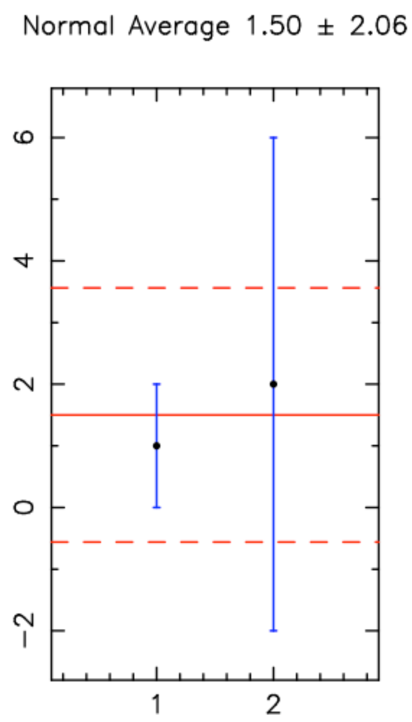
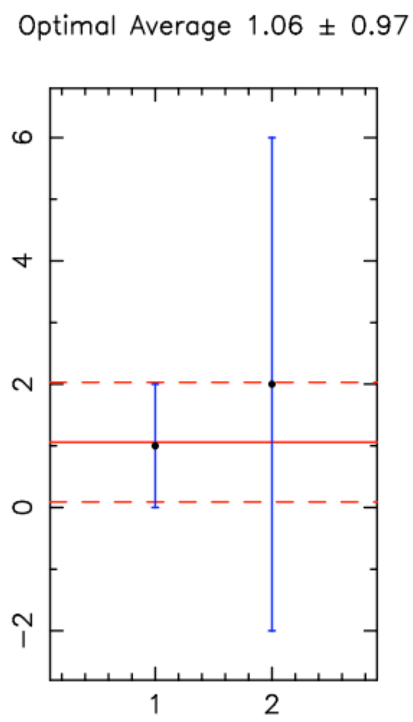
Review: Normal vs Optimal Average

$$\bar{X} \equiv \frac{1}{N} \sum_i X_i$$

$$\sigma^2\left(\bar{X}\right) = \frac{1}{N^2} \sum_i \sigma_i^{\ 2}$$





$$\hat{X} \equiv \frac{\sum_i X_i / \sigma_i^2}{\sum_i 1/\sigma_i^2}$$

$$\sigma^2\left(\hat{X}\right) = \frac{1}{\sum_i 1/\sigma_i^2}$$

Equal weights:
Poor data degrades the result.

Better to ignore “bad” data.

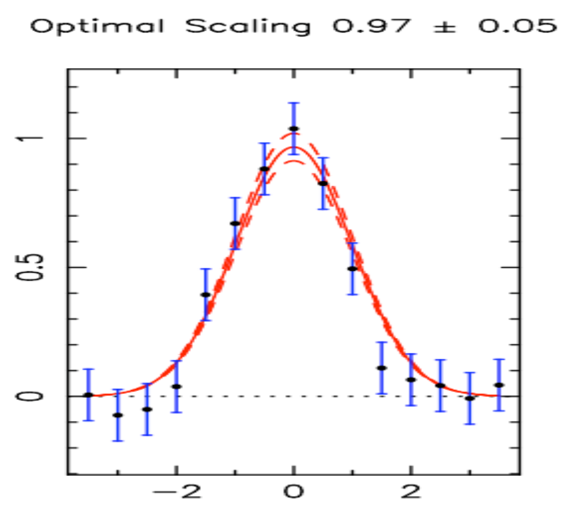
Information lost.

Optimal weights:
New data always improves the result.

Use ALL the data, but with appropriate **1 / Variance** weights.

Must have good error bars.

Measuring a Feature



A = area under the curve,

e.g. flux of the star, strength of a spectral line.

Assume (for now) zero background.

How to measure A ?

