NON-PERTURBATIVE AND TOPOLOGICAL ASPECTS OF QCD — 30th May 2024 QCD Instanton Prospects at the LHC

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In This Talk

- Present ongoing search for gluon-induced QCD instantons in ATLAS
 - Based on work done by V. V. Khoze *et al.* (see previous talk)
 - Very ATLAS oriented
 - A work in progress! No data will be shown.
- But it is difficult! Are there other avenues?
 - Diffractive production?
 - Use flavour tagging?
 - Measure the chirality violation?

LHC Phenomenology of QCD Instantons

Following 't Hooft, do perturbation theory in the instanton background [Khoze *et al.* 1] + [Khoze *et al.* 2, Khoze *et al.* 3, Amoroso *et al.*]

$$\mathcal{A}_{2 \to n_g + 2N_f} = \int d^4 x_0 \int_0^\infty d\rho \, D(\rho) \, e^{-S_I} \prod_{i=1}^{n_g + 2} A_{\text{LSZ}}^{\text{inst}}(p_i; \rho) \prod_{j=1}^{2N_f} \psi_{\text{LSZ}}^{(0)}(p_j; \rho)$$

Event signature

Get cross-section via optical theorem

$$\hat{\sigma}(gg \to X) = \frac{1}{E^2} \text{Im} \mathcal{A}^{I\bar{I}}$$



Predictions for the LHC

$\sqrt{\hat{s}}$ [GeV]	$\hat{\sigma}(gg \rightarrow X)$ [pb]	$\langle 1/\rho \rangle$ [GeV]	$\alpha_{\rm S}(1/\rho)$	$\langle N_{\rm gluons} \rangle$
20	2.01×10^{6}	1.69	0.327	7.81
25	9.49×10^{5}	1.98	0.306	8.58
30	4.64×10^{5}	2.27	0.290	9.07
35	2.32×10^{5}	2.52	0.279	9.61
40	1.25×10^{5}	2.84	0.267	9.67
50	3.89×10^{4}	3.38	0.251	10.56
60	1.38×10^{4}	3.87	0.241	10.89
70	5.45×10^{3}	4.33	0.232	11.38
80	2.36×10^{3}	4.85	0.224	11.67
90	1.08×10^{3}	5.24	0.219	12.31
100	5.44×10^{2}	5.82	0.213	12.10
110	2.79×10^{2}	6.21	0.209	12.62
120	1.53×10^{2}	6.71	0.205	12.77
130	8.56×10^{1}	7.13	0.201	13.04
140	4.99×10^{1}	7.57	0.198	13.25
150	3.01×10^{1}	8.00	0.195	13.45

Table. Partonic cross-section as a function of partonic centre-of-mass energy, √ŝ, taken from 2104.01861.

Theory Inputs to an Experimental Search

$\sqrt{\hat{s}}$ [GeV]	$\hat{\sigma}(gg \to X)$ [pb]	$\langle 1/\rho \rangle$ [GeV]	$\alpha_{\rm S}(1/\rho)$	$\langle N_{\rm gluons} \rangle$
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Nominal factorisation scale choice, μ_{F}

Mean number of gluons to add to each event

Table. Partonic cross-section as a function of partonic

centre-of-mass energy, $\sqrt{\hat{s}}$, taken from 2104.01861.

Mass spectrum

MC Instanton Signal Modelling

- SHERPA 3 for event generation
- RAMBO for phase-space generation
- Final state assembled algorithmically
- Flavour production scheme:
 - Add up to 5 flavours
 - 20 GeV *c*-production threshold
 - 100 GeV *b*-production threshold
- NNPDF3.0 NNLO with $\mu_F = 1 / \rho$ scale choice



Figure from Sherpa 1.1 Manual ('t Hooft vertex embedded) See back-up for a glimpse of Sherpa 3's UE tuning effort

Simulated Mass Spectrum

Interpolate the cross-section data table, generate events with Sherpa in 6 slices



