

Statistical Methods in Particle Physics

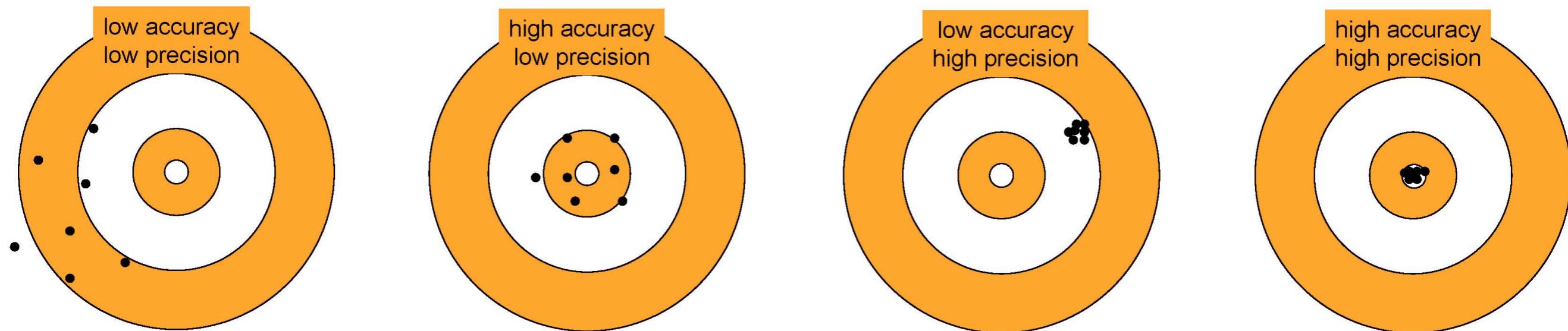
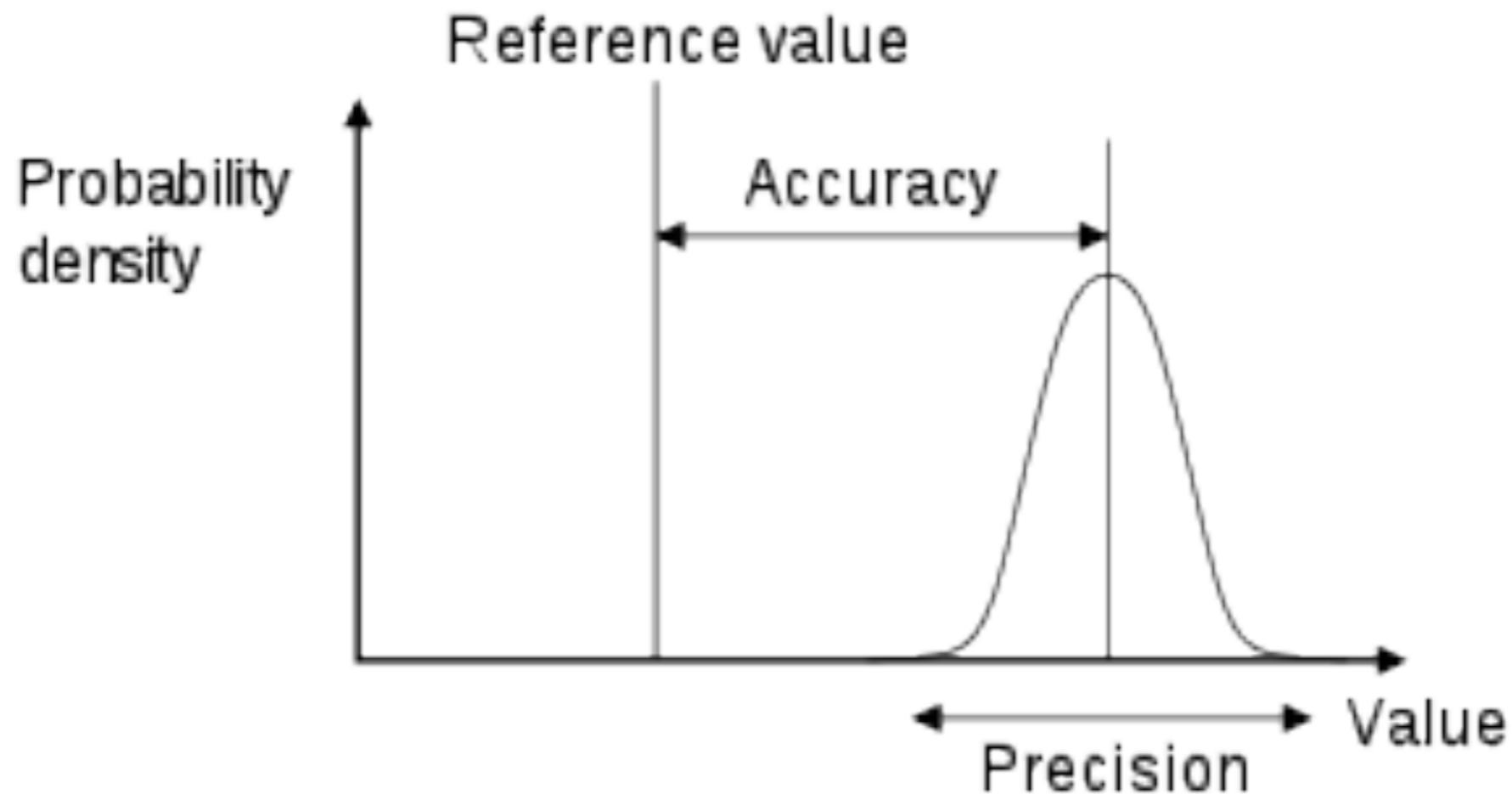
3. Uncertainties

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WS 2017/18

Statistical and Systematic Uncertainties

Precision and Accuracy



Ways to Quote Uncertainties

$$t = (34.5 \pm 0.7) 10^{-3} \text{ s}$$

$$t = 34.5 10^{-3} \text{ s} \pm 2\%$$

$$x = 10.3^{+0.7}_{-0.3}$$

$$m_e = (0.510\,999\,06 \pm 0.000\,000\,15) \text{ MeV}/c^2$$

$$m_e = 0.510\,999\,06 (15) \text{ MeV}/c^2$$

$$m_e = 9.109\,389\,7 10^{-31} \text{ kg} \pm 0.3 \text{ ppm}$$

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

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

Statistical and Systematic Uncertainties

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

quoting stat. and syst. uncertainty separately gives us an idea whether taking more data would be helpful

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 \neq 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 reported 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
- ▶ $\varepsilon = N/N_0 = 0.75$

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

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
- ...

A large fraction of the work in a particle physics analyses is estimating systematic uncertainties!

How to Deal with Systematic Uncertainties?

