Perturbative Theory Uncertainties from Theory Nuisance Parameters.

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Invitation: Meaningful Theory Uncertainties

2 Scale Variations

Theory Nuisance Parameters

Application to Drell-Yan p_T Spectrum

Comparing a measured quantity to its theory prediction to extract POI y $\left[f \pm \Delta f\right]_{\text{measured}} \stackrel{!}{=} \left[f(y) \pm \Delta f\right]_{\text{theory}} \Rightarrow y \pm \Delta y^{\text{exp}} \pm \Delta y^{\text{th}}$

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Theory uncertainty must be as meaningful as experimental one, so it should

- Reflect our level of knowledge
 - Quantify the intrinsic precision of the current prediction
 - It is *not* the distance to the true (or higher-order) result \hat{f}

 $\Delta f
eq |f - \hat{f}|$

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- Have some form of statistical interpretation
 - We want to have some probability or level of confidence that

 $\hat{f} \in [f - \Delta f, f + \Delta f]$

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Have correct correlations

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Theory Correlations.

Correlations can be crucial once several predictions are used in combination

• Prototype example: Ratio of two quantities f and g



• Unc. of ratio depends critically on exact correlation ρ between Δf and Δg

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• Differential spectrum $f(x) \equiv d\sigma/dx$

 Uncertainty on shape of f(x) is encoded in point-by-point correlations ρ_{ij} between Δf(x_i) and Δf(x_j)

\Rightarrow Critical for interpreting differential spectra when relying on shape effects

Scale Variations.

Our Standard Estimation Method.

Consider expansion of quantity f in some small parameter lpha

$$f(\alpha) = f_0 + f_1 \alpha + f_2 \alpha^2 + f_3 \alpha^3 + \mathcal{O}(\alpha^4)$$

• To make a prediction, we calculate first few *true values* \hat{f}_n

NLO:
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Can also perform the expansion in a slightly different way (aka "scheme")

$$\begin{split} \tilde{lpha}(lpha) &= lpha ig[1 + b_0 \, lpha + b_1 \, lpha^2 + b_2 \, lpha^3 + \mathcal{O}(lpha^4) ig] \ \Rightarrow \quad ilde{f}(ilde{lpha}) &= ilde{f}_0 + ilde{f}_1 \, ilde{lpha} + ilde{f}_2 \, ilde{lpha}^2 + ilde{f}_3 \, ilde{lpha}^3 + \mathcal{O}(ilde{lpha}^4) \end{split}$$

- To all orders: $f(\alpha) \equiv \tilde{f}(\tilde{\alpha})$
- Finite-order prediction using $\tilde{f}(\tilde{\alpha})$ differs by higher-order terms

NLO:
$$\tilde{f}(\tilde{\alpha}) = \hat{f}_0 + \hat{f}_1 \tilde{\alpha} = \hat{f}_0 + \hat{f}_1 \alpha + b_0 \hat{f}_1 \alpha^2 + b_1 \hat{f}_2 \alpha^3 + \cdots$$

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Idea: Take the difference between schemes as uncertainty

NLO:
$$\Delta f(\alpha) = b_0 \hat{f}_1 \alpha^2 + b_1 \hat{f}_1 \alpha^3 + \mathcal{O}(\alpha^4)$$

NNLO: $\Delta f(\alpha) = [2b_0(\hat{f}_2 - b_0\hat{f}_1) + b_1\hat{f}_1]\alpha^3 + \mathcal{O}(\alpha^4)$

- We effectively estimate inexactness due to missing terms by approximating them by some linear combination of known lower-order terms, e.g. at NLO $f_2 \approx \hat{f_1} b_0$, $f_3 \approx \hat{f_1} b_1$
- \checkmark Resulting estimated $\Delta f(\alpha)$ is indeed $\mathcal{O}(\alpha^{n+1})$

But nothing guarantees that this is a good approximation (often it is not)

- f_{n+1} often has more complex internal structure than $f_{\leq n}$
- **b**_n are (rather arbitrary) numbers, have a priori nothing to do with f

Scale Variations.



