}) = L(\boldsymbol{\theta}) \quad = \quad \text{the “likelihood function”}$$

Note:

1) For the likelihood we treat the data $\boldsymbol{x}$ as fixed.
2) The likelihood function $L(\boldsymbol{\theta})$ is not a pdf for $\boldsymbol{\theta}$.

The likelihood function for i.i.d.* data

* i.i.d. = independent and identically distributed

Consider n independent observations of x: $x_1, \ldots, x_n$, where x follows $f(x; \theta)$. The joint pdf for the whole data sample is:

$$f(x_1, \ldots, x_n; \theta) = \prod_{i=1}^{n} f(x_i; \theta)$$

In this case the likelihood function is

$$L(\vec{\theta}) = \prod_{i=1}^{n} f(x_i; \vec{\theta}) \qquad (x_i \text{ constant})$$

Parameter estimation

The parameters of a pdf are any constants that characterize it,

$$f(x;\theta) = \frac{1}{\theta} e^{-x/\theta}$$

r.v. parameter

i.e., θ indexes a set of hypotheses.

Suppose we have a sample of observed values: $\boldsymbol{x} = (x_1, \ldots, x_n)$

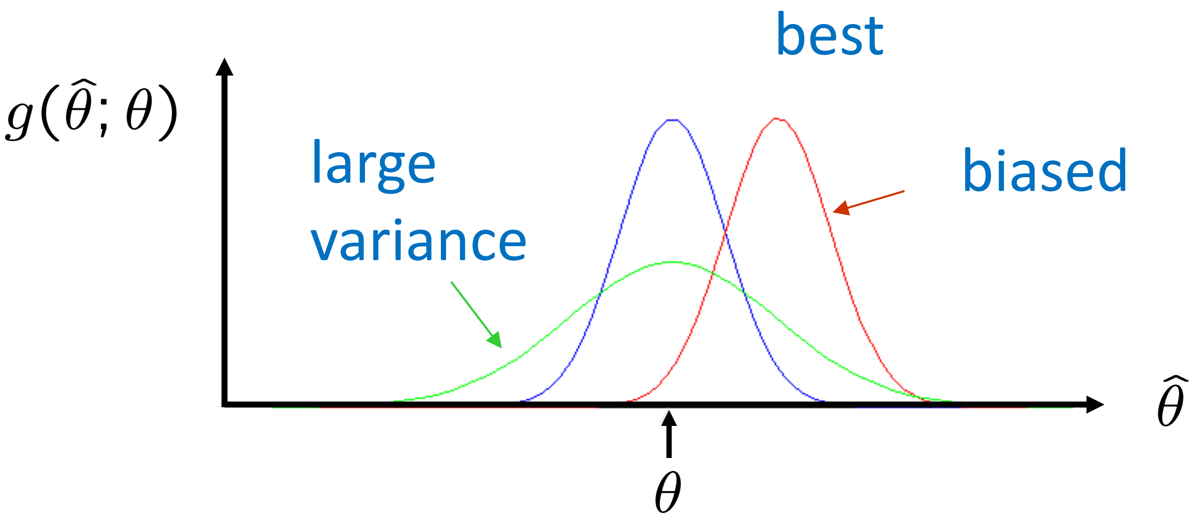
We want to find some function of the data to estimate the parameter(s):

$\boxed{\widehat{\theta}(\vec{x})}$ ← estimator written with a hat

Sometimes we say 'estimator' for the function of $x_1, \ldots, x_n$;
'estimate' for the value of the estimator with a particular data set.

Properties of estimators

If we were to repeat the entire measurement, the estimates from each would follow a pdf:



We want small (or zero) bias (systematic error): $b = E[\widehat{\theta}] - \theta$

$\rightarrow$ average of repeated measurements should tend to true value.

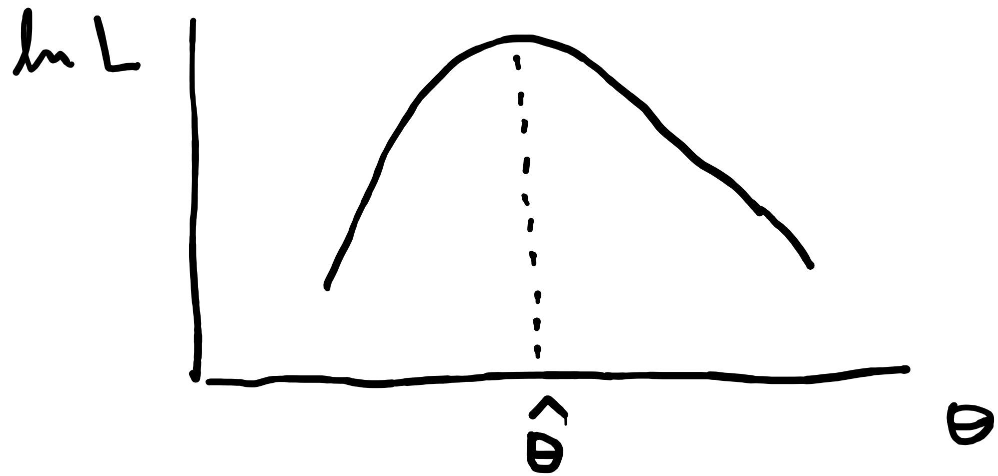
And we want a small variance (statistical error): $V[\widehat{\theta}]$

