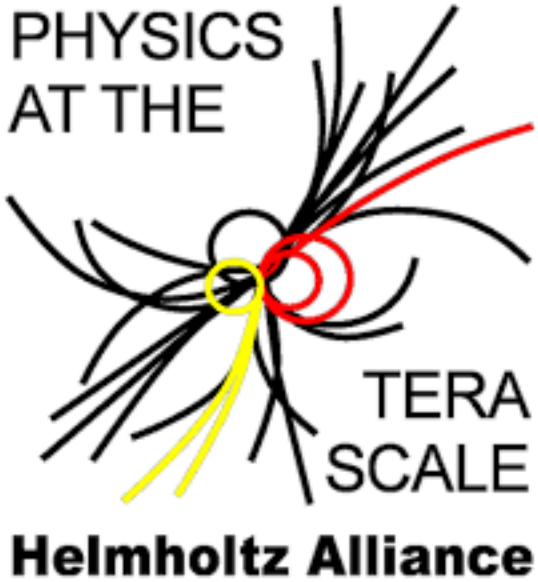
# Statistics for Particle Physics
# "Errors on Errors"




## Terascale Statistics School

https://indico.desy.de/event/46667/

DESY, Hamburg
24-28 Feb 2025



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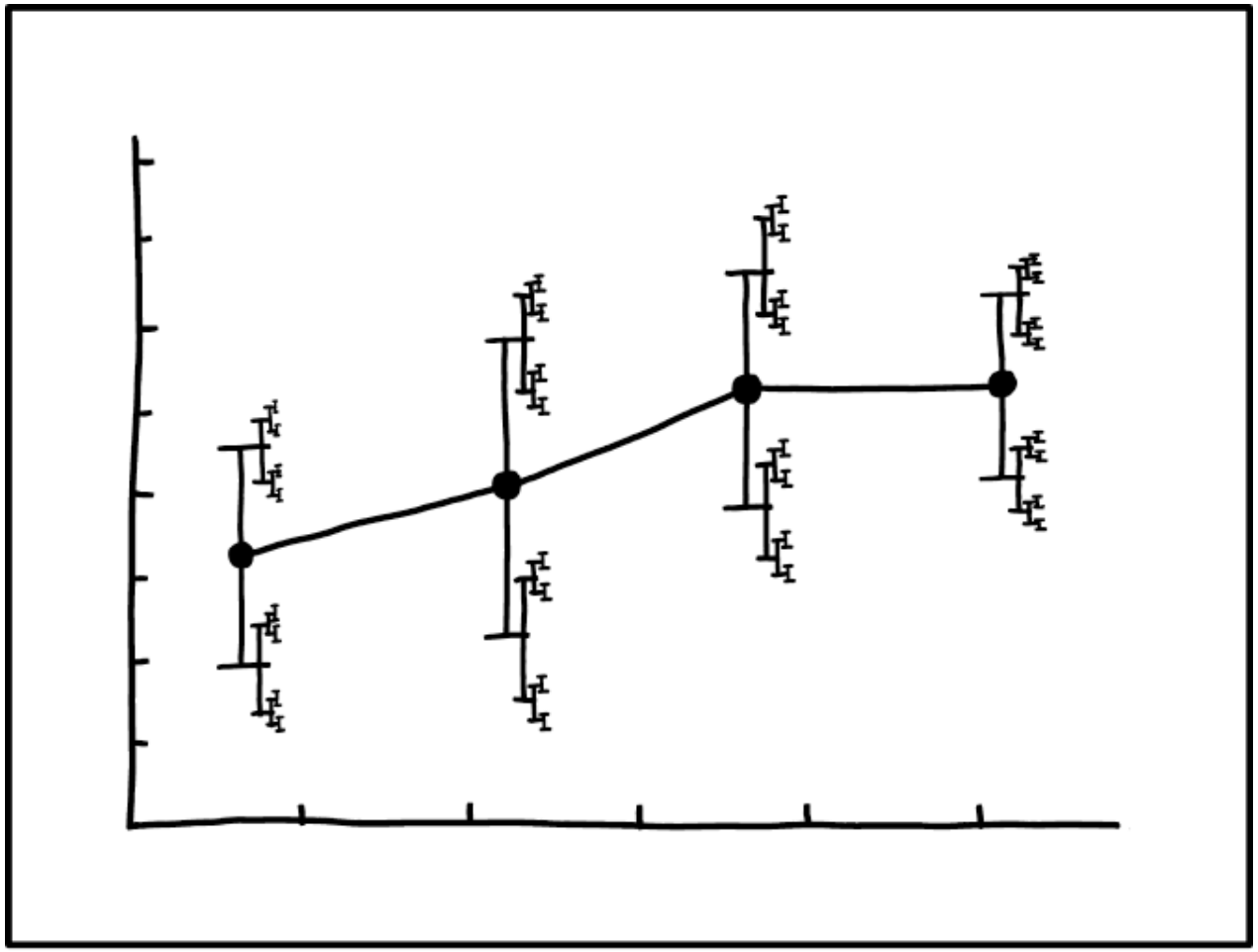
# Outline

| | |
|---|---|
| Monday 15:30 | Hypothesis testing |
| Monday 16:30 | Hypothesis testing tutorial |
| Tuesday 10:30 | Parameter estimation tutorial |
| Tuesday 14:00 | Setting limits |
| Wednesday 9:00 | Bayesian parameter estimation |
| → Wednesday 11:00 | Errors on errors |

## Based on


G. Cowan, Eur. Phys. J. C (2019) 79:133; arXiv:1809.05778
G. Cowan, , EPJ Web of Conferences 258, 09002 (2022); arXiv:2107.02652
E. Canonero, A. Brazzale and G. Cowan, Eur. Phys. J. C (2023) 83:1100; arXiv:2304.10574
E. Canonero, G. Cowan, Eur. Phys. J. C (2025) 85: 156; arXiv:2407.05322

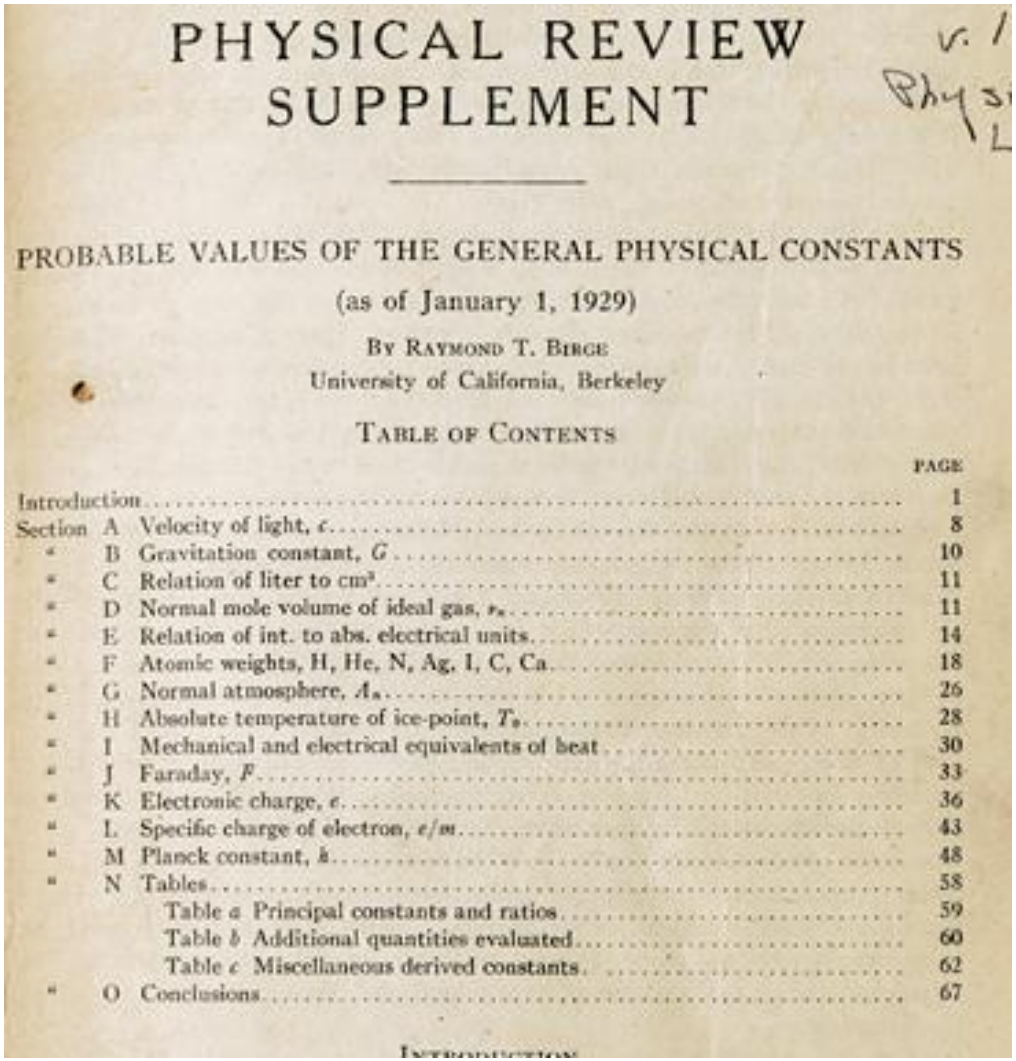


I DON'T KNOW HOW TO PROPAGATE ERROR CORRECTLY, SO I JUST PUT ERROR BARS ON ALL MY ERROR BARS.

http://bancroft.berkeley.edu/Exhibits/physics/learning01.html

# Least Squares for Averaging

= fit of horizontal line



PHYSICAL REVIEW
SUPPLEMENT

PROBABLE VALUES OF THE GENERAL PHYSICAL CONSTANTS

(as of January 1, 1929)

By Raymond T. Birge
University of California, Berkeley

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Raymond T. Birge,
*Probable Values of the General Physical Constants (as of January 1, 1929)*,
Physical Review Supplement, Vol 1, Number 1, July 1929

Forerunner of the Particle Data Group

# Least squares: some issues

The method of least squares requires the standard deviations of the measured quantities, but often these are poorly known.

The uncertainty (e.g. confidence interval) of an LS average does not reflect goodness of fit:

LS average of $9 \pm 1$ and $11 \pm 1$ is $10 \pm 0.71$

LS average of $5 \pm 1$ and $15 \pm 1$ is $10 \pm 0.71$

LS estimators are equivalent to maximum-likelihood assuming Gaussian distributed measurements; but the tails of a Gaussian fall off very fast, not always an appropriate model.

$\rightarrow$ Outliers in LS average have very large influence.

Solution: incorporate the uncertainty in the standard deviations of the measurements into the analysis.

# "Errors on Errors"

*APRIL 15, 1932* *PHYSICAL REVIEW* *VOLUME 40*

## THE CALCULATION OF ERRORS BY THE METHOD OF LEAST SQUARES

By Raymond T. Birge
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(Received February 18, 1932)

Abstract

**Present status of least squares' calculations.**—There are three possible stages in any least squares' calculation, involving respectively the evaluation of (1) the most probable values of certain quantities from a set of experimental data, (2) the reliability or probable error of each quantity so calculated, (3) the reliability or probable error of the probable errors so calculated. Stages (2) and (3) are not adequately treated in most texts, and are frequently omitted or misused, in actual work. The present article is concerned mainly with these two stages.

→ PDG "scale factor method" ≈ scale sys. errors with common factor until $\chi^2_{\text{min}}$ = appropriate no. of degrees of freedom.

# Formulation of the problem

Suppose measurements $\boldsymbol{y}$ have probability (density) $P(\boldsymbol{y}|\boldsymbol{\mu},\boldsymbol{\theta})$,

$\boldsymbol{\mu}$ = parameters of interest

$\boldsymbol{\theta}$ = nuisance parameters

To provide info on nuisance parameters, often treat their best estimates $\boldsymbol{u}$ as indep. Gaussian distributed r.v.s., giving likelihood

$$L(\boldsymbol{\mu},\boldsymbol{\theta}) = P(\mathbf{y},\mathbf{u}|\boldsymbol{\mu},\boldsymbol{\theta}) = P(\mathbf{y}|\boldsymbol{\mu},\boldsymbol{\theta})P(\mathbf{u}|\boldsymbol{\theta})$$

$$= P(\mathbf{y}|\boldsymbol{\mu},\boldsymbol{\theta}) \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma_{u_i}} e^{-(u_i-\theta_i)^2/2\sigma_{u_i}^2}$$

or log-likelihood (up to additive const.)

$$\ln L(\boldsymbol{\mu},\boldsymbol{\theta}) = \ln P(\mathbf{y}|\boldsymbol{\mu},\boldsymbol{\theta}) - \frac{1}{2}\sum_{i=1}^{N} \frac{(u_i-\theta_i)^2}{\sigma_{u_i}^2}$$

# Systematic errors and their uncertainty

Often the $\theta_i$ could represent a systematic bias and its best estimate $u_i$ in the real measurement is zero.

