ADA08 - 9am Thu 29 Sep 2022

Parameter Uncertainties
Confidence Intervals and Regions

Fitting a Linear Trend
Orthogonal vs Correlated Parameters

Summary of the ADA Roadmap:

Algebra of Random Variables

Minimising BoF = χ^2

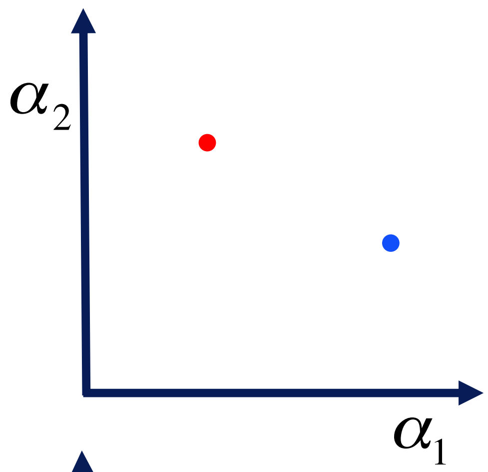
Alternative (Robust) BoFs

Maximum Likelihood (ML) BoF=-2lnL

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

Max Likelihood and Bayesian Inference

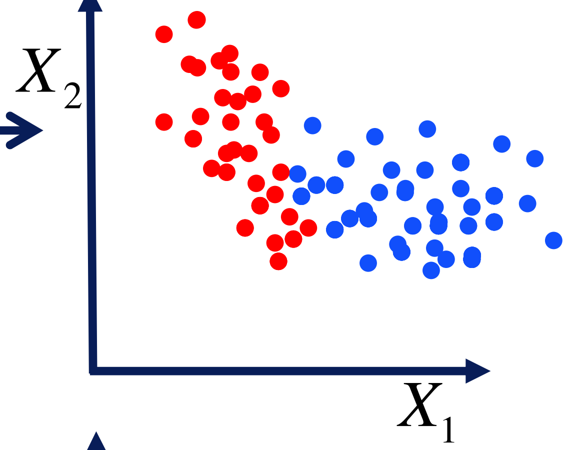
Parameter Space



Model

$$P(X \mid \alpha)$$

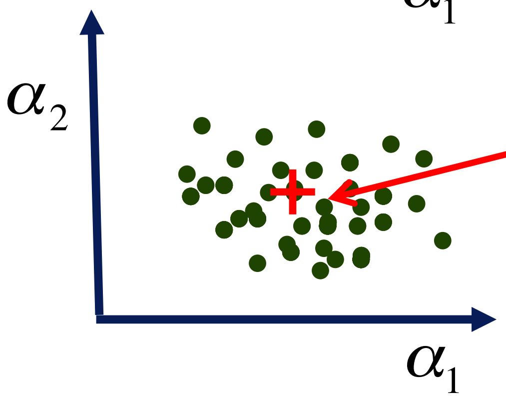
Data Space

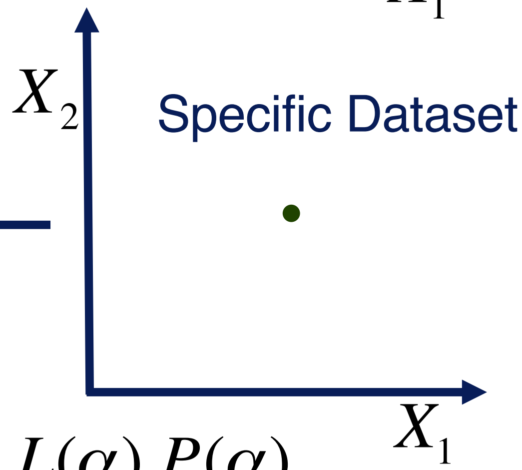


Likelihood Function

$$L(\alpha) \equiv P(X \mid \alpha)$$

$$\alpha_{ML} \;\; \text{maximises} \;\; L(\alpha)$$





Bayesian Inference:

Posterior Probability

$$P(\alpha \mid X) = \frac{P(X \mid \alpha)\, P(\alpha)}{\int P(X \mid \alpha)\, P(\alpha)\, \mathrm{d}\alpha} \propto L(\alpha)\, P(\alpha)$$

$$\alpha_{\mathrm{MAP}} \;\; \text{maximises posterior} : L\left(\alpha\right) P\left(\alpha\right)$$

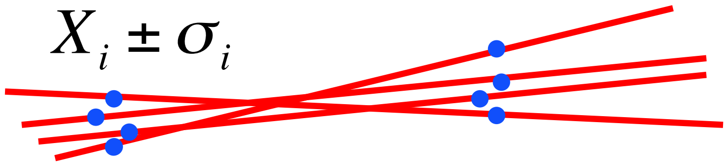
Likelihood updates the Prior.

Monte-Carlo Error Propagation

1. Create **mock datasets**.

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

$X_i \pm \sigma_i$



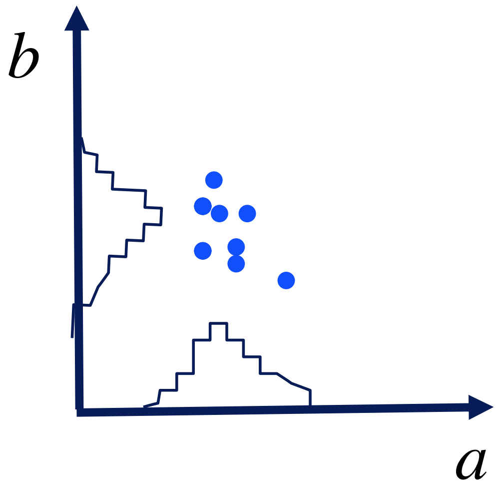
1b. (and/or) "**Bootstrap**" samples:

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**.