Simple method: **Integrate the Data**:

$$\langle X_i \rangle = A\,P_i \qquad \mathrm{Cov}\left[X_i, X_j\right] = \sigma_i^2\,\delta_{ij}$$

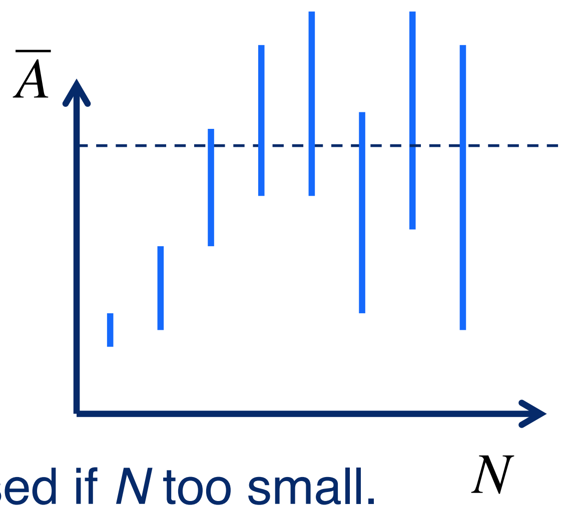
$$\bar{A} \equiv \sum_{i=1}^{N} X_i$$

$$\langle \bar{A} \rangle = A \sum_{i=1}^{N} P_i \qquad \sigma^2\left[\bar{A}\right] = \sum_{i=1}^{N} \sigma_i^2$$

If P_i = fraction of photons in pixel *i* ,

$$\sum_{i=1}^{N} P_i = 1$$

Dilemma:
How many data points to include ?



Biased if *N* too small.

Noisy if *N* too large.

Can we do better? Yes, if the pattern *P* is known.

Optimal Scaling of a Pattern

Scale the pattern P_i by factor A to fit the data.

1: Construct independent unbiased estimates.

2: Optimal average, with $1/\sigma^2$ weights.

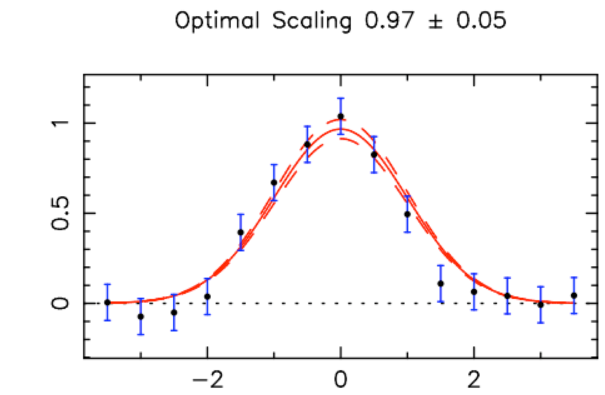
Data : $X_i \pm \sigma_i$
Model : $\langle X_i \rangle \equiv \mu_i = A\, P_i$
Pattern : P_i

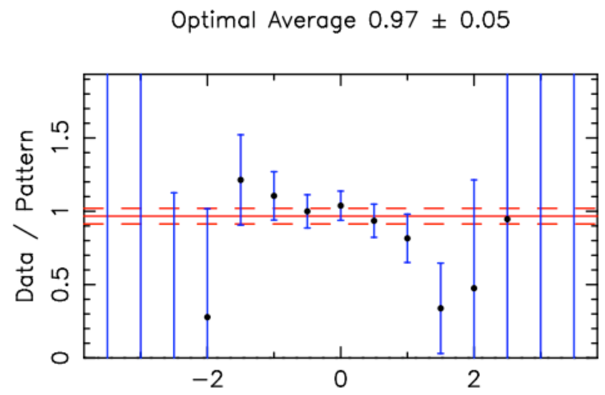
$$A_i \equiv X_i / P_i \quad \text{unbiased:} \quad \langle A_i \rangle = A \qquad \mathrm{Cov}\left[A_i, A_j\right] = \left(\frac{\sigma_i}{P_i}\right)^2 \delta_{ij}$$

$$\text{Optimal average : } w_i = 1/\mathrm{Var}\left[A_i\right] = \left(P_i/\sigma_i\right)^2$$

$$\hat{A} = \frac{\sum_i w_i\, A_i}{\sum_i w_i} = \frac{\sum_i \left(\frac{P_i}{\sigma_i}\right)^2 \left(\frac{X_i}{P_i}\right)}{\sum_i \left(\frac{P_i}{\sigma_i}\right)^2} = \frac{\sum_i X_i\, P_i/\sigma_i^2}{\sum_i P_i^2/\sigma_i^2}$$

$$\mathrm{Var}\left[\hat{A}\right] = \frac{\sum_i \mathrm{Var}\left[X_i\right]\left(P_i/\sigma_i^2\right)^2}{\left(\sum_i P_i^2/\sigma_i^2\right)^2} = \frac{1}{\sum_i P_i^2/\sigma_i^2}$$



