Theoretical uncertainties: selected issues

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HELMHOLTZ
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1. Types of uncertainties
2. Perturbation theory and beyond
3. Uncertainties in parton density fits
4. Summary

Different sources of theoretical uncertainties

"observable = theoretical expression"

1. theoretical expression is only approximate
   often obtained by expansion in small parameter
   $\rightsquigarrow$ estimate size of uncalculated/neglected terms
2. input parameters from standard model:
   α_s, $m_{c,b}$, m_t, $m_{W,Z}$, m_H, CKM matrix elements
   note: running $\alpha_s(\mu)$ depends implicitly on quark masses
3. nonperturbative QCD parameters or functions, e.g.
   parton densities, fragmentation functions,
   decay constants, wave functions (e.g. for $B \to D\ell\nu$, $B \to \pi K$)
   note: PDFs and fragmentation fcts. depend on $\alpha_s(\mu)$ via evolution

quantities in 2., 3. may be obtained from

- comparison "measured observable = theor. expression"
- nonperturbative calculation (e.g. lattice)

Higher orders, power corrections, and all that

observables in high-energy collisions typically evaluated from factorization formula*, e.g.

$$\frac{d\sigma}{d(\text{variables})} = \frac{1}{Q^n}\,\text{PDF}\big(\mu_F, \alpha_s(\mu_F)\big) \underset{x}{\otimes} C\Big(\frac{\mu_F}{Q}, \frac{\mu_R}{Q}, \alpha_s(\mu_R), \ldots\Big) + \mathcal{O}\Big(\frac{1}{Q^{n+1}} \text{ or } \frac{1}{Q^{n+2}}\Big)$$

- $Q =$ hard momentum scale $\qquad x =$ scaling variable
- convolution $f \underset{x}{\otimes} g = \int_x^1 \frac{dz}{z} f\Big(\frac{x}{z}\Big)\, g(z)$
- in $C(\ldots)$ possible dependence on $m_t, m_{W,Z}, m_H$ etc.
- now discuss in turn:
  - higher-order corrections (1st line)
  - power corrections (2nd line)

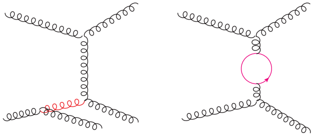
* in some rare cases have factorization theorems

Higher orders

$$\frac{d\sigma}{d(\text{variables})} = \frac{1}{Q^n}\,\text{PDF}\big(\mu_F, \alpha_s(\mu_F)\big) \underset{x}{\otimes} C\Big(\frac{\mu_F}{Q}, \frac{\mu_R}{Q}, \alpha_s(\mu_R), \ldots\Big) + \mathcal{O}(\ldots)$$

- have α_s expansions for C and for $\frac{d}{d\mu_F}\text{PDF}$
- in hard scattering
  - $\mu_R \leftrightarrow$ UV divergences
  - $\mu_F \leftrightarrow$ collinear divergences

  may keep separate



- in general not inconsistent to take different orders in α_s expansion of C and of PDF evolution
  overall accuracy is of course given by least accurate term
  usefulness to be discussed case by case
- analogous comment for order in C and in running of α_s

Renormalization scale dependence

on next slides write μ instead of μ_R for brevity

- renormalization group equation

$$\frac{d}{d\log\mu^2}\,\alpha_s(\mu) = \beta\big(\alpha_s(\mu)\big)$$

with $\beta(\alpha_s) = -\alpha_s^2\big(b_0^{n_f} + b_1^{n_f}\,\alpha_s + b_2^{n_f}\,\alpha_s^2 + b_3^{n_f}\,\alpha_s^3 + \ldots\big)$

- in practice truncate series of $\beta(\alpha_s)$ and solve RGE numerically or by expansion of $\alpha_s(\mu)$ in $\frac{1}{\log(\mu^2/\Lambda^2_{\mathrm{QCD}})}$
- higher-coefficients in α_s expansion of hard-scattering coefficient are μ dependent

$$C = \alpha_s^m(\mu)\,C_0 + \alpha_s^{m+1}(\mu)\,C_1\big(\tfrac{Q}{\mu}\big) + \alpha_s^{m+2}(\mu)\,C_2\big(\tfrac{Q}{\mu}\big) + \ldots$$

but C independent of μ to any given accuracy in α_s:

$$\frac{d}{d\log\mu^2}\,C(\mu) = 0$$

see how this works:

- set $\mu = Q$ in expansion:

$$C = \alpha_s^m(\mu)\,C_0 + \alpha_s^{m+1}(\mu)\,C_1\big(\tfrac{Q}{\mu}\big) + \alpha_s^{m+2}(\mu)\,C_2\big(\tfrac{Q}{\mu}\big) + \ldots$$
$$= \alpha_s^m(Q)\,C_0 + \alpha_s^{m+1}(Q)\,C_1(1) + \alpha_s^{m+2}(Q)\,C_2(1) + \ldots$$

- expand $\alpha_s(Q) = \alpha_s(\mu) + a_1\big(\tfrac{Q}{\mu}\big)\,\alpha_s^2(\mu) + a_2\big(\tfrac{Q}{\mu}\big)\,\alpha_s^3(\mu) + \mathcal{O}(\alpha_s^4)$

$$\frac{d}{d\log Q^2}\,(\text{l.h.s.}) = \beta\big(\alpha_s(Q)\big) = -b_0\,\alpha_s^2(Q) - b_1\,\alpha_s^3(Q) + \mathcal{O}(\alpha_s^4)$$
$$= -b_0\,\alpha_s^2(\mu) - 2a_1 b_0\,\alpha_s^3(\mu) - b_1\,\alpha_s^3(\mu) + \mathcal{O}(\alpha_s^4)$$
$$\frac{d}{d\log Q^2}\,(\text{r.h.s.}) = \frac{da_1}{d\log Q^2}\,\alpha_s^2(\mu) + \frac{da_2}{d\log Q^2}\,\alpha_s^3(\mu) + \mathcal{O}(\alpha_s^4)$$

- compare coefficients of $\alpha_s^n(\mu)$:

$$\frac{da_1}{d\log Q^2} = -b_0 \qquad \Rightarrow \qquad a_1\big(\tfrac{Q}{\mu}\big) = -b_0\,\log\frac{Q^2}{\mu^2}$$
$$\frac{da_2}{d\log Q^2} = -2a_1 b_0 - b_1 \qquad \Rightarrow \qquad a_2\big(\tfrac{Q}{\mu}\big) = +b_0^2\,\log^2\frac{Q^2}{\mu^2} - b_1\,\log\frac{Q^2}{\mu^2}$$

- inserting

$$\alpha_s(Q) = \alpha_s(\mu)\Big[1-\alpha_s(\mu)\, b_0 \log\tfrac{Q^2}{\mu^2} + \alpha_s^2(\mu)\Big(b_0^2 \log^2\tfrac{Q^2}{\mu^2} - b_1 \log\tfrac{Q^2}{\mu^2}\Big) + \ldots\Big]$$

into $\quad C = \alpha_s^m(Q)\,\Big[C_0 + \alpha_s(Q)\, C_1(1) + \alpha_s^2(Q)\, C_2(1) + \ldots\Big]$ get

$$\begin{aligned} C &= \alpha_s^m(\mu) \\ &\quad \times \Big[1 - \alpha_s(\mu)\, m b_0 \log\tfrac{Q^2}{\mu^2} + \alpha_s^2(\mu)\Big(\tfrac{m(m+1)}{2}\, b_0^2 \log^2\tfrac{Q^2}{\mu^2} - m b_1 \log\tfrac{Q^2}{\mu^2}\Big)\Big] \\ &\quad \times \Big[C_0 + \alpha_s(\mu)\, C_1(1) + \alpha_s^2(\mu)\,\Big(C_2(1) - C_1(1)\, b_0 \log\tfrac{Q^2}{\mu^2}\Big)\Big] + \mathcal{O}(\alpha_s^{m+3}) \end{aligned}$$

- in $\quad C = \alpha_s^m(\mu)\, C_0 + \alpha_s^{m+1}(\mu)\, C_1\big(\tfrac{Q}{\mu}\big) + \alpha_s^{m+2}(\mu)\, C_2\big(\tfrac{Q}{\mu}\big) + \ldots$

  have coefficients

$$\begin{aligned} C_1\big(\tfrac{Q}{\mu}\big) &= C_1(1) - m b_0\, C_0 \log\tfrac{Q^2}{\mu^2} \\ C_2\big(\tfrac{Q}{\mu}\big) &= C_2(1) - \Big[(m+1) b_0\, C_1(1) + m b_1\, C_0\Big] \log\tfrac{Q^2}{\mu^2} + \tfrac{m(m+1)}{2}\, b_0^2\, C_0 \log^2\tfrac{Q^2}{\mu^2} \end{aligned}$$