Signal event generator 🖌

Soft QCD Background Models

Background: Soft QCD, $\sigma \sim 111 \text{ mb}$

Nominal model: EPOS LHC

Parton-based Gribov Regge theory with collective hadronisation [1306.0121]

Alternative model: Pythia 8

2 → 2 scatters with MPI based on the Sjöstrand–van Zijl model [PRD], Lund-string fragmentation



Start With a Past Analysis

Charged-particle distributions in $\sqrt{s} = 13$ TeV *pp* interactions measured with the ATLAS detector at the LHC

The ATLAS Collaboration

Featuring

- Low pileup ATLAS data
 - \circ Pile-up values $\langle \mu \rangle \sim 0.035$
 - \circ 1.693 nb⁻¹ ~ $O(10^4)$ instantons
- Minimum Bias triggers
- Charged-particle tracking
- Minimum Bias background models



A Very Simple Analysis

- No jets, flavour tagging, heavy decays,
 ... just tracks.
- Good track reconstruction efficiency
- Small systematic uncertainties
- Enough information to capture isotropy
- Simplified analysis design



Discriminating Variables — Event kinematics



Discriminating Variables — Event kinematics



Discriminating Variables - Event Shapes

Thrust:



Discriminating Variables — Flatenicity

- 'Flatenicity' characterises the uniformity of energy deposits in the detector [2204.13733]
- Sensitive to the number of MPI interactions
- $\eta \phi$ plane partitioned into a uniform 10 x 10 grid of cells
- Total track pT in each cell calculated...then flatenicity given by

$$o = \frac{\sigma_{p_{\rm T}^{\rm cell}}}{\langle p_{\rm T}^{\rm cell} \rangle}$$



Picture of a uniform 'MPI' event taken from [2204.13733]

Correlation Matrices



EPOS LHC

Pythia 8

These matrices factorise into two blocks: Event Shapes and non Event-Shapes

For background estimation, find two independent variables for the 'ABCD' method?

Machine Learning Approach: ABCDisCo

Set up two statistically independent classifiers for ABCD-style background estimation [Kasieczka, Nachman, Schwartz and Shih (2007.14400)]



 $0 \le h_i \le 128, i = 1, 2, 3$



$$\mathcal{L}[f(X), g(X)] = \begin{split} \mathcal{L}_{\mathrm{cl}}[f(X), y] + \mathcal{L}_{\mathrm{cl}}[g(X), y] + \alpha \end{split} \\ \mathcal{L}_{\mathrm{dCorr}_{y=0}^2}[f(X), g(X)] \\ \hline \\ \textbf{Classification terms} \\ \textbf{Modified loss function} \\ \end{split}$$

→ Region definitions and background estimation

Deep Neural Network (DNN) Input Variables

	Γ	Number of tracks	$N_{\rm trk}$			
		Number of tracks above 1 GeV	$N_{\rm trk}(p_{\rm T} > 1 {\rm GeV})$			
		Number of tracks below 1 Gev	$N_{\rm trk}(p_{\rm T} < 1 {\rm GeV})$			
Mass variables		Scalar sum of track $p_{\rm T}$	S_T			
		Transverse mass per track	$m_T/N_{\rm trk}$			
		Mean track $p_{\rm T}$	$\langle p_{\rm T} \rangle$			
		Median track $p_{\rm T}$	med $p_{\rm T}$	Γ		\frown
		Leading track $p_{\rm T}$	$\max p_{\mathrm{T}}$		X	()
		0 11			~ 1	\bigvee
	Г	3d Thrust	T, 3d			_ X
		3 <i>d</i> Thrust major	$T_{\text{major}}, 3d$		V	$\bigcap A$
Event Shape		3d Oblateness	$T_{\rm major} - T_{\rm minor}, 3d$		2	\bigcirc
		3d Sphericity	S, 3d			\backslash
variables		3d Aplanarity	A, 3d			: /x
Variabies		2 <i>d</i> Thrust	T, 2d			1/
		2d Sphericity	S, 2d			
					X	()
	Г	Mean pseudorapidity	$\langle \eta angle$		'n	\bigcirc
Angular		Standard deviation of ϕ	$\sigma(\phi)$			
Aligutai		Standard deviation of η	$\sigma(\eta)$			
• • •		Standard deviation of $\Delta \phi(i, j)$ of all track pairs	$\sigma(\Delta\phi(i,j))$			
variables		Mean of $ \Delta \eta(i, j) $ of all track pairs	$\langle \Delta \eta(i,j) \rangle$			
		Flatenicity on a 10×10 grid	F(10, 10)			

