Systematic Uncertainties in Theory

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Hamburg, 21 March 2013

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
     e.g. in coupling constant $\longrightarrow$ perturbation theory
     $\rightsquigarrow$ estimate size of uncalculated/neglected terms
   - for some situations/aspects do not have systematic theory
     must use models
     $\rightsquigarrow$ may estimate uncertainty by comparing different models

Different sources of theoretical uncertainties

"observable = theoretical expression"

2. input parameters from standard model, e.g.
   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
   - most prominently: parton distributions (PDFs)
     note: PDFs depend on $\alpha_s(\mu)$ via evolution
   - other examples: decay constants, wave functions
     (e.g. for $B \to D\ell\nu$, $B \to \pi K$)

quantities in points 2. and 3. may be obtained from

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

Some parameters and their uncertainties

from: Review of Particles Physics 2012

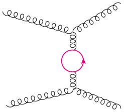
Phys. Rev. D86 (2012) 010001, http://hepdata.cedar.ac.uk/lbl

	relative uncertainty
$m_W = 80.385 \pm 0.015\,\mathrm{GeV}$	1.9×10^{-4}
$m_Z = 91.1876 \pm 0.0021\,\mathrm{GeV}$	2.3×10^{-5}
$m_\tau = 1.77682 \pm 0.00016\,\mathrm{GeV}$	9.0×10^{-5}
$m_b = 4.18 \pm 0.03\,\mathrm{GeV}$	0.72%
$m_t = 160^{+5}_{-4}\,\mathrm{GeV}$	${}^{+3.1\%}_{-2.5\%}$
$1/\alpha_{em} = 137.035999074(44)$	3.2×10^{-9}
$\alpha_s(m_Z) = 0.1184 \pm 0.0007$	0.59%
$= 0.1183 \pm 0.0012$ (without lattice QCD)	1.0%

masses and couplings often appear raised to some power $\rightarrow$ larger uncertainties

m_b and m_t are $\overline{\mathrm{MS}}$ masses at scales $m_b(m_b)$, $m_t(m_t)$

Coupling constants and their running



- due to quantum effects (loop corrections)
  coupling constants depend on renormalization scale μ
  set by "typical momentum scale" of physical process
- electroweak interactions: $\alpha_{em}(0) \approx 0.00730$
  generally quick convergence of pert. series
- strong interactions:
  $\alpha_s(m_Z) \approx 0.118, \quad \alpha_s(m_\tau) \approx 0.33$
  higher order corrections often
  very important (easily factors of 2)
  coupling grows with decreasing μ
  $\rightsquigarrow$ expansion in α_s not useful at low μ

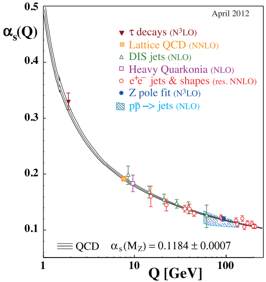


figure: Rev. Part. Phys. 2012

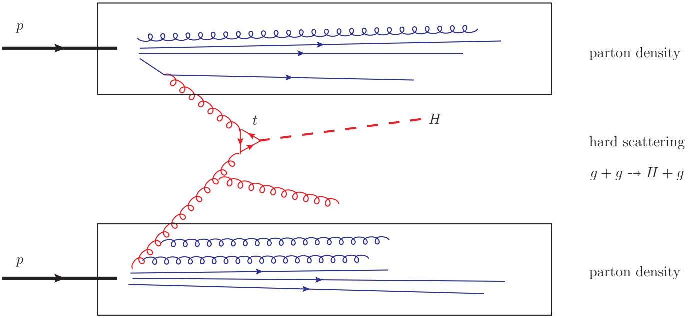
- not everything can be expanded in coupling (e.g. $e^{-\text{const}/\alpha}$)
  non-perturbative effects most ubiquitous in strong interactions

will concentrate on uncertainties due to strong interactions

Factorization: a cornerstone of calculations in QCD

- confinement: quarks and gluons do not exist as free particles; only hadrons are observed
  $\rightsquigarrow$ even at very high energies pp (and ep) collisions involve dynamics at scales $\sim 1\,\mathrm{GeV}$ and below
- idea: separate physics at high and low momentum scales
  - at high scales use expansion in α_s
  - at low scales:
    determine non-perturbative quantities (e.g. parton densities) from experiment, theory or models
    once they are determined, we have predictive power

Example: $p + p \to H + X$ ($X =$ anything)



- factorization formula: parton densities and hard-scattering subprocesses $gg \to H$, $gg \to H + g$, ...

