Can you hear the shape of a jet?

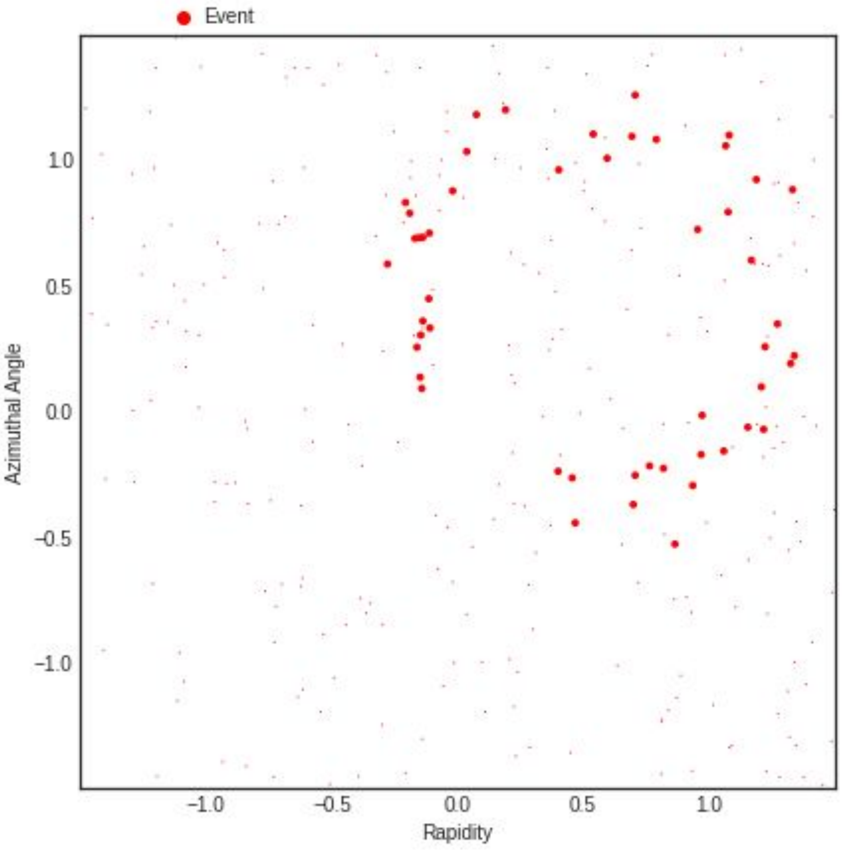
Rikab Gambhir

With Akshunna S. Dogra (),
Demba Ba (),
Abiy Tasissa (),
& Jesse Thaler ()

Email me questions at rikab@mit.edu!

Based on [Ba, Dogra, **RG**, Tasissa, Thaler, 2211.XXXX] (Coming Soon!)

Fundamental Question: What shape is this?

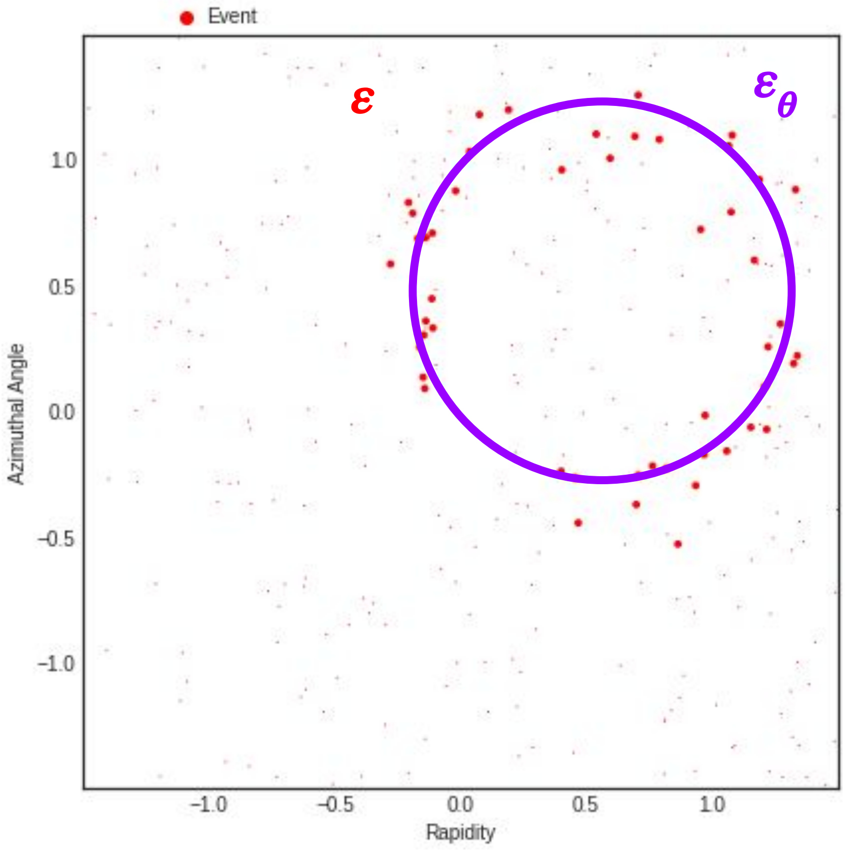


Pictured: (Fake) event that you might have measured at the LHC

Red dots are detector hits on a patch of the LHC cylinder, weighted by energy

Goal: Construct an observable $\mathcal{O}$ that generically answers this question!

Fundamental Question: What shape is this?



Using the **SHAPER** framework …

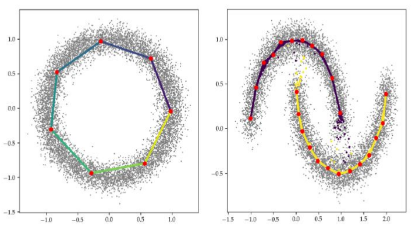
$$\mathcal{O}_{\mathcal{M}}(\mathcal{E}) = \min_{\mathcal{E}'_\theta \in \mathcal{M}} \mathrm{EMD}(\mathcal{E}, \mathcal{E}'_\theta)$$

$$\theta = \operatorname*{argmin}_{\mathcal{E}'_\theta \in \mathcal{M}} \mathrm{EMD}(\mathcal{E}, \mathcal{E}'_\theta)$$

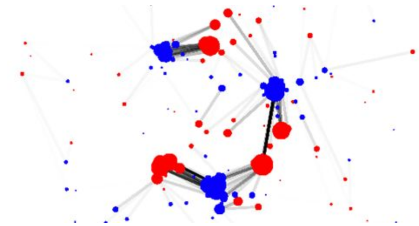
Circle with radius 0.767, center (0.50, 0.36) and a "circle-ness" value of 0.32.

Yes, you *CAN* hear the shape of a jet!

NSF AI Institute for Artificial Intelligence & Fundamental Interactions

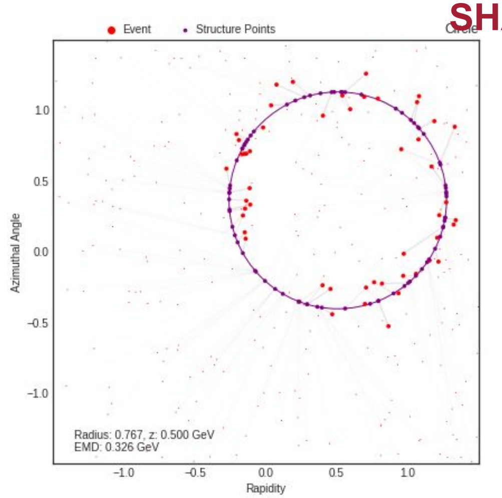


Piecewise-Linear Manifold Approximation with K-Deep Simplices (KDS, 2012.02134)



Well-Defined Metric on Particle Collisions using Energy Mover's Distance (EMD, 2004.04159)

SHAPER: Learning the Shape of Collider Events



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Framework for defining and calculating useful observables for collider physics!

THE UNREASONABLE EFFECTIVENSS OF ~~MATHEMATICS~~ IN ~~THE NATURAL SCIENCES~~

The Wasserstein Metric

Collider Physics

Eugene Wigner

Mathematics, rightly vi s not only truth, b supreme beauty cold and austere, like that of sculpture, w appeal to any part of our weaker nature, without the gorgeous trappings of painting or music, yet sublimely pure, and capable of a stern perfection such as only the greatest art can show. The true spirit of delight, the exaltation, the sense of being more than Man, which is the touchstone of the highest excellence, is to be found in mathematics as surely as in poetry.

