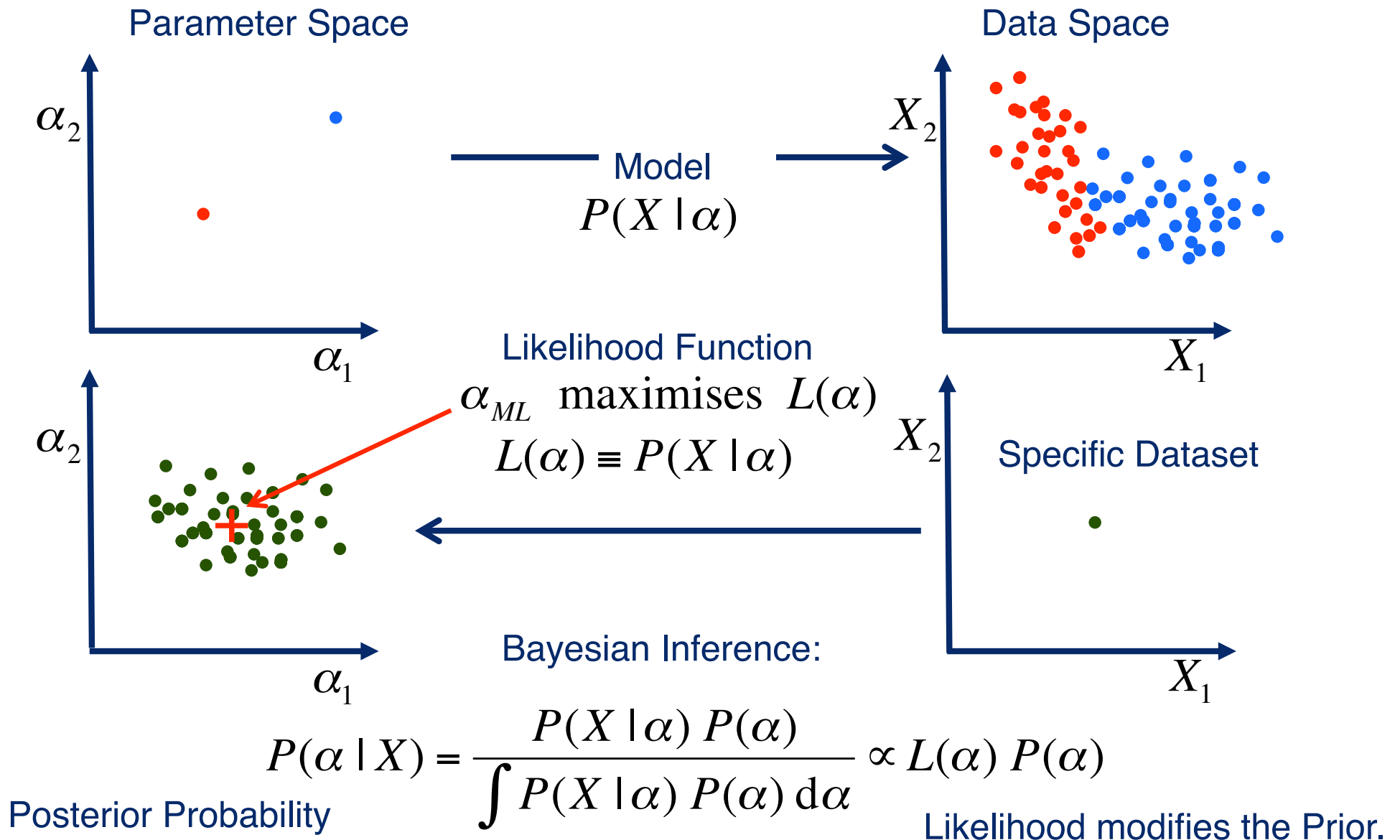


# Review: Max Likelihood and Bayesian Inference

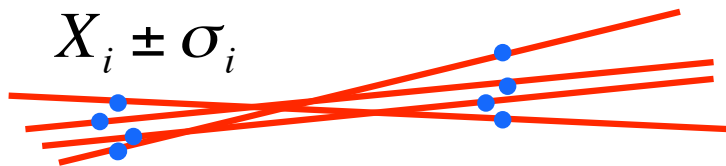


# Monte-Carlo Error Propagation

## 1. Create fake 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).

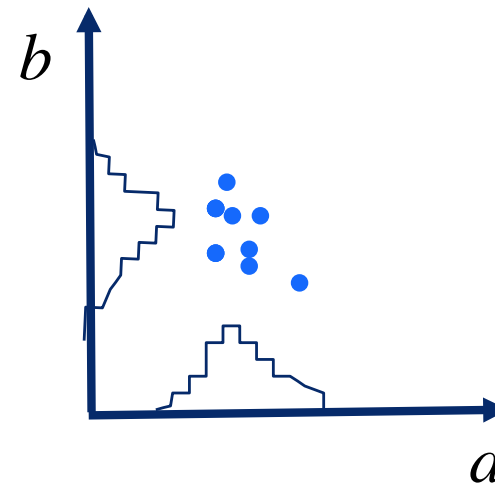
\* Requires more data than parameters (  $N > M$  ).

\* Works with no error bars available.

## 2. Fit the model to each “fake” 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, etc. of the parameters, or **any function of the parameters**.