Confidence interval on a single parameter

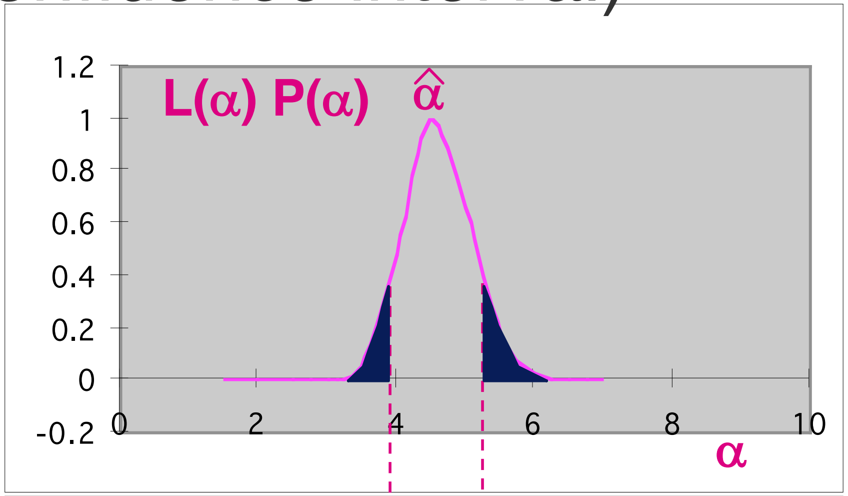
(1-parameter, k-sigma confidence interval)

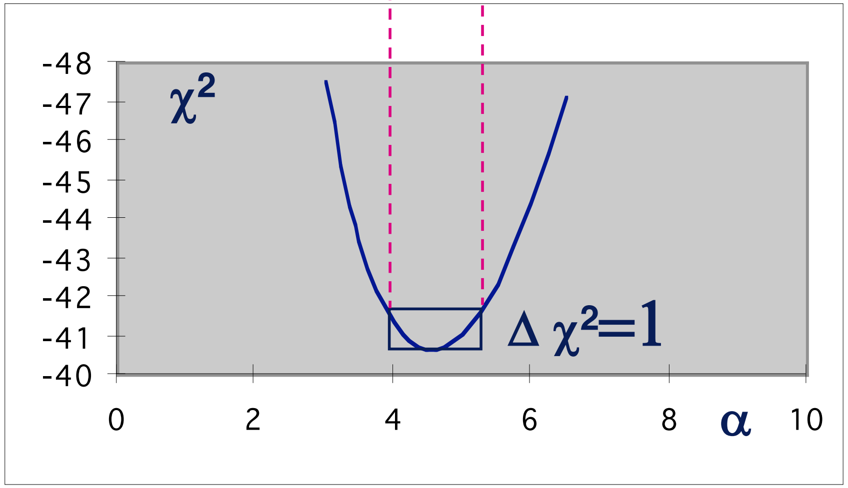
The **1-σ confidence interval** on α includes 68% of the area under the likelihood function:

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

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

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





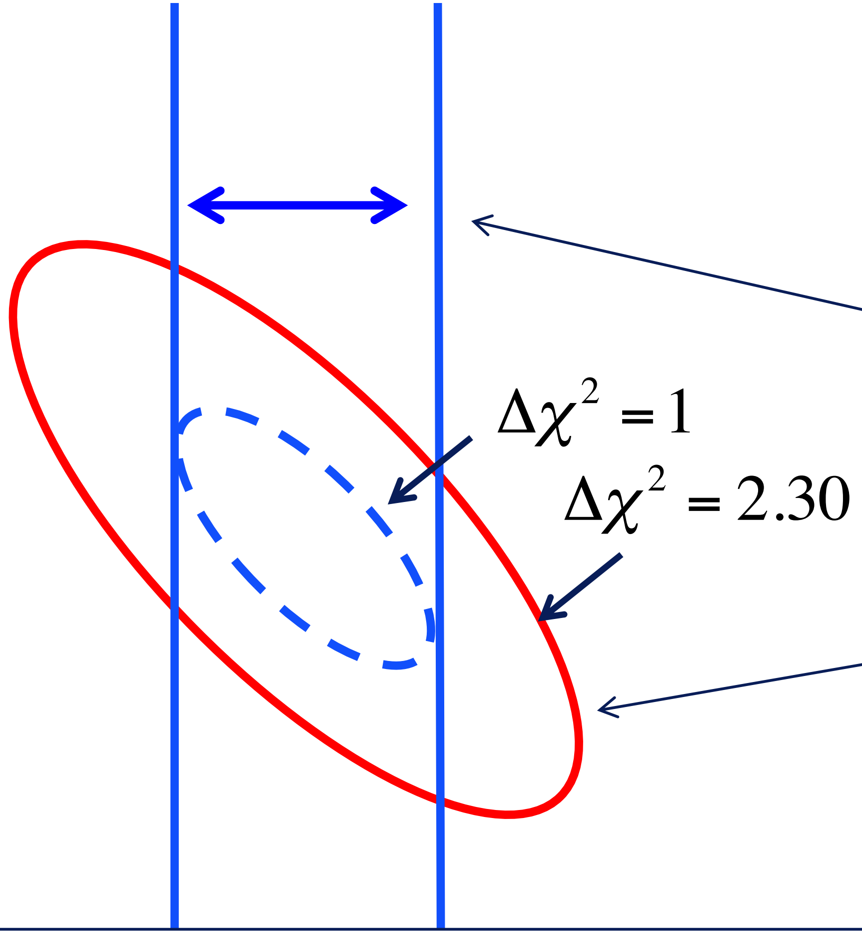
For a k-σ (1-parameter) confidence interval, use $\Delta\chi^2 = k^2$,

$\Delta\chi^2 = 1$ 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:

$\chi^2 \Rightarrow -2\ln(\, L(\alpha)\, P(\alpha)\,)$

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.

