Exploring the (Metric) Space of Jets with CMS Open Data

CERN EP/IT Data Science Seminar

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Joint work with Patrick Komiske, Radha Mastandrea, Preksha Naik, and Jesse Thaler

[1902.02346], to appear in PRL
[19xx.xxxxx]

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Outline

Part I
Introduction

When are two jets similar?
The Energy Mover’s Distance
Movie Time

Part II
Application
Jets in CMS Open Data
Exploring the Space of Jets
Quantifying Detector Effects
Outline

Part I
Introduction

When are two jets similar?

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Movie Time

Part II
Application

Jets in CMS Open Data

Exploring the Space of Jets

Quantifying Detector Effects
When are two jets similar?
When are two jets similar?

These two jets “look” similar, but have different numbers of particles, flavors, and locations.

How do we quantify this?

“Space of Jets”
When are two jets similar?

How a jet gets its shape

Collision

Fragmentation
partons \(g, u, d, \ldots\)

Hadronization
hadrons \(\pi^\pm, K^\pm, \ldots\)

Detection
When are two jets similar?

A jet is…

Theoretically: very complicated

Experimentally: very complicated

However:

The energy flow (distribution of energy) is the information that is robust to: fragmentation, hadronization, detector effects, …

Energy flow $\Leftrightarrow$ Infrared and Collinear (IRC) Safe information

[N.A. Sveshnikov, F.V. Tkachov, 9512370]
[F.V. Tkachov, 9601308]
[P.S. Cherzor, N.A. Sveshnikov, 9710349]
When are two jets similar?

Energy flow is robust information

Treat jets as distributions of energy:

\[ \sum_{i=1}^{M} E_i \delta(\hat{p}_i) \]

\( E_i \) energy
\( \delta(\hat{p}_i) \) direction

Ignoring particle flavor, charge…
When are two jets similar?

When they have similar distributions of energy

The Energy Mover’s Distance

Movie Time

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Quantifying Detector Effects
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Eric M. Metodiev, MIT
The Energy Mover’s Distance

Review: The Earth Mover’s Distance

Earth Mover’s Distance: the minimum “work” (stuff x distance) to rearrange one pile of dirt into another

Metric on the space of (normalized) distributions: symmetric, non-negative, triangle inequality

Distributions are close in EMD ⇔ their expectation values are close.

Also known as the 1-Wasserstein metric.
The Energy Mover’s Distance

Energy Mover’s Distance: the minimum “work” (energy x angle) to rearrange one event (pile of energy) into another

\[ EMD(\varepsilon, \varepsilon') = \min \{ f \} \sum_{i=1}^{M} \sum_{j=1}^{M'} f_{ij} \frac{\theta_{ij}}{R} \]

Difference in radiation pattern

[Komiske, EMM, Thaler, 1902.02346]
The Energy Mover’s Distance

*From Earth to Energy*

**Energy Mover’s Distance:** the minimum “work” \((\text{energy} \times \text{angle})\) to rearrange one event (pile of energy) into another

\[
\text{EMD}(\varepsilon, \varepsilon') = \min \left\{ f \right\} \sum_{i=1}^{M} \sum_{j=1}^{M'} f_{ij} \frac{\theta_{ij}}{R} + \sum_{i=1}^{M} E_i - \sum_{j=1}^{M'} E'_{j}
\]

- Difference in radiation pattern
- Difference in total energy

Eric M. Metodiev, MIT
The Energy Mover’s Distance

*From Earth to Energy*

**Energy Mover’s Distance:** the minimum “work” (energy $\times$ angle) to rearrange one event (pile of energy) into another

\[
\text{EMD}(\mathcal{E}, \mathcal{E}') = \min_{\{f\}} \sum_{i=1}^{M} \sum_{j=1}^{M'} f_{ij} \frac{\theta_{ij}}{R} + \left| \sum_{i=1}^{M} E_i - \sum_{j=1}^{M'} E'_j \right|
\]

- Difference in radiation pattern
- Difference in total energy

**EMD** has dimensions of energy

True metric as long as $R \geq \frac{1}{2} \theta_{\text{max}}$

$R \geq$ the jet radius, for conical jets

Solvable via Optimal Transport problem.

