

STEP: a tool to perform tests of smoothness on differential distributions

Terascale alliance meeting

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Bundesministerium
für Bildung
und Forschung

Introduction

Motivation

STEP library

Smoothness Test with Expansion of Polynomials

→ automated 1D fits with correlations (optional) and early stopping (optional)

Motivation

- Test the **quality** of a differential distribution in terms of the “alignment” of the points around a smooth function.
- Here we will discuss it in the **context** of the QCD interpretation of inclusive jet production^a.
- But **applications** beyond QCD interpretation or even HEP are very likely.

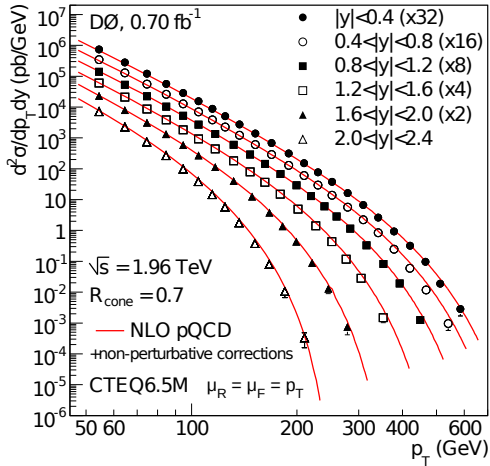
^ae.g. Toni's presentation in which context it was developed.

Applications in this presentation

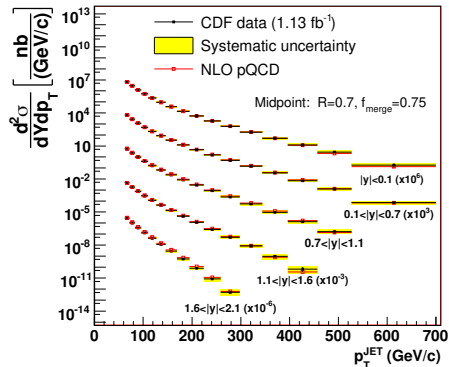
Tevatron DØ & CDF ($p\bar{p}$ at $\sqrt{s} = 1.96$ TeV)

LHC CMS & ATLAS (pp at $\sqrt{s} = 8$ TeV)

→ These data have been used in QCD fits by PDF collaborations [1, 2, 3].



Motivation

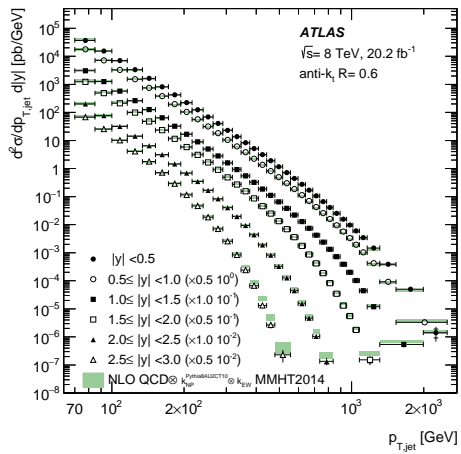


Idea

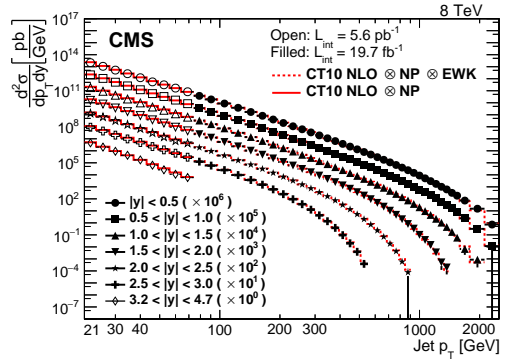
« Physics is smooth. »

« Logarithmic scales can hide monsters. »

→ Relevant for **any differential measurement** with “large” number of bins.



Motivation



Test of smoothness

Find an adequate analytical function to fit the spectrum in order to find deviations **beyond** bin-to-bin fluctuations.

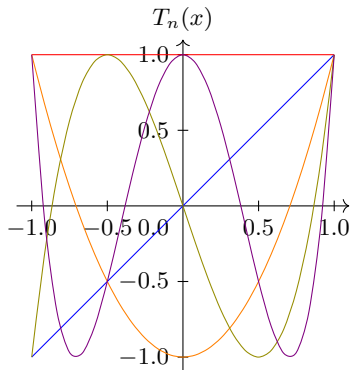
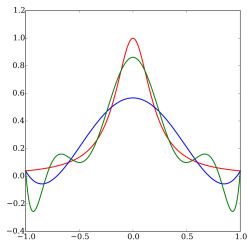
→ Applicable in different circumstances, as for instance:

- Impact from bin-to-bin correlations.
- Check combination of different triggers.
- Smooth systematic uncertainties.
- Smooth binned corrections.