 $lpha \equiv lpha_s(\mu_0)\,, ~~~ ilde lpha \equiv lpha_s(\mu)\,, ~~~ b_0 = 0.85\,L\,, ~~ b_1 = 0.75\,L^2 + 0.34\,L$

Correspond to a continuous scheme change with $L = \ln(\mu/\mu_0) / \ln 2$

• μ (or b_0) is not an actual parameter with a true value that f depends on

- No value for it might ever capture the true result (happens regularly)
- At higher order, uncertainty reduces *only because* μ (or b_0) becomes less relevant and *not because* it somehow becomes better known

What About Correlations?

 $f(\alpha) = \hat{f}_0 + \hat{f}_1 \alpha \pm \Delta f \quad \text{with} \quad \Delta f = \hat{f}_1 b_0 \alpha^2 + \cdots$ $g(\alpha) = \hat{g}_0 + \hat{g}_1 \alpha \pm \Delta g \quad \text{with} \quad \Delta g = g_1 b_0 \alpha^2 + \cdots$

How are Δf and Δg correlated?

- We don't know the method simply does not tell us
 - Correlations require a common uncertain parameter (or more generally a common source of uncertainty)
 - **b**₀, b_1 , ... (or μ) are not common or uncertain parameters
 - X Scale variations *do not* give correct correlations or shape uncertainties
- Best we can do is *assume* some theoretically motivated but still *ad hoc* correlation model that we impose on Δ*f* and Δ*g*
 - Example: Correlating/uncorrelating scale variations
 - ► Another example: Offsetting/scanning over scale variations (→ backup)

\Rightarrow Probably the most severe shortcoming of scale variations

Existing Alternatives to Scale Variations.

There have been precious few efforts to develop alternatives

- Bayesian models [Cacciari, Houdeau '11; Bagnaschi et al. '14; Bonvini '20; Duhr et al. '21]
- Series acceleration [David, Passarino '13]
- Using reference processes [Gosh et al. '22]
- All go in the right direction
 - \checkmark Try to more directly estimate size of missing higher orders
 - ✓ Expose assumptions more explicitly
 - \checkmark Try to address statistical interpretation

However

- Uncertainty estimate still based on the known lower-order terms and/or scale variations
- X Do not address correlations

\Rightarrow Unfortunately, have similar level of arbitrariness and share many limitations of scale variations

Theory Nuisance Parameters.

Parametric Theory Uncertainties.

Let's go back to our expansion of f

$$f(\alpha) = f_0 + f_1 \alpha + f_2 \alpha^2 + f_3 \alpha^3 + \mathcal{O}(\alpha^4)$$

• We calculate first few true \hat{f}_n to make an approximate prediction

LO: $f(\alpha) = \hat{f}_0$ NLO: $f(\alpha) = \hat{f}_0 + \hat{f}_1 \alpha$ NNLO: $f(\alpha) = \hat{f}_0 + \hat{f}_1 \alpha + \hat{f}_2 \alpha^2$

- Q: What is the source of uncertainty in this?
 - The missing terms $f_n \alpha_s^n$?
 - No, actually, it is the unknown series coefficients fn
 - Or more precisely, their unknown true values \hat{f}_n
- \Rightarrow To estimate the theory uncertainty, we need to quantify our limited or lack of knowledge of f_n

Consider f_n as an unknown parameter to be varied in some way

- To evaluate associated uncertainty, we need to propagate this variation into the prediction
- For that, f_n actually has to appear in the prediction, so we include it

$$\begin{split} \mathsf{N}^{1+1}\mathsf{LO:} & f(\alpha,f_2) = \hat{f}_0 + \hat{f}_1 \,\alpha + f_2 \,\alpha^2 \\ \mathsf{N}^{1+2}\mathsf{LO:} & f(\alpha,f_2,f_3) = \hat{f}_0 + \hat{f}_1 \,\alpha + f_2 \,\alpha^2 + f_3 \,\alpha^3 \\ \mathsf{N}^{2+1}\mathsf{LO:} & f(\alpha,f_3) = \hat{f}_0 + \hat{f}_1 \,\alpha + \hat{f}_2 \,\alpha^2 + f_3 \,\alpha^3 \end{split}$$

- And that's basically it!
 - ▶ We explicitly include the (leading) sources of uncertainty in our prediction
 - f_n are well-defined parameters of our prediction with a true but unknown (or imprecisely known) value
 - We simply treat them as such

Theory Nuisance Parameters (TNPs).