$\sim 1\text{ms}$ to compute EMD for two jets with 100 particles.

[ Eric M. Metodiev, MIT ]

[ P.T. Komiske, EMM, J. Thaler, 1902.02346 ]
When are two jets similar?
When they have similar distributions of energy

The Energy Mover’s Distance
Work to rearrange one event into another.

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Jets in CMS Open Data
Exploring the Space of Jets
Quantifying Detector Effects

Outline
Exploring the Space of Jets w. CMS Open Data

When are two jets similar?
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Movie Time

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Quantifying Detector Effects
EMD is the cost of an optimal transport problem.

We also get the shortest path between the events.

Interpolate along path to visualize!
Movie Time: Visualizing Jet Formation

QCD Jets

W Jets

Top Jets

Pythia 8, $R = 1.0$ jets, $p_T \in [500,550] \text{GeV}$
Movie Time: Visualizing QCD Jet Formation

- Quark
- Fragmentation
- Hadronization

fragmentation
EMD: 111.6 GeV

hadronization
EMD: 18.1 GeV
Movie Time: Visualizing $W$ Jet Formation

Eric M. Metodiev, MIT
Movie Time: Visualizing Top Jet Formation

- **Decay Quarks**
- **Fragmentation**
- **Hadronization**

- **Top**
- EMD: 161.1 GeV
- EMD: 47.1 GeV
- EMD: 27.0 GeV
Exploring the Space of Jets w. CMS Open Data

When are two jets similar?
When they have similar distributions of energy

The Energy Mover’s Distance
Work to rearrange one event into another.

Movie Time
Visualize energy movement and jet formation.

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Eric M. Metodiev, MIT
Exploring the Space of Jets w. CMS Open Data
22
When are two jets similar?  
*When they have similar distributions of energy*

The Energy Mover’s Distance  
*Work to rearrange one event into another.*

Movie Time  
*Visualize energy movement and jet formation.*

Jets in CMS Open Data

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CMS Open Data

An amazing resource for physics exploration and proof-of-principle studies.

opendata.cern.ch
CMS Open Data

Many exciting physics applications with the CMS Open Data already.

Exposing the QCD splitting function

[Tripathee, Xue, Larkoski, Marzani, Thaler, 1704.05842]
[Larkoski, Marzani, Thaler, Tripathee, Xue, 1704.05066]

Looking for parity violation in jets

[Lester, Schott, 1904.11195]

Searching for dimuon resonances

[Cesarotti, Soreq, Strassler, Thaler, Xue, 1902.04222]

Analyzing collision data with deep learning techniques

[Madrazo, Cacha, Iglesias, de Lucas, 1708.07034]
[Andrews, Paulini, Gleyzer, Poczos, 1807.11916]
[Andrews, et al., 1902.08276]
CMS 2011A Jet Primary Dataset (+ Simulation)

2.3 fb$^{-1}$ of 7 TeV proton-proton collision data. [link]

$\sim$1 million $R = 0.5$ jets with $p_T \in [375,425]$GeV, $|\eta| < 1.9$

[Komiske, Mastandrea, EMM, Naik, Thaler, to appear]
Jet Substructure Observables

Study jet substructure at truth and detector level.

\[ m^2 = \left( \sum_{i \in \text{Jet}} p^{\mu}_i \right)^2 \]

\[ M = \sum_{i \in \text{Jet}} 1 \]

\[ p_T^D = \frac{\sum_{i \in \text{Jet}} p_{T,i}^2}{\left( \sum_{i \in \text{Jet}} p_{T,i} \right)^2} \]

Similar to: [Larkoski, Marzani, Thaler, Tripathee, Xue, 1704.05066]
Comparing Jets in CMS Open Data

Jets are longitudinally boosted and rotated to \((y, \phi) = (0,0)\).