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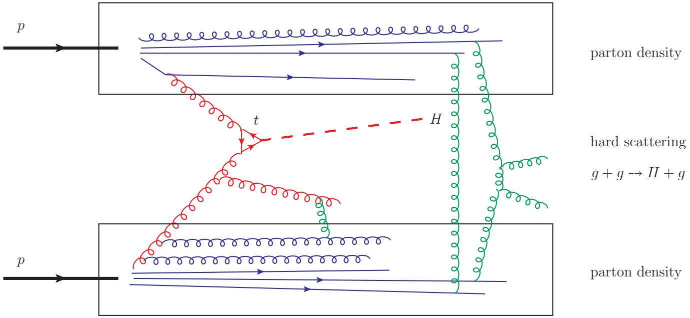
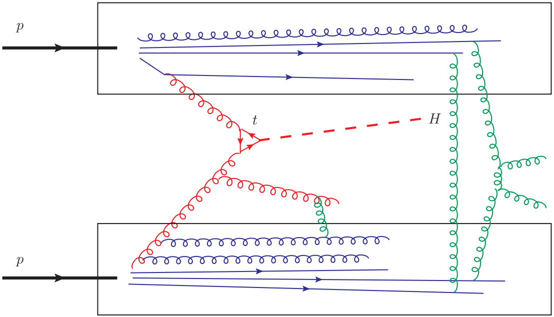


- actual physics more complicated: soft gluon exchange
  - outside domain of perturbation theory $\rightsquigarrow$ must model
  - does not affect sufficiently inclusive observables
  - but does matter for details of final state $\rightsquigarrow$ "underlying event"

Example: $p + p \to H + X$ ($X =$ anything)



- if additional interactions hard ⇝ "multiparton interactions"
  suppressed in sufficiently inclusive observables
  no systematic theory yet ⇝ must model

Factorization formulae

schematic structure for pp collisions

$$\frac{d\sigma}{d(\text{variables})} = f_1(\mu_F) \underset{x_1}{\otimes} \frac{1}{Q^n}\, C\Big\{ \frac{\mu_F}{Q}, \frac{\mu_R}{Q}, \alpha_s(\mu_R), \ldots \Big\} \underset{x_2}{\otimes} f_2(\mu_F)$$
$$+ \mathcal{O}\Big(\frac{1}{Q^{n+1}} \text{ or } \frac{1}{Q^{n+2}} \Big)$$

- $f_1, f_2 =$ parton densities, $\quad C =$ hard-scattering coefficient
- $Q =$ hard momentum scale (e.g. Higgs mass, jet E_T)
  $x_1, x_2 =$ dimensionless variables constructed from kinematics
- convolution $f \underset{x}{\otimes} g = \displaystyle\int_x^1 \frac{dz}{z} f\Big(\frac{x}{z}\Big)\, g(z)$
- in $C(\ldots)$ possible dependence on m_t, m_H etc.
- higher-order corrections (1st line) $\rightarrow$ next slides
  power corrections (2nd line) $\rightarrow$ not discussed here

Factorization formulae

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- have α_s expansions for C and for $df/d\mu_F$
- μ_R = renormalization scale
  separates physics at scale Q from physics at much higher scales (ultraviolet region)

Factorization formulae

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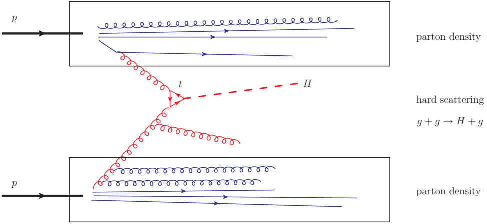


Renormalization scale dependence

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 analytically (possibly approximate)
- 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 is 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:

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

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

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

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

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

- 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

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

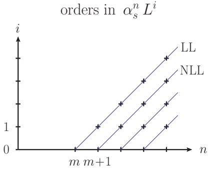
with

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

- 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^{n}LO result get variation at N^{n+1}LO corresponding to

$$\alpha_s^{n+1} \sum_{i=1}^{n+1-m} (\text{known coeff.}) \times \log^i \tfrac{\mu^2}{Q^2} + \mathcal{O}(\alpha_s^{n+2})$$

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



Renormalization scale dependence

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

consequences:

- when calculate higher orders
  expect that scale dependence decreases
- scale variation in N^{n}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?