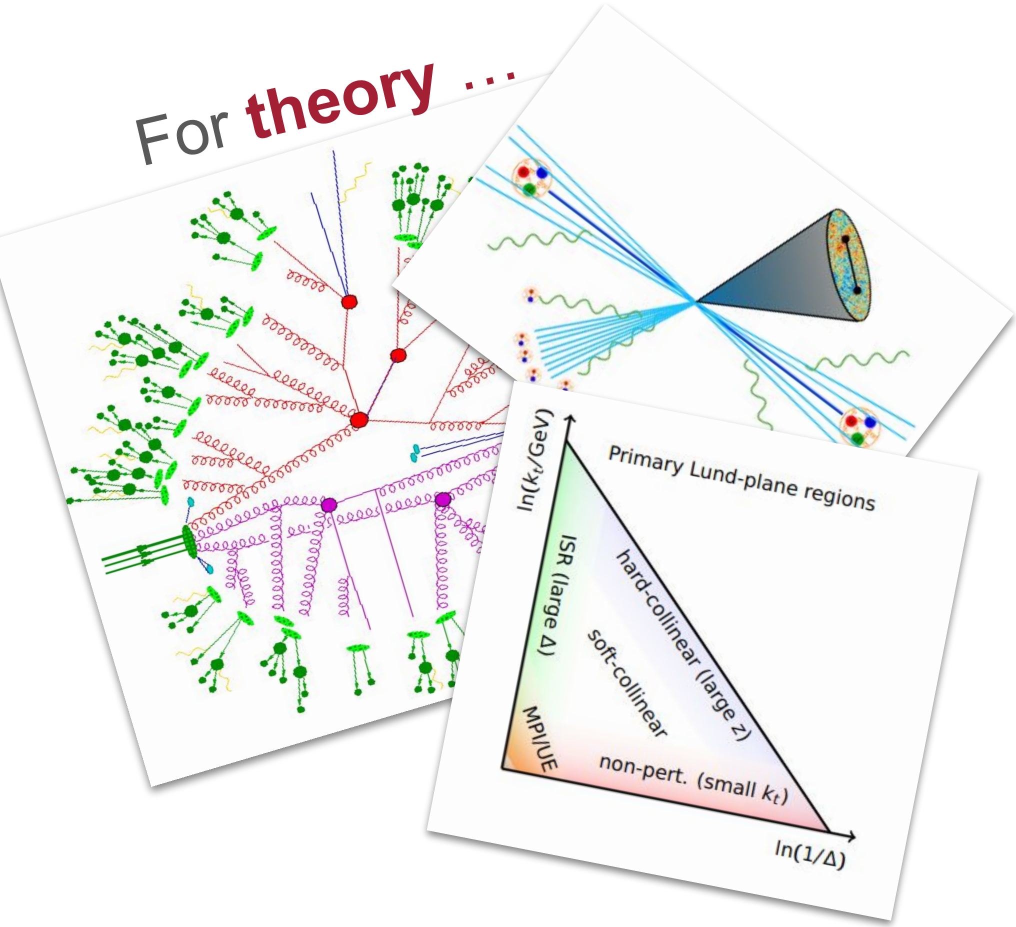
- BERTRAND RUSSELL, Study of Mathematics

Robust Observables

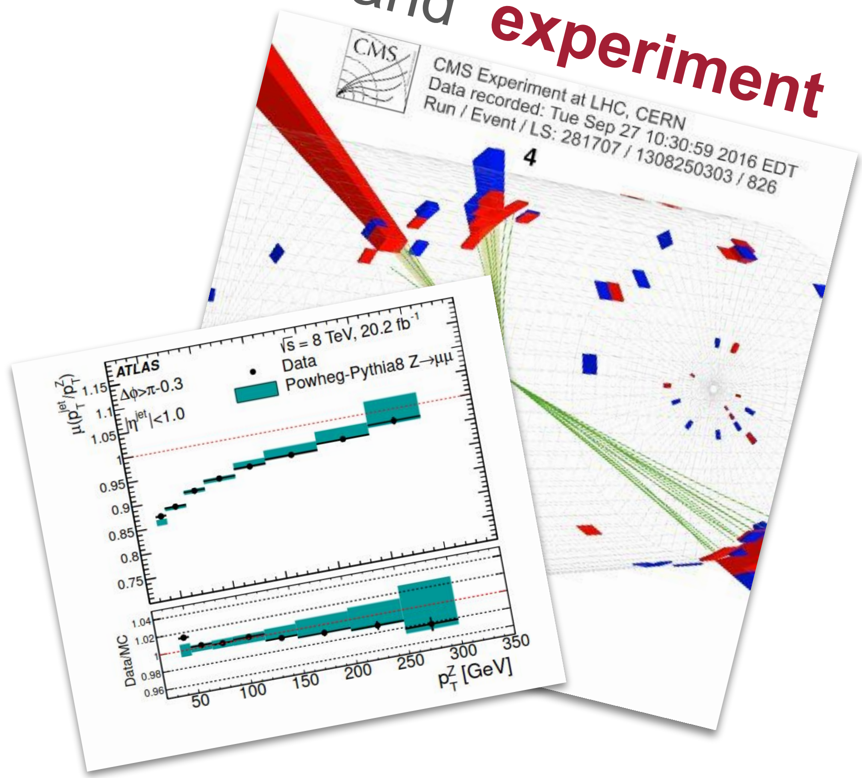
Images from [Bothmann et. al., 1905.09127; Lee, Meçaj, Moult, 2205.03414; Dreyer, Salam, Soyez, 1807.04758 CMS, 1810.10069; ATLAS, 1703.10485]

We want ***Robust Observables***!

For **theory** …



and **experiment**



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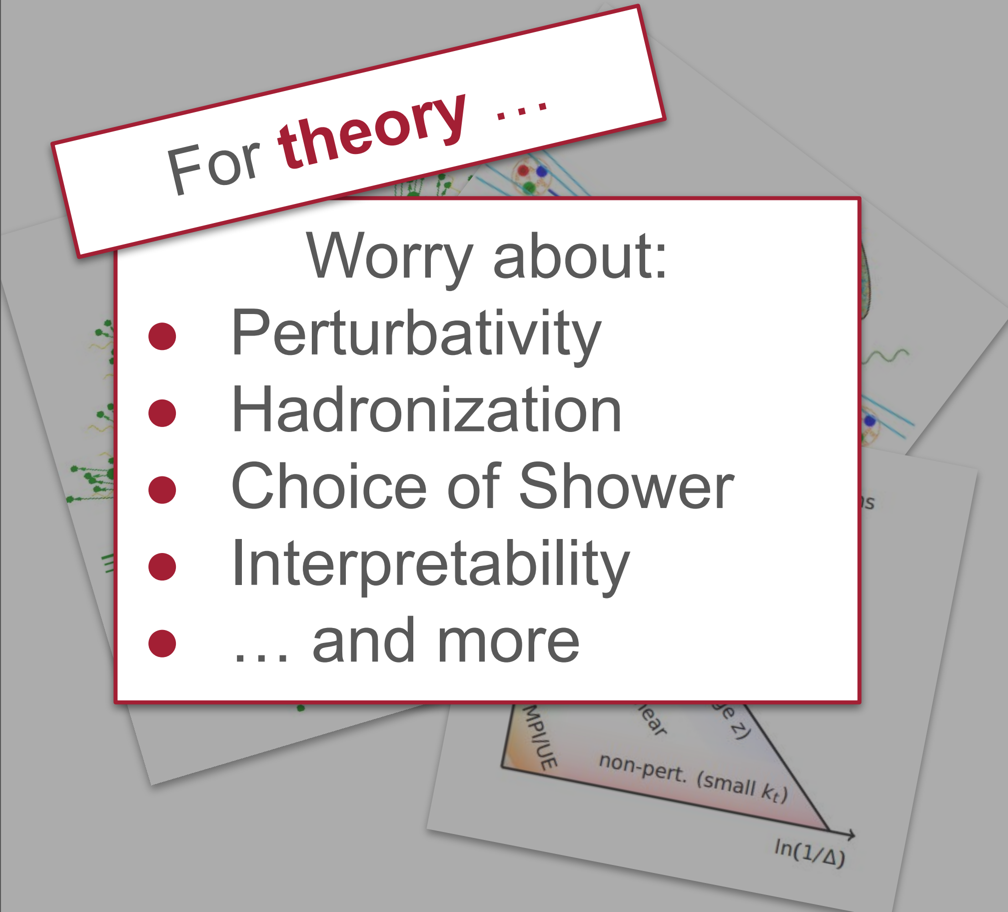
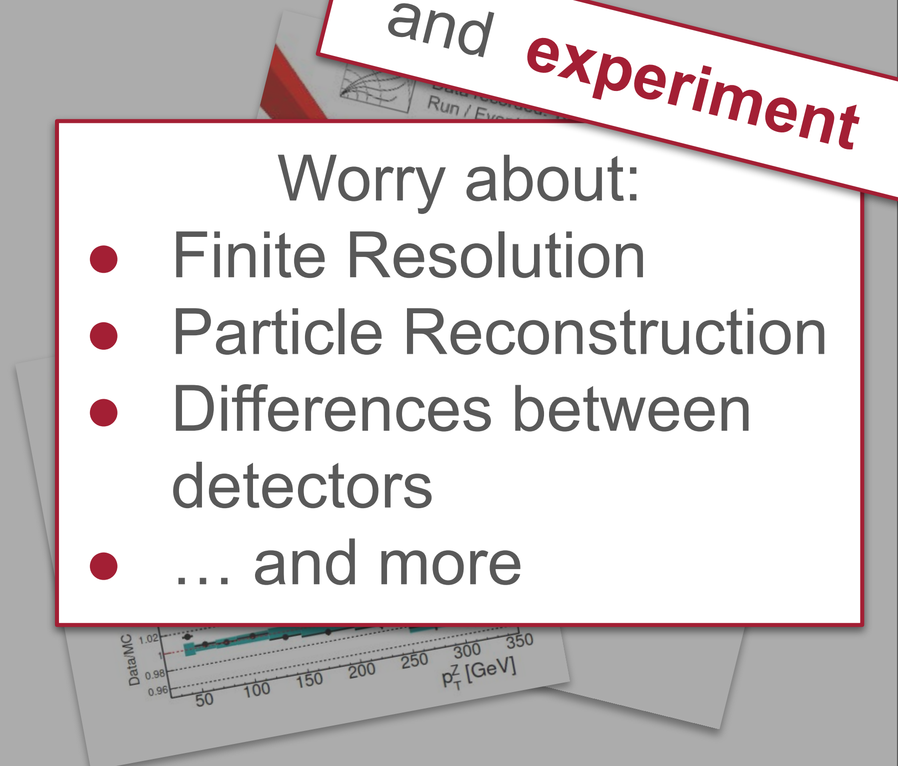