# Confidence interval on a single parameter

(1-parameter, k-sigma confidence interval)

The **1- $\sigma$  confidence interval** on  $\alpha$  includes 68% of the area under the likelihood function:

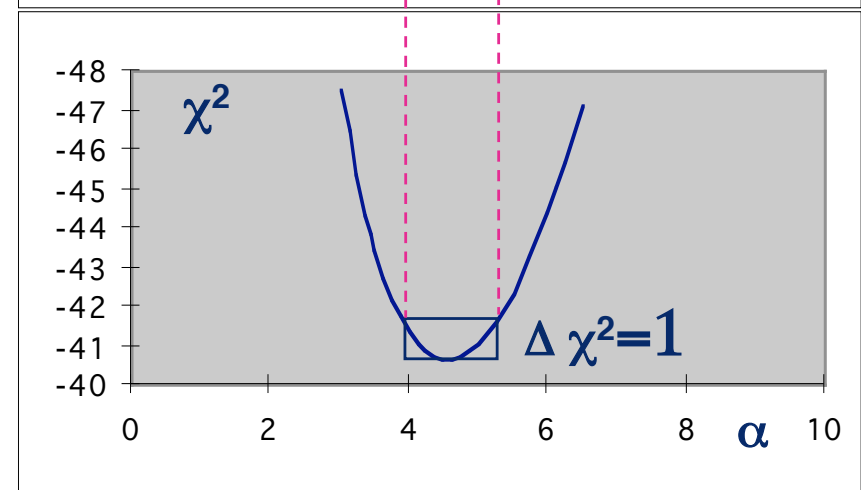
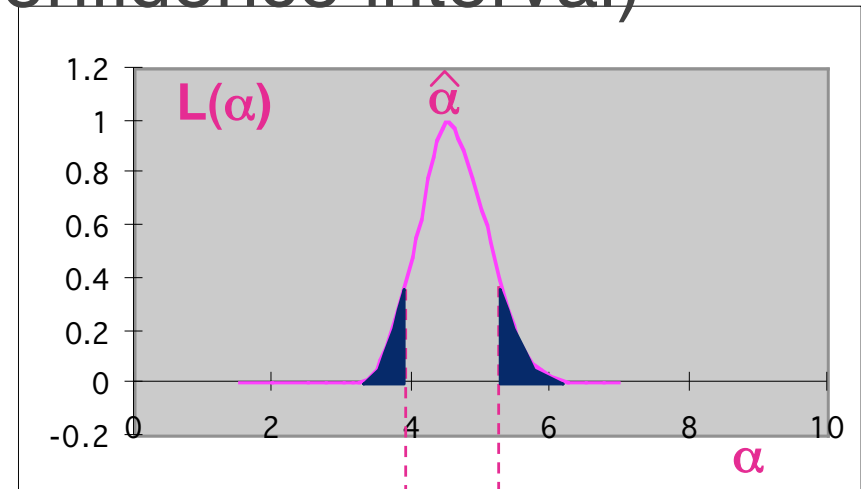
$$L(\alpha) \equiv P(X | \alpha) \propto \frac{e^{-\chi^2/2}}{\prod_i \sigma_i}$$

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

$$P(\alpha | X) \propto L(\alpha) P(\alpha)$$

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

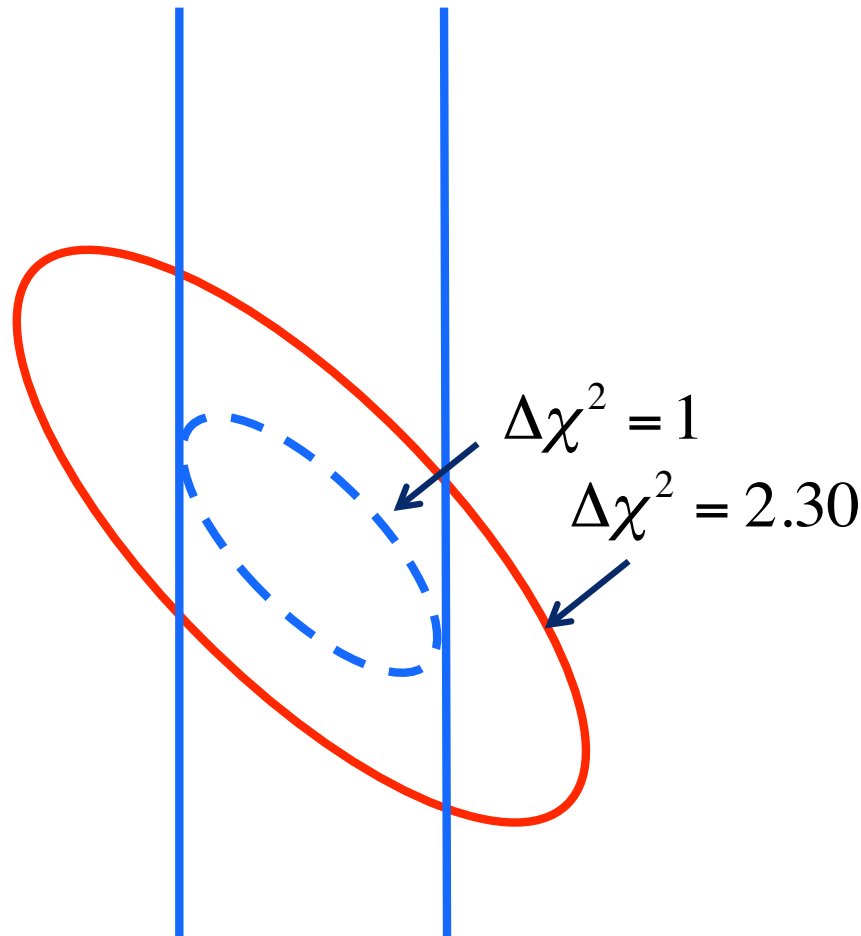
- $\Delta\chi^2 = 1$  for 1- $\sigma$ , 68% probability
- $\Delta\chi^2 = 4$  for 2- $\sigma$ , 95.4% probability
- $\Delta\chi^2 = 9$  for 3- $\sigma$ , 99.73% probability ...



**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  $(X, Y)$ .

The 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  $(X, Y)$ .

The contour encloses 68% probability.