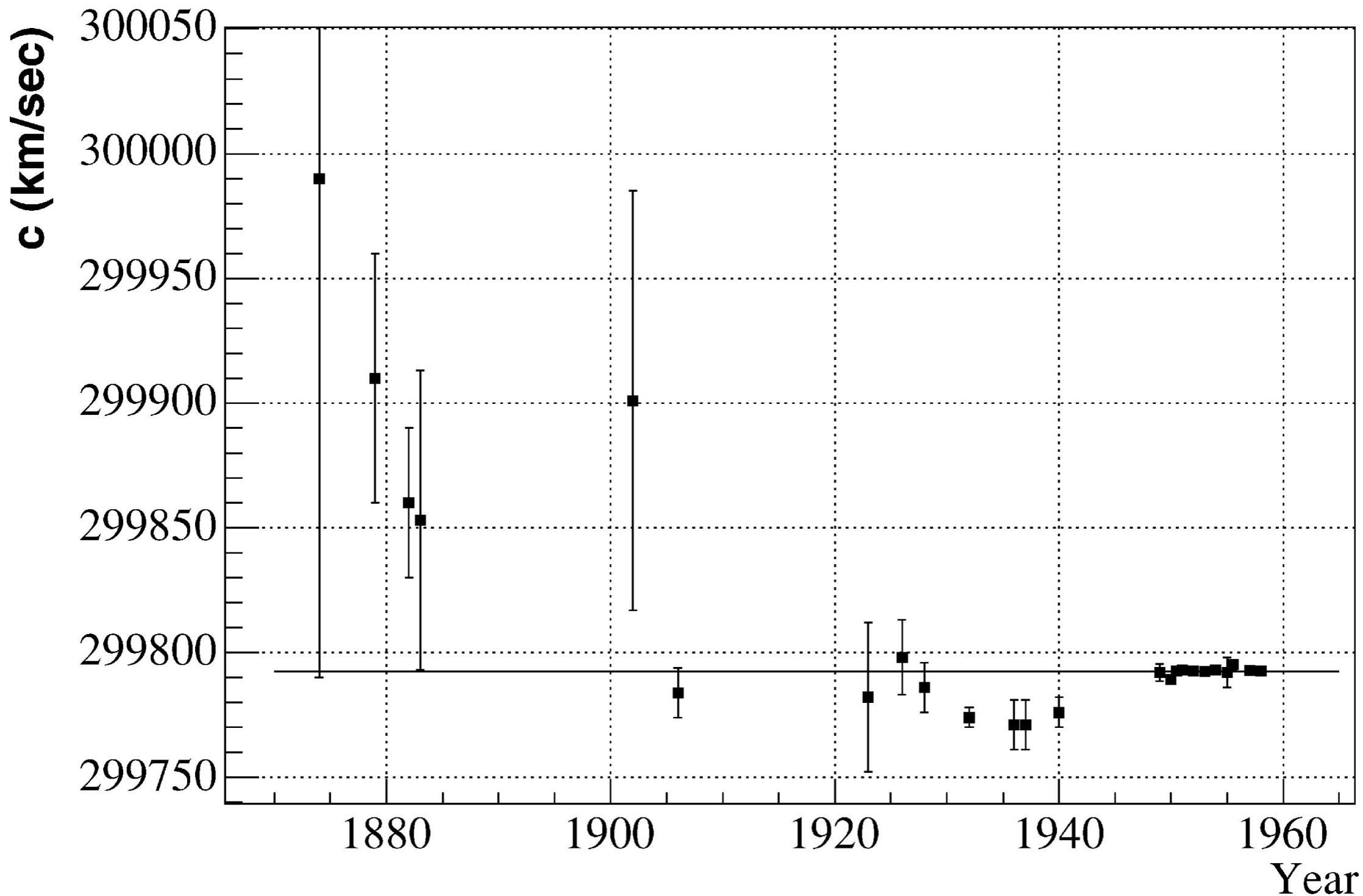
Top-Down Approach

- ▶ Think about all possible sources of potential systematics
- ▶ Requires experience

Bottom-Up Approach

- ▶ Try to find systematic uncertainties not considered in top-down approach
- ▶ Internal cross checks
- ▶ Split data into independent subsets
- ▶ Compare independent analyses if possible
- ▶ Cut variation:
 - helps to identify systematics uncertainties
 - but reasons for possible differences should be understood
 - often difficult to separate statistical fluctuations from real systematic effects

