Statistical Methods in Particle Physics

3. Experimental uncertainties

Heidelberg University, WS 2020/21

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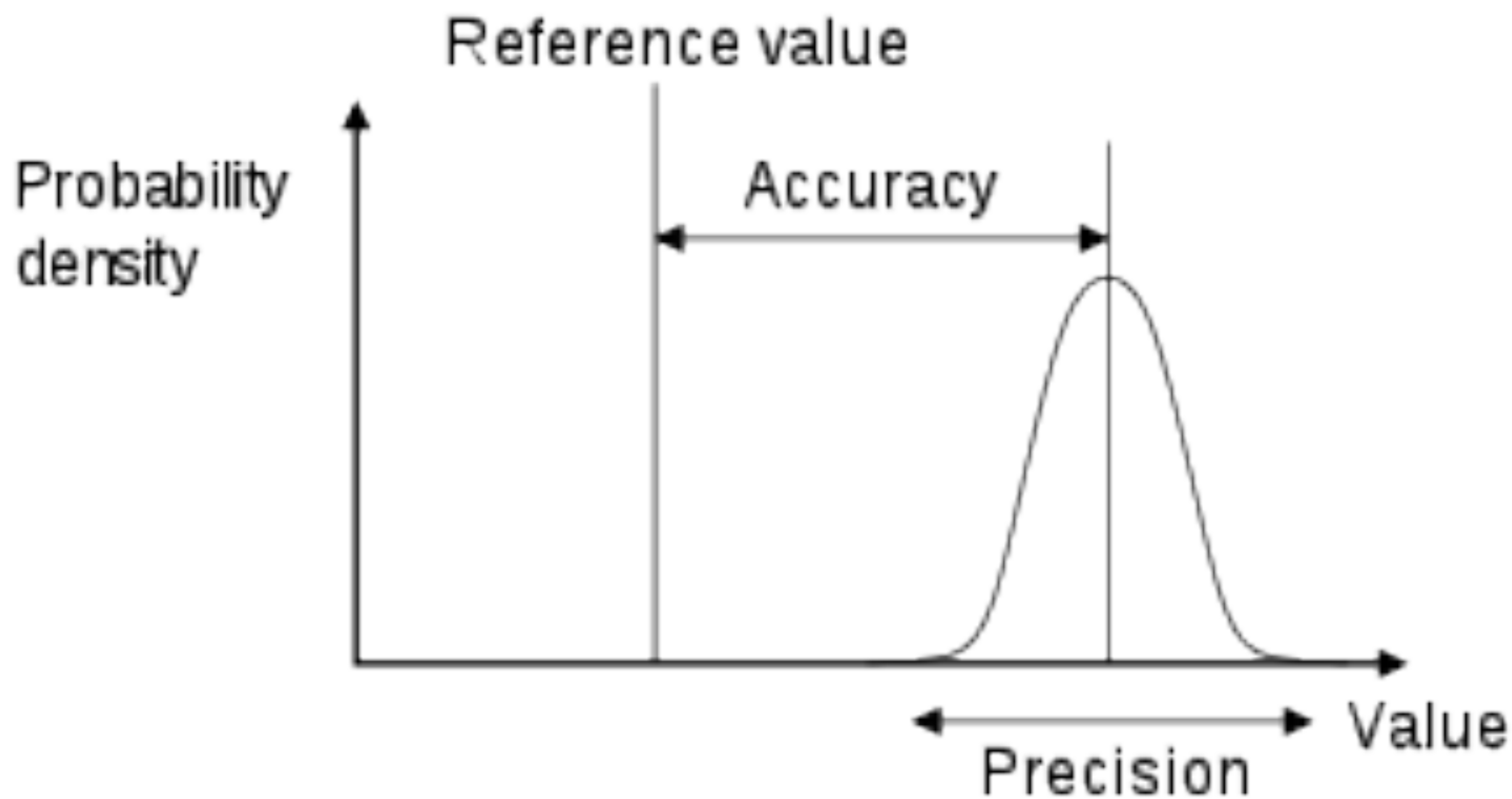
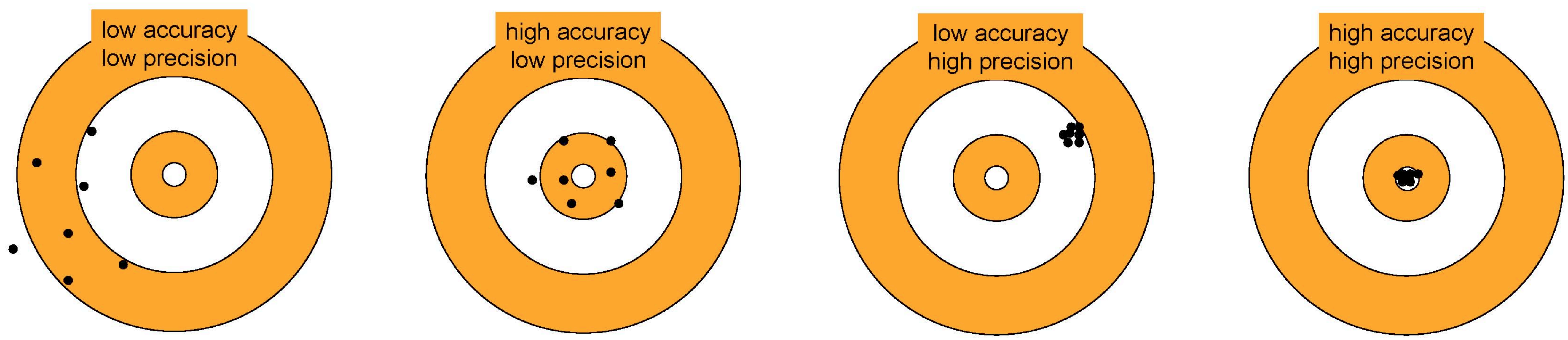
Precision and accuracy





Ways to quote uncertainties

$$t = (34.5 \pm 0.7)\ 10^{-3}\ \mathrm{s}$$
$$t = 34.5\ 10^{-3}\ \mathrm{s} \pm 2\,\%$$
$$x = 10.3^{+0.7}_{-0.3}$$
$$m_e = (0.510\,999\,06 \pm 0.000\,000\,15)\ \mathrm{MeV}/c^2$$
$$m_e = 0.510\,999\,06\ (15)\ \mathrm{MeV}/c^2$$
$$m_e = 9.109\,389\,7\,10^{-31}\,\mathrm{kg}\ \pm 0.3\,ppm$$

An uncertainty σ represents some kind of probability distribution (often a Gaussian, if not stated otherwise)

If no further information is given the interval x ± σ corresponds to a a probability of 68% ("1σ errors")

Statistical and systematic uncertainties

$$x = 2.34 \pm 0.05\,(\mathrm{stat.}) \pm 0.03\,(\mathrm{syst.})$$

- quoting stat. and syst. uncertainty separately gives us an idea whether taking more data would be helpful
- Systematic unc. usually less well known
- important when combining experiments

Statistical or random uncertainties

- Uncertainties that can be reliably estimated by repeating measurements
- They follow a known distribution like a Poisson rate or are determined empirically from the distribution of an unbiased, sufficiently large sample.
- Relative uncertainty reduces as $1/\sqrt{N}$ where N is the sample size

Systematic uncertainties

- Cannot be calculated solely from sampling fluctuations
- In most cases don't reduce as $1/\sqrt{N}$ (but often also become smaller with larger N)
- Difficult to determine, in general less well known than the statistical uncertainty
- Systematic uncertainties ≠ mistakes
  (a bug in your computer code is not a systematic uncertainty)

Statistical uncertainties: Examples

Radioactive decays ($\rightarrow$ Poisson distribution)

- You measure N = 150 decays.
- The result is reports as $N \pm \sqrt{N} \approx 150 \pm 12$

