ADA 12 - 10am Mon 10 Oct 2022

Diagnosis of χ^2_{min} above/below DoF
(Reject model? Clip outliers?
Rescale error bars?)
ML Estimate for Excess Variance

Background Functions
(polynomials, spines, Running Optimal Average (ROA), median filter)

Use χ^2_{min} (or AIC,BIC,…) to reject models

Fit *M* parameters to *N* data points:

$$\chi^2_{\text{min}} = \sum_{i=1}^{N} \left[\frac{X_i - \mu_i(\alpha_{1.},\ldots,\alpha_M)}{\sigma_i} \right]^2 \sim \chi^2_{N-M}$$

$$\left\langle \chi^2_{N-M} \right\rangle = N - M \qquad \sigma^2(\chi^2_{N-M}) = 2(N-M)$$

Why *N* - *M* degrees of freedom?

Fitting *M* = *N* parameters should fit *N* points exactly.

If model is good, then the best-fit χ^2_{min} should be:

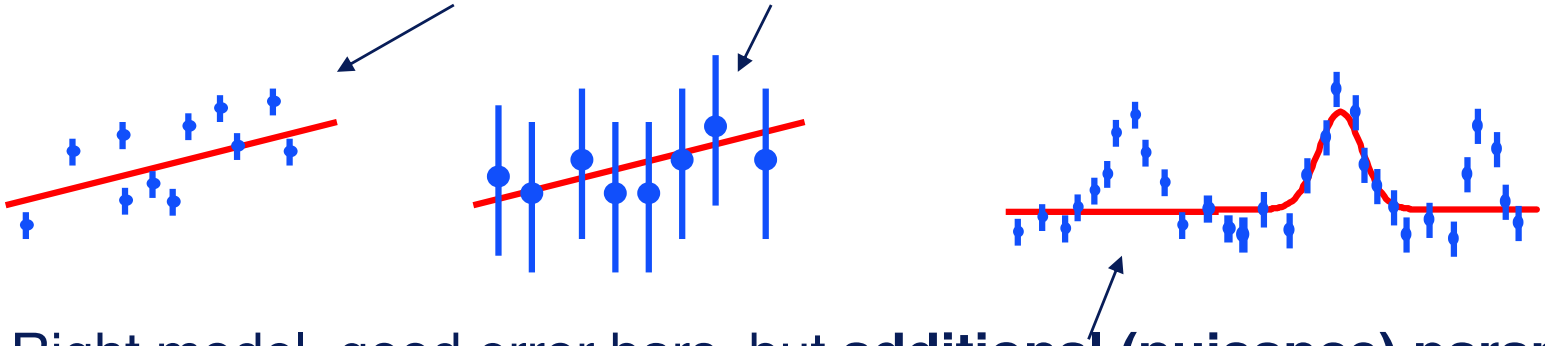
$$\chi^2_{\text{min}} \approx N - M \pm \sqrt{2\,(N-M)}$$

$$\frac{\chi^2_{\text{min}}}{N-M} \approx 1 \pm \sqrt{\frac{2}{N-M}}$$

What if χ^2_{min} is too high (or low)?

Several possibilities:

1. Statistical fluke? Use χ^2_{N-M} distribution to estimate probability (p-value)
2. A few outliers ? Use e.g. sigma-clipping to identify and reject outliers.
3. Wrong model? Use χ^2_{N-M} distribution to reject model (p < threshold)
4. Error bars **too small** or **too large**? Re-scale or adjust σ_i?

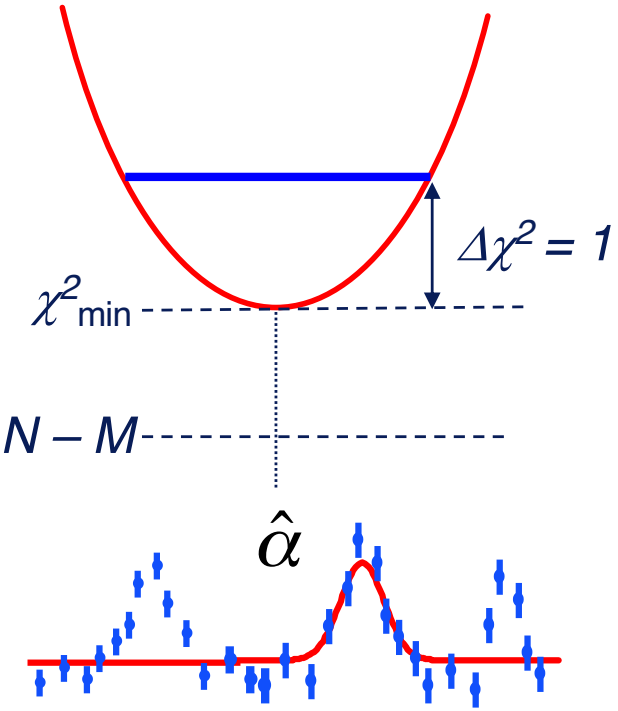


5. Right model, good error bars, but **additional (nuisance) parameters** omitted or not optimised?

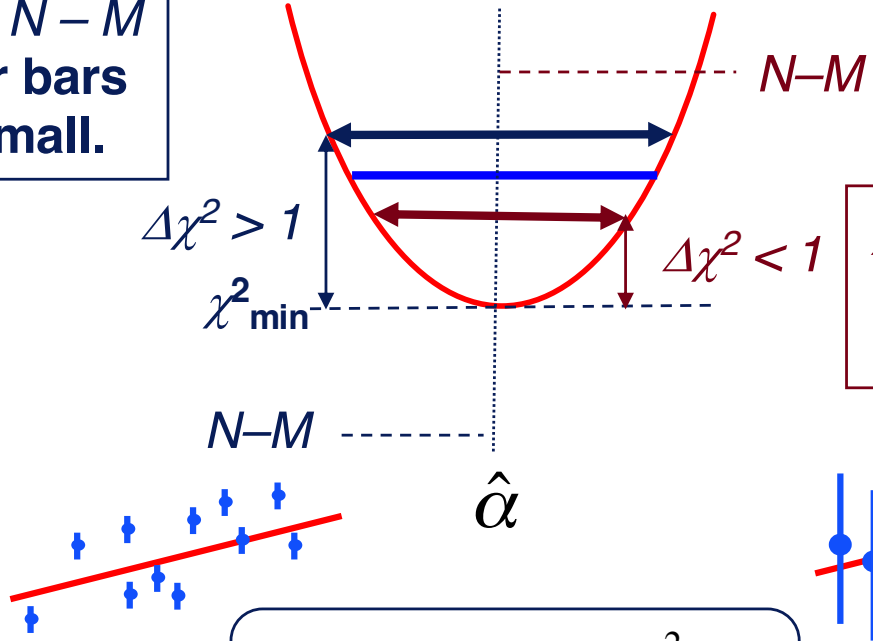
Failure to optimise nuisance parameters increases χ^2_{min} , but may leave the χ^2 curvature the same, **if the nuisance parameters are orthogonal to the parameters of interest**.