Speed of Light vs. Year of Publication

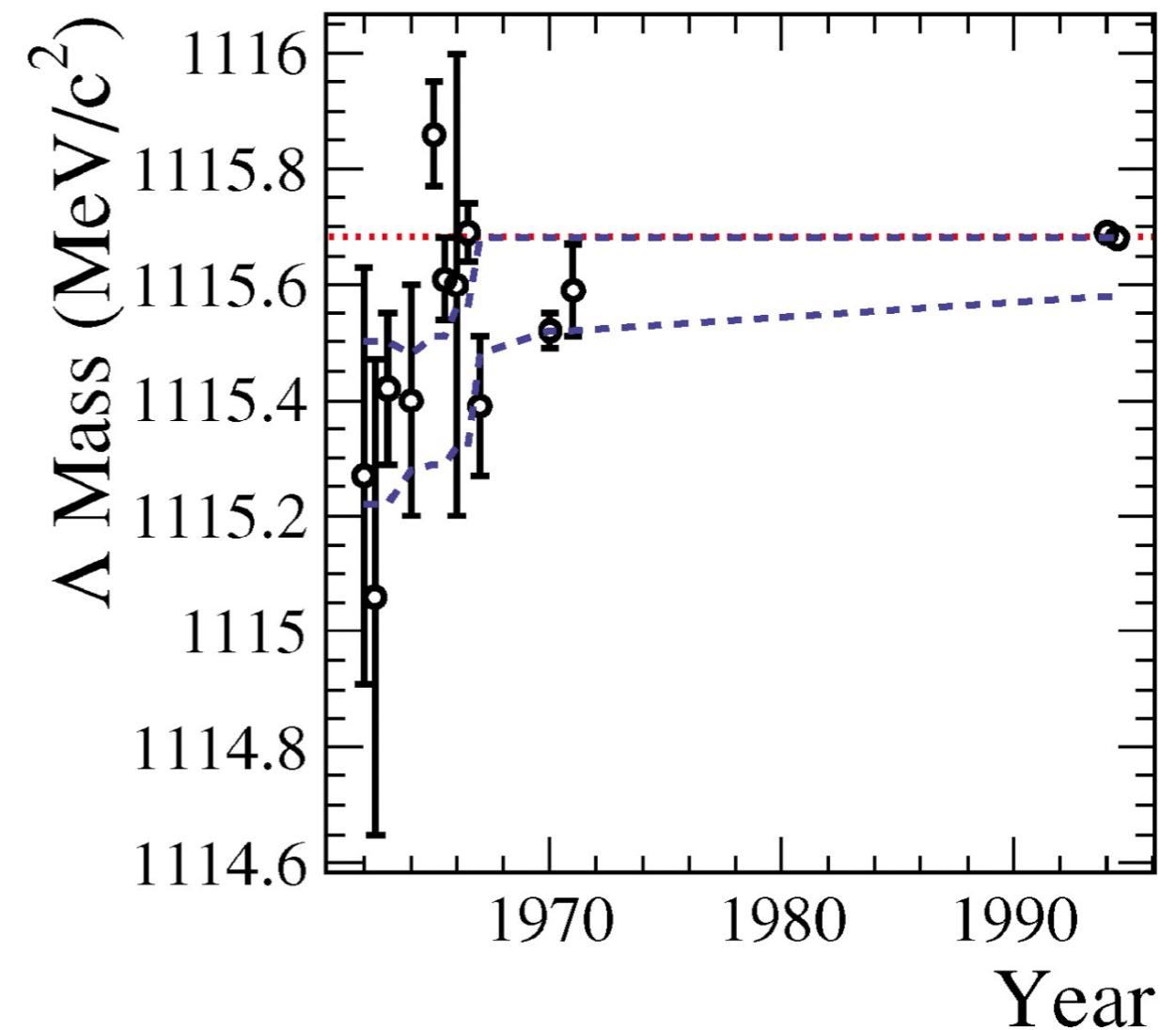
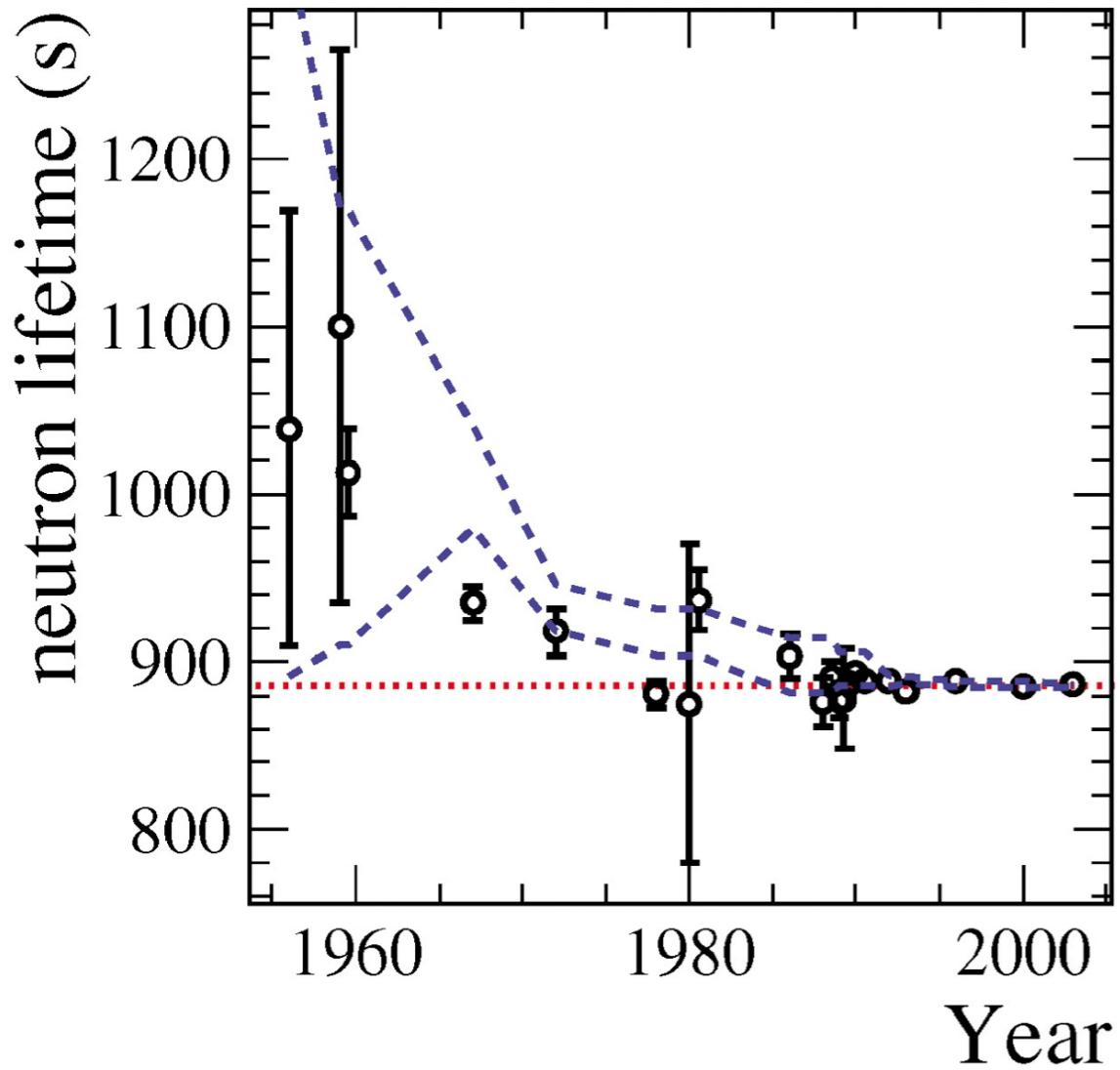


Klein JR, Roodman A. 2005.
Annu. Rev. Nucl. Part. Sci. 55:141–63

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

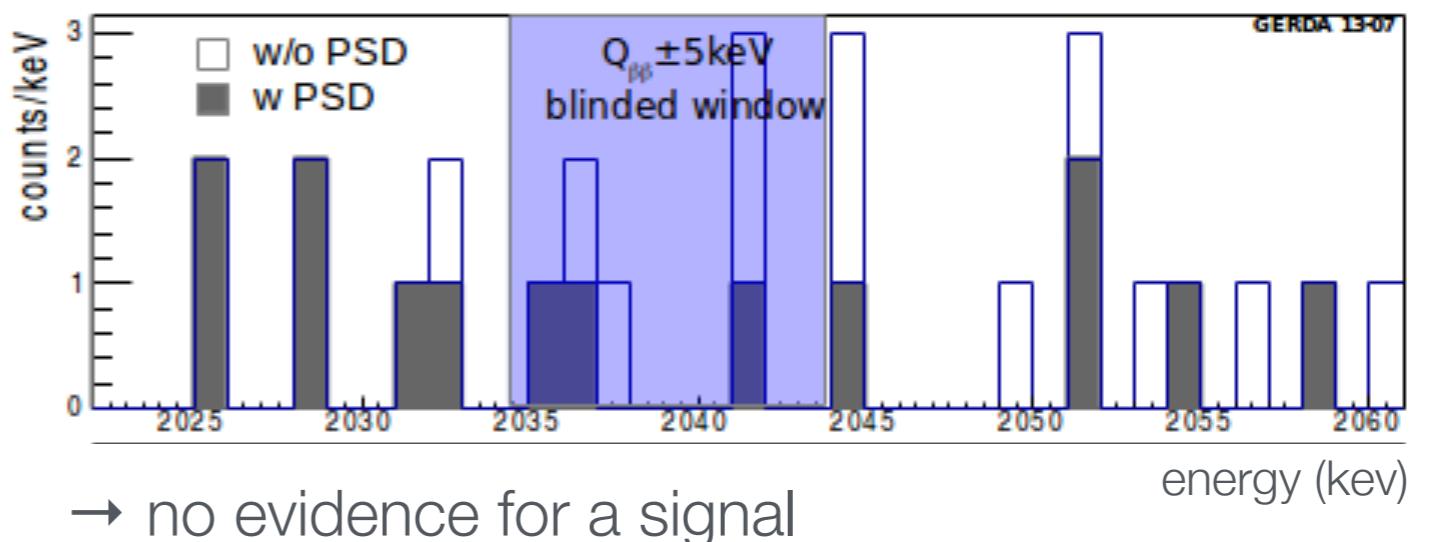
Avoid experimenter's bias by hiding certain aspects of the data.