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

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

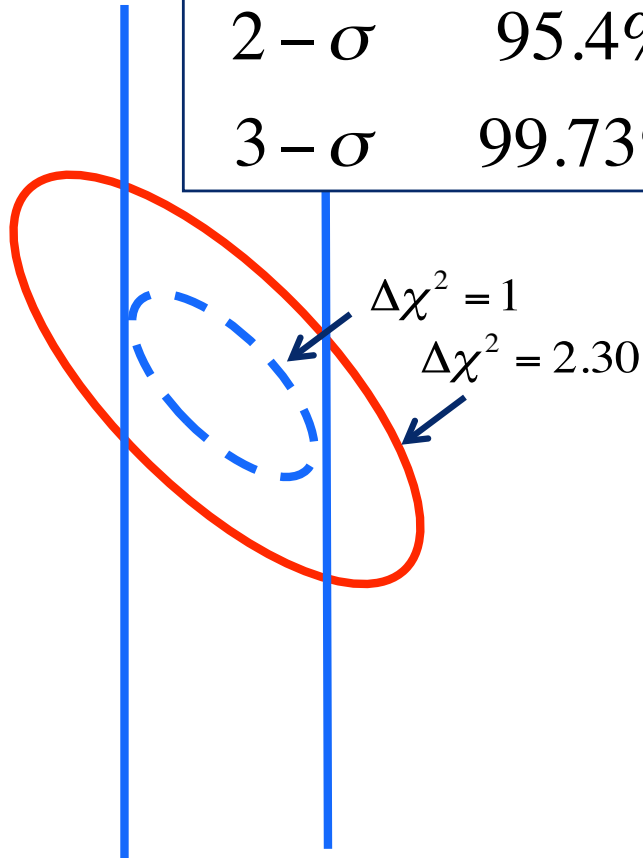
Why?

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

# $M$ - parameter $k - \sigma$ Confidence Regions

$\Delta\chi^2$  thresholds for  $M$ -parameter  $k$ - $\sigma$  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 enclosing 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.

The  $\Delta\chi^2$  in the  $M$ -parameter sub-space has a  $\chi^2_M$  distribution.

# Example: Estimate both $\mu$ and $\sigma$

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

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

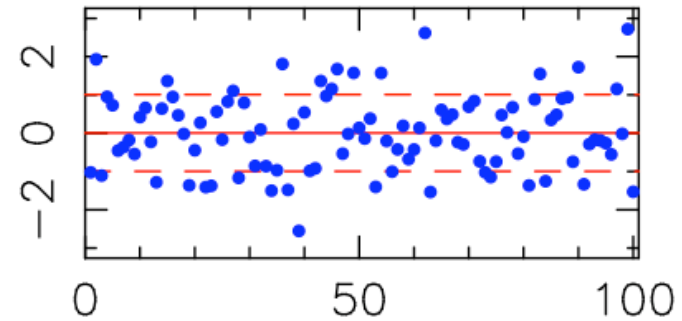
$$0 = \frac{\partial}{\partial \mu} [-2\ln L] = -2 \sum_{i=1}^N \frac{X_i - \mu}{\sigma^2}$$

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

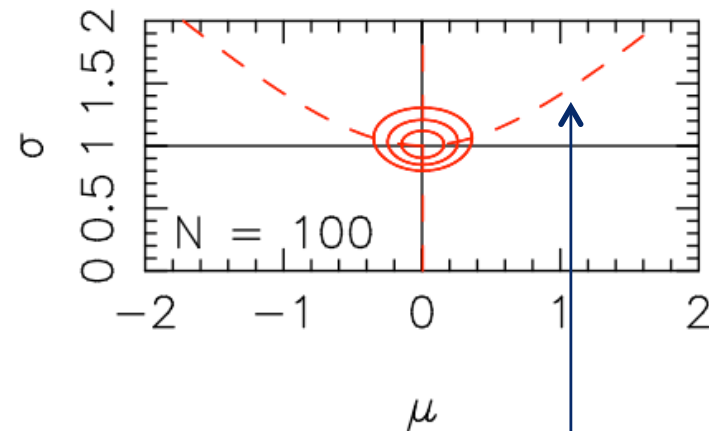
$$\mu_{ML} = \frac{1}{N} \sum_i X_i \quad (\sigma_{ML})^2 = \frac{1}{N} \sum_i (X_i - \mu_{ML})^2$$

Posterior  $\propto$  Likelihood  $\times$  Prior

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

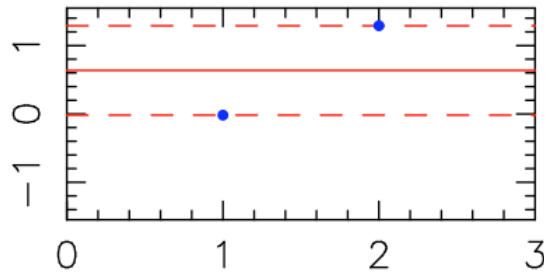


$$L(\mu, \sigma) = P(X | \mu, \sigma)$$

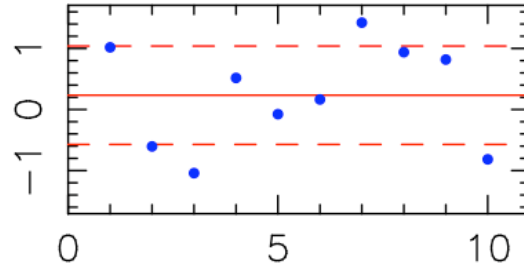


Note: ML gives biased estimate for  $\sigma$ .

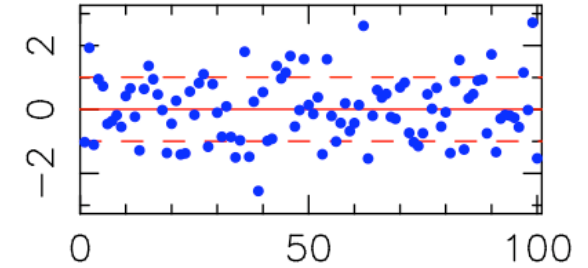
# Example: Estimate both $\mu$ and $\sigma$