For **theory** …

Worry about:

- Perturbativity
- Hadronization
- Choice of Shower
- Interpretability
- … and more



and **experiment**

Worry about:

- Finite Resolution
- Particle Reconstruction
- Differences between detectors
- … and more

Robust Observables

We want ***Robust Observables***!

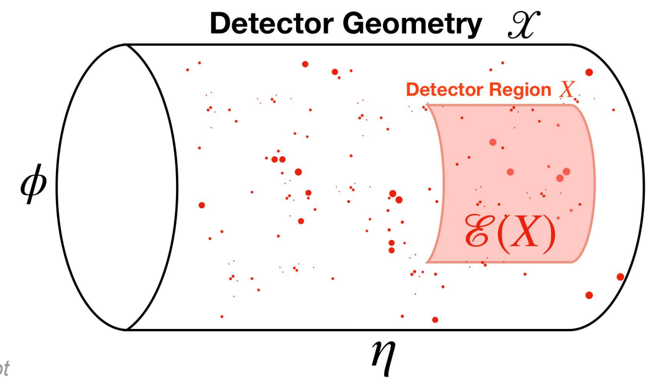
See Ian Moult's Talk from Tuesday!

Build observables out of ***Energy Flows***!

Detector Coordinate (η, ϕ)

$$\mathcal{E}(\vec{y}) = \sum_i z_i \delta(\vec{y} - \vec{y}_i)$$

Energy Fraction E_i / E_{Tot}



- Captures all the IRC-Safe / kinematically accessible calorimeter information in an event.
- Generalizes events - *any* probability distribution of energy could be an event! Events can be **real** or **idealized**

Observables and Wasserstein

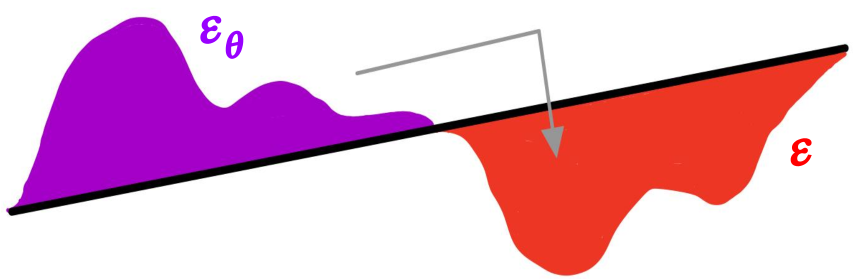
It can be shown that *any* observable on events, that* …

1. … is non-negative and finite
2. … is IRC-safe
3. … is translationally invariant
4. … is invariant to particle labeling
5. … respects the detector metric *faithfully***

… can be written as an optimization of the **Wasserstein Metric (Earth/Energy Mover's Distance)** between the real event and a manifold of idealized energy flows

$$\mathcal{O}_{\mathcal{M}}(\mathcal{E}) = \min_{\mathcal{E}'_\theta \in \mathcal{M}} \mathrm{EMD}(\mathcal{E}, \mathcal{E}'_\theta)$$

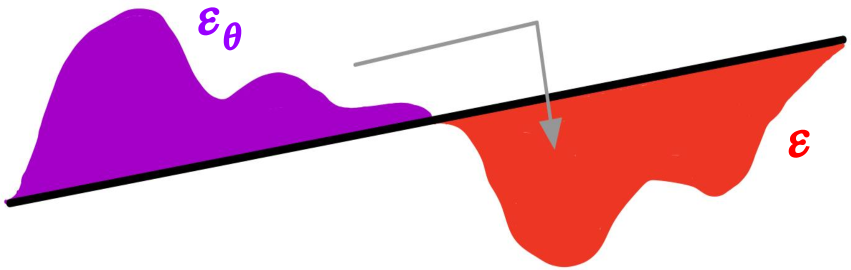
$$\theta = \operatorname*{argmin}_{\mathcal{E}'_\theta \in \mathcal{M}} \mathrm{EMD}(\mathcal{E}, \mathcal{E}'_\theta)$$



EMD = Work done to move "dirt" optimally

*Ask me for more details on this offline!
** Preserves distances between *extended* objects, not just points

Observables and Wasserstein



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4. … is invariant to particle labeling
5. … respects the detector metric *faithfully*

… c

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$$\mathrm{EMD}^{(\beta,R)}(\mathcal{E}, \mathcal{E}') = \min_{\pi_{ij} \geq 0} \left[\frac{1}{\beta R^\beta} \sum_{i=1}^{M} \sum_{j=1}^{N} \pi_{ij} d_{ij}^{\beta} \right] + |\Delta E_{\mathrm{tot}}|$$

$$\sum_{i=1}^{M} \pi_{ij} \leq E'_j, \; \sum_{j=1}^{N} \pi_{ij} \leq E_i \text{ and } \sum_{j=1}^{N} \pi_{ij} = \min(E_{\mathrm{tot}}, E'_{\mathrm{tot}})$$

Ask me for more details on this after!

Hearing Jets

[P. Komiske, E. Metodiev, and J. Thaler, 2004.04159;
J. Thaler, and K. Van Tilburg, 1011.2268;
I. W. Stewart, F. J. Tackmann, and W. J. Waalewijn, 1004.2489.;
S. Brandt, C. Peyrou, R. Sosnowski and A. Wroblewski, PRL 12 (1964) 57-61;
C. Cesarotti, and J. Thaler, 2004.06125]

Observable ⇔ Manifolds

$$\mathcal{O}_{\mathcal{M}}(\mathcal{E}) = \min_{\mathcal{E}'_\theta \in \mathcal{M}} \mathrm{EMD}(\mathcal{E}, \mathcal{E}'_\theta)$$

$$\theta = \operatorname*{argmin}_{\mathcal{E}'_\theta \in \mathcal{M}} \mathrm{EMD}(\mathcal{E}, \mathcal{E}'_\theta)$$

Many existing observables have this form!

Observables ⇔ Manifold of Shapes

- *N*-subjettines ⇔ Manifold of *N*-point events
- *N*-jettiness ⇔ Manifold of *N*-point events with floating total energy
- Thrust ⇔ Manifold of back-to-back point events
- Event Isotropy ⇔ Uniform distribution
- … and more!

All of the form “How much like **[shape]** does my **event** look like?”

We generalize this to build more observables!

Shape Observables

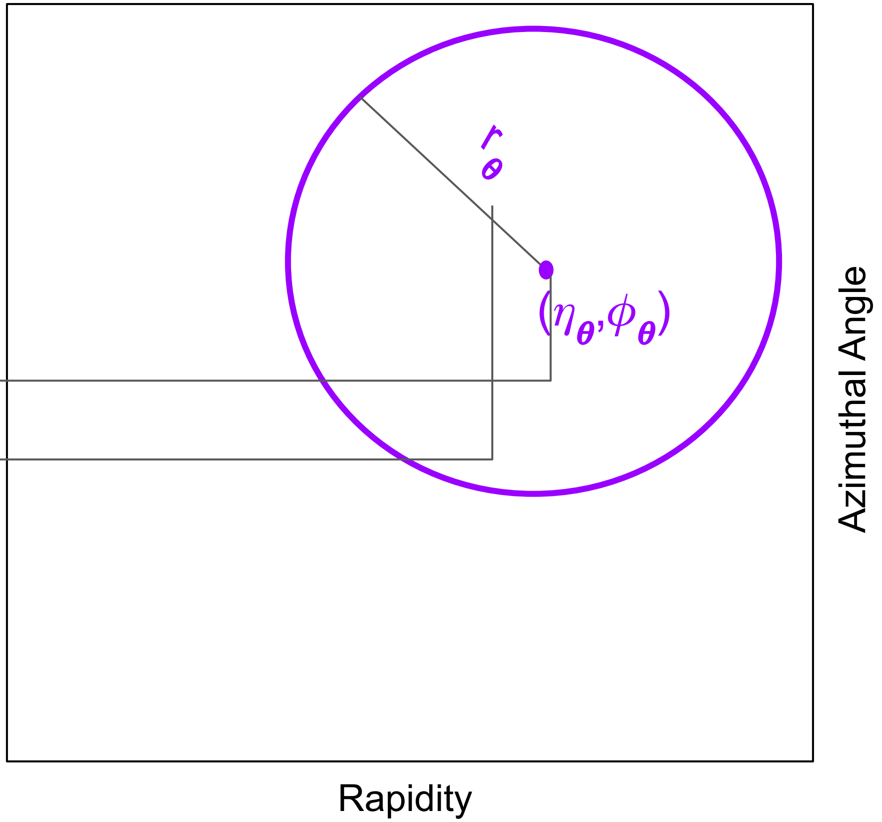
Let's go further! Consider *any* manifold of parameterized energy flows