Method

Chebyshev polynomials

General form



$$T_0(x) = 1, T_1(x) = x, T_2(x) = 2x^2 - 1,$$

$$T_3(x) = 4x^3 - 3x,$$

$$T_4(x) = 8x^4 - 8x^2 + 1, \text{ etc.}$$

Chebyshev polynomials

Difficulties with standard polynomials

- ① Runge phenomenon
- ② Many parameters

→ fits based on standard polynomials $\sum a_i x^i$ difficult...

Definition (first kind)

$$P_n(x) = \sum_{i=0}^n a_i T_i(x) \quad (1)$$

$$\text{where } T_0(x) = 1, \quad T_1(x) = x \quad (2)$$

$$\text{and } T_{i+1}(x) = 2xT_i(x) - T_{i-1}(x) \quad (3)$$

Interesting properties

- ① Fits with Chebyshev polynomials more robust against Runge phenomenon.
- ② P_n is a good approximation of P_{n+1} .

Chebyshev fit of inclusive jet p_T spectrum

$$f_n(p_T) = \exp \left(\sum_{i=0}^n b_i T_i \left(2 \frac{\log p_T / \log p_T^{\min}}{\log p_T^{\max} / \log p_T^{\min}} - 1 \right) \right) \quad (4)$$

- The exponential and the logarithm are used because of the **steeply falling** nature of spectrum^a
- Then **rescaling** is necessary as Chebyshev polynomials only cover $[-1, 1]$.
- n is the **number of parameters** (one unity larger than the degree).

^aThey may of course be removed in case of other differential distributions.

Remark

The **only assumption** is a smooth behaviour...

→ No assumption on the physical nature of the fitted data!

Objective function

$$\chi_n^2 = \min_{b_{i \leq n}} [(\mathbf{x} - \mathbf{y}_{b_{i \leq n}})^T \mathbf{V}^{-1} (\mathbf{x} - \mathbf{y}_{b_{i \leq n}})] \quad (5)$$

- \mathbf{x} corresponds to the binned differential distribution;
- $\mathbf{y}_{b_{i \leq n}}$ corresponds to the values of the smooth fit evaluated at, for instance, the centre of the bins for a given set of parameters $b_{i \leq n}$;
- \mathbf{V} is the covariance matrix of the binned differential distribution.

Algorithm

- 0 The two first parameters are initialised from the first and last points of the spectrum whereas all other parameters are fixed to 0.
- 1 **Fit** with all released parameters.
- 2 **Stop** if one of the following statements is satisfied^a:
 - i the χ^2 is compatible with the number of degrees of freedom (ndf);
 - ii the χ^2/ndf is no longer decreasing;
 - iii or the number of released parameters has reached the maximum allowed.
- 3 **Release** the next parameter and go back to item 1.

^aThe two first criteria can be deactivated.

Application

CDF

DØ

CMS

ATLAS

Comparison

Datasets

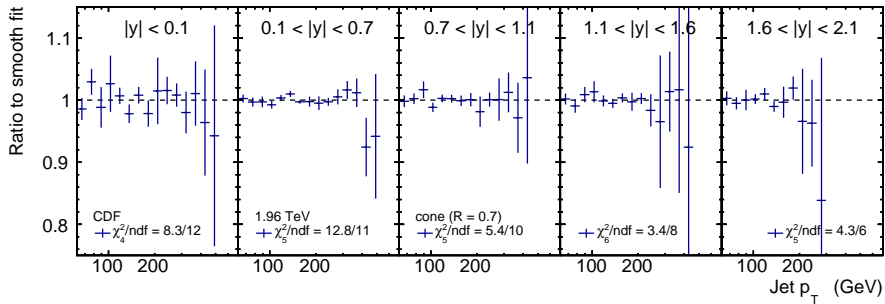
Tevatron Run 2 DØ & CDF ($p\bar{p}$ at $\sqrt{s} = 1.96$ TeV)

LHC Run 1 CMS & ATLAS (pp at $\sqrt{s} = 8$ TeV)

→ These data have been used in QCD fits by PDF collaborations [1, 2, 3].