The $\sigma_{u,i}$ are the corresponding "systematic errors".

Sometimes $\sigma_{u,i}$ is well known, e.g., it is itself a statistical error known from sample size of a control measurement.

Other times the $u_i$ are from an indirect measurement, Gaussian model approximate and/or the $\sigma_{u,i}$ are not exactly known.

Or sometimes $\sigma_{u,i}$ is at best a guess that represents an uncertainty in the underlying model ("theoretical error").

In any case we can allow that the $\sigma_{u,i}$ are not known in general with perfect accuracy.

# Gamma model for variance estimates

Suppose we want to treat the systematic errors as uncertain, so let the $\sigma_{u,i}$ be adjustable nuisance parameters.

Suppose we have estimates $s_i$ for $\sigma_{u,i}$ or equivalently $v_i = s_i^2$, is an estimate of $\sigma_{u,i}^2$.

Model the $v_i$ as independent and gamma distributed:

$$f(v;\alpha,\beta) = \frac{\beta^{\alpha}}{\Gamma(\alpha)} v^{\alpha-1} e^{-\beta v}$$

$$E[v] = \frac{\alpha}{\beta}$$

$$V[v] = \frac{\alpha}{\beta^2}$$

Set $\alpha$ and $\beta$ so that they give desired mean and width for $f(v)$:

$$E[v] = \sigma_u^2 = \alpha/\beta,$$

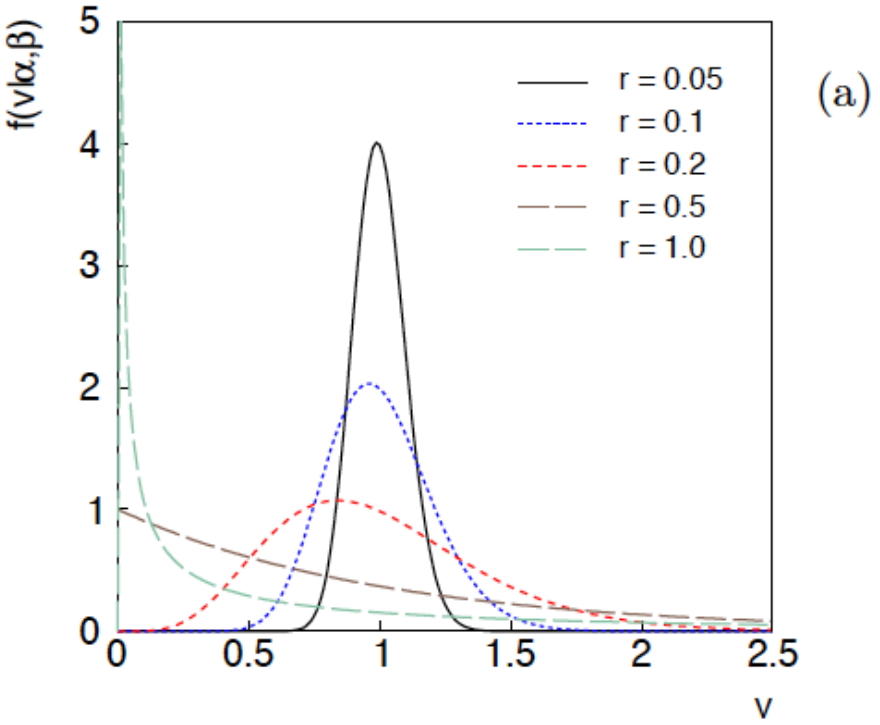
$r = 1/2\sqrt{\alpha} \approx$ relative "error on the error" = $\sigma_s/E[s]$ .

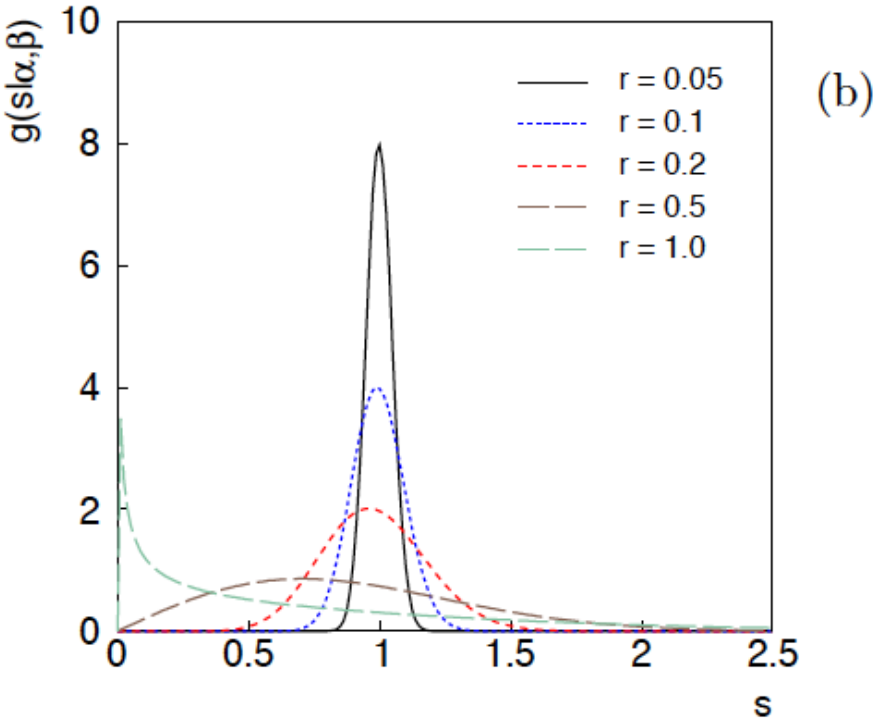
# Distributions of $v$ and $s = \sqrt{v}$

For $\alpha$, $\beta$ of gamma distribution, $\alpha_i = \frac{1}{4r_i^2}$, $\beta_i = \frac{1}{4r_i^2\sigma_{u_i}^2}$

$$r_i \equiv \frac{1}{2}\frac{\sigma_{v_i}}{E[v_i]} = \frac{1}{2}\frac{\sigma_{v_i}}{\sigma_{u_i}^2} \approx \frac{\sigma_{s_i}}{E[s_i]}$$

relative "error on error"



# Motivation for gamma variance model

If one were to have $n$ independent observations $u_1,..,u_n$, with all $u \sim \text{Gauss}(\theta, \sigma_u^2)$, and we use the sample variance

$$v = \frac{1}{n-1}\sum_{i=1}^{n}(u_i - \overline{u})^2$$

to estimate $\sigma_u^2$, then $(n-1)v/\sigma_u^2$ follows a chi-square distribution for $n-1$ degrees of freedom, which is a special case of the gamma distribution ($\alpha = n/2$, $\beta = 1/2$). (In general one doesn't have a sample of $u_i$ values, but if this were to be how $v$ was estimated, the gamma model would follow.)

Furthermore choice of the gamma distribution for $v$ allows one to profile over the nuisance parameters $\sigma_u^2$ in closed form and leads to a simple profile likelihood.

# Likelihood for gamma variance model

$$L(\boldsymbol{\mu}, \boldsymbol{\theta}, \boldsymbol{\sigma}_{\mathbf{u}}^2) = P(\mathbf{y}|\boldsymbol{\mu}, \boldsymbol{\theta}) \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma_{u_i}^2}} e^{-(u_i-\theta_i)^2/2\sigma_{u_i}^2}$$

$$\times \frac{\beta_i^{\alpha_i}}{\Gamma(\alpha_i)} v_i^{\alpha_i - 1} e^{-\beta_i v_i} ,$$

$$\alpha_i = 1/4r_i^2$$
$$\beta_i = \alpha_i/\sigma_{ui}^2$$

Treated like data:
- $y_1,\ldots,y_L$ (the primary measurements)
- $u_1,\ldots,u_N$ (estimates of nuisance par.)
- $v_1,\ldots,v_N$ (estimates of variances of estimates of NP)

Adjustable parameters:
- $\mu_1,\ldots,\mu_M$ (parameters of interest)
- $\theta_1,\ldots,\theta_N$ (nuisance parameters)
- $\sigma_{u,1},\ldots,\sigma_{u,N}$ (sys. errors = std. dev. of of NP estimates)

Fixed parameters:
- $r_1,\ldots,r_N$ (rel. err. in estimate of $\sigma_{u,i}$)

# Profiling over systematic errors

We can profile over the $\sigma_{u,i}$ in closed form

$$\widehat{\widehat{\sigma^2}}_{u_i} = \underset{\sigma^2_{u_i}}{\operatorname{argmax}}\, L(\boldsymbol{\mu}, \boldsymbol{\theta}, \boldsymbol{\sigma}^2_{\mathbf{u}}) = \frac{v_i + 2r_i^2(u_i - \theta_i)^2}{1 + 2r_i^2}$$

which gives the profile log-likelihood (up to additive const.)

$$\begin{aligned} \ln L'(\mu, \boldsymbol{\theta}) &= \ln L(\mu, \boldsymbol{\theta}, \widehat{\widehat{\boldsymbol{\sigma}^2}}_{\mathbf{u}}) \\ &= \ln P(\mathbf{y}|\boldsymbol{\mu}, \boldsymbol{\theta}) - \frac{1}{2}\sum_{i=1}^{N}\left(1 + \frac{1}{2r_i^2}\right)\ln\left[1 + 2r_i^2\frac{(u_i - \theta_i)^2}{v_i}\right] \end{aligned}$$

In limit of small $r_i$ and $v_i \to {\sigma_{u,i}}^2$, the log terms revert back to the quadratic form seen with known $\sigma_{u,i}$.

# Equivalent likelihood from Student's $t$

We can arrive at same likelihood by defining $z_i \equiv \dfrac{u_i - \theta_i}{\sqrt{v_i}}$

Since $u_i$ ~ Gauss and $v_i$ ~ Gamma, $z_i$ ~ Student's $t$

$$f(z_i|\nu_i) = \frac{\Gamma\left(\frac{\nu_i+1}{2}\right)}{\sqrt{\nu_i\pi}\Gamma(\nu_i/2)}\left(1+\frac{z_i^2}{\nu_i}\right)^{-\frac{\nu_i+1}{2}} \quad \text{with} \quad \nu_i = \frac{1}{2r_i^2}$$

Resulting likelihood same as profile $L'(\boldsymbol{\mu},\boldsymbol{\theta})$ from gamma model

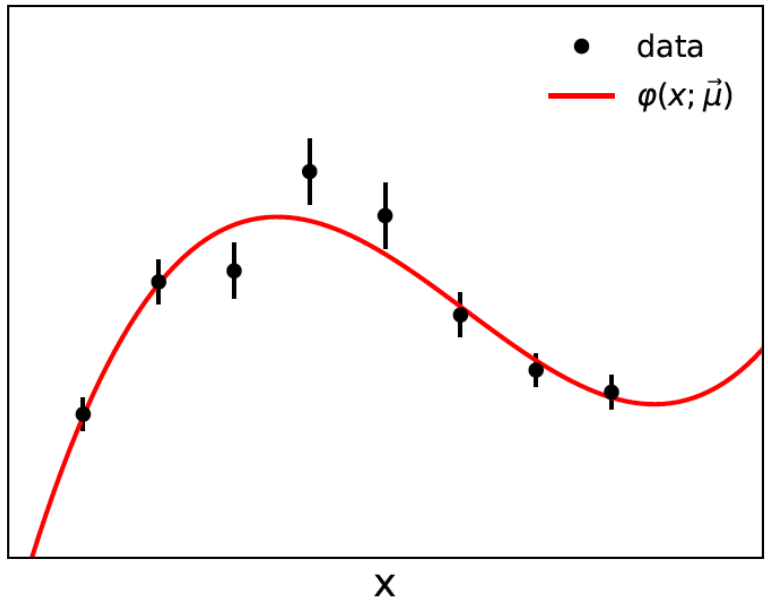
$$L(\boldsymbol{\mu},\boldsymbol{\theta}) = P(\mathbf{y}|\boldsymbol{\mu},\boldsymbol{\theta}) \prod_{i=1}^{N} \frac{\Gamma\left(\frac{\nu_i+1}{2}\right)}{\sqrt{\nu_i\pi}\Gamma(\nu_i/2)}\left(1+\frac{z_i^2}{\nu_i}\right)^{-\frac{\nu_i+1}{2}}$$

# Curve fitting, averages

Suppose independent
$y_i \sim$ Gauss, $i = 1,\ldots,N$, with

$$E[y_i] = \varphi(x_i;\boldsymbol{\mu}) + \theta_i \ ,$$

$$V[y_i] = \sigma^2_{y_i} \quad \text{(known)}.$$




$\boldsymbol{\mu}$ are the parameters of interest in the fit function $\varphi(x;\boldsymbol{\mu})$,

$\boldsymbol{\theta}$ are bias parameters constrained by control measurements
$u_i \sim$ Gauss($\theta_i$, $\sigma_{u,i}$), so that if $\sigma_{u,i}$ are known we have

$$-2\ln L(\boldsymbol{\mu},\boldsymbol{\theta}) = \sum_{i=1}^{N}\left[\frac{(y_i - \varphi(x_i;\boldsymbol{\mu}) - \theta_i)^2}{\sigma^2_{y_i}} + \frac{(u_i - \theta_i)^2}{\sigma^2_{u_i}}\right]$$

# Profiling over $\theta_i$ with known $\sigma_{u,i}$

Profiling over the bias parameters $\theta_i$ for known $\sigma_{u,i}$ gives usual least-squares (BLUE)

$$-2\ln L'(\boldsymbol{\mu}) = \sum_{i=1}^{N} \frac{(y_i - \varphi(x_i;\boldsymbol{\mu}) - u_i)^2}{\sigma_{y_i}^2 + \sigma_{u_i}^2} \equiv \chi^2(\boldsymbol{\mu})$$

Widely used technique for curve fitting in Particle Physics.