Define a *shape* as any parameterized energy flow

For example, for a circle with parameterized radius and center*

$$\mathcal{E}(\vec{y}) = \begin{cases} \frac{1}{2\pi r_\theta} & |\vec{y} - \vec{y}_\theta| = r_\theta \\ 0 & |\vec{y} - \vec{y}_\theta| \neq r_\theta \end{cases}$$

Can then sample points (particles) from this idealized distribution!



Parameterized circle written as an energy flow

*Uniform prior by choice for simplicity. In principle, we can pick any parameterized normalized distribution.

Shape Observables

Given *any* manifold of parameterized energy flows (probability distributions) $\mathcal{M}$, representing shapes, we define the **shape observable** $\mathcal{O}$ and **shape parameters** θ on an event $\mathcal{E}$ as:

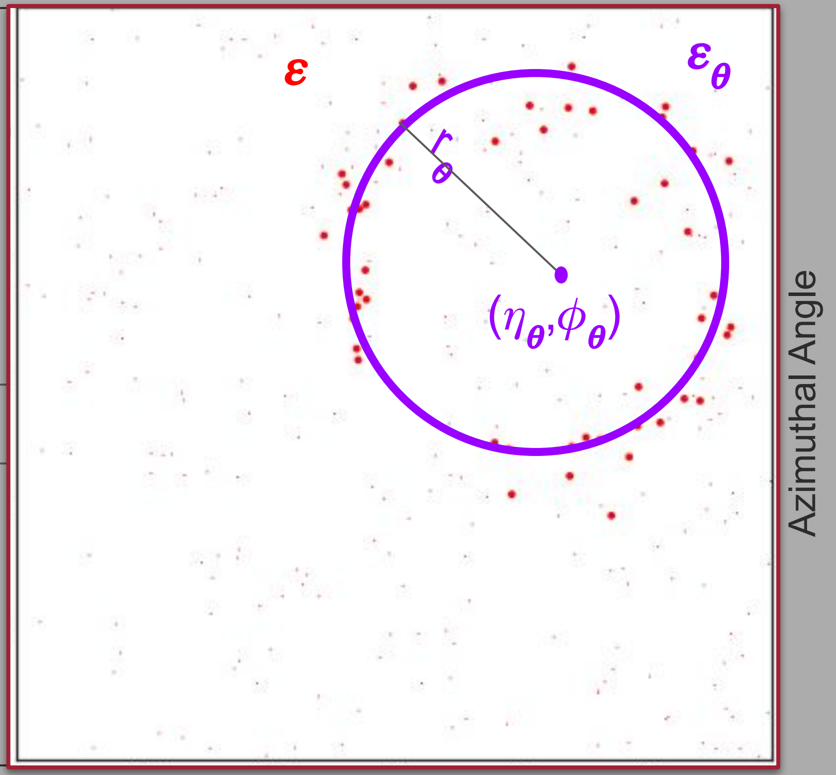
$$\mathcal{O}_{\mathcal{M}}(\mathcal{E}) = \min_{\mathcal{E}'_\theta \in \mathcal{M}} \mathrm{EMD}(\mathcal{E}, \mathcal{E}'_\theta)$$

$$\theta = \underset{\mathcal{E}'_\theta \in \mathcal{M}}{\mathrm{argmin}}\, \mathrm{EMD}(\mathcal{E}, \mathcal{E}'_\theta)$$

Shape observables are the generalization of event and jet shapes like N-(sub)jettiness, thrust, and isotropy!

[Ba, Dogra, **RG**, Tasissa, Thaler, 2211.XXXX]

arameterized energy flows



Parameterized circle written as an energy flow

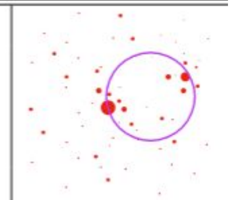
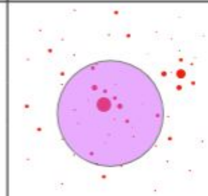
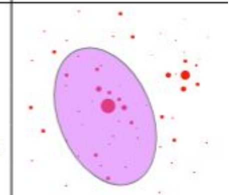
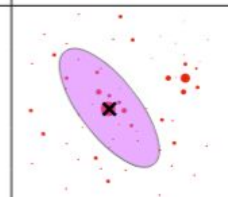
*Uniform prior by choice for simplicity. In principle, we can pick any parameterized normalized distribution.

Hearing Shapes

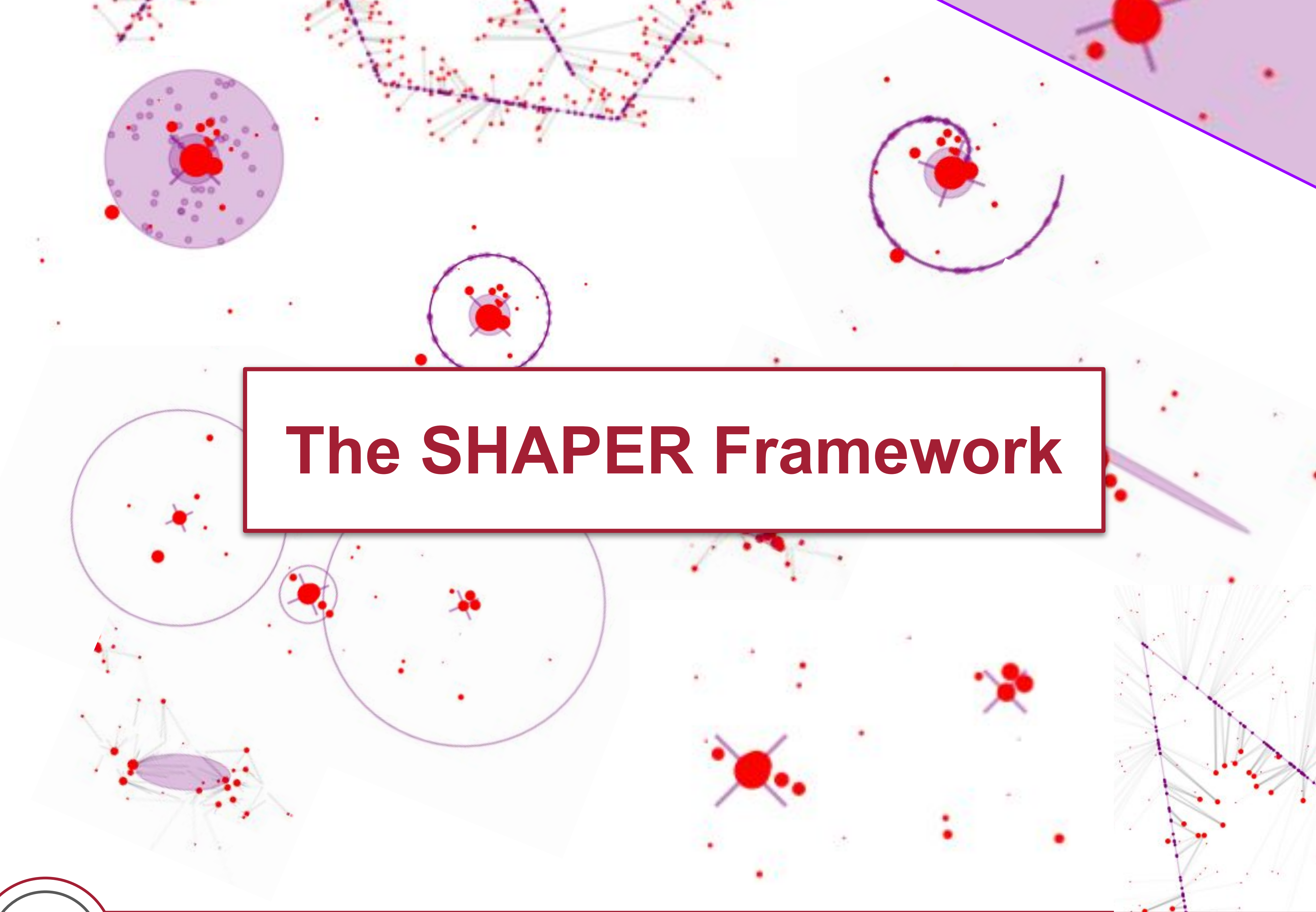
$\mathcal{O}_{\mathcal{M}}(\mathcal{E})$ answers: "How much like a shape in $\mathcal{M}$ does my event $\boldsymbol{\mathcal{E}}$ look like?"