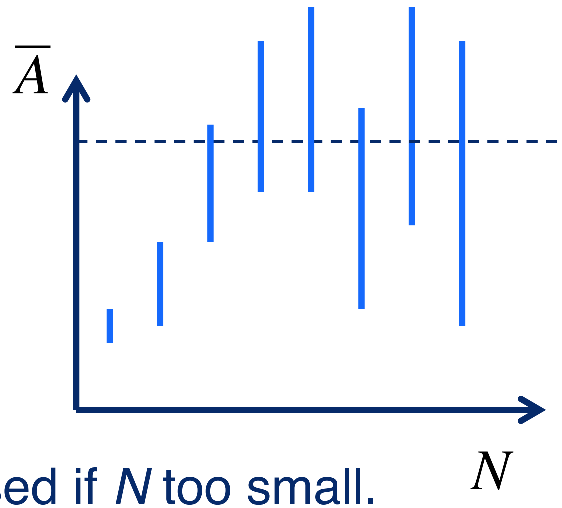


Sum the Data vs Optimal Scaling

Sum up the data.

$$\overline{A} \equiv \sum_{i=1}^{N} X_i$$

$$\left\langle \overline{A} \right\rangle = A \sum_{i=1}^{N} P_i \qquad \sigma^2\left[\overline{A}\right] = \sum_{i=1}^{N} \sigma_i^2$$



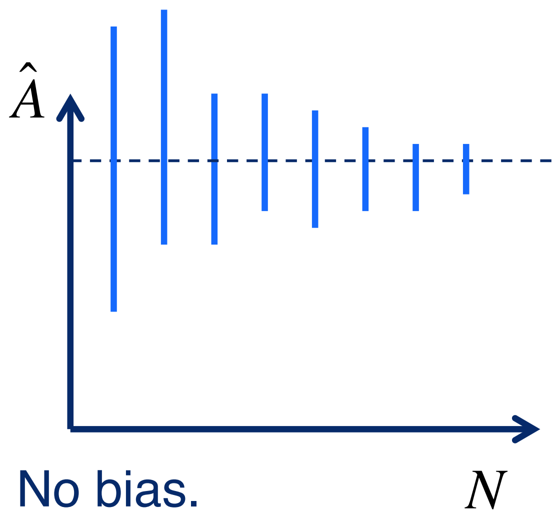
Biased if N too small.

Noisy if N too large.

Optimal Scaling of known Pattern.

$$\hat{A} = \frac{\sum_i X_i \, P_i / \sigma_i^2}{\sum_i P_i^2 / \sigma_i^2}$$

$$\mathrm{Var}\left[\hat{A}\right] = \frac{1}{\sum_i P_i^2 / \sigma_i^2}$$



No bias.

Result improves with N.

Optimal Scaling

The Golden Rule of Optimal Data Analysis:

Data: $X_i \pm \sigma_i$

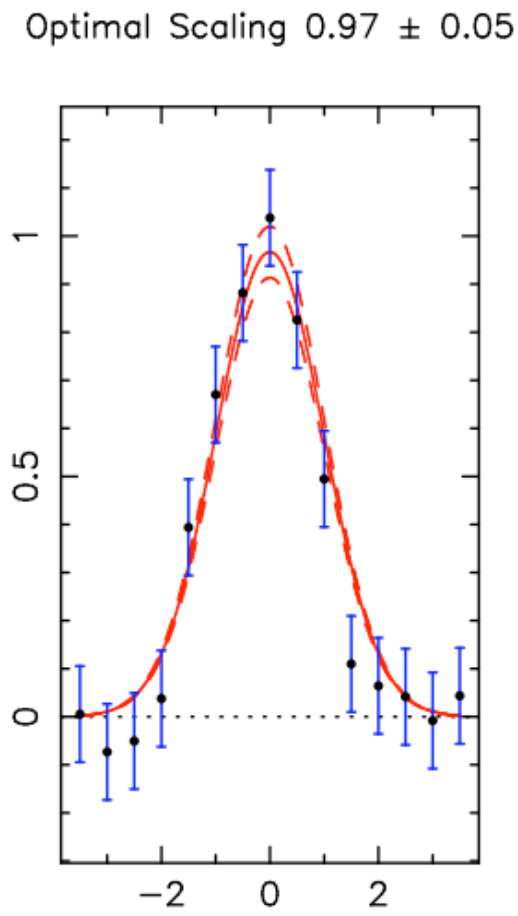
Model: $\langle X_i \rangle \equiv \mu_i = A\,P_i$