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

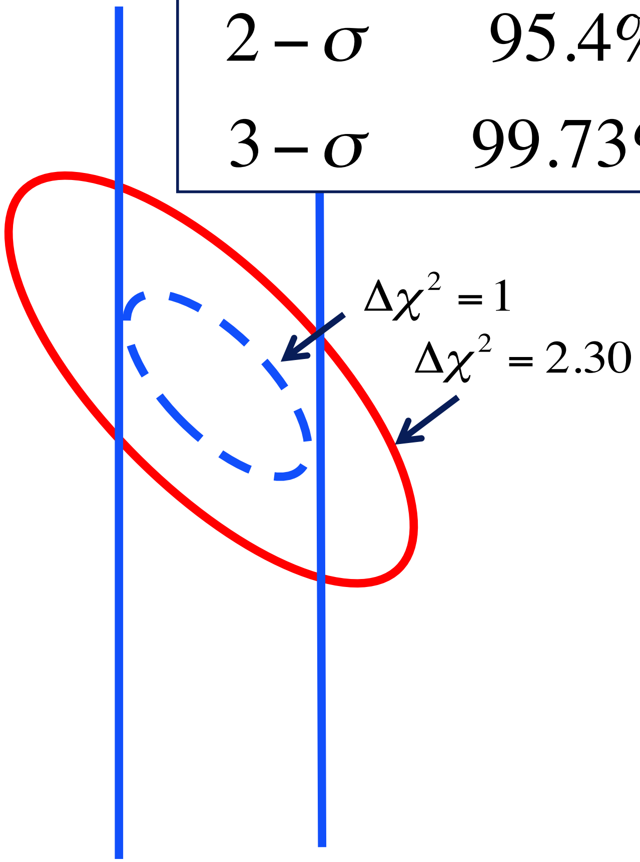
Note: Contour enclosing 68% probability must be **wider** than the 1-parameter confidence interval.

Why?

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.

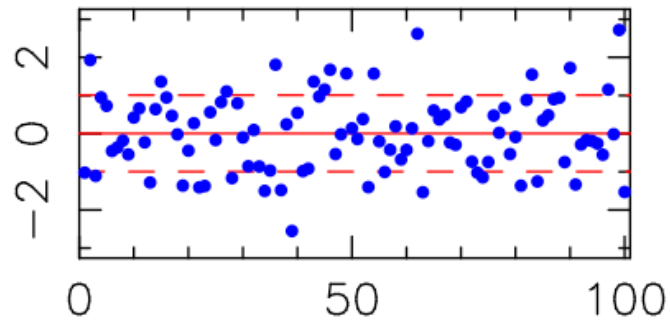
All **nuisance parameters must be re-fitted** (or integrated over) for each set of fixed values for the *M* parameters in the sub-space of interest.

(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.

Example: Estimate both μ and σ

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



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

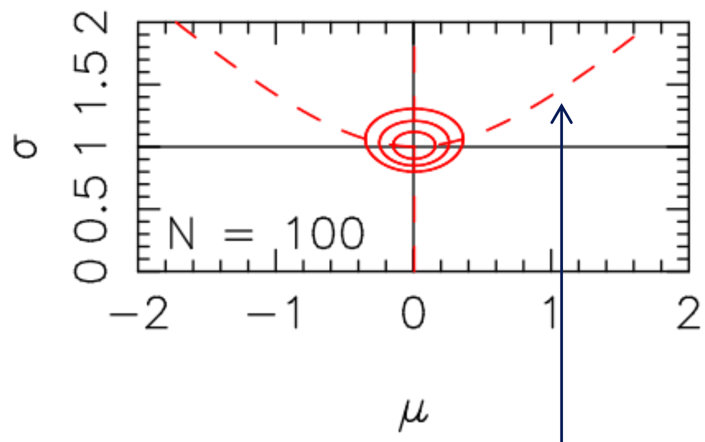
$$0 = \frac{\partial}{\partial\mu}\left[-2\ln L\right] = -2\sum_{i=1}^{N}\frac{X_i-\mu}{\sigma^2}$$

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

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

2-parameter 1,2,3-σ confidence regions:

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

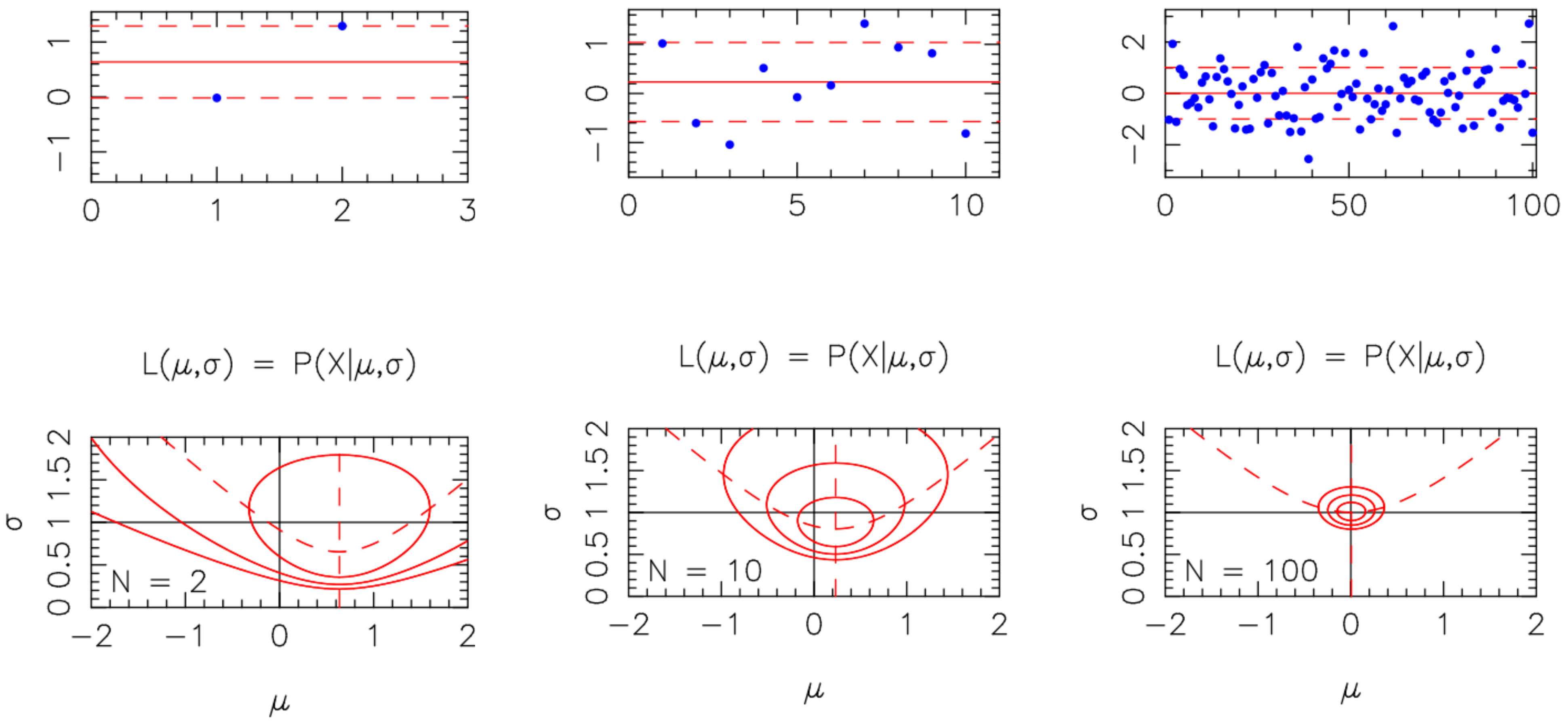


Posterior $\propto$ Likelihood $\times$ Prior

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

Note: ML gives biased estimate for σ.

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}.

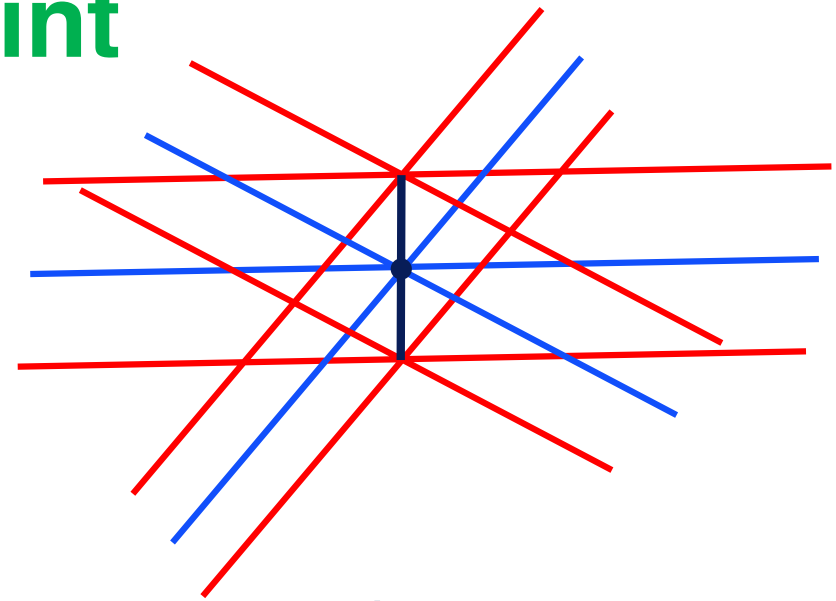
True values: $\mu = 0$ and $\sigma = 1$.

Fit a line to *N=1* data point

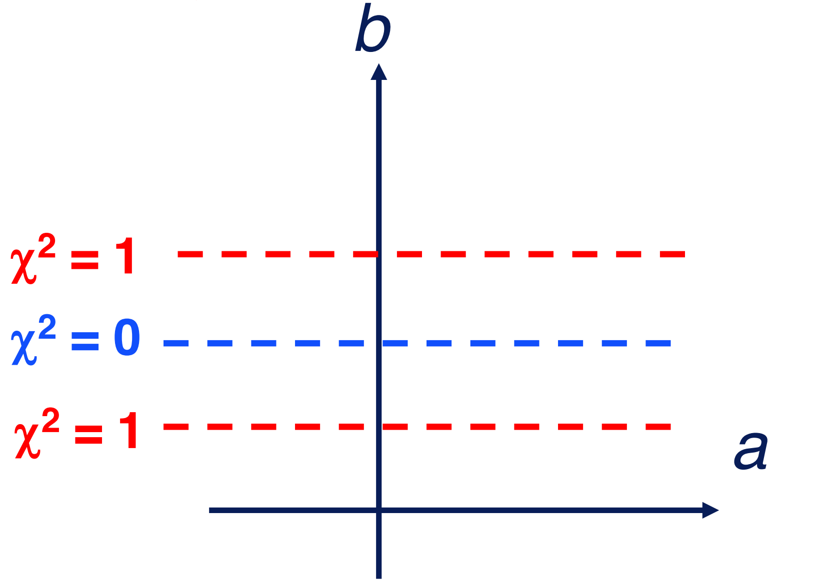
Fit $y = a\,x + b$ to *N=1* data point:

Blue lines : $\chi^2 = 0$

Red lines : $\chi^2 = 1$



χ^2 contours in the *(a,b)* plane:

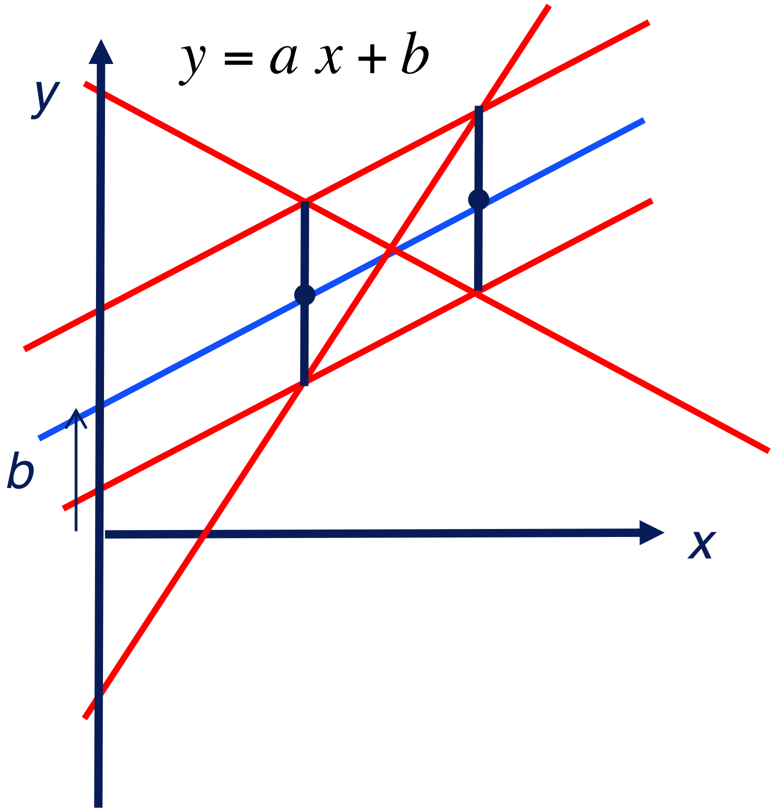


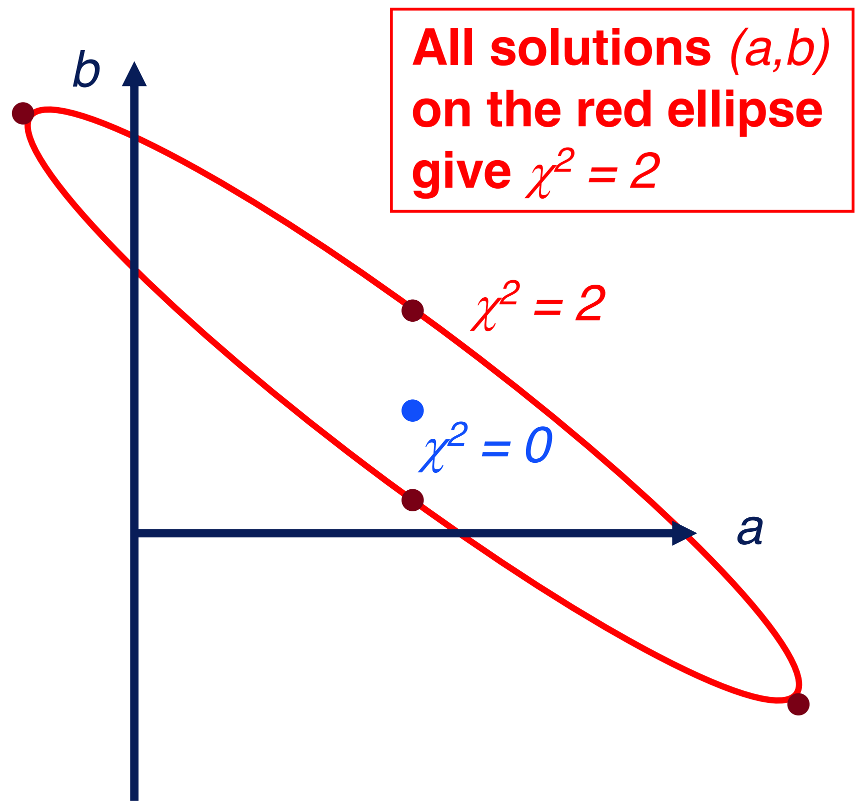
Solution is **degenerate**, since *M=2* parameters are constrained by only *N=1* data point.

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

Fit a line to *N = 2* data points

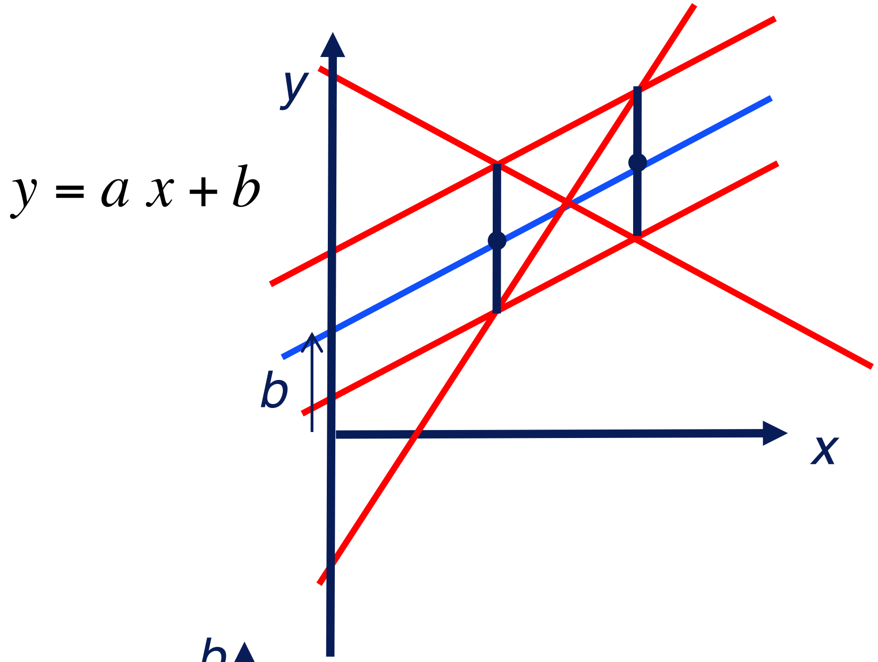
- Fit $y = a\,x + b$ to $N = 2$ data points:
  - red lines give $\chi^2 = 2$
  - blue line gives $\chi^2 = 0$
- Note that *a, b* are not independent.

