

SYSU-PKU Collider Physics Forum
For Young Scientists

3/15/2023

Which Metric on the Space of Collider Events?

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Based on [2008.08604](#), [2102.08807](#), [2111.03670](#), and work in progress.

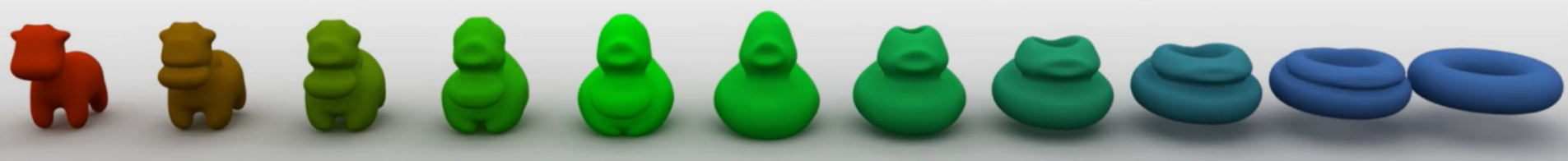
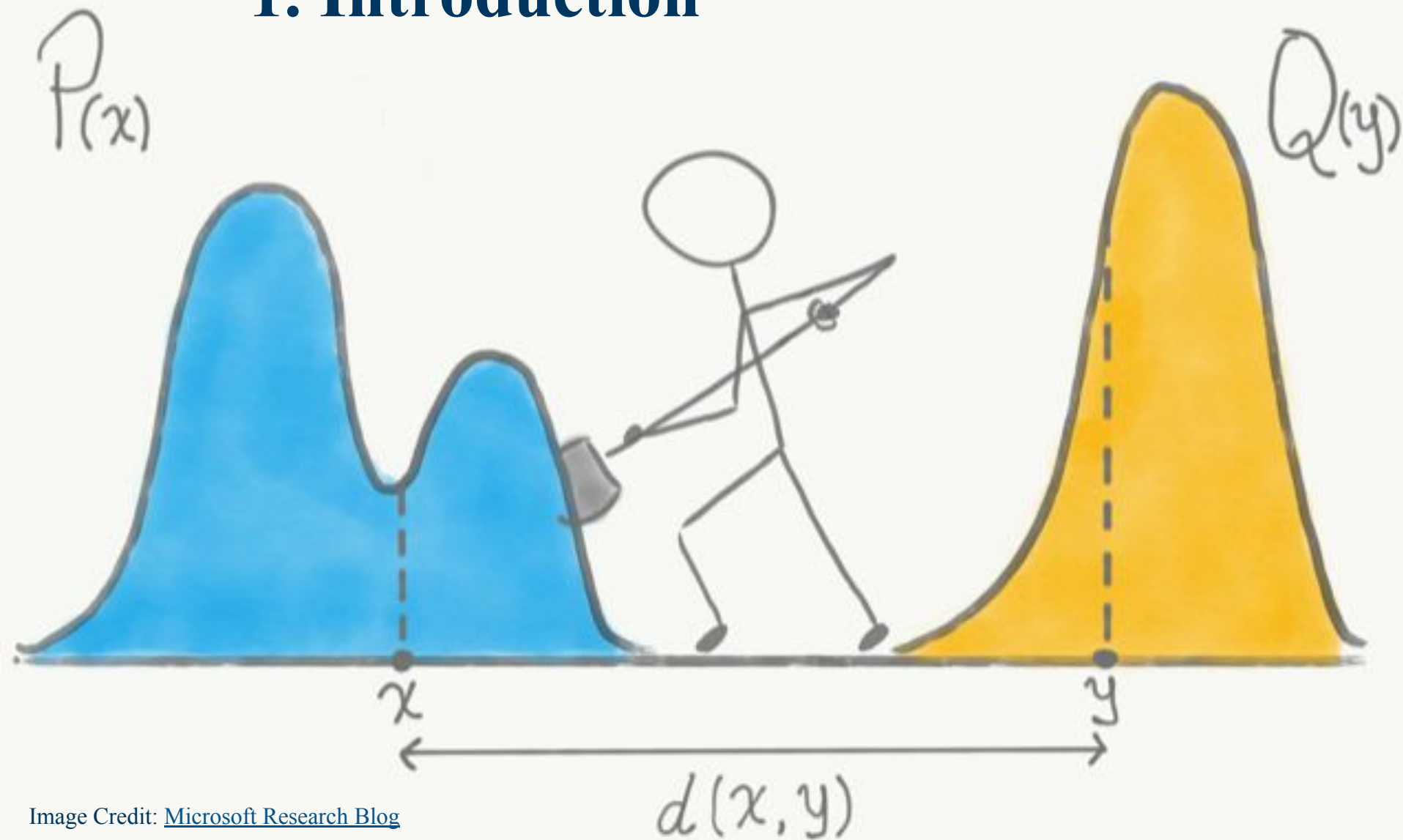


Image Credit: Solomon, et al. SIGGRAPH 2015

Contents

- ❖ **Introduction** — *What is it & Why should we care?*
- ❖ **Theory of Optimal transport (OT)** — *Small doses of not-too-scary math...*
History; Balanced OT; Unbalanced OT; Linearized OT.
- ❖ **Optimal Transport for Collider Physics** — *Successful debut!*
Physics Background; A Unified Framework; Jet Tagging.
- ❖ **Summary & Outlook** — *Let's have more fun.* 🤪

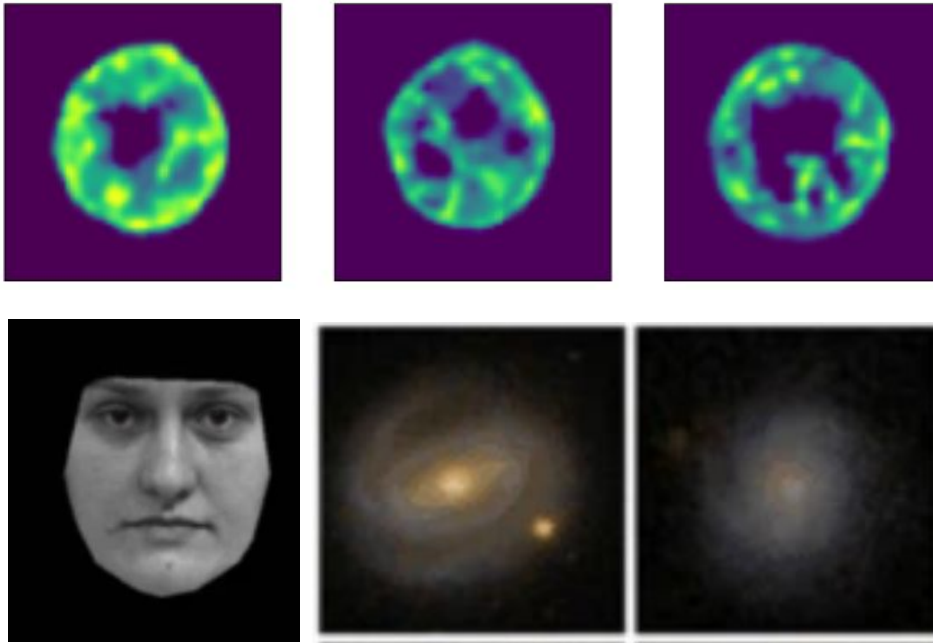
1. Introduction



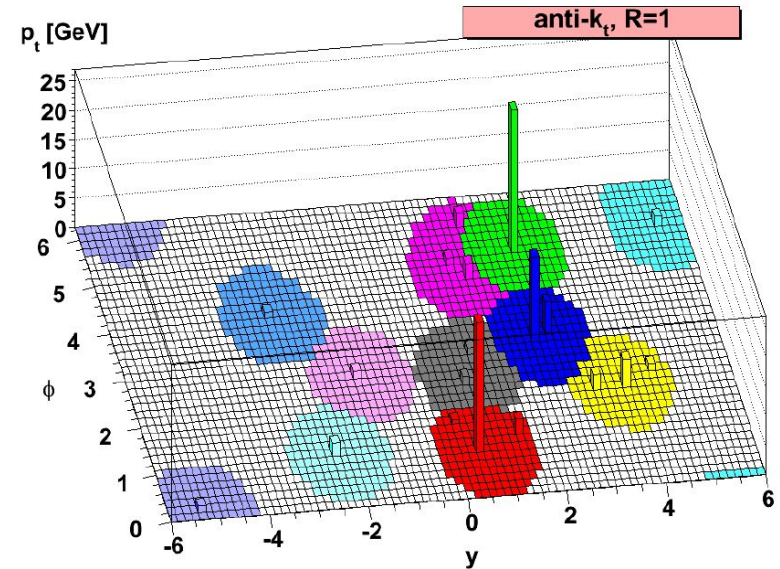
Typical Scenario

Given two distributions, discrete or continuous...

Example images of liver cells, [Fig 5.4](#).



Example facial images and galaxy images, [Fig 6](#).



Example jet image, Fig 2.2 in *Hadronic Jets*.

Q1: How to define a distance between them?