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



Combination of Systematic Uncertainties

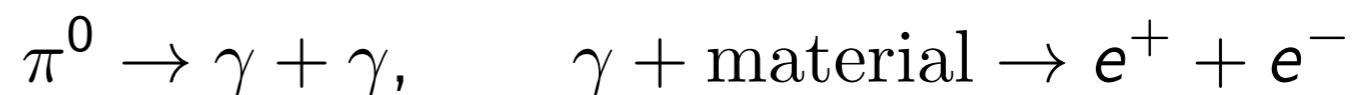
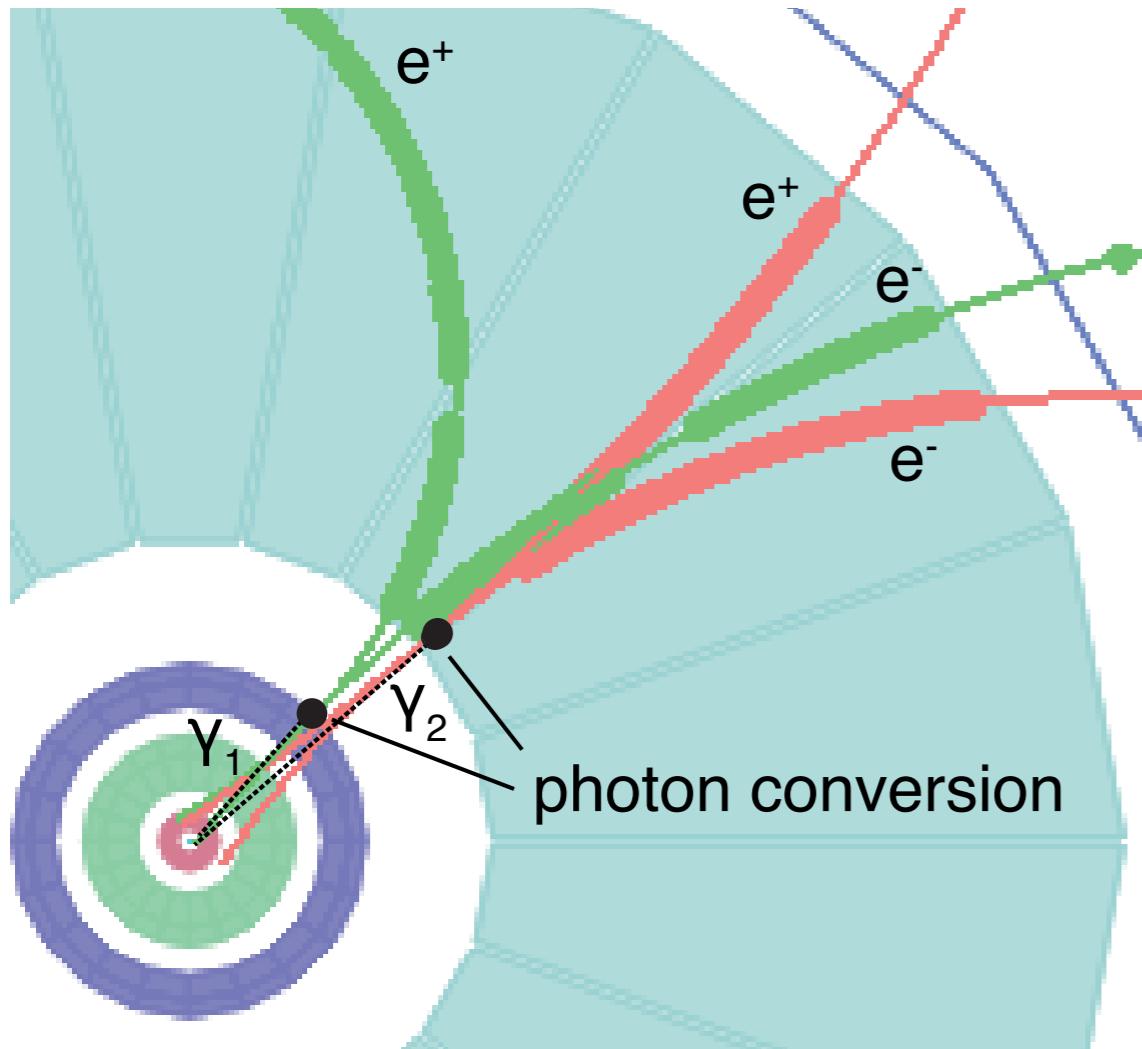
In most cases one tries to find independent sources of systematic uncertainties. These independent uncertainties are therefore added in quadrature:

$$\sigma_{\text{tot}}^2 = \sigma_1^2 + \sigma_2^2 + \dots + \sigma_n^2$$

Often a few source dominate the systematic uncertainty

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

Example: Neutral Pions Yields from Converted Photons in ALICE



PCM		
pp		
	1.1 GeV/c	5.0 GeV/c
Material budget	9.0	9.0
Yield extraction	0.6	2.6
e^+/e^- identification	0.7	1.4
Photon identification ($\chi^2(\gamma)$)	2.4	0.9
π^0 reconstruction efficiency	0.5	3.6
Pile-up correction	1.8	1.8
Total	9.5	10.3

In this measurement the material budget uncertainty dominates the systematic uncertainty

Describing Correlated Systematic Uncertainties (I)

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

$$x_i = x_{\text{true}} + \Delta x_{i,r} + \Delta x_s \quad \begin{aligned} \langle \Delta x_{i,r} \rangle &= 0, & \langle \Delta x_s \rangle &= 0, \\ \langle (\Delta x_{i,r})^2 \rangle &= \sigma_{i,r}^2, & \langle (\Delta x_s)^2 \rangle &= \sigma_s^2 \end{aligned}$$

Variance:

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

Covariance:

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

Describing Correlated Systematic Uncertainties (II)

Covariance matrix for x_1 and x_2 :