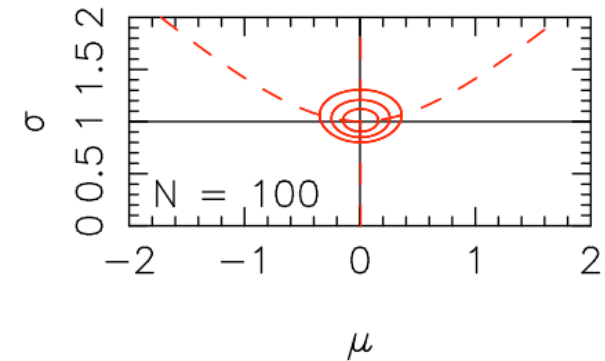
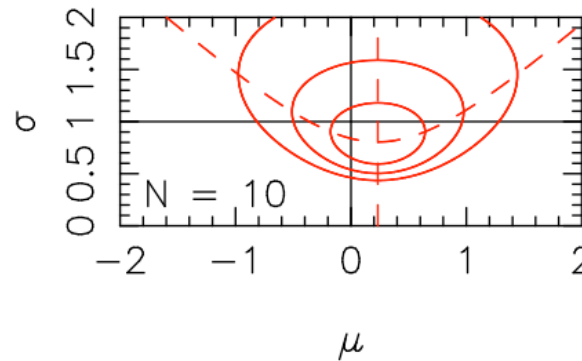
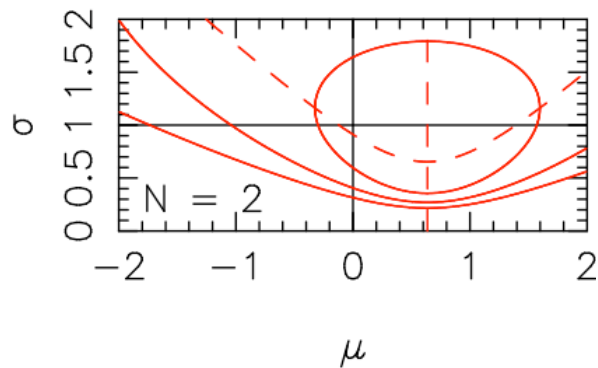
$$L(\mu, \sigma) = P(X|\mu, \sigma)$$



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



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



Contours: 1,2,3-sigma 2-parameter confidence regions for  $\mu$  and  $\sigma$ .

Dashed curves: maximum-likelihood estimates for  $\mu_{ML}$  and  $\sigma_{ML}$ .

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:

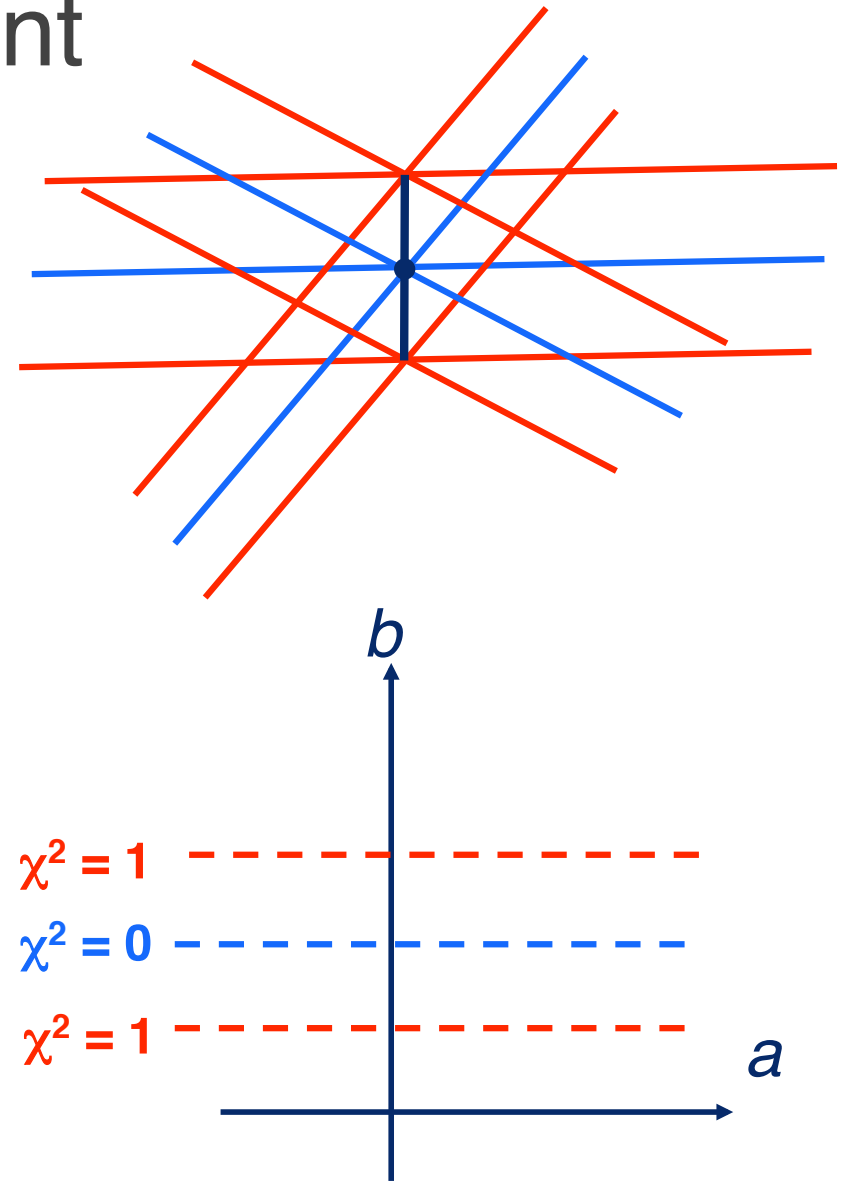
Blue lines :  $\chi^2 = 0$

Red lines :  $\chi^2 = 1$

$\chi^2$  contours in the  $(a,b)$  plane:

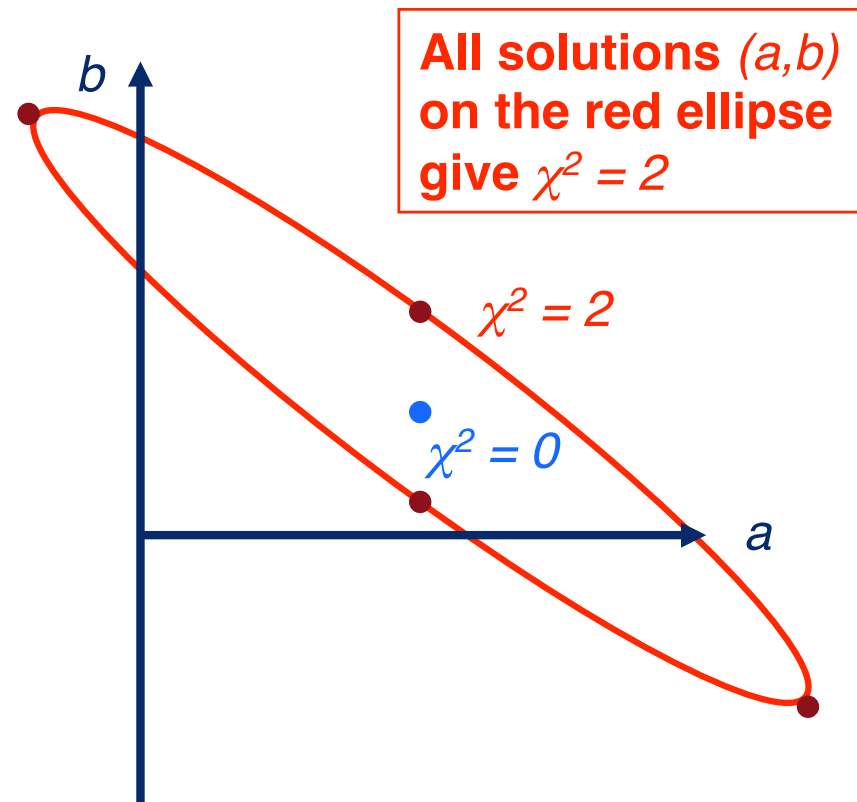
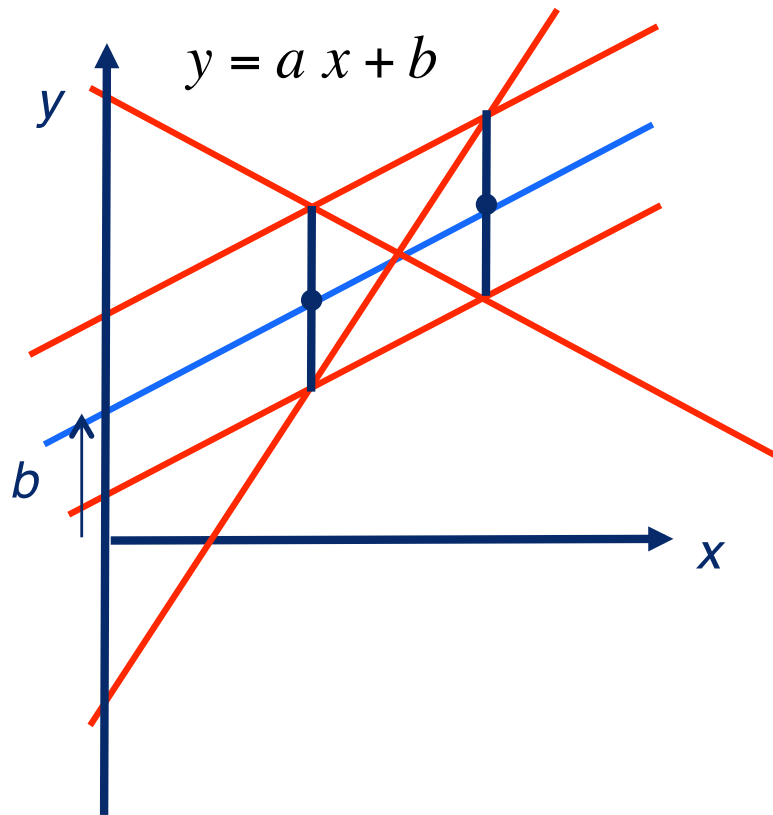
Solution is degenerate, since  $M=2$  parameters are constrained by only  $N=1$  data point.

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



# Fit a line to $N = 2$ data points

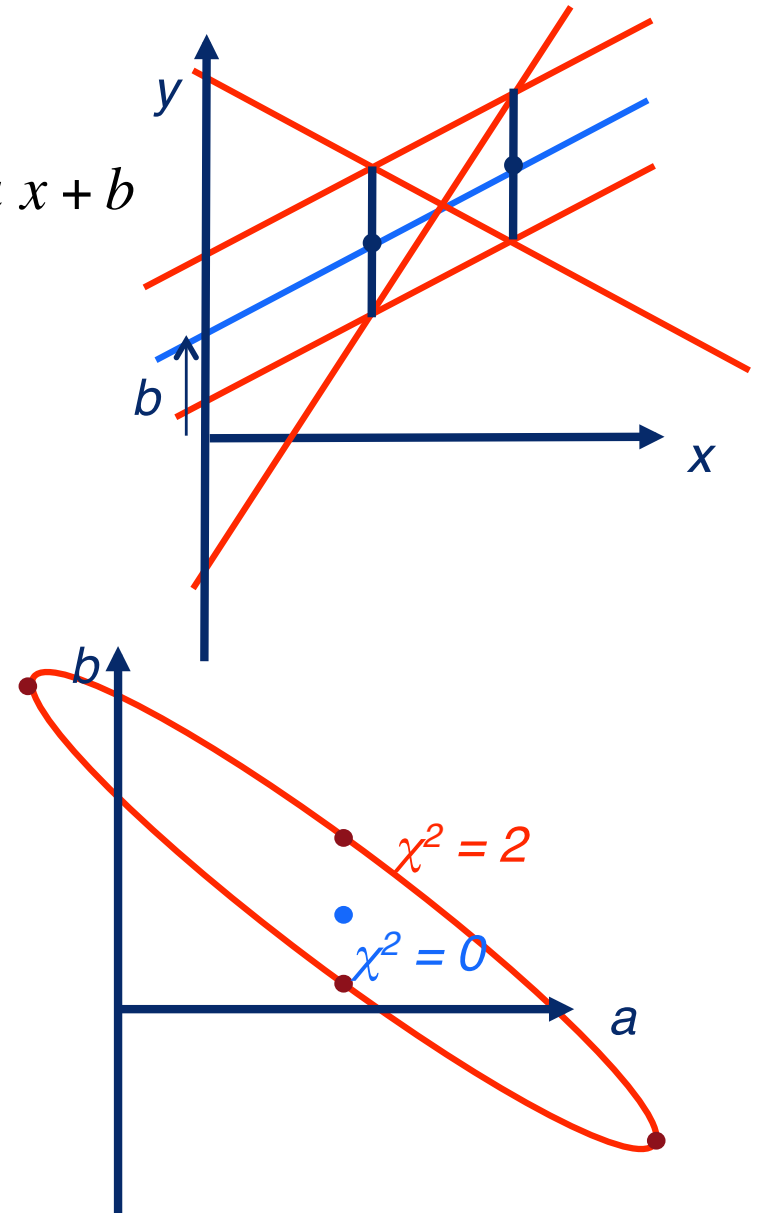
- Fit  $y = a x + b$  to  $N = 2$  data points:
  - red lines give  $\chi^2 = 2$
  - blue line gives  $\chi^2 = 0$
- Note that  $a, b$  are not independent.