Can then still use $\Delta\chi^2$ to set confidence intervals on parameters **orthogonal to the nuisance parameters**.

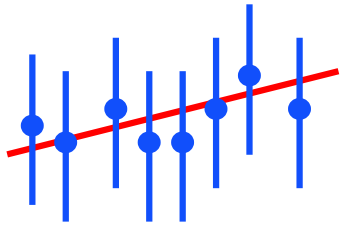
Diagnosis of χ^2_{min} too large or small



$\chi^2_{\text{min}} > N - M$
error bars too small.



$\chi^2_{\text{min}} < N - M$
error bars too large.



$\chi^2_{\text{min}} > N - M$ due to failure to optimise nuisance parameters ?
If these are **orthogonal** to parameters of interest, then the curvature at the minimum is unchanged. Use $\Delta\chi^2 = 1$.

Use: $\Delta\chi^2 = \dfrac{\chi^2_{\text{min}}}{N - M}$

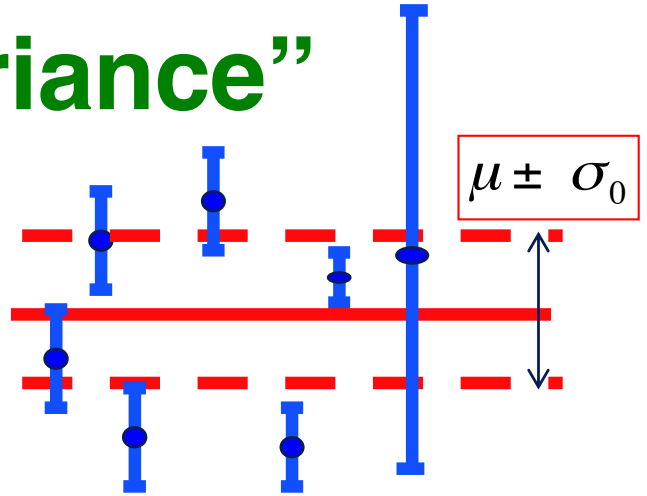
Equivalent to **re-scaling the error bars**

$$\sigma \Rightarrow \sigma \sqrt{\frac{\chi^2_{\text{min}}}{N - M}}$$

ML Estimate for the "Extra Variance"

Assume two independent noise sources:

Errors with known σ_i. Extra variance σ_0^2 .

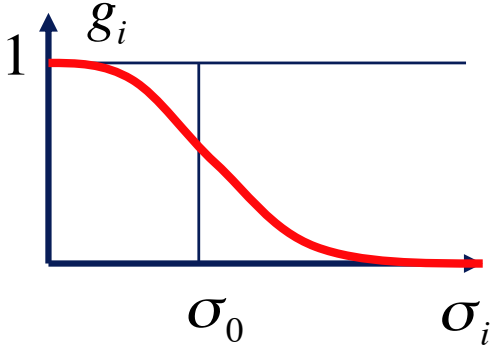


$$\mathrm{Var}[X_i] = \sigma_0^2 + \sigma_i^2 = \frac{\sigma_0^2}{g_i} \qquad g_i \equiv \frac{\sigma_0^2}{\sigma_0^2 + \sigma_i^2} = \frac{1}{1 + (\sigma_i/\sigma_0)^2}$$

$$-2\ln L = \sum_{i=1}^{N} \frac{(X_i - \mu)^2}{\sigma_0^2 + \sigma_i^2} + \sum_{i=1}^{N} \ln\left(\sigma_0^2 + \sigma_i^2\right)$$

$$0 = \frac{\partial(-2\ln L)}{\partial \mu} = -2\sum_{i=1}^{N} \frac{X_i - \mu}{\sigma_0^2 + \sigma_i^2}$$

g_i = "goodness" of X_i for measuring σ_0^2



$$0 = \frac{\partial(-2\ln L)}{\partial \sigma_0^2} = -\sum_{i=1}^{N}\left(\frac{X_i - \mu}{\sigma_0^2 + \sigma_i^2}\right)^2 + \sum_{i=1}^{N} \frac{1}{\sigma_0^2 + \sigma_i^2} = -\sum \frac{(X_i - \mu)^2 g_i^2}{\sigma_0^4} + \sum \frac{g_i}{\sigma_0^2}$$

$$\hat{\mu} = \frac{\sum \frac{X_i}{\sigma_0^2 + \sigma_i^2}}{\sum \frac{1}{\sigma_0^2 + \sigma_i^2}} = \frac{\sum X_i g_i}{\sum g_i} \qquad \mathrm{Var}[\hat{\mu}] = \frac{\sigma_0^2}{\sum g_i} \qquad \hat{\sigma}_0^2 = \frac{\sum (X_i - \mu)^2 g_i^2}{\sum g_i}$$

Need to iterate.

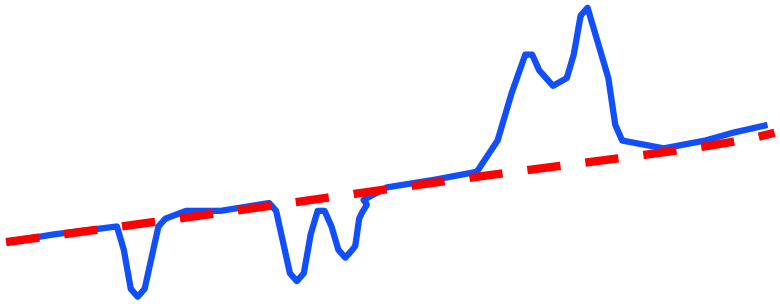
Homework : Work out Var[$\hat{\sigma}_0^2$] .

