ADA08 - 9am Thu 29 Sep 2022

Parameter Uncertainties
Confidence Intervals and Regions

Fitting a Linear Trend
Orthogonal vs Correlated Parameters

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Summary of the ADA Roadmap:

Algebra of Random Variables

Minimising BoF = χ^2

Alternative (Robust) BoFs

Maximum Likelihood (ML) BoF=-2lnL

Bayesian Inference (MAP) BoF=-2ln(L P)

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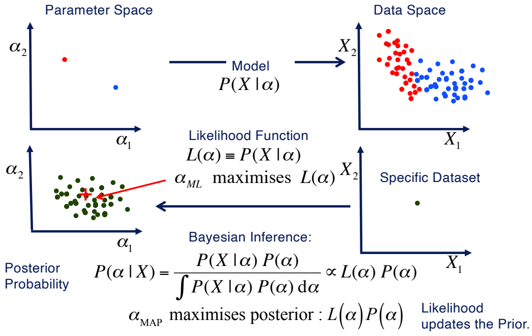
Max Likelihood and Bayesian Inference



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Monte-Carlo Error Propagation

1. Create **mock datasets**.

1a. "Jiggle" the data points (using Gaussian random numbers).
* Requires good error bars.

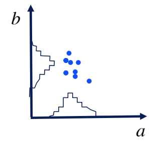
1b. (and/or) "**Bootstrap**" samples:

Pick *N* data points at random, with replacement (some points omitted, some repeated).
* Requires more data than parameters (*N* > *M*).
* Works with no error bars available.

2. Fit the model to each mock dataset.

$$\langle X_i \rangle = a\, t_i + b$$

3. Observe how the best-fit parameter values "dance".



4. Accumulate histograms approximating the parameter probability distributions.

5. Compute mean, median, variance, MAD, etc. of the parameters, or **any function of the parameters**.

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Confidence interval on a single parameter

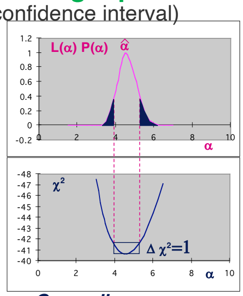
(1-parameter, k-sigma confidence interval)

The **1-σ confidence interval** on α includes 68% of the area under the likelihood function:

$$L(\alpha) \equiv P(X \mid \alpha) \propto \frac{e^{-\chi^2/2}}{\prod_i \sigma_i}$$

or posterior probability distribution, for non-uniform prior $P(\alpha)$:

$$P(\alpha \mid X) \propto L(\alpha)\, P(\alpha)$$



For a *k-σ* (1-parameter) confidence interval, use $\Delta\chi^2 = k^2$,

$\Delta\chi^2 = 1$ for 1-σ, 68% probability
$\Delta\chi^2 = 4$ for 2-σ, 95.4% probability
$\Delta\chi^2 = 9$ for 3-σ, 99.73% probability …

Generalise:

χ^2 => -2 ln($L(\alpha)\, P(\alpha)$)

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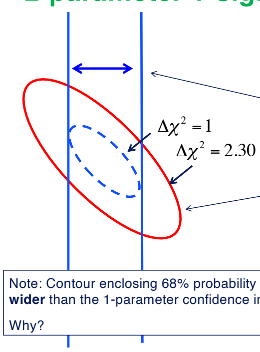
2-parameter 1-sigma Confidence Region



If *Y* is a "**nuisance parameter**", use the **1-parameter 1-sigma confidence interval** in *X*, *tangent to* the $\Delta\chi^2 = 1$ contour in *(X,Y)*.
This interval encloses 68% probability.

If both *X* and *Y* are of interest, use the **2-parameter 1-sigma confidence region**, the $\Delta\chi^2 = 2.30$ contour in *(X,Y)*.
This contour encloses 68% probability.

Use $-2 \ln(L(\alpha)\, P(\alpha))$ instead of χ^2, if needed.

$$L(\alpha) \equiv P(X \mid \alpha) \propto \frac{e^{-\chi^2/2}}{\prod_i \sigma_i}$$

Note: Contour enclosing 68% probability must be **wider** than the 1-parameter confidence interval.

Why?

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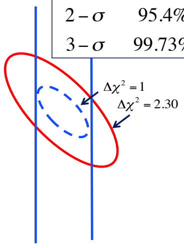
M-parameter k-σ Confidence Regions

$\Delta\chi^2$ thresholds for M-parameter k-σ Confidence Regions

	Prob	$M=1$	2	3	4
$1-\sigma$	68%	1	2.30	3.53	4.72
$2-\sigma$	95.4%	4	6.17	8.02	9.70
$3-\sigma$	99.73%	9	11.8	14.2	16.3



The **M-parameter confidence region** is enclosed by the $\Delta\chi^2$ surface including the desired probability.

