1

- -

Anomaly Detection in Collider Physics via Factorized Observables

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

1

- -

Anomaly Detection in Collider Physics via Factorized Observables

How to Become a FORCE Wielder

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

Introduction

Raymond Wynne - ML4Jets - 07 November 2023

Current set of anomaly detection methods come with specific assumptions

Introduction

Current set of anomaly detection methods come with specific assumptions Examples:

Introduction

Current set of anomaly detection methods come with specific assumptions

Introduction

Examples:

• Comparison between data and simulation [1709.01087, 1806.02350, 1807.06038]

Current set of anomaly detection methods come with specific assumptions

Introduction

Examples:

• Comparison between data and simulation

• New physics appears as resonance [1805.02664, 1902.02634, 2009.02205]

[1709.01087, 1806.02350, 1807.06038]

Current set of anomaly detection methods come with specific assumptions

Introduction

Examples:

- Comparison between data and simulation
- New physics appears as resonance
- Autoencoder operationally defines anomaly

[1709.01087, 1806.02350, 1807.06038]

[1805.02664, 1902.02634, 2009.02205]

[1808.08979, 1903.02032, 2010.05531]

Current set of anomaly detection methods come with specific assumptions

Introduction

Examples:

- Comparison between data and simulation
- New physics appears as resonance

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

[1709.01087, 1806.02350, 1807.06038]

[1805.02664, 1902.02634, 2009.02205]

Current set of anomaly detection methods come with specific assumptions

Introduction

Examples:

Introduce new method with different assumption: **factorization** [1708.02949, 1802.00008, 2002.12376] • Autoencoder operationally defines anomaly [1808.08979, 1903.02032, 2010.05531]

- Comparison between data and simulation
- New physics appears as resonance

[1709.01087, 1806.02350, 1807.06038]

[1805.02664, 1902.02634, 2009.02205]

What is factorization?

Factorization: physics at different energy scales approximately independent

What is factorization?

Factorization: physics at different energy scales approximately independent

What is factorization?

Factorization: physics at different energy scales approximately independent

Given p_T , y , $\mathcal O$, this gives

What is factorization?

Factorization: physics at different energy scales approximately independent

Given p_T , y , $\mathcal O$, this gives

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

What is factorization?

Factorization: physics at different energy scales approximately independent

Given p_T , y , $\mathcal O$, this gives

What is factorization?

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

Marginalizing out y and taking a scale-/boostinvariant O , this gives

Factorization: physics at different energy scales approximately independent

Given p_T , y , $\mathcal O$, this gives

What is factorization?

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

Marginalizing out y and taking a scale-/boostinvariant O , this gives

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

Factorization: physics at different energy scales approximately independent

Given p_T , y , $\mathcal O$, this gives

What is factorization?

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

Marginalizing out y and taking a scale-/boostinvariant O , this gives

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

 $Ex O:$

Factorization: physics at different energy scales approximately independent

Given p_T , y , $\mathcal O$, this gives

What is factorization?

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

Marginalizing out y and taking a scale-/boostinvariant O , this gives

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

Ex $\mathcal{O}:$ $N-$ subjettiness ratios,

[1108.2701]

Factorization: physics at different energy scales approximately independent

Given p_T , y , $\mathcal O$, this gives

What is factorization?

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

Marginalizing out y and taking a scale-/boostinvariant O , this gives

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

Ex *O*: *N* – subjettiness ratios, D_2 ,

[1108.2701] [1401.4458]

Factorization: physics at different energy scales approximately independent

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

What is factorization?

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

Marginalizing out y and taking a scale-/boostinvariant O , this gives

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

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

Factorization: physics at different energy scales approximately independent

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

What is factorization?

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

Marginalizing out y and taking a scale-/boostinvariant O , this gives

Ex $\textcircled{c}: N$ – subjettiness ratios, D_2, D_3, N_i [1108.2701] [1401.4458] [1507.03018] [1609.07483]

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

Signal versus Background Factorization

Signal versus Background Factorization Assume we have a distribution of the form

Signal versus Background Factorization $p(p_T, O) = f_S p_S(p_T) p_S(O) + f_B p_B(p_T) p_B(O)$ Assume we have a distribution of the form

Signal versus Background Factorization $p(p_T, O) = f_S p_S(p_T) p_S(O) + f_B p_B(p_T) p_B(O)$ Assume we have a distribution of the form

Calculate the conditional expectation

Signal versus Background Factorization $(\langle p_T \rangle_S - \langle p_T \rangle_B) L_{S/B}(0)$ $p(p_T, O) = f_S p_S(p_T) p_S(O) + f_B p_B(p_T) p_B(O)$ Calculate the conditional expectation Assume we have a distribution of the form

