10/12/25

ROYAL HOLLOWAY UNIVERSITY OF LONDON

Errors-on-errors in xFitter

Enzo Canonero

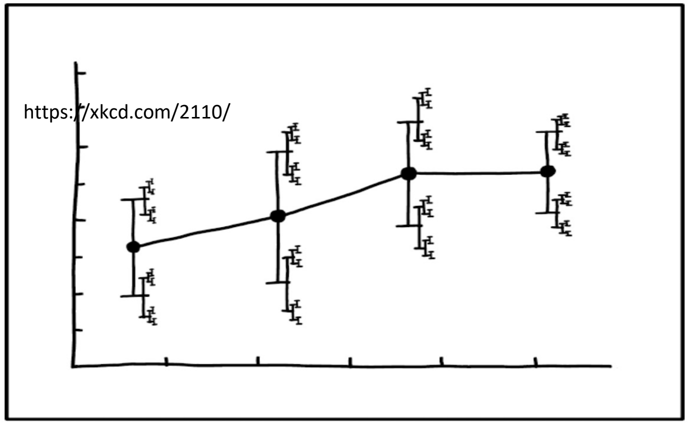
Glen Cowan

Motivation

ROYAL HOLLOWAY UNIVERSITY OF LONDON

1) *Some **systematic uncertainties*** can be well estimated:
   - **Related to stat. error of control measurements**
   - **Related to size of MC event sample**

2) But they can also be ***quite uncertain***:
   - **Theory systematics**
   - **Two points systematics ….**



References:
Full model: Eur. Phys. J. C 85.2 (2025)
My thesis: RHUL pure
Standalone toolkit: GitHub
Higher order asymptotics studies: Eur. Phys. J. C (2023) 83:1100

Motivation

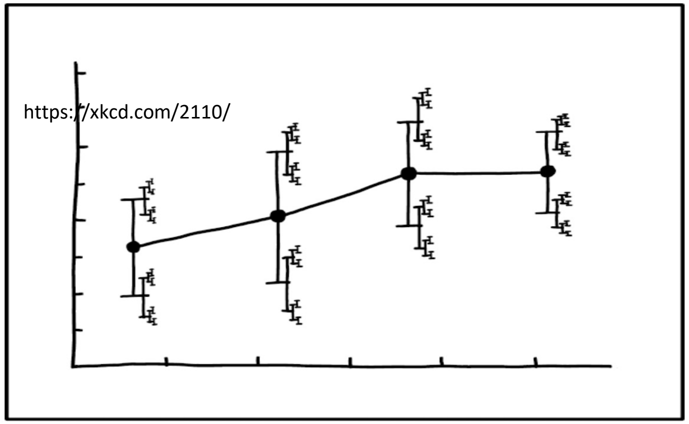
1) *Some* ***systematic uncertainties*** can be well estimated:

- **Related to stat. error of control measurements**
- **Related to size of MC event sample**

2) But they can also be ***quite uncertain***:

- **Theory systematics**
- **Two points systematics ….**

- Non-trivial consequences:
  - **Fits are pulled less by incompatible data**
  - **Incompatible data are treated as an extra source of uncertainty resulting in inflated confidence intervals**



References:
Full model: Eur. Phys. J. C 85.2 (2025)
My thesis: RHUL pure
Standalone toolkit: GitHub
Higher order asymptotics studies: Eur. Phys. J. C (2023) 83:1100

Formulation of the problem

ROYAL HOLLOWAY UNIVERSITY OF LONDON

- Suppose measurements $\boldsymbol{y}$ have a probability density $P(\boldsymbol{y}|\boldsymbol{\mu},\boldsymbol{\theta})$
  - $\boldsymbol{\mu}$ = Parameters of interest
  - $\boldsymbol{\theta}$ = Nuisance parameters

- Auxiliary Measurements $\boldsymbol{u}$ are used to provide info on nuisance parameters and are (often) assumed to be independently Gaussian distributed

- The resulting Likelihood is:

Can be a real measurement or just our best guess based on theoretical reasons

$$L(\boldsymbol{\mu},\boldsymbol{\theta}) = P(\boldsymbol{y},\boldsymbol{u}|\boldsymbol{\mu},\boldsymbol{\theta}) = P(\boldsymbol{y}|\boldsymbol{\mu},\boldsymbol{\theta}) \times \prod_i \frac{1}{\sqrt{2\pi}\sigma_{u_i}} e^{-(u_i-\theta_i)^2/2\sigma_{u_i}^2}$$

Formulation of the problem

- Suppose measurements $\boldsymbol{y}$ have a probability density $P(\boldsymbol{y}|\boldsymbol{\mu},\boldsymbol{\theta})$
  - $\boldsymbol{\mu}$ = Parameters of interest
  - $\boldsymbol{\theta}$ = Nuisance parameters

- Auxiliary Measurements $\boldsymbol{u}$ are used to provide info on nuisance parameters and are (often) assumed to be independently Gaussian distributed

- The resulting Likelihood is:

Can be a real measurement or just our best guess based on theoretical reasons

$$L(\boldsymbol{\mu},\boldsymbol{\theta}) = P(\boldsymbol{y},\boldsymbol{u}|\boldsymbol{\mu},\boldsymbol{\theta}) = P(\boldsymbol{y}|\boldsymbol{\mu},\boldsymbol{\theta})\times\prod_i \frac{1}{\sqrt{2\pi}\sigma_{u_i}} e^{-(u_i-\theta_i)^2/2\sigma_{u_i}^2}$$

- And the log Likelihood:

$$\log L(\boldsymbol{\mu},\boldsymbol{\theta}) = \log P(\boldsymbol{y}|\boldsymbol{\mu},\boldsymbol{\theta}) - \sum \frac{(\boldsymbol{u_i}-\boldsymbol{\theta_i})^2}{\boldsymbol{2\sigma_{u_i}^2}}$$

Formulation of the problem

- Suppose measurements $\boldsymbol{y}$ have a probability density $P(\boldsymbol{y}|\boldsymbol{\mu},\boldsymbol{\theta})$
  - $\boldsymbol{\mu}$ = Parameters of interest
  - $\boldsymbol{\theta}$ = Nuisance parameters

- Auxiliary Measurements $\boldsymbol{u}$ are used to provide info on nuisance parameters and are (often) assumed to be independently Gaussian distributed

- The resulting Likelihood is:

Can be a real measurement or just our best guess based on theoretical reasons

$$L(\boldsymbol{\mu},\boldsymbol{\theta}) = P(\boldsymbol{y},\boldsymbol{u}|\boldsymbol{\mu},\boldsymbol{\theta}) = P(\boldsymbol{y}|\boldsymbol{\mu},\boldsymbol{\theta})\times\prod_i \frac{1}{\sqrt{2\pi}\sigma_{u_i}} e^{-(u_i-\theta_i)^2/2\sigma_{u_i}^2}$$

- And the log Likelihood:

$$\log L(\boldsymbol{\mu},\boldsymbol{\theta}) = \log P(\boldsymbol{y}|\boldsymbol{\mu},\boldsymbol{\theta}) - \sum \frac{(\boldsymbol{u}_i - \boldsymbol{\theta}_i)^2}{2\boldsymbol{\sigma}_{u_i}^2}$$

Let systematic errors be potentially uncertain!

Gamma Variance Model (GVM)

ROYAL HOLLOWAY UNIVERSITY OF LONDON

- The original **quadratic terms** in the log likelihood replaced by **logarithmic terms:**

$$\sum_i \frac{(u_i - \theta_i)^2}{2\sigma_{u_i}^2} \longrightarrow \sum_i \left(1 + \frac{1}{2\varepsilon_i^2}\right) \log\left(1 + 2\varepsilon_i^2 \frac{(u_i - \theta_i)^2}{\sigma_{u_i}^2}\right)$$

ε = error-on-error parameter

ε = 0.3 means 30% uncertainty on σ

Gamma Variance Model (GVM)

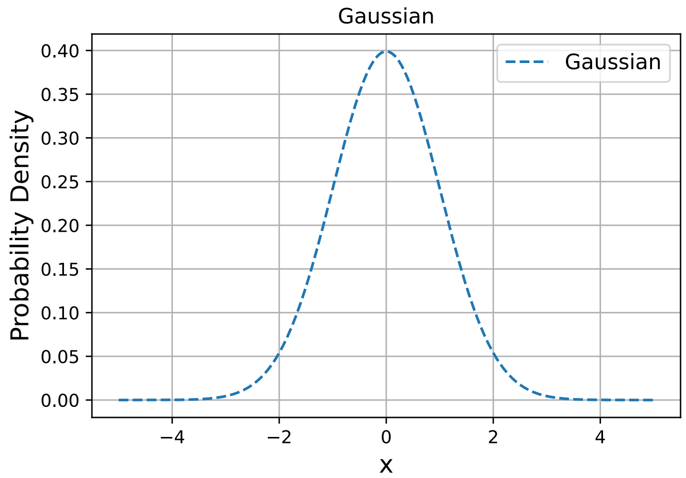
- The original **quadratic terms** in the log likelihood replaced by **logarithmic terms:**