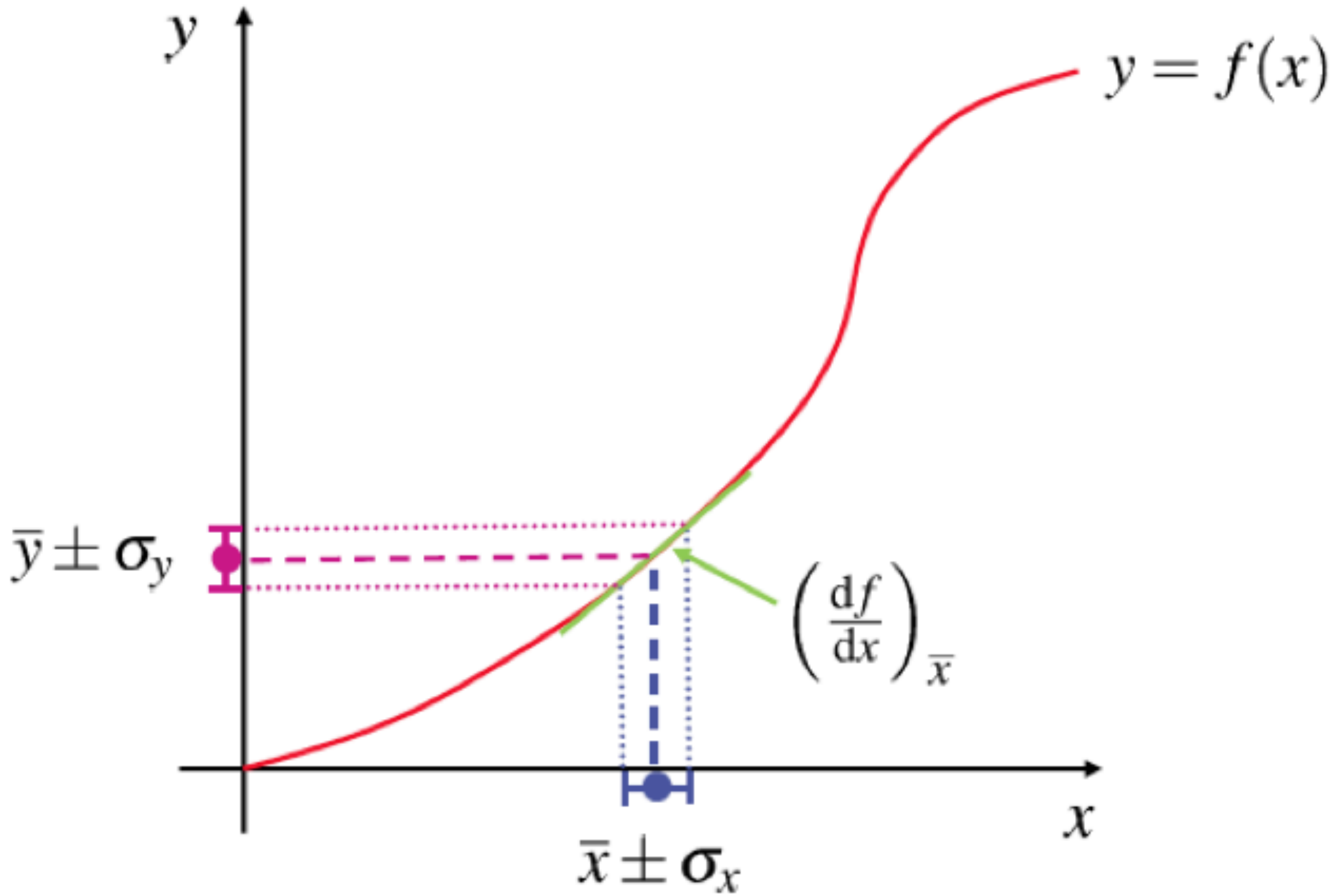
Efficiency of a detector ($\rightarrow$ Binomial distribution)

- From N_0 = 60 particles which traverse a detector, 45 are measured
- $\varepsilon = N/N_0 = 0.75$

$$\sigma_N^2 = N_0 \varepsilon (1 - \varepsilon) \quad \rightsquigarrow \quad \sigma_\varepsilon = \sqrt{\frac{\varepsilon(1-\varepsilon)}{N_0}} = \sqrt{\frac{0.75 \cdot 0.25}{60}} = 0.06$$

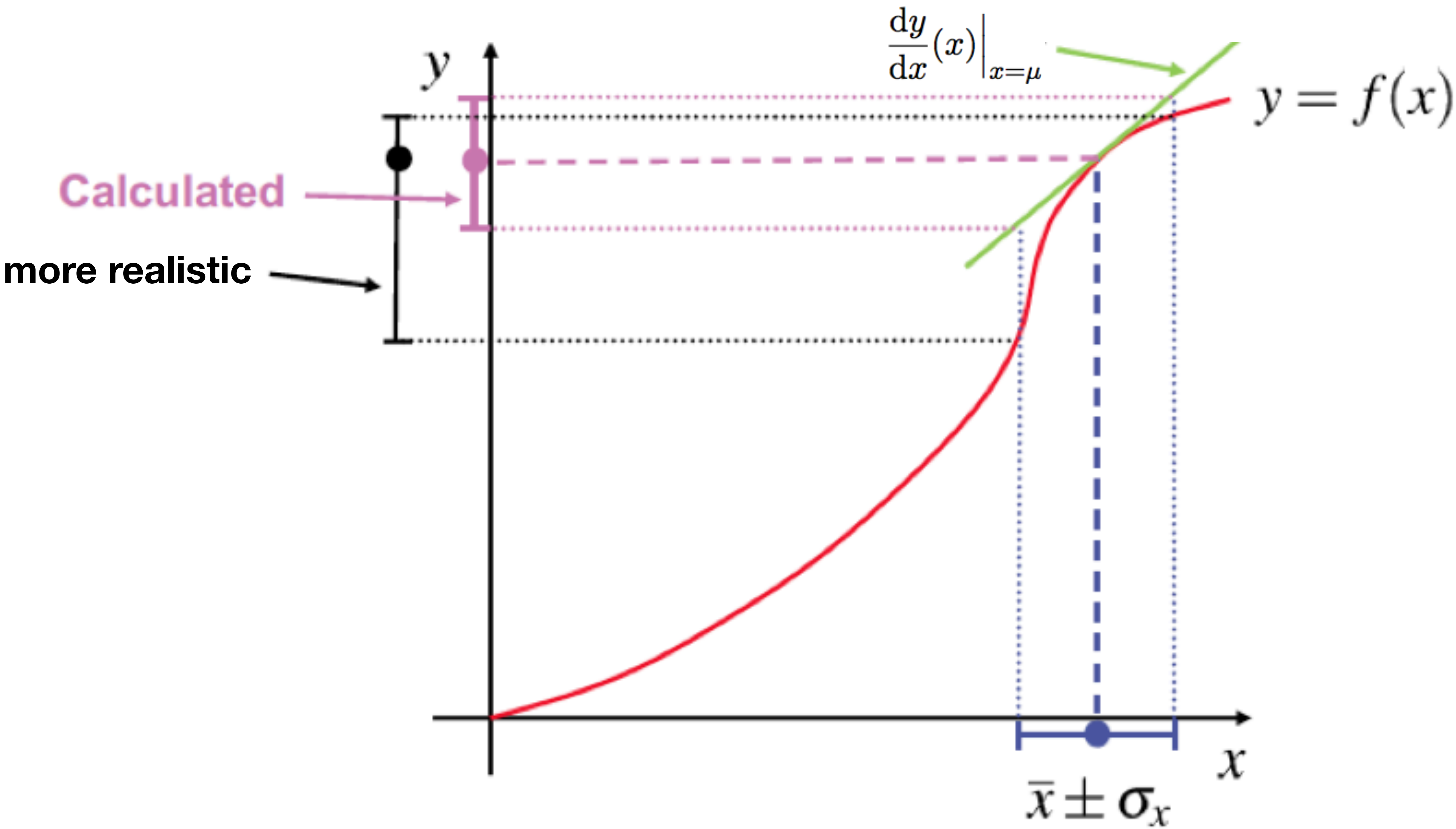
3.1 Error Propagation

Linear error propagation: Sometimes applicable …



Function sufficiently linear within ±σ: linear error propagation applicable

Linear error propagation: Sometimes not applicable …



In this situation linear error propagation is not applicable

Linear error propagation

Consider a measurement of values x_i and their covariances:

$$\vec{x} = (x_1, x_2, ..., x_n) \qquad V_{ij} = \mathrm{cov}[x_i, x_j]$$

Let y be a function of the x_i: $\quad y = f(\vec{x})$

What is the variance of y?

Approach: Taylor expansion of y around $\vec{\mu}$ where $\mu_i = E[x_i]$

In practice we estimate μ_i by measured value x_i

$$V[y] \equiv \sigma_y^2 = E[y^2] - E[y]^2$$

Linear error propagation formula

Taylor expansion:
$$y(\vec{x}) \approx y(\vec{\mu}) + \sum_{i=1}^{n} \left[\frac{\partial y}{\partial x_i}\right]_{\vec{x}=\vec{\mu}} (x_i - \mu_i)$$

$E[y]$ is easy:
$$E[y] \approx y(\vec{\mu}) \qquad \text{as} \quad E[x_i - \mu_i] = 0$$

$E[y^2]$:
$$E[y^2(\vec{x})] \approx y^2(\vec{\mu}) + 2y(\vec{\mu}) \sum_{i=1}^{n} \left[\frac{\partial y}{\partial x_i}\right]_{\vec{x}=\vec{\mu}} E[x_i - \mu_i]$$
$$+ E\left[\left(\sum_{i=1}^{n} \left[\frac{\partial y}{\partial x_i}\right]_{\vec{x}=\vec{\mu}} (x_i - \mu_i)\right)\left(\sum_{j=1}^{n} \left[\frac{\partial y}{\partial x_j}\right]_{\vec{x}=\vec{\mu}} (x_j - \mu_j)\right)\right]$$
$$= y^2(\vec{\mu}) + \sum_{i,j=1}^{n} \left[\frac{\partial y}{\partial x_i}\frac{\partial y}{\partial x_j}\right]_{\vec{x}=\vec{\mu}} V_{ij}$$

Thus:
$$\boxed{\sigma_y^2 = \sum_{i,j=1}^{n} \left[\frac{\partial y}{\partial x_i}\frac{\partial y}{\partial x_j}\right]_{\vec{x}=\vec{\mu}} V_{ij}}$$

Matrix notation

Let vector A be given by $\vec{A} = \vec{\nabla} y, \quad \text{i.e., } A_j = \left(\frac{\partial y}{\partial x_j}\right)_{\vec{x}=\vec{\mu}}$

Then: $$\sigma_y^2 = \sum_{i,j=1}^{n} \left[\frac{\partial y}{\partial x_i}\frac{\partial y}{\partial x_j}\right]_{\vec{x}=\vec{\mu}} V_{ij} \quad = \quad A^{\mathsf{T}} V A$$