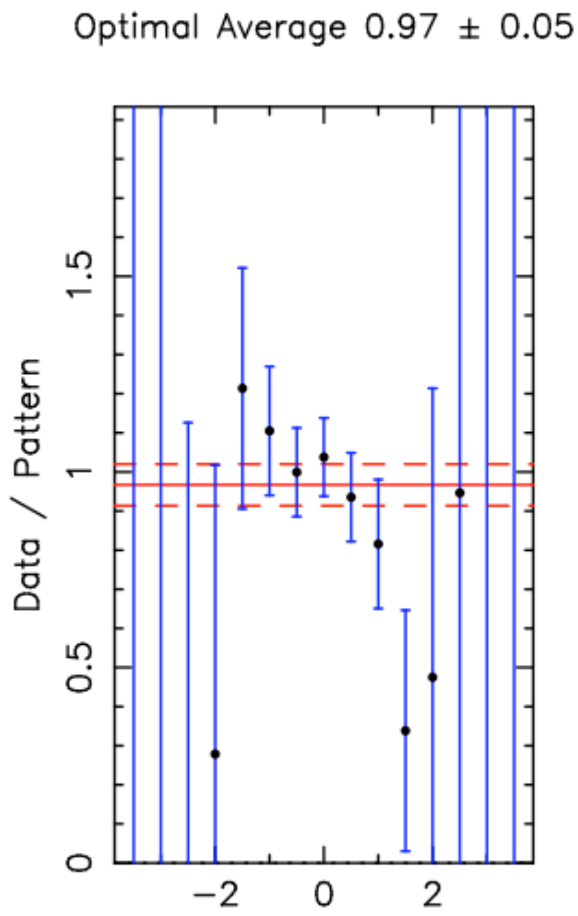
Optimal Scaling:

$$\hat{A} = \frac{\sum_i X_i\,P_i / \sigma_i^2}{\sum_i P_i^2 / \sigma_i^2}$$

$$\mathrm{Var}\left[\hat{A}\right] = \frac{1}{\sum_i P_i^2 / \sigma_i^2}$$

Memorise this result.
Know how to derive it.





Optimal Average is a special case of Optimal Scaling, with pattern $P_i = 1$.

Fitting Models by minimising χ^2

Data: $X_i \pm \sigma_i \quad i = 1 \ldots N$

Model: $\langle X_i \rangle \equiv \mu_i(\alpha)$

Parameters: $\alpha_k \quad k = 1 \ldots M$

Error: $\varepsilon_i \equiv X_i - \mu_i(\alpha)$

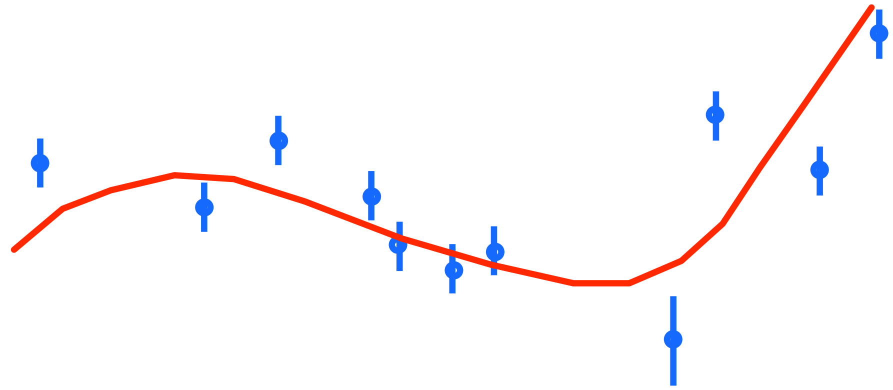
Normalised Error: $\eta_i \equiv \dfrac{\varepsilon_i}{\sigma_i} = \dfrac{X_i - \mu_i(\alpha)}{\sigma_i}$