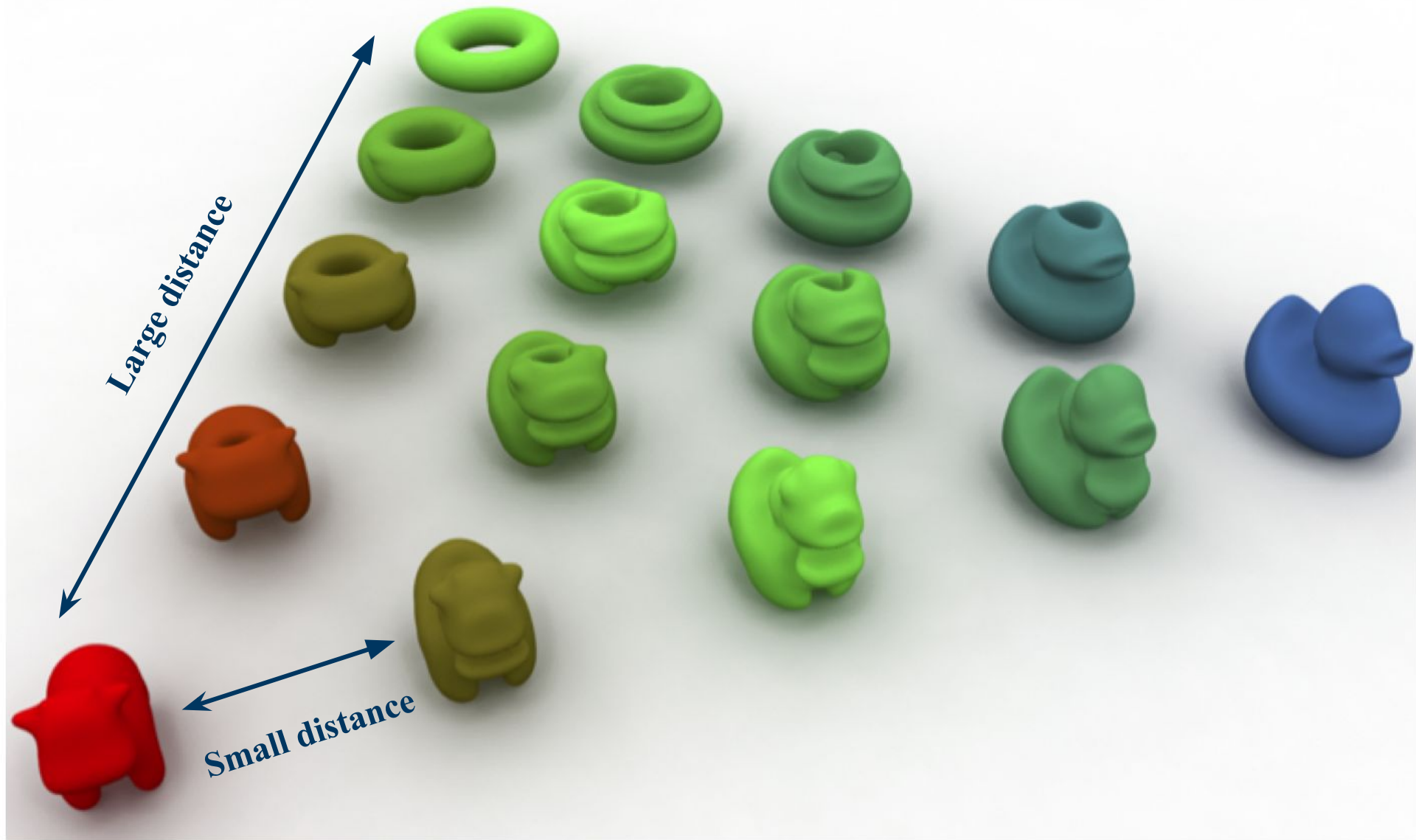


Q2: How to rearrange one to look like the other?

Our Physics Goal here is...

To find a way to quantify the distance between collider events/jets.

How to transform a cow into a duck and into a donut...



Credit: Fig 4 in [paper](#).

Why is the normal Euclidean distance not enough?

Consider two particles with unit energy.

Image-based approach

Bin on N-bin grid, represent energy distribution by vectors in \mathbf{R}^N , compute Euclidean distance between vectors

0	0	0	0	0	0	0
0	1	0	0	0	0	0
0			...			
0		...		1		
0						
0						
0			...			
0						

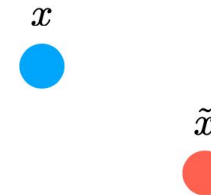
$$\mathbf{v} = [0, \dots, 1, 0, \dots, 0, 0, \dots, 0]$$

$$\mathbf{v}' = [0, \dots, 0, 0, \dots, 1, 0, \dots, 0]$$

$$d_{\ell^2(\mathbb{R}^N)}(\mathcal{E}, \tilde{\mathcal{E}}) = \left(\sum_{i=1}^N |v_i - \tilde{v}_i|^2 \right)^{1/2} = \sqrt{2}$$

regardless of positions

OT-based approach



$$W_p(\mathcal{E}, \tilde{\mathcal{E}}) = \|x - \tilde{x}\|$$

Invaluable if the relative distribution of pixels carries meaning

OT preserves the underlying geometry of the ground space!

$$\beta = 0$$



Monge

Kantorovich

2. Theory of Optimal Transport

Image Credit: N. Papadakis, et al. [10.1137/130920058]

$$\beta = 1$$



$t = 0$

$t = 1/6$

$t = 1/3$

$t = 1/2$

$t = 2/3$

$t = 5/6$

$t = 1$

2.1 A Brief History of Optimal Transport

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Gaspard Monge
1781



M É M O I R E
S U R L A
T H É O R I E D E S D É B L A I S
E T D E S R E M B L A I S.

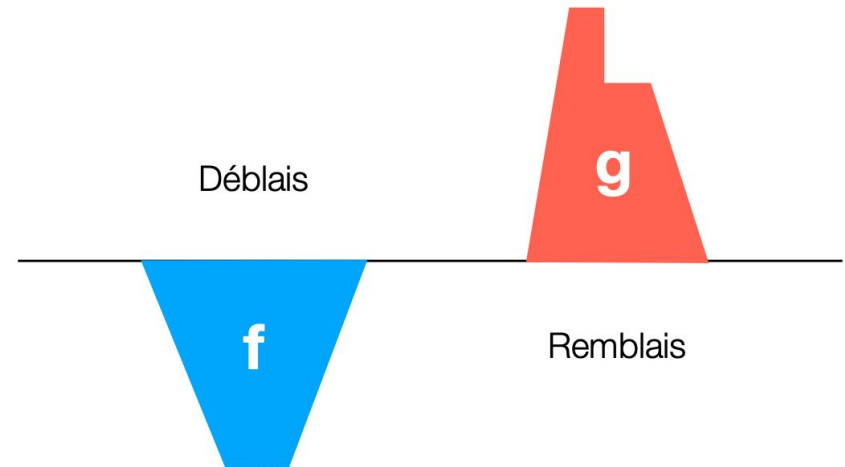
Par M. M O N G E.

LORSQU'ON doit transporter des terres d'un lieu dans un autre, on a coutume de donner le nom de *Déblai* au volume des terres que l'on doit transporter, & le nom de *Remblai* à l'espace qu'elles doivent occuper après le transport.

Le prix du transport d'une molécule étant, toutes choses d'ailleurs égales, proportionnel à son poids & à l'espace qu'on lui fait parcourir, & par conséquent le prix du transport total devant être proportionnel à la somme des produits des molécules multipliées chacune par l'espace parcouru, il s'en suit que le déblai & le remblai étant donnés de figure & de position, il n'est pas indifférent que telle molécule du déblai soit transportée dans tel ou tel autre endroit du remblai, mais qu'il y a une certaine distribution à faire des molécules du premier dans le second, d'après laquelle la somme de ces produits sera la moindre possible, & le prix du transport total fera un *minimum*.

Fundamental problem of **optimal transport**:

How to rearrange **f** to look like **g**
with the **least amount of “work”**?

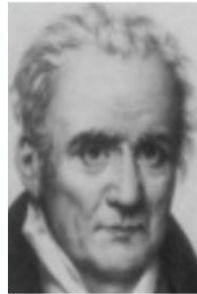


In other words, how can we optimally transport *f* to *g*?

Sounds pretty simple?
Took over 100 years to formulate the problem mathematically!

OT in the Modern Time

1781: Gaspard Monge,
*Mémoire sur la théorie des deblais et
 des remblais*
(On cuttings and embankments)



1942: Leonid Kantorovich,
On the translocation of masses



1999: Felix Otto,
*The geometry of dissipative evolution
 equations: the porous medium
 equation*



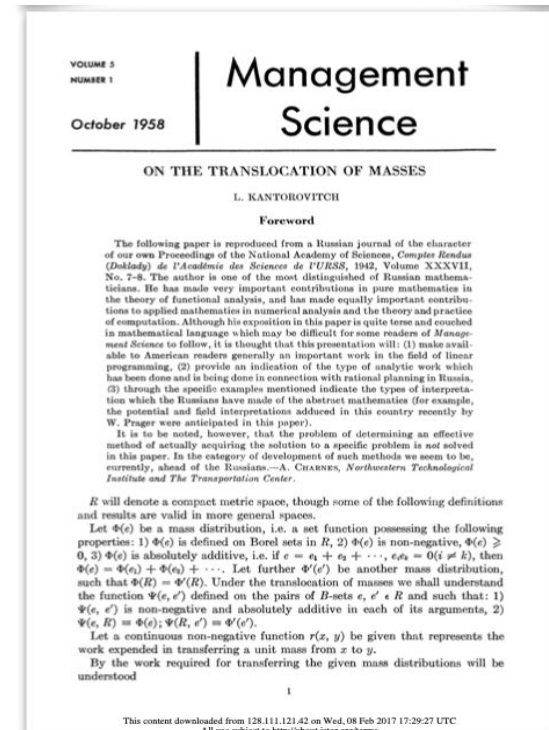
2000: Felix Otto, Cedric Villani,
*Generalization of an inequality by
 Talagrand, as a consequence of the
 logarithmic Sobolev inequality*



2010: Cedric Villani wins Fields medal



2018: Alessio Figalli wins Fields medal



OT gives a family
 of well-defined
 metrics between
 distributions.