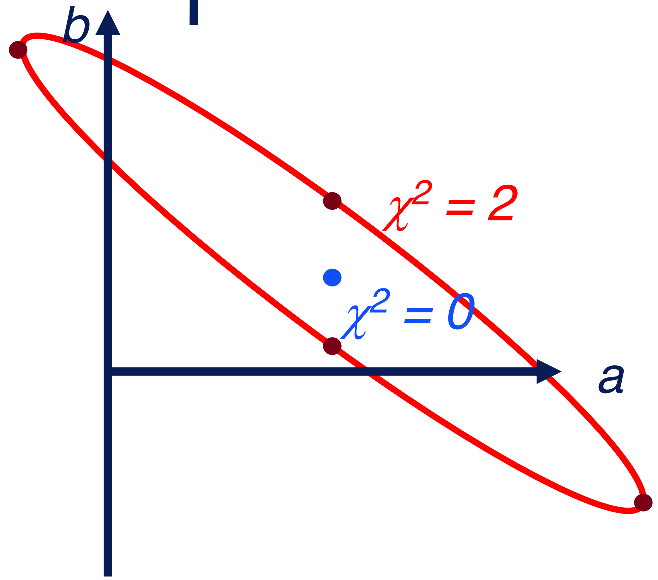




Correlated Parameters ☹

- **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**?



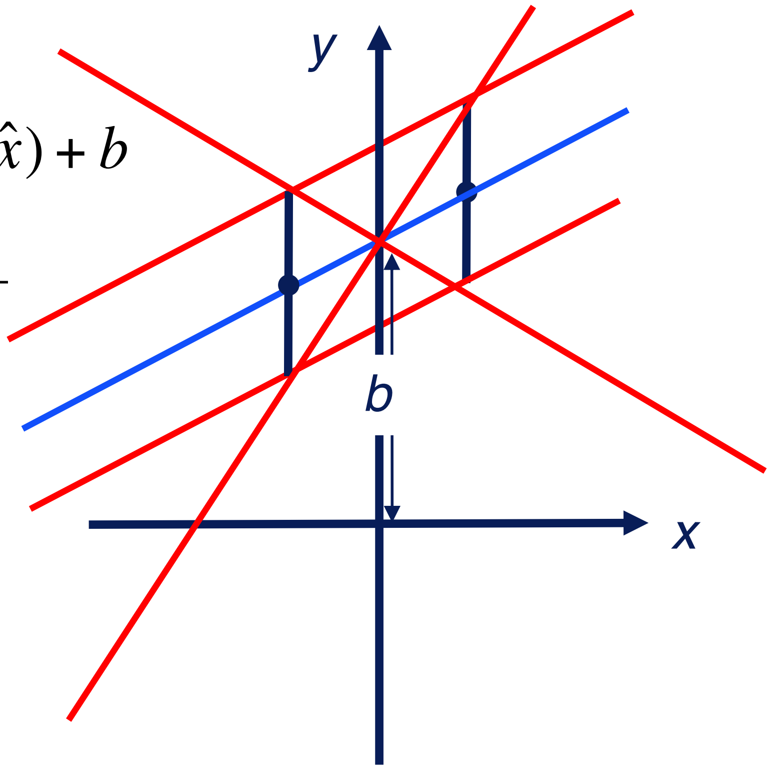


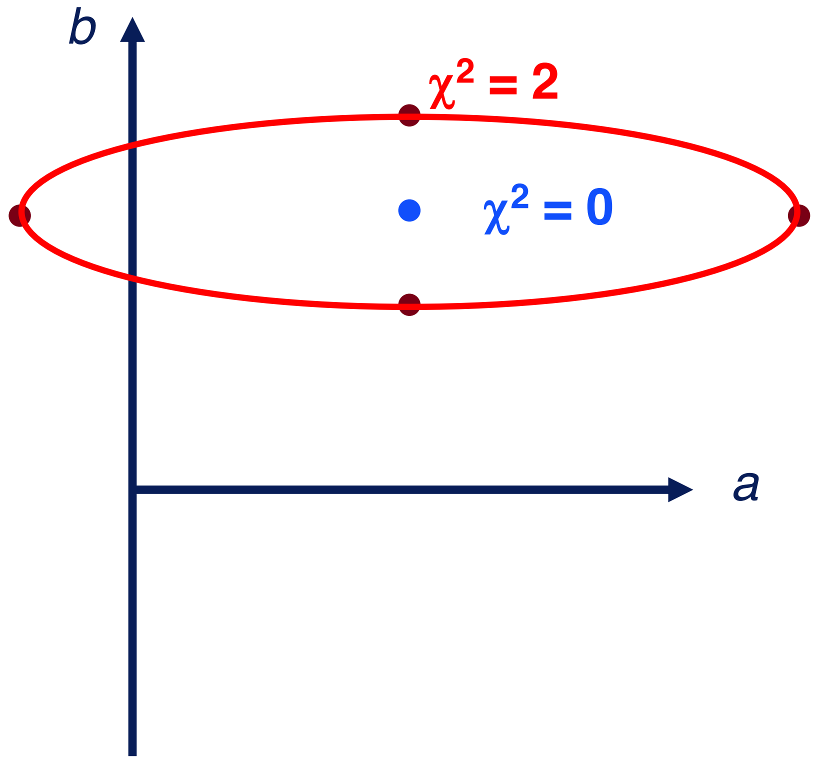
Orthogonal Parameters for fitting a line to *N = 2* data points