- check (exercise): $\frac{d}{d\log\mu^2} C\big(\tfrac{Q}{\mu}, \alpha_s(\mu)\big) = \Big[\frac{\partial}{\partial\log\mu^2} + \beta\,\frac{\partial}{\partial\alpha_s}\Big] C = 0$

- have

$$C = \alpha_s^m(\mu)\, C_0 + \alpha_s^{m+1}(\mu)\, C_1\big(\tfrac{Q}{\mu}\big) + \alpha_s^{m+2}(\mu)\, C_2\big(\tfrac{Q}{\mu}\big) + \ldots$$

with

$$C_1\big(\tfrac{Q}{\mu}\big) = C_1(1) - m b_0\, C_0 \log \tfrac{Q^2}{\mu^2}$$

$$C_2\big(\tfrac{Q}{\mu}\big) = C_2(1) - \Big[(m+1) b_0\, C_1(1) + m b_1\, C_0\Big] \log \tfrac{Q^2}{\mu^2} + \tfrac{m(m+1)}{2}\, b_0^2\, C_0 \log^2 \tfrac{Q^2}{\mu^2}$$

- calculating C_0 (LO) get also terms $\alpha_s^{m+1} \log \frac{Q^2}{\mu^2}, \alpha_s^{m+2} \log^2 \frac{Q^2}{\mu^2}, \ldots$
  calculating $C_1(1)$ (NLO) get also terms $\alpha_s^{m+2} \log \frac{Q^2}{\mu^2}, \alpha_s^{m+3} \log^2 \frac{Q^2}{\mu^2}, \ldots$
  $\rightsquigarrow$ recover logarithmic terms at higher orders, but not coefficients $C_n(1)$
- varying μ in N^{l}LO result get variation at N^{l+1}LO corresponding to

  $$\alpha_s^{l+1} \sum_{i=1}^{l+1} \text{(known coefficient)} \times \log^i \tfrac{\mu^2}{Q^2} + \mathcal{O}(\alpha_s^{l+2})$$

  but no information on $\alpha_s^{l+1}\, C_{l+1}(1)$

Renormalization scale dependence

- varying μ in N^{l}LO result get variation at N^{l+1}LO corresponding to
  $$\alpha_s^{l+1} \sum_{i=1}^{l+1} (\text{known coefficient}) \times \log^i \frac{\mu^2}{Q^2} + \mathcal{O}(\alpha_s^{l+2})$$
  but no information on $\alpha_s^{l+1} C_{l+1}(1)$

consequences:

- when calculate higher orders, expect that scale dependence decreases
- scale variation in N^{l}LO result estimates size of certain higher-order terms, but not of all
  - uncalculated higher orders often estimated by varying μ between $1/2$ and 2 times some central value
    is a conventional choice
  - but what to take for central value?

Renormalization scale choice

- prescriptions for scale choice aiming to minimizing size of higher-order terms

  take NLO calc. of $C(\mu) = \alpha_s^m C_0 + \alpha_s^{m+1} C_1(\mu) + \mathcal{O}(\alpha_s^{m+2})$

  - $\mu =$ typical virtuality in hard-scattering graphs
    useful guidance, but obviously not a well-defined quantity
  - fastest apparent convergence (FAC): $\frac{d}{d\mu^2} \sum_{i=0}^{1} \alpha_s^{m+i} C_i(\mu) = 0$
  - principle of minimal sensitivity (PMS): $C_1(\mu) = 0$
  - Brodsky-Mackenzie-Lepage (BLM): $C_1(\mu)$ independent of n_f
    recall: coefficients b_0, b_1, ... of β function depend on n_f

- how much these reduce higher orders depends on process
  cannot "predict" higher orders without calculating them

Factorization scale dependence

- scale dependence of PDF given by DGLAP equation:

$$\frac{d}{d\log\mu_F^2}\,\mathrm{PDF}(x,\mu_F) = \mathrm{PDF}(\mu_F) \underset{x}{\otimes} P\big(\alpha_s(\mu_F)\big)$$

evolution kernels have perturbative expansion in α_s :

$$P\big(z,\alpha_s(\mu_F)\big) = \alpha_s(\mu_F)\,P_0(z) + \alpha_s^2(\mu_F)\,P_1(z) + \mathcal{O}(\alpha_s^3)$$