2.2 Balanced Optimal Transport

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Let's first look at the Earth Mover's Distance, one simple example of OT distance.

$$EMD(E, E') = \min_{f_{ij} \in \Gamma_{E, E'}} \sum_{ij} f_{ij} \theta_{ij}$$

θ_{ij} : ground metric between particles i and j

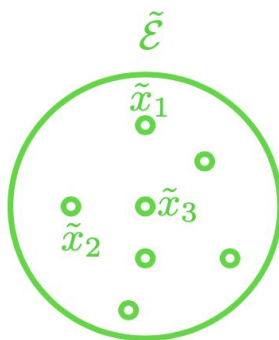
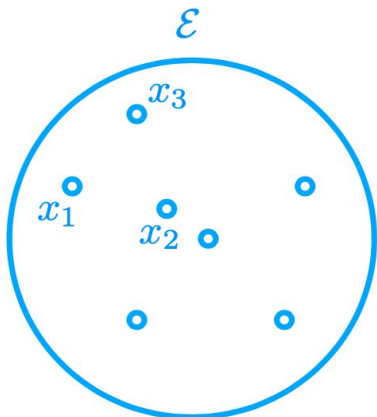
$$\Gamma_{E, E'} = \left\{ f_{ij} : f_{ij} \geq 0, \sum_j f_{ij} = E_i, \sum_i f_{ij} = E'_j \right\}$$

f_{ij} : the amount of mass moved from particle i to particle j .

Consider two "events" $\mathcal{E}, \tilde{\mathcal{E}}$

Collections of particles at locations x_i, \tilde{x}_j in a rectangular domain with masses $E_i, \tilde{E}_j \geq 0$

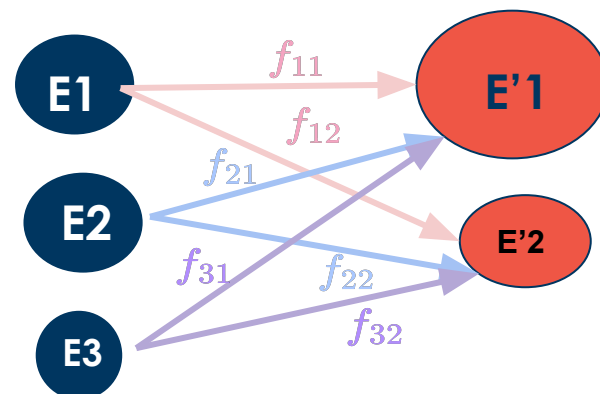
Assume same total mass $\sum_i E_i = \sum_j \tilde{E}_j$



Example:

$$E_1 + E_2 + E_3 = E'_1 + E'_2$$

$$\begin{aligned} f_{11} + f_{12} &= E_1 & f_{11} + f_{21} + f_{31} &= E'_1 \\ f_{21} + f_{22} &= E_2 & f_{12} + f_{22} + f_{32} &= E'_2 \\ f_{31} + f_{32} &= E_3 \end{aligned}$$



Generalize to the p -Wasserstein distances

$$W_p(\mathcal{E}, \tilde{\mathcal{E}}) = \min_{g_{ij} \in \Gamma(\mathcal{E}, \tilde{\mathcal{E}})} \left(\sum_{ij} g_{ij} \|x_i - \tilde{x}_j\|^p \right)^{1/p}$$

$$\Gamma(\mathcal{E}, \tilde{\mathcal{E}}) = \left\{ g_{ij} : g_{ij} \geq 0, \sum_j g_{ij} = E_i, \sum_i g_{ij} = \tilde{E}_j \right\}$$

p=1: Earth Mover's Distance (EMD)

p=2: Monge-Kantorovich Distance /
2-Wasserstein (W_2) Distance

We focus on the W_2 Distance.

Answer: W_2 has a (weak)
Riemannian structure \Rightarrow
can linearize!

Two Equivalent Formulations of W_2 Distance:

**Kantorovich formulation
(static):**

$$W_2(\mathcal{E}, \tilde{\mathcal{E}}) = \min_{r_{ij} \in \Gamma(\mathcal{E}, \tilde{\mathcal{E}})} \left(\sum_{ij} r_{ij} \|x_i - \tilde{x}_j\|^2 \right)^{1/2}$$

Benamou-Brenier formulation (dynamic):

$$\partial_t \rho + \operatorname{div} \omega = 0$$

Continuity Equation

\Leftrightarrow **Charge conservation**

ρ : charge density

ω : current density

No source/sink

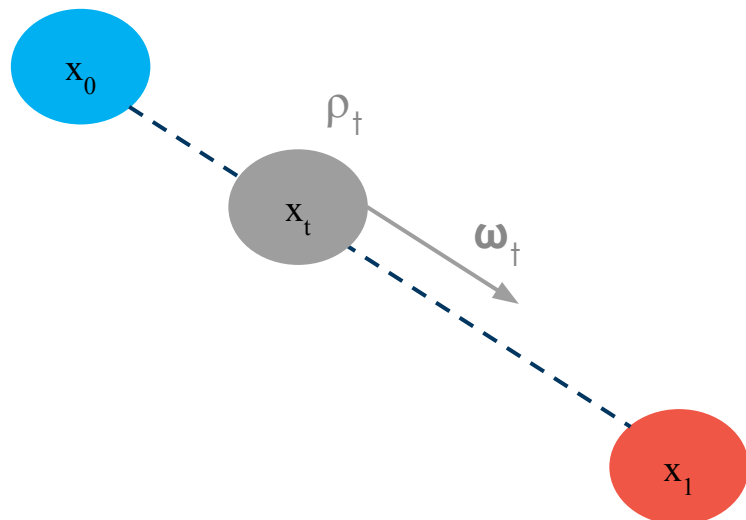
$$J_W(\rho, \omega) := \begin{cases} \int_{[0,1] \times \Omega} \left\| \frac{d\omega}{d\rho} \right\|^2 d\rho & \text{if } \rho \geq 0, \omega \ll \rho \\ +\infty & \text{else.} \end{cases}$$

Cost Functional

$$W_2(\mu_0, \mu_1)^2 := \inf \{ J_W(\rho, \omega) \mid (\rho, \omega) \in \mathcal{CE}(\mu_0, \mu_1) \}$$

Minimizer

Example: Two dirac masses at position x_0 and x_1 .



$$W_2(\delta_{x_0}, \delta_{x_1})^2 = \|x_0 - x_1\|^2.$$

$$\rho_t = \delta_{X(x_0, x_1; t)}$$

$$\omega_t = \delta_{X(x_0, x_1; t)} \cdot \partial_t X(x_0, x_1; t).$$

Let $X(x_0, x_1; t) = (1 - t)x_0 + tx_1$.

A Dirac-to-Dirac geodesic in W_2 consists of a single Dirac traveling along the straight line between them at constant speed.

2.3 Unbalanced Optimal Transport

Balanced Transport: Mass can only be transported, not created or destroyed. Therefore, the total mass of the two distributions must be exactly equal.



Unbalanced Transport: Mass can be transported, created and destroyed. The total mass of the two distributions can be different (but also can be the same too).



Before introducing unbalanced OT, we were doing ... for EMD.

Same as Standard EMD

$$\text{EMD}_R(\mathcal{E}, \mathcal{E}') := \min_{f_{ij} \in \tilde{\Gamma}_{\leq(\mathcal{E}, \mathcal{E}')}} \left[\frac{1}{R} \sum_{ij} f_{ij} \theta_{ij} + \left| \sum_i E_i - \sum_j E'_j \right| \right] \quad (1.2)$$

Extra piece to account for the unequal total mass

$$\tilde{\Gamma}_{\leq(\mathcal{E}, \mathcal{E}')} := \left\{ f_{ij} : f_{ij} \geq 0, \sum_j f_{ij} \leq E_i, \sum_i f_{ij} \leq E'_j, \sum_{ij} f_{ij} = \min \left(\sum_i E_i, \sum_j E'_j \right) \right\}. \quad (1.3)$$

Different conditions for the unbalanced case

Ad-hoc!

Now we can incorporate the total mass difference in a natural way by allowing mass to be created and destroyed in addition to being transported.

Kantorovich type formulation (static):

$$c(x_0, x_1) := \begin{cases} -2 \log(\cos(\|x_0 - x_1\|)) & \text{if } \|x_0 - x_1\| < \frac{\pi}{2} \\ +\infty & \text{else.} \end{cases}$$

$$J_{\text{SM}}(\pi) := \int_{\Omega^2} c \, d\pi + \sum_{i \in \{0,1\}} \text{KL}(\mathbf{P}_{i\#}\pi | \mu_i).$$

$$\text{HK}(\mu_0, \mu_1)^2 = \inf \{ J_{\text{SM}}(\pi) \mid \pi \in \mathcal{M}_+(\Omega^2) \}$$

Bonus: HK also enjoys a (weak) Riemannian structure => can linearize!

Benamou-Brenier-type formulation (dynamic):