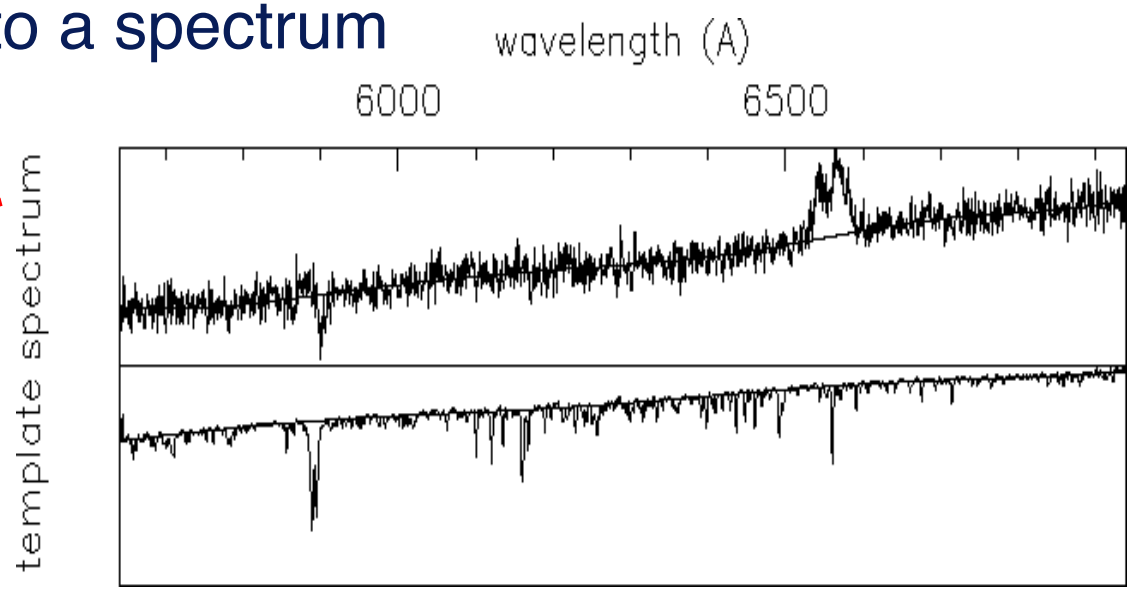
Background Functions

Smooth functions with adjustable flexibility.

- Polynomials
- Splines
- Running Optimal Average
- Any of the above – with sigma clipping.
- Running Median

Example: Continuum fit to a spectrum

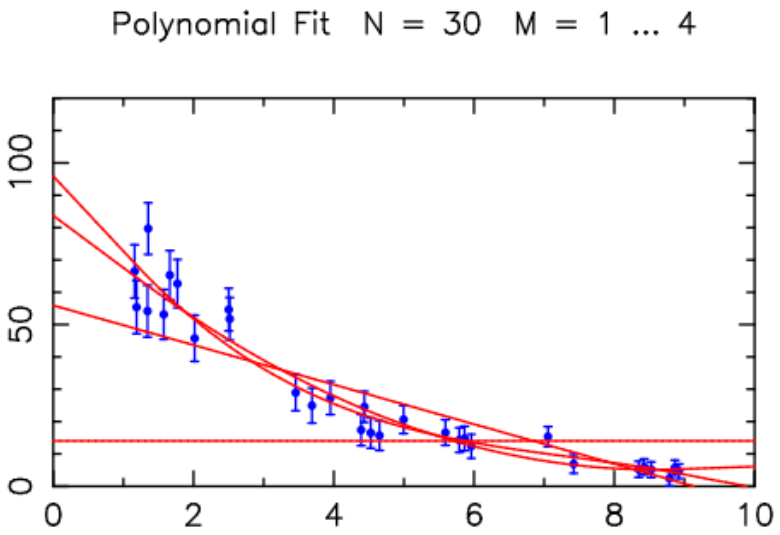




Polynomials

Fit $N = 30$ points with

$M = 1, 2, 3, 4$ polynomial coefficients.



Higher M = more flexible model.

Use lowest M that gives good fit.

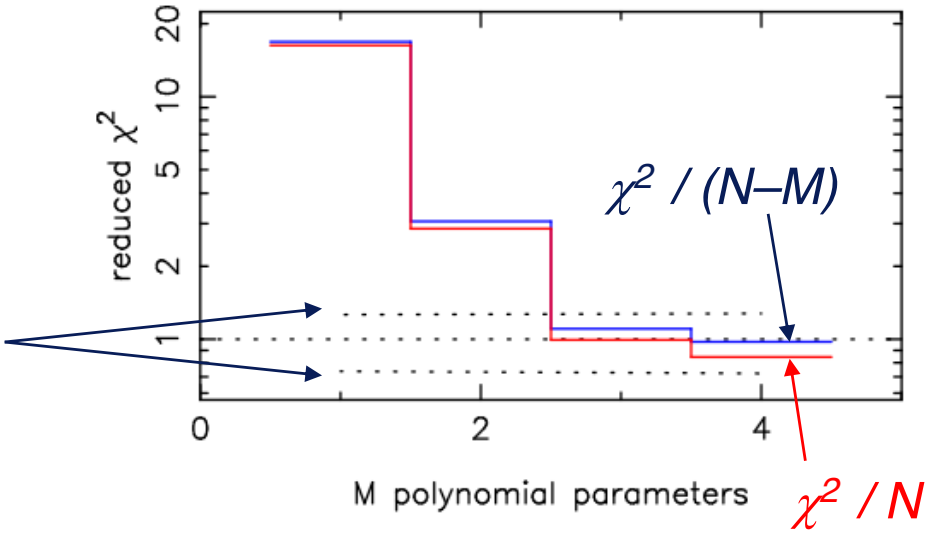
e.g. minimise AIC or BIC

Reject $M = 1, 2.$

Accept $M = 3, 4.$

Based on Reduced χ^2

$$\frac{\chi^2}{N-M} \approx 1 \pm \sqrt{\frac{2}{N-M}}$$



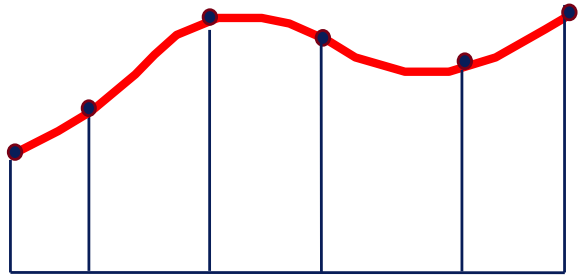
Splines – e.g. piecewise cubic

***N* nodes**: x_i , y_i , $i = 1, \ldots N$. x_i fixed, y_i adjustable.

***4 (N – 1)* parameters** (*4* cubic coefficients for each of the *N - 1* segments)

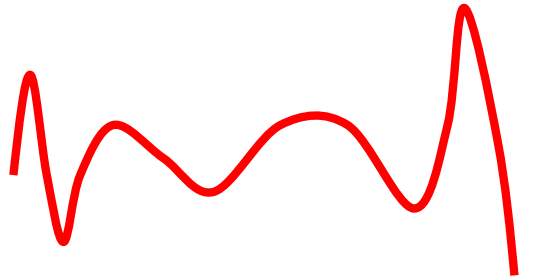
***3 (N – 2)* matching conditions** (value, slope, curvature at each of the *N - 2* internal nodes)

***N + 2* degrees of freedom** (*N* values y_i plus either slope or curvature at 2 end points).



8-parameter cubic spline

- First, **distribute the nodes x_i** , e.g. equally spaced, or equal weight $\Sigma(1/\sigma^2)$ on each segment.
- Then, **fit *N +2* parameters**, e.g. find y_i to minimise χ^2, with endpoint curvatures (or slopes) set to zero.