  - choose approx. of evolution kernel (LO, NLO, NNLO)
  - solve DGLAP equations numerically
    $\Rightarrow$ obtain PDF(μ_1) from PDF(μ_0)

- hard-scattering coefficient contains powers of $\log(\mu_F/Q)$
  μ_F independence of PDF(μ_F) $\otimes\, C(\mu_F)$ implies

$$\frac{d}{d\log\mu_F^2}\,C\big(x,\mu_F,\mu_R,\alpha_s(\mu_R)\big) = -P\big(\alpha_s(\mu_F)\big) \underset{x}{\otimes} C\big(\mu_F,\mu_R,\alpha_s(\mu_R)\big)$$

Factorization scale dependence

$$\frac{d}{d\log\mu_F^2}\, C\big(x, \mu_F, \alpha_s(\mu_R), \ldots\big) = -P\big(\alpha_s(\mu_F)\big) \underset{x}{\otimes} C\big(\mu_F, \mu_R, \alpha_s(\mu_R)\big)$$

using renormalization group equation can rewrite

$$\alpha_s(\mu_R) = \alpha_s(\mu_F) + \sum_{i>1} c_i(\mu_R/\mu_F)\, \alpha_s^i(\mu_F)$$

with expansions

$$C\big(\mu_F, \alpha_s(\mu_F), \mu_R\big) = C_0(\mu_R) + \alpha_s(\mu_F)\, C_1(\mu_F, \mu_R) + \mathcal{O}(\alpha_s^2)$$
$$P\big(\alpha_s(\mu_F)\big) = \alpha_s(\mu_F)\, P_0 + \alpha_s^2(\mu_F)\, P_1 + \mathcal{O}(\alpha_s^3)$$

can match coefficients order by order

$$\Rightarrow \quad C_1(\mu_F, \mu_R) = C_1(Q, \mu_R) - C_0(\mu_R) \otimes P_0\, \log\frac{\mu_F^2}{Q^2} \quad \text{etc.}$$

Factorization scale dependence

- try to chose μ_F such as to avoid large higher-order coefficients
- with C calculated to N^{l}LO have μ_F dependence of order N^{l+1}LO in convolution PDF $\otimes\, C$

  if evolve PDFs with DGLAP kernels up to $\alpha_s^l\, P_{l-1}$ or higher
- as for μ_R may estimate certain higher-order terms by varying μ_F between e.g. $1/2$ and 2 times some central value
- as for μ_R no general solution for finding μ_F that minimizes higher orders

Multi-scale problems

- scale choice even less obvious when have several hard scales
  e.g. Q and p_T, Q and m_c, p_T and m_W, ...
  may try to identify typical virtualities in graphs
- for small/large ratios of hard scales
  (or small/large values of scaling variables, e.g. $x \to 0$ or $x \to 1$)
  then have large logarithms in C for any choice of μ_R, μ_F

Multi-scale problems

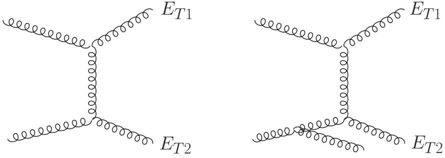
- for certain cases can resum large logarithms to all orders
  e.g. $\alpha_s^n \log^{n+i}$ for all n with given $i = 0, 1, \ldots$
  - transverse-momentum logs: $\log \frac{p_T}{Q}$ $\rightsquigarrow$ Sudakov factors
  - threshold logs: $\log \frac{M^2}{\hat{s}}$
    for production of mass M with partonic collision energy $\sqrt{\hat{s}}$
    $\sigma(ep) \sim \int dz\, \text{PDF}(z)\, C(\hat{s} = zW^2)$
    $\sigma(pp) \sim \int dz_1 dz_2\, \text{PDF}(z_1)\, \text{PDF}(z_2)\, C(\hat{s} = z_1 z_2 s)$
  - high-energy logs: $\log \frac{1}{x}$ $\rightsquigarrow$ BFKL logs
- resummation procedure may have its own uncertainties
  e.g. from integrals of type $\int_0^Q d\mu\, f\big(\alpha_s(\mu)\big)$ $\rightsquigarrow$ Landau pole