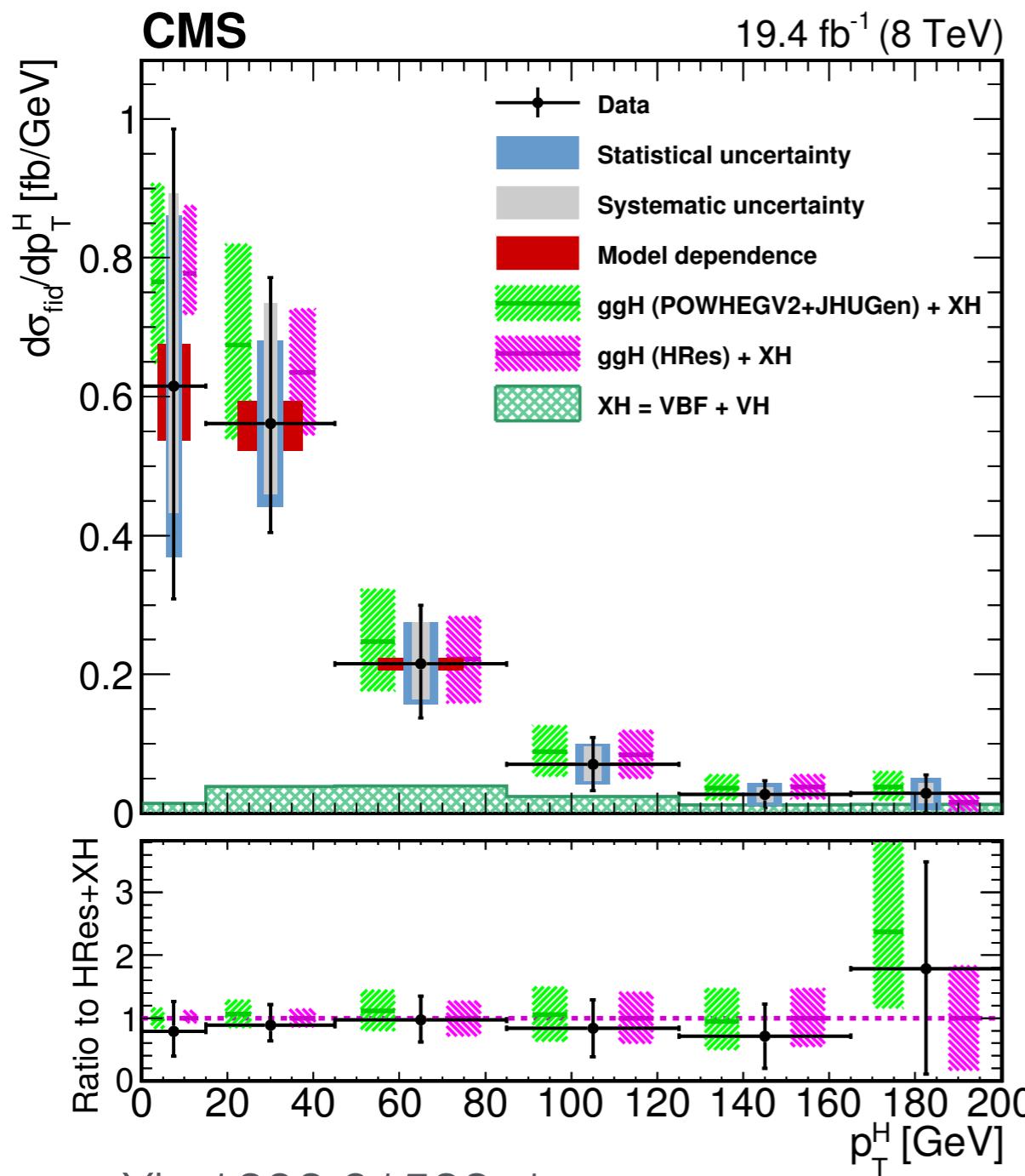
$$V = \begin{pmatrix} \sigma_{1,r}^2 + \sigma_s^2 & \sigma_s^2 \\ \sigma_s^2 & \sigma_{2,r}^2 + \sigma_s^2 \end{pmatrix}$$

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

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

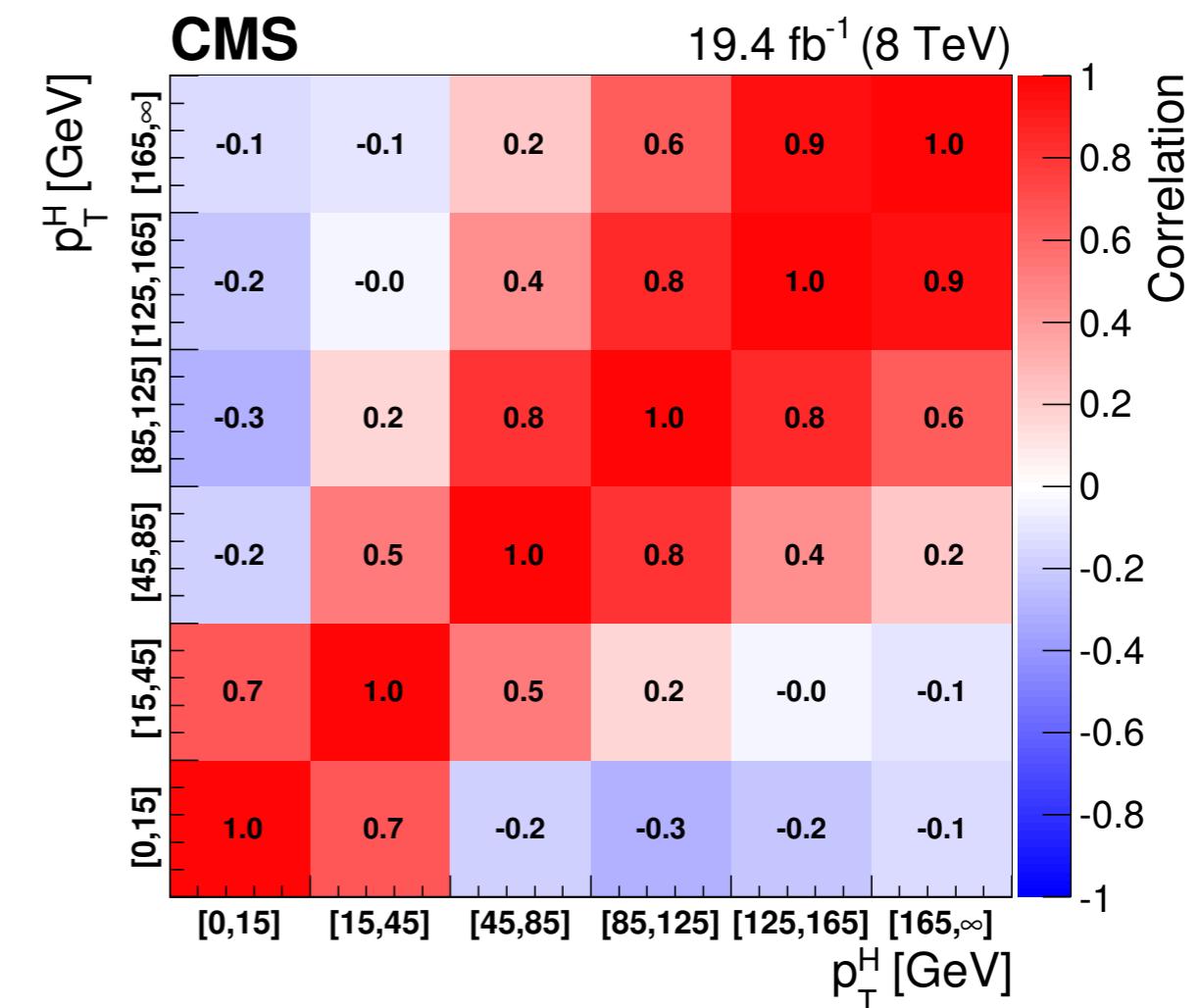
Example:

Transverse Momentum Spectrum of the Higgs-Boson



arXiv:1606.01522v1

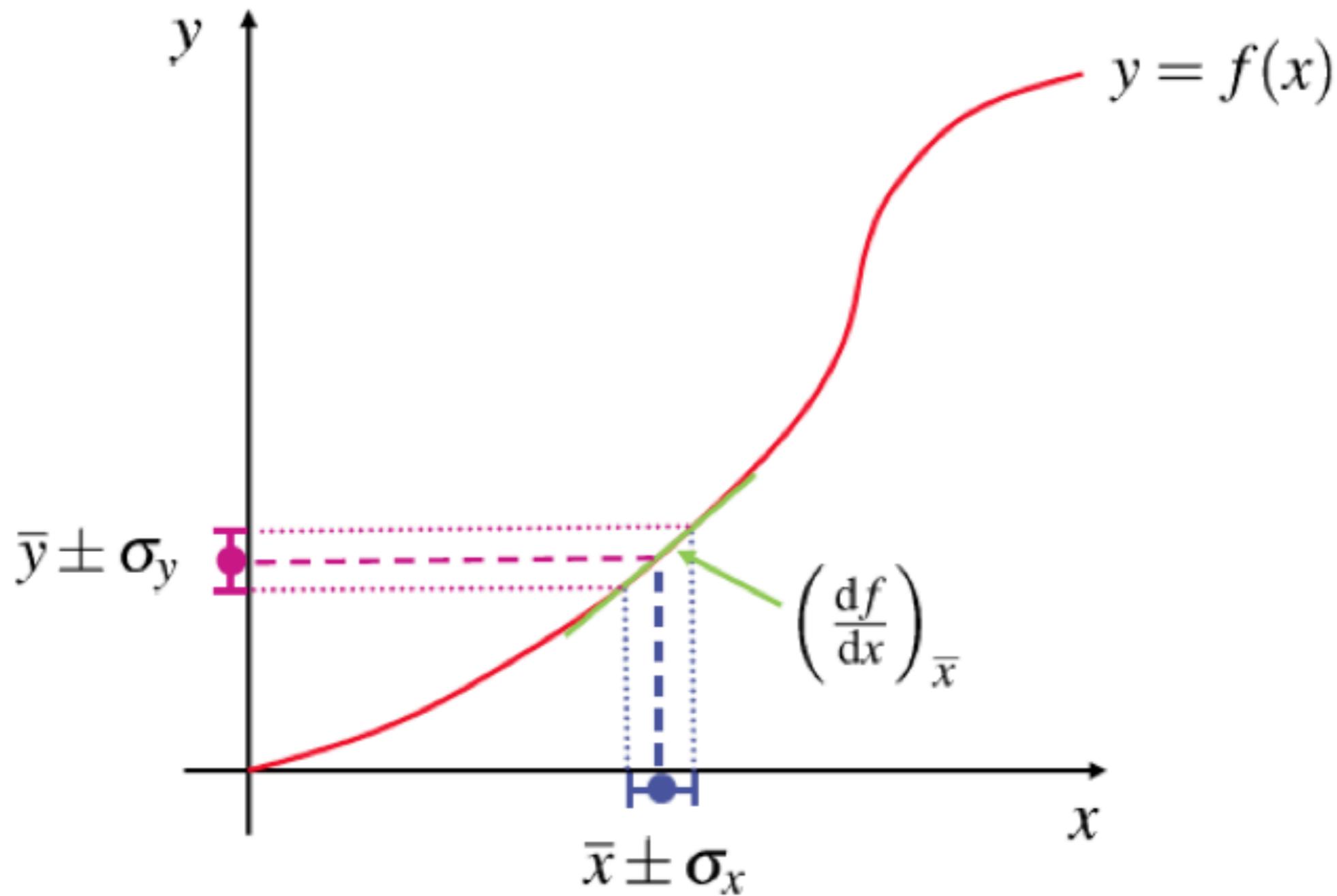
Correlation matrix of the p_T bins:



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

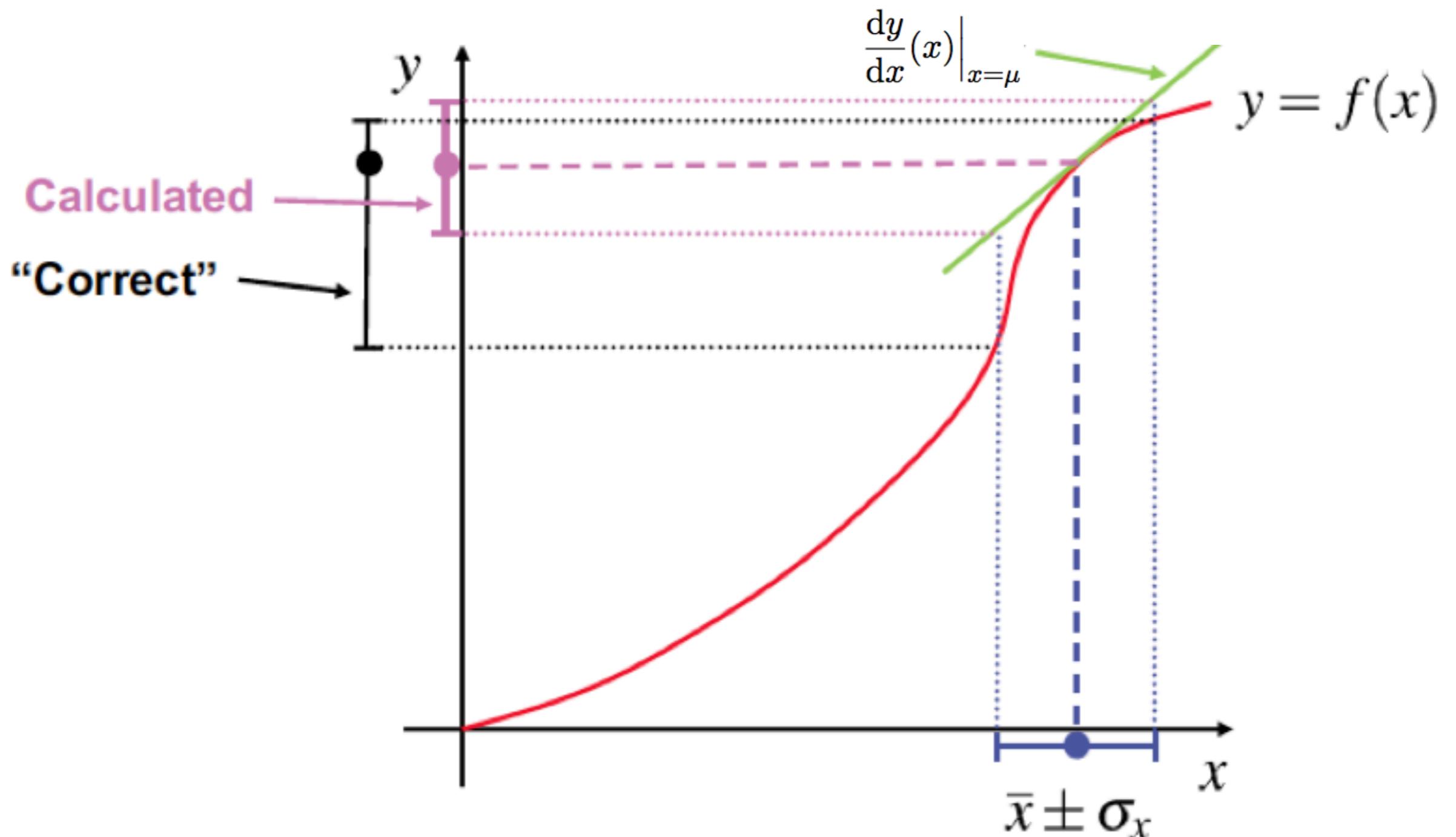
Error Propagation

Linear Error Propagation: Sometimes Applicable ...