$\rightarrow$ small bias & variance are in general conflicting criteria

Maximum Likelihood Estimators (MLEs)

We *define* the maximum likelihood estimators or MLEs to be the parameter values for which the likelihood is maximum.

Maximizing L equivalent to maximizing $\log L$



$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\mathrm{argmax}}\, L(\boldsymbol{\theta})$$

Could have multiple maxima (take highest).

MLEs not guaranteed to have any 'optimal' properties, (but in practice they're very good).

MLE example: parameter of exponential pdf

Consider exponential pdf, $f(t;\tau) = \frac{1}{\tau} e^{-t/\tau}$

and suppose we have i.i.d. data, $t_1, \ldots, t_n$

The likelihood function is $L(\tau) = \prod_{i=1}^{n} \frac{1}{\tau} e^{-t_i/\tau}$

The value of τ for which $L(\tau)$ is maximum also gives the maximum value of its logarithm (the log-likelihood function):

$$\ln L(\tau) = \sum_{i=1}^{n} \ln f(t_i;\tau) = \sum_{i=1}^{n} \left(\ln \frac{1}{\tau} - \frac{t_i}{\tau} \right)$$

MLE example: parameter of exponential pdf (2)

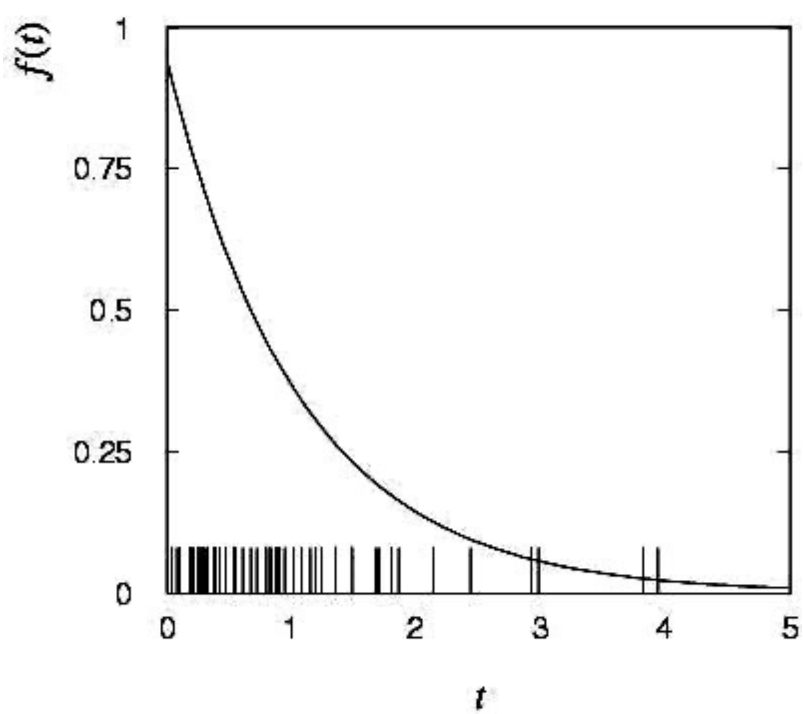
Find its maximum by setting $\dfrac{\partial \ln L(\tau)}{\partial \tau} = 0$,

$$\rightarrow \quad \hat{\tau} = \frac{1}{n} \sum_{i=1}^{n} t_i$$

Monte Carlo test:

generate 50 values

using $\tau = 1$:



We find the ML estimate:

$$\hat{\tau} = 1.062$$

MLE example: parameter of exponential pdf (3)

For the exponential distribution one has for mean, variance:

$$E[t] = \int_0^\infty t \, \frac{1}{\tau} e^{-t/\tau} \, dt = \tau$$

$$V[t] = \int_0^\infty (t - \tau)^2 \, \frac{1}{\tau} e^{-t/\tau} \, dt = \tau^2$$