LO, NLO, and higher

- instead of varying scale(s) may estimate higher orders by comparing N^{l}LO result with N^{l-1}LO
- caveat: comparison NLO vs. LO may not be representative for situation at higher orders

  often have especially large step from LO to NLO

  - certain types of contribution may first appear at NLO
    e.g. terms with gluon density $g(x)$ in DIS, $pp \to W + X$, etc.
  - final state at LO may be too restrictive
    e.g. in inclusive DIS
    or in $\frac{d\sigma}{dE_{T1}\, dE_{T2}}$ for dijet production



Power corrections

- for certain observables (typically those for which have operator product expansion) can identify and estimate size of power-suppressed terms
- example: τ decay $(\mu_R = m_\tau)$

$$R_\tau = \frac{\Gamma(\tau \to \nu_\tau + \text{hadrons})}{\Gamma(\tau \to \nu_\tau + e\nu_e)} = R_0 \left[1 + \frac{\alpha_s}{\pi} + 5.2\,\frac{\alpha_s^2}{\pi^2} + 26.4\,\frac{\alpha_s^3}{\pi^3} + c_2\,\frac{m_q^2}{m_\tau^2} + c_4\,\frac{\langle m\bar{\psi}\psi\rangle}{m_\tau^4} + c_6\,\frac{\langle \bar{\psi}\psi\bar{\psi}\psi\rangle}{m_\tau^6} \right]$$

with (schematically) $m_q^2 =$ combination of squared light quark masses
$\langle m\bar{\psi}\psi\rangle, \langle \bar{\psi}\psi\bar{\psi}\psi\rangle =$ expectation values of quark operators in vacuum

used for determination of $\alpha_s(m_\tau)$ see PDG 2008, sect. 9

Power corrections

- for certain observables (typically those for which have operator product expansion) can identify and estimate size of power-suppressed terms
- example: sum rules for deep inelastic structure functions

  Bjorken sum rule for polarized str. fcts. ($\mu_R = Q$)

$$\int_0^1 dx \left(g_1^p(x,Q^2) - g_1^n(x,Q^2)\right) = \frac{g_A}{6}\left[1 - \frac{\alpha_s}{\pi} - 3.58\,\frac{\alpha_s^2}{\pi^2} - 20.32\,\frac{\alpha_s^3}{\pi^3}\right] + \frac{\langle t\rangle}{Q^2} - \frac{2m_N^2}{9Q^2}\int_0^1 dx\, x^2 \left(g_1^p(x,Q^2) - g_1^n(x,Q^2)\right)$$

$\langle t\rangle$ = defined from expectation values of $\bar\psi G_{\mu\nu}\gamma_\lambda\psi$ between nucleon states

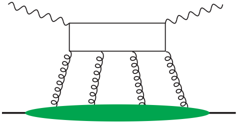
Power corrections

- for factorization formulae of type

$$\frac{d\sigma}{d(\text{variables})} = \frac{1}{Q^n}\,\text{PDF}\big(\mu_F, \alpha_s(\mu_F)\big) \underset{x}{\otimes} C\Big(\frac{\mu_F}{Q}, \frac{\mu_R}{Q}, \alpha_s(\mu_R), \ldots\Big) + \mathcal{O}\Big(\frac{1}{Q^{n+1}} \text{ or } \frac{1}{Q^{n+2}}\Big)$$

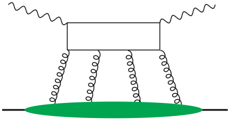
in general have no theoretical expression for power corrections

- exceptions: inclusive DIS and γ^*, W or Z production in pp
  hardly used: too many unknown non-perturbative functions



Power corrections

special case: very small x



- exchange of 4 transverse gluons suppressed by $\frac{1}{Q^2}$ relative to 2 gluons
- but has steeper growth with energy
- at given Q^2 will eventually dominate as x decreases
  $\rightsquigarrow$ change theoretical framework: BFKL, color dipoles, parton saturation
- primary expansion parameter is not $\frac{1}{Q^2}$ but x
  full BFKL contains more than $\log\frac{1}{x}$ resummation at leading twist
- in perturbative accuracy (no full NLO for DIS yet) can presently not compete with collinear factorization
  but allows estimate of power suppressed terms