$\theta_{\mathcal{M}}(\mathcal{E})$ answers: "Which shape in $\mathcal{M}$ does my event $\boldsymbol{\mathcal{E}}$ look like?"

Can define complex manifolds to probe increasingly subtle geometric structure, and even old combine shape observables to create new composite ones!

Shape	Specification	Illustration
Ringiness $\mathcal{O}_R$	**Manifold of Rings** $\mathcal{E}_{x_0,R_0}(x) = \frac{1}{2\pi R_0}$ for $\lvert x - x_0 \rvert = R_0$ $x_0 =$ Center, $R_0 =$ Radius	
Diskiness $\mathcal{O}_D$	**Manifold of Disks** $\mathcal{E}_{x_0,R_0}(x) = \frac{1}{\pi R_0^2}$ for $\lvert x - x_0 \rvert \leq R_0$ $x_0 =$ Center, $R_0 =$ Radius	
Ellipsiness $\mathcal{O}_E$	**Manifold of Ellipses** $\mathcal{E}_{x_0,a,b,\varphi}(x) = \frac{1}{\pi ab}$ for $x \in \text{Ellipse}_{x_0,a,b,\varphi}$ $x_0 =$ Center, $a, b =$ Semi-axes, $\varphi =$ Tilt	
(Ellipse Plus Point)iness	**Composite Shape** $\mathcal{O}_E \oplus \tau_1$ Fixed to same center x_0	
N-(Ellipse Plus Point)iness Plus Pileup	**Composite Shape** $N \times (\mathcal{O}_E \oplus \tau_1) \oplus \mathcal{I}$	

Some examples of shapes you can define!



The SHAPER Framework

SHAPER

Shape-**H**unting **A**lgorithm using
Parameterized **E**nergy
Reconstruction

- Framework for defining and building IRC-safe observables using parameterized objects
- Easy to programmatically define new observables by specifying parameterization, or by combining shapes
- Returns EMD distance and optimal shape parameters

$$\min_{\mathcal{E}'_\theta \in \mathcal{M}} \mathrm{EMD}(\mathcal{E}, \mathcal{E}'_\theta)$$

SHAPER

Sampling Energy Flows
Gradient Descent
Linear Programming
Simplex Projections

Loss and Shape $(\mathscr{O}, \theta)$

Estimating Wasserstein

We need a *differentiable, fast* approximation to the EMD for our minimizations

Sinkhorn Divergence: A strictly convex approximation to EMD! Kantorovich potential formalism::

Algorithm 3.4: Symmetric Sinkhorn algorithm, with debiasing

Parameters: Cost function $\mathbf{C} : (x_i, y_j) \in \mathcal{X} \times \mathcal{X} \mapsto \mathbf{C}(x_i, y_j) \in \mathbb{R}$,
Temperature $\varepsilon > 0$.
Input: Positive measures $\alpha = \sum_{i=1}^{\mathrm{N}} \alpha_i \delta_{x_i}$ and $\beta = \sum_{j=1}^{\mathrm{M}} \beta_j \delta_{y_j}$ with the same mass.

$f_i^{\beta\to\alpha},\ g_j^{\alpha\to\beta},\ f_i^{\alpha\leftrightarrow\alpha},\ g_j^{\beta\leftrightarrow\beta} \leftarrow \mathbf{0}_{\mathbb{R}^{\mathrm{N}}},\ \mathbf{0}_{\mathbb{R}^{\mathrm{M}}},\ \mathbf{0}_{\mathbb{R}^{\mathrm{N}}},\ \mathbf{0}_{\mathbb{R}^{\mathrm{M}}}$ ▷ Dual vectors.
repeat ▷ The four lines below are executed **simultaneously**.
$f_i^{\beta\to\alpha} \leftarrow \frac{1}{2} f_i^{\beta\to\alpha} + \frac{1}{2} \min_{y\sim\beta,\varepsilon} [\mathbf{C}(x_i, y) - g^{\alpha\to\beta}(y)]$, ▷ $\alpha \leftarrow \beta$
$g_j^{\alpha\to\beta} \leftarrow \frac{1}{2} g_j^{\alpha\to\beta} + \frac{1}{2} \min_{x\sim\alpha,\varepsilon} [\mathbf{C}(x, y_j) - f^{\beta\to\alpha}(x)]$, ▷ $\beta \leftarrow \alpha$
$f_i^{\alpha\leftrightarrow\alpha} \leftarrow \frac{1}{2} f_i^{\alpha\leftrightarrow\alpha} + \frac{1}{2} \min_{x\sim\alpha,\varepsilon} [\mathbf{C}(x_i, x) - f^{\alpha\leftrightarrow\alpha}(x)]$, ▷ $\alpha \leftarrow \alpha$
$g_j^{\beta\leftrightarrow\beta} \leftarrow \frac{1}{2} g_j^{\beta\leftrightarrow\beta} + \frac{1}{2} \min_{y\sim\beta,\varepsilon} [\mathbf{C}(y, y_j) - g^{\beta\leftrightarrow\beta}(y)]$. ▷ $\beta \leftarrow \beta$
until convergence up to a set tolerance. ▷ Monitor the updates on the potentials.
return $f_i^{\beta\to\alpha} - f_i^{\alpha\leftrightarrow\alpha},\ g_j^{\alpha\to\beta} - g_j^{\beta\leftrightarrow\beta}$ ▷ Debiased dual potentials $F(x_i)$ and $G(y_j)$.

Implemented using the KerOps+GeomLoss Python Package!

$$\mathcal{O}(\mathcal{E}) = \min_{\mathcal{E}_\theta \in \mathcal{M}} \left[S_\epsilon(\mathcal{E}, \mathcal{E}') \right] \text{ and } \theta(\mathcal{E}) = \operatorname*{argmin}_{\mathcal{E}_\theta \in \mathcal{M}} \left[S_\epsilon(\mathcal{E}, \mathcal{E}') \right], \qquad \text{where}$$

$$S_\epsilon(\mathcal{E}, \mathcal{E}') = \mathrm{OT}_\epsilon(\mathcal{E}, \mathcal{E}_\theta) - \frac{1}{2}\mathrm{OT}_\epsilon(\mathcal{E}, \mathcal{E}) - \frac{1}{2}\mathrm{OT}_\epsilon(\mathcal{E}_\theta, \mathcal{E}_\theta), \qquad \text{and}$$

$$\mathrm{OT}_\epsilon(\mathcal{E}, \mathcal{E}') = \max_{f,g:\mathcal{X}\to\mathbb{R}} \left[\sum_{i=1}^{M} E_i f(x_i) + \sum_{j=1}^{N} E'_j g(y_j) - \epsilon^\beta \log\left(\sum_{ij} E_i E'_j \left(e^{\frac{1}{\epsilon^\beta}\left(f(x_i) + g(y_j) - \frac{d(x_i, y_j)^\beta}{R^\beta}\right)} \right) \right) \right]$$

Can take gradients with respect to the entire event – very useful!

See Ouail Kitouni's talk later for more!

The SHAPER Algorithm

$$\min_{\mathcal{E}'_\theta \in \mathcal{M}} \mathrm{EMD}(\mathcal{E}, \mathcal{E}'_\theta)$$