Example: $$y = \frac{x_1}{x_2}, \quad A = \begin{pmatrix} 1/x_2 \\ -x_1/x_2^2 \end{pmatrix}$$

$$\sigma_y^2 = \left(\frac{1}{x_2}, -\frac{x_1}{x_2^2}\right) \begin{pmatrix} \sigma_1^2 & \mathrm{cov}[x_1, x_2] \\ \mathrm{cov}[x_1, x_2] & \sigma_2^2 \end{pmatrix} \begin{pmatrix} \frac{1}{x_2} \\ -\frac{x_1}{x_2^2} \end{pmatrix}$$

$$= \left(\frac{1}{x_2}, -\frac{x_1}{x_2^2}\right) \begin{pmatrix} \frac{\sigma_1^2}{x_2} - \frac{x_1}{x_2^2}\mathrm{cov}[x_1, x_2] \\ \frac{1}{x_2}\mathrm{cov}[x_1, x_2] - \frac{x_1}{x_2^2}\sigma_2^2 \end{pmatrix} = \frac{1}{x_2^2}\sigma_1^2 + \frac{x_1^2}{x_2^4}\sigma_2^2 - 2\frac{x_1}{x_2^3}\mathrm{cov}[x_1, x_2]$$

$$\rightarrow \quad \frac{\sigma_y^2}{y^2} = \frac{\sigma_1^2}{x_1^2} + \frac{\sigma_2^2}{x_2^2} - 2\frac{\mathrm{cov}[x_1, x_2]}{x_1 x_2} = \frac{\sigma_y^2}{y^2} = \frac{\sigma_1^2}{x_1^2} + \frac{\sigma_2^2}{x_2^2} - 2\frac{\rho\sigma_1\sigma_2}{x_1 x_2}$$

Linear error proportion: Examples

$$y = ax \quad \to \quad \sigma_y^2 = a^2 \sigma_x^2 \qquad \text{i.e. } \sigma_y = |a| \sigma_x$$

$$y = x^n \quad \to \quad \frac{\sigma_y^2}{y^2} = n^2 \frac{\sigma_x^2}{x^2} \qquad \text{i.e. } \frac{\sigma_y}{y} = |n| \frac{\sigma_x}{x}$$

$$y = x_1 + x_2 \quad \to \quad \sigma_y^2 = \sigma_1^2 + \sigma_2^2 + 2\mathrm{cov}[x_1, x_2]$$

$$y = x_1 - x_2 \quad \to \quad \sigma_y^2 = \sigma_1^2 + \sigma_2^2 - 2\mathrm{cov}[x_1, x_2]$$

$$y = x_1 x_2 \quad \to \quad \frac{\sigma_y^2}{y^2} = \frac{\sigma_1^2}{x_1^2} + \frac{\sigma_2^2}{x_2^2} + 2\frac{\mathrm{cov}[x_1, x_2]}{x_1 x_2}$$

Sanity checks:

Average of fully correlated measurements:

$$y = \frac{1}{2}(x_1 + x_2), \; \sigma_1 = \sigma_2 \equiv \sigma, \; \rho = 1 \quad \rightsquigarrow \quad \sigma_y = \sigma$$

Difference of fully correlated measurements:

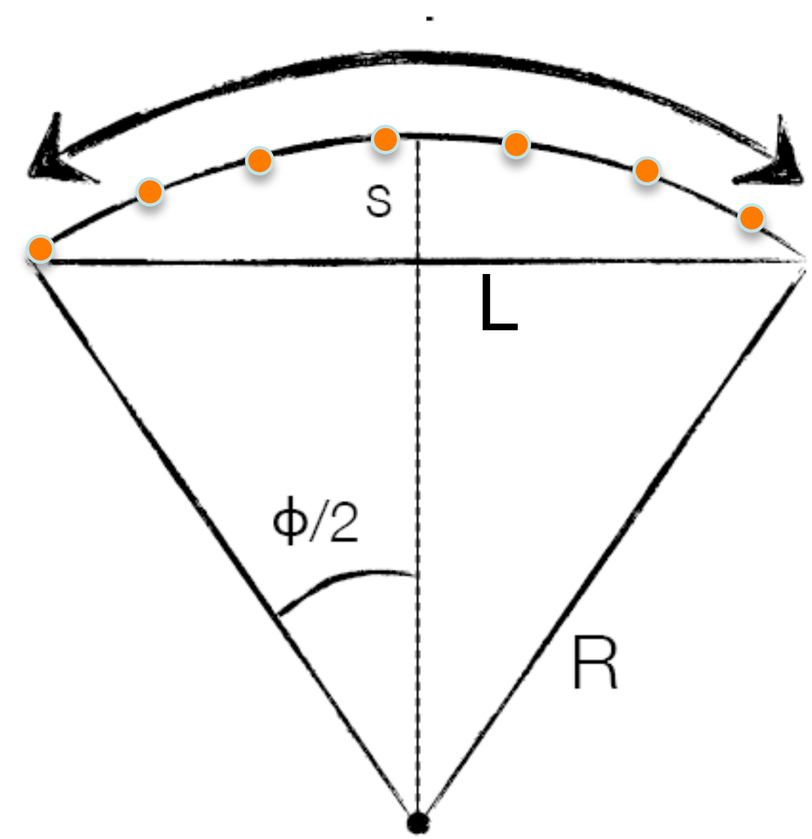
$$y = x_1 - x_2, \; \sigma_1 = \sigma_2 \equiv \sigma, \; \rho = 1$$

$$\rightsquigarrow \quad \sigma_y^2 = 2\sigma^2 - 2\sigma^2 = 0$$

Concrete example: Momentum resolution in tracking

Charged particle moving in constant magnetic field:

$$p_T/\mathrm{GeV} = 0.3 \times B/\mathrm{Tesla} \times R/\mathrm{m}$$



Measurements of space points yields Gaussian uncertainty for sagitta s which is related to p_T as

$$R = \frac{L^2}{8s}, \quad p_T = 0.3B\frac{L^2}{8s}$$

Momentum resolution:

$$\frac{\sigma_{p_T}}{p_T} = \frac{\sigma_s}{s} = \frac{8p_T}{0.3BL^2}\sigma_s$$

Important features:

- Relative momentum uncertainty proportional to momentum
- Relative uncertainty prop. to uncertainty of coordinate measurement

Example:
ATLAS nominal resolution

$$\left(\frac{\sigma_{p_T}}{p_T}\right)^2 = \underbrace{0.001^2}_{\text{multiple scattering}} + \underbrace{(0.0005p_T)^2}_{\text{track uncertainty}}$$

Linear error propagation for uncorrelated measurements

Special case: the x_i are uncorrelated, i.e., $V_{ij} = \delta_{ij}\sigma_i^2$:

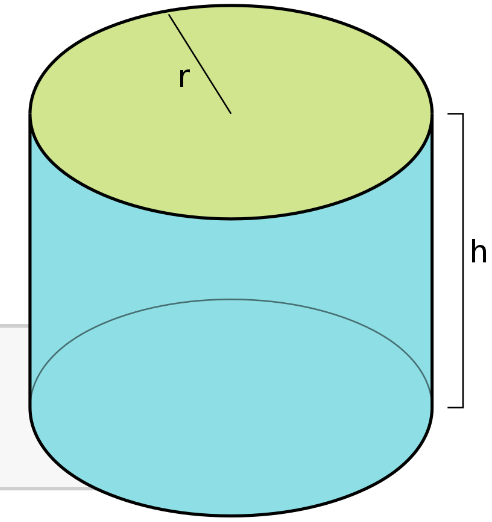
$$\sigma_y^2 = \sum_{i=1}^{n} \left[\frac{\partial y}{\partial x_i}\right]^2_{\vec{x}=\vec{\mu}} \sigma_i^2$$

These formulas are exact only for linear functions.

Approximation breaks down if function is nonlinear over a region comparable in size to the σ_i.

Example of Gaussian error propagation: Volume of a cylinder

[gaussian_error_propagation.ipynb]



[wikipedia]

```
from sympy import *
from IPython.display import display, Latex
```

```
def gaussian_error_propagation(f, vars):
    """
    f: formula (sympy expression)
    vars: list of independent variables and corresponding uncertainties
    [(x1, sigma_x1), (x2, sigma_x2), ...]
    """
    sum = sympify("0") # empty sympy expression
    for (x, sigma) in vars:
        sum += diff(f, x)**2 * sigma**2
    return sqrt(simplify(sum))
```

Show usage for a simple example: Volume of a cylinder with radius r and height h:

```
r, h, sigma_r, sigma_h = symbols('r, h, sigma_r, sigma_h', positive=True)
V = pi * r**2 * h # volume of a cylinder
```

```
sigma_V = gaussian_error_propagation(V, [(r, sigma_r), (h, sigma_h)])
display(Latex(f"$V = {latex(V)}, \, \sigma_V = {latex(sigma_V)}$"))
```

$$V = \pi h r^2, \; \sigma_V = \pi r \sqrt{4h^2\sigma_r^2 + r^2\sigma_h^2}$$

Example of Gaussian error propagation: Volume of a cylinder (now for correlated *r* and *h*)

```python
def gaussian_error_propagation_corr(f, x, V):
    """
    f: function f = f(x[0], x[1], ...)
    x: list of variables
    V: covariance matrix (python 2d list)
    """
    sum = sympify("0") # empty sympy expression
    for i in range(len(x)):
        for j in range(len(x)):
            sum += diff(f, x[i]) * diff(f, x[j]) * V[i][j]
    return sqrt(simplify(sum))
```