$$\partial_t \rho + \text{div } \omega = \boxed{\zeta}$$

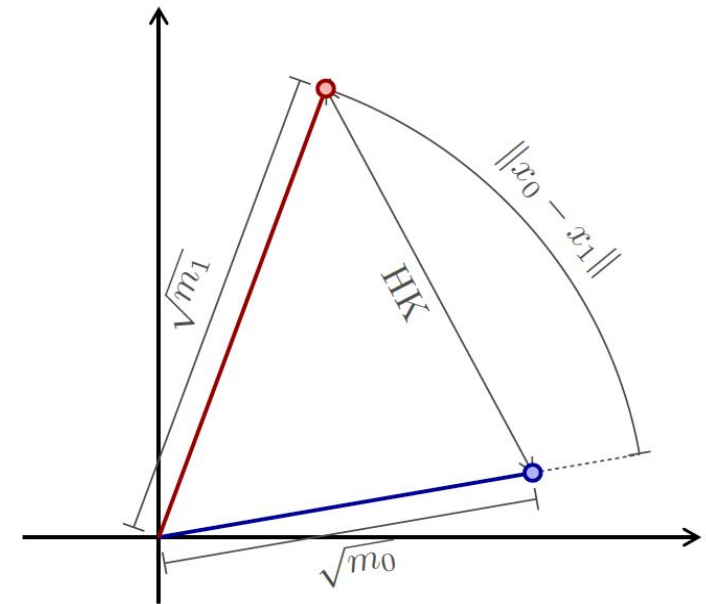
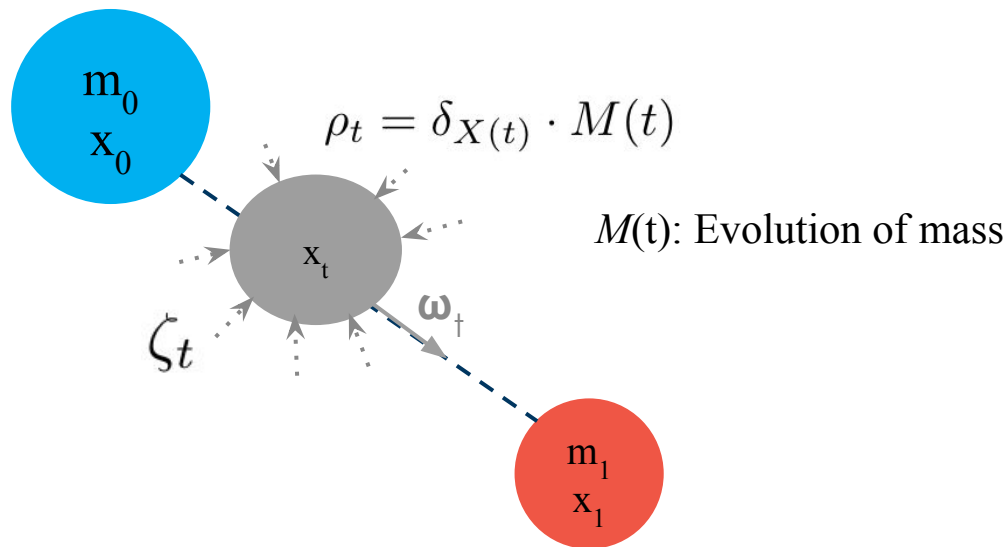
Continuity Equation with Source

$$J_{\text{HK}}(\rho, \omega, \zeta) := \begin{cases} \int_{[0,1] \times \Omega} \left(\left\| \frac{d\omega}{d\rho} \right\|^2 + \boxed{\frac{1}{4} \left(\frac{d\zeta}{d\rho} \right)^2} \right) d\rho & \text{if } \rho \geq 0, \omega, \zeta \ll \rho, \\ +\infty & \text{else.} \end{cases}$$

Additional term takes care of mass creation/destruction

$$\text{HK}(\mu_0, \mu_1)^2 := \inf \{ J_{\text{HK}}(\rho, \omega, \zeta) \mid (\rho, \omega, \zeta) \in \mathcal{CES}(\mu_0, \mu_1) \}$$

Example: Again two dirac masses at position x_0 and x_1 with mass m_0 and m_1 , respectively.



$$\text{HK}(\delta_{x_0} \cdot m_0, \delta_{x_1} \cdot m_1)^2 = m_0 + m_1 - 2\sqrt{m_0 m_1} \overline{\cos}(\|x_0 - x_1\|)$$

where $\overline{\cos}(s) = \cos(\min\{s, \frac{\pi}{2}\})$.

For $\|x_0 - x_1\| \leq \frac{\pi}{2}$

$$\text{HK}(\delta_{x_0} \cdot m_0, \delta_{x_1} \cdot m_1) = \|\sqrt{m_0} - \sqrt{m_1} \exp(i\|x_0 - x_1\|)\|$$

When $\|x_0 - x_1\| > \frac{\pi}{2}$

Mass at x_0 is destroyed, mass at x_1 created. No transport!

HK Distance has an intrinsic length scale κ !

$$J_{\text{HK},\kappa}(\rho, \omega, \zeta) := \begin{cases} \int_{[0,1] \times \Omega} \left(\left\| \frac{d\omega}{d\rho} \right\|^2 + \frac{\kappa^2}{4} \left(\frac{d\zeta}{d\rho} \right)^2 \right) d\rho & \text{if } \rho \geq 0, \omega, \zeta \ll \rho, \\ +\infty & \text{else.} \end{cases}$$

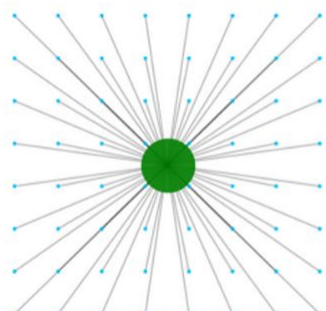
Intrinsic length scale $\kappa > 0$ controls the relative importance of the transport part of the cost and the creation/destruction part.

$$\text{HK}_{\kappa}(\mu_0, \mu_1) \rightarrow W_2(\mu_0, \mu_1)$$

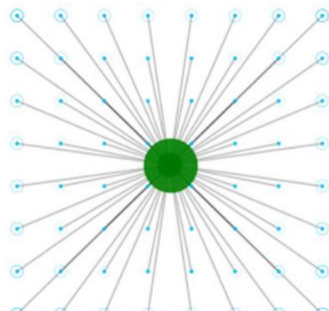
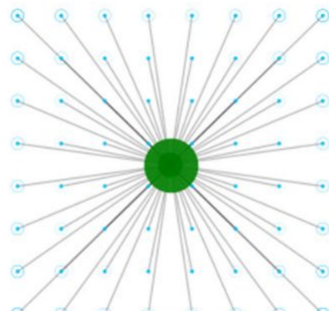
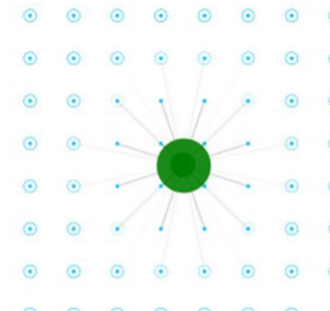
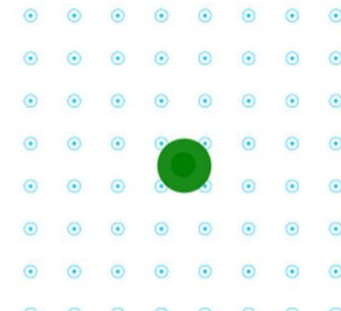
$$\text{HK}_{\kappa}(\mu_0, \mu_1)/\kappa \rightarrow \text{Hellinger distance} \quad (\sim \text{Euclidean})$$

 ∞

0

 κ 

W2: 1.515 GeV

HK($\kappa=100$): 1.515 GeVHK($\kappa=10$): 1.512 GeVHK($\kappa=1$): 1.089 GeVHK($\kappa=0.1$): 0.141 GeV

HK Distance: Normalized vs. Unnormalized Distributions

$$\text{HK}(m_0 \cdot \mu_0, m_1 \cdot \mu_1)^2 = \sqrt{m_0 \cdot m_1} \cdot \text{HK}(\mu_0, \mu_1)^2 + (\sqrt{m_0} - \sqrt{m_1})^2$$

Unnormalized Distributions

Transport plan: $\sqrt{(m_0 \ m_1)}\pi$

Normalized Distributions

Transport plan: π

Unbalanced HK on **unnormalized** measures can be obtained from HK from **normalized** measures.

Local mass discrepancies more **important than** the differences in the **total** mass of the measures.

In analysis, **first normalize** all samples before computing HK, then recover the total mass difference either via the above equation, or keeping the total masses to be separate features.

Practical Limitations of OT Distances:

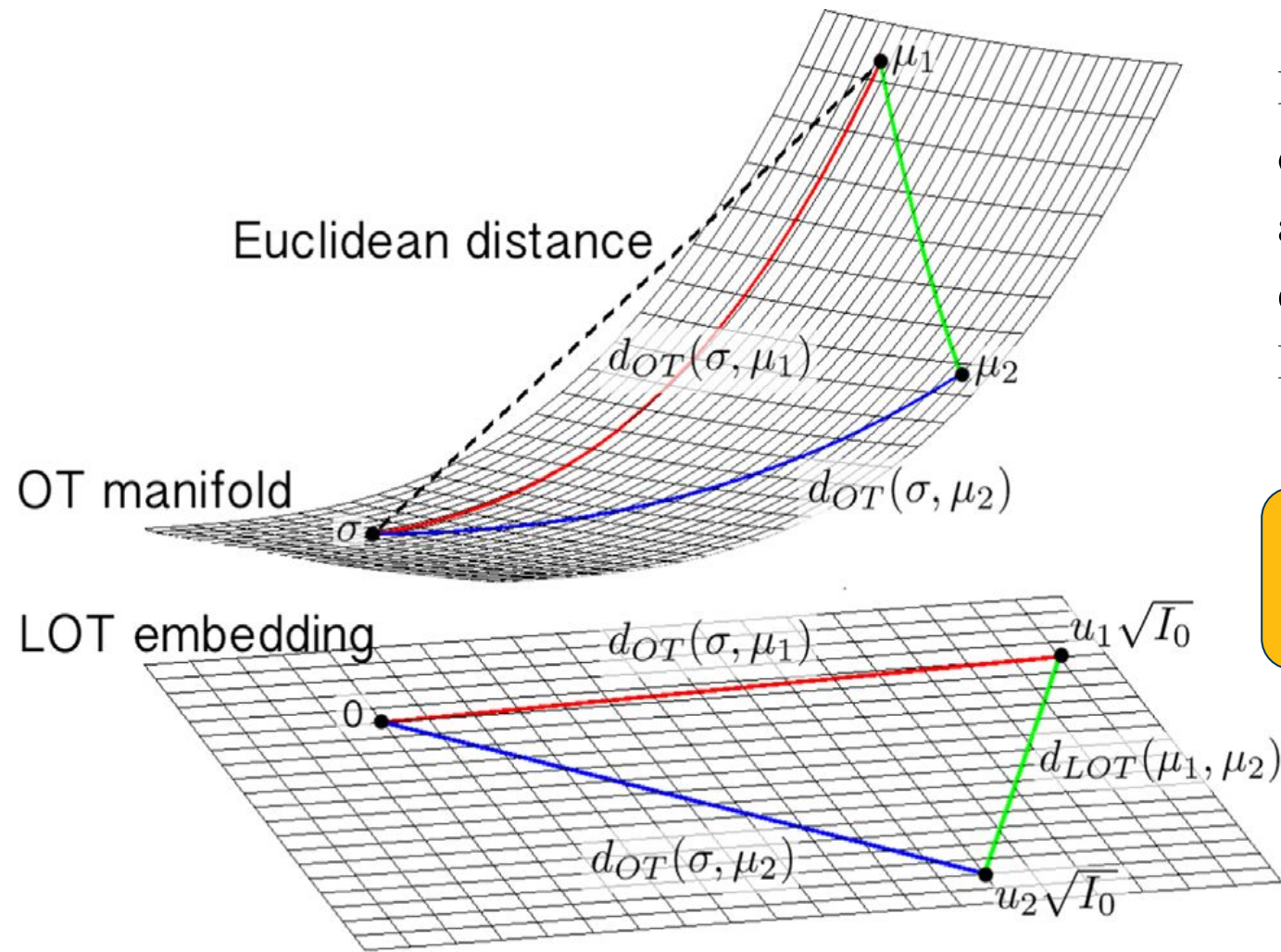
- A dataset with N samples
- T_{OT} : Time to compute one pair of OT distance (~ 0.1 secs)
- T_2 : Time to compute one pair of Euclidean distance ($\sim 10^{-3}$ secs)

