Developing the framework for combined fits of CGC observables

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UNIWERSYTET JAGIELLOŃSKI W KRAKOWIE

work done by Hau Le,

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Developing the framework for combined fits of CGC observables

Explaining the title

- *Developing*: work in progress, partial preliminary results
- *framework*: numerical setup consisting of many small elements with the possible potential for further extensions
- *combined fit*: the goal is to describe simultaneously several sets of experimental data
- *CGC*: Color Glass Condensate is an effective description of processes in pp and pA collisions at high energies $\Longleftrightarrow$ small x
- *observables*: different cross-sections

Developing the framework for combined fits with CGC

Color Glass Condensate framework

- access to unintegrated parton distribution functions
- nonperturbative initial condition - model
- perturbative evolution equation
- predictions of cross-sections at high-energies/small-x

$\ln Q^2$ and $\ln 1/x$ evolution

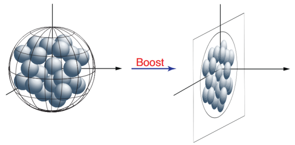
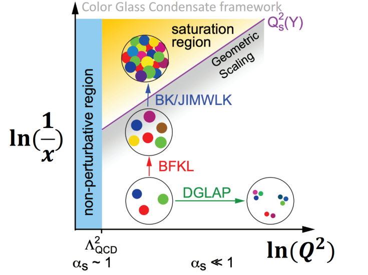


Fig. 2. An ultrarelativistic nucleus appears as a "pancake" with the $A^{1/3}$-enhanced color charge density.



Y. Kovchegov, *Brief Review of Saturation Physics*, Acta Phys. Pol. B, 45 (2014) 2241

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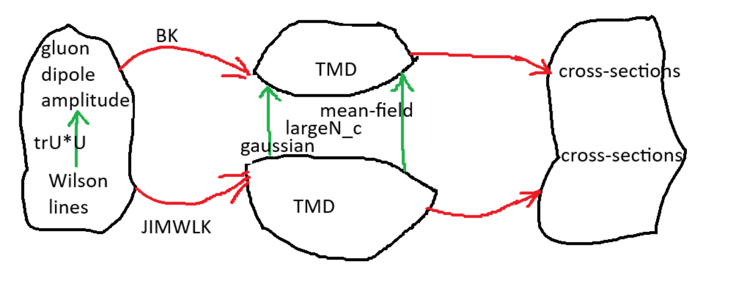
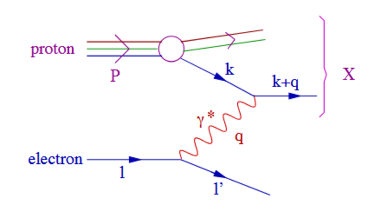
Color Glass Condensate framework



- TMD: Transverse-Momentum-Dependent structure functions
- BK: Balitsky-Kovchegov evolution equation
- JIMWLK: Jalilian-Marian, Iancu, McLerran, Weigert, Leonidov, and Kovner evolution equation

Developing the framework for combined fits with CGC

Virtual photon-proton cross section for transverse (T) and longitudinal (L) polarization of the virtual photon



E. Iancu, *QCD in heavy ions collisions*

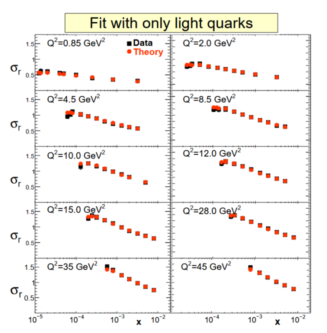
$$x = \frac{-q^2}{(P+q)^2 - q^2 - M^2}$$

$$\sigma_{T,L}(x, Q^2) \quad = \quad \sigma_0 \sum_{f=u,d,s} \int_0^1 dz d\mathrm{r} |\psi^f_{T,L}(e_f, m_f, z, Q^2, \mathrm{r})|^2 N_F(x, \mathrm{r})$$

Initial condition

$$N_F^{\mathrm{MV}}(x = x_0, \mathrm{r}) = 1 - \exp\left[-\frac{\left(r^2 Q_0\right)^\gamma}{4} \ln\left(\frac{1}{r\Lambda} + e\right)\right]$$

Comparison with experimental data for the reduced cross sections in different Q^2 bins