For the MLE $\hat{\tau} = \frac{1}{n} \sum_{i=1}^{n} t_i$ we therefore find

$$E[\hat{\tau}] = E\left[\frac{1}{n}\sum_{i=1}^{n} t_i\right] = \frac{1}{n}\sum_{i=1}^{n} E[t_i] = \tau \quad \longrightarrow \quad b = E[\hat{\tau}] - \tau = 0$$

$$V[\hat{\tau}] = V\left[\frac{1}{n}\sum_{i=1}^{n} t_i\right] = \frac{1}{n^2}\sum_{i=1}^{n} V[t_i] = \frac{\tau^2}{n} \quad \longrightarrow \quad \sigma_{\hat{\tau}} = \frac{\tau}{\sqrt{n}}$$

Variance of estimators: Monte Carlo method

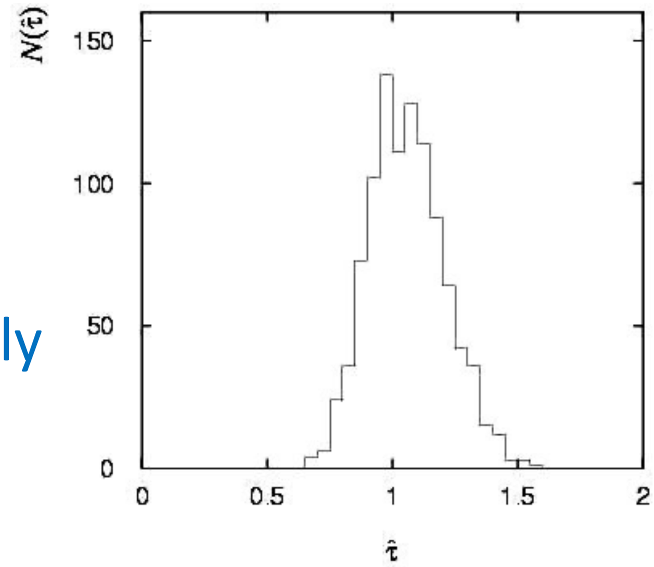
Having estimated our parameter we now need to report its 'statistical error', i.e., how widely distributed would estimates be if we were to repeat the entire measurement many times.

One way to do this would be to simulate the entire experiment many times with a Monte Carlo program (use ML estimate for MC).

For exponential example, from sample variance of estimates we find:

$$\widehat{\sigma}_{\widehat{\tau}} = 0.151$$

Note distribution of estimates is roughly Gaussian − (almost) always true for ML in large sample limit.



Variance of estimators from information inequality

The information inequality (RCF) sets a lower bound on the variance of any estimator (not only ML):

Minimum Variance Bound (MVB)

$$V[\widehat{\theta}] \geq \left(1 + \frac{\partial b}{\partial \theta}\right)^2 \Big/ E\left[-\frac{\partial^2 \ln L}{\partial \theta^2}\right] \qquad (b = E[\widehat{\theta}] - \theta)$$

Often the bias b is small, and equality either holds exactly or is a good approximation (e.g. large data sample limit). Then,

$$V[\widehat{\theta}] \approx -1 \Big/ E\left[\frac{\partial^2 \ln L}{\partial \theta^2}\right]$$

Estimate this using the 2nd derivative of $\ln L$ at its maximum:

$$\widehat{V}[\widehat{\theta}] = -\left(\frac{\partial^2 \ln L}{\partial \theta^2}\right)^{-1}\Bigg|_{\theta=\widehat{\theta}}$$

MVB for MLE of exponential parameter

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

We found for the exponential parameter the MLE $\hat{\tau} = \frac{1}{n}\sum_{i=1}^{n} t_i$

and we showed $b = 0$, hence $\partial b/\partial\tau = 0$.

We find $$\frac{\partial^2 \ln L}{\partial \tau^2} = \sum_{i=1}^{n}\left(\frac{1}{\tau^2} - \frac{2t_i}{\tau^3}\right)$$

and since $E[t_i] = \tau$ for all i, $E\left[\frac{\partial^2 \ln L}{\partial \tau^2}\right] = -\frac{n}{\tau^2}$,

and therefore $\mathrm{MVB} = \frac{\tau^2}{n} = V[\hat{\tau}]$. (Here MLE is "efficient").

