ADA05 - 9am Thu 22 Sep 2022

Optimal Scaling

Fitting models by minimizing χ^2
Parameter uncertainty from $\Delta\chi^2=1$

Dancing χ^2 Landscape
χ^2_{min} and $\Delta\chi^2$
Degrees of Freedom

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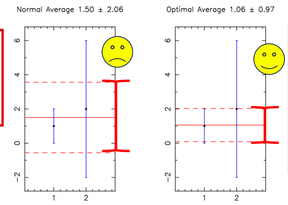
Review: Sample Mean vs Optimal Average

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



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

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.

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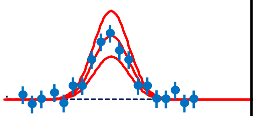
Measuring a Feature

A = area under the curve,
e.g. flux of a star, strength of a spectral line.

Assume (for now) zero background, known pattern.

Model: $\mu_i \equiv \langle X_i \rangle = A\,P_i \qquad \mathrm{Cov}[X_i, X_j] = \sigma_i^2\,\delta_{ij}$



How to measure A ?

Simple method: **Integrate the Data**:

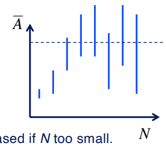
$$\bar{A} = \sum_{i=1}^{N} X_i$$

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

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.

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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.

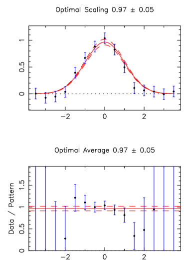
Data: $X_i \pm \sigma_i$
Model: $\mu_i \equiv \langle X_i \rangle = A\,P_i$
Pattern: P_i

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

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

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

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



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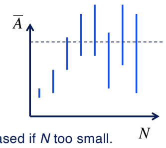
Sum the Data vs Optimal Scaling

Sum up the data.

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

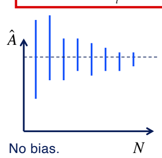
$$\langle \bar{A} \rangle = A \sum_{i=1}^{N} P_i \qquad \sigma^2[\bar{A}] = \sum_{i=1}^{N} \sigma_i^2$$



Biased if N too small.
Noisy if N too large.

Optimal Scaling of known Pattern.

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



No bias.
Result improves with N.

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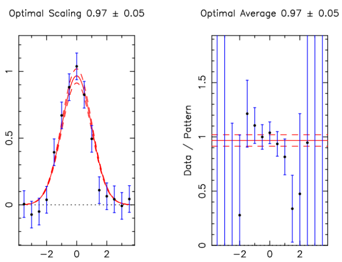
Optimal Scaling

"Golden Rule" of Optimal Data Analysis:

Data : $X_i \pm \sigma_i$
Model : $\langle X_i \rangle = \mu_i = A\,P_i$
Optimal Scaling :

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

Memorise this result.
Know how to derive it.



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

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Fitting Models by minimising χ^2

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

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

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

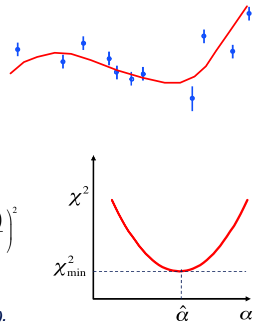
Error: $\varepsilon_i = X_i - \mu_i(\alpha)$

Normalised Error: $\chi_i = \frac{\varepsilon_i}{\sigma_i} = \frac{X_i - \mu_i(\alpha)}{\sigma_i}$

"**Badness-of-Fit**" statistic:

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

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



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

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

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

Badness-of-Fit statistic:

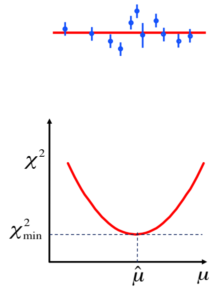
$$\chi^2 = \sum_i \left(\frac{X_i - \mu}{\sigma_i} \right)^2$$

Minimise χ^2:

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

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

The Optimal Average minimises χ^2 !



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Parameter Error Bar: $1-\sigma$ at $\Delta\chi^2 = 1$

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

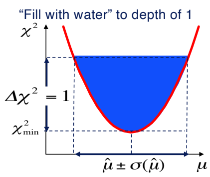
Must have $\sigma^2(\hat{\mu}) = \sigma^2(\hat{X}) = \frac{1}{\sum_i 1/\sigma_i^2}$

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

$$\chi^2 = \chi^2_{\min} + \frac{1}{2} \frac{\partial^2 \chi^2}{\partial \mu^2} \Big|_{\mu = \hat{\mu}} (\mu - \hat{\mu})^2 + \dots$$

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

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



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

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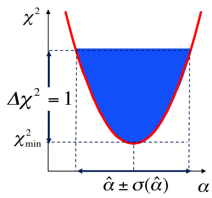
Parameter Error Bar: 1-σ from χ^2 Curvature

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

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

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



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

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

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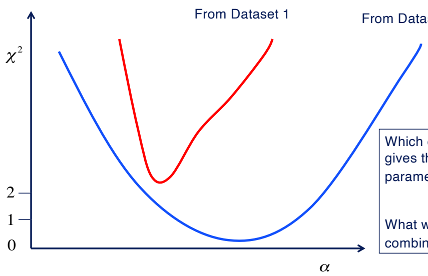
Test Understanding



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

What would $\chi^2(\alpha)$ be if you combined these 2 datasets ?