Generally in real measurement, $u_i = 0$.

Generalized to case of correlated $y_i$ and $u_i$ by summing statistical and systematic covariance matrices.

# Curve fitting with uncertain $\sigma_{u,i}$

Suppose now $\sigma_{u,i}{}^2$ are adjustable parameters with gamma distributed estimates $v_i$.

Retaining the $\theta_i$ but profiling over $\sigma_{u,i}{}^2$ gives

$$-2\ln L'(\boldsymbol{\mu},\boldsymbol{\theta}) = \sum_{i=1}^{N}\left[\frac{(y_i-\varphi(x_i;\boldsymbol{\mu})-\theta_i)^2}{\sigma_{y_i}^2} + \left(1+\frac{1}{2r_i^2}\right)\ln\left(1+2r_i^2\frac{(u_i-\theta_i)^2}{v_i}\right)\right]$$

Profiled values of $\theta_i$ from solution to cubic equations:

$$\theta_i^3 + [-2u_i - y_i + \varphi_i]\,\theta_i^2 + \left[\frac{v_i+(1+2r_i^2)\sigma_{y_i}^2}{2r_i^2} + 2u_i(y_i-\varphi_i) + u_i^2\right]\theta_i$$

$$+ \left[(\varphi_i - y_i)\left(\frac{v_i}{2r_i^2}+u_i^2\right) - \frac{(1+2r_i^2)\sigma_{y_i}^2 u_i}{2r_i^2}\right] = 0\,, \quad i = 1,\ldots,N\,,$$

# Goodness of fit

Can quantify goodness of fit with statistic

$$q = -2 \ln \frac{L'(\hat{\boldsymbol{\mu}}, \hat{\hat{\boldsymbol{\theta}}})}{L'(\hat{\boldsymbol{\varphi}}, \hat{\boldsymbol{\theta}})}$$

$$= \min_{\boldsymbol{\mu},\boldsymbol{\theta}} \sum_{i=1}^{N} \left[ \frac{(y_i - \varphi(x_i;\boldsymbol{\mu}) - \theta_i)^2}{\sigma_{y_i}^2} + \left(1 + \frac{1}{2r_i^2}\right) \ln \left(1 + 2r_i^2 \frac{(u_i - \theta_i)^2}{v_i}\right) \right]$$

where $L'(\boldsymbol{\varphi},\boldsymbol{\theta})$ has an adjustable $\varphi_i$ for each $y_i$ (the saturated model).

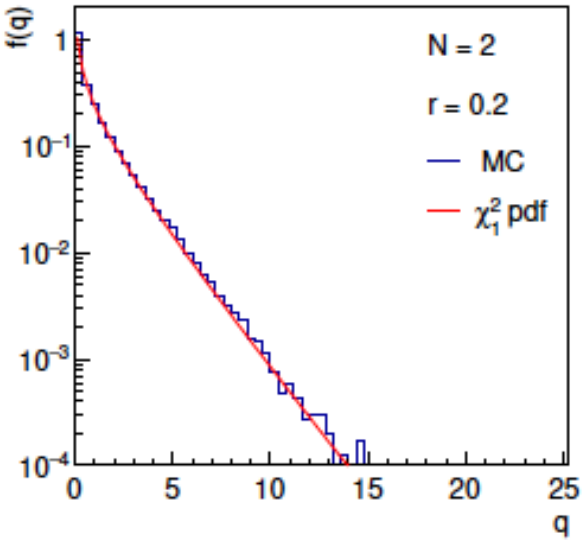
Asymptotically should have $q \sim$ chi-squared($N$–$M$).

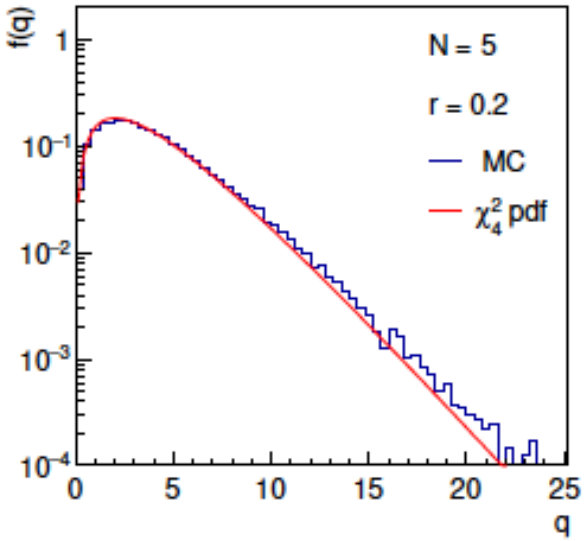
For increasing $r_i$, asymptotic distribution no longer valid.

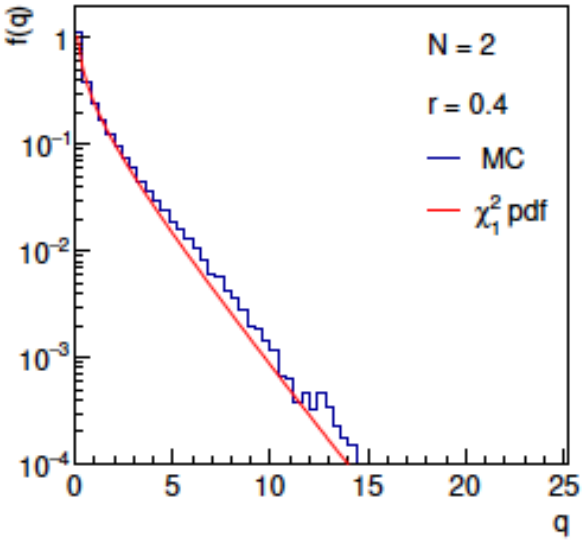
Bartlett (1937) defines modified statistic: $q' = \dfrac{n_\mathrm{d}}{E[q]} q$

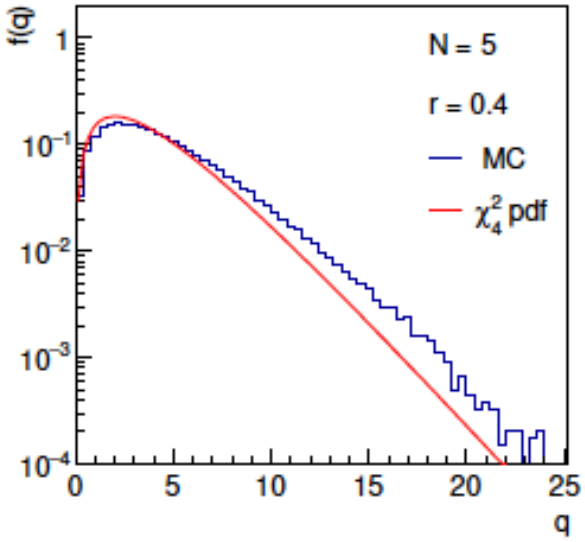
By construction $q'$ has mean $n_\mathrm{d} = N$-$M$ and turns out to have a distribution significantly closer to the asymptotic chi-square. (See Canonero et al., Eur. Phys. J. C (2023) 83:1100.)