Variance of estimators: graphical method

Expand $\ln L(\theta)$ about its maximum:

$$\ln L(\theta) = \ln L(\hat{\theta}) + \left[\frac{\partial \ln L}{\partial \theta}\right]_{\theta=\hat{\theta}} (\theta - \hat{\theta}) + \frac{1}{2!}\left[\frac{\partial^2 \ln L}{\partial \theta^2}\right]_{\theta=\hat{\theta}} (\theta - \hat{\theta})^2 + \ldots$$

First term is $\ln L_{\max}$, second term is zero, for third term use information inequality (assume equality):

$$\ln L(\theta) \approx \ln L_{\max} - \frac{(\theta - \hat{\theta})^2}{2\widehat{\sigma^2}_{\hat{\theta}}}$$

i.e., $$\ln L(\hat{\theta} \pm \hat{\sigma}_{\hat{\theta}}) \approx \ln L_{\max} - \frac{1}{2}$$

$\rightarrow$ to get $\hat{\sigma}_{\hat{\theta}}$, change θ away from $\hat{\theta}$ until $\ln L$ decreases by 1/2.

Example of variance by graphical method

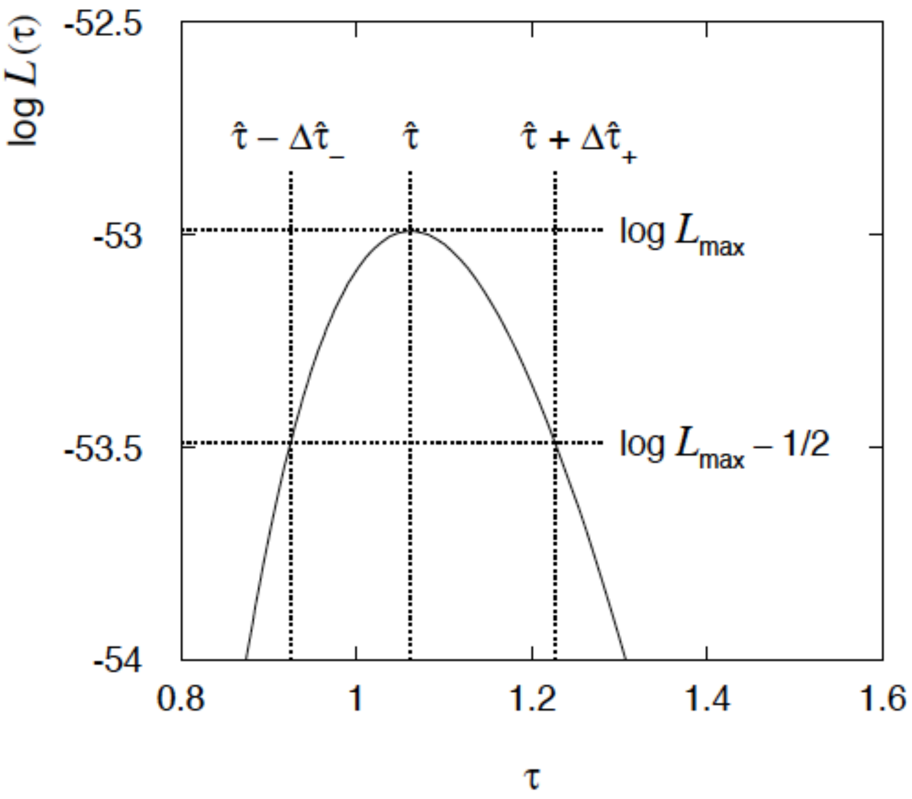
ML example with exponential:

$$\hat{\tau} = 1.062$$

$$\Delta\hat{\tau}_- = 0.137$$

$$\Delta\hat{\tau}_+ = 0.165$$

$$\hat{\sigma}_{\hat{\tau}} \approx \Delta\hat{\tau}_- \approx \Delta\hat{\tau}_+ \approx 0.15$$



Not quite parabolic $\ln L$ since finite sample size (n = 50).

Information inequality for N parameters

Suppose we have estimated N parameters $\boldsymbol{\theta} = (\theta_1,\ldots,\theta_N)$

The *Fisher information matrix* is

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

and the covariance matrix of estimators $\hat{\boldsymbol{\theta}}$ is $V_{ij} = \mathrm{cov}[\hat{\theta}_i, \hat{\theta}_j]$

The information inequality states that the matrix

$$M_{ij} = V_{ij} - \sum_{k,l} \left(\delta_{ik} + \frac{\partial b_i}{\partial\theta_k}\right) I_{kl}^{-1} \left(\delta_{lj} + \frac{\partial b_l}{\partial\theta_j}\right)$$

is positive semi-definite:

$\boldsymbol{z}^{\mathrm{T}} M \boldsymbol{z} \geq 0$ for all $\boldsymbol{z} \neq 0$, diagonal elements ≥ 0

Information inequality for N parameters (2)

In practice the inequality is ~always used in the large-sample limit:

bias $\rightarrow$ 0

inequality $\rightarrow$ equality, i.e, $M = 0$, and therefore $V^{-1} = I$

That is, $$V_{ij}^{-1} = -E\left[\frac{\partial^2 \ln L}{\partial\theta_i \partial\theta_j}\right]$$

This can be estimated from data using $$\widehat{V}_{ij}^{-1} = -\left.\frac{\partial^2 \ln L}{\partial\theta_i \partial\theta_j}\right|_{\hat{\boldsymbol{\theta}}}$$

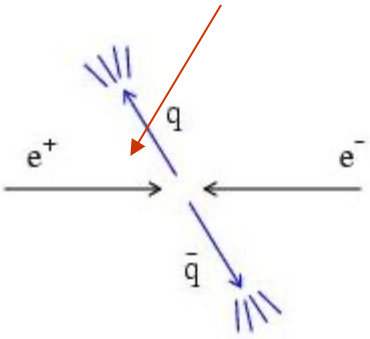
Find the matrix V^{-1} numerically (or with automatic differentiation), then invert to get the covariance matrix of the estimators

$$\widehat{V}_{ij} = \widehat{\mathrm{cov}}[\hat{\theta}_i, \hat{\theta}_j]$$

Example of ML with 2 parameters

Consider a scattering angle distribution with $x = \cos\theta$,

$$f(x;\alpha,\beta) = \frac{1+\alpha x+\beta x^2}{2+2\beta/3}$$



or if $x_{\min} < x < x_{\max}$, need to normalize so that

$$\int_{x_{\min}}^{x_{\max}} f(x;\alpha,\beta)\,dx = 1 \ .$$

Example: $\alpha = 0.5$, $\beta = 0.5$, $x_{\min} = -0.95$, $x_{\max} = 0.95$, generate $n = 2000$ events with Monte Carlo.

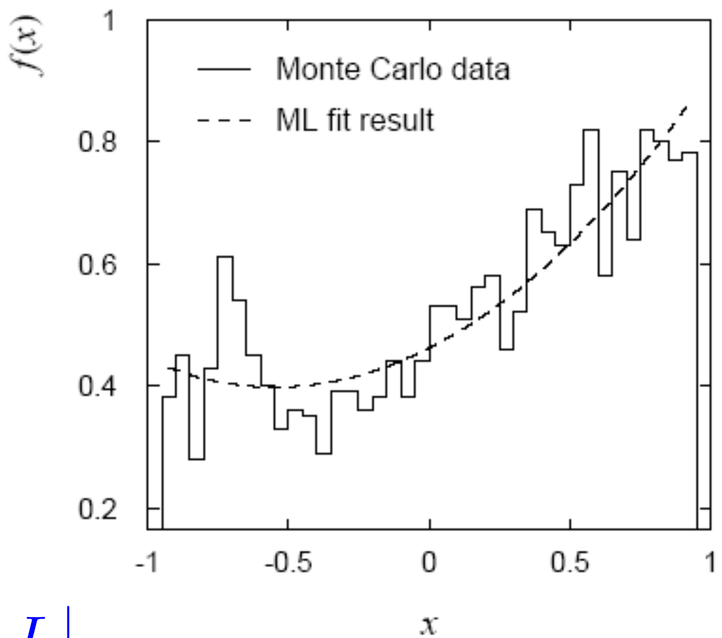
$$\ln L(\alpha,\beta) = \sum_{i=1}^{n} \ln f(x_i;\alpha,\beta)$$