$Q^2_{s0} = 0.164$ GeV^2 at $x_0 = 0.01$, $\sigma_0 = 32.324$, $\gamma = 1.123$, $C = 2.48$ and $m_l = 0.0182$

J. L. Albacete, N. Armesto, J.G. Milhano, P. Quiroga Arias, C.A. Salgado, *AAMQS: A non-linear QCD analysis of new HERA data at small-x including heavy quarks*, Eur. Phys. J. C 71, 1705 (2011)

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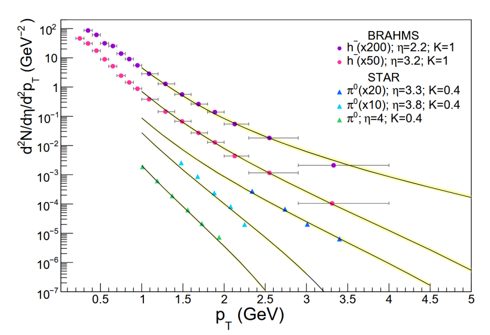
Negatively charged hadron and π^0 yields in proton-proton collisions at $\sqrt{S_{NN}} = 200$ GeV



$Q_{s0}^2 = 0.4$ GeV^2 at $x_0 = 0.02$ was the only fitted parameter

J. Albacete, C. Marquet, *Single inclusive hadron production at RHIC and the LHC from the Color Glass Condensate*, Phys.Lett.B687:174-179,2010

Negatively charged hadron and π^0 yields in proton-proton collisions at $\sqrt{S_{NN}} = 200$ GeV

$$\frac{dN_h}{dy_h d^2 p_t} = \frac{K}{(2\pi)^2} \int_{x_F}^{1} \frac{dz}{z^2} \left\{ \sum_q \left[x_1 f_{q/p}(x_1, p_t^2) N_F(x_2, \frac{p_t}{z}) D_{h/q}(z, p_t^2) \right] + \right.$$
$$\left. + \left[x_1 f_{g/p}(x_1, p_t^2) N_A(x_2, \frac{p_t}{z}) D_{h/g}(z, p_t^2) \right] \right\}$$

J. Albacete, C. Marquet, *Single inclusive hadron production at RHIC and the LHC from the Color Glass Condensate*, Phys.Lett.B687:174-179,2010

Developing the framework for combined fits with CGC

Framework: requirements

- evolution equation
- initial condition
- access to gluon dipole amplitude in position and momentum spaces
- minimization algorithm $\Rightarrow$ levmar library
- access to fragmentation functions and PDFs $\Rightarrow$ LHAPDF library

Framework: features

- BK evolution equation with kinematical constraint
- Balitsky/daughter/mother dipole prescription for the running coupling
- Euler/Runge integration scheme
- uncertainty estimation
- parallelization $\Rightarrow$ short running time
- ...

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Balitsky-Kovchegov evolution equation

The LO BK equation reads

$$\frac{\partial S_{\bar{\boldsymbol{x}}_\perp \bar{\boldsymbol{y}}_\perp}(\eta)}{\partial \eta} = \frac{\bar{\alpha}_s}{2\pi} \int d^2\bar{\boldsymbol{z}}_\perp \, \mathscr{M}_{\bar{\boldsymbol{x}}_\perp \bar{\boldsymbol{y}}_\perp \bar{\boldsymbol{z}}_\perp} \left[S_{\bar{\boldsymbol{x}}_\perp \bar{\boldsymbol{z}}_\perp}(\eta) S_{\bar{\boldsymbol{z}}_\perp \bar{\boldsymbol{y}}_\perp}(\eta) - S_{\bar{\boldsymbol{x}}_\perp \bar{\boldsymbol{y}}_\perp}(\eta) \right],$$

where

$$\mathscr{M}_{\bar{\boldsymbol{x}}_\perp \bar{\boldsymbol{y}}_\perp \bar{\boldsymbol{z}}_\perp} = \frac{(\bar{\boldsymbol{x}}_\perp - \bar{\boldsymbol{y}}_\perp)^2}{(\bar{\boldsymbol{x}}_\perp - \bar{\boldsymbol{z}}_\perp)^2 (\bar{\boldsymbol{z}}_\perp - \bar{\boldsymbol{y}}_\perp)^2}.$$