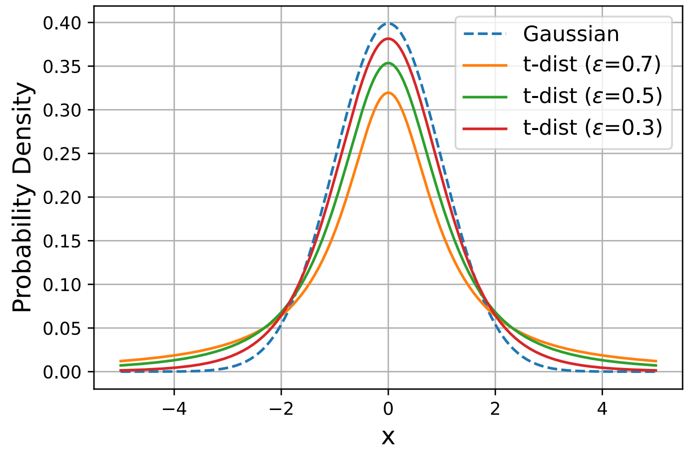
$$\sum_i \frac{(u_i - \theta_i)^2}{2\sigma_{u_i}^2} \longrightarrow \sum_i \left(1 + \frac{1}{2\varepsilon_i^2}\right) \log\left(1 + 2\varepsilon_i^2 \frac{(u_i - \theta_i)^2}{\sigma_{u_i}^2}\right)$$

ε = error-on-error parameter

ε = 0.3 means 30% uncertainty on σ

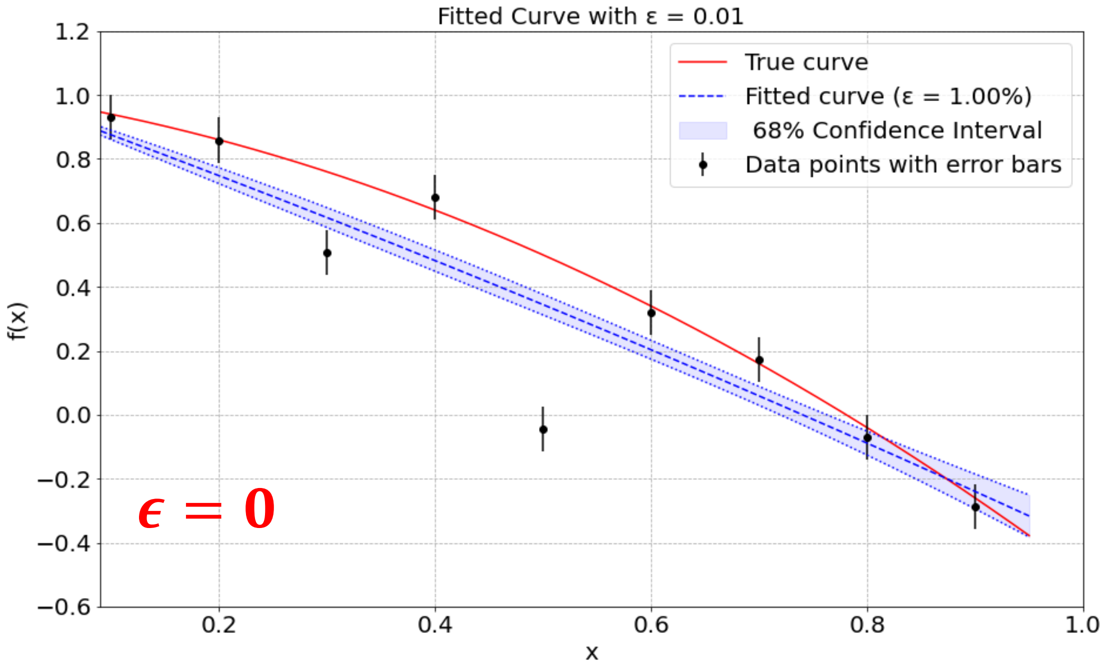
- Equivalent to switch from **Gaussian constraints** to **Student's t constraints** for systematics:





Fitting of a curve: compatible measurements

- Fit of a quadratic function with ***two outliers***



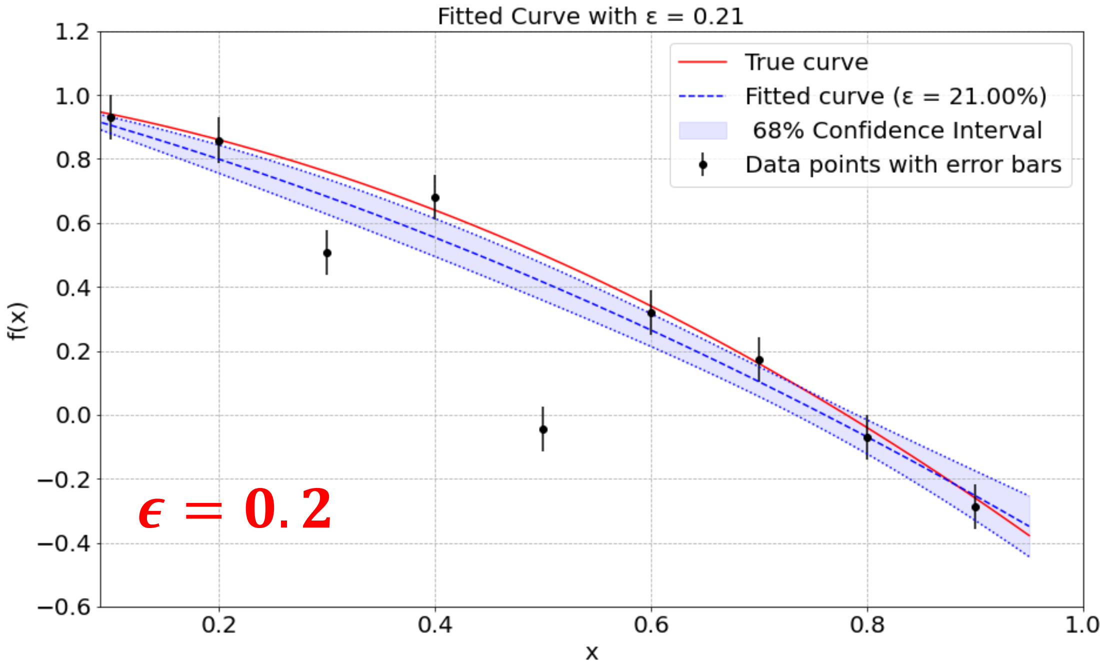
$$y_i \sim f(x_i) + \theta_i$$

Params of interest

$$f(x_i) = \boldsymbol{a}x_i^2 + \boldsymbol{b}x + \boldsymbol{c}$$

Fitting of a curve: compatible measurements

- Fit of a quadratic function with ***two outliers***



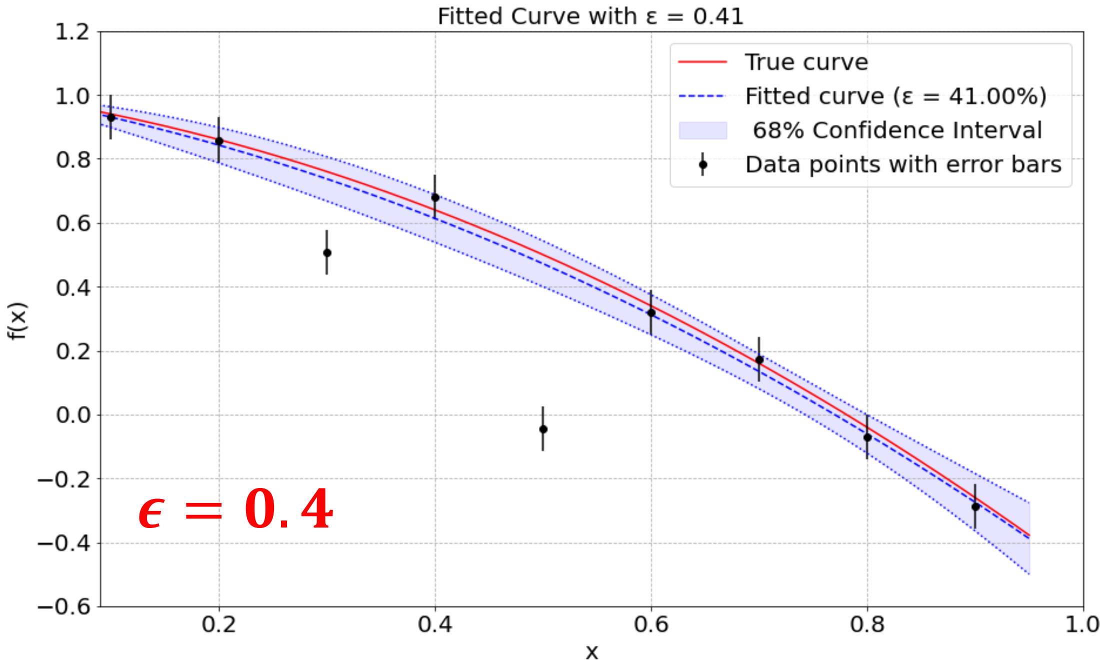
$$y_i \sim f(x_i) + \theta_i$$

Params of interest

$$f(x_i) = ax_i^2 + bx + c$$

Fitting of a curve: compatible measurements

- Fit of a quadratic function with ***two outliers***



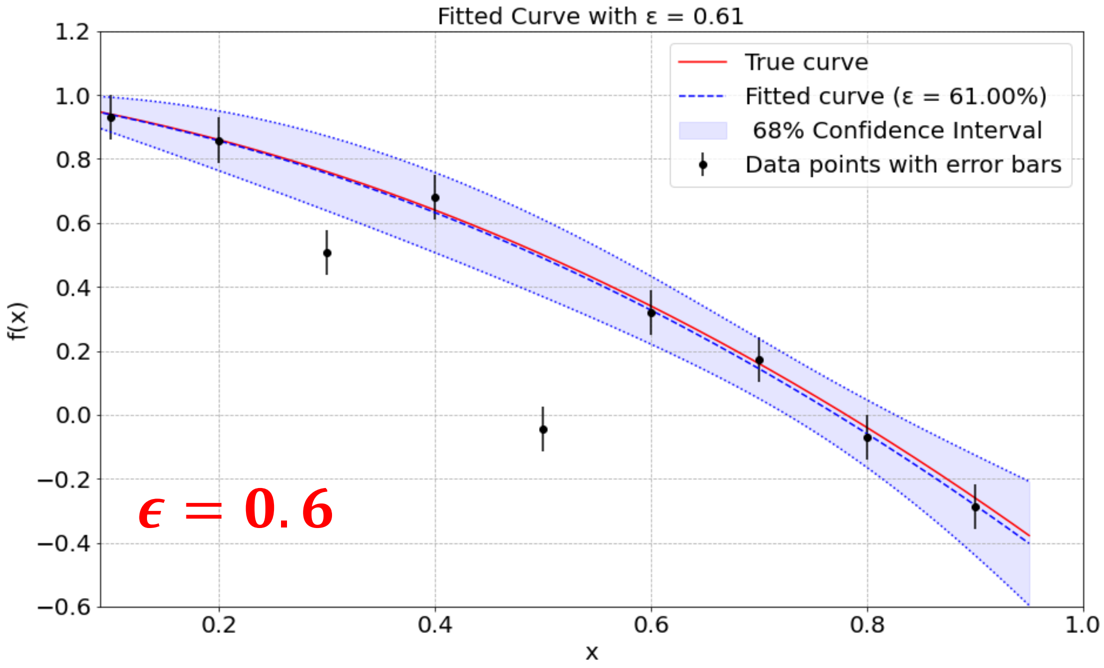
$$y_i \sim f(x_i) + \theta_i$$

Params of interest

$$f(x_i) = a x_i^2 + b x + c$$

Fitting of a curve: compatible measurements

- Fit of a quadratic function with <u>*two outliers*</u>



$$y_i \sim f(x_i) + \theta_i$$

Params of interest

$$f(x_i) = \boldsymbol{a} x_i^2 + \boldsymbol{b} x + \boldsymbol{c}$$

Complete model

- Gamma Variance Model:

$$\chi^2 = \sum_i \frac{(y_i - f_i(\boldsymbol{a}) - \sum_s \Gamma_i^s \theta_s)^2}{\sigma_i^2} + \sum_s \left(\mathbf{1} + \frac{\mathbf{1}}{\mathbf{2}\boldsymbol{\varepsilon}_i^2}\right) \mathbf{log}\left(\mathbf{1} + \mathbf{2}\boldsymbol{\varepsilon}_i^2 \boldsymbol{\theta}_i{}^2\right)$$

- Appliable both to addictive and multiplicative systematics as only the systematic terms in the chi2 are being changed

ROYAL HOLLOWAY UNIVERSITY OF LONDON

$$\chi^2 = \sum_i \frac{(y_i - f(\boldsymbol{a}) - \sum_s \Gamma_i^s \theta_s)^2}{\sigma_i^2} + \sum_s \left(\mathbf{1} + \frac{\mathbf{1}}{\mathbf{2}\boldsymbol{\varepsilon}_i^2}\right) \mathbf{log}\left(\mathbf{1} + \mathbf{2}\boldsymbol{\varepsilon}_i^2 \boldsymbol{\theta}_i{}^2\right)$$

- How do I minimize with respect to θ?
  - Numerically -> Treat θ as external
  - Analytically -> Expand the log in $\boldsymbol{\varepsilon}$

- In general just a subsample of systematics need a numerical minimization (only those with Large pulls)

- All the others can be minimized with the analytical approach

Bartlett correction

- Correction factors needed to account for the non-Gaussianity of the χ^2 (log-terms)

  - Goodness-of-fit: $\chi^2 \rightarrow \frac{\chi^2}{\boldsymbol{b}_{\chi^2}}$

  - Covariance matrix $V \rightarrow V * \boldsymbol{b}_V$

- In general $\boldsymbol{b}_{\chi^2} \neq \boldsymbol{b}_V$

- Non-negligible if number EonE > ~10

- **Steering.txt**
  - Specify whether to treat each systematic uncertainty as **External** or **Nuisance** (already implemented).
  - Specify the **error-on-error** value.
  - Specify the number of **iterations** for the analytical procedure.
  - Specify whether to enable **Bartlett corrections**.

```
&Systematics
  ListOfSources = 'sysHZComb1053:E', 'proc_tb21:E'

  Epsilon = 0.61, 0.61
  n_iterations = 4
  Enable_Bartlett = .true.

&End
```

- **Systematics.inc**
  - Initialize errors-on-errors related variables

```
C  Errors-on-Errors settings
      logical          EoEEnabled
      integer          EoE_n_iterations
      logical          EoEActive(NSYSMAX)
      double precision EoEEpsilon(NSYSMAX)

      common/CEonE/ EoEEnabled, EoE_n_iterations, EoEActive, EoEEpsilon

C --- Bartlett corrections for EoE
      logical BartlettEnabled
      double precision BartlettLRFactor
      double precision BartlettGoFFactor
      double precision BartlettSysFactor(NSysMax)
      common/CBartlett/ BartlettEnabled, BartlettLRFactor, BartlettGoFFactor, BartlettSysFactor
```

- Read_steer.f
  1. Set defaults (Set_Defaults)
  2. Read steering file (read_systematics)

```
C E-on-E defaults
      EoEEnabled       = .false.
      EoE_n_iterations = 2
      do i=1,NSYSMAX
        EoEActive(i)  = .false.
        EoEEpsilon(i) = 0.0D0
      enddo

C Bartlett defaults
      BartlettEnabled          = .true.
      BartlettLRFactor         = 0.0D0
      BartlettGoFFactor        = 0.0D0
      do i=1,NSYSMAX
        BartlettSysFactor(i)   = 0.0D0
      enddo
```

```
C --- Inspect Epsilon() from &Systematics
      neps = 0
      do i=1,nsys
         if (Epsilon(i) .gt. -1.0D98) then
            if (Epsilon(i) .lt. 0.0D0) then
               call hf_errlog(29092502,'F: Epsilon(i) must be >= 0 or unset')
               call hf_stop
            endif
            neps = neps + 1
         endif
      enddo

C Only proceed if there is at least one non-negative value
      if (neps .gt. 0) then
         if (neps .eq. nsys) then
            do i=1,nsys
               if (Epsilon(i) .gt. 0.0D0) then
                  EoEEpsilon(i) = Epsilon(i)
                  EoEActive(i)  = .true.
               else
                  EoEEpsilon(i) = 0.0D0
                  EoEActive(i)  = .false.
               endif
            enddo
         else
            call hf_errlog(29092501,
     $ 'F: Systematics/Epsilon must be length(NSources)')
            call hf_stop
         endif
      endif
```