# Correlated Parameters

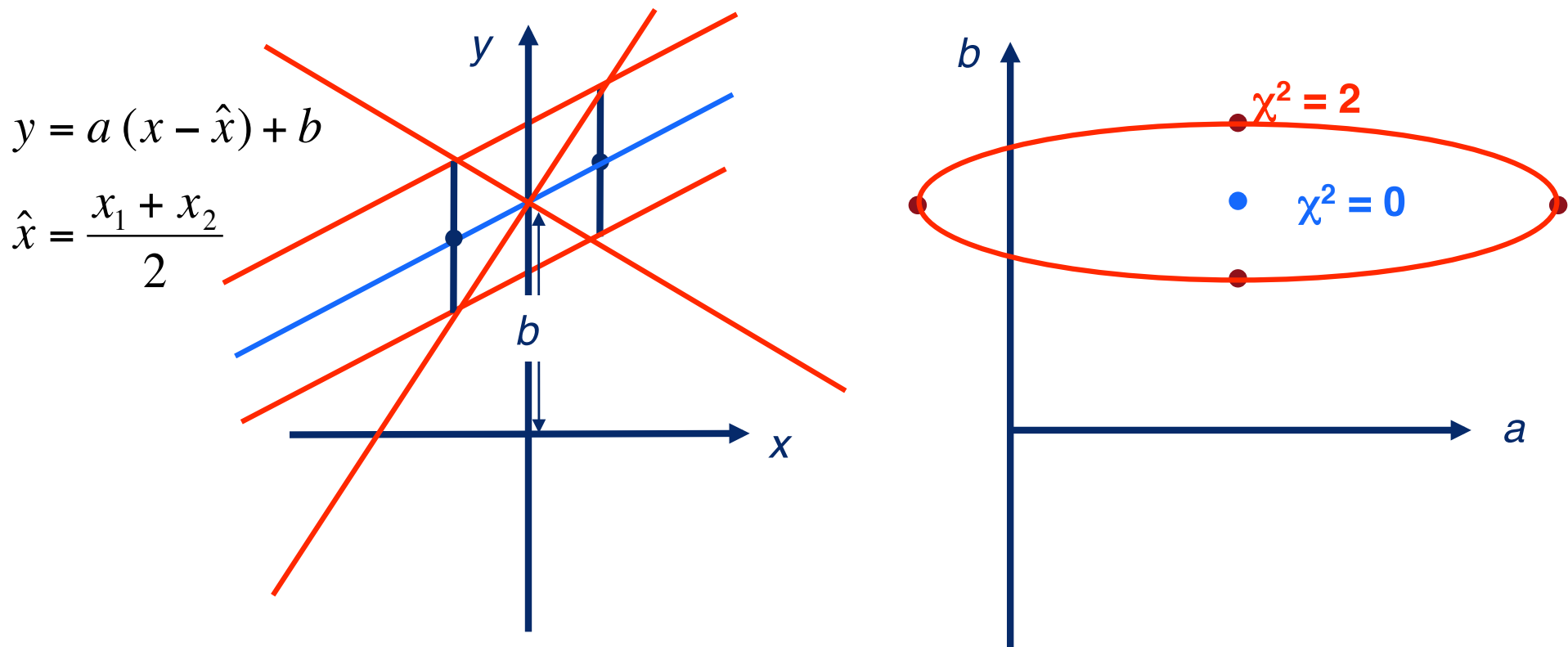
- $a$  and  $b$  are correlated :
- To find the optimal  $(a,b)$  we must:
  - minimize  $\chi^2$  with respect to  $a$  at a sequence of fixed  $b$
  - then minimise the resulting  $\chi^2$  values with respect to  $b$ .
- If  $a$  and  $b$  were independent, then all slices through the  $\chi^2$  surface 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?