Rewritten in radial variables

$$\frac{\partial S(r,\eta)}{\partial \eta} = \frac{\bar{\alpha}_s}{2\pi} \int d\phi \, dr_z \, r_z \, \frac{r^2}{r_z^2 (r^2 + r_z^2 - 2 r r_z \cos\phi)} \times$$
$$\times \left[S(r_z,\eta) \, S\left(\sqrt{r^2 + r_z^2 - 2 r r_z \cos\phi}, \eta \right) - S(r,\eta) \right].$$

Balitsky-Kovchegov evolution equation

Account for several additional physical effects, such as the running of the coupling constant with the energy scale, resummation of subleading corrections [Ducloue et al., 2019]

$$\frac{\partial S(r,\eta)}{\partial \eta} = \int d\phi\, dr_z\, r_z \times$$
$$\times \left[\frac{\bar{\alpha}_s(r)}{2\pi r_z^2} \left(\frac{r^2}{r_{zy}^2 + \varepsilon^2} + \frac{\bar{\alpha}_s(r_z)}{\bar{\alpha}_s(r_{zy})} - 1 + \frac{r_z^2}{r_{zy}^2 + \varepsilon^2} \left(\frac{\bar{\alpha}_s(r_{zy})}{\bar{\alpha}_s(r_z)} - 1 \right) \right) \right] \times$$
$$\times \left[S(r_z, \eta - \delta_{r_z;r}) S(r_{zy}, \eta - \delta_{r_{zy};r}) - S(r,\eta) \right],$$

where $r_{zy} = \sqrt{r^2 + r_z^2 - 2 r r_z \cos\phi}$. The shifts in η in the dipole amplitudes are given by $\delta_{r_z;r} = \max\left\{0, 2\log\frac{r}{r_z}\right\}$ and similarly $\delta_{r_{zy};r} = \max\left\{0, 2\log\frac{r}{r_{zy}}\right\}$.

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Automatic Differentiation in a nutshell

Allows to evaluate 'analytic' derivatives of a computer program with respect to external parameters.

- numbers are promoted to vectors

$$x \to \begin{pmatrix} x \\ \partial_A \\ \partial_B \\ \partial_A^2 \\ \partial_A \partial_B \\ \vdots \end{pmatrix}$$

- all arithmetic operators are overloaded
- functions with derivatives have to be provided
- works for most algorithms

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Automatic Differentiation for the Balitsky-Kovchegov evolution equation

$$S(r,\eta) \to \begin{pmatrix} S(r,\eta) \\ \partial_{Q_0} S(r,\eta) \\ \partial_r S(r,\eta) \\ \partial^2_{Q_0} S(r,\eta) \\ \partial^2_r S(r,\eta) \end{pmatrix}$$

Then

$$\frac{\partial S(r,\eta)}{\partial \eta} = \int d\phi \, dr_z \, r_z \times$$
$$\times \left[\frac{\bar{\alpha}_s(r)}{2\pi r_z^2} \left(\frac{r^2}{r_{zy}^2 + \varepsilon^2} + \frac{\bar{\alpha}_s(r_z)}{\bar{\alpha}_s(r_{zy})} - 1 + \frac{r_z^2}{r_{zy}^2 + \varepsilon^2} \left(\frac{\bar{\alpha}_s(r_{zy})}{\bar{\alpha}_s(r_z)} - 1 \right) \right) \right] \times$$
$$\times \left[S(r_z, \eta - \delta_{r_z;r}) S(r_{zy}, \eta - \delta_{r_{zy};r}) - S(r,\eta) \right],$$

gives $S(r,\eta)$ together with the evolved derivatives.

F. Cougoulic, P. Korcyl, T. Stebel, *Improving the solver for the Balitsky-Kovchegov evolution equation with Automatic Differentiation*, Comput.Phys.Commun. 313 (2025) 109616

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Automatic Differentiation for the Balitsky-Kovchegov evolution equation

Benefits:

- faster convergence of the fit
  - fewer iterations
  - less computer time
  - can test more parameters in the initial condition
- access to the Hessian matrix allows easy estimation of uncertainties
- more reliable estimation of some TMD functions with long tails
- can tell how the initial condition is sensitive to the given experimental data

Costs:

- slower code, but less than naively expected

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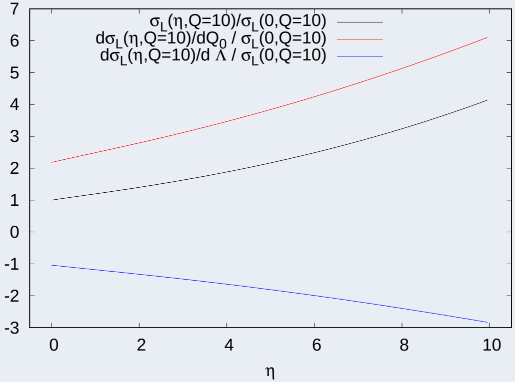
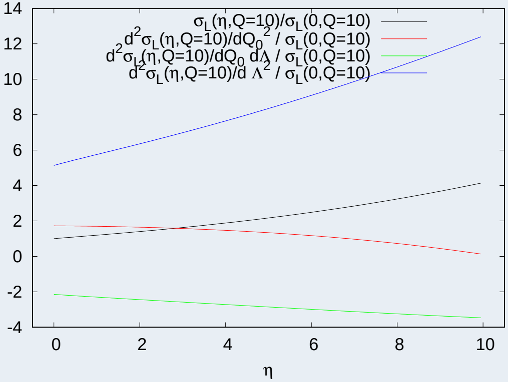
First derivatives of the longitudinal cross-section $\sigma_L^{\gamma^*,p}(x, Q^2 = 10\,\mathrm{GeV}^2)$



Sensitivity of the observable to the parameters of the initial condition

Second derivatives of the cross-section $\sigma_L^{\gamma^*,p}(x, Q^2 = 10\,\mathrm{GeV}^2)$



Immediate access to the exact Hessian matrix at the minimum

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Hessian method

Assume that $\chi^2_{\rm global}$ is quadratic about the global minimum

$$\Delta\chi^2_{\rm global} \equiv \chi^2_{\rm global} - \chi^2_{\rm min} = \sum_{i,j=1}^{n} H_{ij}\left(a_i - a_i^0\right)\left(a_j - a_j^0\right),$$

where

$$H_{ij} = \frac{1}{2}\frac{\partial^2\chi^2_{\rm global}}{\partial a_i \partial a_j}\bigg|_{\rm min}$$

We can diagonalize the covariance matrix $C \equiv H^{-1}$,

$$\sum_{j=1}^{n} C_{ij} v_{jk} = \lambda_k v_{ik},$$

$$a_i - a_i^0 = \sum_{k=1}^{n}\left(\sqrt{\lambda_k}\, v_{ik}\right) z_k \quad \Rightarrow \quad \Delta\chi^2_{\rm global} = \sum_{k=1}^{n} z_k^2 \equiv T^2$$

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Comparison of the uncertainties obtained from the Hessian and Monte Carlo methods for the PDFs

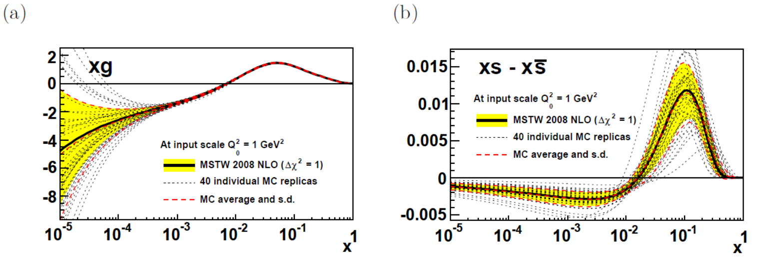

Figure 1. Comparison of Hessian and Monte Carlo results at the input scale of $Q_0^2 = 1$ GeV^2 for the (a) gluon distribution and (b) strange asymmetry. Both results allow $n = 20$ free PDF parameters and do not apply a tolerance (i.e. $T = 1$ in the Hessian case). The best-fit (solid curves) and Hessian uncertainty (shaded region) are in good agreement with the average and standard deviation (thick dashed curves) of the $N_{\text{rep}} = 40$ Monte Carlo replica PDF sets (thin dotted curves).