# Distributions of $q$

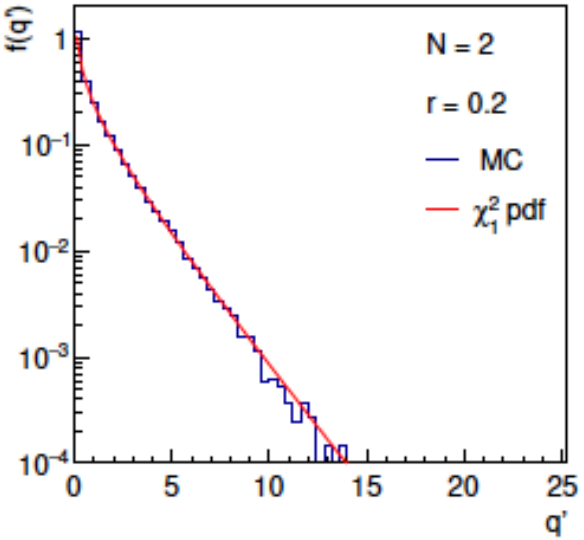


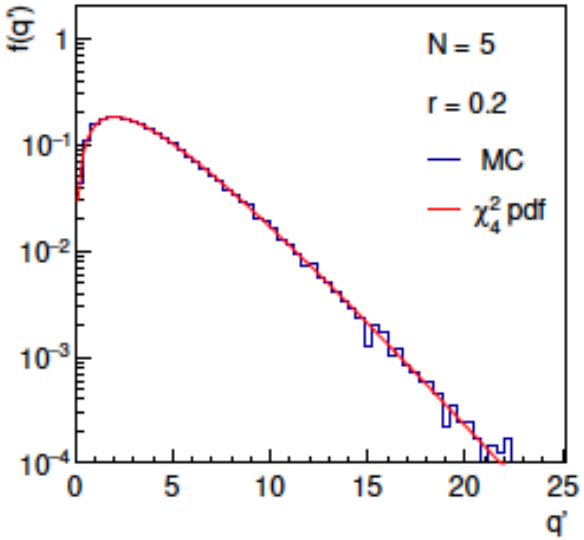



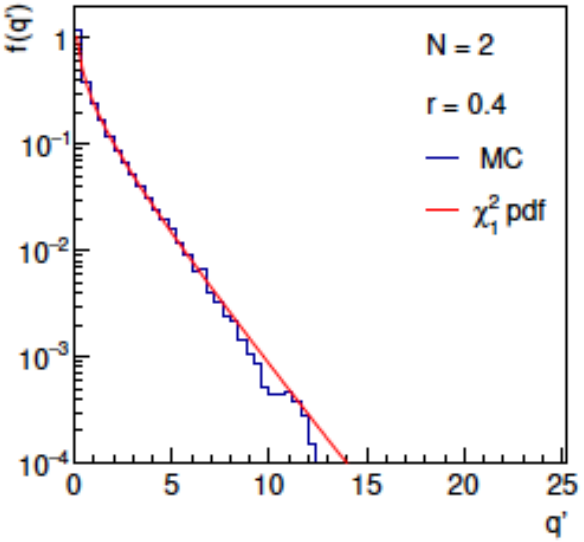



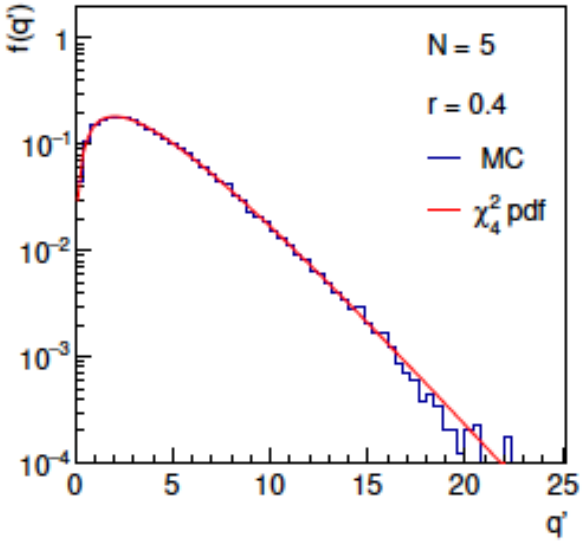



# Distributions of Bartlett-corrected $q'$



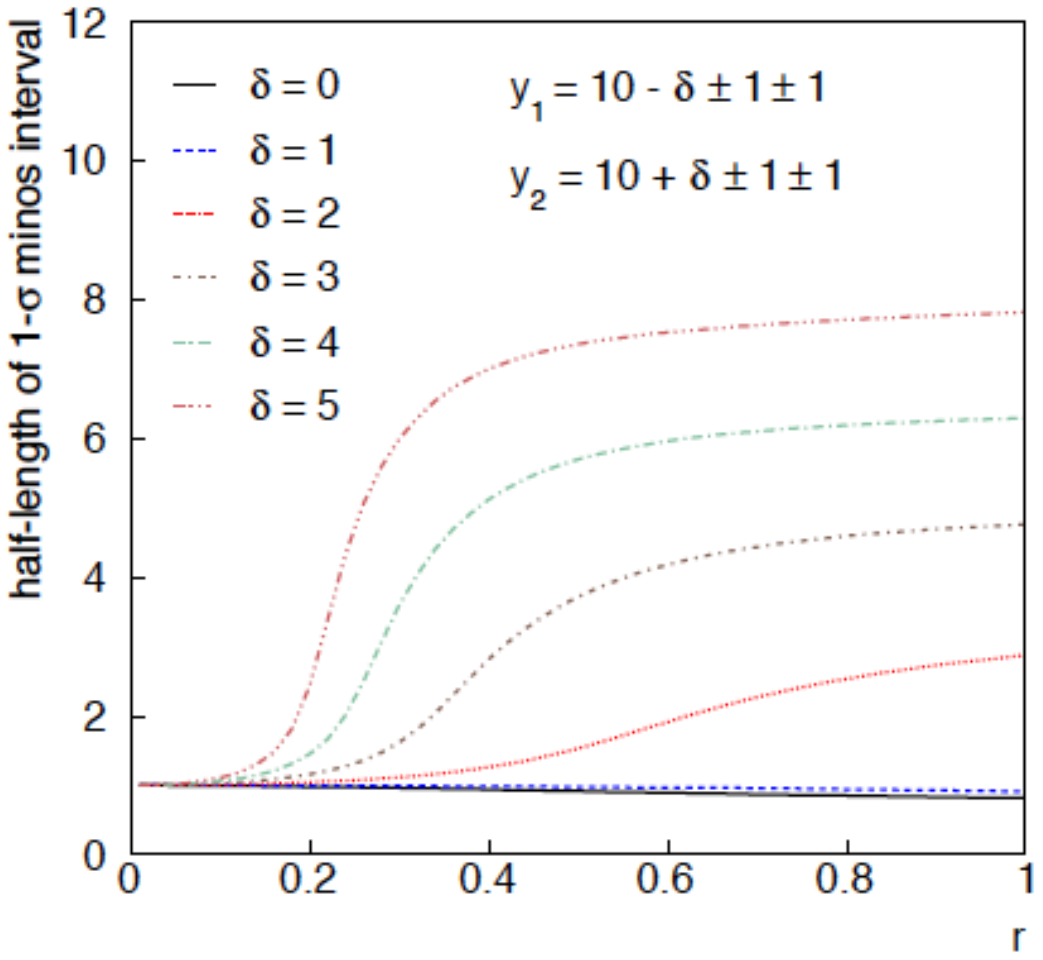



# Example: average of two measurements

Approximate ("MINOS") confidence interval based on

$$\ln L'(\mu) = \ln L'(\hat{\mu}) - Q_\alpha/2 \quad \text{with} \quad Q_\alpha = F^{-1}_{\chi^2}(1-\alpha; n)$$



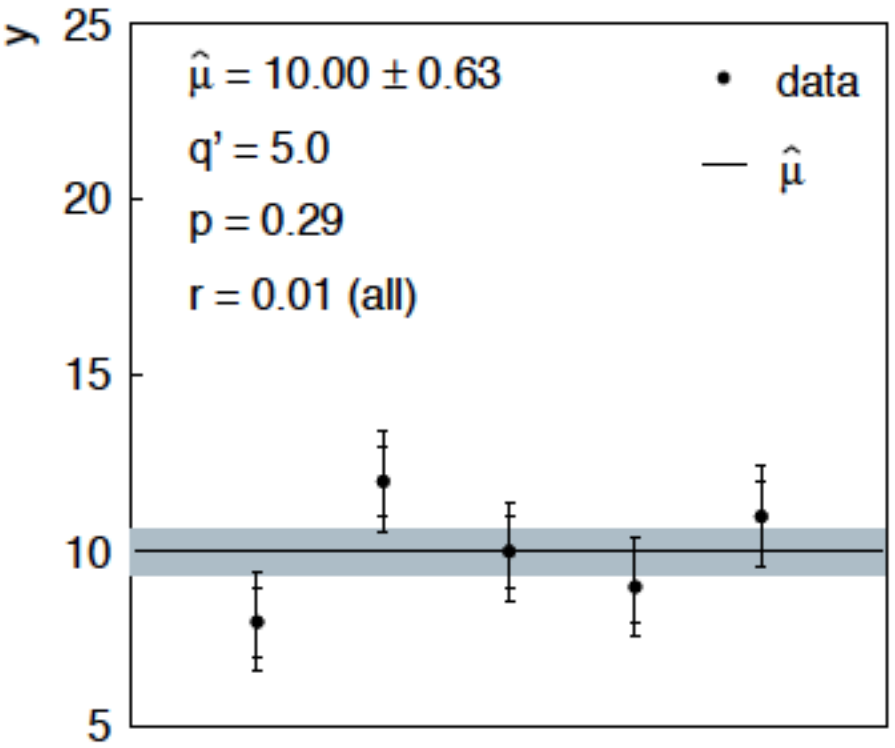

Increased discrepancy between values to be averaged gives larger interval.

Interval length saturates at ~level of absolute discrepancy between input values.

relative error on sys. error

# Sensitivity of average to outliers

Suppose we average 5 values, $y = 8, 9, 10, 11, 12$, all with stat. and sys. errors of 1.0, and suppose negligible error on error (here take $r = 0.01$ for all).

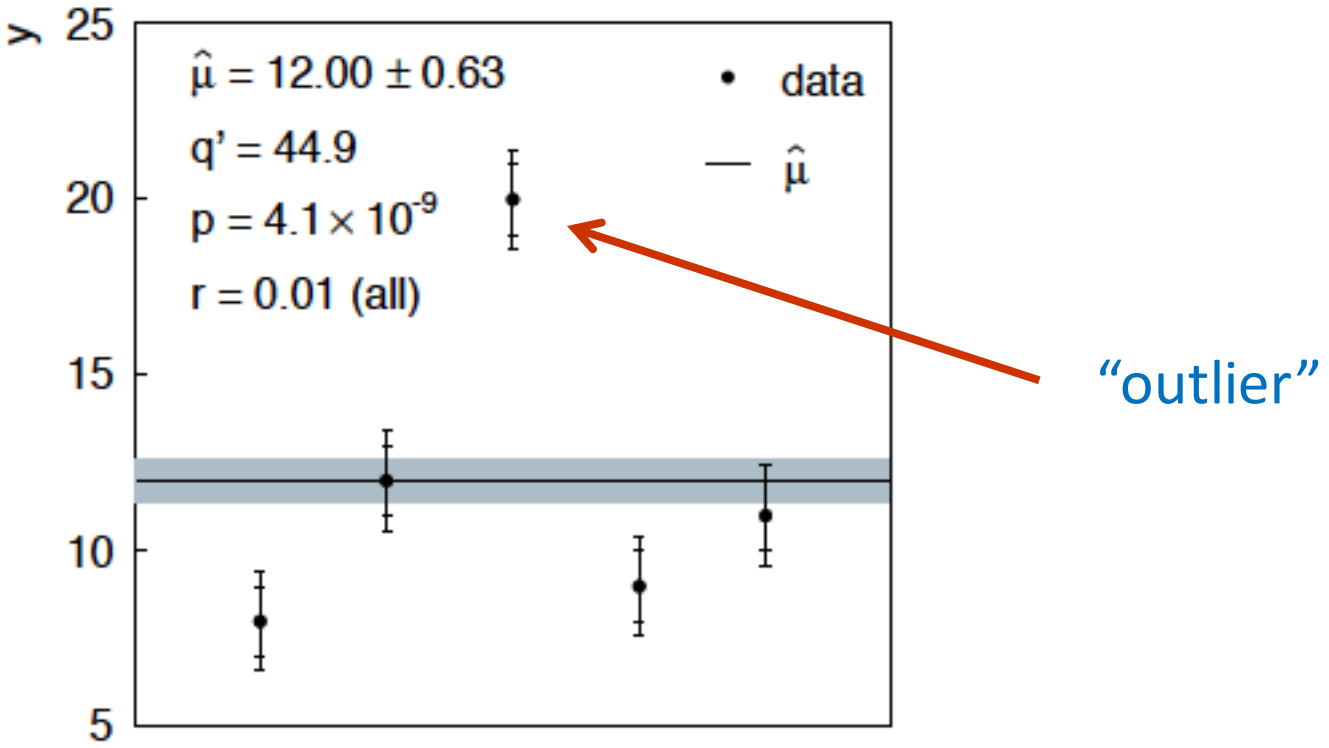



inner error bars
$= \sigma_{y,i}$

outer error bars
$= (\sigma_{y,i}^2 + \sigma_{u,i}^2)^{1/2}$

# Sensitivity of average to outliers (2)

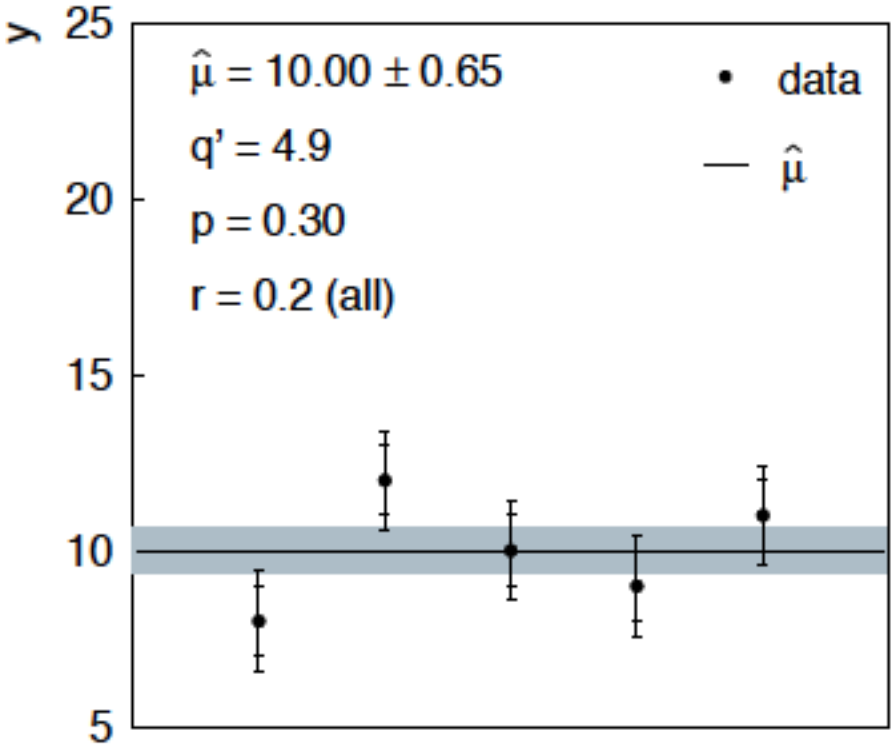
Now suppose the measurement at 10 had come out at 20:




Estimate pulled up to 12.0, size of confidence interval ~unchanged (would be exactly unchanged with $r \to 0$).