$$y = a x + b$$



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

- Fit  $y = a(x - \hat{x}) + b$
- Note:  $a, b$  are now independent ! 😊

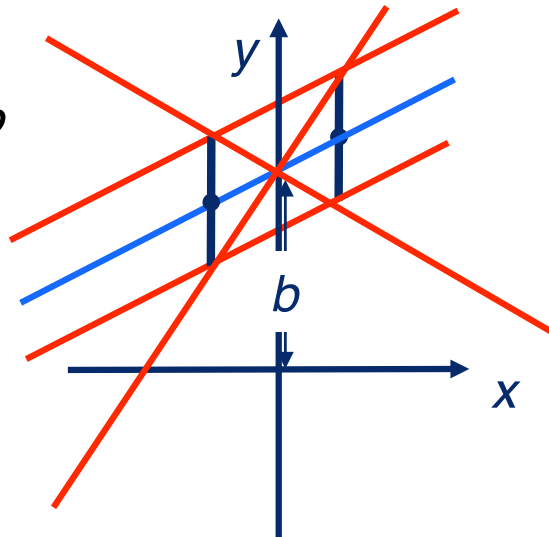


# Orthogonal slope and intercept

**Analysis using the algebra of random variables:**

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

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



$$\hat{b} = \hat{y} = \frac{y_1 + y_2}{2}$$

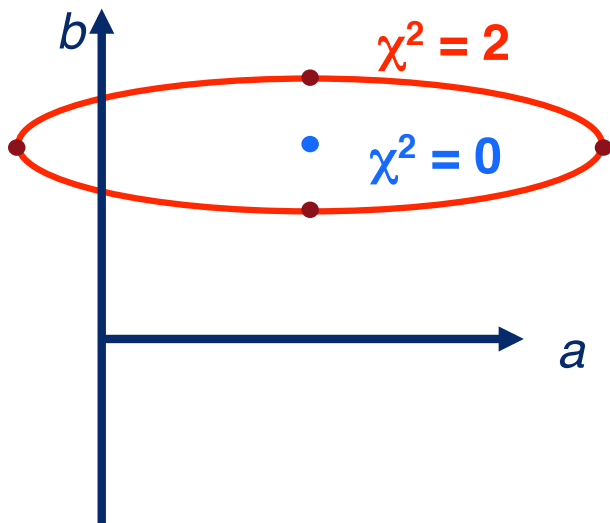
$$\hat{a} = \frac{y_2 - y_1}{(x_2 - x_1)}$$

$$\sigma^2(\hat{y}) = \frac{2\sigma^2}{4}$$

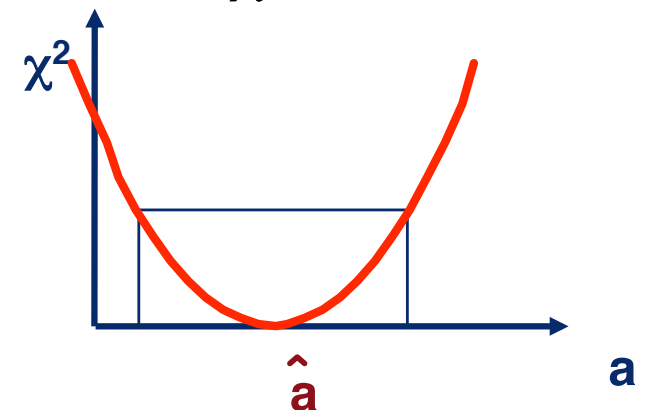
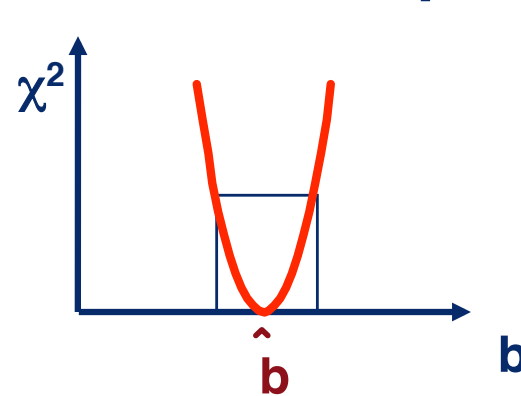
$$\sigma^2(\hat{a}) = \frac{2\sigma^2}{(x_2 - x_1)^2}$$

$$\sigma(\hat{y}) = \frac{\sigma}{\sqrt{2}}$$

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

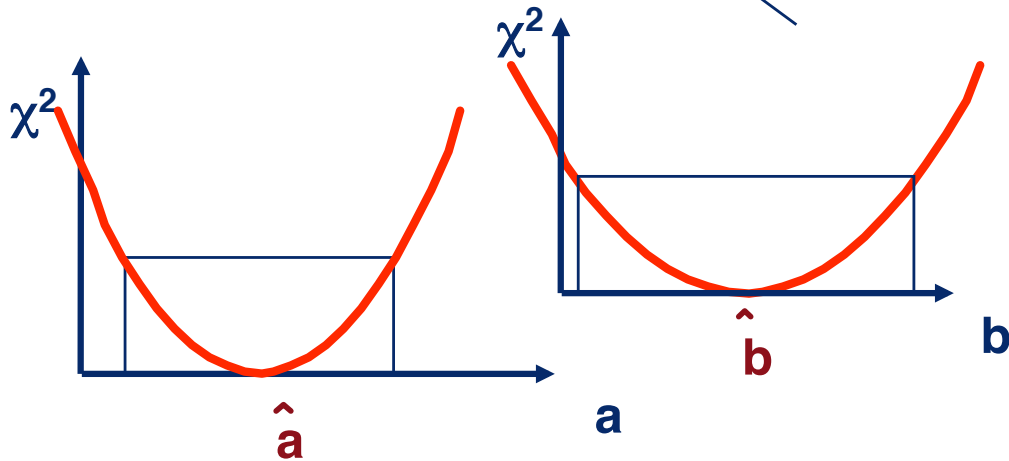
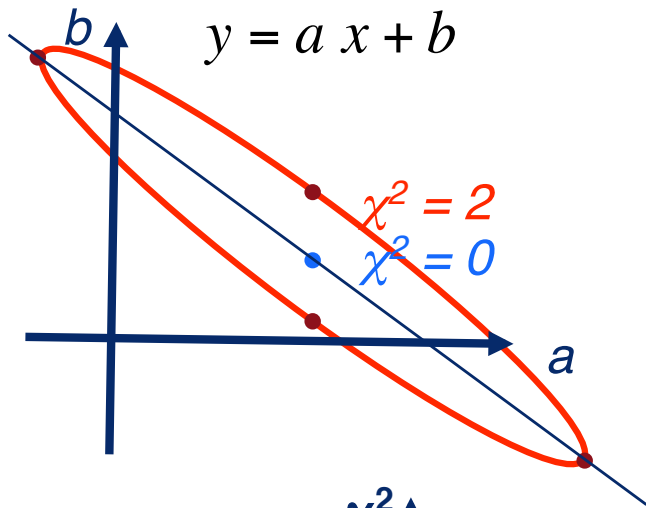