G. Watt, R. Thorne, *Study of Monte Carlo approach to experimental uncertainty propagation with MSTW2008 PDFs*, JHEP 1208:052, 2012

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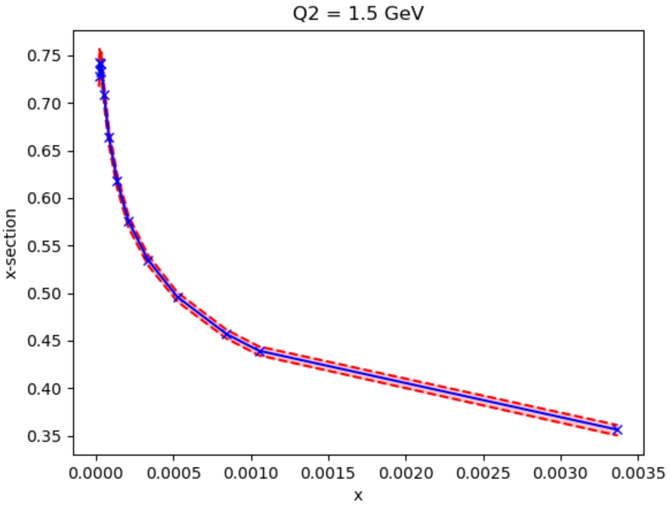
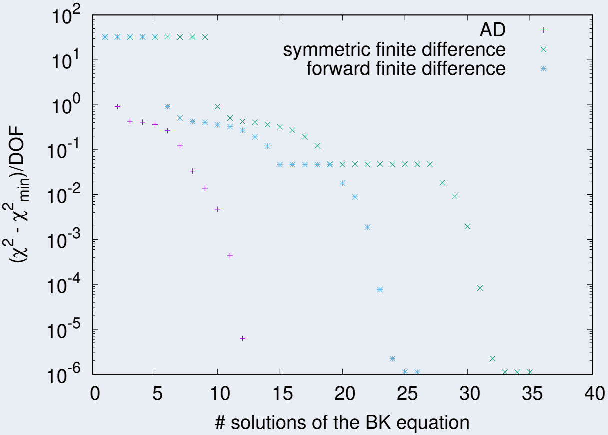
Uncertainty of the DIS cross-section obtained with the Hessian method



Increased efficiency of the Levenberg-Marquard optimization algorithm



Fitting 4 parameters to the DIS HERA data

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Logarithmic Fourier Transform

Popular in geophysics, cosmology, and signal processing.

- It allows for the Fourier transform of data sampled on a logarithmic scale rather than linear,
- fits perfectly into our setup as we solve the BK equation on a logarithmic grid,
- more reliable than an ordinary 2D Fourier transform,
- Bessel function is not needed,
- order of magnitude more efficient in computer time.

Main idea:

$$\tilde{f}(k) = C(k)\, \mathrm{FT}_{1D}^{\tau\to k}\left[\, B(\tau)\, \mathrm{FT}_{1D}^{x\to\tau}\left[\, A(x)\; f(x)\,\right]\right]$$

where $A(x)$, $B(\tau)$, and $C(k)$ are known functions that can be precomputed. $\mathrm{FT}_{1D}^{x\to k}$ is an ordinary, linear, one-dimensional FT.

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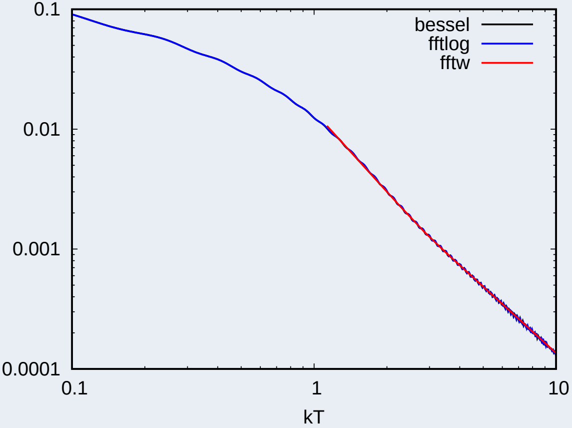
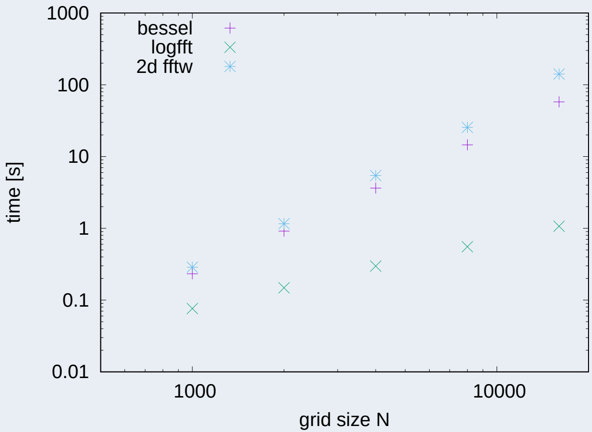
Logarithmic Fourier Transform



The WW TMD structure function obtained with three different methods with MV model, $N = 2000$

Logarithmic Fourier Transform



Time comparison: the logfft approach, numerical integration of the Bessel functions, and a 2D Fourier transform evaluated using the FFTW3 library.