Show usage for a simple example: Volume of a cylinder with radius r and height h:

```python
r, h, sigma_r, sigma_h = symbols('r, h, sigma_r, sigma_h', positive=True)
rho = Symbol("rho", real=True) # correlation coefficient
V = pi * r**2 * h # volume of a cylinder
```

```python
vars = [r, h]
cov_matrix = [[sigma_r**2, rho * sigma_r * sigma_h],
              [rho * sigma_r * sigma_h, sigma_h**2]]
Matrix(cov_matrix)
```

$$\begin{bmatrix} \sigma_r^2 & \rho\sigma_h\sigma_r \\ \rho\sigma_h\sigma_r & \sigma_h^2 \end{bmatrix}$$

```python
sigma_V = gaussian_error_propagation_corr(V, vars, cov_matrix)
display(Latex(f"$V = {latex(V)}, \, \sigma_V = {latex(sigma_V)}$"))
```

$$V = \pi h r^2, \ \sigma_V = \pi r \sqrt{4h^2\sigma_r^2 + 4hr\rho\sigma_h\sigma_r + r^2\sigma_h^2}$$

$$r = 3\,\mathrm{cm},\ \sigma_r = 0.1\,\mathrm{cm}$$
$$h = 5\,\mathrm{cm},\ \sigma_h = 0.1\,\mathrm{cm}$$
$$V = \pi r^2 h = 141.4\,\mathrm{cm}^3$$

Uncertainty of the cylinder volume *V* depends on the correlation coefficient ρ:

ρ	σ_V
–1	6.6 cm³
0	9.8 cm³
1	12.3 cm³

[gaussian_error_propagation_correlated_variables.ipynb]

Linear error propagation: Generalization from $\mathbb{R}^n \rightarrow \mathbb{R}$ to $\mathbb{R}^n \rightarrow \mathbb{R}^m$

Generalization: Consider set of *m* functions:

$$\vec{y}(\vec{x}) = (y_1(\vec{x}), y_2(\vec{x}), \ldots, y_m(\vec{x}))$$

Then:

$$\mathrm{cov}[y_k, y_l] \equiv U_{kl} \approx \sum_{i,j=1}^{n} \left[\frac{\partial y_k}{\partial x_i} \frac{\partial y_l}{\partial x_j} \right]_{\vec{x}=\vec{\mu}} V_{ij}$$

In matrix notation:

$$U = A\, V\, A^{\mathrm{T}} \qquad A_{ij} = \left[\frac{\partial y_i}{\partial x_j} \right]_{\vec{x}=\vec{\mu}}$$

Reduction of the standard deviation for repeated independent measurements

Consider the average of n independent observation x_i:

$$\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$$

Expectation values and variance of the measurements:

$$E[x_i] = \mu_i \qquad V[x_i] = \sigma^2$$

Standard deviation of the mean:

$$V[\bar{x}] = \frac{1}{n^2} \sum_{i=1}^{n} \sigma_i^2 = \frac{1}{n} \sigma^2 \qquad \rightarrow \qquad \sigma_{\bar{x}} = \frac{\sigma}{\sqrt{n}}$$

Standard deviation of the mean decreases as $1/\sqrt{n}$

Example: Photon energy measurements

The energy resolution of a γ-ray detector used to investigate a decaying nuclear isotope is 50 keV.

- If only one photon is detected the energy of the decay is known to 50 keV
- 100 collected decays: energy of the decay known to 5 keV
- To reach 1 keV one needs to observe 2500 decays

Averaging uncorrelated measurements

Consider two uncorrelated measurements: $x_1 \pm \sigma_1, \; x_2 \pm \sigma_2$

Linear combination:

$$y = w_1 x_1 + w_2 x_2 \qquad \sigma_y^2 = w_1^2 \sigma_1^2 + w_2^2 \sigma_2^2$$

Now choose the weights such that σ_y^2 is minimal (under the condition $w_1 + w_2 = 1$):

$$\frac{\partial}{\partial w_i} \sigma_y^2 = 0 \quad \rightarrow \quad w_i = \frac{1/\sigma_i^2}{1/\sigma_1^2 + 1/\sigma_2^2}$$

And for the uncertainty of y we obtain (linear error propagation):

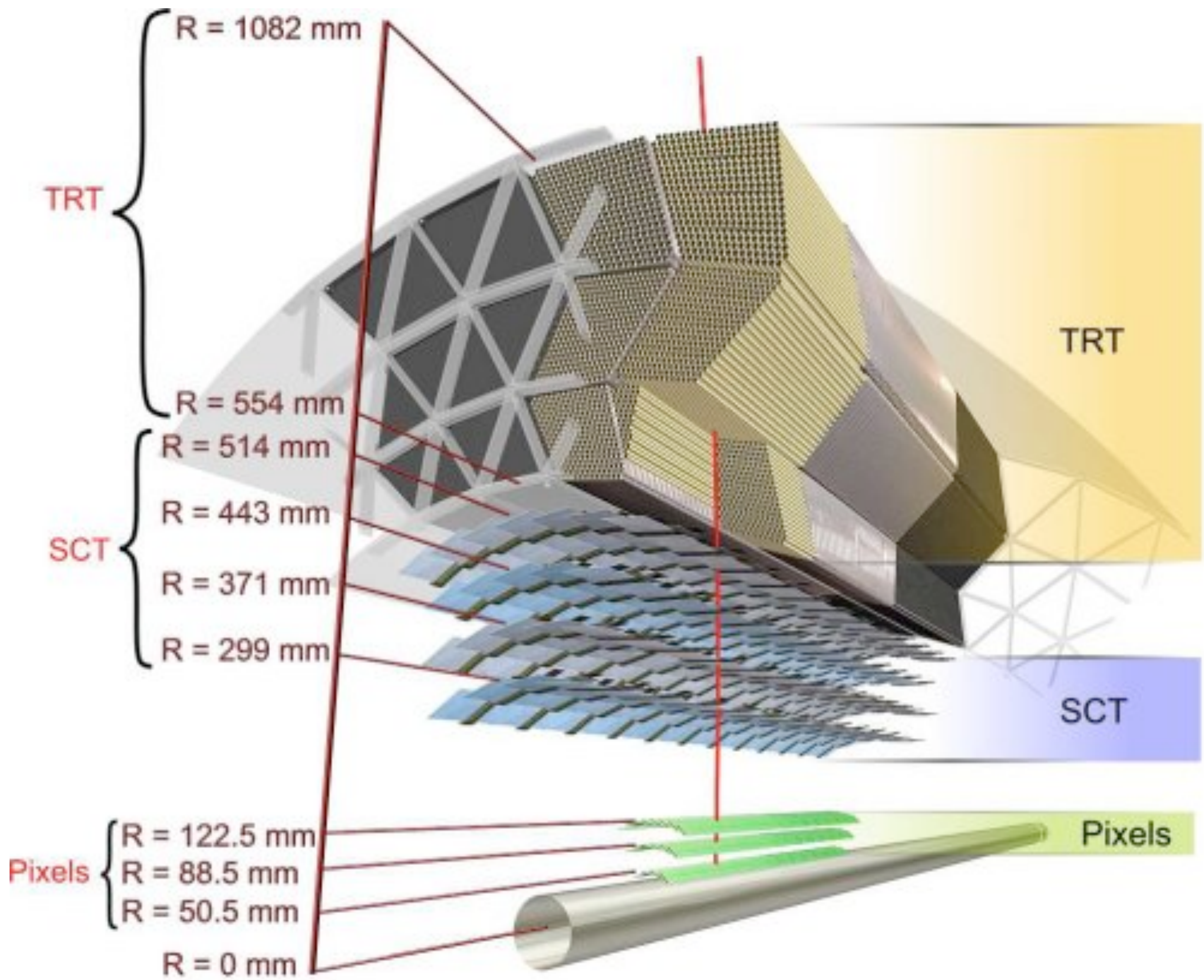
$$\frac{1}{\sigma_y^2} = \frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}$$

In general, for n uncorrelated measurements:

$$y = \sum_{i=1}^{n} w_i x_i, \qquad w_i = \frac{1/\sigma_i^2}{\sum_{j=1}^{n} 1/\sigma_j^2}, \qquad \frac{1}{\sigma_y^2} = \sum_{j=1}^{n} \frac{1}{\sigma_j^2}$$

Example: Averaging uncorrelated measurements

p_T of a particle in three subsystems of the ATLAS detector:



detector	p_T (GeV)
pixel detector	20 ± 2
semiconductor tracker	21 ± 1
transition radiation tracker	22 ± 4

Weighted average:

$$(20.86 \pm 0.87)\ \text{GeV}$$

$$p_T = \frac{\frac{20\ \text{GeV}}{4\ \text{GeV}^2} + \frac{21\ \text{GeV}}{1\ \text{GeV}^2} + \frac{22\ \text{GeV}}{16\ \text{GeV}^2}}{\frac{1}{4\ \text{GeV}^2} + \frac{1}{1\ \text{GeV}^2} + \frac{1}{16\ \text{GeV}^2}} = 20.86\ \text{GeV}$$

$$\sigma_{p_T} = \left[\frac{1}{4\ \text{GeV}^2} + \frac{1}{1\ \text{GeV}^2} + \frac{1}{16\ \text{GeV}^2}\right]^{-1/2} = 0.87\ \text{GeV}$$

Weighted average from Bayesian approach

Consider two measurements x_1 and x_2 with Gaussian uncertainties σ_1 and σ_2. In a Bayesian approach the probability distribution for the true value μ is given by

$$p(\mu) \propto L(x_1, x_2|\mu)\pi(\mu)$$

Assuming a flat prior $\pi(\mu) \equiv 1$ and independence of the two measurements one obtains

$$\begin{aligned} p(\mu) &\propto L(x_1|\mu)L(x_2|\mu) \\ &= G(x_1; \mu, \sigma_1)G(x_2; \mu, \sigma_2) \\ &\propto \exp\left[-\frac{1}{2}\left(\frac{(\mu - x_1)^2}{\sigma_1^2} + \frac{(\mu - x_2)^2}{\sigma_2^2}\right)\right] \end{aligned}$$

The product of the two Gaussians gives a Gaussian with mean

$$\mu = w_1 x_1 + w_2 x_2 \quad \text{where } w_i = \frac{1/\sigma_i^2}{1/\sigma_1^2 + 1/\sigma_2^2}$$

and standard deviation

$$\frac{1}{\sigma^2} = \frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}$$

→ same result as before

Asymmetric Errors

R. Barlow, arXiv:physics/0406120

Sometimes measurements are quoted with asymmetric errors: $x_i{}^{+\sigma_{i,+}}_{-\sigma_{i,-}}$

How to combine such measurements?