# Average with all $r = 0.2$

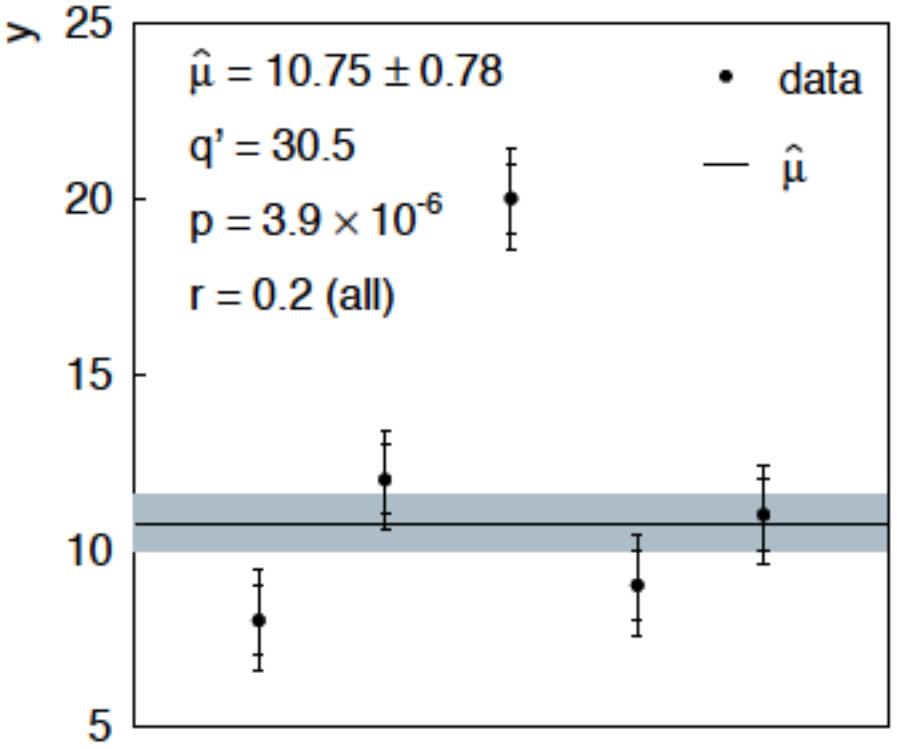
If we assign to each measurement $r = 0.2$,




Estimate still at 10.00, size of interval moves 0.63 → 0.65

# Average with all $r = 0.2$ with outlier

Same now with the outlier (middle measurement $10 \to 20$)




Estimate $\to 10.75$ (outlier pulls much less).

Half-size of interval $\to 0.78$ (inflated because of bad g.o.f.).

# Naive approach to errors on errors

Naively one might think that the error on the error in the previous example could be taken into account conservatively by inflating the systematic errors, i.e.,

$$\sigma_{u_i} \to \sigma_{u_i}(1 + r_i)$$

But this gives

$\hat{\mu} = 10.00 \pm 0.70$ without outlier (middle meas. 10)

$\hat{\mu} = 12.00 \pm 0.70$ with outlier (middle meas. 20)

So the sensitivity to the outlier is not reduced and the size of the confidence interval is still independent of goodness of fit.

# Discussion / Conclusions

Gamma model for variance estimates gives confidence intervals that increase in size when the data are internally inconsistent, and gives decreased sensitivity to outliers (known property of Student's $t$ based regression).

Equivalence with Student's $t$ model, $\nu = 1/2r^2$ degrees of freedom.

Simple profile likelihood – quadratic terms replaced by logarithmic:

$$\frac{(u_i - \theta_i)^2}{\sigma_{u_i}^2} \quad \rightarrow \quad \left(1 + \frac{1}{2r_i^2}\right) \ln\left[1 + 2r_i^2 \frac{(u_i - \theta_i)^2}{v_i}\right]$$

# Discussion / Conclusions (2)

Asymptotics can break for increased error-on-error, may need Bartlett correction, higher-order asymptotics or MC.

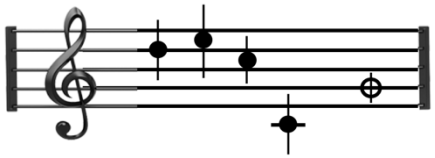
Method assumes that meaningful $r_i$ values can be assigned and is valuable when systematic errors are not well known but enough "expert knowledge" is available to do so.

Alternatively, one could try to fit a global $r$ to all systematic errors, analogous to PDG scale factor method or meta-analysis à la DerSimonian and Laird. ($\longrightarrow$ current work).

Could also use e.g. as "stress test" – crank up the $r_i$ values until significance of result degrades and ask if you really trust the assigned systematic errors at that level.

Ongoing studies (with E. Canonero): application to averages of top mass, W mass; general software framework.

# Tutorial: Student's *t* average



Software:
https://www.pp.rhul.ac.uk/~cowan/stat/exercises/stave/stave.py

The program stave.py implements the Gamma Variance Model (GVM) described in Lecture 3 for averaging $N$ measurements.

For details see G. Cowan, EPJC (2019) 79:133.

In this version the model does not distinguish between statistical and systematic errors.

Confidence interval for the mean $\mu$ becomes sensitive to goodness-of-fit (increases if data internally inconsistent).

Estimated mean less sensitive to outliers.

# Least Squares vs Gamma Variance Model

Quadratic terms from Least Squares replaced by logarithmic ones:

$$\frac{(y_i - \mu)^2}{\sigma_i^2} \quad \rightarrow \quad \left(1 + \frac{1}{2r_i^2}\right) \ln\left[1 + 2r_i^2 \frac{(y_i - \mu)^2}{v_i}\right]$$

where

$y_i$ = measured value

$v_i = s_i^2$ = estimated variance

$r_i$ = relative uncertainty on estimate of variance

Equivalent to replacing Gauss pdf for measurements by Student's $t$, number of degrees of freedom $= 1/2r_i^2$

# A quick look at stave.py

## Set measured values, estimates of std. dev., errors on errors:

```
y = np.array([17., 19., 15., 3.])       # measured values
s = np.array([1.5, 1.5, 1.5, 1.5])      # estimates of std. dev
v = s**2                                # estimates of variances
r = np.array([0.2, 0.2, 0.2, 0.2])      # relative errors on errors
```

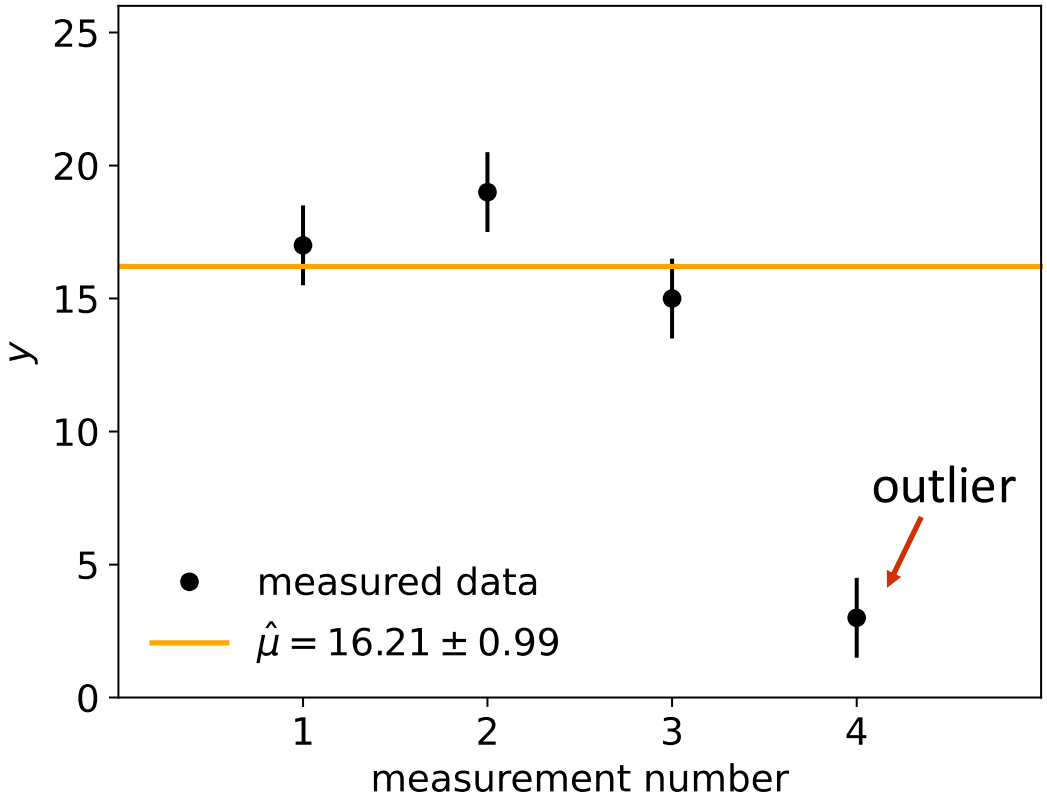
## log-likelihood:

```
class NegLogL:

    def __init__(self, y, s, r):
        self.setData(y, s, r)

    def setData(self, y, s, r):
        self.data = y, s, r

    def __call__(self, mu):
        y, s, r = self.data
        v = s ** 2
        lnf = -0.5*(1. + 1./(2.*r**2))*np.log(1. + 2.*(r*(y-mu))**2/v)
        return -np.sum(lnf)
```

# Example average with GVM

Suppose four measurements of the parameter $\mu$.

Each reports an estimated standard dev. of $s = 1.5$ and a "relative error on the error" $r = 0.2$.




Suggested exercise:

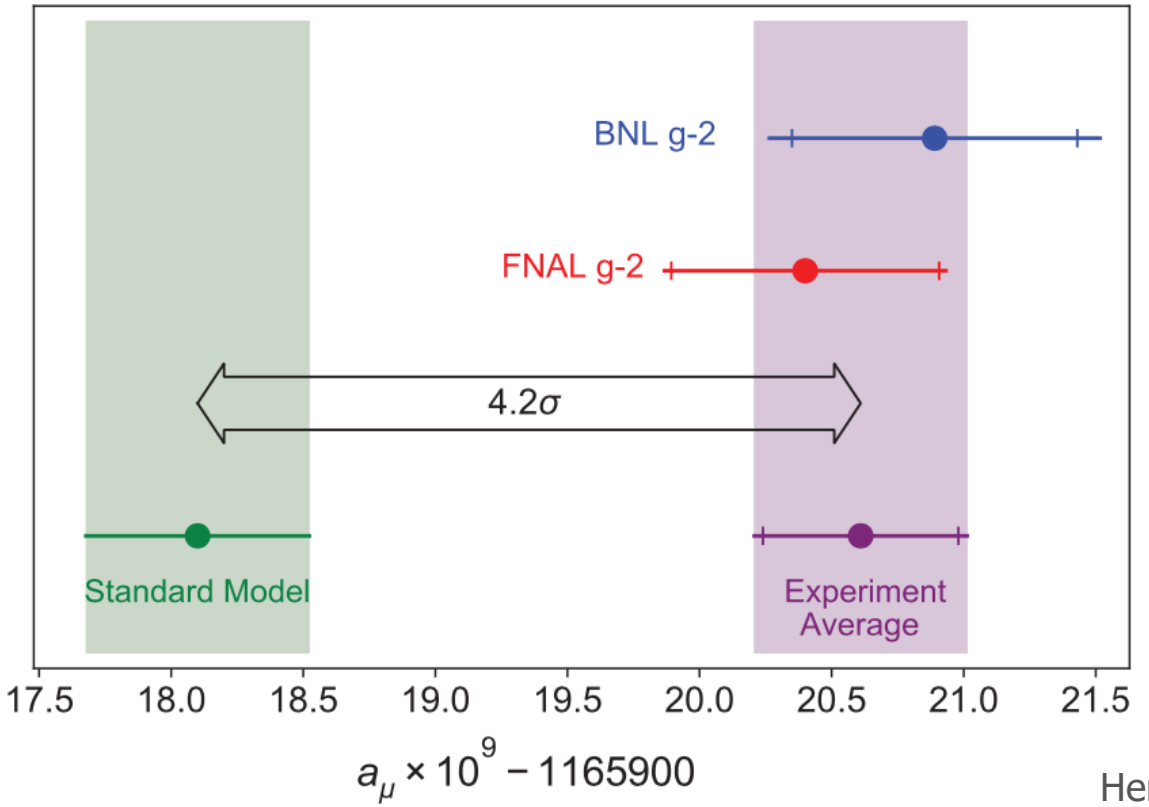
Experiment with different numbers of measurements, different levels of internal consistency, different values for the std. dev. and error on error.

# Extra Slides

# Application to the muon $g-2$ anomaly

The recently measured muon $g-2$ (ave. of 2006, 2021) disagrees with the Standard Model prediction with a significance of 4.2σ.

Muon g-2 Collab., PRL 126, 141801 (2021)




Discrepancy significantly reduced by 2021 lattice-based prediction of Borsanyi et al. (BMW).

Current goal is to investigate sensitivity of significance to error assumptions, so for now focus on the 4.2σ problem.

Here using 2021 meausrement; see also D. P. Aguillard *et al.* (The Muon g−2 Collaboration) Phys. Rev. Lett. **131**, 161802 (2023)

# Muon $g-2$ ingredients

Using $a_\mu = (g-2)/2$ $\qquad y = a_\mu \times 10^9 - 1165900$

the ingredients of the 4.2σ effect are:

$$y_{\text{exp}} = 20.61 \pm 0.41$$

(ave. of BNL 2006 and FNAL 2021)

0.37 (stat.) ± 0.17 (sys.)

B. Abi et al. (Muon $g-2$ Collaboration), *Measurement of the Positive Muon Anomalous Magnetic Moment to 0.46 ppm*, Phys. Rev. Lett. 126, 141801 (2021).