Jet production

- fundamental problem: factorization formulae are for prod'n of high-p_T partons, not high-p_T hadrons
  note: due to collinear and soft radiation "momentum of final-state parton" is only defined at LO
- if apply jet algorithm to partons in theory formula and to hadrons in measurement
  $\rightsquigarrow$ kinematical ambiguities: energy vs. momentum
  (light quarks and gluons taken as massless, hadrons are not)
- event generators model the parton $\rightarrow$ hadron transition
  uncertainty of "hadronization corrections" typically determined by comparing different models
- may instead use fragmentation functions (theory $\sim$ for PDFs) if measure individual hadrons
  e.g. $\gamma^* p \to D^* + X$ instead of $\gamma^* p \to c + X$

Parton density fits

Principle of PDF determinations:

- compare data with factorization formulae for selected processes and kinematics
- specify PDF at reference scale Q_0
  use DGLAP to evolve to scales used in fact. formulae

  e.g. CTEQ : $Q_0 = 1.3\,\mathrm{GeV}$ use data with $Q > 2\,\mathrm{GeV}$
  MSTW : $Q_0 = 1\,\mathrm{GeV}$ use data with $Q > 1.4\,\mathrm{GeV}$
- conventional determinations parameterize PDFs at Q_0 and determine parameters by χ^2 fit to data

  NNPDF collab. uses neural networks, avoids choice of function
  claims "unbiased" representation of PDFs

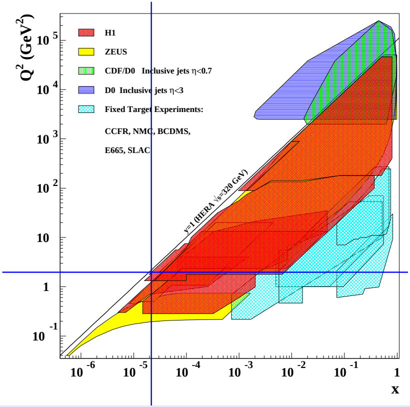
  however, theoretical bias regarding shape and smoothness of PDFs is not illicit

Evolution

$$\frac{d}{d\log \mu_F^2} \mathsf{PDF}(x, \mu_F) = \int_x^1 \frac{dz}{z} \mathsf{PDF}(z, \mu_F)\, P\Big(\frac{x}{z}\Big)$$

$\Rightarrow$ specifying PDF(x, μ_F) for all $x > x_0$ at one μ_F
fixes PDF for $x > x_0$ at all other μ_F

- no inform'n about PDFs at $x < x_0$ without data at $x < x_0$
- indirect inform'n about PDFs at large x via convolution integrals



Uncertainties on extracted PDFs

- selection of data sets and kinematics
- perturbative order of evolution and hard-scattering coefficients
- values of α_s and m_c, m_b and possibly other constants
  if taken as external parameters i.e. not fitted
  some PDF sets available for different values of α_s
- fine details of perturbative calculations
  e.g. treatment of heavy quarks, resummation
- power corrections (typically try to avoid by minimal Q in data)
- corrections for data with nuclear targets

errors on fitted parameters

- reflect errors (stat. and syst.) of fitted data
  discuss on the following slides

Parametric errors in PDF fits

see e.g. hep-ph/0201195 (CTEQ6), arXiv:0802.0007 (CTEQ6.6)
arXiv:0901.0002 (MSTW 2008)

- errors obtained in χ^2 fit

simplest version: $$\chi^2 = \sum_i \frac{\big[D_i - T_i(\boldsymbol{p})\big]^2}{\sigma_{i,\,\mathsf{stat}}^2 + \sigma_{i,\,\mathsf{syst}}^2}$$

$D_i =$ data point number i

$T_i =$ corresponding theory prediction

$\boldsymbol{p} = \{p_1, \ldots, p_k\} =$ set of fitting parameters

more sophisticated treatment for correlated systematic errors, i.e. overall normalization

$$\chi^2 = \sum_i \frac{\left[D_i - T_i(\boldsymbol{p})\right]^2}{\sigma^2_{i,\,\mathsf{stat}} + \sigma^2_{i,\,\mathsf{syst}}}$$

if assume that errors of D_i follow a Gaussian distribution, then

- fitted $\boldsymbol{p}$ follow a k-dim. Gaussian dist. around true values $\boldsymbol{p}_0$
- have k-dim. χ^2 distribution for

  $$\Delta\chi^2(\boldsymbol{p}) = \chi^2(\boldsymbol{p}) - \chi^2_{\mathsf{min}} = \textstyle\sum_{ij} (p - p_0)_i \, H_{ij} \, (p - p_0)_j$$