Table. List of our ABCDisCo network input variables.

"Mass" Binning



Truth mass bins: (20, 40), (100, 150), (60, 80) GeV

- Principled choice: do the analysis in reconstructed mass bins
 - Decouple somewhat from cross-section modelling
 - Enhance sensitivity with a shape fit
 - Also, it aids the DNN training

Classifier Output Planes (Or 'ABCD' Planes)



Classifier Output Distributions: Low Mass



Classifier Output Distributions: Medium Mass



Classifier Output Distributions: High Mass



 \rightarrow Pretty good! But how good?

Classifier ROC Curves for Comparison



Classification performance improves from low to high-mass

*Area Under the [ROC] Curve (AUC)

NPTA Ynyr Harris — 30 May 2024

A Particularly Interesting Variable: $\langle |\Delta \eta(i, j)| \rangle$



- Mean magnitude of Δη over all pairs of tracks
- Immediately important for the classifiers (right)
- Captures the so-called 'instanton band'
 - T. Carli et al., 'Soft Bombs' paper (2016)



^Network input variable-ranking plot based on SHAP values



^Mean classifier outputs as functions of the input

'Instanton Band' Idea



$$\eta = -\ln\left(\tan\frac{\theta}{2}\right)$$

Figure from 1612.00850

- Isotropy in polar angles \rightarrow band in pseudorapidity (or z in the figure)
- Longitudinal boost of the centre of mass \rightarrow displacement along z
- More activity concentrated in the band in signal events!
- The DNNs seek out the 'instanton band' using the $\langle |\Delta \eta(i, j)| \rangle$ variable!

Background Model Reweighting / "Tracking Corrections"



The Principle of Our Background Estimation



Statistical Analysis: One-Bin Counting Experiment

- Three mass categories, and ABCD regions in each
- Standard ATLAS treatment based on a profile likelihood ratio
 - One-bin cut-and-count analysis in each mass category
 - Simple extension: statistical combination





ATLAS Results

< Insert ATLAS results here >

(Spoiler: expected sensitivity is currently not fantastic)

The Main Problem: Irreducible 'Minimum Bias' Background

VS





Minimum Bias background		Instanton signal	
σ ~ 111 mb	VS	σ ~ 26 μb	S / B ~ O(10 ⁻⁵)

Signal and background final state kinematics are *very similar* And the small S / B is difficult to combat (even with our DNNs)

Other Production Modes? Central Exclusive Production...?



Instantons in Diffractive Production

V. V. Khoze et al. again [PRD 104, 054013 (2021), PRD 105, 036008 (2022)]



- Same calculational technique as for the $gg \rightarrow X$ cross-section
- Cross-sections of up to 10⁵ pb for [very] low masses [with no Q₊ cut]

CEP is a Possible Search Avenue For ATLAS



Figure from M. Trzebiński, CERN Detector Seminar (2017)

- ALFA: Absolute Luminosity For Atlas [JINST **11** P11013]
- AFP: Atlas Forward Proton [ATLAS-TDR-024]
 - Study performed by Marek Tasevsky [EPJC 83, 35 (2023)]

QCD Instanton Searches With Forward Proton Tags

Tasevsky *et al.* looked at ATLAS sensitivity to M > 60 GeV instantons in AFP-tagged events



A very comprehensive study, considering single and double-AFP tags • four luminosity scenarios • multi-parton interactions • pile-up and combinatorial background protons • plus efficiency reductions from detector effects.