G. W. Bennett et al. (Muon $g-2$ Collaboration), *Final report of the E821 muon anomalous magnetic moment measurement at BNL*, Phys. Rev. D 73, 072003 (2006).

$$y_{\text{SM}} = 18.10 \pm 0.43$$

(SM pred. by Muon $g-2$ theory initiative)

0.40 (Had. Vac. Pol.) ± 0.18 (Had. Light-by-Light)

T. Aoyama, N. Asmussen, M. Benayoun, J. Bijnens, and T. Blum et al., *The anomalous magnetic moment of the muon in the standard model*, Phys. Rep. 887, 1 (2020).

# Suppose $\sigma_{\rm SM}$ uncertain

Suppose measurement errors well known, but that the SM theory error $\sigma_{\rm SM}$ (estimated 0.43) could be uncertain.

This is the largest systematic and probably hardest to estimate.

Treat estimate $v_{\rm SM} = (0.43)^2$ of variance $\sigma^2_{\rm SM}$ as gamma distributed, width from relative uncertainty parameter $r_{\rm SM}$.

Maximum-likelihood for mean from minimum of

$$Q(\mu) = -2 \ln \frac{L(\mu)}{L_{\rm sat}}$$

$$= \frac{(y_{\rm exp} - \mu)^2}{\sigma^2_{\rm exp}} + \left(1 + \frac{1}{2r^2_{\rm SM}}\right) \ln \left[1 + 2r^2_{\rm SM} \frac{(y_{\rm SM} - \mu)^2}{v_{\rm SM}}\right]$$

# $p$-value/significance of common-mean hypothesis

Significance (goodness of fit) from $q = Q(\hat{\mu})$.

Because of non-quadratic term in $Q(\mu)$, distribution of $q$ departs from chi-square(1) for increasing $r_{\rm SM}$.

Best to get distribution of $q$ from Monte Carlo (and speed up with Bartlett correction – see EPJC (2019) 79:133).

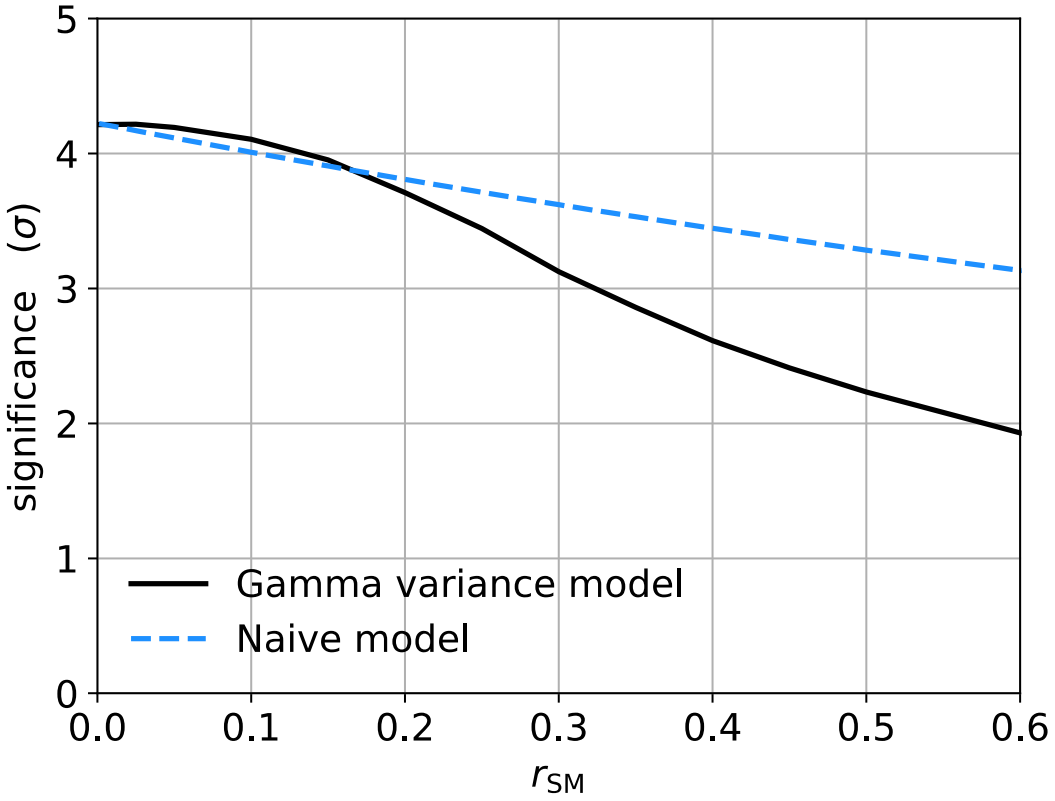
For $r_{\rm SM} > 0$ distribution of $q$ depends on $\sigma^2_{\rm SM}$. For MC use Maximum-Likelihood estimate ("profile construction"):

$$\widehat{\sigma^2}_{\rm SM} = \frac{v_{\rm SM} + 2r_{\rm SM}^2(y_{\rm SM} - \hat{\mu})^2}{1 + 2r_{\rm SM}^2}$$

$$\text{MC} \;\rightarrow\; f(q) \;\rightarrow\; p = \int_{q,\text{obs}}^{\infty} f(q)\,dq \;\rightarrow\; \text{significance } Z = \Phi^{-1}(1 - p/2)$$

# of sigmas

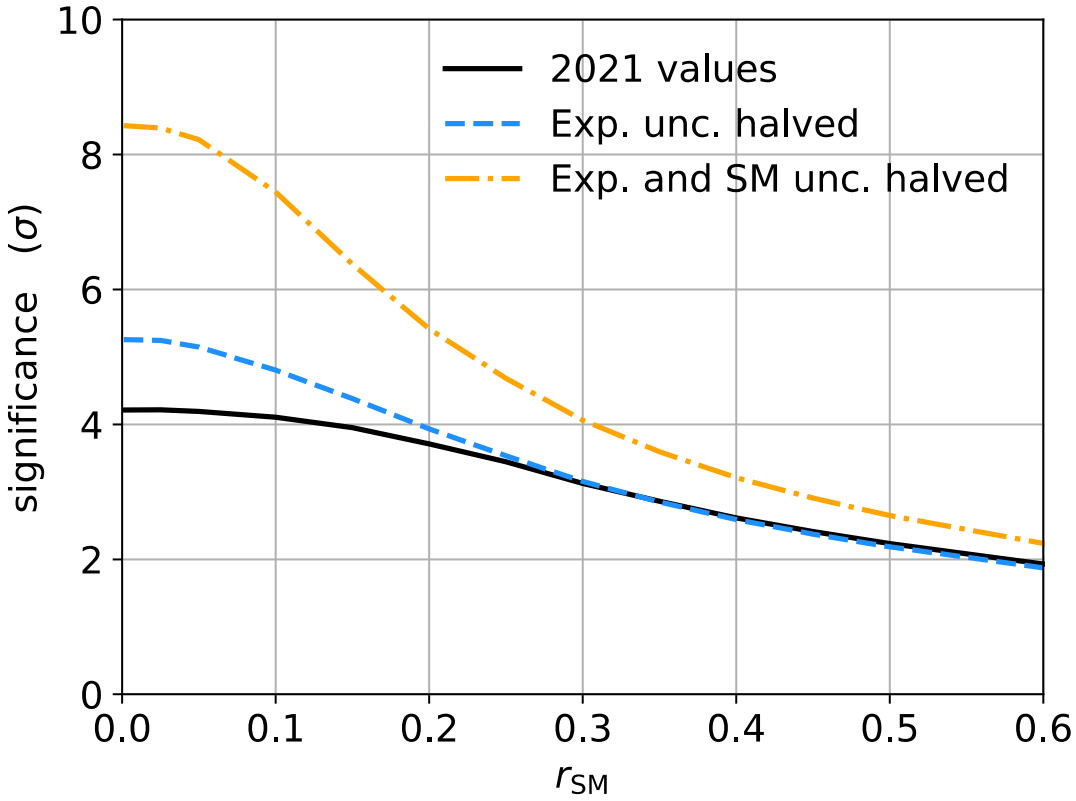
# Significance of discrepancy versus $r_{\mathrm{SM}}$




Naive model: use least squares but let $\sigma_{\mathrm{SM}} \to (1 + r_{\mathrm{SM}})\sigma_{\mathrm{SM}}$

Gamma variance model gives greater decrease in significance for $r_{\mathrm{SM}} \gtrsim 0.2$, e.g., $3.1\sigma$ for $r_{\mathrm{SM}} = 0.3$, $2.0\sigma$ for $r_{\mathrm{SM}} = 0.6$.

# Significance of discrepancy versus $r_{\mathrm{SM}}$




Establishing $4\sigma$ effect requires $r_{\mathrm{SM}} \lesssim 0.3$ even if nominal exp. and SM uncertainties become half of present values.

# Discussion on muon $g-2$

Including uncertainties on estimates of uncertainties can have large effect on hypothesis test, esp. for high significance.

To establish e.g. a $5\sigma$ effect it is crucial to have both:

small uncertainties

accurate estimates of those uncertainties (~ 20% level)

This is ultimately because the tails of the Gaussian fall off so quickly.

Gamma Variance Model ~ Student's $t$ likelihood with $\nu = 1/2r^2$ degrees of freedom $\longrightarrow$ longer tails than Gaussian.

Ongoing discussion with Bogdan Malaescu of Muon g-2 Theory Initiative on the HVP uncertainty, see, e.g.,

B. Malaescu et al., https://indico.him.uni-mainz.de/event/11/contributions/80/attachments/50/51/amuWorkshop_Correlations_Malaescu.pdf

M. Davier et al., Eur. Phys. J. C 80 (2020) 241 , arXiv:1908.00921

# Developments of LS for Averaging

Much work in HEP and elsewhere on application/extension of least squares to the problem of averaging or meta-analysis, e.g.,

A. C. Aitken, *On Least Squares and Linear Combinations of Observations*, Proc. Roy. Soc. Edinburgh **55** (1935) 42.

L. Lyons, D. Gibaut and P. Clifford, *How to Combine Correlated Estimates of a Single Physical Quantity*, Nucl. Instr. Meth. **A270** (1988) 110.

A. Valassi, *Combining Correlated Measurements of Several Different Physical Quantities*, Nucl. Instr. Meth. **A500** (2003) 391.

R. Nisius, *On the combination of correlated estimates of a physics observable*, Eur. Phys. J. C **74** (2014) 3004.

R. DerSimonian and N. Laird, *Meta-analysis in clinical trials*, Controlled Clinical Trials **7** (1986) 177-188.

# Errors on theory errors, e.g., in QCD

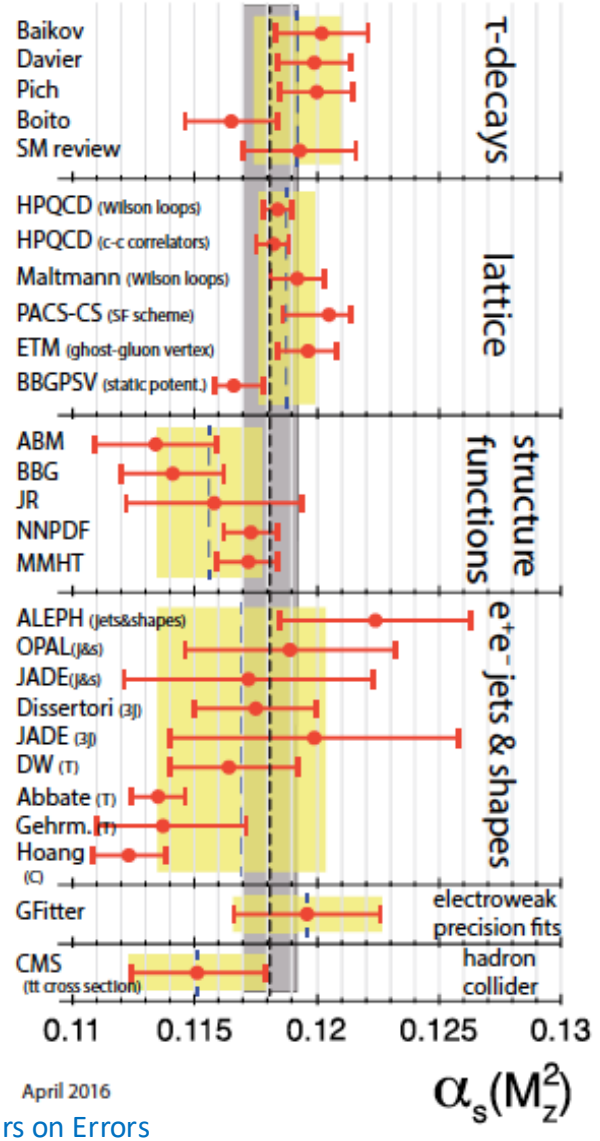
Uncertainties related to theoretical predictions are notoriously difficult to quantify, e.g., in QCD may come from variation of renormalization scale in some "appropriate range".