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

-
-
- $= \mathscr{M}(L_{S/B}(\mathcal{O}))$
-

Signal versus Background Factorization $(\langle p_T \rangle_S - \langle p_T \rangle_B) L_{S/B}(0)$ $p(p_T, O) = f_S p_S(p_T) p_S(O) + f_B p_B(p_T) p_B(O)$ Calculate the conditional expectation Assume we have a distribution of the form

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

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

-
-
-
-

Signal versus Background Factorization $[p_T | \mathcal{O}] = \langle p_T \rangle_B + f_S$ $(\langle p_T \rangle_S - \langle p_T \rangle_B) L_{S/B}(0)$ $1 - f_S + f_S L_{S/B}(\mathcal{O})$ $p(p_T, O) = f_S p_S(p_T) p_S(O) + f_B p_B(p_T) p_B(O)$ $= \mathscr{M}(L_{S/B}(\mathcal{O}))$ Calculate the conditional expectation Assume we have a distribution of the form

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

How do we extract $E[p_T | 0]$?

How do we extract $E[p_T | 0]$?

$E[p_T | 0]$ minimizes the mean-squared error loss!

Raymond Wynne - ML4Jets - 07 November 2023

$E[p_T|\mathcal{O}]$ minimizes the mean-squared error loss! How do we extract $E[p_T | 0]$? Enter machine learning!

$\mathbb{E}[p_T|\mathcal{O}]$ minimizes the mean-squared error loss! How do we extract $E[p_T | 0]$? Enter machine learning!

 $\overline{}$

$\mathbb{E}[p_T|\mathcal{O}]$ minimizes the mean-squared error loss! How do we extract $E[p_T]$ 0]? Enter machine learning!

… really just need →

$\mathbb{E}[p_T|\mathcal{O}]$ minimizes the mean-squared error loss! How do we extract $E[p_T]$ 0]? Enter machine learning!

… really just need →

The FORCE Method

Factorized **O**bservables for **R**egressing Conditional Expectation
Define approximately factorized objects (e.g.~jets)

The FORCE Method

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

The FORCE Method

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

- $-$ kinematics p_T
- scale-/boost-invariant substructure O

pT pT q $X \nvert p_T$

The FORCE Method

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

- $-$ kinematics p_T
- scale-/boost-invariant substructure 6

Train a machine-learning model to predict p_T from 0

The FORCE Method

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

- $-$ kinematics p_T
- scale-/boost-invariant substructure O

<u>Frain</u> a machine-learning model to predict p_T **E** p_T *p* from \odot with the mean-squared error loss

The FORCE Method

-
-
- *X* p_T $E[p_T | \mathcal{O}]$ $q \searrow p$ $E[P]$ $E[p_T|\mathcal{O}]$

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

- $-$ kinematics p_T
- scale-/boost-invariant substructure O

Train a machine-learning model to predict p_T from \odot with the mean-squared error loss

The FORCE Method

-
-
-

Classify anomalous objects via cutting on the model output

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

- $-$ kinematics p_T
- scale-/boost-invariant substructure O

Train a machine-learning model to predict p_T from \odot with the mean-squared error loss

The FORCE Method

-
-
-
-

Classify anomalous objects via cutting on the model output

Find anomalies by predicting kinematics from substructure

Use the FORCE Luke

"Use the Force, Luke."

Demonstrations of FORCE:

Use the FORCE Luke

"Use the Force, Luke."

Demonstrations of FORCE:

Use the FORCE Luke

"Use the Force, Luke."

Demonstrations of FORCE:

1. Toy Gaussian Dataset

Use the FORCE Luke

"Use the Force, Luke."

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

Gaussian Simulation

Gaussian Simulation

1 kinematic variable, 1 substructure variable

Gaussian Simulation

1 kinematic variable, 1 substructure variable

1 million draws from background model

Gaussian Simulation

1 kinematic variable, 1 substructure variable 1 million draws from background model *f_S* · 1 million draws from signal model