Bin-to-bin uncertainties

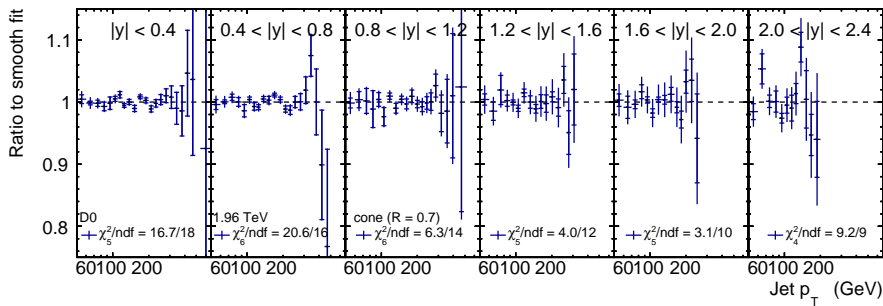
detector	stat. corr.	syst. unc.
CDF [4]		
DØ [5]		×
CMS [6]	×	×
ATLAS [7]	×	



Figure

Steps due to the trigger strategy visible at 146 GeV (96 GeV) in 2nd (3rd) y bin.
→ Seems to be negligible in front of the statistical uncertainties.

	$ y < 0.1$	$0.1 < y < 0.7$	$0.7 < y < 1.1$	$1.1 < y < 1.6$	$1.6 < y < 2.1$
2	163.16 ± 0.38	1896.56 ± 0.38	1165.27 ± 0.39	1441.15 ± 0.41	1224.13 ± 0.47
3	7.03 ± 0.39	97.04 ± 0.39	67.30 ± 0.41	62.69 ± 0.43	41.67 ± 0.50
4	0.70 ± 0.41	8.82 ± 0.41	9.89 ± 0.43	1.69 ± 0.45	1.97 ± 0.53
5	0.56 ± 0.43	1.17 ± 0.43	0.54 ± 0.45	0.43 ± 0.47	0.72 ± 0.58
6	0.55 ± 0.45	0.65 ± 0.45	0.60 ± 0.47	0.42 ± 0.50	0.42 ± 0.63

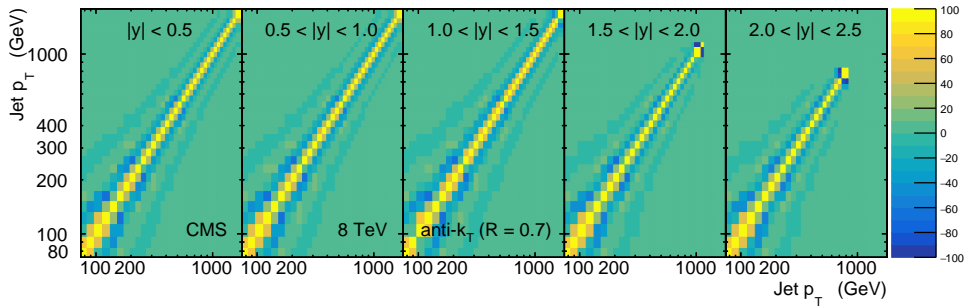
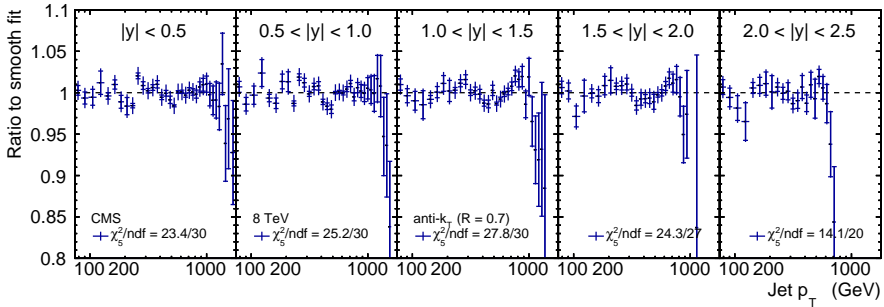


Figure

Additional bin-to-bin uncorrelated systematic uncertainty seems slightly overestimated at $|y| > 0.8$.

	$ y < 0.4$	$0.4 < y < 0.8$	$0.8 < y < 1.2$	$1.2 < y < 1.6$	$1.6 < y < 2.0$	$2.0 < y < 2.4$
2	811.57 ± 0.31	1016.79 ± 0.32	795.84 ± 0.33	432.24 ± 0.37	386.47 ± 0.39	329.43 ± 0.43
3	59.47 ± 0.32	76.89 ± 0.32	54.23 ± 0.34	35.55 ± 0.38	27.01 ± 0.41	14.65 ± 0.45
4	6.45 ± 0.32	7.31 ± 0.33	3.35 ± 0.35	1.47 ± 0.39	2.04 ± 0.43	1.02 ± 0.47
5	0.93 ± 0.33	1.44 ± 0.34	0.50 ± 0.37	0.33 ± 0.41	0.31 ± 0.45	0.42 ± 0.50
6	0.88 ± 0.34	1.29 ± 0.35	0.45 ± 0.38	0.35 ± 0.43	0.32 ± 0.47	0.42 ± 0.53