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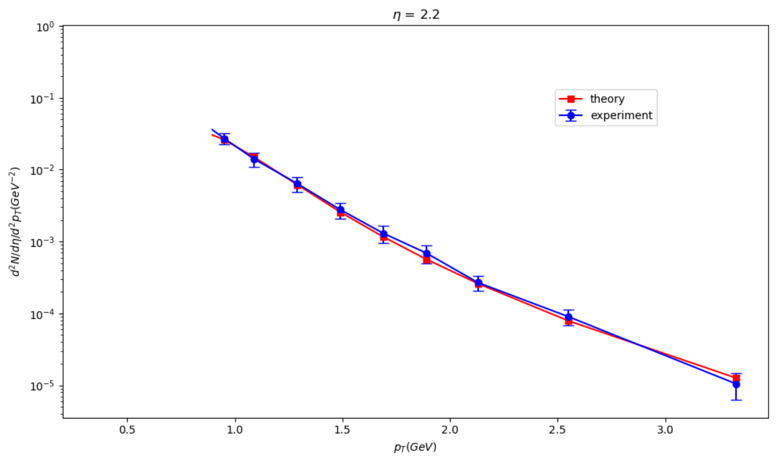
Preliminary results for combined fit



Back to BRAMHS data: negatively charged hadron and π^0 yields in proton-proton collisions at $\sqrt{S_{NN}} = 200$ GeV

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Going further

$$\frac{d\sigma(pA \to qgX)}{d^2P_t d^2k_t dy_1 dy_2} = \frac{\alpha_s^2}{2C_F}\frac{z(1-z)}{P_t{}^4} x_1 q(x_1,\mu^2) P_{gq}(z) \times \left\{ \left[(1-z)^2 - \frac{z^2}{N_c^2} \right] \mathcal{F}_{qg}^{(1)}(x_2,k_t) + \mathcal{F}_{qg}^{(2)}(x_2,k_t) \right\}, \tag{2.12}$$

$$\frac{d\sigma(pA \to q\bar{q}X)}{d^2P_t d^2k_t dy_1 dy_2} = \frac{\alpha_s^2}{2C_F}\frac{z(1-z)}{P_t{}^4} x_1 g(x_1,\mu^2) P_{qg}(z) \left\{ [(1-z)^2 + z^2] \mathcal{F}_{gg}^{(1)}(x_2,k_t) + 2z(1-z)\mathrm{Re}\, \mathcal{F}_{gg}^{(2)}(x_2,k_t) - \frac{1}{N_c^2}\mathcal{F}_{gg}^{(3)}(x_2,k_t) \right\}, \tag{2.13}$$

$$\frac{d\sigma(pA \to ggX)}{d^2P_t d^2k_t dy_1 dy_2} = \frac{\alpha_s^2}{2C_F}\frac{z(1-z)}{P_t{}^4} x_1 g(x_1,\mu^2) P_{gg}(z) \times \left\{ [(1-z)^2 + z^2] \mathcal{F}_{gg}^{(1)}(x_2,k_t) + 2z(1-z)\mathrm{Re}\, \mathcal{F}_{gg}^{(2)}(x_2,k_t) + \mathcal{F}_{gg}^{(6)}(x_2,k_t) + \frac{1}{N_c^2}\left[\mathcal{F}_{gg}^{(4)}(x_2,k_t) + \mathcal{F}_{gg}^{(5)}(x_2,k_t) - 2\mathcal{F}_{gg}^{(3)}(x_2,k_t) \right] \right\}, \tag{2.14}$$

C. Marquet, E. Petreska, C. Roiesnel, *Transverse-momentum-dependent gluon distributions from JIMWLK evolution*, JHEP10 (2016) 065