SHAPER

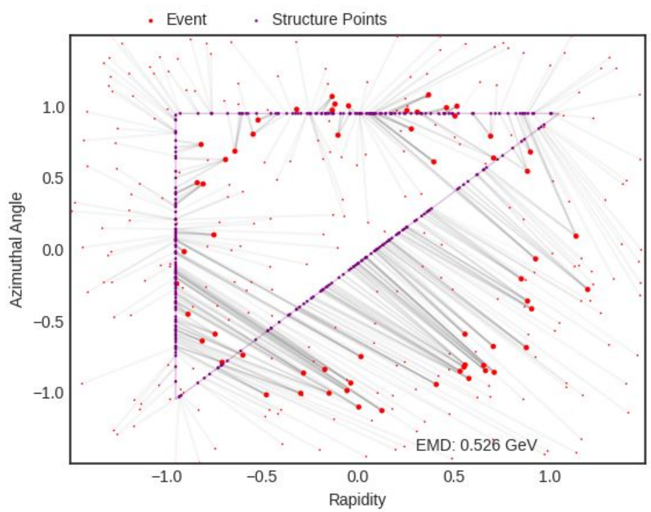
To estimate a shape observable …

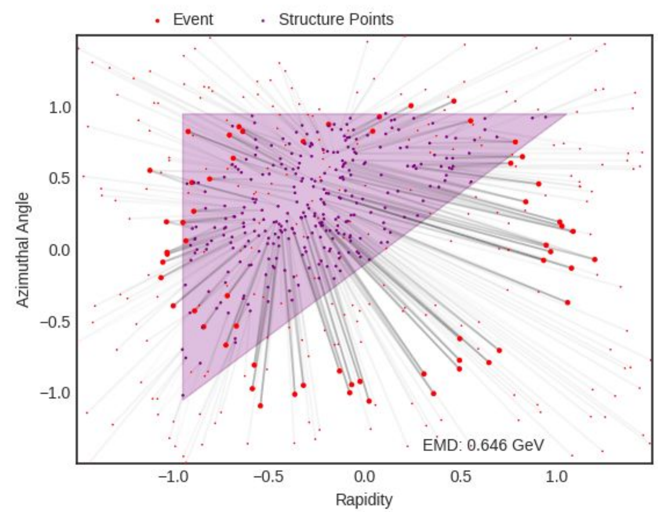
1. Define a parameterized distribution that can be sampled $\Leftrightarrow$ **Manifold** $\mathcal{M}$
2. Initialize the parameters $\boldsymbol{\theta}$ in an IRC-safe way (Usually k_T)
3. Use the Sinkhorn Algorithm to estimate the EMD between your **event** $\boldsymbol{\mathcal{E}}$ and **shape** $\boldsymbol{\mathcal{E}_\theta}$
4. Calculate the gradients of the EMD using the Kantorovich potentials
5. Use the gradients to update $\boldsymbol{\theta}$ (using ADAM or another optimizer)
6. Repeat 3-5 until convergence
7. Return the loss $\mathcal{O}_\mathcal{M}$ and the optimal parameters $\theta_\mathcal{M}$

Loss and Shape ($\mathcal{O}$, θ)

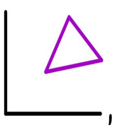
Fun Animations

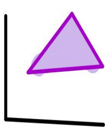
How **triangle-y** is an event? (Boundary or filled in)?





Red: Event
Purple: Shape ε_θ
Grey: Matrix f_{ij} connecting *particles* and *triangle*

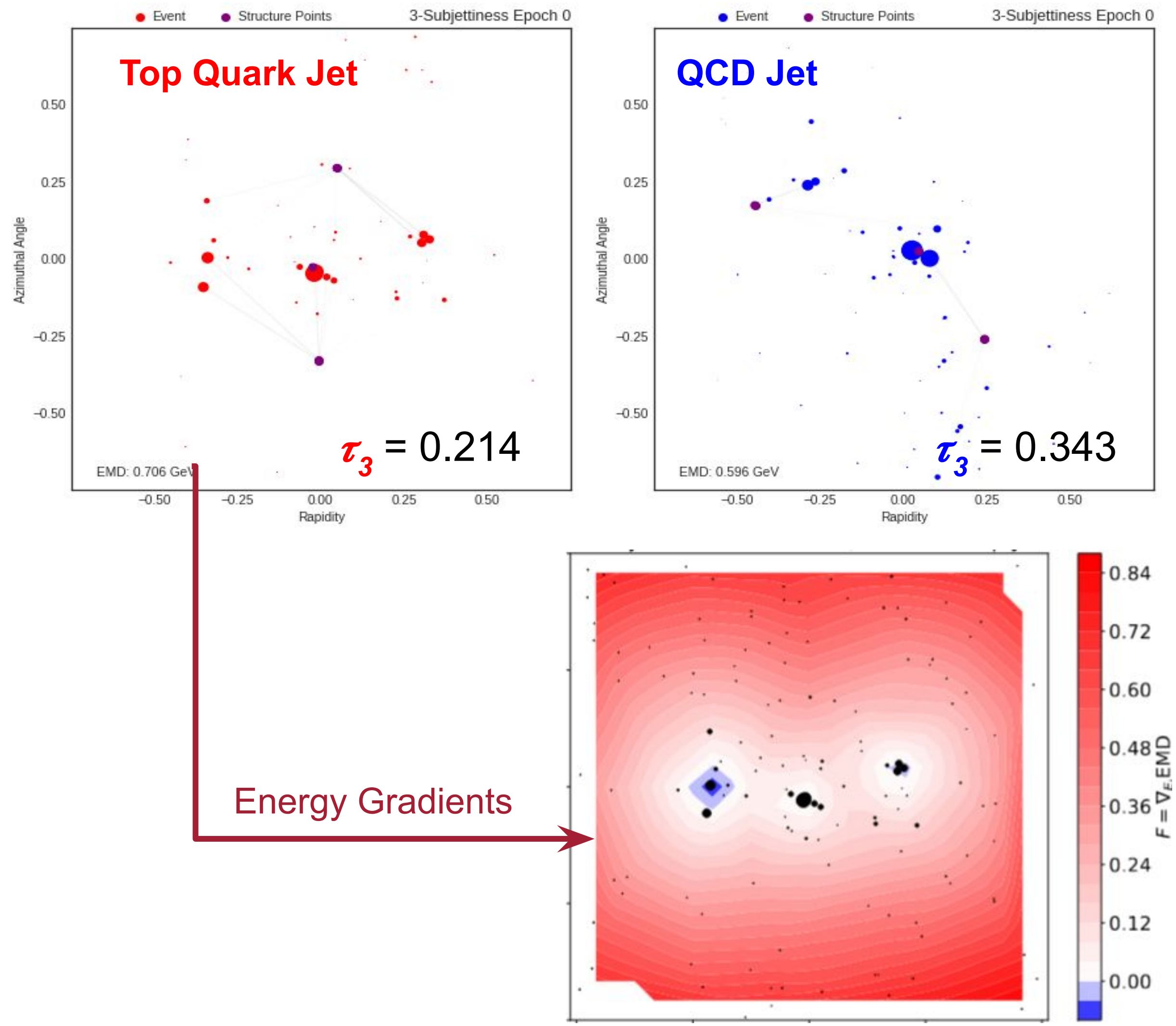
Left: ε_θ =  , EMD = 0.245

Right: ε_θ =  EMD = 0.279

N-Subjettiness

Easy to compute your favorite classic jet observables!

We can even get *gradients* of our observables with respect to the events!



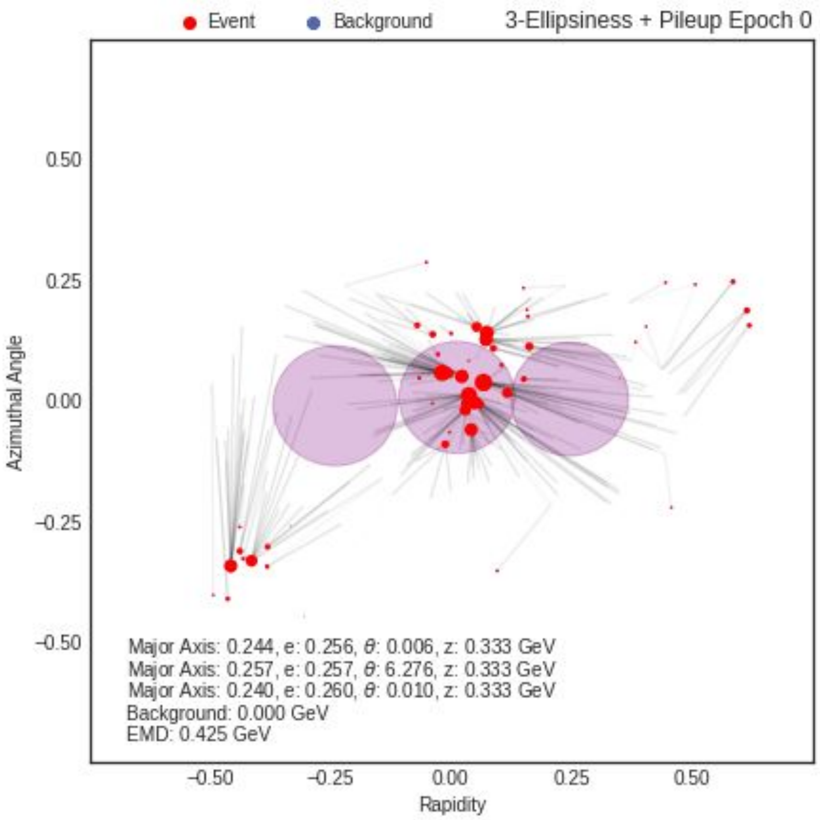
New IRC-Safe Observables

The **SHAPER** framework makes it easy to invent new jet observables!

e.g. ***N*-Ellipsiness+Pileup** as a jet algorithm.

- Learn jet centers
- Dynamic jet radii (no *R* hyperparameter)
- Dynamic eccentricities and angles
- Dynamic jet energies
- Learned parameters for discrimination

Can design custom specialized jet algorithms to learn jet substructure!