need to find maximum numerically

Example of ML with 2 parameters: fit result

Finding maximum of $\ln L(\alpha, \beta)$ numerically gives

$$\widehat{\alpha} = 0.508$$
$$\widehat{\beta} = 0.47$$



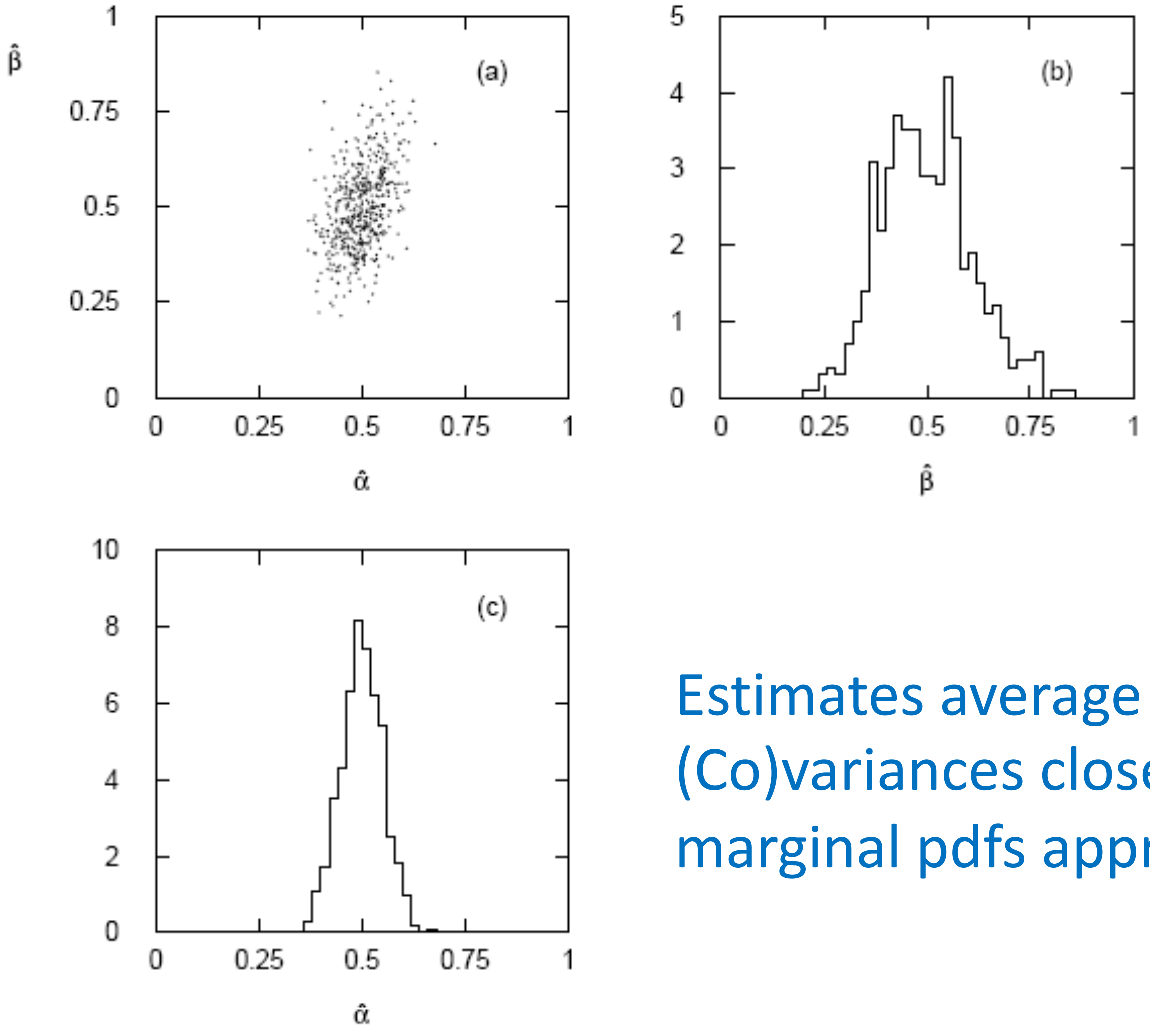
N.B. No binning of data for fit, but can compare to histogram for goodness-of-fit (e.g. 'visual' or χ^2).

(Co)variances from $\widehat{(V^{-1})}_{ij} = -\left.\frac{\partial^2 \ln L}{\partial\theta_i \partial\theta_j}\right|_{\vec{\theta}=\widehat{\vec{\theta}}}$

$$\widehat{\sigma}_{\widehat{\alpha}} = 0.052 \qquad \mathrm{cov}[\widehat{\alpha}, \widehat{\beta}] = 0.0026$$
$$\widehat{\sigma}_{\widehat{\beta}} = 0.11 \qquad r = 0.46$$ = correlation coefficient

Two-parameter fit: MC study

Repeat ML fit with 500 experiments, all with $n = 2000$ events:



$$
\begin{aligned}
\overline{\hat{\alpha}} &= 0.499 \\
s_{\hat{\alpha}} &= 0.051 \\
\overline{\hat{\beta}} &= 0.498 \\
s_{\hat{\beta}} &= 0.111 \\
\widehat{\mathrm{cov}}[\hat{\alpha}, \hat{\beta}] &= 0.0024 \\
r &= 0.42
\end{aligned}
$$

Estimates average to ~true values;
(Co)variances close to previous estimates;
marginal pdfs approximately Gaussian.