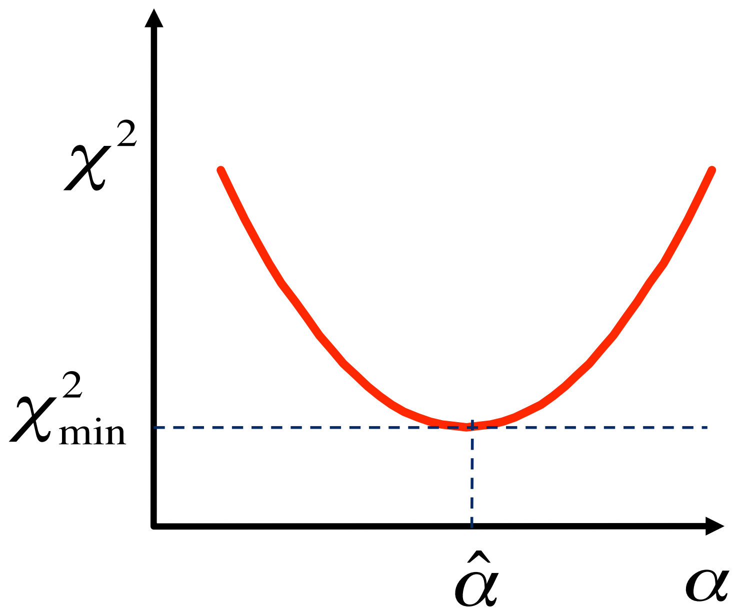
"Badness-of-Fit" statistic:

$$\chi^2(X, \sigma, \alpha) \equiv \sum_{i=1}^{N} \eta_i^2 = \sum_{i=1}^{N} \left(\frac{X_i - \mu_i(\alpha)}{\sigma_i} \right)^2$$

Best-fit parameters $\hat{\alpha}$ minimise χ^2.

(BoF a.k.a. "Goodness-of-Fit" statistic).



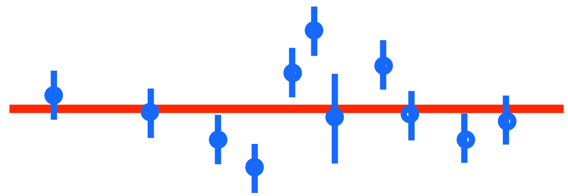


Example: Estimate $< X >$ by χ^2 Fitting

Model: $\langle X_i \rangle = \mu$ $\quad \mathrm{Cov}\left[X_i, X_j\right] = \sigma_i^2\, \delta_{ij}$

Badness-of-Fit statistic:

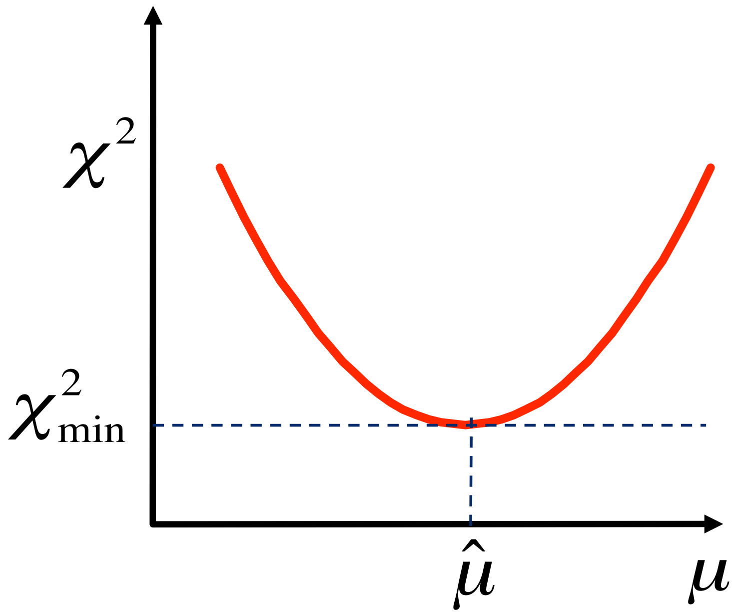
$$\chi^2 = \sum_i \left(\frac{X_i - \mu}{\sigma_i} \right)^2$$



Minimise χ^2 :

$$0 = \frac{\partial \chi^2}{\partial \mu} = -2 \sum_i \frac{X_i - \mu}{\sigma_i^2} \qquad \text{at} \quad \mu = \hat{\mu}$$

$$\sum_i \frac{X_i}{\sigma_i^2} = \sum_i \frac{\hat{\mu}}{\sigma_i^2} \quad \Rightarrow \quad \hat{\mu} \;=\; \frac{\sum_i X_i / \sigma_i^2}{\sum_i 1/\sigma_i^2} = \hat{X}.$$



The Optimal Average minimises χ^2 !