A Note on Theory Systematics

- Factorisation scale uncertainty
 - \circ Factor of 2^{±1} variations
 - Comparison with alternative choice, $\sqrt{\hat{s}} / N_{gluons}$
- Renormalisation scale uncertainty
 - Implement custom μ_R reweighting in MC
- Uncertainty on order of α_s
 - \circ Somewhat captured by α_s variations and different PDF sets

In principle, there is an O(100) uncertainty on the instanton cross-section [2101.02719] (but this is why we should measure it!)

 $\frac{(\mu_{\rm r}^v)^{2b_0}}{(\mu_{\rm r}^0)^{2b_0}} \frac{\exp\left[-4\pi/\alpha_S(\mu_{\rm r}^v)\right]}{\exp\left[-4\pi/\alpha_S(\mu_{\rm r}^0)\right]}$

Conclusion

- ATLAS search for QCD instantons is underway
 - But struggles with background modelling and rejection
- Can we improve our strategy?
 - Use forward proton tags
 - Use flavour tagging?
 - Target the chirality violation?









BACKUP

Much of My PhD Experience



The ATLAS Experiment (A Toroidal LHC Apparatus)



[Detector paper (2008), Higgs boson discovery (2012), 1000 publications (2021)]

Previous ATLAS Soft QCD Measurements



Minimum Bias (MB)

13 TeV, tracks-based: 1602.01633 13 TeV, 100 MeV tracks-based: 1606.01133 ≤ 7 TeV, tracks-based: 1012.5104, etc.



Underlying Event (UE) 13 TeV, tracks-based: 1701.05390 13 TeV in Z-events: 1905.09752 7 TeV with jets: 1406.0392, etc.



Total Inelastic *pp* **Cross-Section** @ 13 TeV: 1606.02625 @ 7 TeV: 1104.0326, etc.

Performed for insights into low energy strong interactions

(Inputs to MC event generator tuning, understanding for pileup modelling, etc.)

Tracking Systematics

Impact parameter resolution

- Smear d0 and z0 within resolution
- + TRK_RES_D0_MEAS
- + TRK_RES_Z0_MEAS

Residual alignment uncertainties

- Use central η - ϕ maps of the residual biases
- + TRK_BIAS_D0_WM
- + TRK_BIAS_Z0_WM
- + TRK_BIAS_QOVERP_SAGITTA_WM

Efficiency uncertainties

- Account for difference of efficiency in data/MC from material uncertainty, based on truth-matching
- + TRK_EFF_<WP>_OVERALL
- + TRK_EFF_<WP>_IBL
- + TRK_EFF_<WP>_pp0
- + TRK_EFF_<WP>_PHYSMODEL



Efficiency of the Single-Arm Minimum Bias Trigger



1602.01633

Signal-Modelling Systematics

Assess by performing reasonable variations of the event generation, e.g.



- Not sure how to treat the scale choice variation (1 / $\rho \rightarrow \sqrt{s'}$ / N_{gluons}), which is large
 - In principle the signal cross-section and its shape have to be recalculated

Flatenicity Calculated on a 10 x 10 Grid in η x φ



What Does a DNN Learn?

Look at 2d classifier output vs input histograms, e.g.



What Does a DNN Learn?

Even better: look at the profiles of the classifier outputs in classifier inputs, e.g.