Code is thoroughly commented

ROYAL HOLLOWAY UNIVERSITY OF LONDON

- **getchisquare.f**

chi2_calc_chi2: Set log-constrain if EonE are active for systematic K

```
C Correlated chi2 part:
      fcorchi2_in = 0.d0
      do k=1, NSys
         if (SysForm(k) .eq. isNuisance .or. SysForm(k) .eq. isExternal) then
            if (EoEEnabled .and. EoEActive(k)) then
               temp_val = 2.0D0 * EoEEpsilon(k)**2 * rsys_in(k)**2 * SysPriorScale(k)
               fcorchi2_in = fcorchi2_in
     $            + (1.0D0 + 1.0D0/(2.0D0*EoEEpsilon(k)**2))
     $              * log(1.0D0 + temp_val)
            else
               fcorchi2_in = fcorchi2_in + rsys_in(k)**2 * SysPriorScale(k)
            endif
         endif
```

ROYAL HOLLOWAY UNIVERSITY OF LONDON

chi2_calc_syst_shifts: Iterate to minimize analytically sources with active EonE

```
C EoE (errors-on-errors) iterations for nuisance sources
      if (EoEEnabled) then
         do iter = 1, EoE_n_iterations

C reset incremental shifts
            do i=1,nsys
               shift1(i) = 0.0D0
            enddo

C rebuild A and C; diagonal = prior
            do i=1,nsys
               C(i) = 0.0D0
               do j=1, nsys
                  A(i,j) = 0.0D0
               enddo
C quadratic prior by default; switch to EoE log prior if active (nuisance only)
               if ( SysForm(i) .eq. isNuisance ) then
                  if (EoEActive(i)) then
                     Numerator_eps   = 1.0D0 + 2.0D0 * EoEEpsilon(i)**2
                     Denominator_eps = ( 1.0D0 / SysPriorScale(i) )
     $                               + 2.0D0 * EoEEpsilon(i)**2 * shift0(i)**2
```

ROYAL HOLLOWAY UNIVERSITY OF LONDON

chi2_calc_syst_shifts: Compute Bartlett factors, if **EnableBartlett** is set to **True**

```
C Account for Bartlett factors
      if (iflag.eq.3) then
        if (BartlettEnabled .and. EoEEnabled) then
          do i = 1, nsys
            if (SysForm(i) .eq. isNuisance) then
              BartlettSysFactor(i) = 0.0D0
              if (EoEActive(i)) then
                eps2 = EoEEpsilon(i)*EoEEpsilon(i)
                j_ii = A(i,i)
                sigma_u2 = ( 1.0D0 / SysPriorScale(i) ) + ( 2.0D0*eps2*shift0(i)*shift0(i) ) / ( 1.0D0 + 2.0D0*eps2 )

                ratio   = j_ii / sigma_u2

                b_theta = ( 4.0D0*ratio - ratio*ratio ) * eps2
                BartlettSysFactor(i) = b_theta
              endif
            endif
          enddo
        endif
      endif

C Apply Bartlett factors to ersys_in
      do l=1,nsys
        if ( SysForm(l) .eq. isNuisance ) then
          rsys_in(l) = shift0(l)
          if (iflag.eq.3) then
            ersys_in(l) = sqrt(A(l,l)) * ( 1 + BartlettSysFactor(l))
          endif
        endif
      enddo
```

ROYAL HOLLOWAY UNIVERSITY OF LONDON

- fcn.f

Process Bartlett factors

```
   ! ----- Bartlett-only-for-printing scaling -----
   nExtSyst = 0
   do i=1,nsys
      if ( SysForm(i) .eq. isExternal) then
         nExtSyst = nExtSyst + 1
      endif
   enddo

   nPOI = nparFCN - nExtSyst
   print *, 'External systs = ', nExtSyst
   c_bart_chi2 = 1.0D0
   c_bart_ci = 1.0D0
   if (BartlettEnabled .and. EoEEnabled) then
      if (ndf .gt. 0) then
         c_bart_chi2 = 1.0D0 / ( 1.0D0 + BartlettGoFFactor / dble(ndf) )
         c_bart_ci   = sqrt(1.0D0 + BartlettLRFactor / dble(nPOI))
         ! Warn only when Bartlett is active and reduces printed values
         if (c_bart_chi2 .lt. 1.0D0) then
            call hf_errlog(25100101,
$'W: c_bart_chi2 < 1; mathematically should be <=1, consider setting Enable_Bartlett = .false.')
         endif
      endif
   endif
```

Apply Bartlett factors only when printing the results. The function's return value is left unchanged, so other methods that call it are not affected.

```
! Scale ONLY what we print:
chi2out_print = chi2out * c_bart_chi2
```

- **error_bands_pumplin.f**

Error_Bands_Pumplin: Compute Bartlett factors to rescale confidence intervals

```
nExtSyst = 0
do i=1,nsys
   if ( SysForm(i) .eq. isExternal) then
      nExtSyst = nExtSyst + 1
   endif
enddo

nPOI = nparFCN - nExtSyst
c_BartLR    = 1.0D0
bart_scale = 1.0D0
if (BartlettEnabled .and. EoEEnabled) then
   if (nPOI .gt. 0) then
      c_BartLR = 1.0D0 + BartlettLRFactor/dble(nPOI)
      bart_scale = sqrt(c_BartLR)
   endif
endif
```

Error_Bands_Pumplin: Apply these factors to the eigen-vector shifts

```
C
C Shift parameters by the j-th de-correlated error:
C
            do i=1,npar
               a(i) = pkeep(i)
               iint = iunint(i)
               if (iint.gt.0) then
                  if(doOffset) then
                    shift = shift_dir * DecorVarShift(iint, j)
                  else
                    call MNSTAT(fmin, fedm, errdef, npari, nparx, istat)   !> MW&FG for scaling with DeltaChi2>1.0
                    shift = shift_dir * GetUmat(iint,j)*SQRT(errdef)       !> MW&FG for scaling with DeltaChi2>1.0
                  endif
                  shift = shift * bart_scale
                  a(i) = a(i) + shift
               endif
            enddo  ! i
```

ErrBandsSym: same implementation

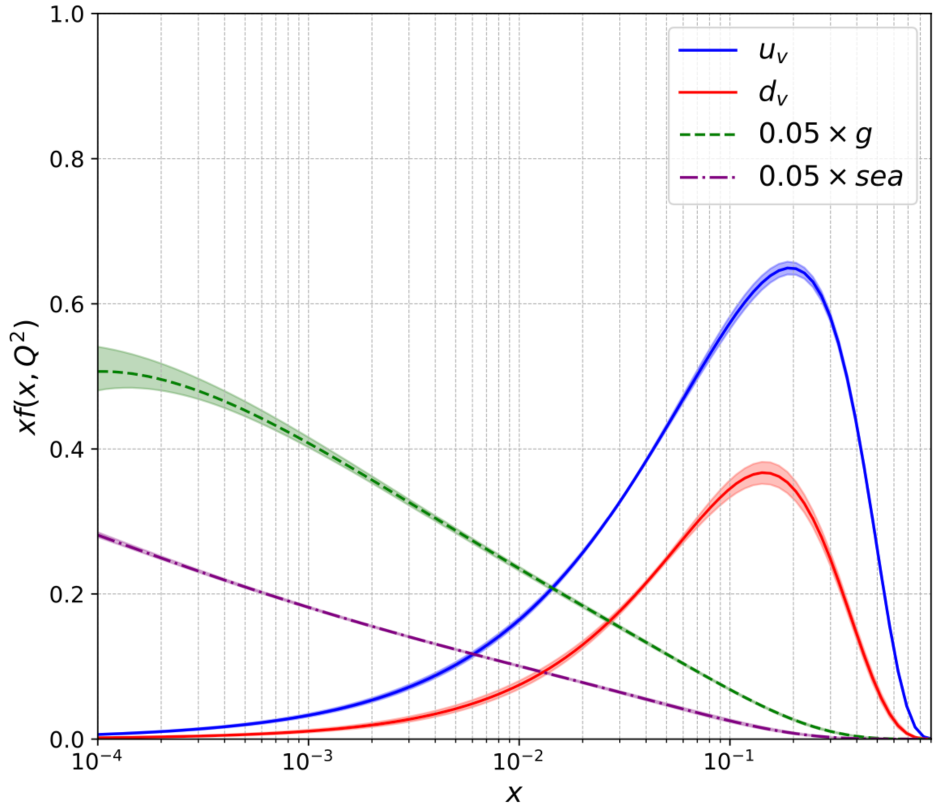
PDF fits

PDF fits determine the parton momentum distributions inside hadrons from a global set of experimental cross-section data.