Scaling \(\sum_{i=1}^{M} p_{T,i} \rightarrow 400\) GeV to focus on substructure.
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*Work to rearrange one event into another.*

Movie Time
*Visualize energy movement and jet formation.*

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Jets in CMS Open Data
*A great resource for physics exploration*

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Exploring the Space of Jets

Quantifying Detector Effects
Most Representative Jets: K-medoids

Jet Mass

AK5 Jets, $|\eta^{\text{jet}}| < 1.9$
$p_T^{\text{jet}} \in [375, 425]$ GeV, CHS
CMS 2011 Open Data
$p_T^{\text{PFC}} > 1$ GeV, Tracks
Rotated, Scaled to 400 GeV

Preliminary
Most Representative Jets: K-medoids

AK5 Jets, $|\eta^{\text{jet}}| < 1.9$
$p_T^{\text{jet}} \in [375, 425] \text{ GeV}$, CHS
CMS 2011 Open Data
$p_T^{\text{PFC}} > 1 \text{ GeV}$, Tracks
Rotated, Scaled to 400 GeV

PRELIMINARY
Towards Anomaly Detection

Complements recent developments in anomaly detection for collider physics.

[Collins, Howe, Nachman, 1805.02664]
[Heimel, Kasieczka, Plehn, Thompson, 1808.08979]
[Farina, Nakai, Shih, 1808.08992]
[Cerri, Nguyen, Pierini, Spiropulu, Vlimant, 1811.10276]
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[Cerri, Nguyen, Pierini, Spiropulu, Vlimant, 1811.10276]
Exploring the Space of Jets: Visualizing the Manifold

Visualize the space of events with t-Distributed Stochastic Neighbor Embedding (t-SNE).

Finds an embedding into a low-dimensional manifold that respects distances.

What does the space of jets look like?
Exploring the Space of Jets: Visualizing the Manifold

What does the space of jets look like?
Exploring the Space of Jets: Correlation Dimension

Intuition:

\[ N_{\text{neighboring}}(r) \propto r^{\text{dim}} \]

\[ \text{dim}(r) = r \frac{\partial}{\partial r} \ln N_{\text{neighbors}}(r) \]

Correlation dimension:

\[ \text{dim}(Q) = Q \frac{\partial}{\partial Q} \ln \left( \sum_{i=1}^{N} \sum_{j=1}^{N} \theta[\text{EMD}(\varepsilon_i, \varepsilon_j) < Q] \right) \]

Energy scale \( Q \) dependence

Count neighbors in ball of radius \( Q \)
Exploring the Space of Jets: Correlation Dimension

**EMD: Intrinsic Dimension**

PYTHIA 8.235, $\sqrt{s} = 14$ TeV

$R = 1.0$, $p_T \in [500, 550]$ GeV

QCD jets are simplest.

W jets are more complicated.

Top jets are most complex.

“Decays” have ~constant dimension.
Exploring the Space of Jets: Correlation Dimension

**EMD**: Intrinsic Dimension
PYTHIA 8.235, $\sqrt{s} = 14$ TeV
$R = 1.0$, $p_T \in [500, 550]$ GeV

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“Decays” have $\sim$constant dimension.

Fragmentation becomes more complex at lower energy scales.
Exploring the Space of Jets: Correlation Dimension

QCD jets are simplest.

W jets are more complicated.

Top jets are most complex.

“Decays” have ∼constant dimension.

Fragmentation becomes more complex at lower energy scales.

Hadronization becomes relevant at scales around 20 GeV.
Exploring the Space of Jets: Correlation Dimension

Can we understand this analytically?

Pileup & Detector Effects

AK5 Jets, $|\eta^{\text{jet}}| < 1.9$

$P_T^{\text{jet}} \in [375, 425] \text{ GeV}$

Scaled to 400 GeV

PRELIMINARY

Dimension blows up at low energies.