- Show that classifiers A and B make different use of the input variables
- Show where discrimination power comes from, e.g. here edges vs center of track $\sigma(\eta)$

Module	Model parameter
	$p_{T,\min}$
	$p_{T, 0}$
AMISIC	ξ
MIDIO	$f_{ m mat}$
	r_1
	r_2
	$\langle k_T angle$
	σ
Primordial_KPerp	k_T^{\max}
	η
	α
AHADIC	
	-

Sj\"ostrand-van Zijl model [Phys. Rev. **D** 36, 2019]

$$P_{\rm no}(p_{T,\rm min}) = \exp\left(-\frac{1}{\xi\sigma_{\rm ND}}\int\limits_{p_{T,\rm min}^2} dp_T^2 \frac{d\hat{\sigma}}{dp_T^2}\right)$$

Transverse momentum regulator

$$p_T^2 \to p_T^2 + p_{T,0}^2$$

Double Gaussian matter density profile assumption

$$\rho(r) \propto (1 - f_{\text{mat}}) \frac{1}{r_1^3} \exp\left(-\frac{r^2}{r_1^2}\right) + f_{\text{mat}} \frac{1}{r_2^3} \exp\left(-\frac{r^2}{r_2^2}\right)$$

Intrinsic transverse momentum of partons in hadrons

$$\Pr(k_T) \propto \exp\left(-\frac{(k_T - \langle k_T \rangle)^2}{\sigma^2}\right) \times \left[1 - \left(\frac{k_T}{k_T^{\max}}\right)^{\eta}\right]$$

AHADIC model: *A modified cluster-hadronization model*, 0311085

Sherpa 2.2 manual, 1905.09127



Tracks-based UE at 7 TeV 🖌

[ATLAS_2010_S889472, 1012.0791]







UE at 7 TeV with leading jet 🖌

[ATLAS_2014_I1298811, 1406.0392]



Fitted SHERPA UE Parameters

Parameter	Prior Value	Scan Range	Tuned Value	Relative Change
AMISIC::PT_0(ref)	2.5	0.1 - 1	0.716 ± 0.008	-71.4%
AMISIC::PT_Min(ref)	3	2.5 - 5	4.260 ± 0.009	+42.0%
AMISIC::SIGMA_ND_NORM	0.4	0.4 - 1	0.458 ± 0.003	+14.5%
AMISIC::MATTER_FRACTION1	0.5	0.1 - 0.4	0.187 ± 0.003	-62.6%
AMISIC::RADIUS1	0.4	0.0-0.5	0.157 ± 0.002	-60.8%
AMISIC::RADIUS2	1	0.8 - 1.5	0.890 ± 0.005	-11.0%
AMISIC::Eta	0.16	<u>(x)</u>	0.16	
INTRINSIC_KPERP::MEAN	0	0 - 1.2	1.004 ± 0.009	$+\infty\%$
INTRINSIC_KPERP::SIGMA	1.5	0.5 - 3	$1.10 \hspace{0.1in} \pm \hspace{0.1in} 0.03$	-27%
INTRINSIC_KPERP::MAX	3	2-5	2.69 ± 0.03	-10%
INTRINSIC_KPERP::CUT_EXPO	5	3 - 6	5.12 ± 0.04	+2%
AHADIC::ALPHA_B	2.5		15	
AHADIC::BETA_B	0.25		0.9	
AHADIC::GAMMA_B	0.5		15	

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The background is modelled using the RAPGAP and DJANGOH Monte Carlo programs. The RAPGAP Monte Carlo program [32] incorporates the $\mathcal{O}(\alpha_s)$ QCD matrix elements and models higher order parton emissions to all orders in α_s using the concept of parton showers [33] based on the leading-logarithm DGLAP equations [34], where QCD radiation can occur before and after the hard subprocess. An alternative treatment of the perturbative phase is implemented in DJANGOH [35] which uses the Colour Dipole Model [36] with QCD matrix element corrections as implemented in ARIADNE [37]. In both MC generators hadronisation is modelled with the LUND string fragmentation [38, 39] using the ALEPH tune [40]. QED radiation and electroweak effects are simulated using the HERACLES [41] program, which is interfaced to the RAPGAP and DJANGOH event generators. The parton density functions of the proton are taken from the CTEQ6L set [42].