There is no statistical justification for adding the positive and negative uncertainties in quadrature separately:

$$y = \sum_i x_i, \quad \cancel{\sigma_{y,+}^2 = \sum_i \sigma_{i,+}^2, \quad \sigma_{y,-}^2 = \sum_i \sigma_{i,-}^2}$$

Gaussian likelihood in case of symmetric uncertainties for observation $\hat{x} \pm \sigma$:

$$L(\hat{x}; x) \propto \exp\left[-\frac{1}{2}\frac{(x-\hat{x})^2}{\sigma^2}\right]$$

If no further information is provided in case of asymmetric uncertainties, Barlow proposes to use the following likelihood:

$$L(\hat{x}; x) \propto \exp\left[-\frac{1}{2}\left(\frac{(x-\hat{x})^2}{\sigma_-\sigma_+ + (\sigma_+ - \sigma_-)(x-\hat{x})}\right)\right]$$

Based on this one can come up with a procedure for combining measurements with asymmetric errors, see Barlow's paper

Monte Carlo error propagation

Example:
Ratio of two Gaussian distributed quantities

$$x = 5 \pm 1$$

$$y = 5 \pm 1$$

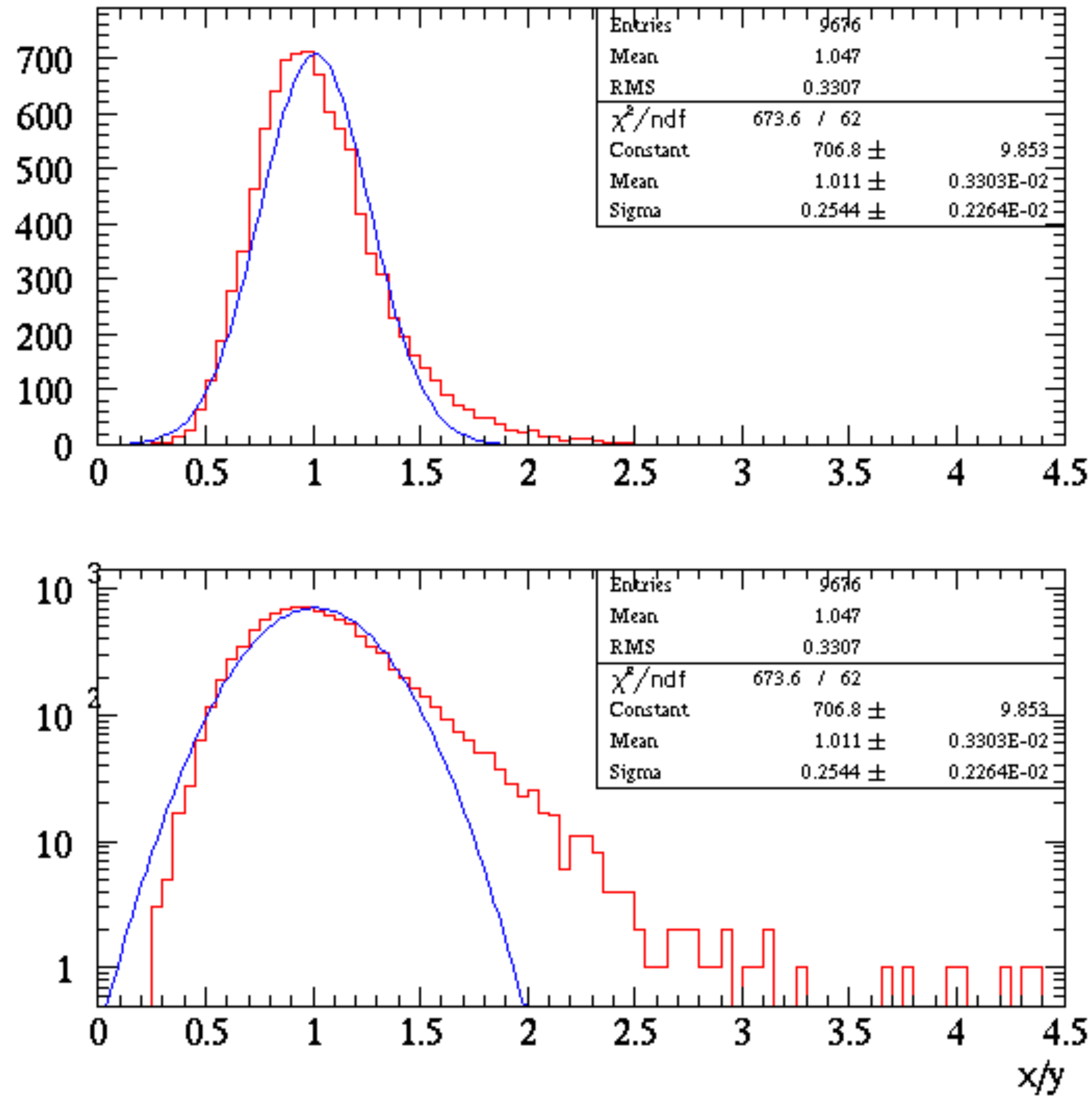
Approach: draw values for *x* and *y* many times and fill histogram with ratios

Standard linear error prop.:

$$R = 1 \pm 0.28$$

Mean and rms of histogram:

$$R = 1.05 \pm 0.33$$



Rule of thumb: ratio of two Gaussians will be approximately Gaussian if fractional uncertainty is dominated by numerator, and denominator cannot be small compared to numerator

3.2 Systematic Uncertainties

Systematic uncertainties: Examples

Calibration uncertainties of the measurement apparatus

- E.g., energy scale uncertainty of a calorimeter

Uncertainty of the detector resolution

Detector acceptance

Limited knowledge about background processes

Uncertainties of auxiliary quantities

- E.g. reference branching ratios uses as input
- Uncertainty of theoretical quantities

…

The uncertainty in the estimation of such a systematic effect is called a systematic uncertainty.

How to deal with systematic uncertainties?

Top-Down Approach

- Think about all possible sources of potential systematics
- Can/should be done at the planning stage of an experiment
- Requires experience

Bottom-Up Approach

- Try to find systematic uncertainties not considered in top-down approach
- Internal cross checks
- Compare independent analyses if possible
- see next slides

Sanity / Consistency checks

R. Barlow
"Systematic Errors, Fact and Fiction," hep-ex/0207026

Look for systematic effects by repeating the analysis with changes which *should* make no difference:

Data subsets

Magnet up/down

Different selection cuts

Different histogram bin sizes and fit ranges

Different Event Generator for efficiency calculation

Look for impossibilities

If a check passes the test:
move on and do not add the discrepancy to the systematic uncertainty

If a check fails: try to identify the reason. Only as very last resort, add contribution to total systematic uncertainty. This might underestimate the real uncertainty.