Jets are “more than fractal”

Can we understand this analytically?
Exploring the Space of Jets: Correlation Dimension

At LL: \[ \text{dim}_{q/g}(Q) = - \frac{8\alpha_s C_{q/g}}{\pi} \ln \frac{Q}{p_T/2} \]

+ 1-loop running of \( \alpha_s \)

\[ C_q = C_F = \frac{4}{3} \]
\[ C_g = C_A = 3 \]

**EMD: Intrinsic Dimension**
PYTHIA 8.235, \( \sqrt{s} = 14 \text{ TeV} \)
\( R = 1.0, p_T \approx 500 \text{ GeV} \)

**MC**
- Quark Jets
- Gluon Jets
- Hadrons
- Partons
- Theory, LL

Dimension blows up at low energies.

Jets are “more than fractal”
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Work to rearrange one event into another.

Movie Time

Visualize energy movement and jet formation.

Part II
Application

Jets in CMS Open Data

A great resource for physics exploration

Exploring the Space of Jets

New ways to visualize and probe collider data

Quantifying Detector Effects
Exploring the Space of Jets w. CMS Open Data

New ways to visualize and probe collider data

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Eric M. Metodiev, MIT
Exploring the Space of Jets w. CMS Open Data
EMD and IRC-Safe Observables

Events close in EMD are close in any infrared and collinear safe observable!

Additive IRC-safe observables:

$$\mathcal{O}(\mathcal{E}) = \sum_{i=1}^{M} E_i \Phi(\hat{n}_i)$$

Energy Mover’s Distance

$$\text{EMD}(\mathcal{E}, \mathcal{E}') \geq \frac{1}{RL} \left| \mathcal{O}(\mathcal{E}) - \mathcal{O}(\mathcal{E}') \right|$$

“Lipschitz constant” of $\Phi$

i.e. bound on its derivative

Additive IRC-safe observables:

Difference in observable values

e.g. jet angularities:

For $\beta \geq 1$ jet angularities:

$$\left| \lambda(\beta)(\mathcal{E}) - \lambda(\beta)(\mathcal{E}') \right| \leq \beta \text{ EMD}(\mathcal{E}, \mathcal{E}')$$

[C. Berger, T. Kucs, and G. Sterman, 0303051]
[A. Larkoski, J. Thaler, and W. Waalewijn, 1408.3122]
Old Observables in a New Language

**Thrust** is the EMD between the event and two back-to-back particles.

\[
t(\mathcal{E}) = E - \max_{\hat{n}} \sum_i |\hat{p}_i \cdot \hat{n}|
\]

\[
t(\mathcal{E}) = \min_{|\mathcal{E}'|=2} \text{EMD}(\mathcal{E}, \mathcal{E}')
\]

with \(\theta_{ij} = \hat{p}_i \cdot \hat{p}_j, \hat{p} = \tilde{p}/E\)

\[\tau_N(\mathcal{E}) = \min_{|\mathcal{E}'|=N} \text{EMD}(\mathcal{E}, \mathcal{E}').\]

\[\tau_N(\mathcal{E}) = \min_{|\mathcal{E}'|=N} \text{EMD}(\mathcal{E}, \mathcal{E}').\]

\(N\)-**(sub)**jettiness is the EMD between the event and the closest \(N\)-particle event.

\[
\tau_N^{(\beta)}(\mathcal{E}) = \min_{N \text{ axes}} \sum_{i=1}^M E_i \min_k \{\theta_{1,k}^{\beta}, \theta_{2,k}^{\beta}, \ldots, \theta_{N,k}^{\beta}\}
\]

\(\beta \geq 1\) is \(p\)-Wasserstein distance with \(p = \beta\).
Quantifying Detector Effects