Mutual tension:

- PDFs from different experiments often disagree at the level of their quoted experimental uncertainties
- When combined they often yield values $\chi^2/DOF > 1$

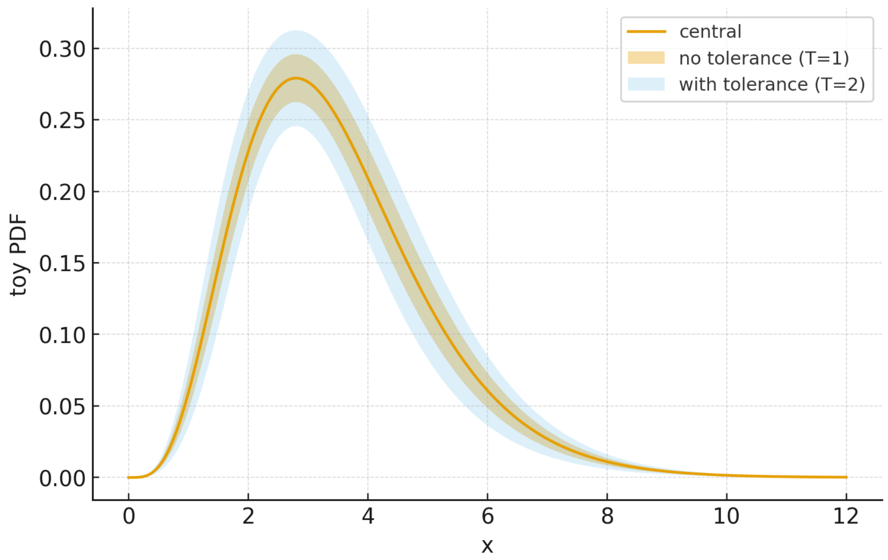
- **AIm**: assign "errors on errors" to the experimental uncertainties of the fit dataset



PDF fits

Problem: Often in PDF fits one finds values of $\frac{\chi^2}{Dof} > 1$ due to tensions among diverse datasets

Solution: In PDF fits a tolerance[*] $T > 1$ replaces $\Delta\chi^2 = 1$ by $\Delta\chi^2 = T^2$ so that the quoted confidence intervals have correct coverage



Why $T > 1$:

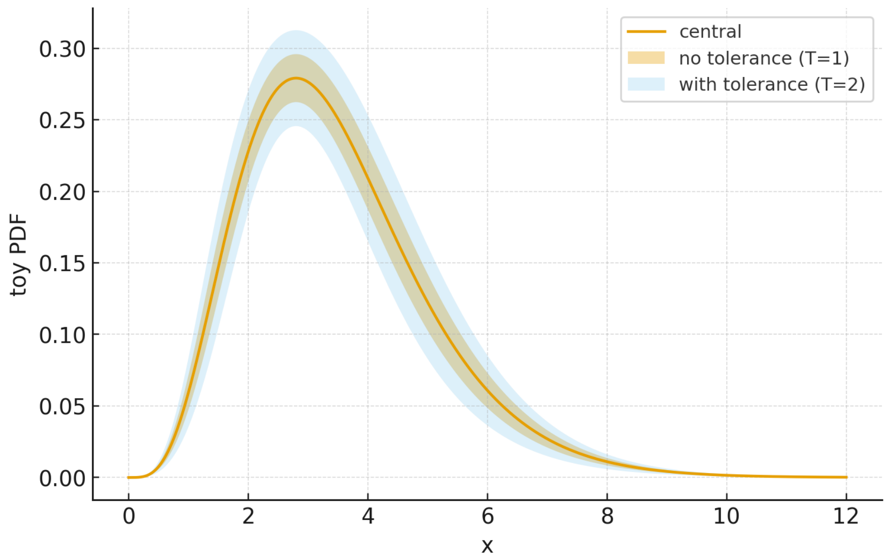
- Misestimated errors/correlations
- Parametrization/fit
- Theoretical predictions
- Non-Gaussian likelihoods

[*] Eur. Phys. J. C 63 (2009)

PDF fits

Problem: Often in PDF fits one finds values of $\frac{\chi^2}{Dof} > 1$ due to tensions among diverse datasets

Solution: In PDF fits a tolerance[*] $T > 1$ replaces $\Delta\chi^2 = 1$ by $\Delta\chi^2 = T^2$ so that the quoted confidence intervals have correct coverage



Why $T > 1$:

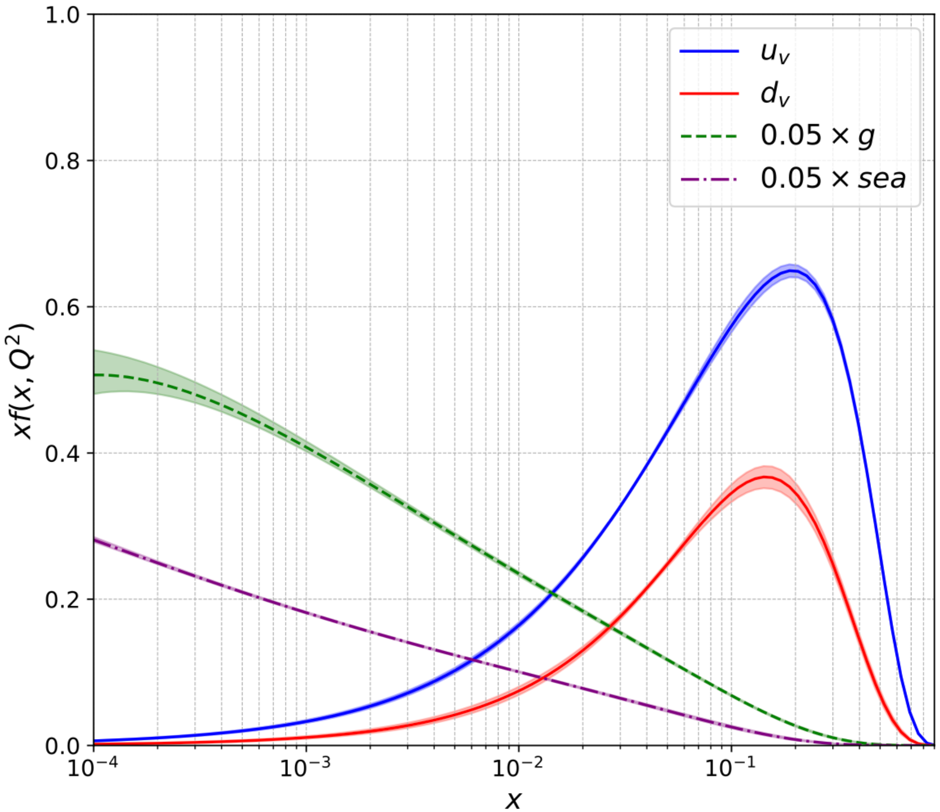
- **Misestimated errors**/correlations
- Parametrization/fit
- Theoretical predictions
- **Non-Gaussian likelihoods**

These two points are addressed by the errors-on-errors framework simultaneously

[*] Eur. Phys. J. C 63 (2009)

HERA combined dataset

$Q^2 = 10\ \text{GeV}^2$



- With $\epsilon = 0$, we reproduce the results of the Hera fit:

$$\frac{\chi^2}{DOF} = \frac{1363}{1131}$$

- We use the fit setup and parametrization of the combined HERA dataset paper[*]

[*]: Eur. Phys. J. C 75.12 (2015)

HERA combined dataset

- 169 systematic sources in the fit (Bartlett factor matters!)

- Group them in three categories[*]
  - ”Ugly” systematics $\boldsymbol{\epsilon_s = 0.6}$ (32)
  - ”Bad” systematics $\boldsymbol{\epsilon_s = 0.3}$ (12)
  - ”Good” systematics $\boldsymbol{\epsilon_s = 0.0}$ (125)