All **nuisance parameters must be re-fitted** (or integrated over) for each set of fixed values for the M parameters in the sub-space of interest.

(a.k.a. "marginalise over the nuisance parameters".)

The $\Delta\chi^2$ in the M-parameter sub-space has a χ^2_M distribution, with M degrees of freedom.

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Example: Estimate both μ and σ

$$L(\mu,\sigma) \equiv P(X\,|\,\mu,\sigma) = \frac{e^{-\chi^2/2}}{(2\pi)^{N/2}\,\sigma^N}$$

$$-2\ln L = \sum_{i=1}^{N}\left(\frac{X_i-\mu}{\sigma}\right)^2 + 2N\ln\sigma + \text{const}$$

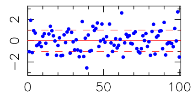
$$0 = \frac{\partial}{\partial\mu}\left[-2\ln L\right] = -2\sum_{i=1}^{N}\frac{X_i-\mu}{\sigma^2}$$

$$0 = \frac{\partial}{\partial\sigma}\left[-2\ln L\right] = -2\sum_{i=1}^{N}\frac{(X_i-\mu)^2}{\sigma^3} + \frac{2N}{\sigma}$$

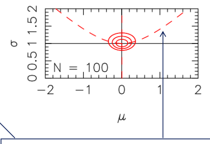
$$\mu_{\text{ML}} = \frac{1}{N}\sum_i X_i \qquad \sigma^2_{\text{ML}} = \frac{1}{N}\sum_i\left(X_i-\mu_{\text{ML}}\right)^2$$

Posterior $\propto$ Likelihood $\times$ Prior

$$P(\mu,\sigma\,|\,X) \propto L(\mu,\sigma)\,P(\mu,\sigma)$$



2-parameter 1,2,3-σ confidence regions:
$L(\mu,\sigma) = P(X|\mu,\sigma)$



Note: ML gives biased estimate for σ.

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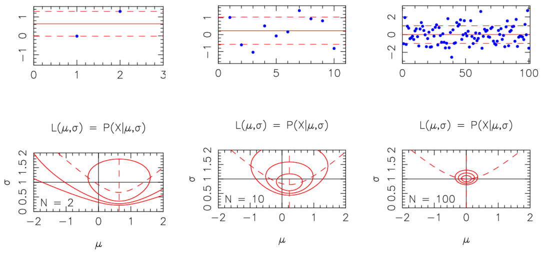
Example: Estimate both μ and σ



Contours: 1,2,3-sigma 2-parameter confidence regions for μ and σ.
Dashed curves: maximum-likelihood estimates for μ_{ML} and σ_{ML}.
True values: $\mu=0$ and $\sigma=1$.

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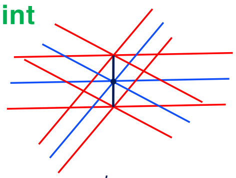
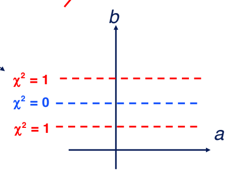
Fit a line to $N=1$ data point

Fit $y=a\,x+b$ to $N=1$ data point:
Blue lines : $\chi^2=0$
Red lines : $\chi^2=1$



χ^2 contours in the (a,b) plane:



Solution is **degenerate**, since $M=2$ parameters are constrained by only $N=1$ data point.

Bayes: prior $P(a,b)$ needed to determine a unique solution.

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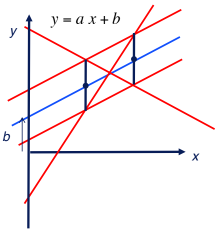
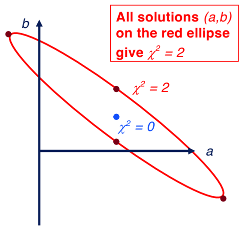
Fit a line to $N=2$ data points

- Fit $y=a\,x+b$ to $N=2$ data points:
  - red lines give $\chi^2=2$
  - blue line gives $\chi^2=0$
- Note that a, b are not independent.