Handling discrete systematic uncertainties

Example: choice of model used to determine a correction *R*

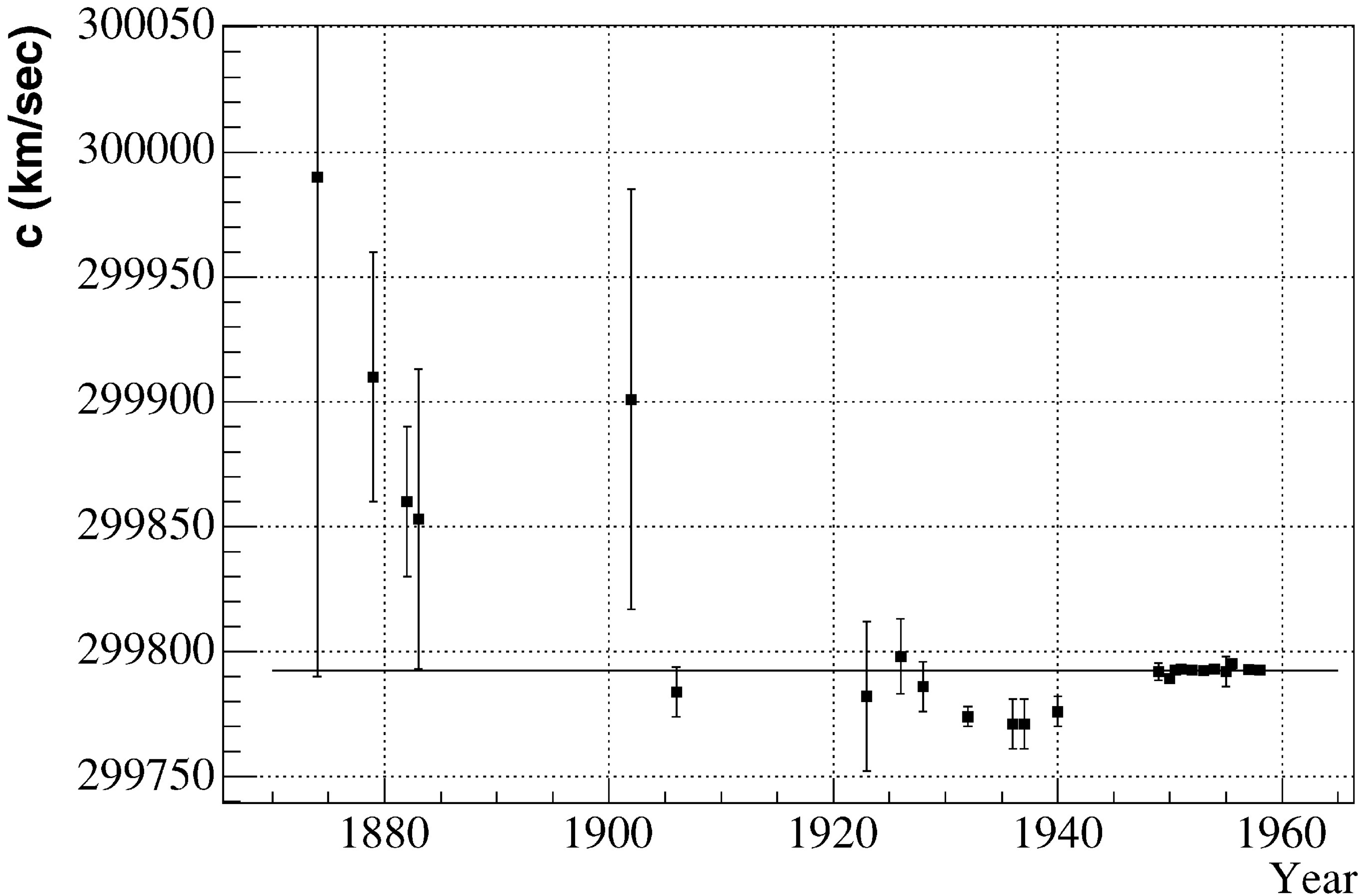
With 1 preferred model and one other, quote $R_1 \pm |R_1 - R_2|$

With 2 models of equal status, quote $\dfrac{R_1 + R_2}{2} \pm \dfrac{|R_1 - R_2|}{\sqrt{2}}$

n equal models, quote $\bar{R} \pm \sqrt{\dfrac{1}{n-1}\displaystyle\sum_{i=1}^{n}(R_i - \overline{R})^2} = \sqrt{\dfrac{n}{n-1}(\overline{R^2} - \overline{R}^2)}$

Two extreme models, quote $\dfrac{R_1 + R_2}{2} \pm \dfrac{|R_1 - R_2|}{\sqrt{12}}$

Speed of Light vs. Year of Publication

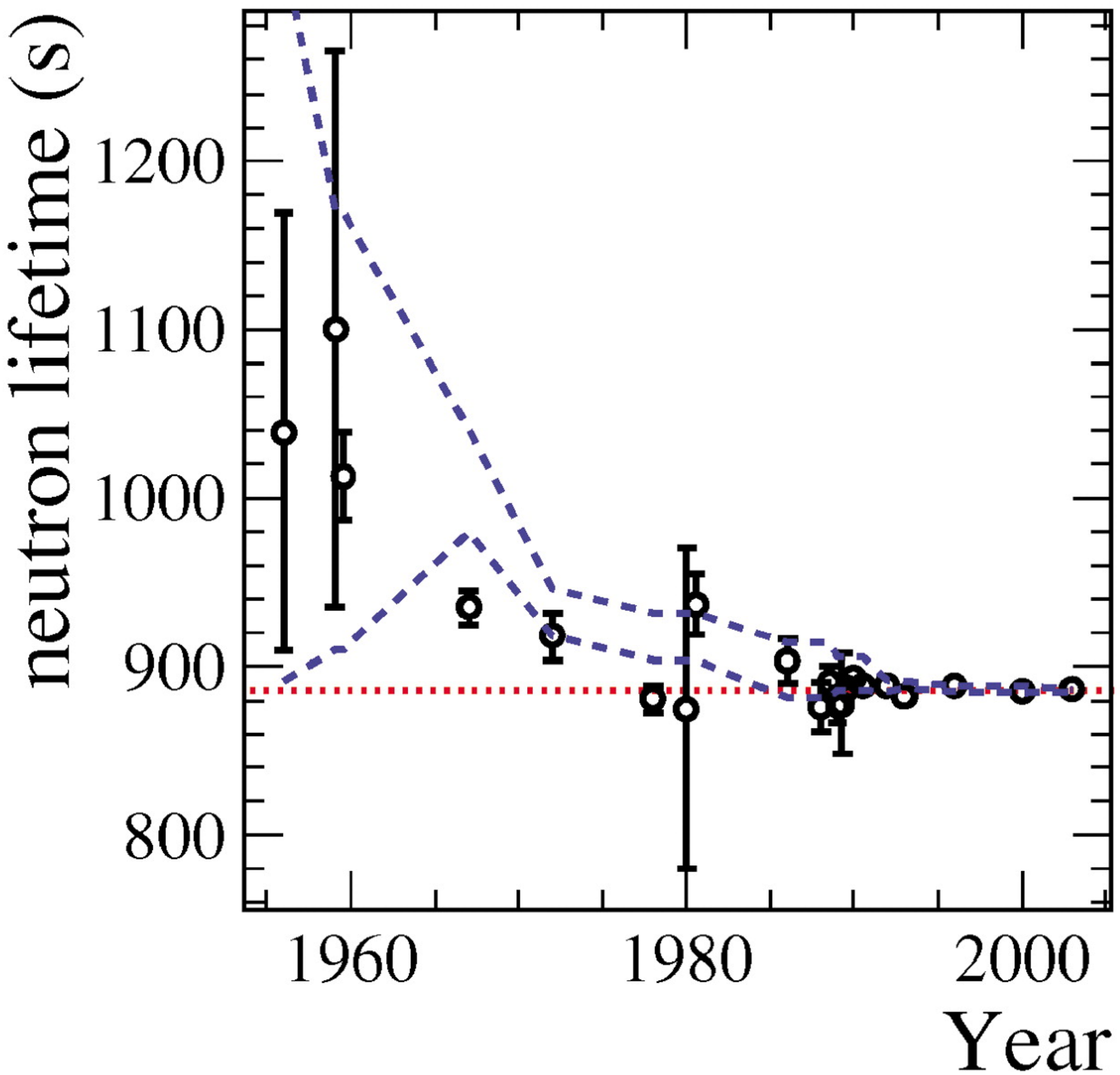


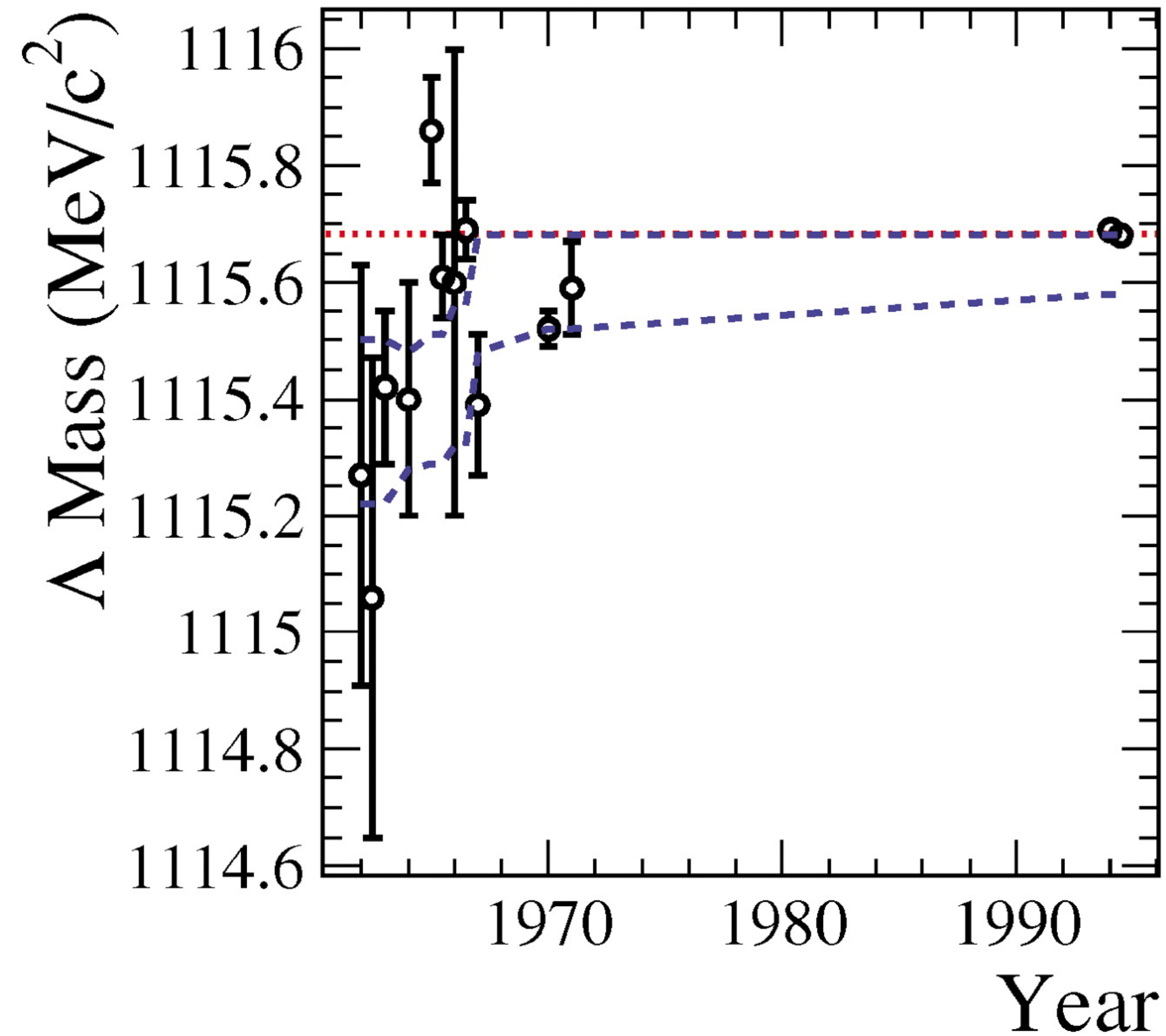
Klein JR, Roodman A. 2005.
Annu. Rev. Nucl. Part. Sci. 55:141–63