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

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

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

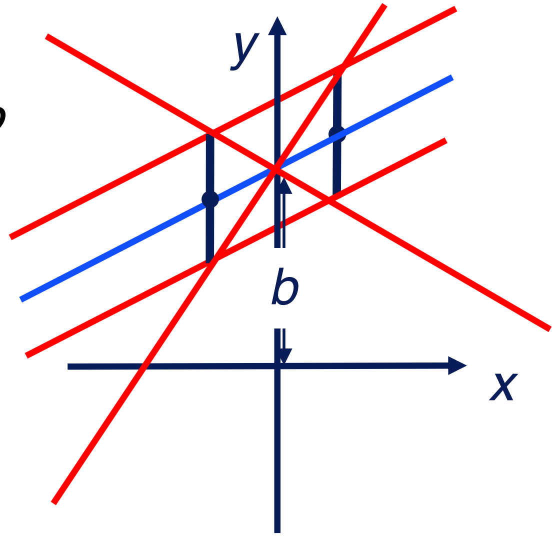




Orthogonal slope and intercept

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

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

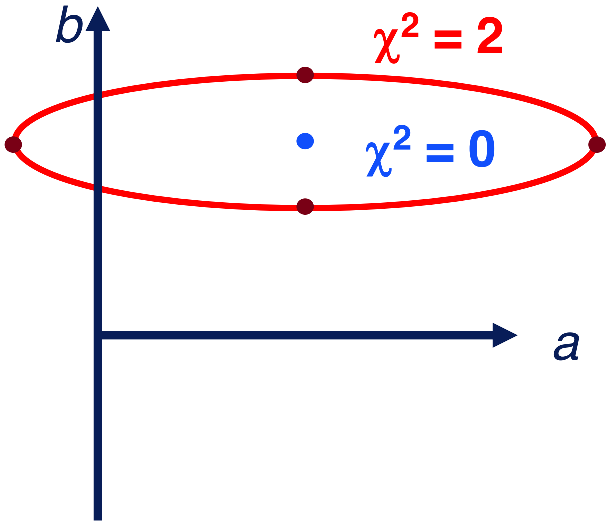


Analysis using the algebra of random variables:

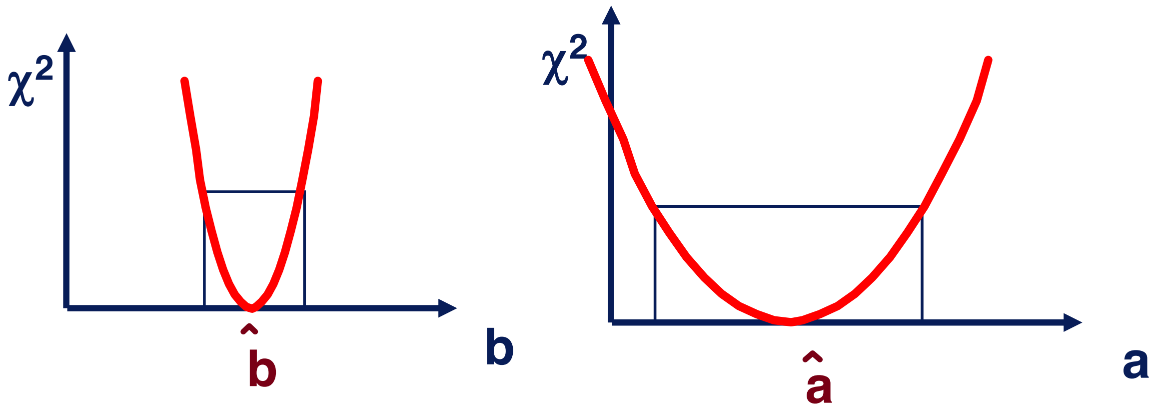
$$\hat{b} = \hat{y} = \frac{y_1 + y_2}{2} \qquad \hat{a} = \frac{y_2 - y_1}{(x_2 - x_1)}$$

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

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

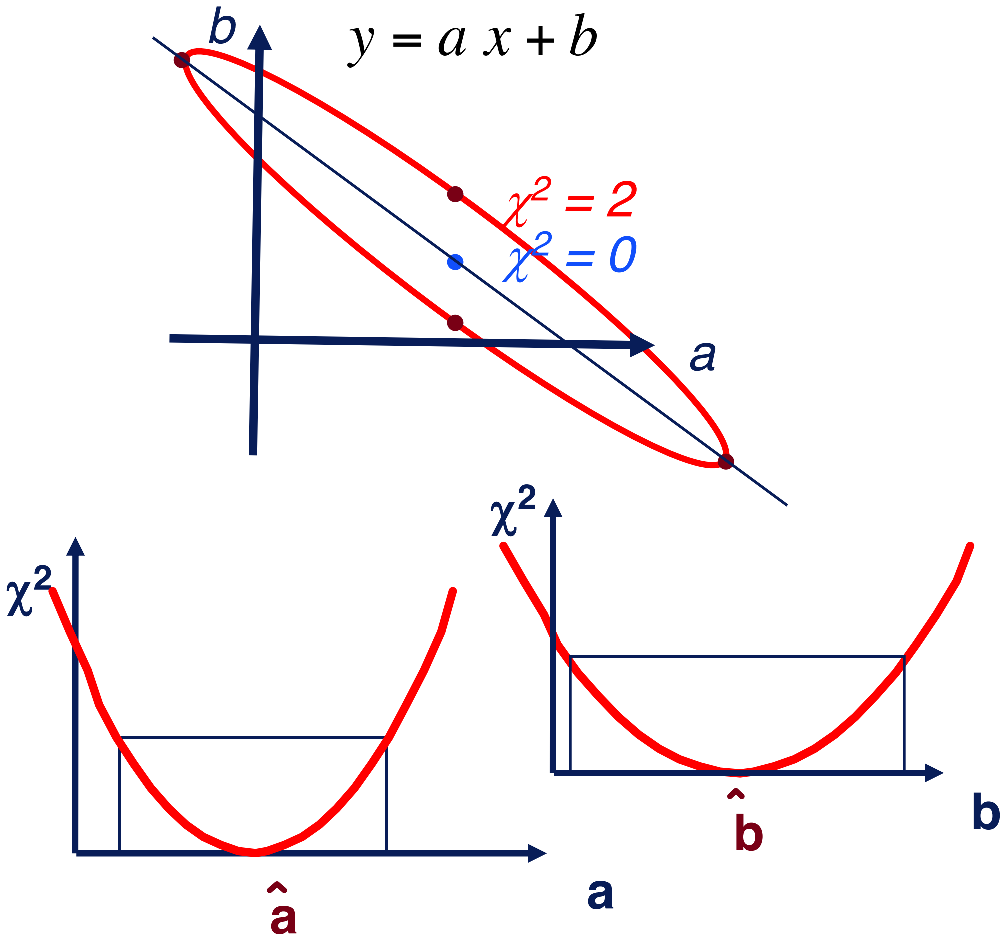


Corresponds to $\Delta\chi^2 = 1$.