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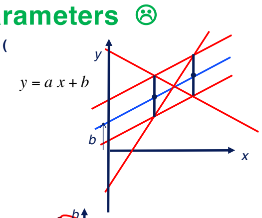
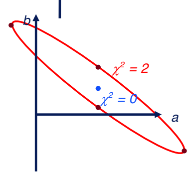
Correlated Parameters ☹

- **Parameters a and b are correlated** :(
- To find the optimal (a, b) we must:
  - minimize χ^2 with respect to a at a sequence of fixed b values
  - then minimise the resulting χ^2 values with respect to b.
- If a and b were independent, then all slices through the χ^2 surface at each fixed b would have same shape and minimum.
- Similarly for a.
- We could then optimize a and b independently, saving a lot of calculation
- **How to make a and b independent of each other?**





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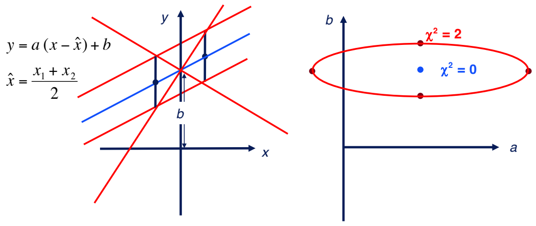
Orthogonal Parameters for fitting a line to $N = 2$ data points

- Fit $y = a\,(x - \hat{x}) + b$
- Different parameters for same model.
- Note: a, b are now independent ! ☺



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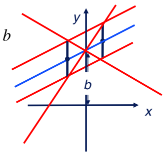
Orthogonal slope and intercept

Analysis using the algebra of random variables:

$y = a\,(x - \hat{x}) + b$

$\hat{x} = \frac{x_1 + x_2}{2}$

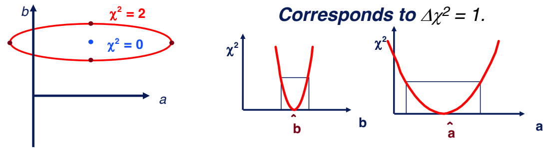


$\hat{b} = \hat{y} = \frac{y_1 + y_2}{2}$ $\qquad \hat{a} = \frac{y_2 - y_1}{(x_2 - x_1)}$

$\sigma^2(\hat{b}) = \frac{2\sigma^2}{4}$ $\qquad \sigma^2(\hat{a}) = \frac{2\sigma^2}{(x_2 - x_1)^2}$

$\sigma(\hat{b}) = \frac{\sigma}{\sqrt{2}}$ $\qquad \sigma(\hat{a}) = \sqrt{2}\,\frac{\sigma}{(x_2 - x_1)}$

Corresponds to $\Delta\chi^2 = 1$.



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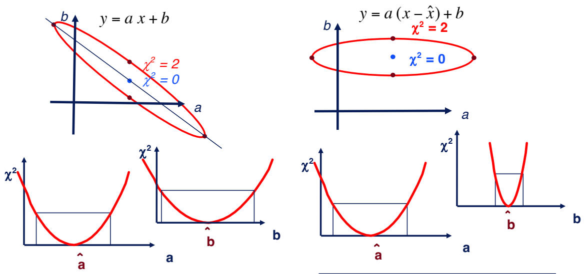
Orthogonal vs Correlated Parameters

Correlated Parameters ☹ $\qquad$ **Orthogonal Parameters** ☺



For each a, a different b minimises χ^2.
For each b, a different a minimises χ^2.

For any a, the same b minimises χ^2.
For any b, the same a minimises χ^2.

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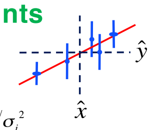
Fit a line to N data points



- If we use $y = a\,x + b$ then a, b are correlated.
- Make a, b orthogonal: $y = a\,(x - \hat{x}) + b$ $\qquad \hat{x} = \frac{\sum x_i/\sigma_i^2}{\sum 1/\sigma_i^2}$ (to be proven later)
- Intercept: Set $a = 0$ and optimise b:
  optimal average: $\hat{b} = \hat{y} = \frac{\sum y_i/\sigma_i^2}{\sum 1/\sigma_i^2}$, $\qquad \mathrm{Var}[\hat{b}] = \frac{1}{\sum 1/\sigma_i^2}$
- Slope: Set $b = 0$ and optimise a:
  optimal scaling of pattern: $P_i = x_i - \hat{x}$

$$\hat{a} = \frac{\sum y_i\,(x_i - \hat{x})/\sigma_i^2}{\sum (x_i - \hat{x})^2/\sigma_i^2}, \qquad \mathrm{Var}[\hat{a}] = \frac{1}{\sum (x_i - \hat{x})^2/\sigma_i^2}$$

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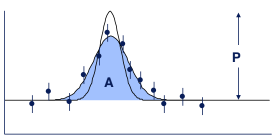
Choose Orthogonal Parameters

- Good practice (when possible).
- Results for any one parameter don't depend on values of other parameters.
- Example: fit a gaussian profile. 2 fit parameters:
  - Width, w
  - Area or peak value. Which is best?

Peak value depends on width – bad

$$f(x) = P e^{-\frac{1}{2}\left(\frac{x - x_0}{w}\right)^2}$$



$$g(x) = \frac{A}{w\sqrt{2\pi}}\, e^{-\frac{1}{2}\left(\frac{x - x_0}{w}\right)^2}$$

Area is (more nearly) independent of width – good

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