Anomaly Detection in Collider Physics via Factorized Observables

Raymond Wynne Based on work with Eric Metodiev and Jesse Thaler Preprint and code coming soon! ML4Jets 2023 - 07 November 2023





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How to Become a FORCE Wielder

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 Autoencoder operationally defines anomaly [1808.08979, 1903.02032, 2010.05531] Introduce new method with different assumption:

Current set of anomaly detection methods come with specific assumptions

Examples:

- Comparison between data and simulation [1709.01087, 1806.02350, 1807.06038]
- New physics appears as resonance [1805.02664, 1902.02634, 2009.02205]

• Autoencoder operationally defines anomaly [1808.08979, 1903.02032, 2010.05531] Introduce new method with different assumption: factorization [1708.02949, 1802.0008, 2002.12376]

Current set of anomaly detection methods come with specific assumptions





Factorization: physics at different energy scales approximately independent



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Given p_T , y, \mathcal{O} , this gives

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Factorization: physics at different energy scales approximately independent

Given p_T , y, \mathcal{O} , this gives

 $p(p_T, y, \mathcal{O}) \approx \sum f_i p_i(p_T, y) p_i(\mathcal{O} | p_T)$

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Factorization: physics at different energy scales approximately independent

Given p_T , y, \mathcal{O} , this gives

$$p(p_T, y, \mathcal{O}) \approx \sum_{i} f_i p_i(p_T, y) p_i(\mathcal{O} \mid p_T)$$

Marginalizing out y and taking a scale-/boostinvariant \mathcal{O} , this gives



Canonical example: jets





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$$p(p_T, \mathcal{O}) \approx \sum_i f_i p_i(p_T) p_i(\mathcal{O})$$

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Ex *1*:

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Ex \mathcal{O} : N – subjettiness ratios,

[1108.2701]

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Ex \mathcal{O} : N – subjettiness ratios, D_2 ,

[1108.2701]

[1401.4458]

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Ex \mathcal{O} : N – subjettiness ratios, D_2 , D_3 , [1401.4458] [1507.03018] [1108.2701]



Canonical example: jets





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Marginalizing out y and taking a scale-/boostinvariant \mathcal{O} , this gives

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Ex \mathcal{O} : N – subjettiness ratios, D_2 , D_3 , N_i [1108.2701] [1401.4458] [1507.03018] [1609.07483]

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Signal versus Background Factorization

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Calculate the conditional expectation

Signal versus Background Factorization Assume we have a distribution of the form $p(p_T, \mathcal{O}) = f_S p_S(p_T) p_S(\mathcal{O}) + f_B p_B(p_T) p_B(\mathcal{O})$ Calculate the conditional expectation

 $\mathbb{E}[p_T \mid \mathcal{O}] = \langle p_T \rangle_B + f_S \frac{(\langle p_T \rangle_S - \langle p_T \rangle_B) L_{S/B}(\mathcal{O})}{1 - f_S + f_S L_{S/B}(\mathcal{O})}$

Signal versus Background Factorization Assume we have a distribution of the form $p(p_T, \mathcal{O}) = f_S p_S(p_T) p_S(\mathcal{O}) + f_B p_B(p_T) p_B(\mathcal{O})$ Calculate the conditional expectation

Monotonically related to $L_{S/B}(O)$, the optimal classifier!

- $\mathbb{E}[p_T|\mathcal{O}] = \langle p_T \rangle_B + f_S \frac{(\langle p_T \rangle_S \langle p_T \rangle_B) L_{S/B}(\mathcal{O})}{1 f_S + f_S L_{S/B}(\mathcal{O})} = \mathcal{M}(L_{S/B}(\mathcal{O}))$

Signal versus Background Factorization Assume we have a distribution of the form $p(p_T, \mathcal{O}) = f_S p_S(p_T) p_S(\mathcal{O}) + f_B p_B(p_T) p_B(\mathcal{O})$ Calculate the conditional expectation $\mathbb{E}[p_T|\mathcal{O}] = \langle p_T \rangle_B + f_S \frac{(\langle p_T \rangle_S - \langle p_T \rangle_B) L_{S/B}(\mathcal{O})}{1 - f_S + f_S L_{S/B}(\mathcal{O})} = \mathcal{M}(L_{S/B}(\mathcal{O}))$

Monotonically related to $L_{S/B}(O)$, the optimal classifier! For $f_S = 0$, we get a random classifier

How do we extract $\mathbb{E}[p_T | \mathcal{O}]$?

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$\mathbb{E}[p_T | \mathcal{O}]$ minimizes the mean-squared error loss!

How do we extract $\mathbb{E}[p_T | \mathcal{O}]$? $\mathbb{E}[p_T \mid \mathcal{O}]$ minimizes the mean-squared error loss! Enter machine learning!