8-parameter polynomial

Low-order polys are good for simple background fits.

Splines better than high-order polys. Better control over the *x* distribution of the degrees of freedom.

Running Optimal Average (ROA)

Time-series data: $X_i \pm \sigma_i$ at times t_i

$$\hat{X}(t) = \frac{\sum X_i \, w_i(t)}{\sum w_i(t)} \qquad \sigma^2\left(\hat{X}(t)\right) = \frac{1}{\sum w_i(t)}$$

$$w_i(t) = \frac{G(t - t_i)}{\sigma_i^2}$$

Memory function *G(t)* expands the error bars as time-difference increases.

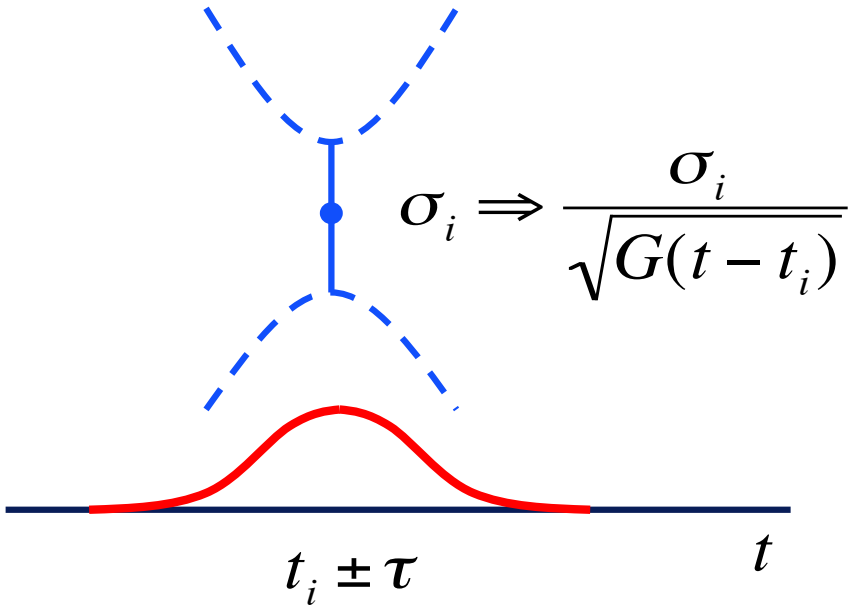
Parameter τ controls time interval over which the data point retains its $1/\sigma^2$ weight.

Memory functions:

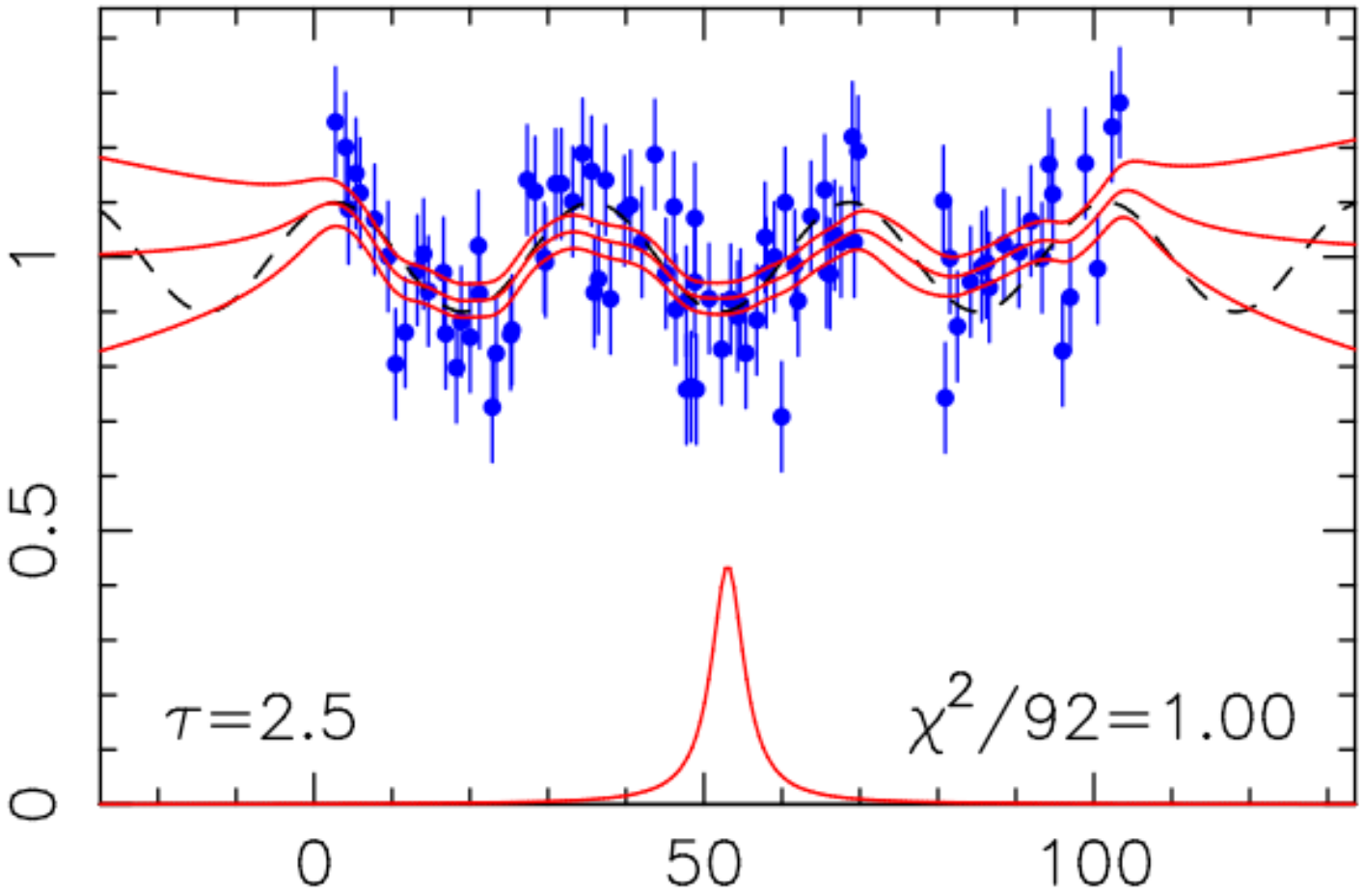
boxcar: $G(t) = \begin{cases} 1 & |t| < \tau \\ 0 & |t| > \tau \end{cases}$