OT for the whole dataset takes time on the order of $N(N-1)/2 \times T_{OT}$.
=> Too long for large datasets!

Compute the OT distances between **100k** events takes
~16 years on a desktop.

2.4 Linearized Optimal Transport

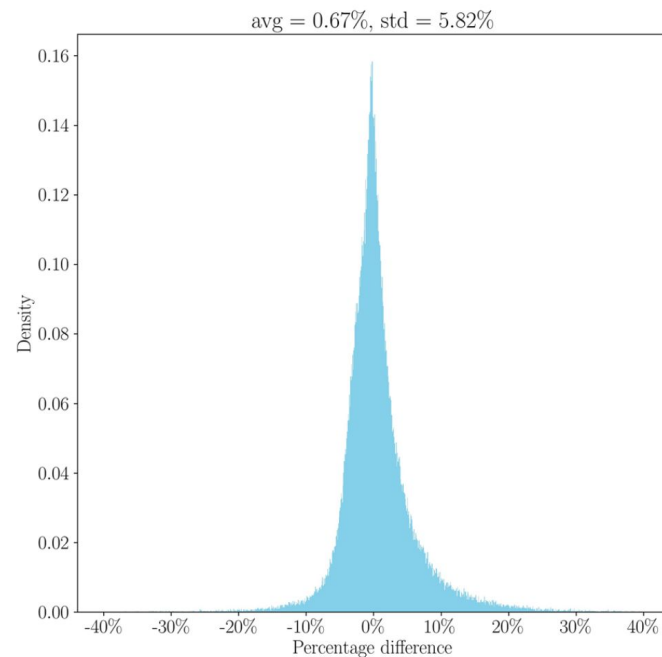
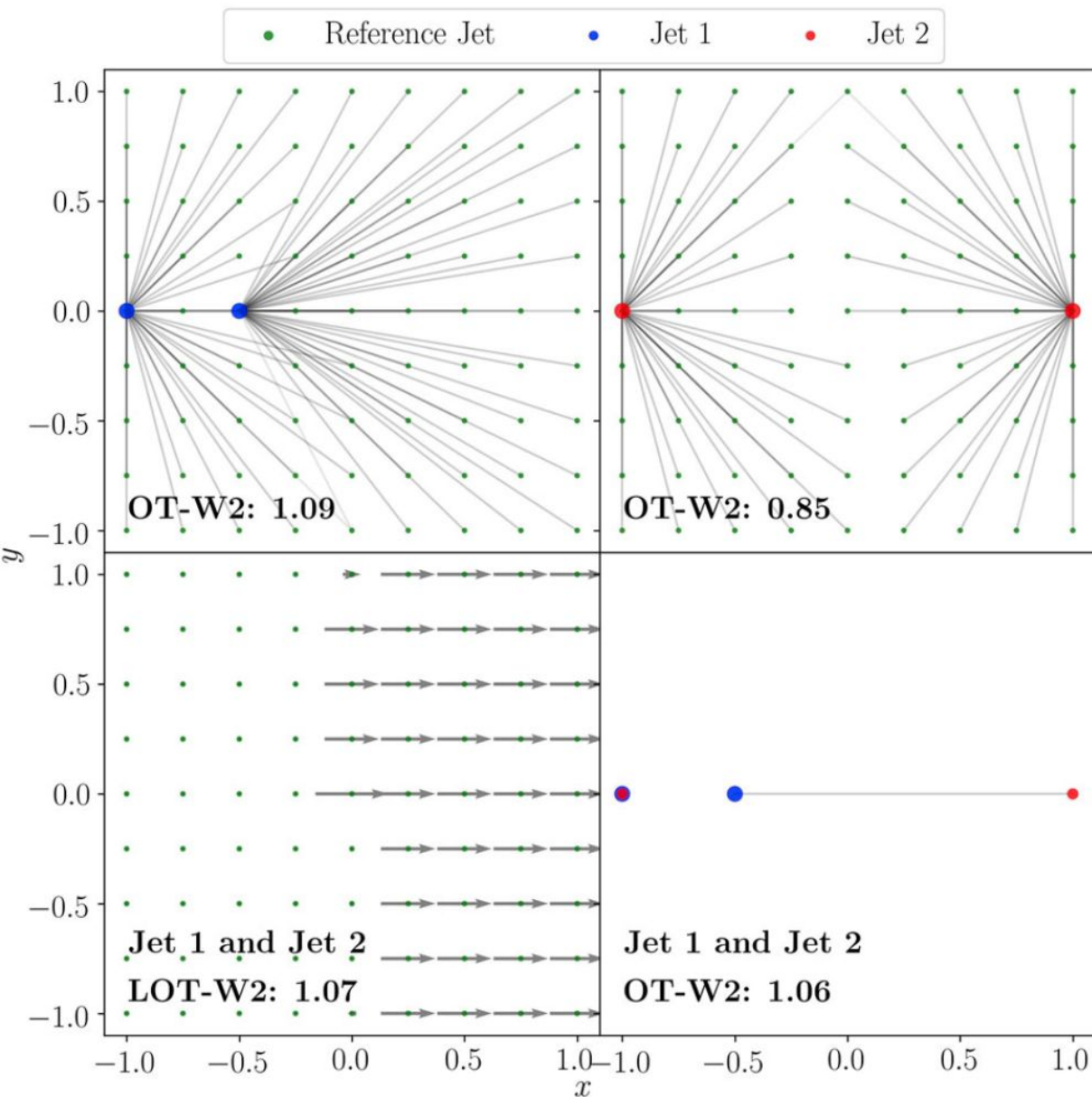
Goal: Reduce computation to $N \times T_{OT} + N(N-1)/2 \times T_2$ by using **Linearized Optimal Transport (LOT)**. [\[Wang et al.\]](#)



Basic Idea: Project onto the tangent plane at a chosen reference event, then compute Euclidean distances.

Now only minutes on your desktop!

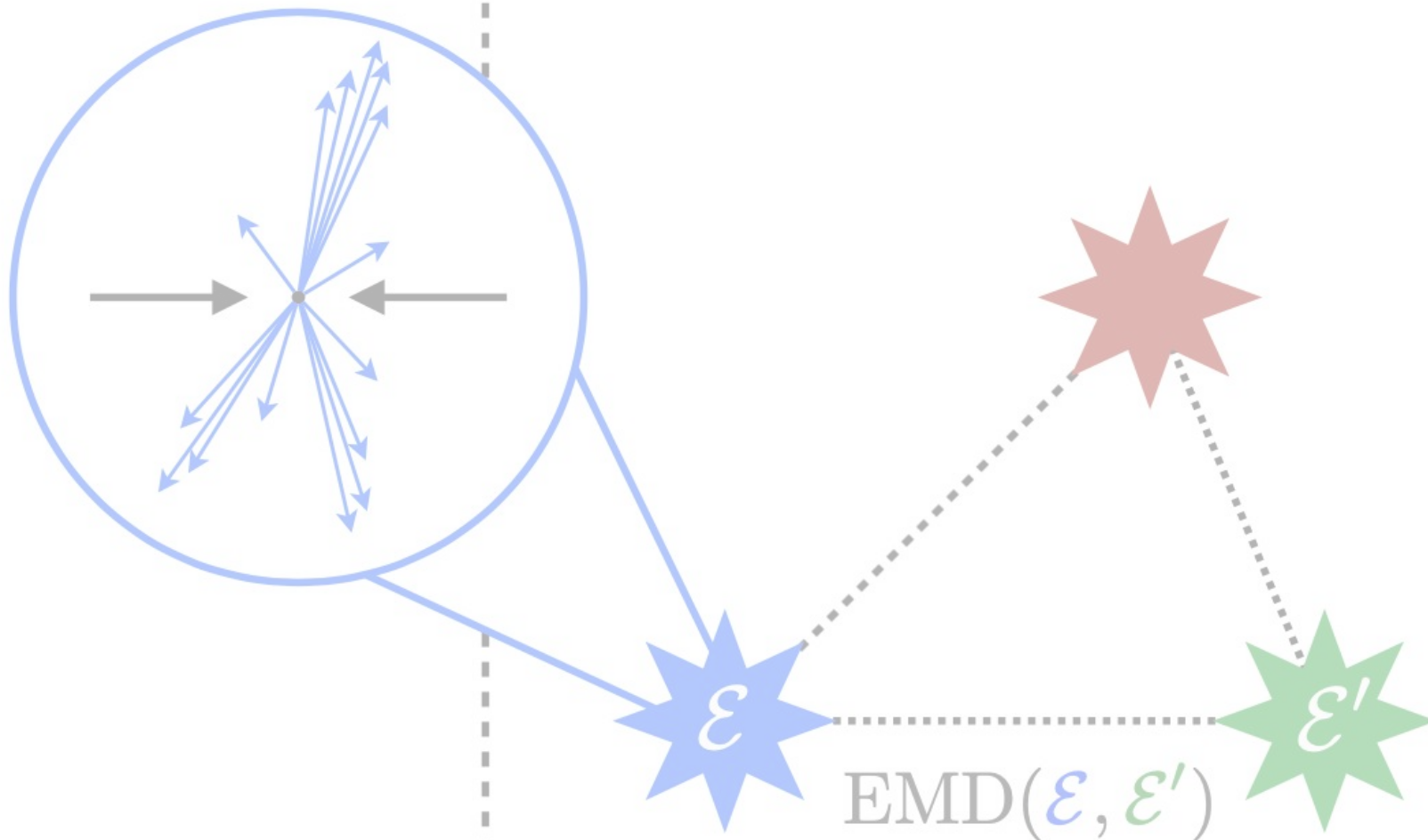
A Simple Example



Percentage difference between linearized W_2 and W_2 distances for 500 W and QCD jets.