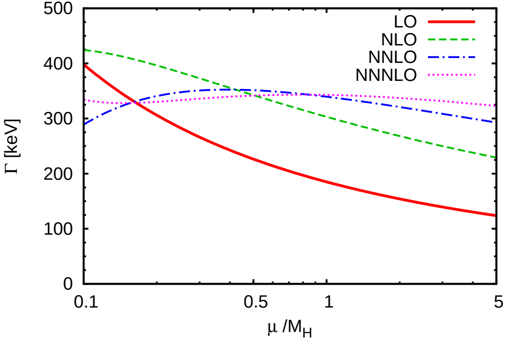
Renormalization scale choice

- 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
  - principle of minimal sensitivity (PMS): $\frac{d}{d\mu^2} \sum_{i=0}^{1} \alpha_s^{m+i} C_i(\mu) = 0$
  - fastest apparent convergence (FAC): $C_1(\mu) = 0$
  - Brodsky-Mackenzie-Lepage (BLM): more complicated
- how much these reduce higher orders depends on process
  cannot "predict" higher orders without calculating them

Renormalization scale dependence

- example: inclusive hadronic decay of Higgs boson via top quark loop (i.e. without direct coupling to $b\bar{b}$)
- in perturbation theory: $H \to 2g$, $H \to 3g$, ... known to N^{3}LO Baikov, Chetyrkin, hep-ph/0604194



plot for $m_H = 125\,\mathrm{GeV}$

Factorization scale dependence

- scale dependence of PDF given by DGLAP equation:

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

  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

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

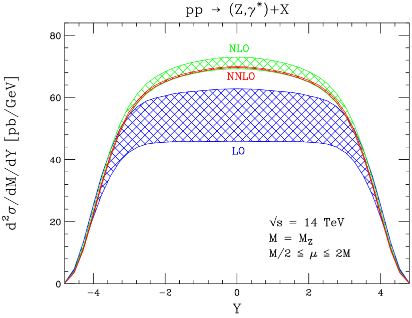
Factorization scale dependence

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

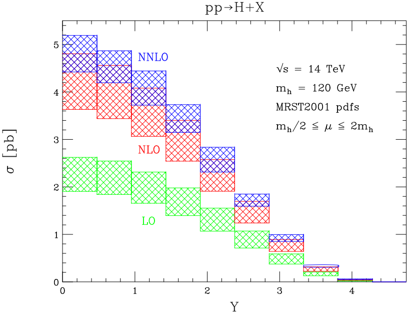
  if evolve PDFs with DGLAP kernels up to $\alpha_s^n\, P_{n-1}$ or higher
- as for μ_R may estimate certain higher-order terms by varying μ_F between e.g. $1/2$ and 2 times some central value
- as for μ_R no general solution for finding μ_F that minimizes higher orders
- often set $\mu_F = \mu_R$ (and vary them) together
  but can also set and vary them separately

Scale dependence

examples: rapidity distributions in Z/γ^* and in Higgs production



Anastasiou, Dixon, Melnikov, Petriello, hep-ph/0312266



Anastasiou, Melnikov, Petriello, hep-ph/0501130

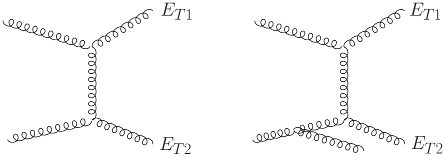
$\mu_F = \mu_R = \mu$ varied within factor 1/2 to 2

LO, NLO, and higher

- instead of varying scale(s) may estimate higher orders by comparing N^{n}LO result with N^{n-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 $\frac{d\sigma}{dE_{T1}\, dE_{T2}}$ for dijet production



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

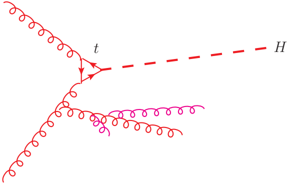
Multi-scale problems

- 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: $\log \frac{p_T}{Q}$ for $p_T \ll Q$ $\rightsquigarrow$ Sudakov factors
  - threshold logs: $\log \frac{M^2}{\hat{s}}$ for $\hat{s} \to M^2$
    for production of mass M with partonic collision energy $\sqrt{\hat{s}}$
    $\sigma(pp) \sim \int dz_1 dz_2 \, \mathsf{PDF}(z_1) \, \mathsf{PDF}(z_2) \, C(\hat{s} = z_1 z_2 s)$
  - high-energy logs: $\log \frac{Q^2}{s}$ for $s \gg Q^2$ $\rightsquigarrow$ BFKL equation
- resummation procedure may have its own uncertainties

  e.g. from integrals of type $\int_0^Q d\mu \, \mathsf{fct.}\big(\alpha_s(\mu)\big)$ $\rightsquigarrow$ Landau pole