Gaussian: $= \exp\left\{-\frac{1}{2}\left(\frac{t}{\tau}\right)^2\right\}$

Lorentzian: $= \frac{1}{1 + (t/\tau)^2}$



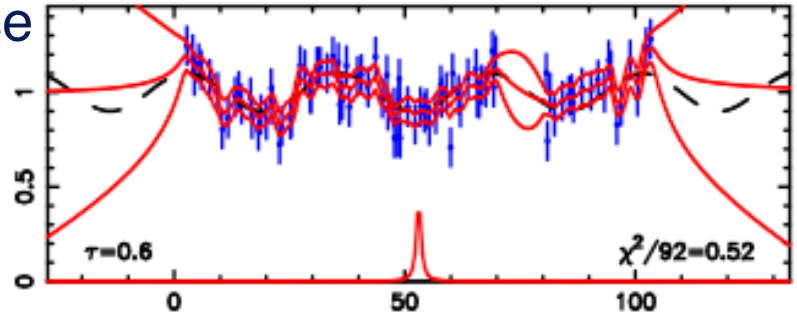
Running Optimal Average (ROA)

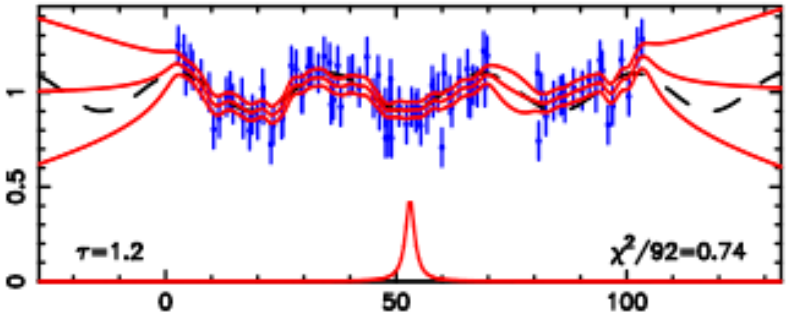


Smooth curve, with error bars, running thru the data.