Developing the framework for combined fits with CGC

TMD approximated in terms of the dipole amplitude S

$$\mathscr{F}_{qg}^{(1)}(\boldsymbol{k}_\perp, x) = \frac{N_c}{2\pi^2}\int \frac{r_\perp \mathrm{d}r_\perp}{2\pi} J_0(k_\perp r_\perp)\nabla_\perp^2\left[1 - S(r_\perp, x)\right]$$

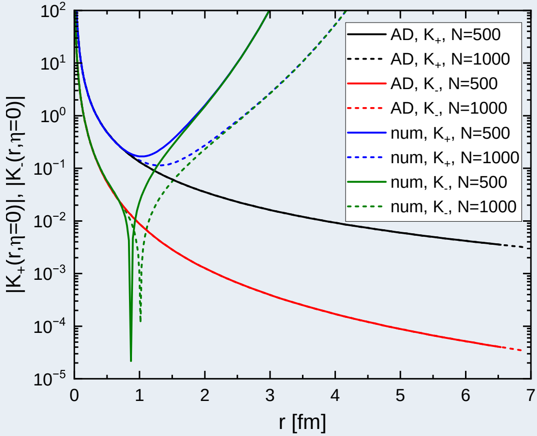
$$\mathscr{F}_{gg}^{(3)}(\boldsymbol{k}_\perp, x) = \frac{C_F}{2\pi^2}\int \frac{r_\perp \mathrm{d}r_\perp}{2\pi} J_0(k_\perp r_\perp)\mathscr{K}(r_\perp, x)\left[1 - (S(r_\perp, x))^{N_c/C_F}\right]\times \\ \times (S(r_\perp, x))^2$$

$$\mathscr{F}_{WW}(\boldsymbol{k}_\perp, x) = \frac{C_F}{2\pi^2}\int \frac{r_\perp \mathrm{d}r_\perp}{2\pi} J_0(k_\perp r_\perp)\mathscr{K}(r_\perp, x)\left[1 - (S(r_\perp, x))^{N_c/C_F}\right]$$

$$\nabla_\perp^2 = \frac{\partial^2}{\partial r_\perp^2} + \frac{1}{r_\perp}\frac{\partial}{\partial r_\perp}$$

$$\mathscr{K}(r_\perp, x) = \frac{\nabla_\perp^2 \Gamma(r_\perp, x)}{\Gamma(r_\perp, x)} \quad \text{where} \quad \Gamma(r_\perp, x) = -\log\left[S(r_\perp, x)\right]$$

Back to Automatic Differentiation again



Functions $|\mathscr{K}_{+}(r_{\perp})|$ and $|\mathscr{K}_{-}(r_{\perp})|$ at initial condition $\eta = 0$

Next steps

- uncertainty analysis and model selection: Bayesian analysis based on the calculation of evidence; comparison of uncertainties from the Hessian method, Markov Chain Monte Carlo, and Nested Sampling algorithms
- testing the stability: impact of different running coupling prescriptions, different implementations of the kinematical constraint
- inclusion of other data/cross-section
- TMD functions from JIMWLK

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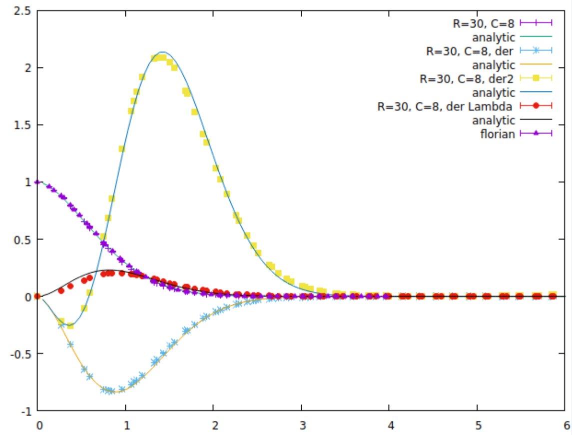
Automatic Differentiation for JIMWLK



Gluon dipole amplitude obtained from JIMWLK, together with the first and second derivatives with respect to Q_0

Summary

- I have presented elements of the framework that allow for the efficient fitting of several observables
- I have discussed the benefits of using automatic differentiation
- I have shown how to increase the performance by employing the logarithmic Fourier transform
- I have presented preliminary results of the fit to the DIS from HERA and single inclusive hadron production from BRAHMS
- I have highlighted future steps

Thank you very much for your attention!