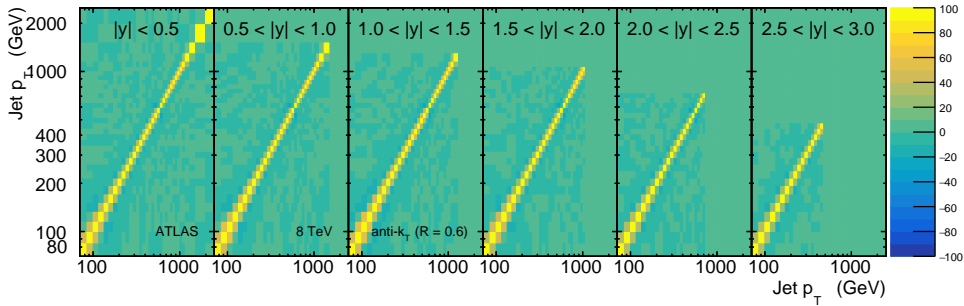
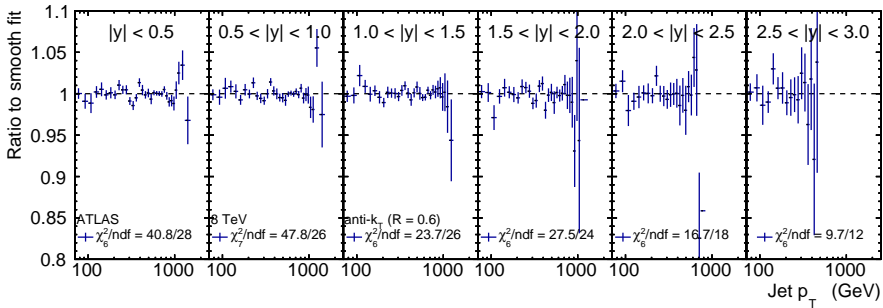
- Introduction
- Method
- Application
- CDF
- DØ
- CMS
- ATLAS
- Comparison
- Reference
- Summary & Conclusions
- Back-up



Figure

- Only the **phase space** relevant for QCD interpretation has been considered.
- **Statistical correlations** are provided directly by CMS and accounted for in each fit.
- Steps related to the **unfolding** may still be seen but are more difficult to find due to correlations and to the unfolding.
- The additional 1% **bin-to-bin uncorrelated systematic uncertainty** is necessary but likely too conservative (wavy shape).

	$ y < 0.5$	$0.5 < y < 1.0$	$1.0 < y < 1.5$	$1.5 < y < 2.0$	$2.0 < y < 2.5$
2	841.51 ± 0.25	1019.44 ± 0.25	1442.31 ± 0.25	1965.81 ± 0.26	1943.62 ± 0.29
3	47.77 ± 0.25	66.72 ± 0.25	115.51 ± 0.25	185.72 ± 0.26	187.95 ± 0.30
4	7.52 ± 0.25	7.55 ± 0.25	14.07 ± 0.25	21.57 ± 0.27	17.79 ± 0.31
5	0.78 ± 0.26	0.84 ± 0.26	0.93 ± 0.26	0.90 ± 0.27	0.70 ± 0.32
6	0.76 ± 0.26	0.65 ± 0.26	0.50 ± 0.26	0.47 ± 0.28	0.41 ± 0.32

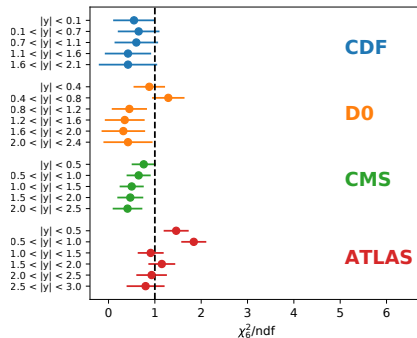
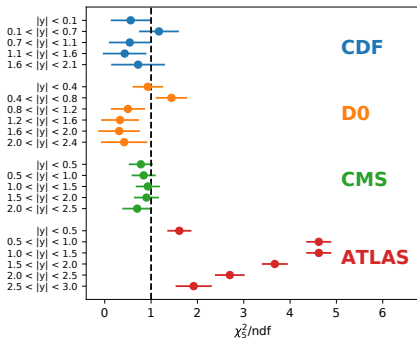


Figure

- **Statistical correlations** are accounted for using replica method.
- The statistical uncertainties seem insufficient to cover the **deviations** from a smooth behaviour in the two first rapidity bins, and no additional bin-to-bin uncorrelated systematic uncertainties are provided.
- This might be related to the issues observed by several PDF collaborations [1, 2, 3].