Parameter Error Bar: 1−σ at $\Delta\chi^2 = 1$

From χ^2 fit : $\hat{\mu} = \hat{X} =$ Optimal Average

Must have $\sigma^2(\hat{\mu}) = \sigma^2(\hat{X}) = \dfrac{1}{\sum_i 1/\sigma_i^2}$

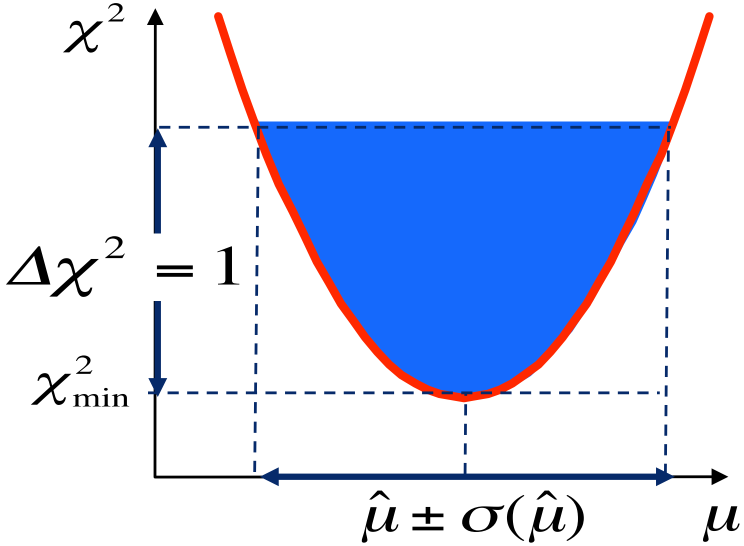
$$\frac{\partial \chi^2}{\partial \mu} = -2 \sum_i \frac{X_i - \mu}{\sigma_i^2}$$

$$\frac{\partial^2 \chi^2}{\partial \mu^2} = +2 \sum_i \frac{1}{\sigma_i^2}$$

$$\chi^2 = \chi^2_{\min} + \frac{1}{2} \left.\frac{\partial^2 \chi^2}{\partial \mu^2}\right|_{\mu = \hat{\mu}} (\mu - \hat{\mu})^2 + \ldots$$

$$= \chi^2_{\min} + \left(\sum_i \frac{1}{\sigma_i^2} \right) (\mu - \hat{\mu})^2 + \ldots$$

$$= \chi^2_{\min} + \left(\frac{\mu - \hat{\mu}}{\sigma(\hat{\mu})} \right)^2 + \ldots$$



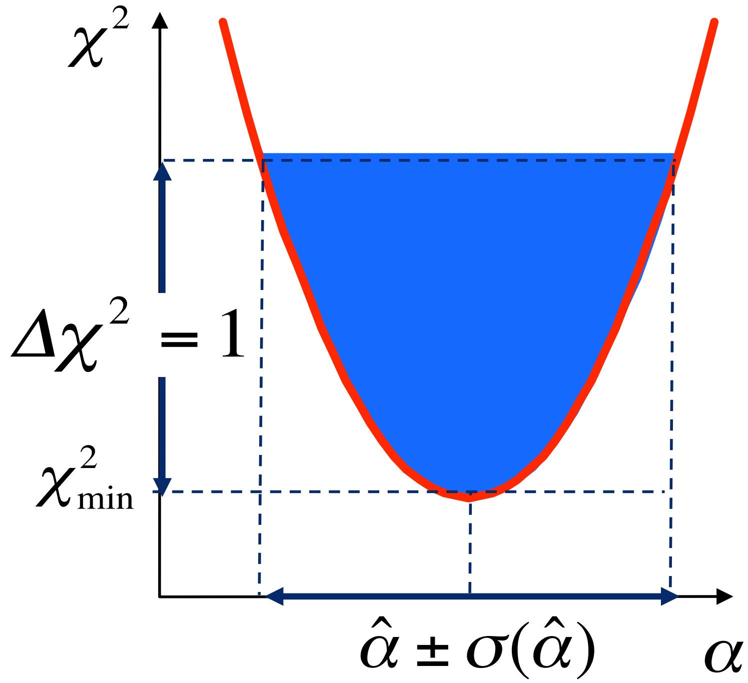
$$\therefore \quad \Delta\chi^2 \equiv \chi^2 - \chi^2_{\min} \approx \left(\frac{\mu - \hat{\mu}}{\sigma(\hat{\mu})} \right)^2 = 1 \quad \text{for} \quad \mu = \hat{\mu} \pm \sigma(\hat{\mu})$$