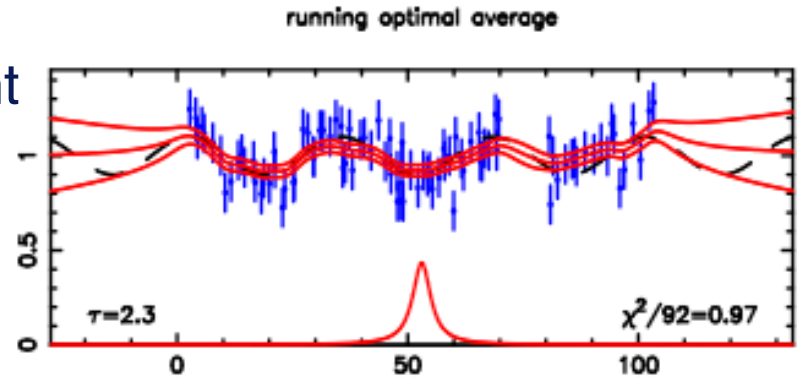
ROA timescale τ controls flexibility

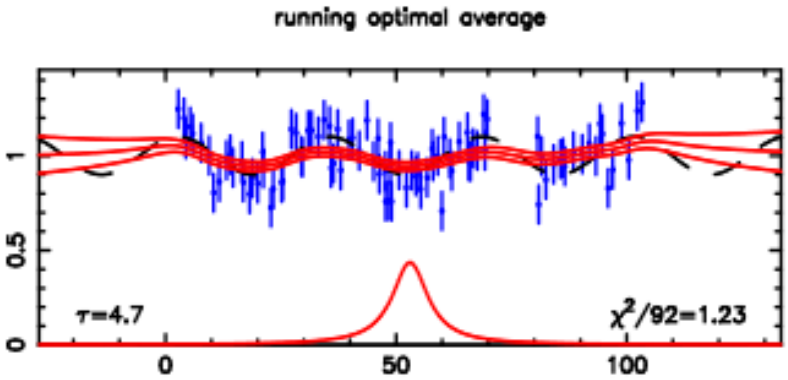
Too loose



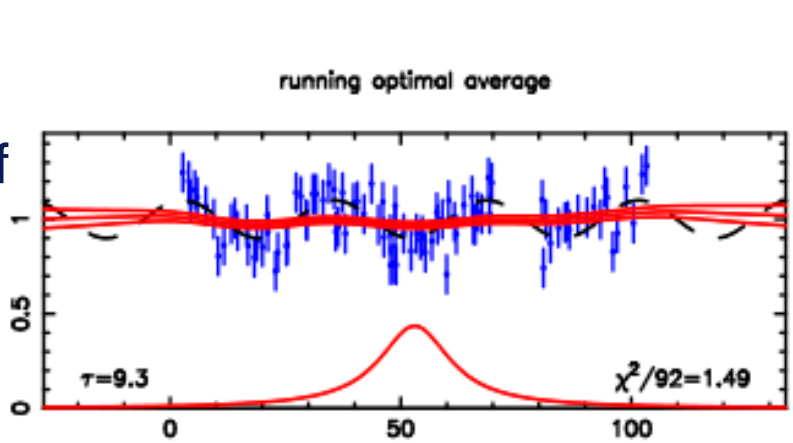


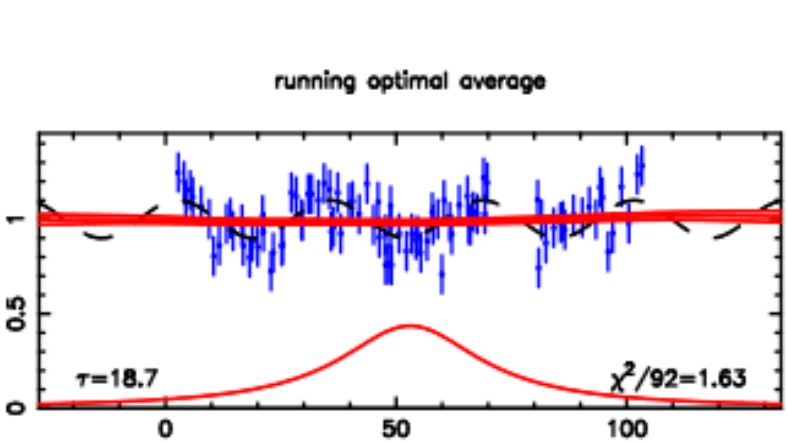
Just right



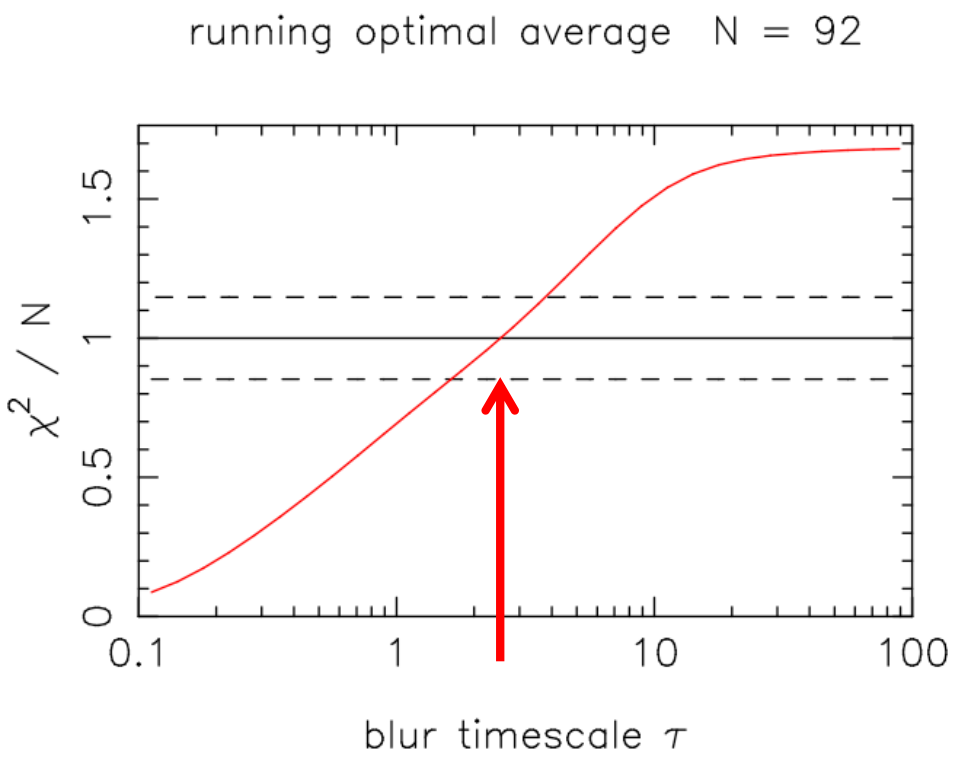


Too stiff



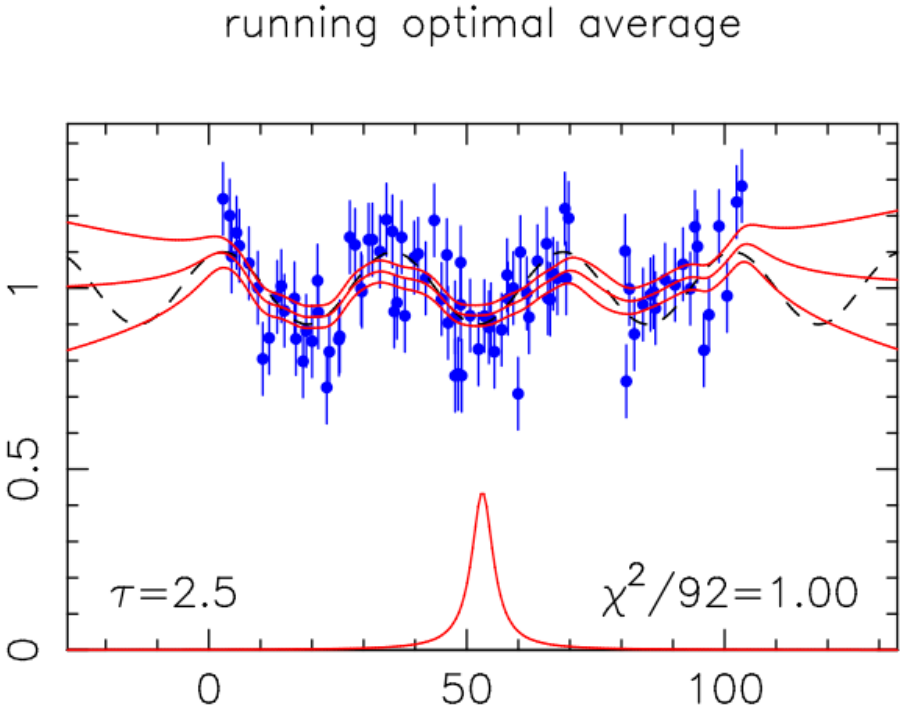


Running Optimal Average (ROA)



Blur timescale τ can be chosen to make $\chi^2 / N \sim 1$.

Can also define the effective number of parameters, and minimise BIC.

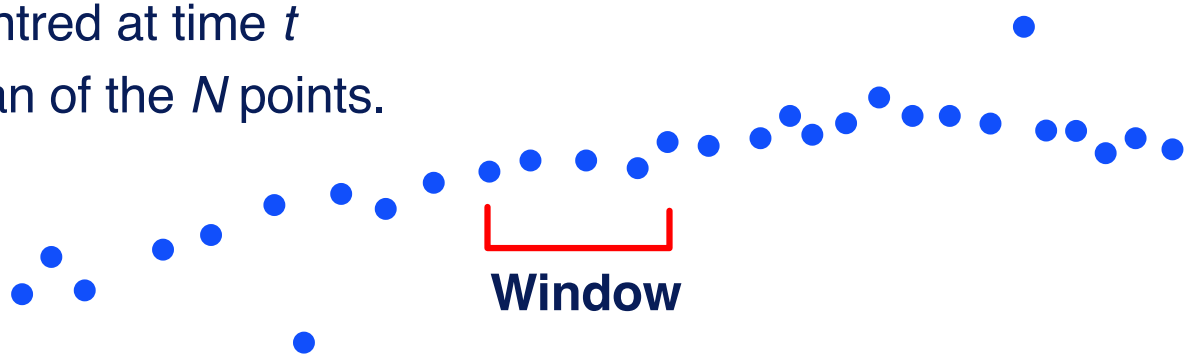


Interpolates across gaps.
Extrapolates past ends.
Averages appropriately.
Error bars provided.
(Almost) model-free.