Experimenter's Bias?

Klein JR, Roodman, A. 2005,
Annu. Rev. Nucl. Part. Sci. 55:141–63

Do researches unconsciously work toward a certain value?





Possible bias:

the investigator searches for the source or sources of such errors, and continues to search until he gets a result close to the accepted value.

Then he/she stops!

Blind analyses

Klein JR, Roodman, A. 2005,
Annu. Rev. Nucl. Part. Sci. 55:141–63

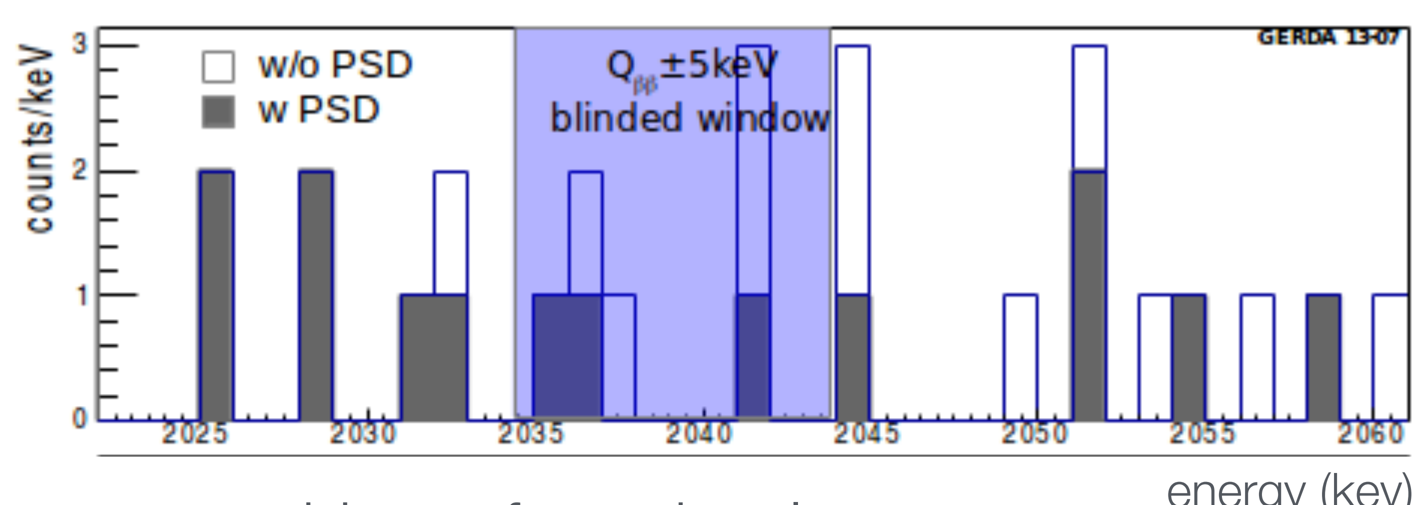
Avoid experimenter's bias by hiding certain aspects of the data.

Things that can be hidden in the analysis:

- The signal events, when the signal occurs in a well-defined region of the experiment's phase space.
- The result, when the numerical answer can be separated from all other aspects of the analysis.
- The number of events in the data set, when the answer relies directly upon their count.
- A fraction of the entire data set.

Example: GERDA experiment

- search for neutrinoless double beta decay
- Signal: sharp peak
- Background model fixed prior to unblinding of signal region



→ no evidence for a signal

Combination of systematic uncertainties

Systematic uncertainties are usually given as standard deviations ($x \pm \sigma_x$), corresponding to a 68% probability.

Other meaning (e.g. maximum extent uncertainty) this should be explicitly stated.

In most cases one tries to find independent sources of systematic uncertainties. These independent uncertainties are therefore added in quadrature:

$$\sigma_{\mathrm{tot}}^2 = \sigma_1^2 + \sigma_2^2 + \ldots + \sigma_n^2$$

Often a few source dominate the systematic uncertainty

→ No need to work to hard on correctly estimating the small uncertainties

Systematic uncertainties: Covariance matrix approach (I)

Consider two measurement x_1 and x_2 with with individual random uncertainties $\sigma_{1,r}$ and $\sigma_{2,r}$ and a common systematic uncertainty σ_s:

$$x_i = x_{\text{true}} + \Delta x_{i,\text{r}} + \Delta x_{\text{s}}$$

$$\langle \Delta x_{i,\text{r}} \rangle = 0, \quad \langle \Delta x_{\text{s}} \rangle = 0,$$
$$\langle (\Delta x_{i,\text{r}})^2 \rangle = \sigma_{i,\text{r}}^2, \quad \langle (\Delta x_{\text{s}})^2 \rangle = \sigma_s^2$$

Variance:

$$\begin{aligned} V[x_i^2] &= \langle x_i^2 \rangle - \langle x_i \rangle^2 \\ &= \langle (x_{\text{true}} + \Delta x_{i,\text{r}} + \Delta x_{\text{s}})^2 \rangle - \langle x_{\text{true}} + \Delta x_{i,\text{r}} + \Delta x_{\text{s}} \rangle^2 \\ &= \langle (\Delta x_{i,\text{r}} + \Delta x_{\text{s}})^2 \rangle \\ &= \sigma_{i,r}^2 + \sigma_s^2 \end{aligned}$$

Covariance:

$$\begin{aligned} \text{cov}[x_1, x_2] &= \langle x_1 x_2 \rangle - \langle x_1 \rangle \langle x_2 \rangle \\ &= \ldots \\ &= \sigma_s^2 \end{aligned}$$

Systematic uncertainties: Covariance matrix approach (II)

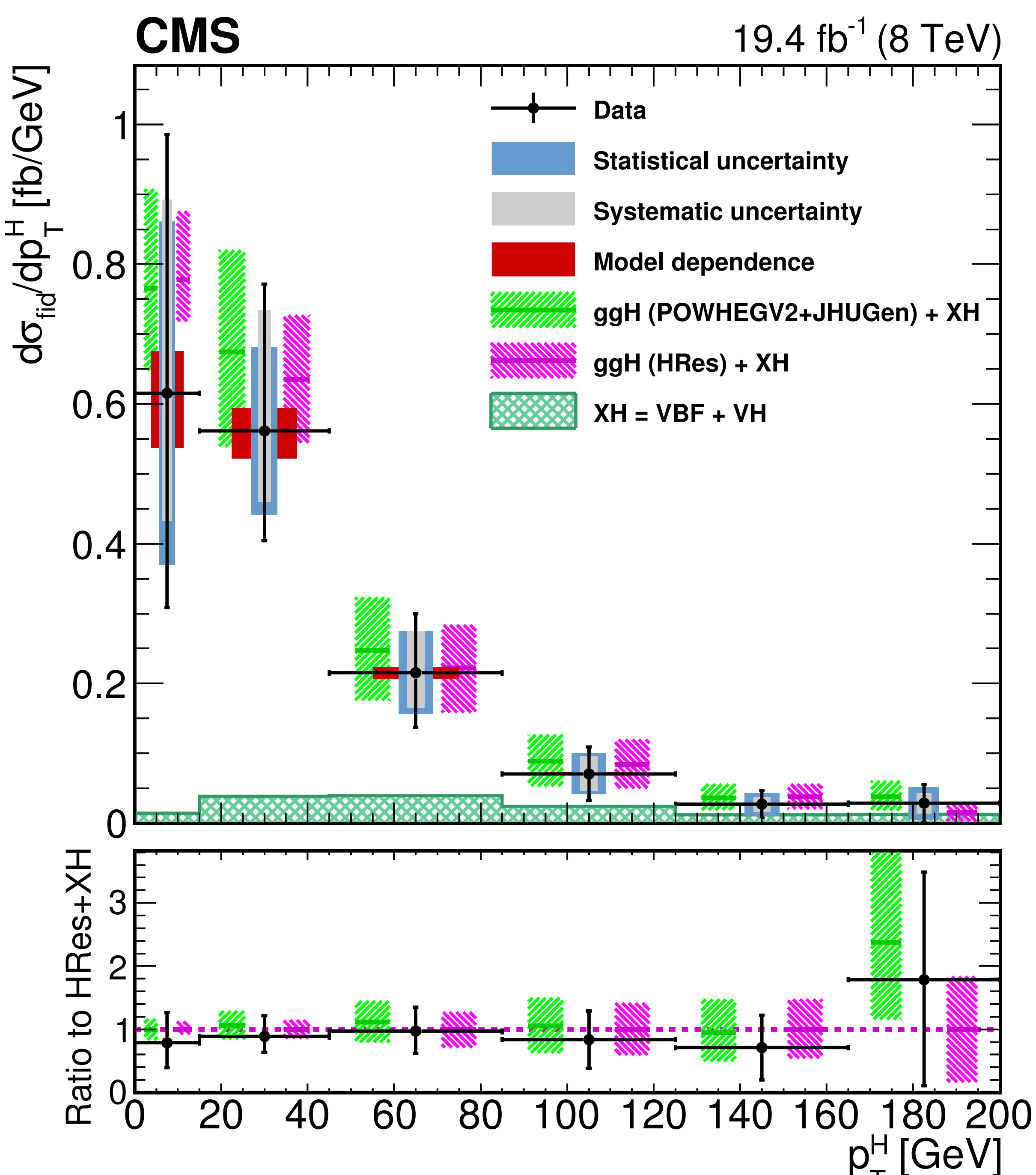
Covariance matrix for x_1 and x_2:

$$V = \begin{pmatrix} \sigma_{1,r}^2 + \sigma_s^2 & \sigma_s^2 \\ \sigma_s^2 & \sigma_{2,r}^2 + \sigma_s^2 \end{pmatrix}$$

This also works when the uncertainties are quoted as relative uncertainties:

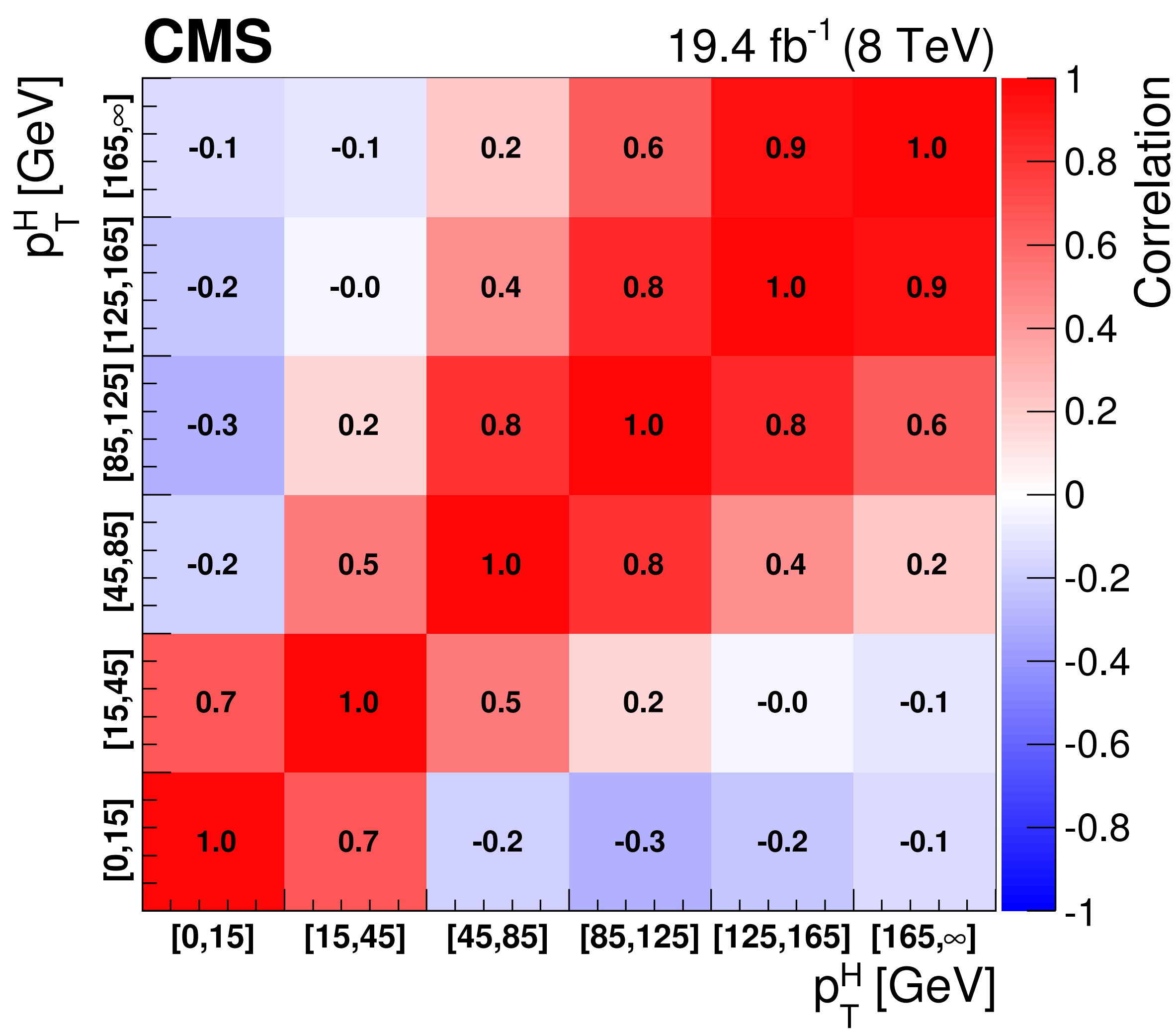
$$\sigma_s = \varepsilon x \qquad \rightsquigarrow \qquad V = \begin{pmatrix} \sigma_{1,r}^2 + \varepsilon^2 x_1^2 & \varepsilon^2 x_1 x_2 \\ \varepsilon^2 x_1 x_2 & \sigma_{2,r}^2 + \varepsilon^2 x_1^2 \end{pmatrix}$$

Example:
Transverse momentum spectrum of the Higgs boson



arXiv:1606.01522v1

Correlation matrix of the p_T bins:



$$\rho_{i,j} = \frac{V_{i,j}}{\sigma_i \sigma_j}, \qquad V = \text{covariance matrix}$$

Weighted average of correlated data points

Consider n data points y_i with covariance matrix V: $\vec{y} = (y_1, y_2, \ldots, y_n)$

One can calculate a weighted average λ by minimizing

$$\chi^2(\lambda) = (\vec{y} - \vec{\lambda})^\mathsf{T} V^{-1} (\vec{y} - \vec{\lambda})$$

$$\vec{\lambda} := (\lambda, \lambda, \ldots, \lambda)$$

One obtains (here without calculation):

$$\hat{\lambda} = \sum_{i=1}^{N} w_i y_i \qquad w_i = \frac{\sum_{j=1}^{n} (V^{-1})_{i,j}}{\sum_{k,l=1}^{n} (V^{-1})_{k,l}}$$

Variance results from error propagation:

$$\sigma^2_{\hat{\lambda}} = \vec{w}^\mathsf{T} V \vec{w} = \sum_{i,j=1}^{n} w_i V_{ij} w_j$$

Minimizing the χ^2 gives the *best linear unbiased estimate* (BLUE) → linear unbiased estimator with the lowest variance

- BLUE combination may be biased if uncertainties not known or are estimated from measured values
- Improvement: iterative approach (rescaling uncertainties based on previous iteration)

Special case: Weighted average of two correlated measurements

Consider two measurements with covariance matrix V (ρ = correlation coeff.):

$$y_1, \ y_2 \qquad V = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$$

Applying the formulas from the previous slide:

$$V^{-1} = \frac{1}{1-\rho^2} \begin{pmatrix} \frac{1}{\sigma_1^2} & \frac{-\rho}{\sigma_1\sigma_2} \\ \frac{-\rho}{\sigma_1\sigma_2} & \frac{1}{\sigma_2^2} \end{pmatrix} \qquad \hat{\lambda} = w y_1 + (1-w) y_2$$

$$w = \frac{\sigma_2^2 - \rho\sigma_1\sigma_2}{\sigma_1^2 + \sigma_2^2 - 2\rho\sigma_1\sigma_2} \qquad V[\hat{\lambda}] = \sigma^2 = \frac{(1-\rho^2)\sigma_1^2\sigma_2^2}{\sigma_1^2 + \sigma_2^2 - 2\rho\sigma_1\sigma_2}$$

equivalently:

$$\frac{1}{\sigma^2} = \frac{1}{1-\rho^2}\left[\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2} - \frac{2\rho}{\sigma_1\sigma_2}\right]$$

Bayesian approach to systematic uncertainties

"Bayesians lose no sleep over systematics" (lecture S. Oser)

Quantity of interest: θ, prior knowledge: $\pi(\theta)$

Likelihood depends parameter ν ("nuisance parameter")

We simply treat θ and ν as an unknown parameters:

$$P(\theta, \nu | \mathrm{data}) \propto L(\mathrm{data} | \theta, \nu) \pi(\theta, \nu)$$

As we are only interested in θ, we marginalize by integrating over ν:

$$P(\theta) = \int P(\theta, \nu) \, d\nu$$

Prior knowledge on ν often is the result of a calibration measurement.