Parameter Error Bar: 1-σ from χ^2 Curvature

$$\Delta\chi^2 \equiv \chi^2 - \chi^2_{\min} \approx \frac{1}{2}\left(\frac{\partial^2\chi^2}{\partial\alpha^2}\right)\Bigg|_{\alpha=\hat{\alpha}} (\alpha-\hat{\alpha})^2$$

$$= \left(\frac{\alpha-\hat{\alpha}}{\sigma(\hat{\alpha})}\right)^2 = 1 \quad \text{for} \quad \alpha = \hat{\alpha} \pm \sigma(\hat{\alpha})$$

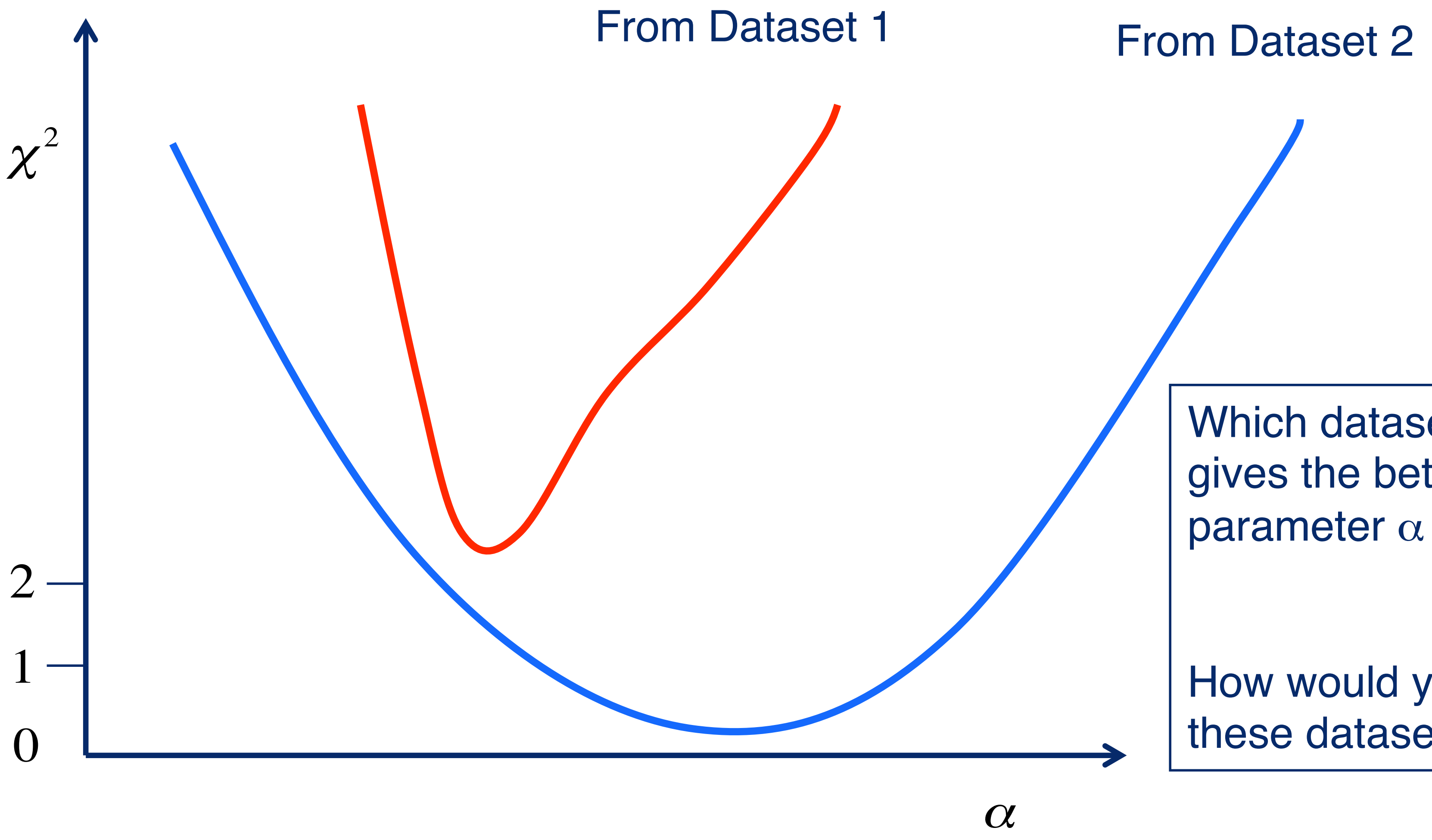
$$\therefore \quad \sigma^2(\hat{\alpha}) = \frac{2}{\left(\frac{\partial^2\chi^2}{\partial\alpha^2}\right)\Big|_{\alpha=\hat{\alpha}}}$$



Exact for linear models, BoF(α) quadratic in α.