In reality, $f_n \equiv f_n(x)$ has (lots of) nontrivial internal structure "x"

- Parameterize it in terms of TNPs: $f_n(x, \theta_n)$ where $\theta_n \equiv \{\theta_n^i\}$
 - N¹⁺¹LO: $f(\alpha, x, \theta_2) = \hat{f}_0(x) + \hat{f}_1(x)\alpha + \frac{f_2(x, \theta_2)\alpha^2}{f_1(x)\alpha^2}$

N¹⁺²LO: $f(\alpha, x, \theta_{2,3}) = \hat{f}_0(x) + \hat{f}_1(x)\alpha + f_2(x, \theta_2)\alpha^2 + f_3(x, \theta_3)\alpha^3$

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- Key condition: There must be true values $\hat{\theta}_n$ such that

$$\hat{f}_n(x) = f_n(x, \hat{\theta}_n)$$

This makes TNPs well-defined parameters with true but unknown value
 Theory uncertainties become truly parametric with all the implied benefits

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- This makes TNPs well-defined parameters with true but unknown value
- Theory uncertainties become truly parametric with all the implied benefits
- ⇒ Step 1: Derive an appropriate TNP parameterization $f_n(x, \theta_n)$ and implement it in all the predictions

Step 1: TNP Parameterization.

$f_n(x)$ are functions of various x dependences

- Discrete: partonic channels, quantum numbers, ...
- Continuous but discrete values: n_f , N_c , E_{cm} , ...
- Fully continuous: Kinematic variables (p_T^Z, Y, q^2) , particle masses, ...
- Q: Which dependences do we need to account for and parameterize?
 - All those in which we need correlations
 - Plus those that help to obtain better theory constraints

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To satisfy key condition $f_n(x, \theta_n)$ must encode correct x dependence

 $\hat{f}_n(x) = f_n(x, \hat{\theta}_n)$

- Requires expert knowledge on underlying structure (functional form in *x*)
 - Deriving $f_n(x, \theta_n)$ means deriving correct theory correlation structure in x

X This is where scale variations, Pythia variations, etc. fail:

Do not yield a correct parameterization, cannot give correct correlations

Step 1: Parameterization Strategies.

General strategy

 \Rightarrow Break down internal structure until remaining unknowns $f_{n,i}$ are numbers

Specific strategy depends on what we know about functional form of $f_n(x)$

- We know it well enough to parameterize it explicitly For example:
 - Dependence on partonic channels is always known exactly
 - We might know from theory that $f_n(x)$ is a polynomial in $\ln x$

$$\Rightarrow \qquad f_n(x) = \sum_{i=0}^k f_{n,i} \, \ln^i x$$

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- We know it well enough to parameterize it explicitly
- We know it well enough to apply 1) in some limit and can expand around that limit

$$f_n(x) = f_{n0}(x) + f_{n1}(x) \varepsilon + f_{n2}(x) \varepsilon^2 + \mathcal{O}(\varepsilon^3)$$

For example:

- Drell-Yan p_T spectrum at small p_T : $\varepsilon = p_T^2/Q^2$
- $f_{n0}(p_T)$ can be obtained from p_T resummation with strategy 1)

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- We know it well enough to parameterize it explicitly
- We know it well enough to apply 1) in some limit
- If we don't have sufficient knowledge for either strategy 1 or 2, we can always expand in a suitable, complete functional basis {\(\phi_i\)}\)

$$f_n(x) = \sum_{i=0}^{\infty} f_{n,i} \phi_i(x) \quad
ightarrow \quad f_n(x, heta_n) = \sum_{i=0}^k heta_{n,i} \phi_i(x)$$

- A good basis is one that we can truncate after a few terms with high confidence that we can neglect truncated terms as a subleading source of uncertainty
- There are various ways for designing good bases

Constraining the TNPs.