Collision

Fragmentation
partons $\bar{q}, u, d, \ldots$

Hadronization
hadrons $\pi^\pm, K^\pm, \ldots$

Detection
Quantifying Detector Effects with EMD

Gen./Sim. EMD: 28.3 GeV

Gen./Sim. EMD: 27.0 GeV

Gen./Sim. EMD: 11.6 GeV

+ charged hadron subtraction
+ $p_T^{PFC} > 1$ GeV cut

Tracks only
Quantifying Detector Effects with EMD

AK5 Jets, CHS
$p_T^{jet} \in [375, 425]$ GeV
Scaled to 400 GeV

better

All PFCs
with CHS
with $p_T^{PFC} > 2$ GeV
with Tracks Only
Quantifying event modifications: Pileup

HL-LHC \(t\bar{t}\) event in ATLAS ITK at \(<\mu>=200\)
Pileup Mitigation

Can use vertex information in CMS Open Data to find charged pileup particles. Allows us to study the effect of pileup on radiation pattern and observables.

+ pileup
EMD = 28 GeV
Pileup Mitigation

Can use vertex information in CMS Open Data to find charged pileup particles. Allows us to study the effect of pileup on radiation pattern and observables.

- Quantify pileup mitigation performance with EMD (more in backup).
- Optimize machine learning-based pileup mitigation methods to minimize EMD?

[Komiske, EMM, Nachman, Schwartz, 1707.08600]
[Martinez, Cerri, Pierini, Spiropulu, Vlimant, 1810.07988]
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Work to rearrange one event into another.

Movie Time

Visualize energy movement and jet formation.

Jets in CMS Open Data

A great resource for physics exploration

Exploring the Space of Jets

New ways to visualize and probe collider data

Quantifying Detector Effects

Robust bounds for pileup and detector effects
Going Beyond

Clustering sets of events

New observables through EMD geometry

EMD for density estimation

“Event” mover’s distance between ensembles?

Model (in)dependent anomaly detection?

Train ML models to optimize EMD directly?

Include flavor information?

Eric M. Metodiev, MIT
EnergyFlow

https://energyflow.network

Welcome to EnergyFlow

EnergyFlow is a Python package containing a suite of particle physics tools. Originally designed to compute Energy Flow Polynomials (EFPs), as of version 0.10.0 the package expanded to include implementations of Energy Flow Networks (EFNs) and Particle Flow Networks (PFN)s. As of version 0.11.0, functions for facilitating the computation of the Energy Mover’s Distance (EMD) on particle physics events are included. To summarize the main features:

- **Energy Flow Polynomials**: EFPs are a collection of jet substructure observables which form a complete linear basis of IRC-safe observables. EnergyFlow provides tools to compute EFPs on events for several energy and angular measures as well as custom measures.

- **Energy Flow Networks**: EFNs are infrared- and collinear-safe models designed for learning from collider events as unordered, variable-length sets of particles. EnergyFlow contains customizable Keras implementations of EFNs.

- **Particle Flow Networks**: PFNs are general models designed for learning from collider events as unordered, variable-length sets of particles. EnergyFlow provides tools to compute PFNs on events for several energy and angular measures as well as custom measures.
The End
Thank you!
Extra Slides
Jet Kinematic Distributions

CMS 2011 Open Data
CMS 2011 Simulation
PYTHIA 6 Generation

AK5 Jets, $|\eta^{\text{jet}}| < 1.9$
$p_T^{\text{jet}} \geq 375$ GeV

Ratio to Sim.

Jet Transverse Momentum $p_T$ [GeV]

Differential Cross Section [nb/GeV]

CMS 2011 Open Data
CMS 2011 Simulation
PYTHIA 6 Generation

AK5 Jets
$p_T^{\text{jet}} \geq 375$ GeV

Ratio to Sim.