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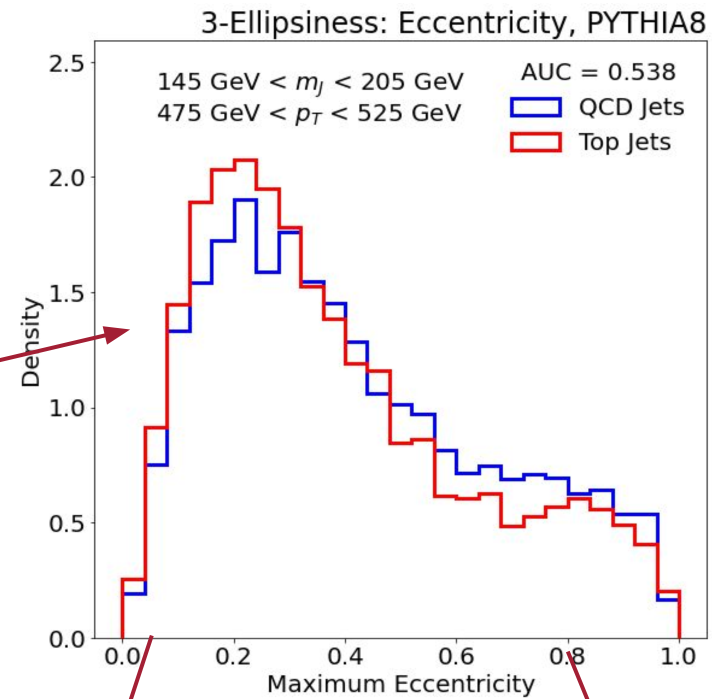
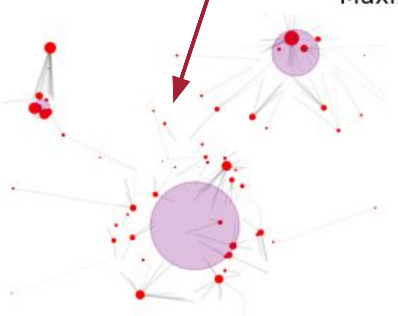
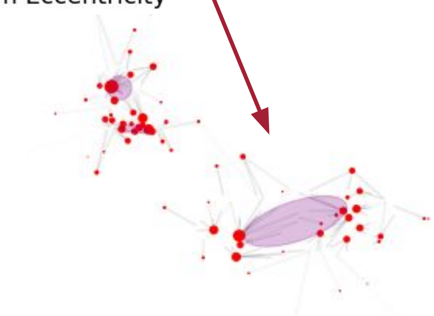




Low Max Eccentricity (.001)



High Max Eccentricity (.972)

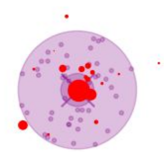
Grooming with Shapes

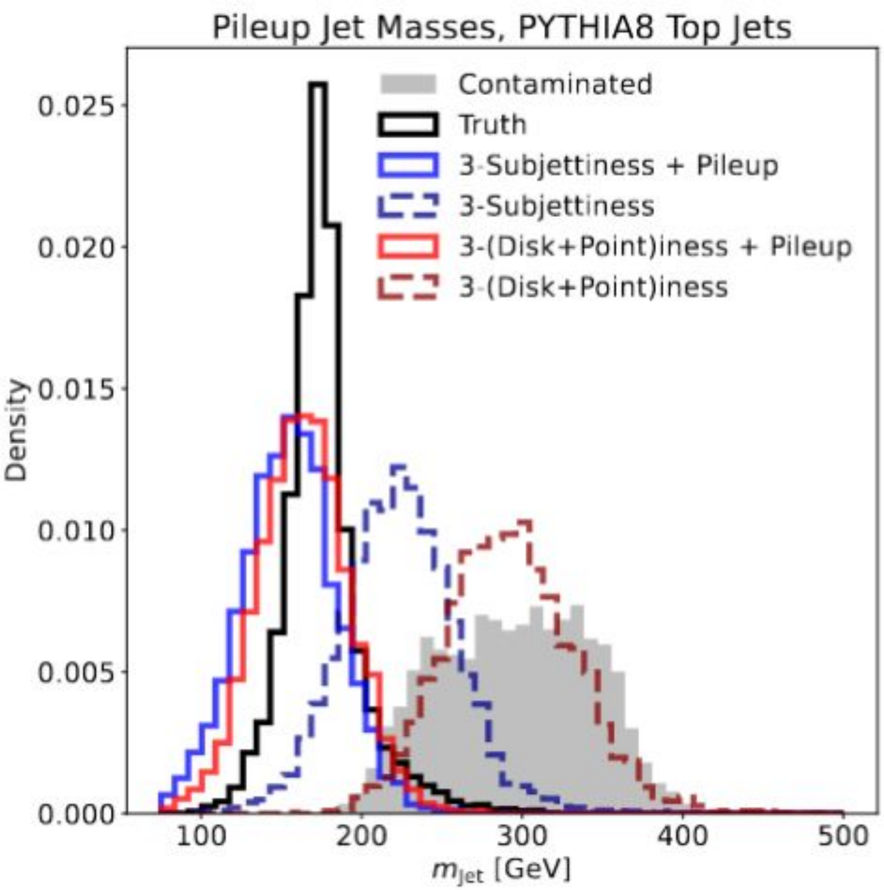
Use shapes to approximate events and extract masses - model **pileup** with a uniform background with floating weight!

Contaminate top jets with 5-30% extra energy spread uniformly in an 0.8x0.8 plane

Consider 4 shapes:

- 3-Subjettiness
- 3-Subjettiness + Uniform
- 3-(Disk+Point)iness
- 3-(Disk+Point)iness + Uniform





Probing **collinear** (δ-function) and **soft** (shape) structure!

Outlook

- The Wasserstein metric is ***the*** natural language for jet observables, based on IRC-safety and geometry!
- **SHAPER** is a machine learning framework for calculating generalized observables programmatically!
- Playground for defining and building custom observables and jet algorithms!

$$\mathcal{O}_{\mathcal{M}}(\mathcal{E}) = \min_{\mathcal{E}'_\theta \in \mathcal{M}} \mathrm{EMD}(\mathcal{E}, \mathcal{E}'_\theta)$$

$$\theta = \operatorname*{argmin}_{\mathcal{E}'_\theta \in \mathcal{M}} \mathrm{EMD}(\mathcal{E}, \mathcal{E}'_\theta)$$

Outlook

- The Wasserstein metric is ***the*** natural language for jet observables, based on IRC-safety and geometry!
- **SHAPER** is a machine learning framework for calculating generalized observables programmatically!
- Playground for defining and building custom observables and jet algorithms!

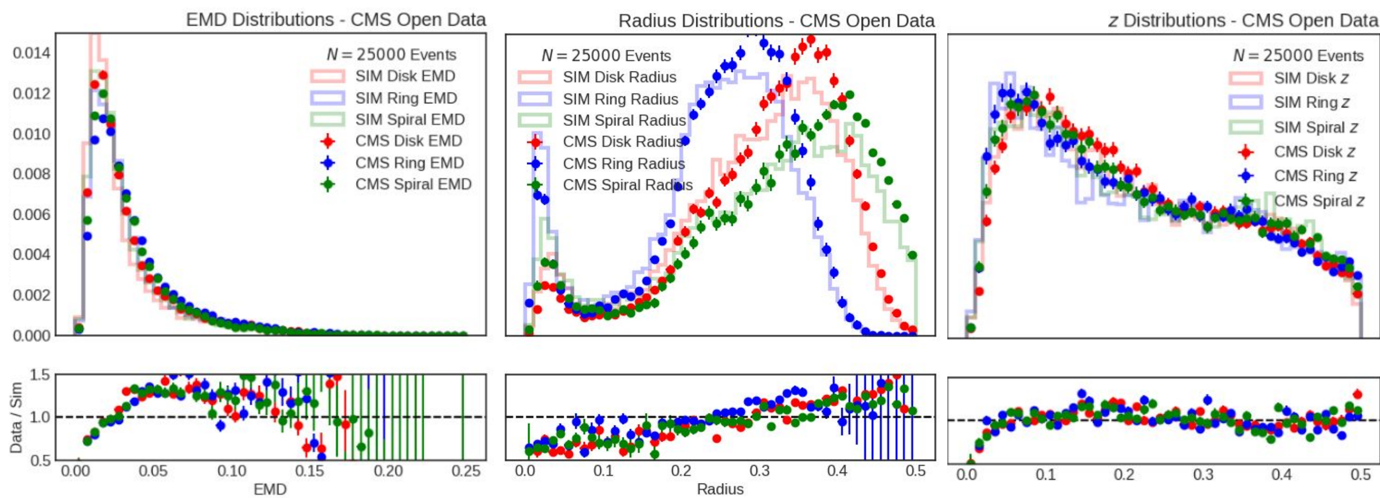
$$\boxed{\begin{aligned} \mathcal{O}_{\mathcal{M}}(\mathcal{E}) &= \min_{\mathcal{E}'_\theta \in \mathcal{M}} \text{EMD}(\mathcal{E}, \mathcal{E}'_\theta) \\ \theta &= \underset{\mathcal{E}'_\theta \in \mathcal{M}}{\text{argmin}}\, \text{EMD}(\mathcal{E}, \mathcal{E}'_\theta) \end{aligned}}$$

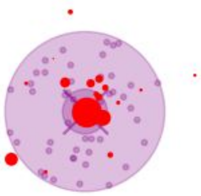
Using **SHAPER**, you ***CAN*** hear the shape of a jet!