Since θ_n are proper parameters, they can have proper estimates/constraints

$$heta_n = u_n \pm \Delta u_n$$

Can come from

- From theory: Can be modelled as "imagined" auxiliary measurement
- From experiment: Real auxiliary or nominal measurement

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- Could profile them as a free nuisance parameter in fit to data
 - No dependence on theory prejudice on how much to vary/assumptions
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 - From experiment: Real auxiliary or nominal measurement
- Could profile them as a free nuisance parameter in fit to data
 - No dependence on theory prejudice on how much to vary/assumptions
 - If the data is sensitive to a θ_n , it will constrain it, otherwise it doesn't matter
- Nevertheless, still worthwhile/useful to have a theory constraint
 - Leaving them completely free in a fit may not always be possible or practical
 - Important to know their expected "natural" size to check data constraints
 - We do like to know the uncertainty of a prediction without having to fit to data
- \Rightarrow Step 2: Obtain suitable constraints on θ_n

Step 2: Theory Constraints for Scalar Series.

Assume everything has been broken down to scalar series (in QCD)

$$f(lpha_s) = 1 + \sum_{n=1} f_n \Big(rac{lpha_s}{4\pi}\Big)^n$$

Parameterize coefficients f_n (numbers) as

 $f_n(\theta_n) = N_n \,\theta_n$

- Normalization N_n from expected "natural size" of f_n : $|\hat{f}_n| \lesssim N_n$
- Expect θ_n to have $\mathcal{O}(1)$ natural size: $|\hat{\theta}_n| \lesssim 1$
- Impose a theory constraint

$$heta_n = u_n \pm \Delta u_n = 0 \pm 1$$

• Default assumption: Model u_n as normal distributed random variable

⇒ Defines a specific "theory estimator": Validate it on known pert. series

Let's take as an example: $q ar q o V, \, q ar q o H, \, gg o H$ form factors

$f(lpha_s)$	N_n	\hat{f}_1/N_1	\hat{f}_2/N_2	\hat{f}_3/N_3	\hat{f}_4/N_4
$c_{qar{q}V}(lpha_s)$	1	-8.47	-48.6	-1387	-42015

1	-0.47	+87.1	+2309	+76100
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	4^n	-0.12	+5.44	+36.1	+297
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	$4^n C_F C_A^{n-1}$	-1.59	-0.76	-1.81	-4.56
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	$4^n C_A C_A^{n-1} (n-1)!$	+0.41	-0.17	-1.18	-1.00
\Rightarrow Let's pick: $N_n = 4C_r(4C_A)^{n-1}(n-1)!$					

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Step 2: Validation on Known Series.



Consider set of QCD series $F = \{f\}$ of a common type/category

- Identify $P_{ heta_n^f}(x)$ with population distribution of $\hat{ heta}_n^f \in F_n$ (assumption)
 - For any given θ_n^f , its unknown $\hat{\theta}_n^f$ comes from a QCD bag of coefficients
- Estimate population distribution from a sample of known series
 - Good fit to normal distribution ("central-limit theorem of Feynman diagrams")
 - Note: Distribution is a property of this specific estimator

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Application to Drell-Yan p_T Spectrum.

TNP Parameterization for $V p_T$ Spectrum.

Consider dependence on $x \equiv q_T = p_T^V$ (where $V = Z/\gamma, W$)

1) Apply strategy 2: Expand in $\,arepsilon = q_T^2/Q^2\,$ (where $Q\equiv m_{\ell\ell}$)

$$\frac{\mathrm{d}\sigma}{\mathrm{d}q_{T}} = \frac{\mathrm{d}\sigma^{(0)}}{\mathrm{d}q_{T}} \times \left[1 + \mathcal{O}\left(\frac{q_{T}^{2}}{Q^{2}}\right)\right]$$

▶ $\mathcal{O}(q_T^2/Q^2)$ corrections stay below $\lesssim 5\%$ up to $q_T \lesssim Q/3...Q/2$

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▶ $\mathcal{O}(q_T^2/Q^2)$ corrections stay below $\lesssim 5\%$ up to $q_T \lesssim Q/3...Q/2$

2) Apply strategy 1 to $\mathrm{d}\sigma^{(0)}/\mathrm{d}q_T$

$$rac{\mathrm{d}\sigma^{(0)}}{\mathrm{d}q_T} = \left[\sum_{a,b} H_{ab} imes B_a \otimes B_b \otimes S
ight](L = \ln q_T/Q)$$
 $F(lpha_s, L) = F(lpha_s) \exp \int_0^L \mathrm{d}L' \left\{\Gamma_{\mathrm{cusp}}[lpha_s(L')] \, L' + \gamma_F[lpha_s(L')]
ight\}$

- q_T dependence is predicted by resummation in terms of several independent (scalar) series
- Boundary conditions and anomalous dimensions of RGE for each function

TNPs for p_T Spectrum: After the Dust has Settled.