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Scaling a Pattern by χ^2 minimization

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

Badness-of-fit:

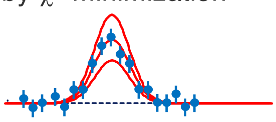
$$\chi^2 = \sum_i \left(\frac{X_i - A\, P_i}{\sigma_i} \right)^2$$

Minimise χ^2:

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

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

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



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

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

Same result as Optimal Scaling.

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Summary: Optimal Average/Scaling is equivalent to Minimise χ^2

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

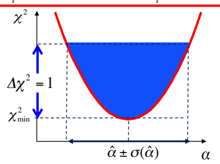
$$\hat{X} = \frac{\sum_i X_i/\sigma_i^2}{\sum_i 1/\sigma_i^2} \qquad \sigma^2\left(\hat{X}\right) = \frac{1}{\sum_i 1/\sigma_i^2}$$

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

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

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

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



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$\chi^2_{\min}$ = "Badness of Fit" statistic

$\chi^2_{\min}$ is a statistic.
It has a probability distribution:

To fit N data points, adjust M parameters to minimise χ^2.

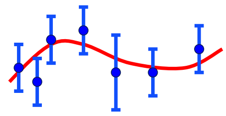
$$\chi^2 \equiv \sum_{i=1}^{N}\left(\frac{X_i - \mu_i(\alpha)}{\sigma_i}\right)^2 \sim \chi^2_{N-M}$$

X_i = data values $i = 1 \ldots N$

σ_i = 1 - σ error bar

$\mu_i(\alpha)$ = model predicted data value

α_k = parameters of the model $k = 1 \ldots M$



N = number of data points

M = number of fitted parameters

$N - M$ = degrees of freedom

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Review : Constructing χ^2_N from N Gaussians

- Sum of squares of N independent Gaussian random variables

$\chi^2_N \equiv$ Chi - squared with N degrees of freedom

X and Y are independent Gaussian random variables.

$X \sim G(0,1) \qquad Y \sim G(0,1)$

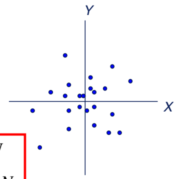
$X^2 \sim \chi^2_1 \qquad Y^2 \sim \chi^2_1$

$X^2 + Y^2 \sim \chi^2_2$

and so on for each new degree of freedom:

$$\chi^2_N + \chi^2_M \sim \chi^2_{N+M}$$

$$\langle \chi^2_N \rangle = N \qquad \sigma^2\left(\chi^2_N\right) = 2N$$



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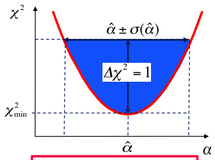
Dancing Data => Dancing χ^2 Landscape

Fit M parameters to N data points.

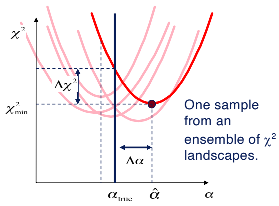
$$\chi^2(X,\sigma,\alpha) = \sum_{i=1}^{N}\left(\frac{X_i - \mu_i(\alpha)}{\sigma_i}\right)^2$$

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



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

Caveat: Assumes orthogonal parameters. Generalise to correlated parameters later.



$$\hat{\alpha} \sim G\left(\alpha_{\text{true}}, \sigma^2(\hat{\alpha})\right)$$

$$\chi^2\left(\alpha_{true}\right) \sim \chi^2_N$$

$$\chi^2_{\min} \equiv \chi^2\left(\hat{\alpha}\right) \sim \chi^2_{N-M}$$

$$\Delta\chi^2 \equiv \chi^2\left(\alpha_{\text{true}}\right) - \chi^2_{\min} \sim \chi^2_M$$

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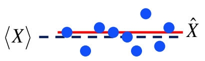
Degrees of Freedom (DoF)

N data : $\langle X_i \rangle = \langle X \rangle \quad \text{Cov}\left(X_i, X_j\right) = \sigma_i^2\,\delta_{ij}$

$$\sum_{i=1}^{N}\left(\frac{X_i - \langle X \rangle}{\sigma_i}\right)^2 \sim \chi^2_N. \quad N \text{ degrees of freedom.}$$

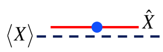
If $\langle X \rangle$ unknown, use $\hat{X}$ instead:



$$\sum_{i=1}^{N}\left(\frac{X_i - \hat{X}}{\sigma_i}\right)^2 \sim \chi^2_{N-1}. \quad N-1 \text{ degrees of freedom.}$$

For a single datum : $N = 1, \quad \hat{X} = X_1$

$$\left(\frac{X_1 - \langle X \rangle}{\sigma_1}\right)^2 \sim \chi^2_1. \quad 1 \text{ degree of freedom}$$



$$\left(\frac{X_1 - \hat{X}}{\sigma_1}\right)^2 = 0. \quad 0 \text{ degrees of freedom.}$$

Fit M parameters to N data :

$$\sum_{i=1}^{N}\left(\frac{X_i - \mu_i(\alpha)}{\sigma_i}\right)^2 \sim \chi^2_{N-M}. \quad N-M \text{ degrees of freedom.}$$

Each fitted parameter removes 1 degree of freedom from the residuals.

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