Multiparameter graphical method for variances

Expand $\ln L(\boldsymbol{\theta})$ to 2nd order about MLE:

$$\ln L(\boldsymbol{\theta}) \approx \ln L(\hat{\boldsymbol{\theta}}) + \sum_i \left.\frac{\partial \ln L}{\partial \theta_i}\right|_{\hat{\boldsymbol{\theta}}} (\theta_i - \hat{\theta}_i) + \frac{1}{2!} \sum_{i,j} \left.\frac{\partial^2 \ln L}{\partial \theta_i \partial \theta_j}\right|_{\hat{\boldsymbol{\theta}}} (\theta_i - \hat{\theta}_i)(\theta_j - \hat{\theta}_j)$$

$\ln L_{\max}$

zero

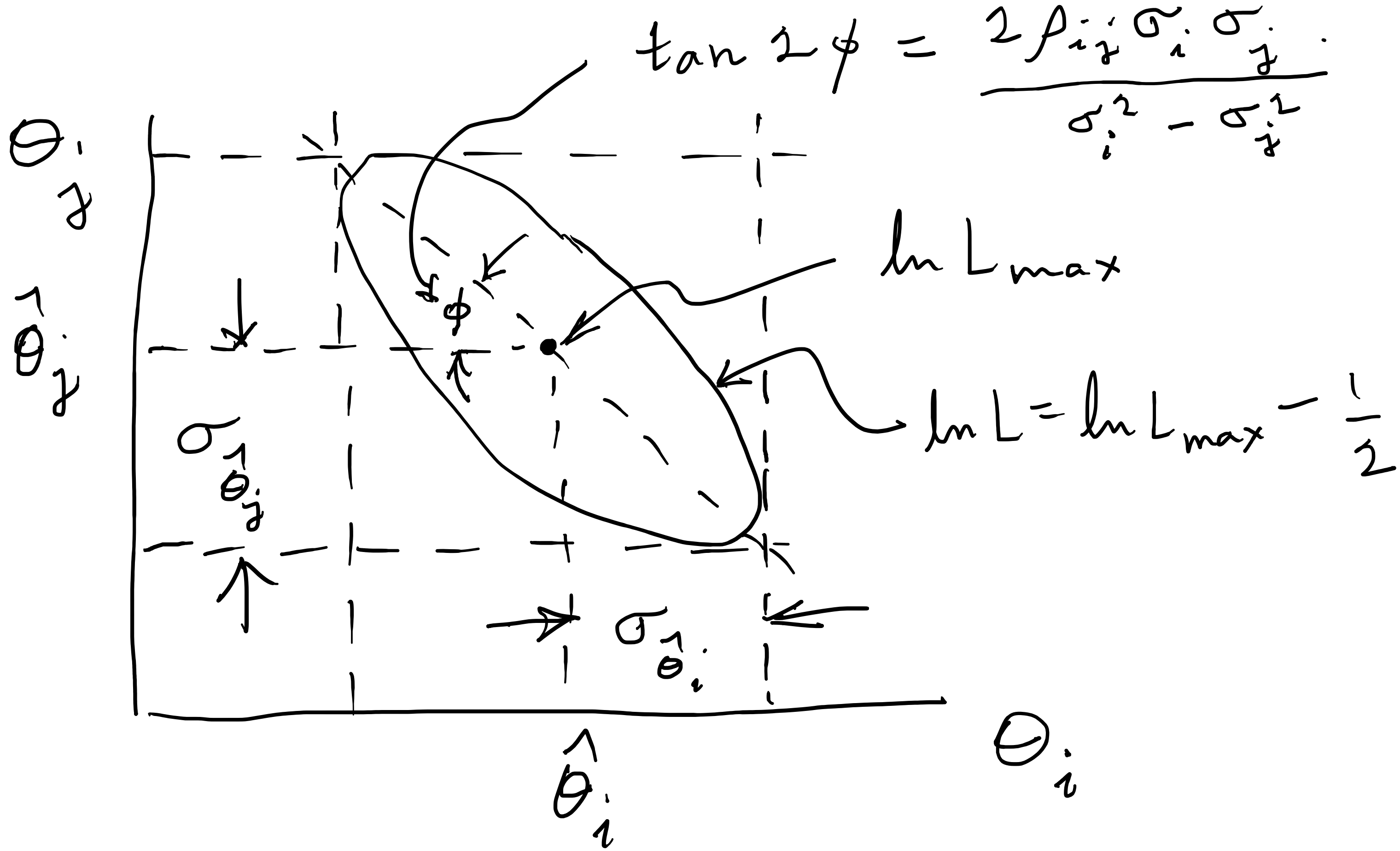
relate to covariance matrix of MLEs using information (in)equality.