	$ y < 0.5$	$0.5 < y < 1.0$	$1.0 < y < 1.5$	$1.5 < y < 2.0$	$2.0 < y < 2.5$	$2.5 < y < 3.0$
2	2188.98 ± 0.25	3033.97 ± 0.25	4115.24 ± 0.26	3860.63 ± 0.27	2722.43 ± 0.30	1142.21 ± 0.35
3	99.77 ± 0.25	178.11 ± 0.26	325.30 ± 0.26	322.57 ± 0.27	261.13 ± 0.31	92.98 ± 0.37
4	17.57 ± 0.26	27.64 ± 0.26	49.63 ± 0.27	37.35 ± 0.28	17.49 ± 0.32	9.03 ± 0.38
5	1.61 ± 0.26	4.62 ± 0.27	4.62 ± 0.27	3.67 ± 0.28	2.70 ± 0.32	1.92 ± 0.39
6	1.46 ± 0.27	1.84 ± 0.27	0.91 ± 0.28	1.15 ± 0.29	0.93 ± 0.33	0.80 ± 0.41
7	1.46 ± 0.27	1.84 ± 0.28	0.92 ± 0.28	1.18 ± 0.29	0.73 ± 0.34	0.86 ± 0.43

Comparison



Interpretation

- Steps due to the **triggers** are visible (e.g. CDF & CMS).
- Certain **bin-to-bin decorrelated uncertainties** are likely overestimated (DØ in forward region; CMS in all regions) or underestimated (ATLAS).
- Need for higher number of parameters in central region of ATLAS measurement might be related to difficulties encountered in QCD interpretation.

Reference

Article

Source code

arXiv:2111.09968v1 [hep-ph] 18 Nov 2021

STEP: a tool to perform tests of smoothness on differential distributions based on Chebyshev polynomials of the first kind

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Abstract: We motivate and describe a method based on fits with Chebyshev polynomials to test the smoothness of differential distributions. We also provide a header-only tool in C++ called *Step* to perform such tests. As a demonstration we use the tool in the context of the measurement of inclusive double-differential cross sections in the jet transverse momentum and rapidity at the Tevatron and LHC.

Keywords: smoothness, step, Chebyshev polynomials, inclusive jet, correlations, D0, CDF, CMS, ATLAS, library, C++

^{*}Corresponding author

Outline

- Motivation and description of the method
 - Application on real data
- Essentially the content of this presentation.

Status

- Posted on arXiv [8].
- Plan to submit it to a journal in the coming hours/days.

How-to

- Just download the header `Step.h` from the GitLab repository [9], then the following call is enough to get a ROOT TF1 object:

```
TF1 * f = Step::GetSmoothFit<log,exp>(hist,n);
```

- Here is an example of a more advanced call (but more complex isn't possible):

```
TF1 * f = Step::GetSmoothFit (h,cov,im,iM,n,1,true,cout);
```

- Most general prototype:

```
TF1 * GetSmoothFit (TH1 * h, TH2 * cov, int im, int iM,  
    int maxdegree, double nSigmaStop = 1, bool autoStop = true,  
    std::ostream& stream = std::cout);
```

→ Additional information on the fit performance is available using the static STL container `Step::chi2s`.

Examples

All results shown in the presentation and in the article may be reproduced.

Summary & Conclusions

Summary & Conclusions

- We have presented an original method to test the quality of a differential distribution.
- We have applied the method to several measurements used by PDF collaborations.
- We have provided a package and briefly instructed how to use it.

Thank you for your attention!

Back-up

Acronyms I

ATLAS A Toroidal LHC ApparatuS. 3, 11, 18

CDF Collider Detector at Fermilab. 3, 11, 18

CMS Compact Muon Solenoid. 3, 11, 15, 18

DØ after the location of the detector. 3, 11, 18

HEP High-Energy Physics. 3

PDF Parton Distribution Function. 3, 11, 17, 23

QCD Quantum Chromodynamics. 3, 11, 15, 18

STL Standard Template Library. 21

References I



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Patrick L. S. Connor and Radek Žlebčik. **Step: a tool to perform tests of smoothness on differential distributions based on Chebyshev polynomials of the first kind**. 2021. arXiv: 2111.09968 [hep-ph].



Patrick L.S. Connor and Radek Žlebčik. **Step repository**. <https://gitlab.cern.ch/step>. 2021.

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