  $H =$ Hesse matrix $=$ inverse of covariance matrix V
- observable $\mathcal{O}(\boldsymbol{p})$ follows Gaussian dist. with error

$$\Delta\mathcal{O} = T \sqrt{\textstyle\sum_{ij} \frac{\partial\mathcal{O}}{\partial p_i} \, H^{-1}_{ij} \, \frac{\partial\mathcal{O}}{\partial p_j}}$$

with $T = 1$ for 68% C.L., $T = 2.71$ for 95% C.L. etc.
readily generalizes to several obs. and their correlated errors
$\rightsquigarrow$ complicated in practice, would need derivatives $\partial\mathcal{O}/\partial p_i$

$$\Delta\mathcal{O} = T\sqrt{\sum\nolimits_{ij} \frac{\partial\mathcal{O}}{\partial p_i}\, H^{-1}_{ij}\, \frac{\partial\mathcal{O}}{\partial p_j}}$$

- diagonalize Hesse matrix H and rescale eigenvectors
  $\Rightarrow$ linear combinations z_i of $(p - p_0)_j$ satisfying

$$\Delta\chi^2 = \sum_i z_i^2$$

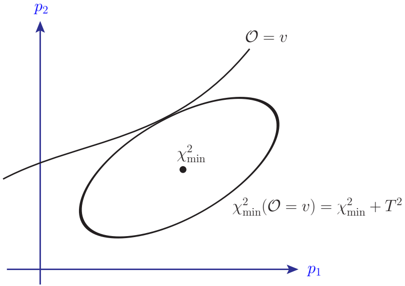
$$\Delta\mathcal{O} = T\sqrt{\sum\nolimits_i \frac{\partial\mathcal{O}}{\partial z_i}\, \frac{\partial\mathcal{O}}{\partial z_i}} = \sqrt{\sum\nolimits_i \left[\frac{\mathcal{O}(S_i^+) - \mathcal{O}(S_i^-)}{2}\right]^2}$$

  with eigenvector PDF sets $S_i^{\pm}$
  corresponding to parameters $z_i = \pm T$ and $z_j = 0$ for $j \neq i$
  in last step have linearized $\mathcal{O}$ around $\boldsymbol{z} = 0$

- for large errors $\Delta\chi^2$ not quadratic in $(p - p_0)_i$ or z_i
  $\rightsquigarrow$ linear error propagation not reliable
  $\rightsquigarrow$ Legendre multiplier method

Legendre multiplier method

- minimize $\chi^2(\boldsymbol{p})$ with constraint $\mathcal{O} = v$ — uses Legendre mult.
- determine values v with $\chi^2_{\text{min}}(\mathcal{O} = v) = \chi^2_{\text{min}} + T^2$
  min/max of $v - \mathcal{O}_{\chi^2_{\text{min}}}$ gives lower/upper error on $\mathcal{O}$
- equiv. to Hesse method if χ^2 quadratic and $\mathcal{O}$ linear in $\boldsymbol{p}$
- requires separate fits for each considered observable $\mathcal{O}$



The tolerance criterion

- if data points D_i follow Gaussian dist.
  then for experiment with N_j data points
  expect contribution $\chi^2_{j,\text{min}} \sim N_j$ to global χ^2_{min}
- often not seen in practice: for some cases
  - $\chi^2_{j,\text{min}}$ significantly below or above N_j
  - $\chi^2_{j,\text{min}}$ much larger than χ^2 minimized separately for experiment
  - get inconsistent errors on $\boldsymbol{p}$ when fitting subsets of data

  indicates that some data sets not consistent with each other
  in such a case standard χ^2 errors misrepresent uncertainty
- modified criterion for T CTEQ: $T^2 \sim 100$, MSTW: $T^2 \approx 50$
  - obtained by procedure/algorithm looking at χ^2 from individual experiments
  - may be seen as ad hoc deviation from "standard statistics"
    but "standard criterion" for T requires that all data points
    have Gaussian dist. with quoted uncertainties

Summary

- estimating theoretical uncertainties $\neq$ an exact science
- "scale uncertainty" based on renormalization group eq.
  estimates certain higher-order terms in α_s
  prescriptions for scale choice = educated guesses
- higher-order terms not the only source of uncertainty
  power corrections, hadronization corrections, ... more difficult to assess
- errors of PDF fits reflect uncertainties of fitted data
  (not a straightforward exercise in textbook statistics)
  do not include uncertainties of theory used to fit data