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... really just need \rightarrow



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The FORCE Method

<u>Factorized</u> <u>Observables</u> for <u>Regressing</u> <u>Conditional</u> <u>Expectation</u>


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Define approximately factorized objects (e.g.~jets)







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Define approximately factorized objects (e.g.~jets) - kinematics p_T







Factorized Observables for **R**egressing **C**onditional **Expectation**

Define approximately factorized objects (e.g.~jets)

- kinematics p_T
- scale-/boost-invariant substructure 0



<u>Factorized</u> <u>Observables</u> for <u>Regressing</u> <u>Conditional</u> <u>Expectation</u>

Define approximately factorized objects (e.g.~jets)

- kinematics p_T
- scale-/boost-invariant substructure 0

Train a machine-learning model to predict p_T from 0





<u>Factorized</u> <u>Observables</u> for <u>Regressing</u> <u>Conditional</u> <u>Expectation</u>

Define approximately factorized objects (e.g.~jets)

- kinematics p_T
- scale-/boost-invariant substructure 0

Train a machine-learning model to predict p_T from *(i)* with the mean-squared error loss

 $\mathbb{E}\left[\begin{array}{c} p_T \\ \mathcal{O} \end{array} \right]$ $\mathbb{E}[p_T|\mathcal{O}]$



<u>Factorized</u> <u>Observables</u> for <u>Regressing</u> <u>Conditional</u> <u>Expectation</u>

Define approximately factorized objects (e.g.~jets)

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Classify anomalous objects via cutting on the model output



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- kinematics p_T
- scale-/boost-invariant substructure 0

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Classify anomalous objects via cutting on the model output

Find anomalies by predicting kinematics from substructure





Demonstrations of FORCE:

"Use the Force, Luke."

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Demonstrations of FORCE:

1. Toy Gaussian Dataset

"Use the Force, Luke."

Demonstrations of FORCE: 1. Toy Gaussian Dataset 2. LHC Olympics R&D Dataset

"Use the Force, Luke."







1 kinematic variable, 1 substructure variable





1 kinematic variable, 1 substructure variable

1 million draws from background model





1 kinematic variable, 1 substructure variable 1 million draws from background model $f_S \cdot 1$ million draws from signal model



- Fully connected network
- 3 layers of 100 nodes
- ReLU Activation

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Optimal performance in high signal limit



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Optimal performance in high signal limit Random classifier in low signal limit



Convergence for Gaussian Simulation



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Since we constructed from Gaussians, can compute $\mathbb{E}[p_T | \mathcal{O}]$ analytically



Convergence for Gaussian Simulation

Since we constructed from Gaussians, can compute $\mathbb{E}[p_T | \mathcal{O}]$ analytically

Find solid convergence in large signal limit, with decaying performance as signal fraction decreases



LHC Olympics **R&D** Dataset









Energy flow polynomials - systematic expansion in energy and angle

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Energy flow polynomials - systematic expansion in energy and angle

Take EFPs $d \leq 3 \Longrightarrow$ 13 features



Energy flow polynomials - systematic expansion in energy and angle

Take EFPs $d \leq 3 \implies$ 13 features

Transverse boosts scale



Energy flow polynomials - systematic expansion in energy and angle

Take EFPs $d \leq 3 \implies$ 13 features

Transverse boosts scale Energy: γ



Energy flow polynomials - systematic expansion in energy and angle

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Transverse boosts scale Energy: γ Angle: $1/\gamma$



Energy flow polynomials - systematic expansion in energy and angle

Take EFPs $d \leq 3 \implies$ 13 features

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Introduce normalized EFPs


What's our scale-/boost-invariant substructure observables?

Energy flow polynomials - systematic expansion in energy and angle

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 $13 \rightarrow 8$ independent observables





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- Dropout and L2 Regularization
- Mean across 10 models



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Non-trivial discrimination power for $f_S = 0$



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Near optimal in high signal limit

Non-trivial discrimination power for $f_S = 0$ *More on that later*



Let's go on a bump hunt!

Let's go on a bump hunt!

We find the Z'





Let's go on a bump hunt!

We find the Z'



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and the X and Y!



Explicitly construct factorized distribution by separately shuffling signal and background

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Explicitly construct factorized distribution by separately shuffling signal and background

Optimal performance in high signal limit



Explicitly construct factorized distribution by separately shuffling signal and background

Optimal performance in high signal limit Smooth decay of statistical power



Explicitly construct factorized distribution by separately shuffling signal and background

Optimal performance in high signal limit Smooth decay of statistical power Random classifier in low signal limit



How does shuffling affect the bump hunt?





How does shuffling affect the bump hunt?



We see comparable results to non-shuffled features, motivating original feature set



GIVE YOURSELF TO THE DARK SIDE



GIVE YOURSELF TO THE DARK SIDE



Integrate with existing anomaly detection methods



GIVE YOURSELF TO THE DARK SIDE



Integrate with existing anomaly detection methods

Generalize to more than 1 kinematic feature and more than 2 event categories



Integrate with existing anomaly detection methods

Generalize to more than 1 kinematic feature and more than 2 event categories

Make method more sensitive to small signal fractions





Integrate with existing anomaly detection methods

Generalize to more than 1 kinematic feature and more than 2 event categories

Make method more sensitive to small signal fractions

Interrogate conditional expectation to recover $f_S, \langle p_T \rangle_B, \langle p_T \rangle_S, \text{ and } L_{S/B}(\mathcal{O})$



Key Takeaways:



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Train ML model to predict kinematics from substructure \implies powerful classifier



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Shift discussion from specific models to factorized structure



Key Takeaways:

Train ML model to predict kinematics from substructure \implies powerful classifier

Shift discussion from specific models to factorized structure

Focused on jets, but works for any factorized objects







Thank you!







Thank you!



Backup Slides

Interrogating the Normalization EFPs vs p_T Mutual Information






Interrogating the Normalization EFPs vs *m*_J Mutual Information



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Bump Hunt w/ $f_S = 0$



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