The linear approx for both W_2 and HK is pretty good! 🤩

[Komiske, Metodiev, Thaler 2004.04159]



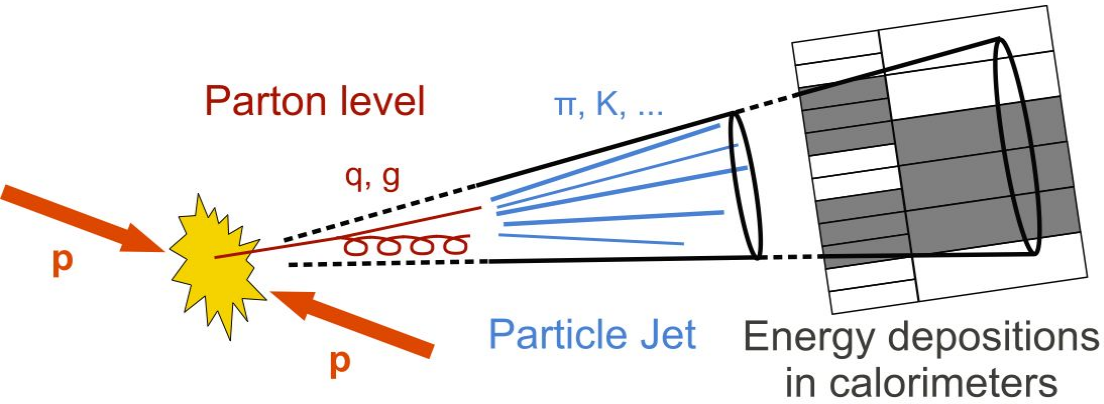
3. Optimal Transport for Collider Physics

3.1 Physics Background

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Simplified Perspective: Events as energy flow on calorimeters.

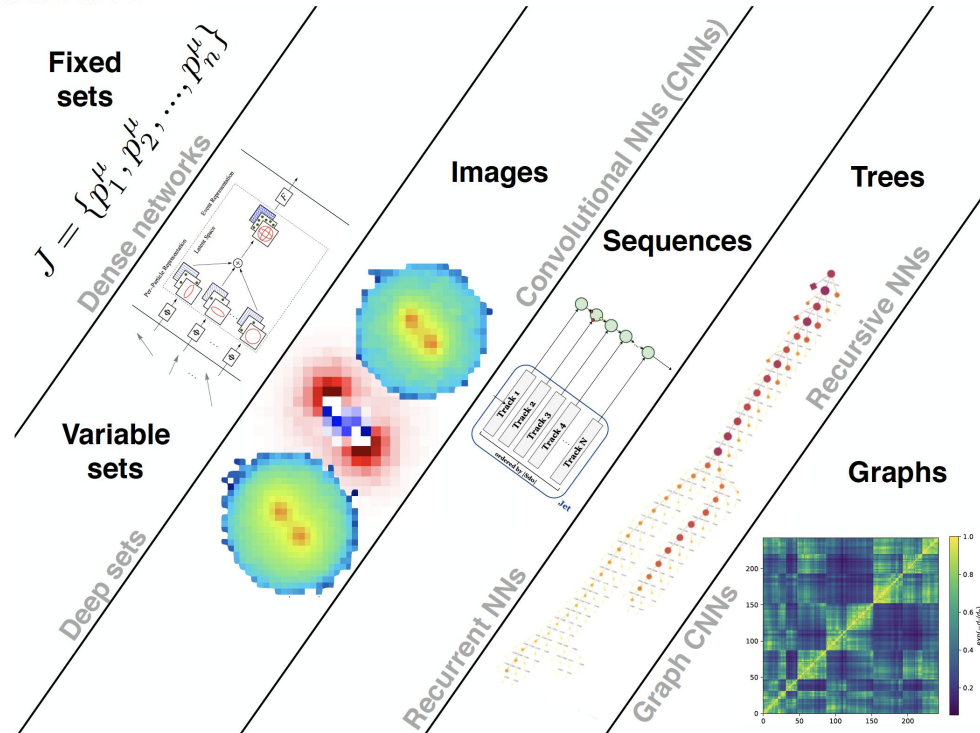
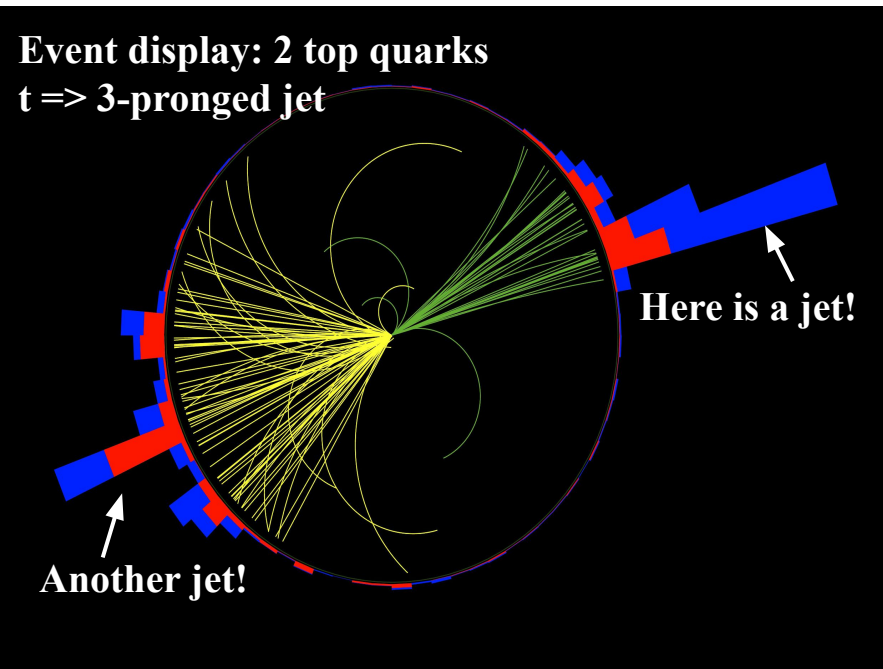
Phenomenological Tool: Jets and Jet substructure.



$$\mathcal{E}(\hat{n}) = \sum_{i \in J} E_i \delta(\hat{n} - \hat{n}_i)$$

Common ML Methods

Source: [CMS website, 1709.04464v2](https://cms.cern/1709.04464v2).



Why optimal transport as the metrics on jets?

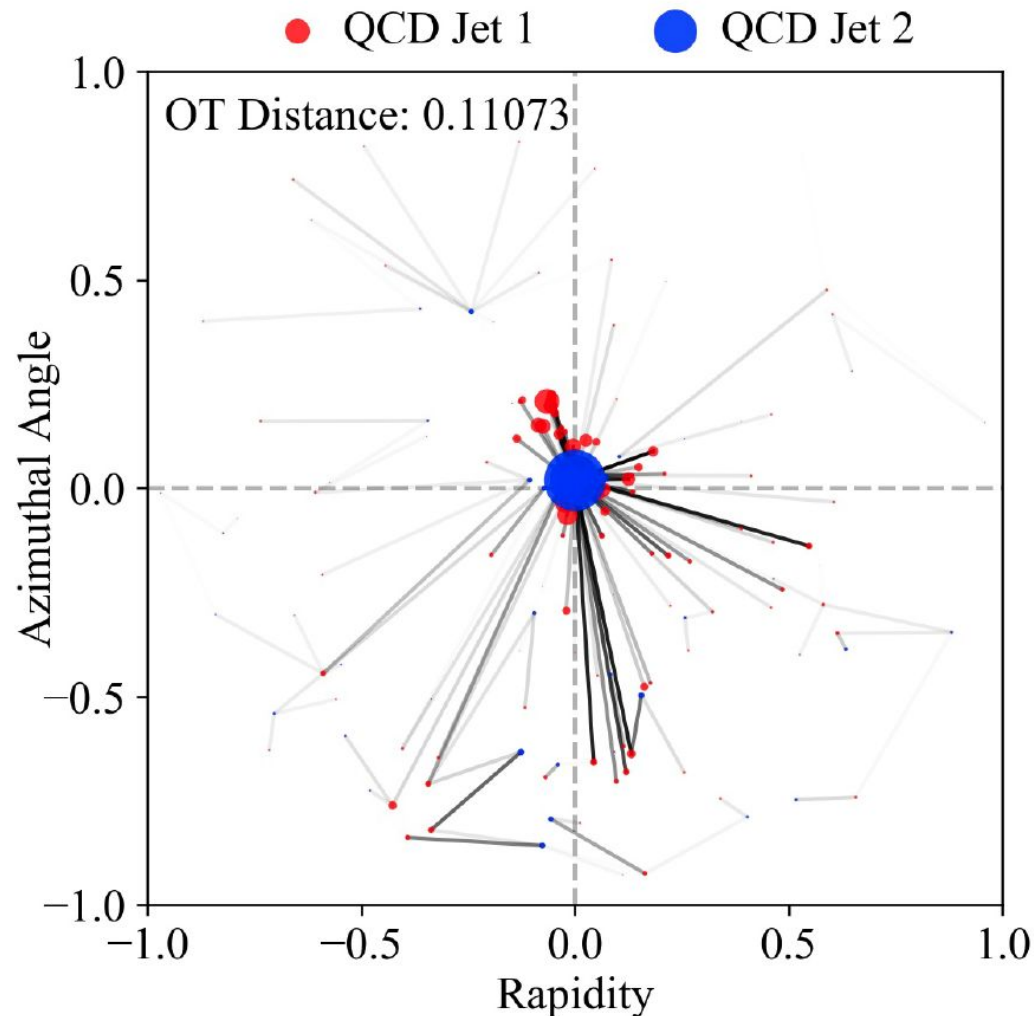
Goal: Give the space of collider events a physically meaningful metric.