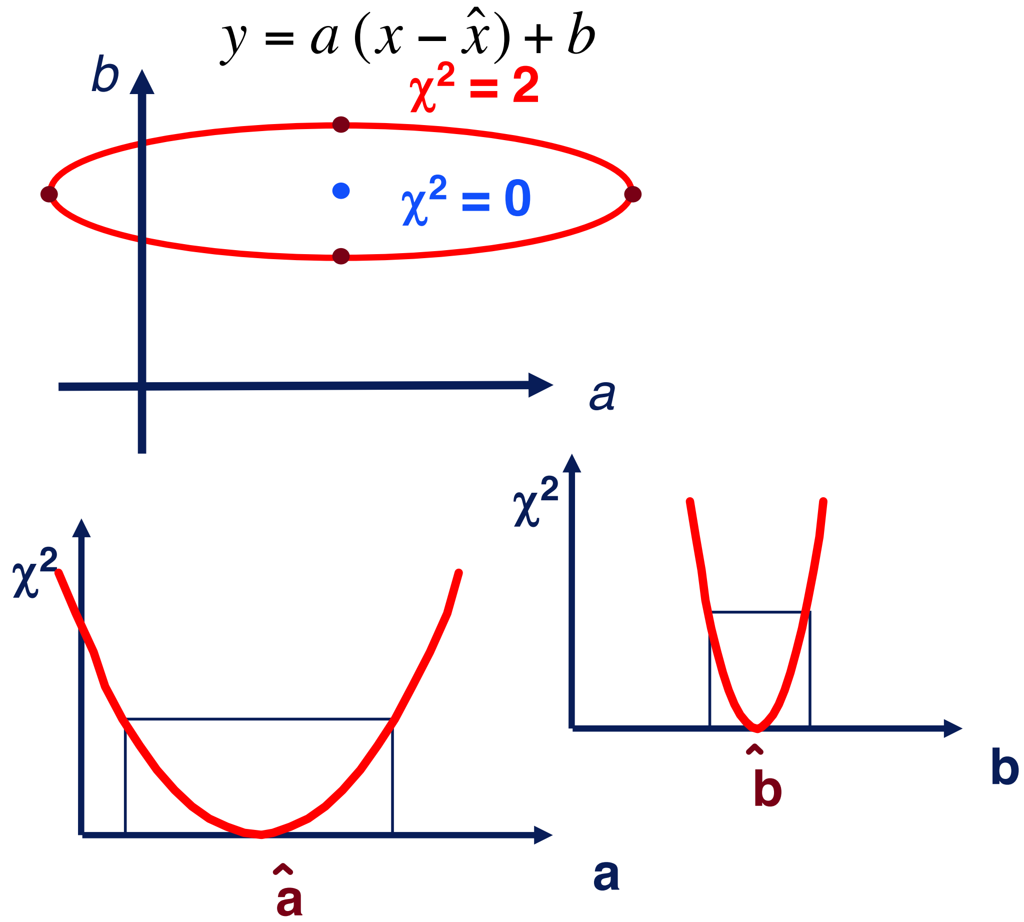
Orthogonal vs Correlated Parameters

Correlated Parameters ☹



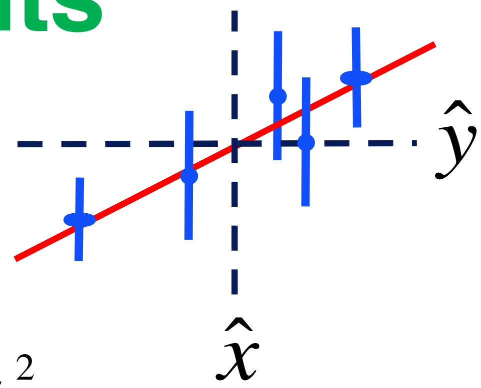
For each *a*, a different *b* minimises χ^2.
For each *b*, a different *a* minimises χ^2.

Orthogonal Parameters ☺



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

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:

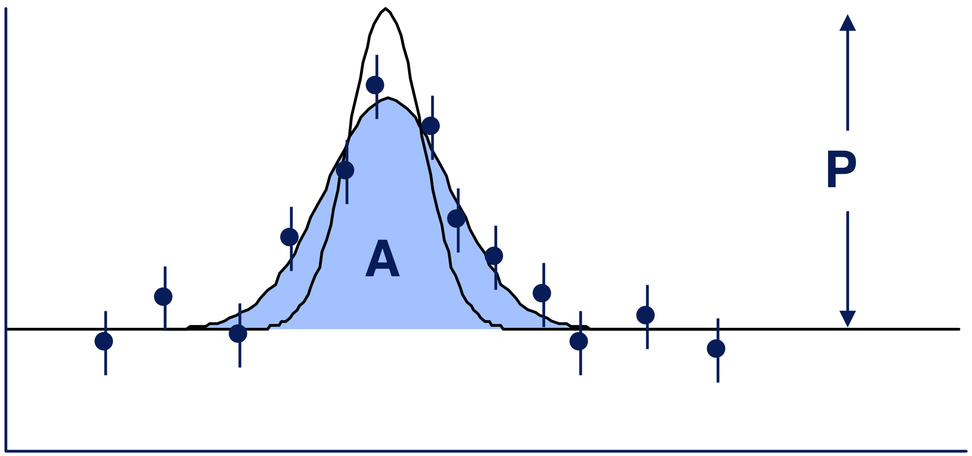
$$\hat{b} = \hat{y} = \frac{\sum y_i / \sigma_i^2}{\sum 1/\sigma_i^2}, \qquad \mathrm{Var}\left[\hat{b}\right] = \frac{1}{\sum 1/\sigma_i^2}$$

- Slope: Set *b = 0* and optimise *a*:
  optimal scaling of pattern: $P_i = x_i - \hat{x}$

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

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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