More questions? Email me at rikab@mit.edu
Appearing on arXiv soon! (Plus code!)

Appendices

Observables on CMS OpenData





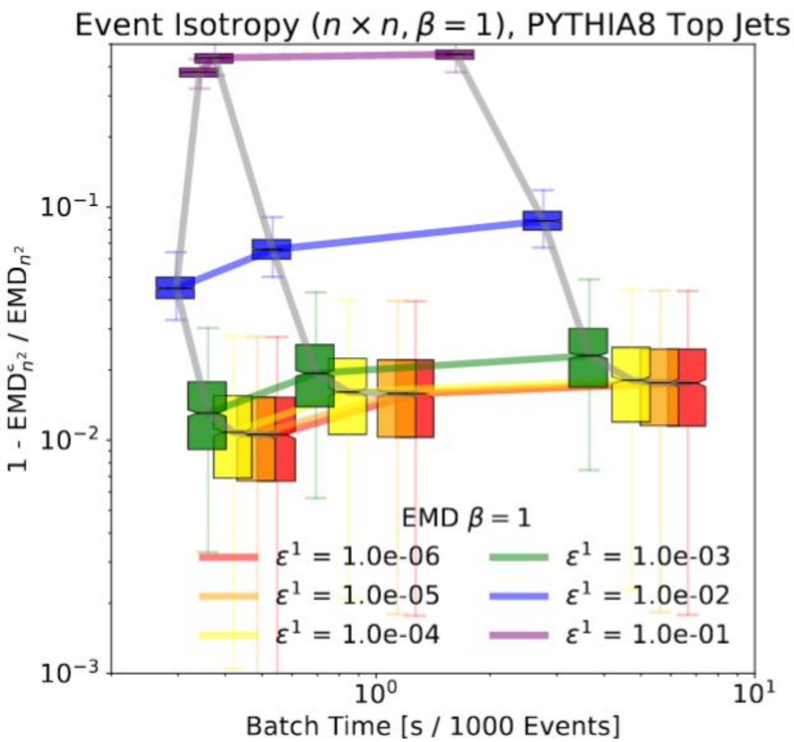
Disk + δ-function

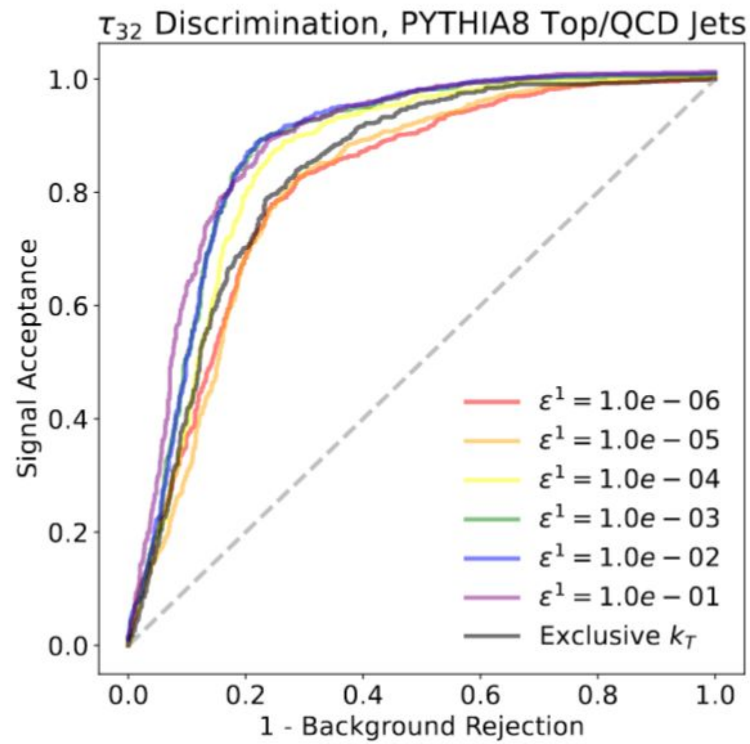
Ring + δ-function

Spiral + δ-function

Probing **collinear** (δ-function) and **soft** (shape) structure!

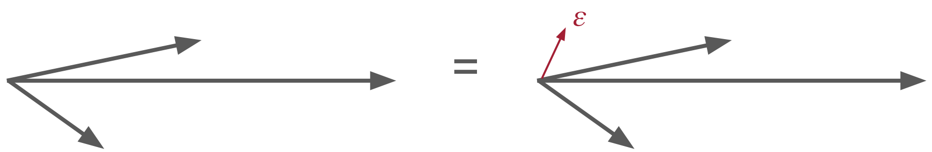
Performance Benchmarks



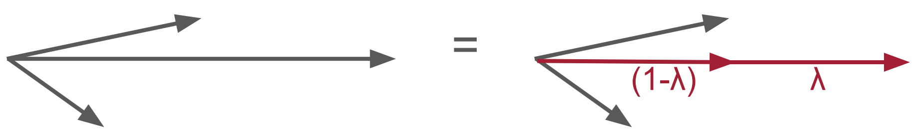


IRC Safety

Infrared Safety: An observable is unchanged under a soft emission



Collinear Safety: An observable is unchanged under a collinear splitting



[P. Tankala, A. Tasissa, J. M. Murphy, D. Ba, 2012.02134;
see also F.Dornaika, L.Weng, DOI: 0.1007/s13042-019-01035-z;
see also S. Roweis and L.Saul, DOI: 10.1126/science.290.5500.2323]

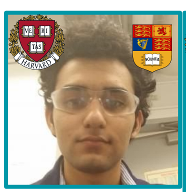
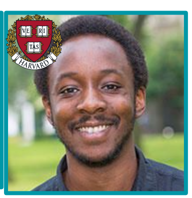
Building SHAPER

Key Component: The Loss function! Step 1: Manifold Learning

$$\mathcal{L}_R(\mathcal{E},\mathcal{E}') = \min_{\pi_{ij}\geqslant 0}\left[\sum_{i=1}^{M}\sum_{j=1}^{M'}\pi_{ij}\frac{|x_i - x_j'|}{R}\right],$$

$$\text{where } \sum_{i=1}^{M}\pi_{ij} = 1$$

Dogra **Ba**

K-Deep Simplices, Dictionary Learning, & Manifold Learning

[P. Komiske, E. Metodiev, J. Thaler, 1902.02346;
see also T. Cai, J. Cheng, K. Craig, N. Craig, 2111.03670;
see also C. Zhang, Y. Cai, G. Lin, C. Shen, 2003.06777;
see also L. Hou, C. Yu, D. Samaras, 1611.05916;
see also M. Arjovsky, S. Chintala, L. Bottou, 1701.07875]

Building SHAPER

Key Component: The Loss function! Step 2: Physical Principles

$$\mathcal{L}_R(\mathcal{E},\mathcal{E}') = \min_{\pi_{ij}\geqslant 0}\left[\sum_{i=1}^{M}\sum_{j=1}^{M'}\pi_{ij}\frac{|x_i - x'_j|}{R}\right] + \left|\sum_{i=1}^{M} z_i - \sum_{j=1}^{M'} z'_j\right|,$$

$$\text{where} \sum_{i=1}^{M}\pi_{ij} \leqslant z'_j, \quad \sum_{j=1}^{M'}\pi_{ij} \leqslant z_i, \quad \sum_{i,j}^{M,M'}\pi_{ij} = \min\left(\sum_{i=1}^{M} z_i, \sum_{j=1}^{M'} z'_j\right)$$

Dogra Ba

K-Deep Simplices,
Dictionary Learning, &
Manifold Learning

IRC Safety,
Unclustered Radiation, &
Wasserstein Geometry

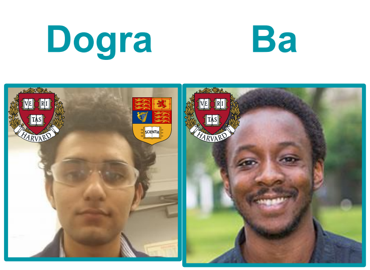
Gambhir Thaler


Building SHAPER

Key Component: The Loss function! Step 3: Synthesis

$$\mathcal{L}_R(\mathcal{E},\mathcal{E}') = \min_{\pi_{ij}\geq 0}\left[\sum_{i=1}^{M}\sum_{j=1}^{M'}\pi_{ij}\frac{|x_i - x'_j|}{R}\right] + \left|\sum_{i=1}^{M} z_i - \sum_{j=1}^{M'} z'_j\right|,$$

$$\text{where } \sum_{i=1}^{M}\pi_{ij} \leqslant z'_j, \quad \sum_{j=1}^{M'}\pi_{ij} \leqslant z_i, \quad \sum_{i,j}^{M,M'}\pi_{ij} = \min\left(\sum_{i=1}^{M} z_i, \sum_{j=1}^{M'} z'_j\right)$$



K-Deep Simplices, Dictionary Learning, & Manifold Learning

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IRC Safety, Unclustered Radiation, & Wasserstein Geometry