Motive 1: Jet tagging with fast, simple-to-use, easy-to-interpret machine learning models.

Motive 2: Unify the concepts and techniques in QFT and jet physics through the geometric language of a metricized collider space.

Related Works: Jesse Thaler's group at MIT.

Jets are discrete distributions on the y - ϕ plane. We want a distance between them. \Rightarrow **Of course OT!**



3.2 A Unified Framework

IRC safety: EMD continuity everywhere except a negligible set of events.

Collider observables: the distance of closest approach between an event and a manifold of events.

Jet algorithm: approximates an M-particle event with $N < M$ objects called jet.

Pileup mitigation: finds the event that, when combined with an amount ρ of uniform radiation U , is closest to the given event.

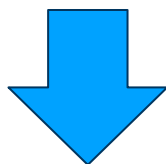
A distance between theories: EMD as the ground metric and cross sections as weights.

Source: Table 1, [2004.04159](#).

Concept	Equation	Illustration
Infrared and Collinear Safety [27–39]	$\text{EMD}(\mathcal{E}, \mathcal{E}') < \delta \implies \mathcal{O}(\mathcal{E}) - \mathcal{O}(\mathcal{E}') < \epsilon$	
Observables Event Shapes [40–45] Jet Shapes [46–48]	$\mathcal{O}(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{M}} \text{EMD}(\mathcal{E}, \mathcal{E}')$	
Jets Cone Finding [49, 50] Seq. Rec. [51–54]	$\mathcal{J}(\mathcal{E}) = \arg \min_{\mathcal{J} \in \mathcal{P}_N} \text{EMD}(\mathcal{E}, \mathcal{J})$	
Pileup Subtraction [55–61]	$\mathcal{E}_C(\mathcal{E}, \rho) = \arg \min_{\mathcal{E}' \in \Omega} \text{EMD}(\mathcal{E}, \mathcal{E}' + \rho \mathcal{U})$	
Theory Space	$\mathcal{T}(\mathcal{E}) = \sum_{i=1}^N \sigma_i \delta(\mathcal{E} - \mathcal{E}_i)$	

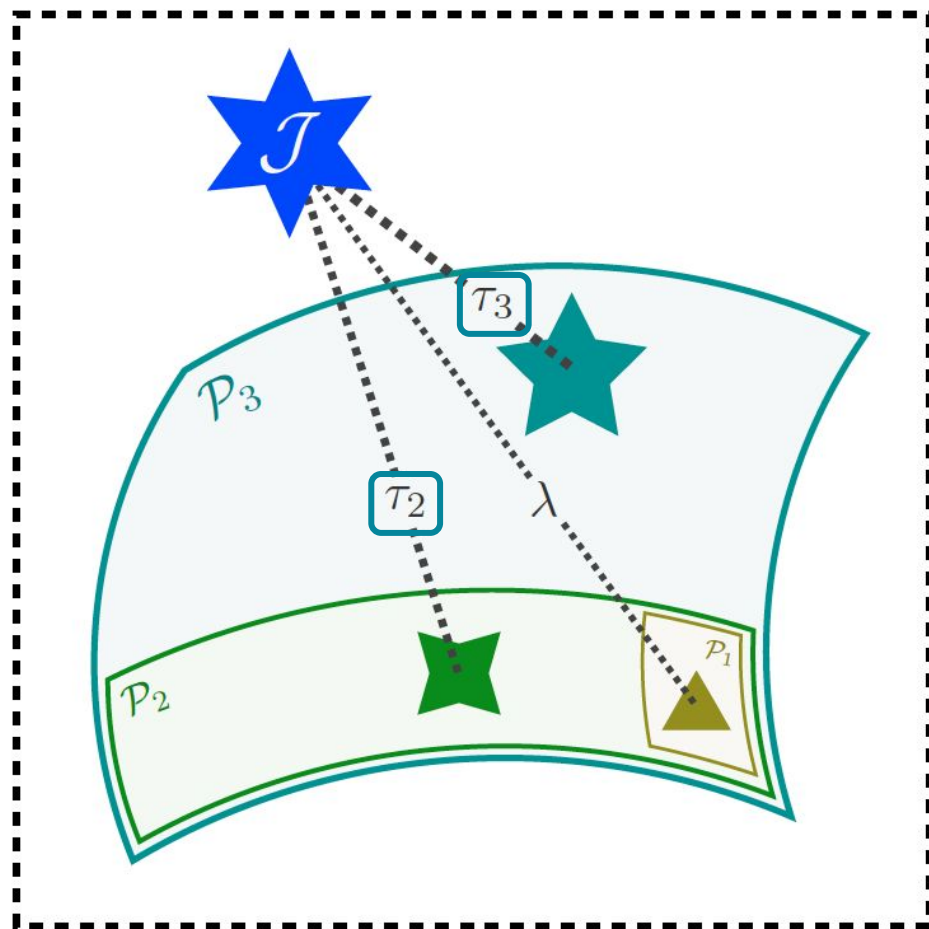
For example, N -subjettiness can be defined using the EMD distance.

$$\tau_N^{(\beta)}(\mathcal{J}) = \min_{\hat{n}_1, \dots, \hat{n}_N} \sum_{i=1}^M E_i \min(\theta_{i1}^\beta, \theta_{i2}^\beta, \dots, \theta_{iN}^\beta)$$



$$\tau_N^{(\beta)}(\mathcal{J}) = \min_{\mathcal{J}' \in \mathcal{P}_N} \text{EMD}_\beta(\mathcal{J}, \mathcal{J}').$$

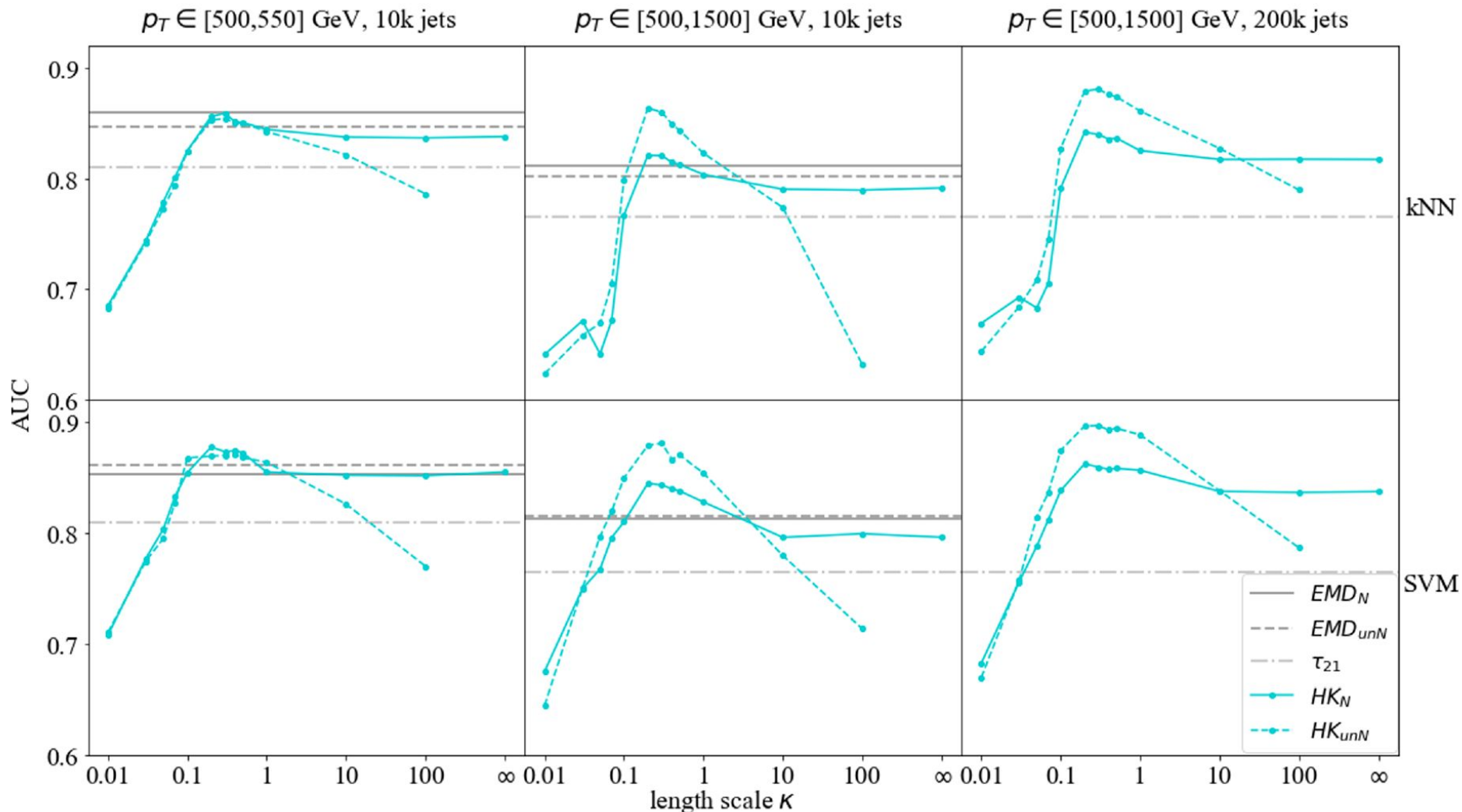
$$\tau_{N,N-1}^{(\beta)} = \frac{\tau_N^{(\beta)}}{\tau_{N-1}^{(\beta)}}$$