Approximate for non-linear models, BoF(α) not quadratic in α.

Test Understanding



Which dataset (1 or 2) gives the better estimate of parameter α ?

How would you combine these datasets ?

Scaling a Pattern by χ^2 minimization

Model: $\mu_i = \langle X_i \rangle = A\, P_i$

Badness-of-fit:

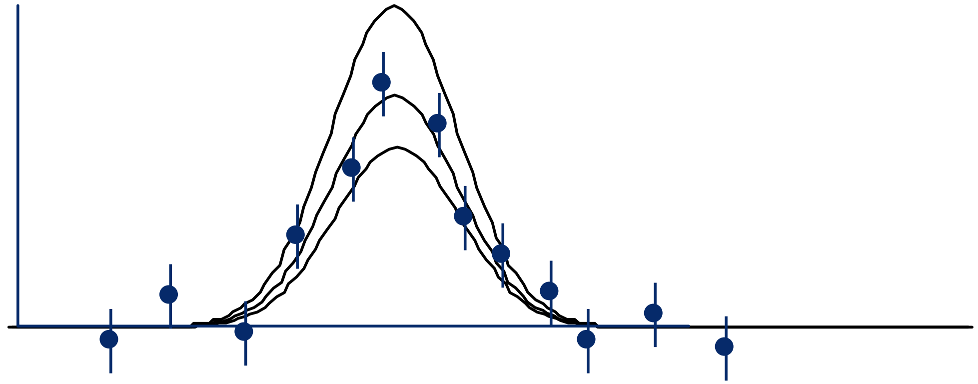
$$\chi^2 = \sum_i \left(\frac{X_i - A\, P_i}{\sigma_i} \right)^2$$

Minimise:

$$0 = \frac{\partial \chi^2}{\partial A} = -2 \sum_i \frac{(X_i - A\, P_i)\, P_i}{\sigma_i^2}$$

$$\Rightarrow \quad \sum_i \frac{X_i\, P_i}{\sigma_i^2} = \sum_i \frac{\hat{A}\, P_i^2}{\sigma_i^2}$$

$$\hat{A} = \frac{\sum_i X_i\, P_i / \sigma_i^2}{\sum_i P_i^2 / \sigma_i^2} .$$



$$\frac{\partial^2 \chi^2}{\partial A^2} = +2 \sum_i \frac{P_i^2}{\sigma_i^2}$$

$$\sigma^2\left(\hat{A}\right) = \frac{2}{\dfrac{\partial^2 \chi^2}{\partial A^2}} = \frac{1}{\sum_i P_i^2 / \sigma_i^2}$$

Same result as Optimal Scaling.

Summary

- Two 1-parameter models:
  - Estimating < X > : $\mu_i = \langle X_i \rangle = \mu$
  - Scaling a pattern: $\mu_i = \langle X_i \rangle = A\, P_i$
- Two equivalent methods:
  - **Algebra of Random Variables: Optimal Average and Optimal Scaling**

$$\hat{X} = \frac{\sum_i X_i / \sigma_i^2}{\sum_i 1/\sigma_i^2} \qquad \sigma^2\left(\hat{X}\right) = \frac{1}{\sum_i 1/\sigma_i^2}$$

$$\hat{A} = \frac{\sum_i X_i\, P_i / \sigma_i^2}{\sum_i P_i^2 / \sigma_i^2} \qquad \sigma^2\left(\hat{A}\right) = \frac{1}{\sum_i P_i^2 / \sigma_i^2}$$

  - **Minimising χ^2** gives same result:

$$\Delta\chi^2 \equiv \chi^2 - \chi^2_{\min} = \left(\frac{\alpha - \hat{\alpha}}{\sigma\left(\hat{\alpha}\right)} \right)^2 + \ldots$$

$$\sigma^2\left(\hat{\alpha}\right) = \frac{2}{\left(\frac{\partial \chi^2}{\partial \alpha^2} \right) \Bigg|_{\alpha = \hat{\alpha}}}$$