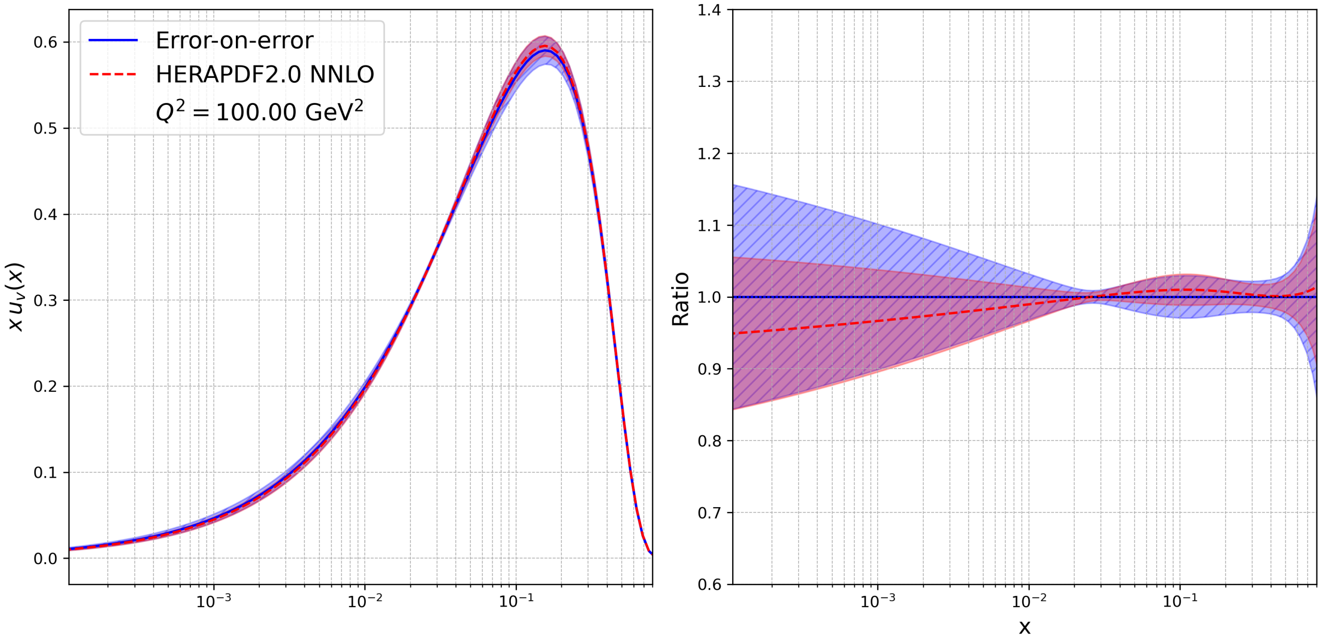
$$\frac{\chi^2}{DOF} = \frac{1363}{1131} \longrightarrow \frac{1315}{1131}$$

[*] backup

HERA combined dataset (preliminary)

1. Valence up-quark PDF

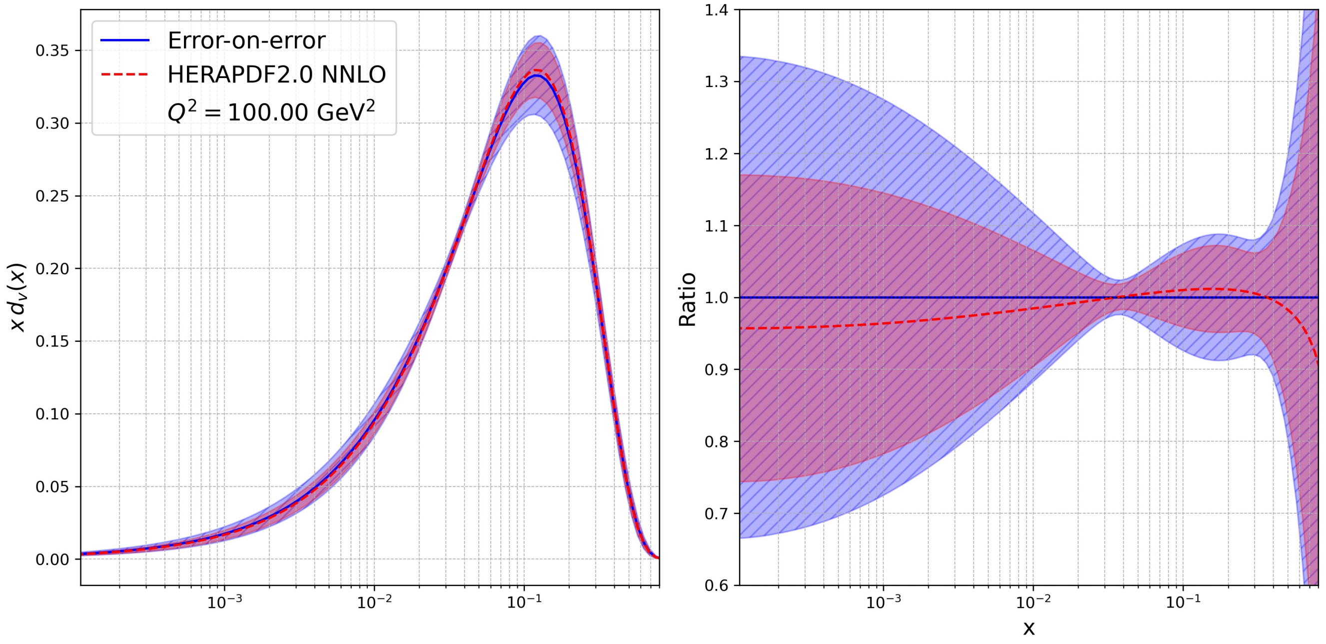
$Q^2 = 1.9$ GeV²



HERA combined dataset (preliminary)

1. Valence down-quark PDF

$Q^2 = 1.9$ GeV^2

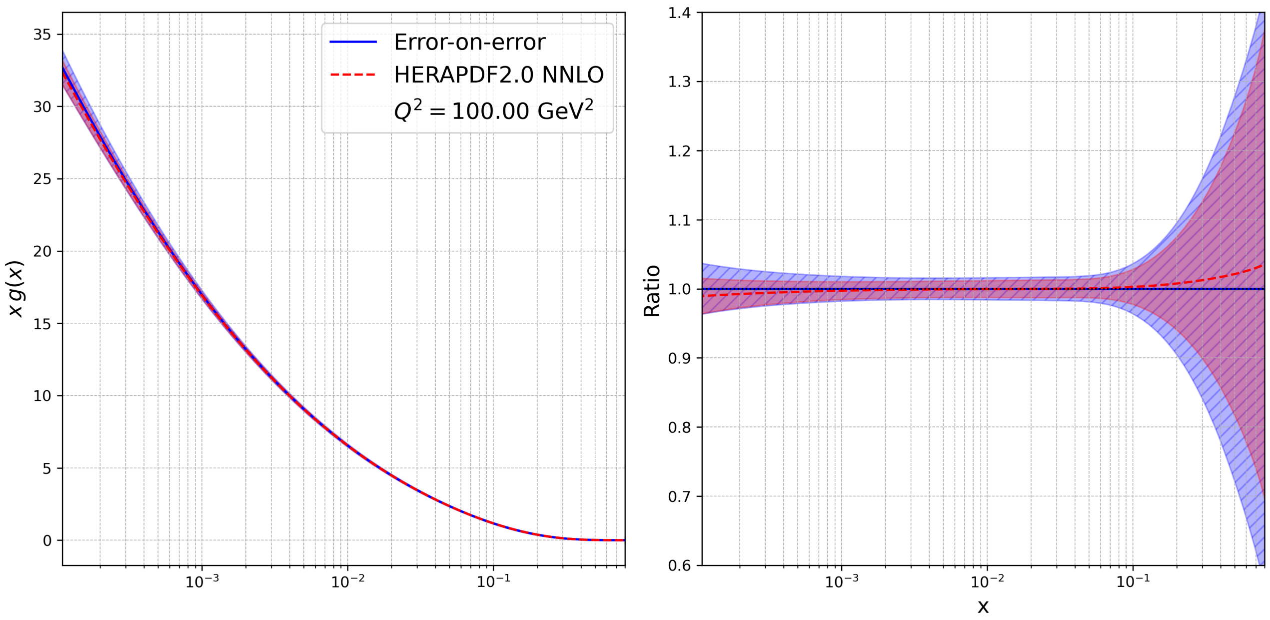


HERA combined dataset (preliminary)