Jet production

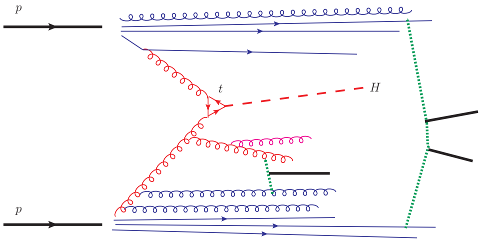
- fundamental problem: factorization formulae are for prod'n of high-p_T partons, not high-p_T hadrons
- parton $\rightarrow$ hadron transition non-perturbative $\rightsquigarrow$ need model
- to minimize theory uncertainties:
  - define hadronic jets using an algorithm that is not sensitive to collinear and soft radiation (beyond perturbative control)



  - apply algorithm to partons in computation and to hadrons in measurement
  - hadronization corrections should then be moderate and typically decrease with jet E_T

Monte Carlo generators e.g. HERWIG, PYTHIA, SHERPA

- build on structure of factorization formulae
- but compute fully exclusive final states (no unspecified "$+X$")



- ingredients:
  - parton densities and hard-scattering matrix elements
  - parton showers: small-angle radiation from partons in initial and final state in perturbative region
  - models for hadronization, underlying event, multiparton int's

Parton density fits

Principle of PDF determinations:

- compare data with factorization formulae for selected processes and kinematics
- specify PDF at reference scale μ_0

  use DGLAP eqs. to evolve to scales μ used in fact. formulae
- conventional determinations parameterize PDFs at μ_0 and determine parameters by χ^2 fit to data

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

Recent PDF sets

PDF set	order	fitted PDF parameters	μ_0^2 [GeV^2]	Q^2_{min} [GeV^2]	$\alpha_s(m_Z)$	
JR09	NNLO	20	0.55	2	$0.1124(20)$	fitted
ABKM09	NNLO	21	9	2.5	$0.1135(14)$	fitted
MSTW08	LO	28	1	2	0.139	
	NLO				0.120	
	NNLO				0.117	
HERAPDF1.0	NLO	10	1.9	3.5	0.1176	
CT10	NLO	26	1.69	4	0.118	
NNPDF2.1	LO	259	2	3	$0.119, 0.130$	
	NLO				0.119	
	NNLO				0.119	

Q_{min} = minimum Q for fitted data on deep inelastic scattering
updates: ABKM09 $\to$ ABM10, HERAPDF1.0 $\to$ 1.5, NNPDF2.1 $\to$ 2.3

Recent PDF sets

PDF set	m_c	m_b	tolerance T	
	[GeV]	[GeV]	68% CL	90% CL
JR09	1.3	4.2	4.54	
ABKM09	1.5	4.5	1	
MSTW08	1.4	4.75	≈ 1 to 6.5	≈ 2.5 to 11
HERAPDF1.0	1.4	4.75	1	
CT10	1.3	4.75		10
NNPDF2.1	1.414	4.75	–	–

m_c and m_b are pole masses

T will be explained later

Uncertainties on extracted PDFs

“systematic theory uncertainties”

- 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 are 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

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

  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

$$\Delta\chi^2 = \sum\nolimits_i z_i^2$$

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

  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
  $\rightsquigarrow$ Lagrange multiplier method (not discussed here)
  see e.g. CTEQ, hep-ph/0101051

The tolerance criterion

- if data points D_i follow Gaussian distribution then experiment with N_j data points contributes $\chi^2_{j,\text{min}} \sim N_j$ to global χ^2_{min}
- not always 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

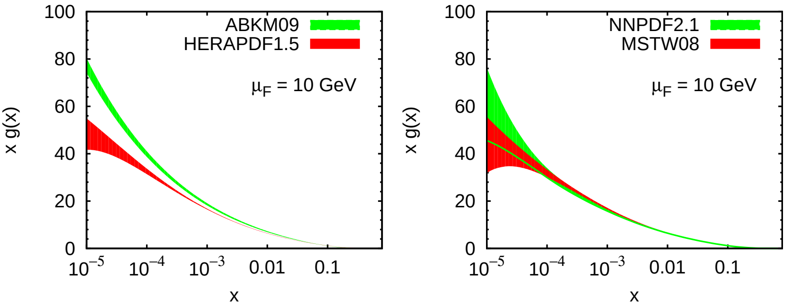
  may be due to inconsistent data sets, shortcomings of theory description or of PDF parameterization
  in such a case standard χ^2 errors misrepresent uncertainty
- modified criterion for T adopted by groups CT, MSTW, JR
  - obtained by procedure/algorithm looking at χ^2 from individual experiments
  - 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