Result: $$\ln L(\boldsymbol{\theta}) = \ln L_{\max} - \frac{1}{2} \sum_{i,j} (\theta_i - \hat{\theta}_i) V_{ij}^{-1} (\theta_j - \hat{\theta}_j)$$

So the surface $\ln L(\boldsymbol{\theta}) = \ln L_{\max} - \frac{1}{2}$ corresponds to

$(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^T V^{-1} (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) = 1$, which is the equation of a (hyper-) ellipse.

Multiparameter graphical method (2)



Distance from MLE to tangent planes gives standard deviations.

The $\ln L_{\max} - 1/2$ contour for two parameters

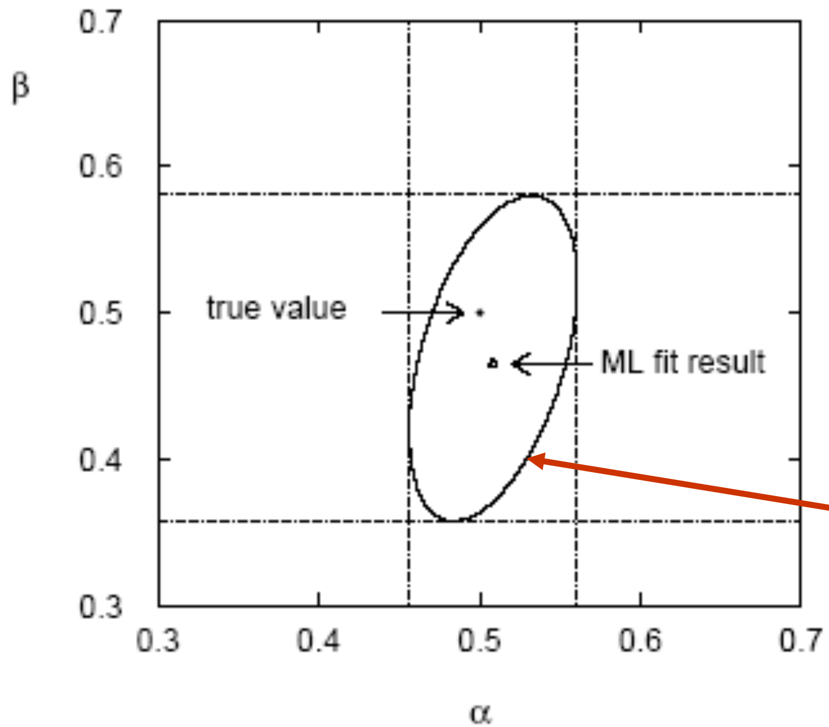
For large n, $\ln L$ takes on quadratic form near maximum:

$$\ln L(\alpha, \beta) \approx \ln L_{\max} - \frac{1}{2(1-\rho^2)} \left[\left(\frac{\alpha - \hat{\alpha}}{\sigma_{\hat{\alpha}}} \right)^2 + \left(\frac{\beta - \hat{\beta}}{\sigma_{\hat{\beta}}} \right)^2 - 2\rho \left(\frac{\alpha - \hat{\alpha}}{\sigma_{\hat{\alpha}}} \right) \left(\frac{\beta - \hat{\beta}}{\sigma_{\hat{\beta}}} \right) \right]$$

The contour $\ln L(\alpha, \beta) = \ln L_{\max} - 1/2$ is an ellipse:

$$\frac{1}{(1-\rho^2)} \left[\left(\frac{\alpha - \hat{\alpha}}{\sigma_{\hat{\alpha}}} \right)^2 + \left(\frac{\beta - \hat{\beta}}{\sigma_{\hat{\beta}}} \right)^2 - 2\rho \left(\frac{\alpha - \hat{\alpha}}{\sigma_{\hat{\alpha}}} \right) \left(\frac{\beta - \hat{\beta}}{\sigma_{\hat{\beta}}} \right) \right] = 1$$

(Co)variances from ln *L* contour



The α, β plane for the first MC data set

$$\ln L(\alpha, \beta) = \ln L_{\max} - 1/2$$

$\longrightarrow$ Tangent lines to contours give standard deviations.

$\longrightarrow$ Angle of ellipse φ related to correlation: $\tan 2\phi = \dfrac{2\rho\sigma_{\hat{\alpha}}\sigma_{\hat{\beta}}}{\sigma_{\hat{\alpha}}^2 - \sigma\hat{\beta}^2}$

Extra slides