Median Filter and Sigma-Clip

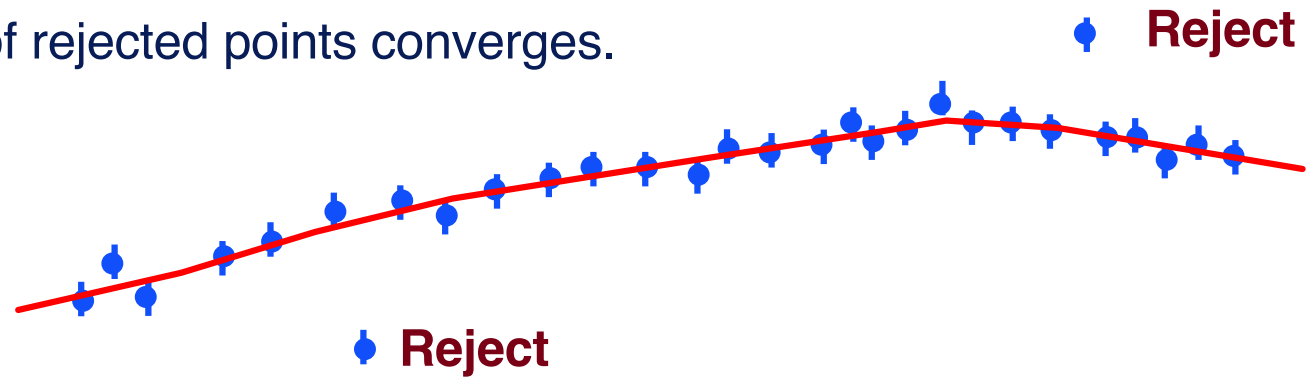
Median filter:

- window of N points centred at time t
- medfilt(t) is the median of the N points.



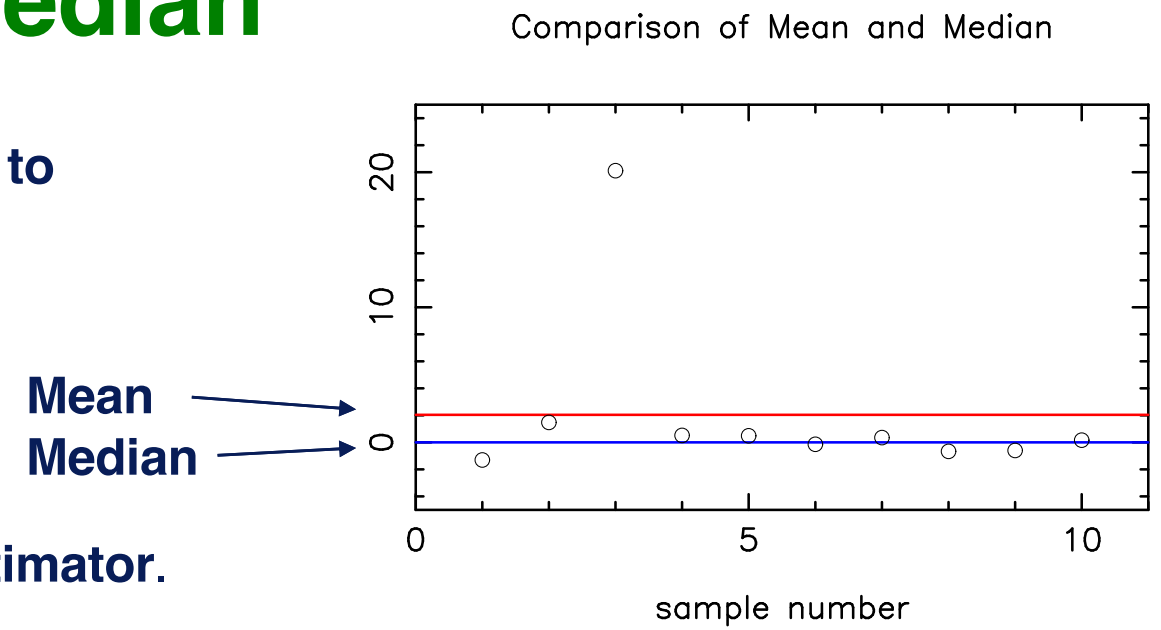
Sigma-clip:

- Fit all points by minimising χ^2
- Set threshold K and check for outliers at $\pm K\,\sigma$ or more
- Repeat fit omitting **largest** outlier
- Iterate until set of rejected points converges.



Mean vs Median

- The median is **less sensitive to outliers** than the mean.



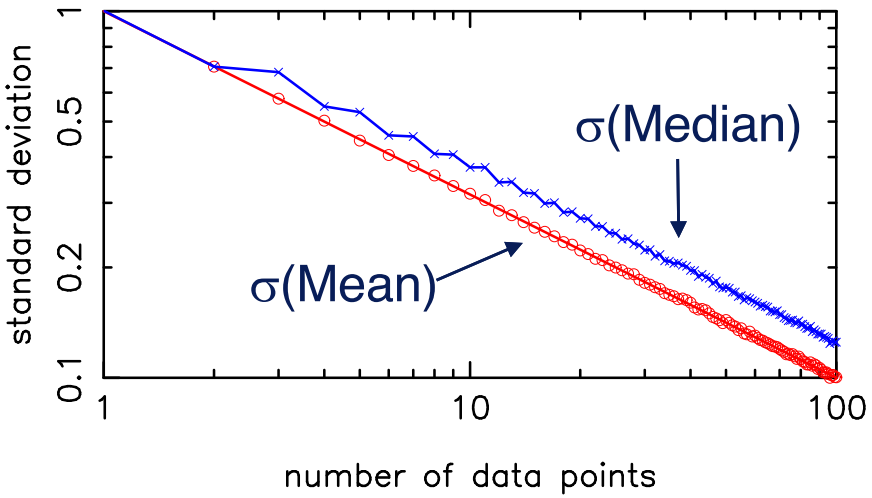
- The median is **unbiased** but **not a minimum-variance estimator.**

- Note how **standard deviation of the median** varies with sample size *N* in comparison to **standard deviation of the mean.**

$$\mathrm{Var}[\bar{X}] = \sigma^2/N$$

$$\mathrm{Var}[X_{\mathrm{med}}] \to (\pi/2)\,(\sigma^2/N)$$

Variance of the Median exceeds the Variance of the Mean by a factor $\pi/2 = 1.57$ (for large *N*).