ROC-AUC for Gaussian Simulation

ROC-AUC for Gaussian Simulation

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

ROC-AUC for Gaussian Simulation

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

⟹

ROC-AUC for Gaussian Simulation

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

⟹

ROC-AUC for Gaussian Simulation

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

Optimal performance in high signal limit

ROC-AUC for Gaussian Simulation

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

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

Convergence for Gaussian Simulation

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

Convergence for Gaussian Simulation

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

LHC Olympics R&D Dataset

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

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

Energy flow polynomials - systematic expansion in energy and angle

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

Energy flow polynomials - systematic expansion in energy and angle

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

Energy flow polynomials - systematic expansion in energy and angle

Take EFPs *d* ≤ 3 → 13 features

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

Energy flow polynomials - systematic expansion in energy and angle

Take EFPs *d* ≤ 3 → 13 features

Transverse boosts scale

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

Energy flow polynomials - systematic expansion in energy and angle

Take EFPs *d* ≤ 3 → 13 features

Transverse boosts scale Energy: *γ*

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

Energy flow polynomials - systematic expansion in energy and angle

Take EFPs *d* ≤ 3 → 13 features

Transverse boosts scale Energy: *γ* Angle: 1/*γ*

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

Energy flow polynomials - systematic expansion in energy and angle

Take EFPs *d* ≤ 3 → 13 features

Transverse boosts scale Energy: *γ* Angle: 1/*γ*

Introduce normalized EFPs

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

Energy flow polynomials - systematic expansion in energy and angle

Take EFPs *d* ≤ 3 → 13 features

Transverse boosts scale Energy: *γ* Angle: 1/*γ*

Introduce normalized EFPs

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

Energy flow polynomials - systematic expansion in energy and angle

Take EFPs *d* ≤ 3 → 13 features

Transverse boosts scale Energy: *γ* Angle: 1/*γ*

Introduce normalized EFPs

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

Energy flow polynomials - systematic expansion in energy and angle

Take EFPs *d* ≤ 3 → 13 features

Transverse boosts scale Energy: *γ* Angle: 1/*γ*

Introduce normalized EFPs

 $13 \rightarrow 8$ independent observables

ROC-AUC for LHCO

ROC-AUC for LHCO

- Fully connected network
- 3 layers of 100 nodes
- ReLU Activation
- Dropout and L2 Regularization
- Mean across 10 models

ROC-AUC for LHCO

- Fully connected network
- 3 layers of 100 nodes
- ReLU Activation
- Dropout and L2 Regularization
- Mean across 10 models

ROC-AUC for LHCO

- Fully connected network
- 3 layers of 100 nodes
- ReLU Activation
- Dropout and L2 Regularization
- Mean across 10 models

 \rightarrow

ROC-AUC for LHCO

Near optimal in high signal limit

 \rightarrow

- Fully connected network
- 3 layers of 100 nodes
- ReLU Activation
- Dropout and L2 Regularization
- Mean across 10 models

ROC-AUC for LHCO

Near optimal in high signal limit

Non-trivial discrimination power for $f_{\!S}^{} \! = 0$

 \rightarrow

- Fully connected network
- 3 layers of 100 nodes
- ReLU Activation
- Dropout and L2 Regularization
- Mean across 10 models

ROC-AUC for LHCO

Non-trivial discrimination power for $f_{\!S}^{} \! = 0$ *More on that later*

 \rightarrow

Near optimal in high signal limit

- Fully connected network
- 3 layers of 100 nodes
- ReLU Activation
- Dropout and L2 Regularization
- Mean across 10 models

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*′ and the *X* and *Y*!

FORCE-ing Factorization with Shuffling

FORCE-ing Factorization with Shuffling

Explicitly construct factorized distribution by separately shuffling signal and background

FORCE-ing Factorization with Shuffling

Explicitly construct factorized distribution by separately shuffling signal and background

⟹

FORCE-ing Factorization with Shuffling

Explicitly construct factorized distribution by separately shuffling signal and background

⟹

FORCE-ing Factorization with Shuffling

Explicitly construct factorized distribution by separately shuffling signal and background

⟹

Optimal performance in high signal limit

FORCE-ing Factorization with Shuffling

Explicitly construct factorized distribution by separately shuffling signal and background

⟹

Optimal performance in high signal limit Smooth decay of statistical power

FORCE-ing Factorization with Shuffling

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

Come to the dark side: Future Work

GIVE YOURSELF TO THE DARK SIDE

Come to the dark side: Future Work

GIVE YOURSELF TO THE DARK SIDE

Come to the dark side: Future Work

GIVE YOURSELF TO THE DARK SIDE

Integrate with existing anomaly detection methods

Come to the dark side: Future Work

Integrate with existing anomaly detection methods

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

Come to the dark side: Future Work

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 , $\langle p_T \rangle_B$, $\langle p_T \rangle_S$, and $L_{S/B}(0)$

Come to the dark side: Future Work

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

Conclusion

Key Takeaways:

Conclusion

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

Key Takeaways:

Conclusion

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

Key Takeaways:

Shift discussion from specific models to factorized structure

Conclusion

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

Key Takeaways:

Shift discussion from specific models to factorized structure

Focused on jets, but works for any factorized objects

Thank you!

Raymond Wynne - ML4Jets - 07 November 2023

Thank you!

Raymond Wynne - ML4Jets - 07 November 2023

Backup Slides

Interrogating the Normalization EFPs vs p_T **Mutual Information**

Raymond Wynne - ML4Jets - 07 November 2023

Interrogating the Normalization EFPs vs m_J **Mutual Information**

Bump Hunt w/ *f ^S* = 0

Raymond Wynne - ML4Jets - 07 November 2023