ROYAL HOLLOWAY UNIVERSITY OF LONDON

2. Gluon PDF

$Q^2 = 1.9\ \text{GeV}^2$

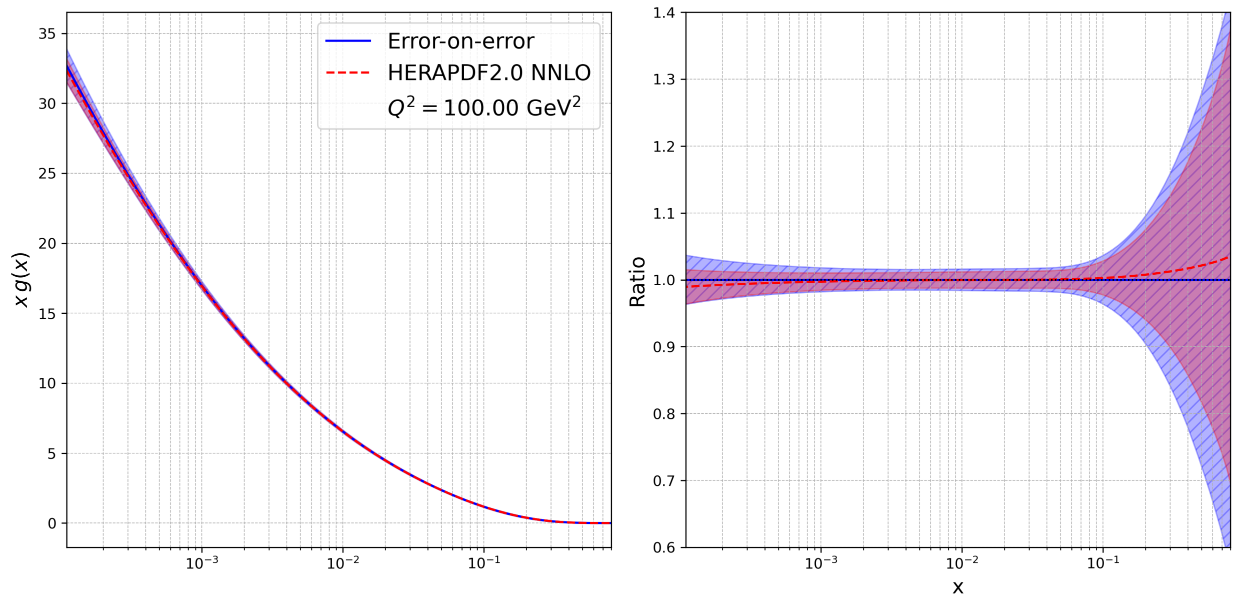


HERA combined dataset (preliminary)

ROYAL HOLLOWAY UNIVERSITY OF LONDON

2. Gluon PDF

$Q^2 = 1.9$ GeV²



Comments:

- PDFs are modified in regions where the data are less well modelled or exhibit tensions
- Specifically, low Q^2 region $(3.5 < Q^2 < 10)$ GeV²

ROYAL HOLLOWAY UNIVERSITY OF LONDON

Thank you for your attention

Back-up slides

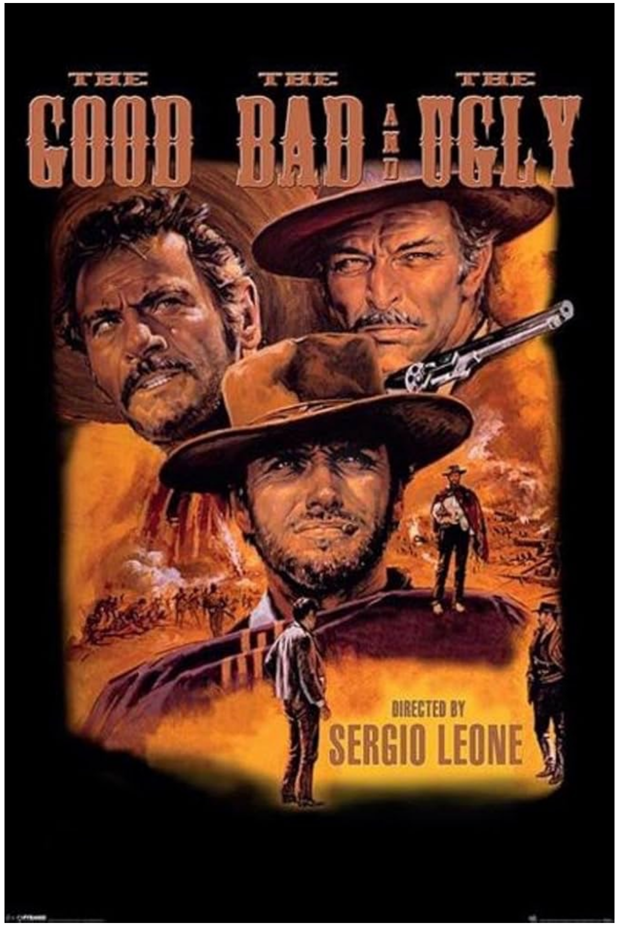
Motivation

Particle physics experiments face a vast variety of systematic uncertainties*:

- **"Good" Systematics:**
  - Statistically driven uncertainties (your own calibrations)
  - Clear probabilistic model

- **"Bad" Systematics:**
  - Do not reliably improve with more data
  - E.g: external results, analysis methodology biases, …

- **"Ugly" Systematics:**
  - Theory uncertainties
  - No well-defined sampling distribution
  - Treated via ad-hoc prescriptions



*Pekka Sinervo – PHYSTAT 2003, Nicholas Wardle

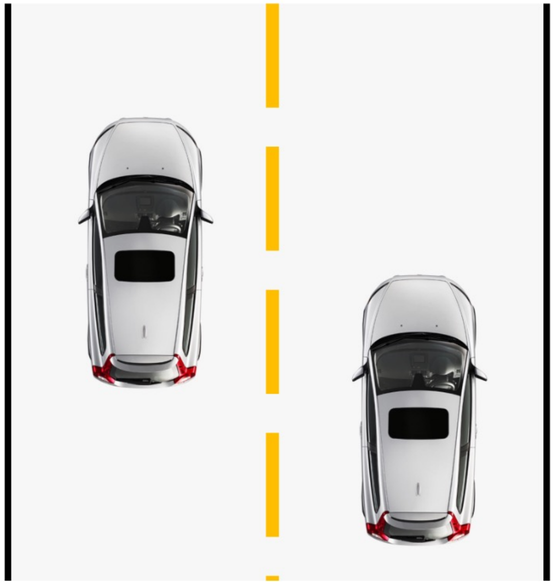
Ugly systematics: discrete choices

ROYAL HOLLOWAY UNIVERSITY OF LONDON

Compare two models $\mathcal{O}_1$ and $\mathcal{O}_2$ and define:

$$\hat{\mathcal{O}} = \frac{\mathcal{O}_1 + \mathcal{O}_2}{2} \qquad \Delta\mathcal{O} = \frac{|\mathcal{O}_1 - \mathcal{O}_2|}{\sqrt{2}}$$

- The average prediction $\hat{\mathcal{O}}$ may have no physical meaning (Phillip Litchfield two lane traffic example)



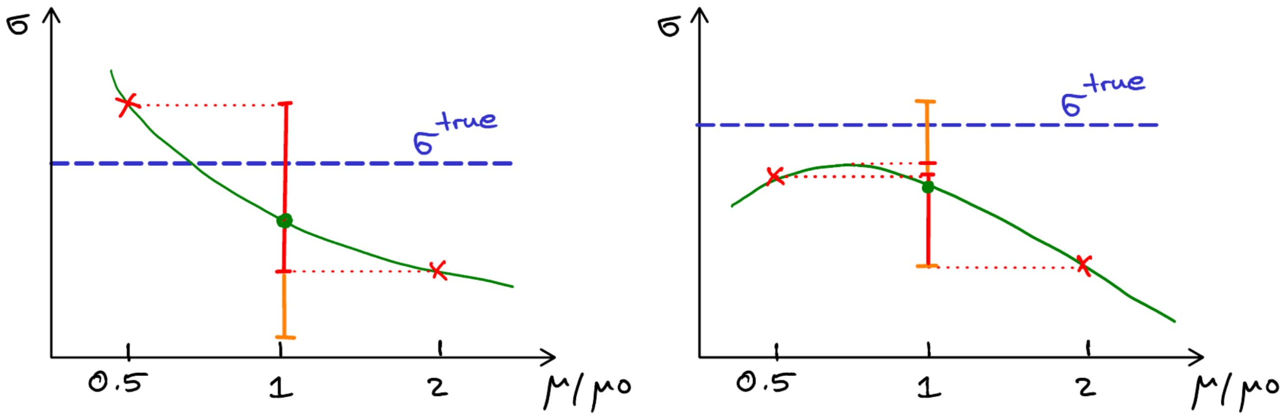
- If $\mathcal{O}_1$ and $\mathcal{O}_2$ are both biased in the same way → $\Delta\mathcal{O}$ **underestimated**
- If $\mathcal{O}_1$ accurate and $\mathcal{O}_2$ is poor → $\Delta\mathcal{O}$ **overestimated**

Ugly systematics: parameter variation

- Some systematics uncertainties have a parametric description
- We model an observable as $\mathcal{O}(\theta)$:

$$\mathcal{O}_{true} = \mathcal{O}(\theta_0) \pm \Delta\mathcal{O}$$

- We vary θ to estimate $\Delta\mathcal{O}$
- Ex: Renormalization scale variation