Brake things down to independent perturbative series, e.g. at $N^{2+1}LL$

• 5 scalar series (plus a few more we can neglect here for simplicity)

$$\begin{split} &\Gamma(\alpha_s) = \alpha_s \,\hat{\Gamma}_0 + \alpha_s^2 \,\hat{\Gamma}_1 + \alpha_s^3 \,\hat{\Gamma}_2 + \alpha_s^4 \,\Gamma_3(\theta_3^{\Gamma}) \\ &\gamma_\mu(\alpha_s) = \alpha_s \,\hat{\gamma}_{\mu 0} + \alpha_s^2 \,\hat{\gamma}_{\mu 1} + \alpha_s^3 \,\gamma_{\mu 2}(\theta_2^{\gamma_\mu}) \\ &\gamma_\nu(\alpha_s) = \alpha_s \,\hat{\gamma}_{\nu 0} + \alpha_s^2 \,\hat{\gamma}_{\nu 1} + \alpha_s^3 \,\gamma_{\nu 2}(\theta_2^{\gamma_\nu}) \\ &H(\alpha_s) = \left| \hat{c}_0 + \alpha_s \,\hat{c}_1 + \alpha_s^2 \,c_2(\theta_2^H) \right|^2 \\ &\tilde{S}(\alpha_s) = \left[\hat{\tilde{S}}_0 + \alpha_s \,\hat{\tilde{S}}_1 + \alpha_s^2 \,\tilde{S}_2(\theta_2^S) \right]^2 \end{split}$$

 Up to 5 one-dimensional functional series for beam functions (plus several more for DGLAP splitting functions)

$$ilde{b}_i(x,lpha_s) = \sum_j \int\! rac{\mathrm{d}z}{z} \left[\hat{I}_{ij,0}(z) + \hat{I}_{ij,1}(z) + I_{ij,2}(z, heta_2^{B_{ij}})
ight] f_j\!\left(rac{x}{z}
ight),$$

• Currently use known functional form: $I_{ij,n}(z, \theta_n^{B_{ij}}) = \frac{3}{2} \theta_n^{B_{ij}} \hat{I}_{ij,n}(z)$

In the future use strategy 2 to parameterize z dependence

2025-07-01 | Frank Tackmann

Results for Drell-Yan p_T Spectrum.

Comparing different orders at 95% "theory CL" ($\Delta \theta_n = 2$)



Uncertainties reduce as we go to higher order (by construction)

Uncertainty Breakdown.



Separately varying each TNP by $\pm \Delta \theta_n = 1$

- TNPs provide breakdown into independent uncertainty sources with correct shape
 - Encodes correct point-by-point correlations
 - lmportantly, carries over to p_T^{ℓ} and other decay kinematics

Correlations between W and Z.



relative impacts for W



- Caveats apply: These are only the (formerly) leading perturbative unc.
- Subleading effects can become important (or even dominant) now
 - Quark mass effects
 - EW corrections
 - Power corrections

Profiling TNPs.



- Include prior Gaussian theory constraint $heta_n = 0 \pm 1$
- Data provides nontrivial constraints on TNPs
 - Post-fit prediction has reduced theory uncertainties
 - Induces nontrivial post-fit correlations

Profile against True Higher Order.



- Simulates fit to real data (which contains all-order result)
 - TNPs are pulled toward their true values
 - Post-fit prediction gets corrected toward true result

Relaxing the Prior Theory Constraint.



Data is able to sufficiently constrain TNPs by itself

- Reduces dependence on prior theory constraint (and associated potential bias)
 - Post-fit constraints on TNPs become even more consistent with true values
- Uncertainty on final result almost unchanged

Bonus: Including Nonperturbative Effects.



$$ilde{f}_i(x,b_T,\mu,Q) = ilde{f}_i^{(0)}(x,b_T,\mu,Q) iggl\{ 1+b_T^2 \Big[oldsymbol{\Lambda}_{2,i}(x)+oldsymbol{\lambda}_2\,\lnrac{b_TQ}{b_0} \Big] + \mathcal{O}(oldsymbol{\Lambda}_{ ext{QCD}}^4b_T^4) iggr\}$$

Also include quadratic and quartic OPE coefficients in the fit

TNPs still pulled toward their true values but less constrained 2025-07-01 | Frank Tackmann

26/27.