The NNPDF approach

- to avoid bias due to functional form of PDFs, use very flexible functions (called "neural networks") with large number of free parameters (about $10\times$ more than in standard approach)
- standard χ^2 fit then not possible, instead
  - generate Monte Carlo ensemble of replicas of original data (typically $N_{\text{rep}} = 100$ or 1000), according to central values and errors of measurement
  - in each replica divide data into "training" and "validation" set
  - for each replica minimize χ^2 on training set until χ^2 of validation set starts to increase (thus avoiding to fit "noise in the data")
- central values and uncertainties on observable (or on PDFs themselves) given by ensemble average etc.

$$\overline{\mathcal{O}} = \frac{1}{N_{\text{rep}}} \sum_{r}^{N_{\text{rep}}} \mathcal{O}_r \qquad (\Delta\mathcal{O})^2 = \frac{1}{N_{\text{rep}} - 1} \sum_{r}^{N_{\text{rep}}} (\mathcal{O}_r - \overline{\mathcal{O}})^2$$

Illustration of PDF sets and their errors



error bands for 68% CL

- spread between different parameterizations often larger than error bands of single parameterization
- error bands propagate uncertainties of fitted data into PDFs but do not reflect "systematic theory uncertainties" of PDF extraction

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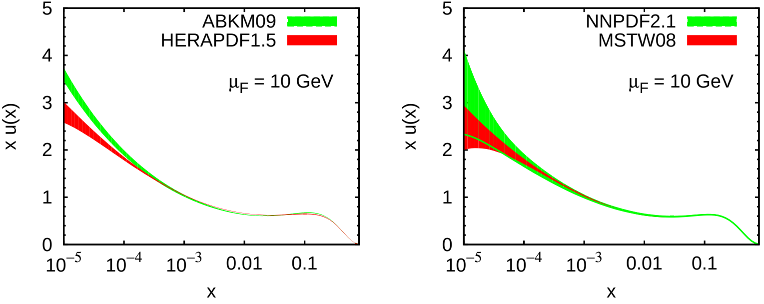

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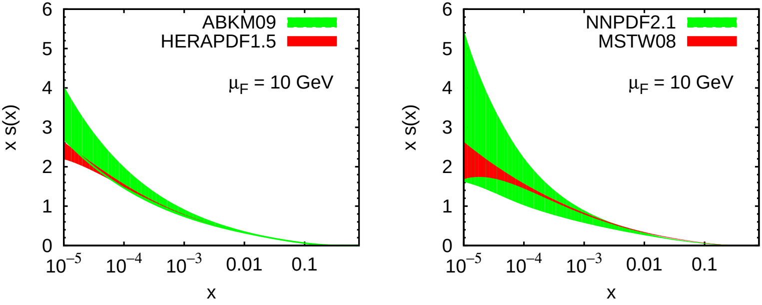

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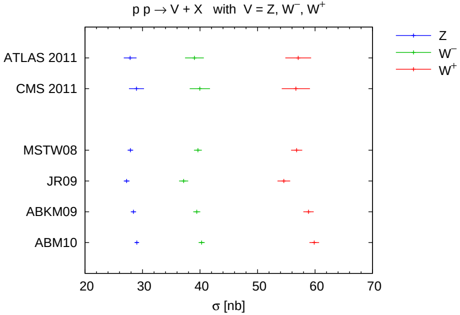

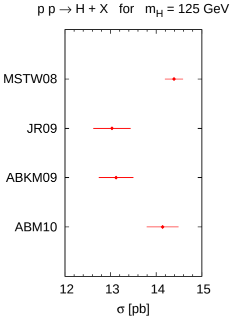

benchmark NNLO cross sections at $\sqrt{s} = 7\,\mathrm{TeV}$ from Alekhin et al., arXiv:1011.6259

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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 orders in pert. theory not the only source of uncertainty
  full final state details, hadronization corrections, ...
  are more difficult to quantify
- errors of PDF fits reflect uncertainties of fitted data
  (not always a straightforward exercise in textbook statistics)
  do not include uncertainties of theory used to fit data