Problematic e.g. for $\alpha_s$ $\longrightarrow$

If, e.g., some (theory) errors are underestimated, one may obtain poor goodness of fit, but size of confidence interval from usual recipe will not reflect this.

An outlier with an underestimated error bar can have an inordinately strong influence on the average.

M. Tanabashi et al. (Particle Data Group), Phys. Rev. D 98, 030001 (2018)



# Correlated uncertainties

The phrase "correlated uncertainties" usually means that a single nuisance parameter affects the distribution (e.g., the mean) of more than one measurement.

For example, consider measurements $\boldsymbol{y}$, parameters of interest $\boldsymbol{\mu}$, nuisance parameters $\boldsymbol{\theta}$ with

$$E[y_i] = \varphi_i(\boldsymbol{\mu}, \boldsymbol{\theta}) \approx \varphi_i(\boldsymbol{\mu}) + \sum_{j=1}^{N} R_{ij}\theta_j$$

That is, the $\theta_i$ are defined here as contributing to a bias and the (known) factors $R_{ij}$ determine how much $\theta_j$ affects $y_i$.

As before suppose one has independent control measurements $u_i \sim$ Gauss($\theta_i$, $\sigma_{ui}$).

# Correlated uncertainties (2)

The total bias of $y_i$ can be defined as $$b_i = \sum_{j=1}^{N} R_{ij}\theta_j$$

which can be estimated with $$\hat{b}_i = \sum_{j=1}^{N} R_{ij}u_j$$

These estimators are correlated having covariance

$$U_{ij} = \mathrm{cov}[\hat{b}_i, \hat{b}_j] = \sum_{k=1}^{N} R_{ik}R_{jk}V[u_k]$$

In this sense the present method treats "correlated uncertainties", i.e., the control measurements $u_i$ are independent, but nuisance parameters affect multiple measurements, and thus bias estimates are correlated.

# Single-measurement model

As a simplest example consider

$y \sim \text{Gauss}(\mu, \sigma^2)$,

$v \sim \text{Gamma}(\alpha, \beta)$, $\qquad \alpha = \frac{1}{4r^2}, \qquad \beta = \frac{1}{4r^2\sigma^2}$

$$L(\mu, \sigma^2) = f(y, v|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(y-\mu)^2/2\sigma^2} \frac{\beta^\alpha}{\Gamma(\alpha)} v^{\alpha-1} e^{-\beta v}$$

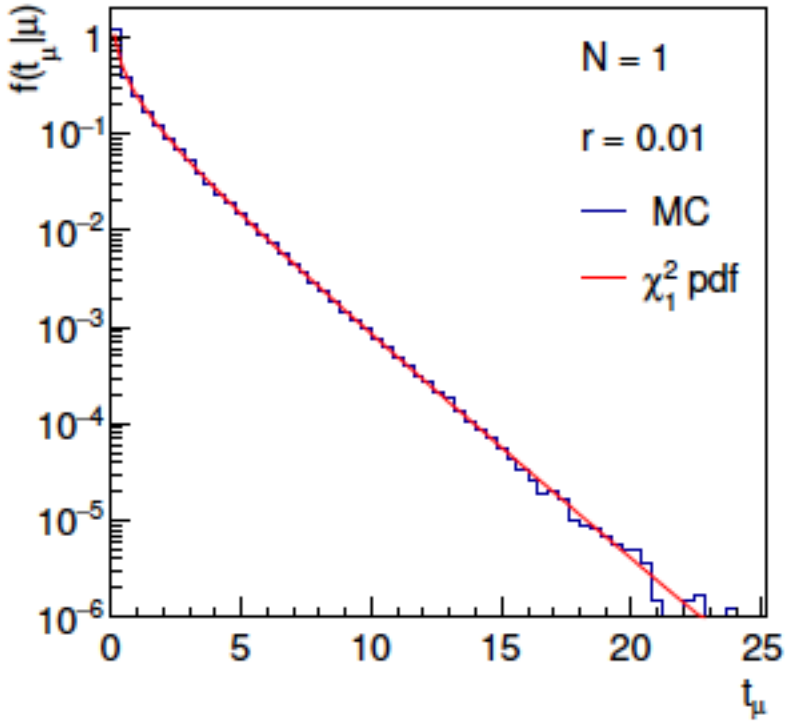
Test values of $\mu$ with $t_\mu = -2 \ln \lambda(\mu)$ with $\quad \lambda(\mu) = \dfrac{L(\mu, \widehat{\widehat{\sigma^2}}(\mu))}{L(\hat{\mu}, \widehat{\sigma^2})}$

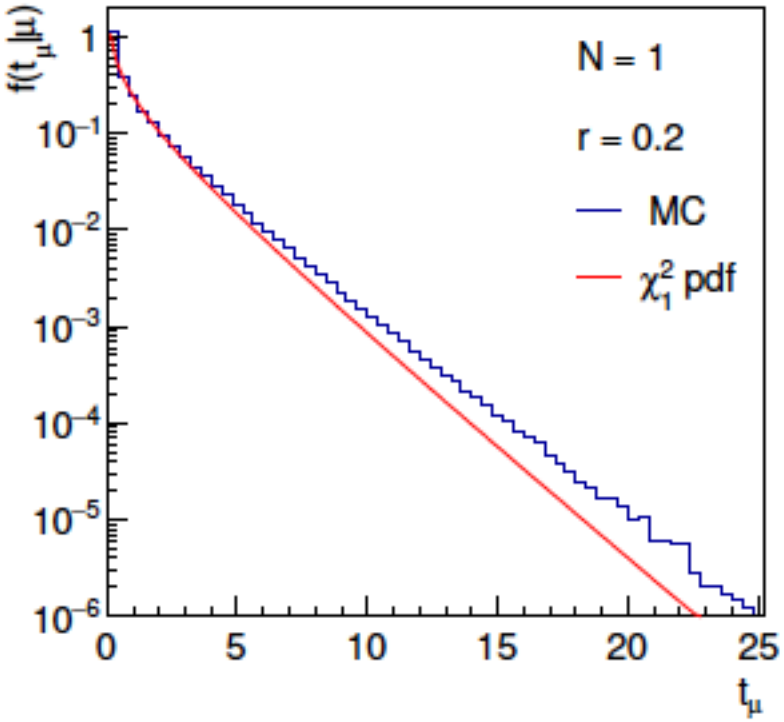
$$t_\mu = \left(1 + \frac{1}{2r^2}\right) \ln \left[1 + 2r^2 \frac{(y-\mu)^2}{v}\right]$$

# Distribution of $t_\mu$

From Wilks' theorem, in the asymptotic limit we should find $t_\mu$ ~ chi-squared(1).

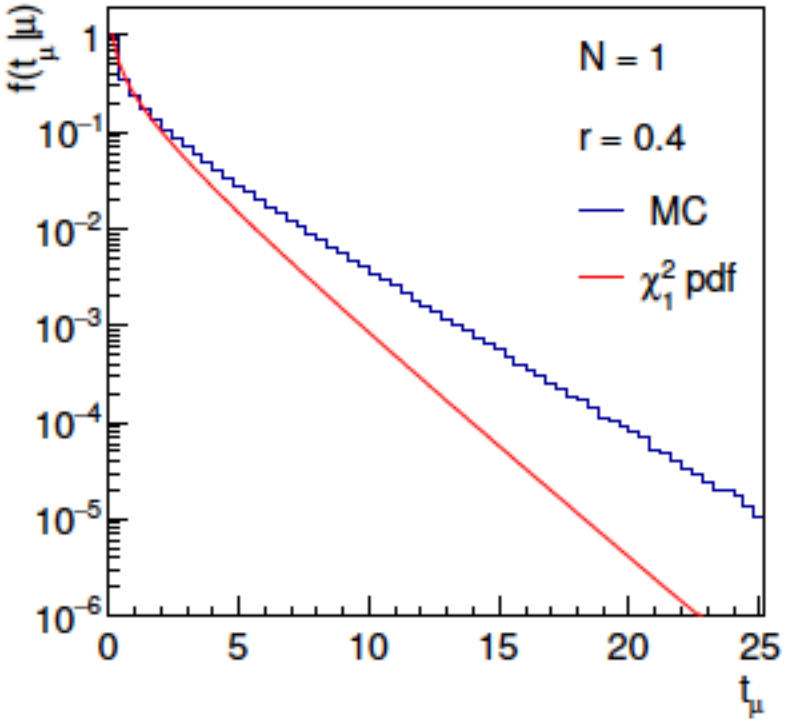
Here "asymptotic limit" means all estimators ~Gauss, which means $r \to 0$. For increasing $r$, clear deviations visible:

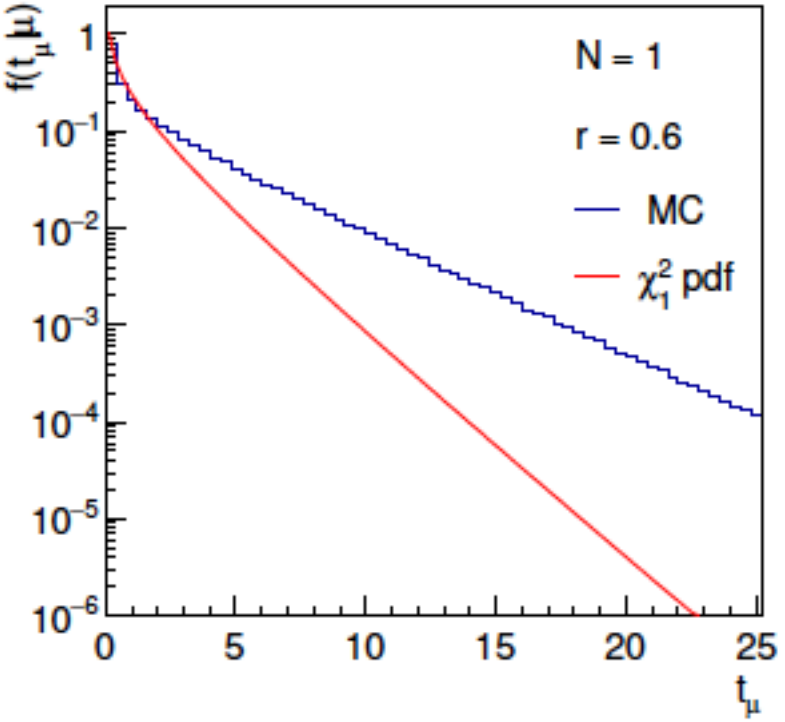


# Distribution of $t_\mu$ (2)

For larger $r$, breakdown of asymptotics gets worse:



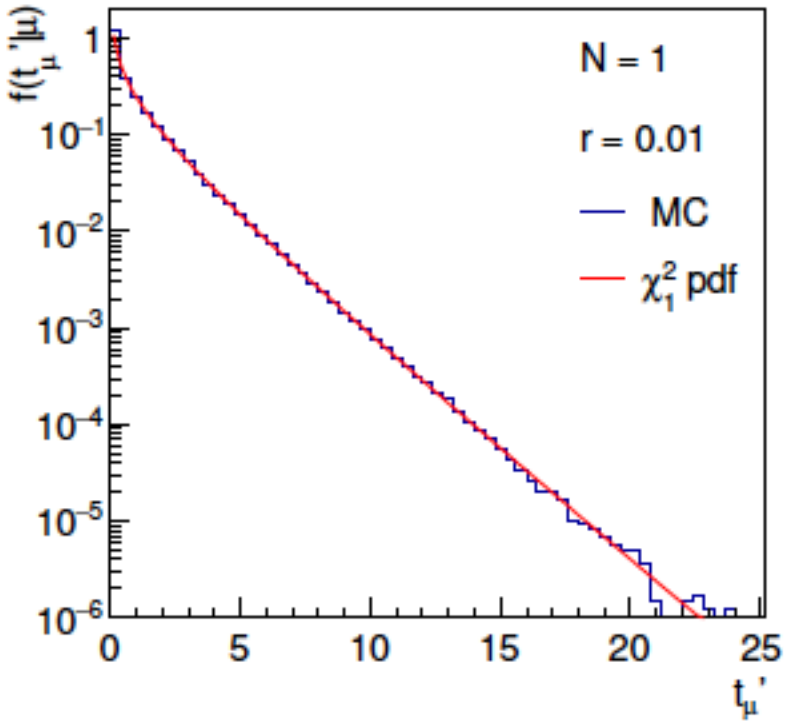

Values of $r \sim$ several tenths are relevant so we cannot in general rely on asymptotics to get confidence intervals, $p$-values, etc.