Jet Pseudorapidity $\eta$

Differential Cross Section [nb]
Quantifying event modifications: Hadronization

$$\lambda(\beta=1) = \sum_{i=1}^{M} E_i \theta_i$$

$$\lambda(\beta=1) = 111.1 \text{GeV}$$  $$\lambda(\beta=1) = 111.6 \text{GeV}$$

EMD: QCD Jet Angularity
PYTHIA 8.235, $\sqrt{s} = 14 \text{ TeV}$
$R = 1.0$, $p_T \in [500, 550] \text{ GeV}$

$\mathcal{E} = \mathcal{E}_{\text{partons}}$
$\mathcal{E}' = \mathcal{E}_{\text{hadrons}}$

$$\left| \lambda(\beta=1)(\mathcal{E}) - \lambda(\beta=1)(\mathcal{E}') \right| \leq \text{EMD}(\mathcal{E}, \mathcal{E}')$$
Exploring the Space of Events: $k$-medoids

**EMD**: QCD Jets, $k=3$-medoids

*PYTHIA 8.235, $\sqrt{s} = 14$ TeV
$R = 1.0$, $p_T \in [500, 550]$ GeV*
Exploring the Space of Events: Jet Classification

Classify $W$ jets vs. QCD jets

Look at a jet's nearest neighbors (kNN) to predict its class.

Optimal IRC-safe classifier with enough data.

Nearing performance of ML.
Exploring the Space of Events

Use EMD as a measure of event similarity

Unsupervised clustering algorithms can be used to cluster events

Jets are clusters of particles

???? are clusters of jets

VP Tree: $O(\log(N))$ neighbor query time

Much more to explore.
Exploring the Space of Events: $W$ jets

$W$ jets are 2-pronged:

\( z \): Energy Sharing of Prongs

\( \theta \): Angle between Prongs

\( \varphi \): Azimuthal orientation

Constrained by $W$ mass:

\[
z(1 - z)\theta^2 = \frac{p_{\mu J}^2}{p_T^2} = \frac{m_W^2}{p_T^2}
\]

Hence we expect a **two-dimensional** space of $W$ jets.

After $\varphi$ rotation: **one-dimensional**

$W$ jets, $R = 1.0$

\( p_T \in [500,510] \text{GeV} \)
Quantifying event modifications: Pileup

Leading Vertex Jet

How can we quantify pileup mitigation?

[Eric M. Metodiev, MIT]

[Eric M. Metodiev, MIT]

[Eric M. Metodiev, MIT]

[Eric M. Metodiev, MIT]
Quantifying event modifications: Pileup

Compare on a collection of observables?

Requires ad hoc choices of observables.

Compare calorimeter images pixel by pixel?

Discontinuous under physically-sensible single-pixel perturbations. Undesirable behavior with increasing resolution.
Quantifying event modifications: Pileup

Measure pileup mitigation performance with EMD!

Guarantees performance on IRC safe observables.
Stable under physically-sensible perturbations.
Train to optimize EMD with machine learning?
Integrated Luminosity

![Graph showing Integrated Luminosity over time, with dates from March 14 to August 22, 2011. The graph includes lines for LHC 2011A Delivered Luminosity, CMS 2011A Recorded Luminosity, Jet300 Effective Luminosity, and a PRELIMINARY note.]
Exploring the Space of Jets: Correlation Dimension

Sketch of leading log (one emission) calculation:

\[
\dim_{q/g}(Q) = Q \frac{\partial}{\partial Q} \ln \sum_{i=1}^{N} \sum_{j=1}^{N} \Theta[\text{EMD}(\varepsilon_i, \varepsilon_j) < Q]
\]

\[
= Q \frac{\partial}{\partial Q} \ln \Pr[\text{EMD} < Q]
\]

\[
= Q \frac{\partial}{\partial Q} \ln \Pr[\lambda(\beta=1) < Q; C_{q/g} \rightarrow 2 C_{q/g}]
\]

\[
= Q \frac{\partial}{\partial Q} \ln \exp \left( -\frac{4\alpha_s C_{q/g}}{\pi} \ln^2 \frac{Q}{p_T/2} \right)
\]

\[
= -\frac{8\alpha_s C_{q/g}}{\pi} \ln \frac{Q}{p_T/2}
\]

+ 1-loop running of \(\alpha_s\)

\[
C_q = C_F = \frac{4}{3}
\]

\[
C_g = C_A = 3
\]
When are two collider events similar?

How an event gets its shape: Experiment
Pileup Mitigation with PUMML