**Corresponds to  $\Delta\chi^2 = 1$ .**



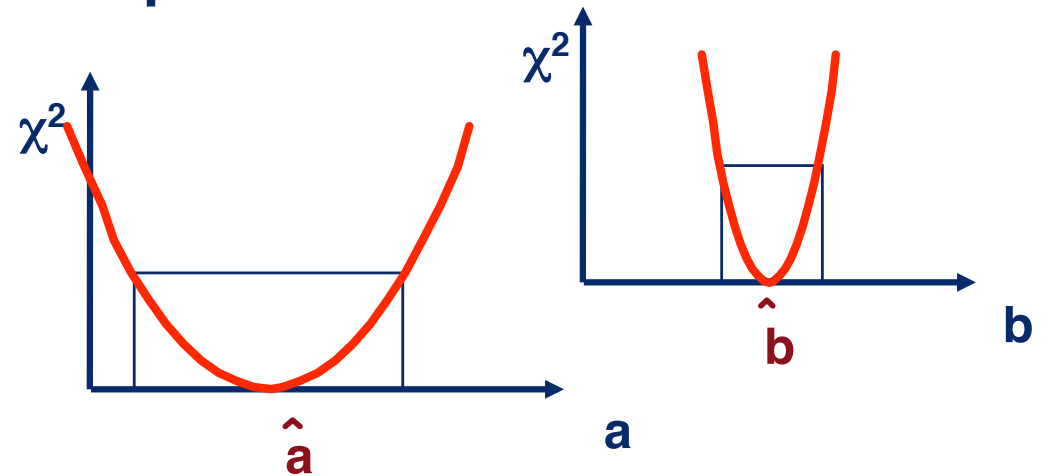
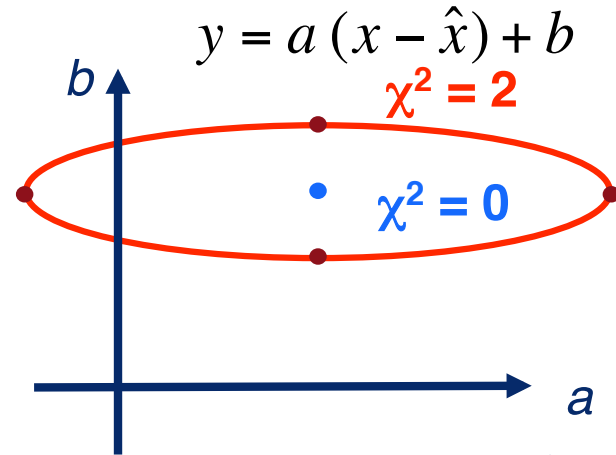
# Orthogonal vs Correlated Parameters:

## Correlated Parameters:



For each  $a$ , a different  $b$  minimises  $\chi^2$ .  
For each  $b$ , a different  $a$  minimises  $\chi^2$ .

## Orthogonal Parameters:



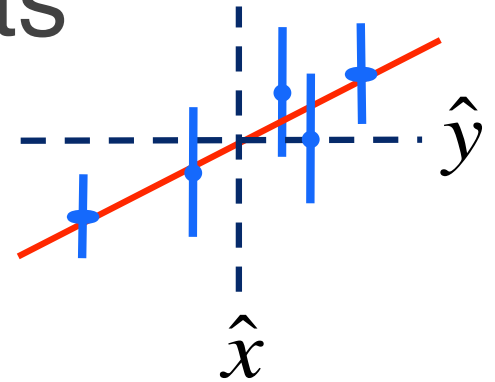
For any  $a$ , the same  $b$  minimises  $\chi^2$ .  
For any  $b$ , the same  $a$  minimises  $\chi^2$ .

# Fit a line to $N$ data points

- If we use  $y = a x + b$  then  $a, b$  are correlated.
- To make  $a, b$  orthogonal:

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

$$\hat{x} = \frac{\sum x_i / \sigma_i^2}{\sum 1 / \sigma_i^2}$$



- Intercept: **optimal average:**

$$\hat{b} = \hat{y} = \frac{\sum y_i / \sigma_i^2}{\sum 1 / \sigma_i^2},$$

$$\text{Var}[\hat{b}] = \frac{1}{\sum 1 / \sigma_i^2}$$

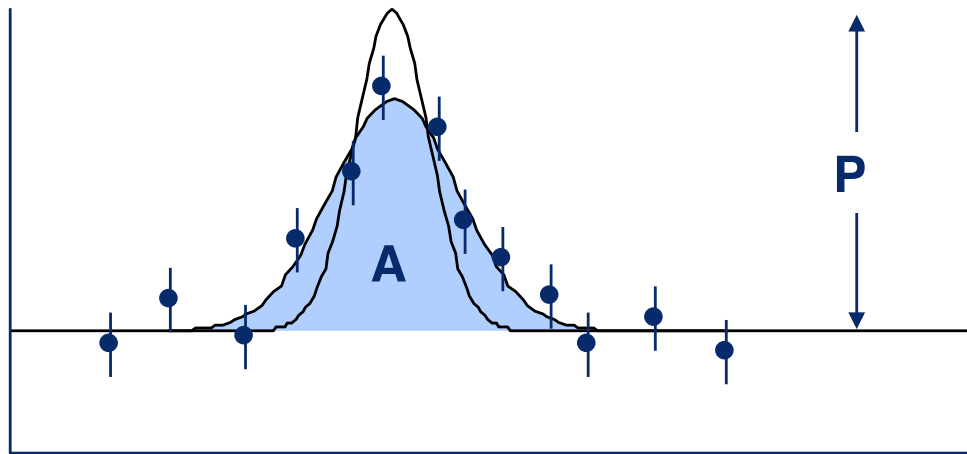
- Slope: **optimal scaling:**

$$\hat{a} = \frac{\sum (y_i - \hat{y})(x_i - \hat{x}) / \sigma_i^2}{\sum (x_i - \hat{x})^2 / \sigma_i^2},$$

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

# 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