Var[Median] = (π/2) Var[Mean]

N gaussian random numbers:

$$\langle X_i \rangle = \mu \quad \mathrm{Var}[X_i] = \sigma^2 \quad i = 1 \ldots N$$

$$f(x) = F'(x) = \frac{1}{\left(2\pi\sigma^2\right)^{1/2}} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$

P = fraction of positive errors :

$$p_i = \begin{cases} 1 & X_i > \mu \\ 0 & X_i < \mu \end{cases} \qquad \langle p_i \rangle = \frac{1}{2} \quad \sigma^2(p_i) = \frac{1}{4}$$

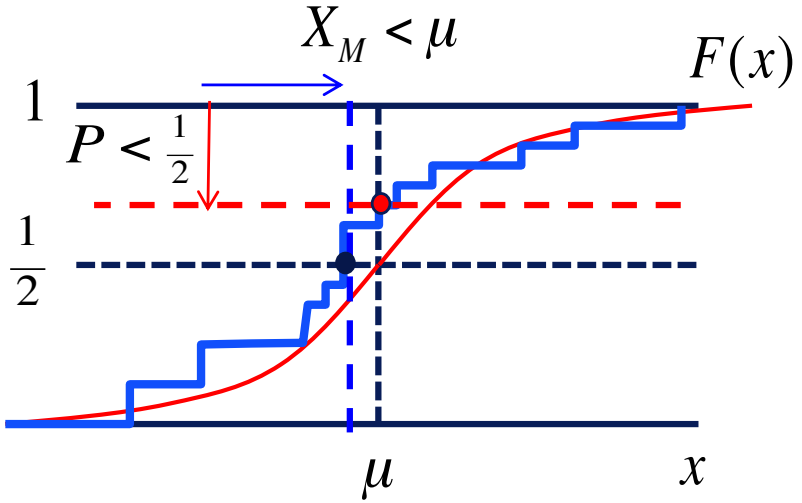
$$P \equiv \frac{1}{N}\sum_{i=1}^{N} p_i \qquad \langle P \rangle = \frac{1}{2} \quad \sigma^2(P) = \frac{1}{4N}$$

Median: $X_M - \mu \approx \dfrac{P - \langle P \rangle}{F'(\mu)} = \dfrac{P - \frac{1}{2}}{f(\mu)}$

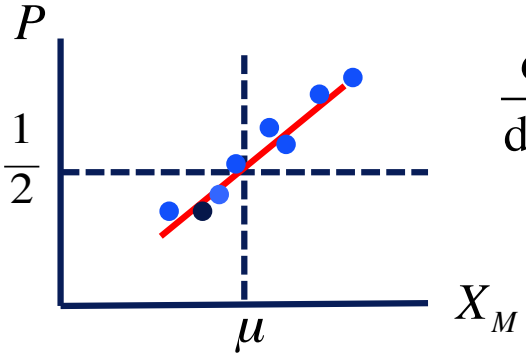
$$\frac{\partial X_M}{\partial P} = \frac{1}{f(\mu)} = \left(2\pi\sigma^2\right)^{1/2}$$

$$\sigma^2(X_M) = \sigma^2(P)\left|\frac{\partial X_M}{\partial P}\right|^2 = \frac{1}{4N\left(f(\mu)\right)^2} = \frac{2\pi\sigma^2}{4N} = \frac{\pi}{2}\frac{\sigma^2}{N}$$

$$\sigma^2(\bar{X}) = \frac{\sigma^2}{N}$$



P co-varies with X_M :



$$\frac{dP}{dX_M} \approx F'(\mu)$$

Variance of the Median is larger by a factor *π / 2 = 1.57* (for large *N*) than the Variance of the Mean.

Var[Median] = (π/2) Var[Mean]

N gaussian random numbers:

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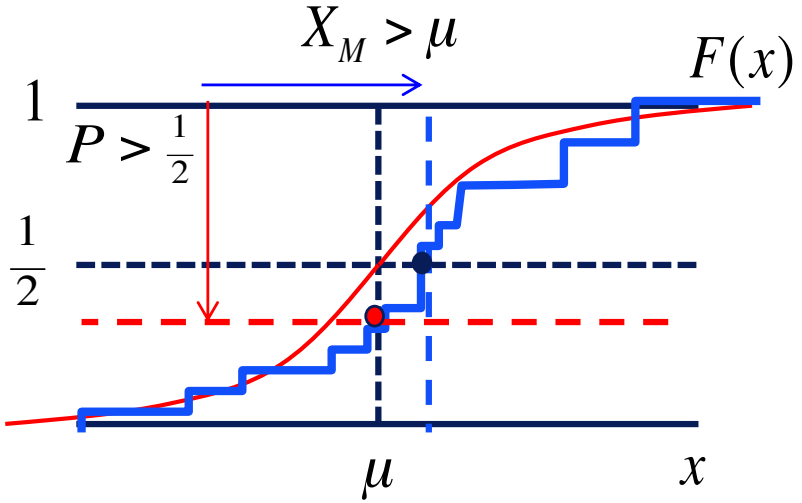
Median: $X_M - \mu \approx \dfrac{P - \langle P \rangle}{F'(\mu)} = \dfrac{P - \frac{1}{2}}{f(\mu)}$

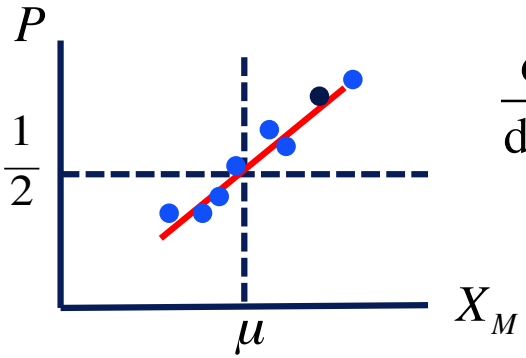
$$\frac{\partial X_M}{\partial P} = \frac{1}{f(\mu)} = \left(2\pi\sigma^2\right)^{1/2}$$

$$\sigma^2(X_M) = \sigma^2(P)\left|\frac{\partial X_M}{\partial P}\right|^2 = \frac{1}{4N\left(f(\mu)\right)^2} = \frac{2\pi\sigma^2}{4N} = \frac{\pi}{2}\frac{\sigma^2}{N}$$

$$\sigma^2(\bar{X}) = \frac{\sigma^2}{N}$$



P co-varies with X_M :



$$\frac{dP}{dX_M} \approx F'(\mu)$$

Variance of the Median is larger by a factor *π / 2 = 1.57* (for large *N*) than the Variance of the Mean.

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