# Bartlett corrections

One can modify $t_\mu$ defining $$t'_\mu = \frac{n_\mathrm{d}}{E[t_\mu]} t_\mu$$

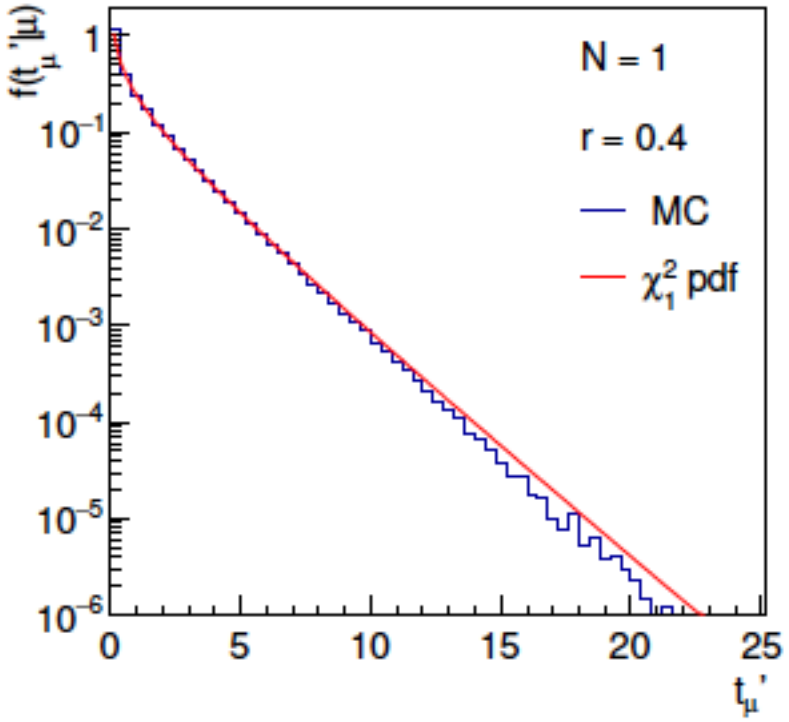
such that the new statistic's distribution is better approximated by chi-squared for $n_d$ degrees of freedom (Bartlett, 1937).

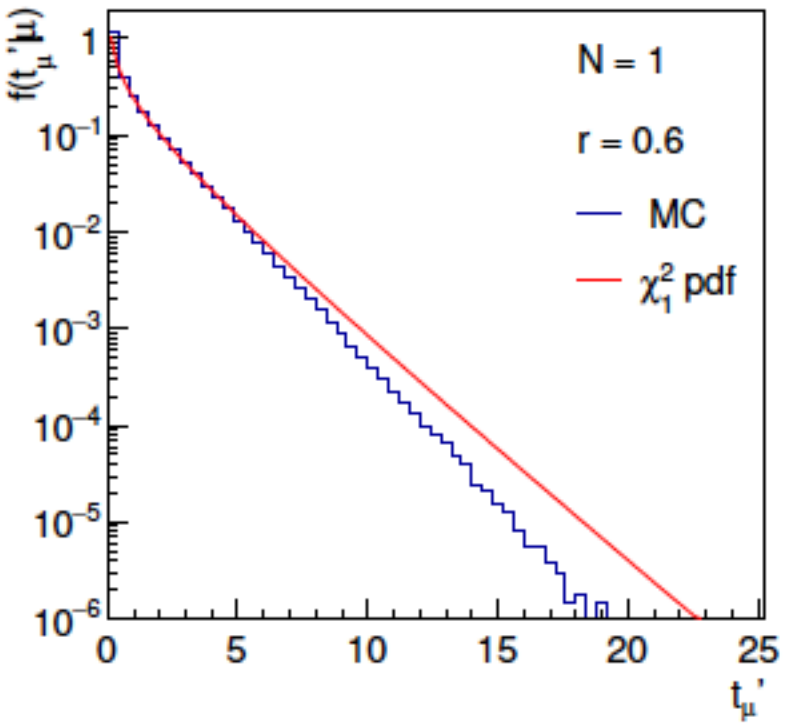
For this example $E[t_\mu] \approx 1 + 3r^2 + 2r^4$ works well:



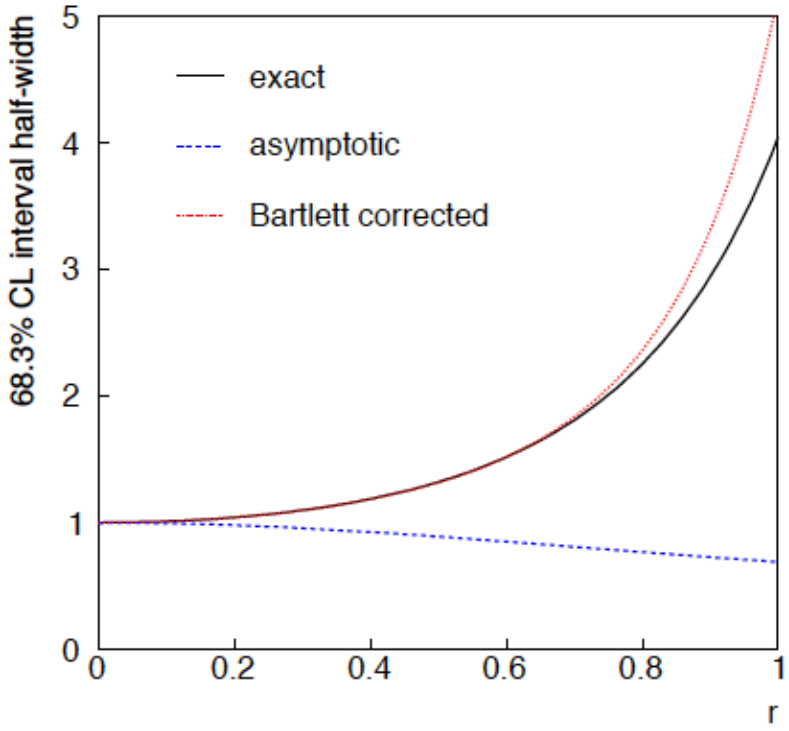
# Bartlett corrections (2)

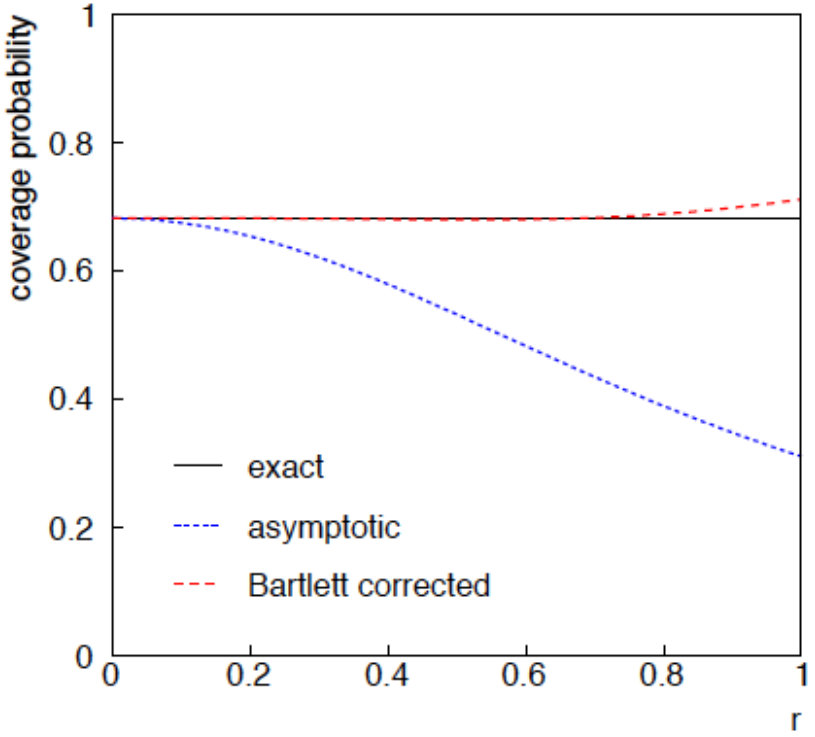
Good agreement for $r$ ~ several tenths out to $\sqrt{t_\mu'}$ ~ several, i.e., good for significances of several sigma:



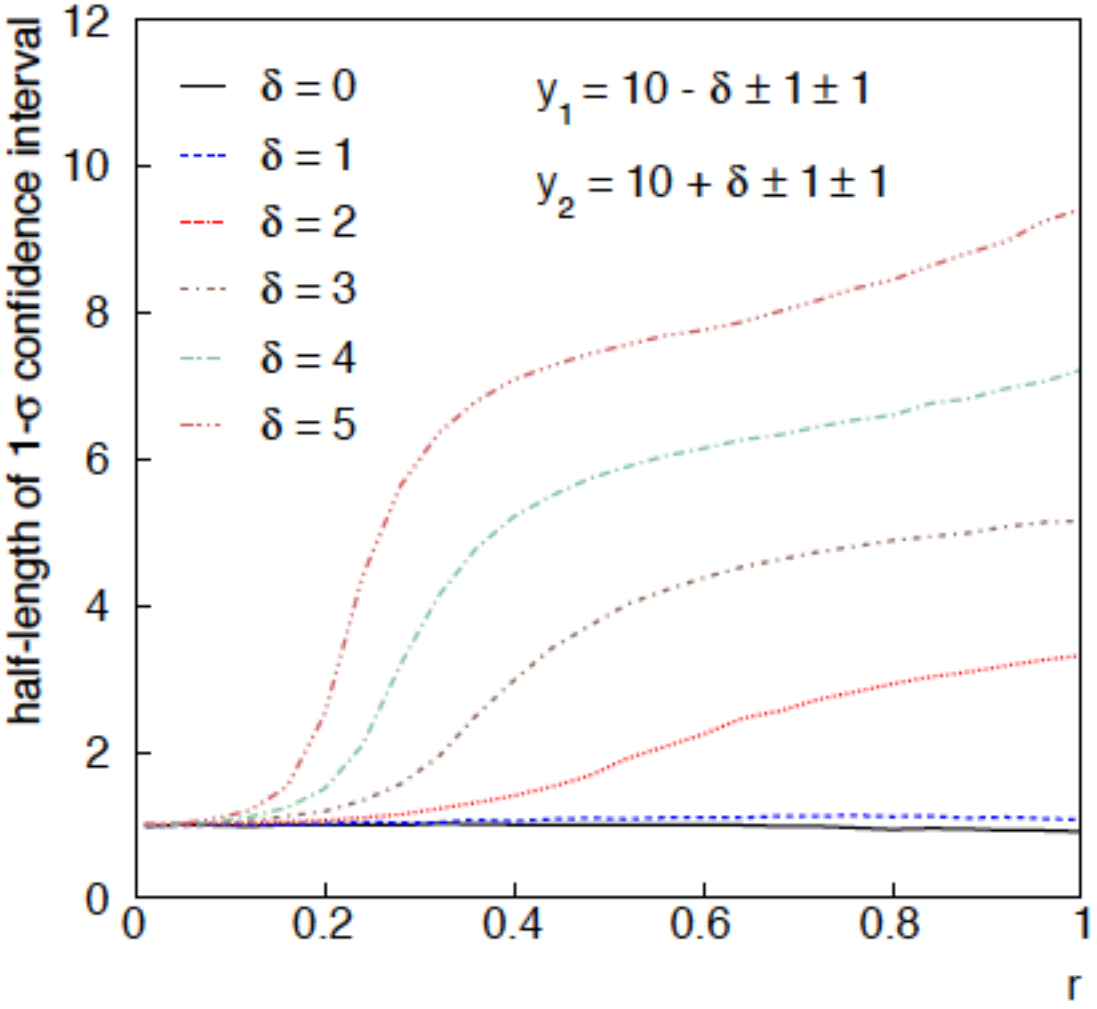



# 68.3% CL confidence interval for $\mu$



# Same with interval from $p_\mu = \alpha$ with nuisance parameters profiled at $\mu$



# Coverage of intervals

Consider previous average of two numbers but now generate for $i = 1, 2$ data values

$$y_i \sim \text{Gauss}(\mu, \sigma_{y,i})$$

$$u_i \sim \text{Gauss}(0, \sigma_{u,i})$$

$$v_i \sim \text{Gamma}(\sigma_{u,i}, r_i)$$

$$\sigma_{y,i} = \sigma_{u,i} = 1$$

and look at the probability that the interval covers the true value of $\mu$.

Coverage stays reasonable to $r \sim 0.5$, even not bad for Profile Construction out to $r \sim 1$.