Function sufficiently linear within $\pm\sigma$: 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:

$$\vec{x} = (x_1, x_2, \dots, x_n) \quad V_{ij} = \text{cov}[x_i, x_j]$$

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

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

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

Thus:

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

Matrix Notation

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

Then:

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

Example:

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

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

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

Linear Error Propagation: Examples

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

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

$$y = x_1 + x_2 \rightarrow \sigma_y^2 = \sigma_1^2 + \sigma_2^2 + 2\text{cov}[x_1, x_2]$$

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

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

Sanity checks:

Average of fully correlated measurements:

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

Difference of fully correlated measurements:

$$y = x_1 - x_2, \sigma_1 = \sigma_2 \equiv \sigma, \rho = 1 \\ \rightsquigarrow \sigma_y^2 = 2\sigma^2 - 2\sigma^2 = 0$$

Concrete Example: Momentum Resolution in Tracking

Charged particle moving in constant magnetic field:

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

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

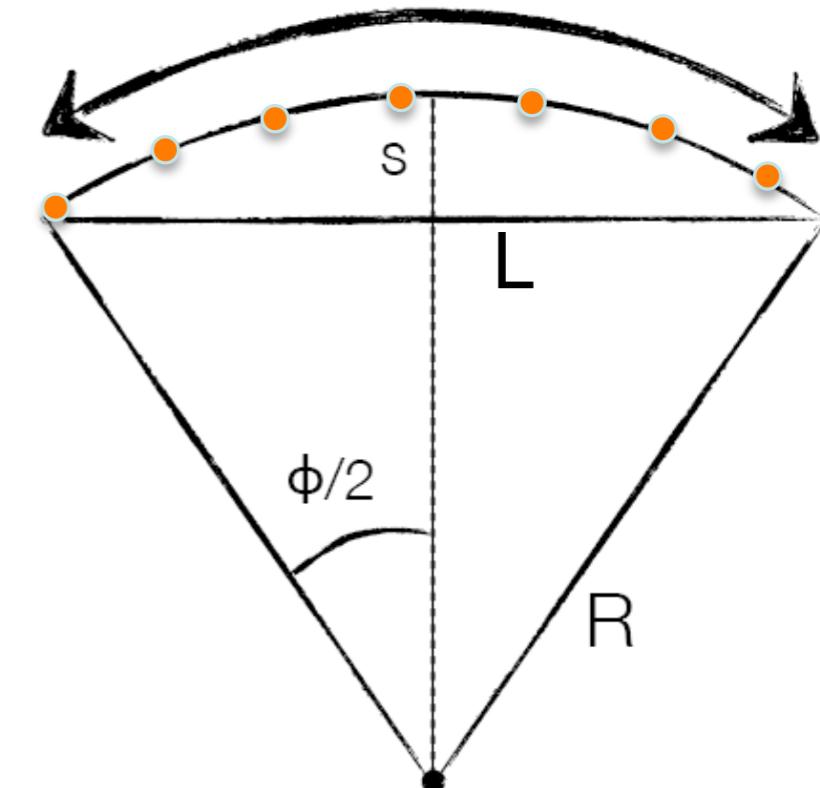
$$R = \frac{L^2}{8s}, \quad p_T = 0.3B \frac{L^2}{8s}$$

Momentum resolution:

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

Important features:

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



Example:

ATLAS nominal resolution

$$\left(\frac{\sigma_{p_T}}{p_T} \right)^2 = \boxed{0.001^2} + \boxed{(0.0005p_T)^2}$$

multiple scattering track uncertainty

Linear Error Propagation for Uncorrelated Measurements

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

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

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 .

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:

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

Then:

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

In matrix notation:

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

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:

$$E[x_i] = \mu; \quad V[x_i] = \sigma^2$$

Standard deviation of the mean:

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

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:

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

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):

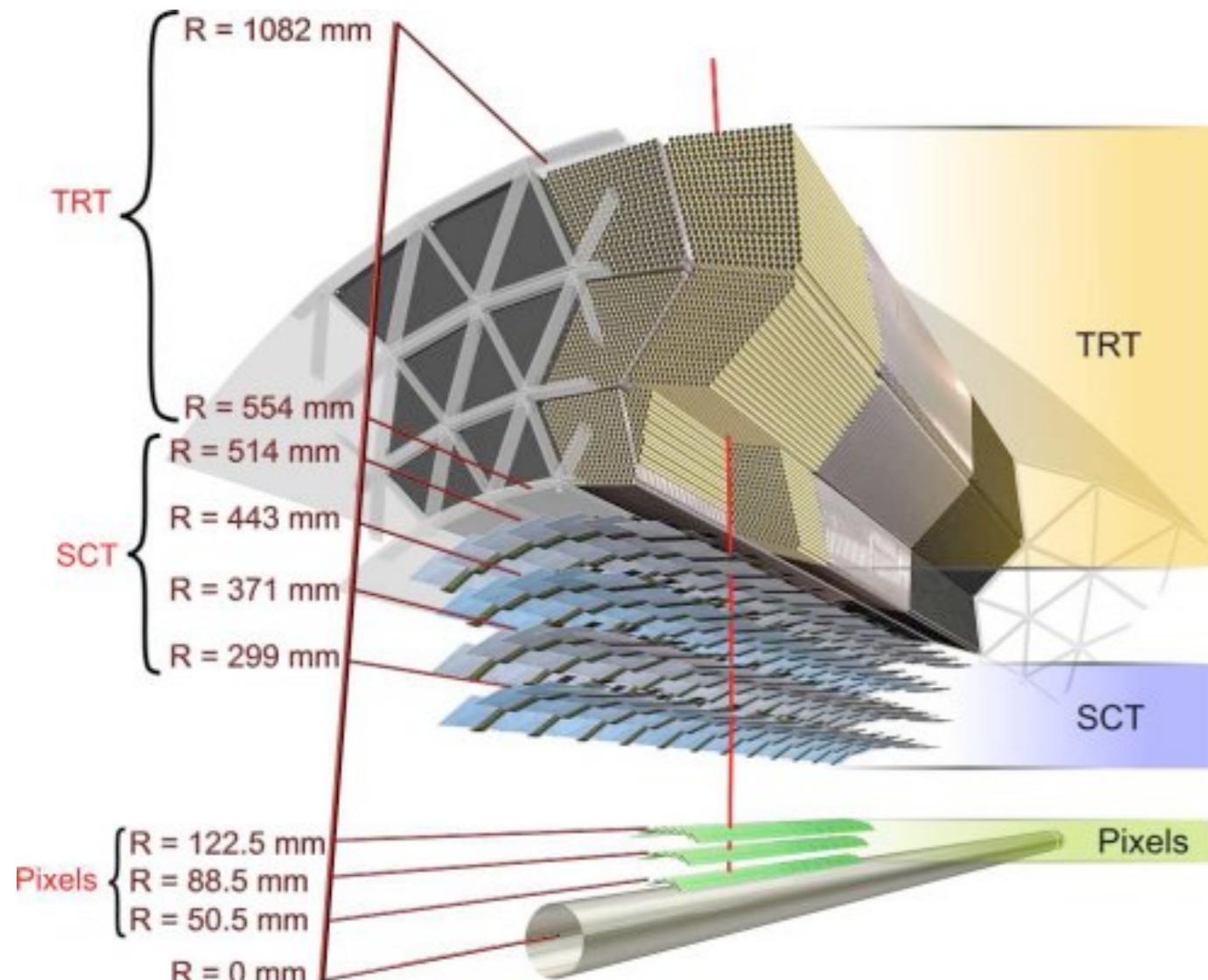
$$\frac{1}{\sigma_y^2} = \frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}$$

In general, for n uncorrelated measurements:

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

Example: Averaging Uncorrelated Measurements

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



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

detector	$p_T (\text{GeV})$
pixel detector	20 ± 2
semiconductor tracker	21 ± 1
transition radiation tracker	22 ± 4

Weighted average:

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

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

Weighted Average from Bayesian Approach

Consider two measurements μ_1 and μ_2 with Gaussian uncertainties σ_1 and σ_2 . In a Bayesian approach the probability distribution for the true value x is given by

$$p(x) \propto L(\mu_1, \mu_2|x)\pi(x)$$

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

$$\begin{aligned} p(x) &\propto L(\mu_1|x)L(\mu_2|x) \\ &= G(\mu_1; x, \sigma_1)G(\mu_2; x, \sigma_2) \\ &\propto \exp\left[-\frac{1}{2}\left(\frac{(x - \mu_1)^2}{\sigma_1^2} + \frac{(x - \mu_2)^2}{\sigma_2^2}\right)\right] \end{aligned}$$

The product of the two Gaussians gives a Gaussian with mean

$$\mu = w_1\mu_1 + w_2\mu_2 \quad \text{where } w_i = \frac{1/\sigma_i^2}{1/\sigma_1^2 + 1/\sigma_2^2}$$

and standard deviation

$$\frac{1}{\sigma^2} = \frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2} \quad \rightarrow \text{same result as before}$$

Monte Carlo Error Propagation

Example:

Ratio of two Gaussian distributed quantities

$$x = 5 \pm 1$$

$$y = 5 \pm 1$$

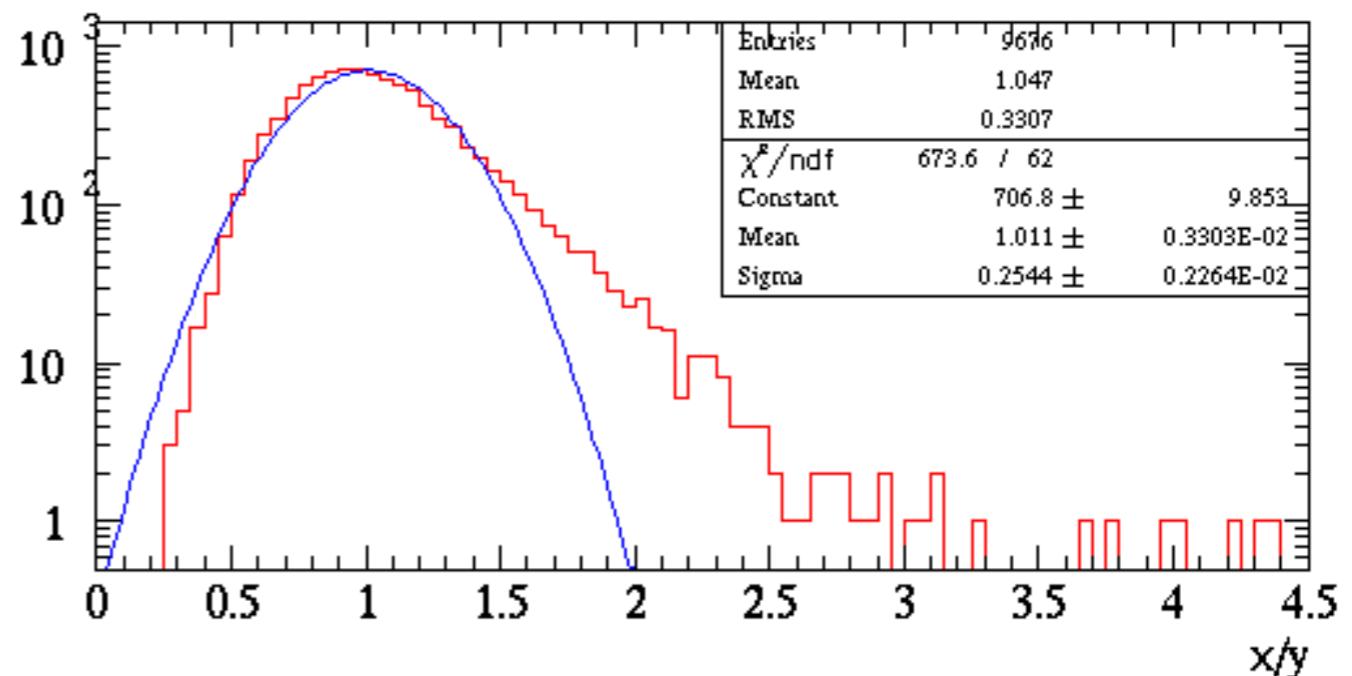
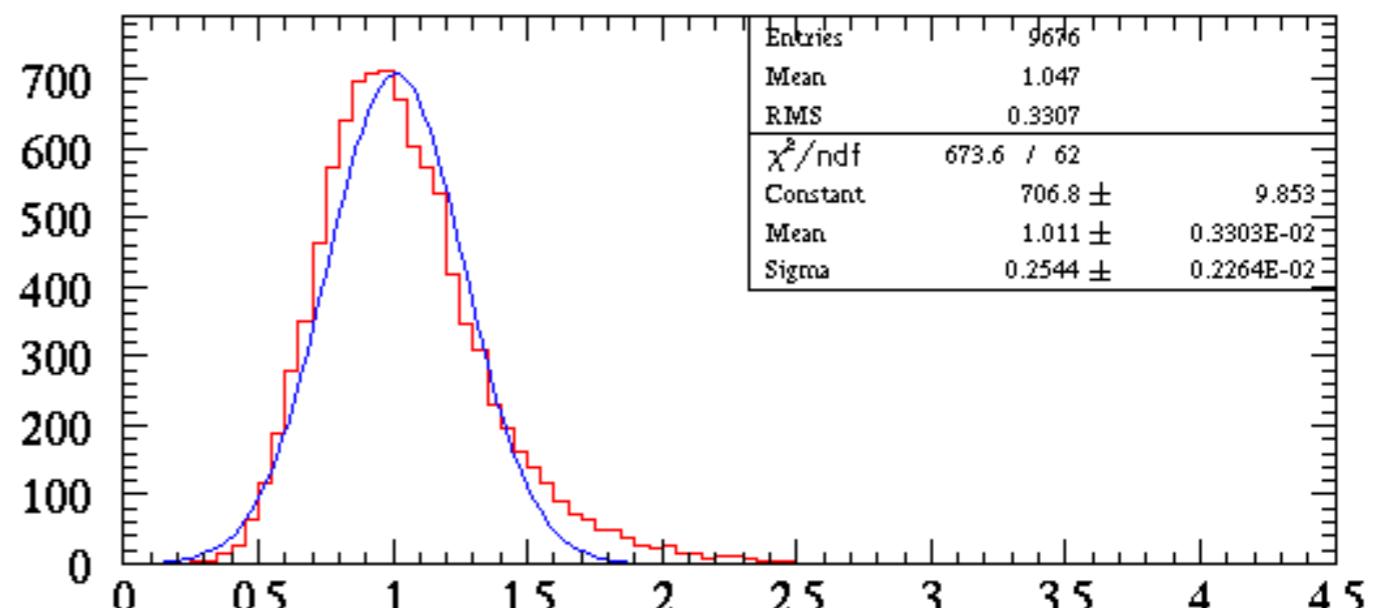
Approach: draw values for x and y many times and fill histogram with ratios

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