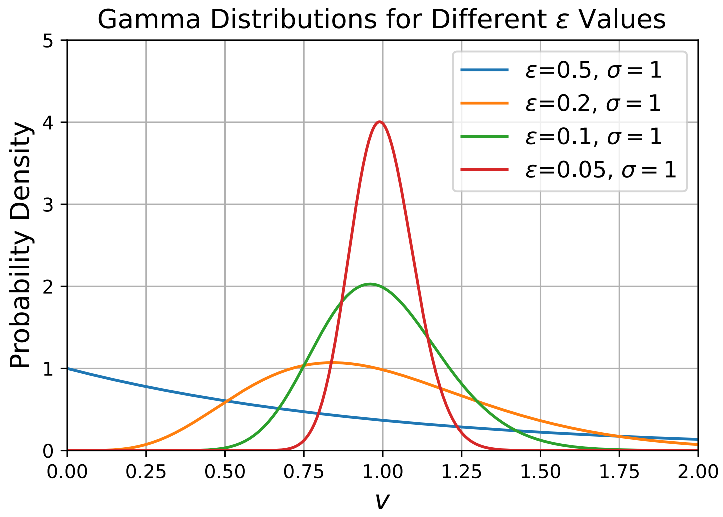
*Frank Tackmann example

Gamma Distributions

- Treat the systematic variances $\sigma_{u_i}^2$ are *adjustable parameters* (*nuisance parameter*).
- Suppose their best estimates v_i are gamma distributed:

$$v \sim \frac{\beta^\alpha}{\Gamma(\alpha)} v^{\alpha-1} e^{-\beta v}$$

$$\alpha = \frac{1}{4\varepsilon_i^2} \qquad \beta = \frac{1}{4\varepsilon_i^2 \sigma_{u_i}^2}$$



- σ_{u_i} Systematic Error
- $\varepsilon_i = \frac{1}{2}\frac{\sigma_{v_i}}{\sigma_{u_i}^2} \cong \frac{\sqrt{v_i}}{\sigma_{u_i}}$ relative error on σ_{u_i}: "***Error on error***"

Gamma Variance Model (GVM)

- The likelihood is modified as follows:

$$L(\boldsymbol{\mu}, \boldsymbol{\theta}, \boldsymbol{\sigma}_{\boldsymbol{u}_i}^2) = P(\boldsymbol{y}|\boldsymbol{\mu}, \boldsymbol{\theta}) \times \prod_i \frac{1}{\sqrt{2\pi}\sigma_{u_i}} e^{-(u_i-\theta_i)^2/2\sigma_{u_i}^2} \times \frac{\boldsymbol{\beta}_i^{\alpha_i}}{\boldsymbol{\Gamma}(\boldsymbol{\alpha}_i)} \boldsymbol{v}_i^{\alpha_i - 1} \boldsymbol{e}^{-\beta_i v_i}$$

- One can profile over $\boldsymbol{\sigma}_{\boldsymbol{u}_i}^2$ in closed form:

$$\log L_P(\boldsymbol{\mu}, \boldsymbol{\theta}) = \log P(\boldsymbol{y}|\boldsymbol{\mu}, \boldsymbol{\theta}) - \frac{1}{2} \sum_i \left(\mathbf{1} + \frac{\mathbf{1}}{\mathbf{2}\varepsilon_i^2} \right) \mathbf{log} \left(\mathbf{1} + \mathbf{2}\varepsilon_i^2 \frac{(\boldsymbol{u}_i - \boldsymbol{\theta}_i)^2}{\boldsymbol{v}_i} \right)$$

- We call this model the Gamma Variance Model (GVM)

(see: G. Cowan, Eur. Phys. J. C (2019) 79:133; arXiv:1809.05778)

Motivation for the GVM

- Gamma distributions allow to parametrize distributions of positive defined variables (like estimates of variances)

- Using Gamma distributions it is possible to profile in close form over σ_i^2

Motivation for the GVM

- Gamma distributions include the case where the variance is estimate from a real dataset of control measurements:

$$v_i = \frac{1}{n_i - 1} \sum \left(u_{i,j} - \bar{u_i}\right)^2$$

- $(n-1)v_i/\sigma_{u_i}^2$ follows a χ_{n-1}^2 distribution and v_{i} a Gamma distribution with:

$$\alpha_i = \frac{n_i - 1}{2}$$

$$\beta_i = \frac{n_i - 1}{2\sigma_{u_i}^2}$$

From BLUE to the Gamma Variance Model

- BLUE (Best Linear Unbiased Estimators) approach to combinations:

$$\chi^2 = \sum_i \big(y_i - f(\boldsymbol{a})\big) V_{ij}^{-1} (y_j - f(\boldsymbol{a}))$$

$$V_{ij} = V_{ij}^{(stat)} + V_{ij}^{(syst)}$$

- $V_{ij}^{(stat)}$: Statistical covariance matrix.
- $V_{ij}^{(syst)}$: Covariance matrix induced by systematic source.
- $V_{ij}^{(syst)} = \sum_s V_{ij}^{(s)}$

ROYAL HOLLOWAY UNIVERSITY OF LONDON

- Nuisance parameters approach:

Magnitude of the bias induced by the systematic source *s*

$$\chi^2 = \sum_i \frac{(y_i - f(\boldsymbol{a}) - \sum_s \Gamma_i^s \theta_s)^2}{\sigma_i^2} + \sum_s \theta_S^2$$

From BLUE to the Gamma Variance Model

- Nuisance parameters approach:

Magnitude of the bias induced by the systematic source *s*

$$\chi^2 = \sum_i \frac{(y_i - f(\boldsymbol{a}) - \sum_s \Gamma_i^s \theta_s)^2}{\sigma_i^2} + \sum_s \theta_S^2$$

- Connection:

$$V_{ij}^{(syst)} = \sum_s V_{ij}^{(s)}$$

$$V_{ij}^{(s)} = \Gamma_i^s \Gamma_j^s$$

- Gamma Variance Model:

$$\chi^2 = \sum_i \frac{(y_i - f(\boldsymbol{a}) - \sum_s \Gamma_i^s \theta_s)^2}{\sigma_i^2} + \sum_s \left(\mathbf{1} + \frac{\mathbf{1}}{\mathbf{2}\boldsymbol{\varepsilon}_i^2}\right) \mathbf{log}\left(\mathbf{1} + \mathbf{2}\boldsymbol{\varepsilon}_i^2 \boldsymbol{\theta}_i{}^2\right)$$

- What to do if we do not have access to the factors Γ_i^s (we only know $V_{ij}^{(syst)}$)?

$$V_{ij}^{(syst)} = \sum_s V_{ij}^{(s)}$$

From BLUE to the Gamma Variance Model

- Switch to a nuisance parameters approach:

Proof is non-trivial!

$$\chi^2 = \sum_i \frac{(y_i - \mu - \theta_i)^2}{\sigma_i^2} + \sum_{ij} \theta_i C_{ij}^{-1} \theta_j$$

$$C_{ij} = V_{ij}^{(s)}$$

- Substitute quadratic term with log-constraint:

$$\sum_{ij} \theta_i C_{ij}^{-1} \theta_j \longrightarrow \sum_i \left(N + \frac{1}{2\varepsilon_i^2} \right) \log\left(1 + 2\varepsilon_i^2 \theta_i C_{ij}^{-1} \theta_j\right)$$

Bartlett Correction

- The Hessian method is based on the assumption that the χ^2 follows a χ^2 distribution.

- Our "goodness-of-fit" statistics q *is* is not a χ^2 so will will not follow exactly a χ^2 for large values of ϵ^2

Large literature on the topic:

- *Bartlett, M. S. (1937) Proceedings of the Royal Society A, 160, 268–282)*
- *Applied Asymptotics Case Studies in Small-Sample Statistics by A. R. Brazzale, A. C. Davison and N. Reid)*
- Canonero, E., Brazzale, A.R. & Cowan, *Eur. Phys. J. C* **83**, 1100 (2023).

Bartlett Correction

ROYAL HOLLOWAY UNIVERSITY OF LONDON

- Modify the test statistic q so that its distribution is closer to a χ^2 :

$$q \longrightarrow q^* = q\frac{N_{dof}}{E[q]}$$

Bartlett Correction

ROYAL HOLLOWAY UNIVERSITY OF LONDON

- Modify the test statistic q so that its distribution is closer to a χ^2 :

$$q \longrightarrow q^* = q\frac{N_{dof}}{E[q]}$$

Expectation value in the asymptotic limit (degrees of freedom of χ^2)

Exact expectation value

Bartlett Correction

- Modify the test statistic q so that its distribution is closer to a χ^2 :

$$q \longrightarrow q^* = q\frac{N_{dof}}{E[q]}$$

Expectation value in the asymptotic limit (degrees of freedom of χ^2)

Exact expectation value

$$q \sim \chi^2 + \mathcal{O}(\epsilon^2)$$

$$q^* \sim \chi^2 + \mathcal{O}(\epsilon^4)$$