Summary.

Interpretation of precision measurements requires *meaningful* theory uncertainties which includes in particular proper theory correlations

Scale variations become insufficient once theory unc. \sim experimental unc

Neither particularly reliable nor can they do correlations

Theory nuisance parameters

- Provide truly parametric theory uncertainties that
 - ✓ Encode correct correlations
 - ✓ Can be consistently propagated everywhere (fits, MCs, neural networks, ...)
 - $\checkmark\,$ Can be consistently profiled and constrained by data
- Bonus: Can fully benefit from all known partial higher-order information
- First successful applications to resummed Drell-Yan p_T spectrum
 - Implemented in SCETlib (available upon request, hopefully fully public soon)
 - Precision W-mass measurement by CMS [→ see Kenneth's talk]
- First promising applications to PDF fits and fixed-order predictions [MSHT20aN3LO (Gowan et al.) '22; Poncelet, Lim '24]

Additional Slides

Scanning over Scale Variations.



Repeat fit for each individual scale variation and take envelope of results

- Amounts to trying out various correlation models for the same total uncertainty band
 - None of the trial variations provides a realistic correlation model
 - Individual variations are not meaningful (which is why we take their envelope)
- Best we can do with scale variations
 - Perform as many variations as we can to "fill out" the band, hoping to include at least one that happens to give sufficiently conservative estimate
 - And/or identify conceptually "independent" subsets of variations and add their envelopes

TNPs for Drell-Yan p_T Spectrum: More Details.

Apply strategy 2 with
$$arepsilon = q_T^2/Q^2$$
 ($Q \equiv \sqrt{m_{\ell\ell}}$) $rac{\mathrm{d}\sigma}{\mathrm{d}^4 q} = rac{\mathrm{d}\sigma^{(0)}}{\mathrm{d}^4 q} imes \left[1 + \mathcal{O}\!\left(rac{q_T^2}{Q^2}
ight)
ight]$

- Power corrections stay below $\lesssim 5\%$ up to $q_T \lesssim Q/3...Q/2$
- Leading-power term is subject of q_T factorization and resummation

- $\blacktriangleright \text{ Here } VV' = \{\gamma\gamma, \gamma Z, Z\gamma, ZZ, W^+W^+, W^-W^-\}$
- Factorization allows us to apply strategy 1 to $q_T(b_T)$, q^2 , V
- Also allows us to factorize $x_{a,b}$ dependence and apply strategy 2 to it

Results for Drell-Yan p_T Spectrum: Other Ratios.



[For details see Cridge, Marinelli, FT; arXiv:2506.13874]

We perform Asimov fits to (unfluctuated) pseudodata

- Standard method to study expected uncertainties in a controlled setting
 - Unobscured by statistical fluctuations and subleading effects
- Goals: Demonstrate TNPs and estimate expected uncertainties in $lpha_s(m_Z)$
 - Can consistently drop subleading effects in both pseudodata and theory model (power corrections, quark mass effects, EW corrections)
 - They are needed to fit the real data, but are irrelevant for estimating the dominant uncertainties

Pseudodata

- Central value given by central SCETlib prediction with $lpha_s(m_Z)=0.118$
- Exp. uncertainties and correlations from ATLAS 8 TeV inclusive $Z p_T$ measurement [Eur. Phys. J. C 84 (2024) 315 [arXiv: 2309.09318]]
- Same bins and cuts as used by ATLAS $lpha_s(m_Z)$ determination [arXiv:2309.12986]

Results for α_s with Profiling TNPs.

[For details see Cridge, Marinelli, FT; arXiv:2506.13874]

different pert. orders

relaxing theory constraint



Important: Not all sources of theory uncertainties included yet

α_s Results with TNPs and Nonpert. Parameters.

[For details see Cridge, Marinelli, FT; arXiv:2506.13874]



Important: Not all sources of theory uncertainties included yet

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