QCDINS [11,43] is a Monte Carlo package to simulate QCD instanton-induced scattering processes in DIS. The hard process generator is embedded in the HERWIG [44] program and is implemented as explained in section [2]. The number of flavours is set to $n_f = 3$. Outside the allowed region defined by Q'_{\min}^2 and x'_{\min} the instanton cross section is set to zero. The CTEQ5L [45] parton density functions are employed. Besides the hard instanton subprocess, subleading QCD emissions are simulated in the leading-logarithm approximation, using the coherent branching algorithm implemented in HERWIG. The hadronisation is performed according to the Lund string fragmentation.

Search at High-Q² by the H1 Collaboration

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No evidence for QCD Instantons found, but predictions challenged for the first time.

Possibly not the final word from the HERA data...

Cross-sections of Central Instanton Production

V. V. Khoze et al, Central Instanton Production, 2111.02159



M_{inst} [GeV]	$d\sigma_{pp}^{(1a)}[{ m pb}]$	$d\sigma_{pp}^{(1b)}[{ m pb}]$	$d\sigma_{pp}^{(2a)}[\mathrm{pb}]$	$d\sigma_{pp}^{(2b)}[\mathrm{pb}]$	$d\sigma_{pp}^{(2b)}, Q_t > 20 \text{GeV}$
15	13.3	$4.56 \cdot 10^4$	$3.72 \cdot 10^3$	$1.83 \cdot 10^5$	-
35	$6 \cdot 10^{-3}$	$1.69 \cdot 10^2$	8.10	$2.28 \cdot 10^3$	$1.99 \cdot 10^{-3}$
55	$3.82 \cdot 10^{-5}$	3.27	$1.19 \cdot 10^{-1}$	$8.96 \cdot 10^{1}$	$2.95 \cdot 10^{-3}$
75	$8.8 \cdot 10^{-7}$	$1.61 \cdot 10^{-1}$	$4.72 \cdot 10^{-3}$	7.06	$1.70 \cdot 10^{-3}$
95	$4.27 \cdot 10^{-8}$	$1.38 \cdot 10^{-2}$	$3.42 \cdot 10^{-4}$	$8.58 \cdot 10^{-1}$	$7.26 \cdot 10^{-4}$
115	$3.37 \cdot 10^{-9}$	$1.74 \cdot 10^{-3}$	$3.68 \cdot 10^{-5}$	$1.39 \cdot 10^{-1}$	$2.80 \cdot 10^{-4}$
135	$3.77 \cdot 10^{-10}$	$2.86 \cdot 10^{-4}$	$5.29 \cdot 10^{-6}$	$2.75 \cdot 10^{-2}$	$1.04 \cdot 10^{-4}$

Table 1: Instanton cross-sections at the 14 TeV LHC. The differential cross-sections for the process in Figs.1a, 1b and 2a, 2b, given by Eqs. (5.1) and (5.2), are computed for a range of instanton masses M_{inst} .

QCD Instanton Searches With Forward Proton Tags

$(\langle \mu angle, \mathcal{L}[\mathrm{fb}^{-1}])$	$M_{\rm inst} > 60 { m ~GeV}$	$M_{\rm inst} > 100 { m ~GeV}$
(0, 0.1)	19.0/(0.4+3.5)	5.8/(0.2+3.5)
(1.0, 0.1)	8.7/(6.5+0.2)	3.2/(4.7+0.2)
(2.0, 1.0)	52.2/(58.1+2.5)	15.4/(55.3+2.2)
(5.0,10.0)	56.2/(205.6+13.3)	23.8/(137.1+7.6)

Table 1 Summary of event yields after applying cuts in Eq. (9) and Eq. (10) for the single-tag search approach for $M_{\text{inst}} > 60$ GeV and $M_{\text{inst}} > 100$ GeV, respectively, and for four luminosity scenarios ($\langle \mu \rangle$, \mathcal{L}). For each scenario, a ratio of number of signal to background events, $N_{\text{S}}/(N_{\text{ND}} + N_{\text{SD}})$, is shown.