3.3 Jet Tagging

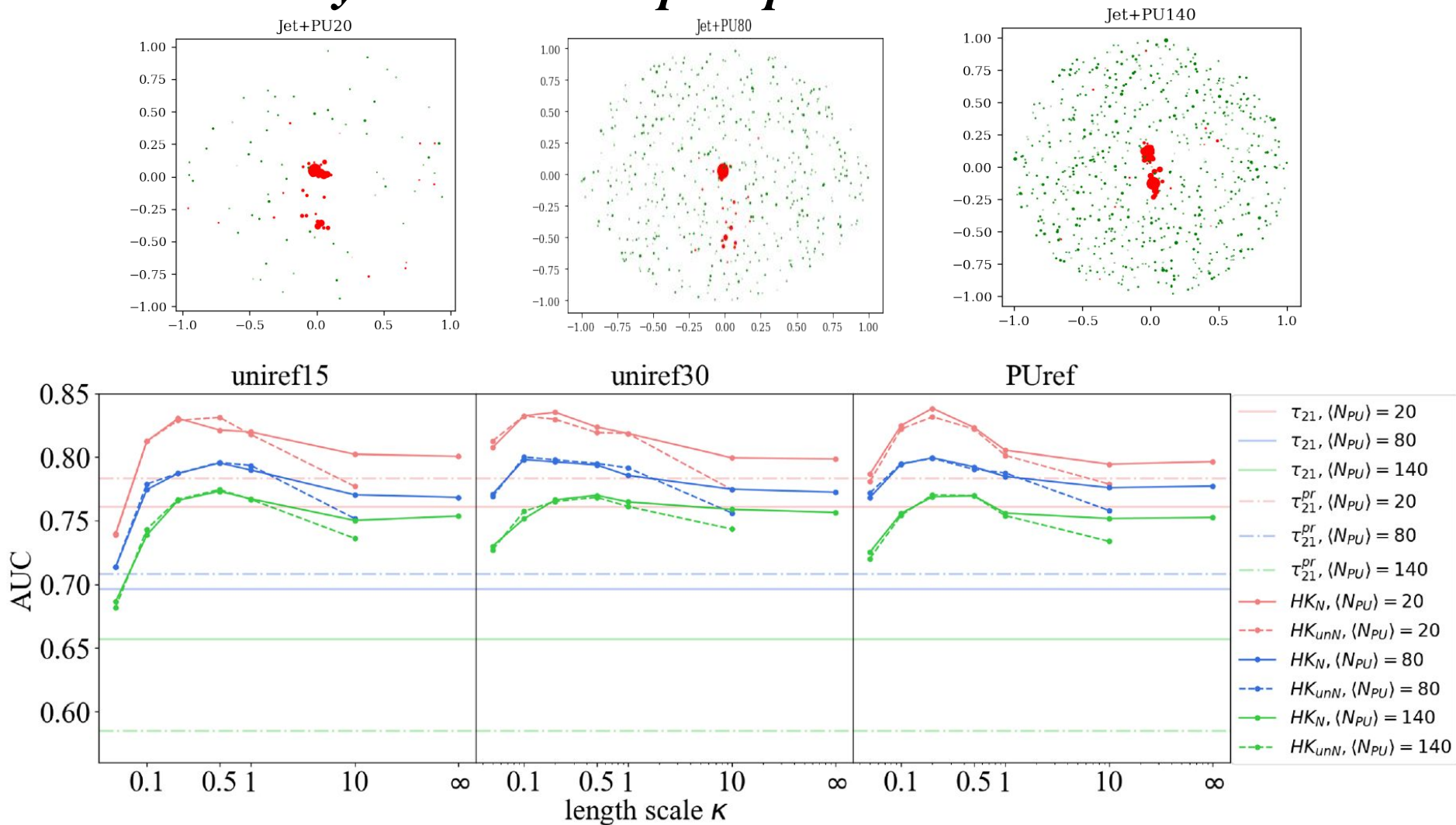
- Task is to classify simulated QCD vs. W boson jets.
- Linearized W_2 and HK distances with various κ
- Apply simple ML models such as kNN and SVM to classify the jets.

Please refer to our [paper](#) for more details.

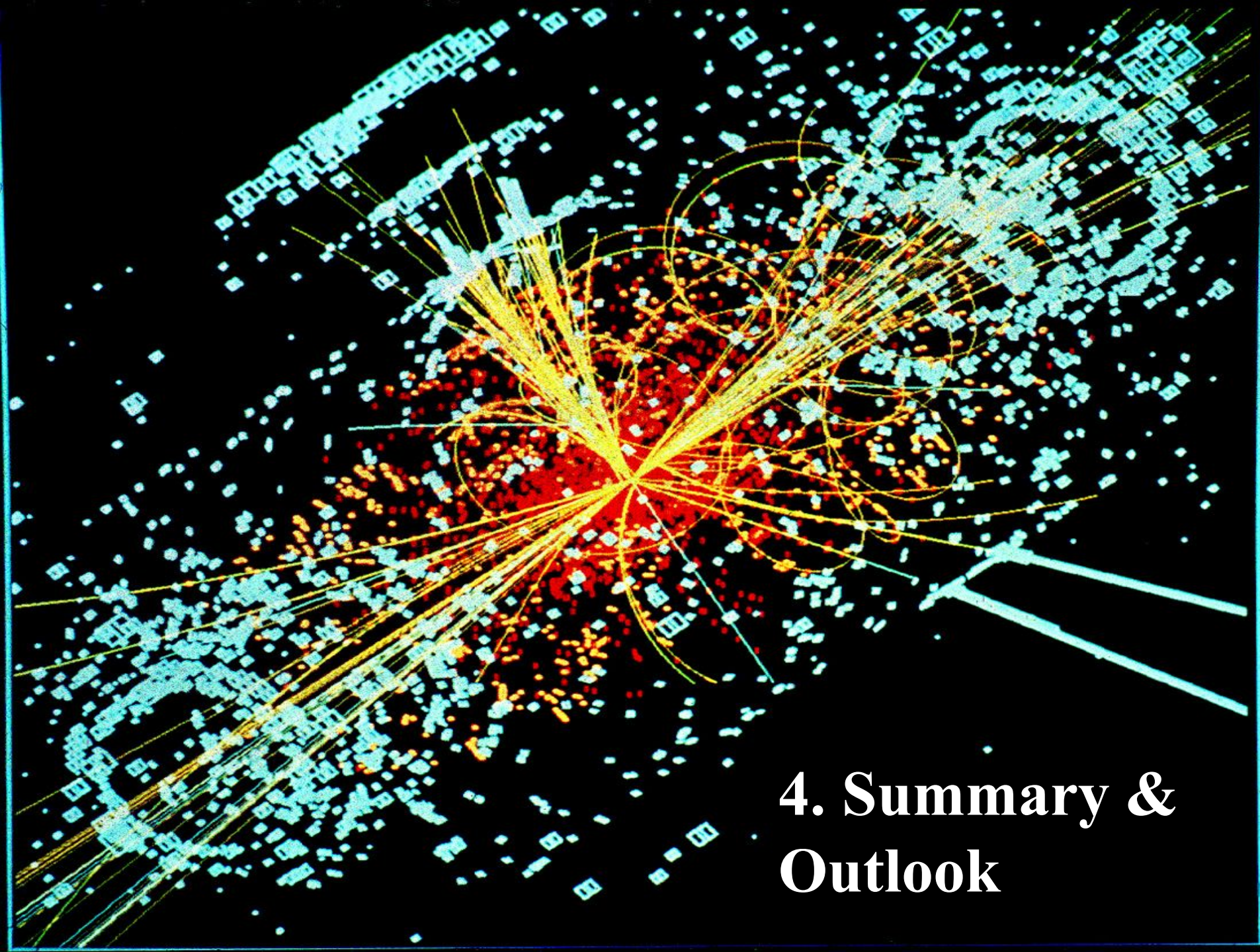


Is OT relatively insensitive to pileup?

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Linearized W_2 and HK distances on 10k WQCD jets with different pileups (Poisson distributions with mean $N_{PU} = 20, 80, 140$) compared with τ_{21} on pruned jets in the same dataset.



4. Summary & Outlook

Take-home Messages

Optimal Transport is GREAT!

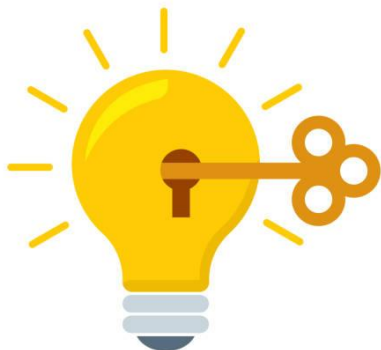
Especially suitable whenever you want to define a distance between two distributions with rich substructures.

One example of such distributions is LHC jets, immensely important to collider physics.

Potentially many other use cases in physics and beyond.

OT also has many theoretical implications, e.g., Renormalization Group Flow as OT.

It's now your turn to play with OT!



Future Directions Along the Current Lines of Research

More Developments of the OT framework

Multi-species OT

*OT with
Invariances*

*OT on Multi-scaled
Distributions*

...

OT for Collider Physics

*OT for Anomaly
Detection*

*Study the OT
Manifold*

*OT for a Theory
Space*

...

OT for Other HEP Fields

OT for Dark Matter

Your turn now!

...



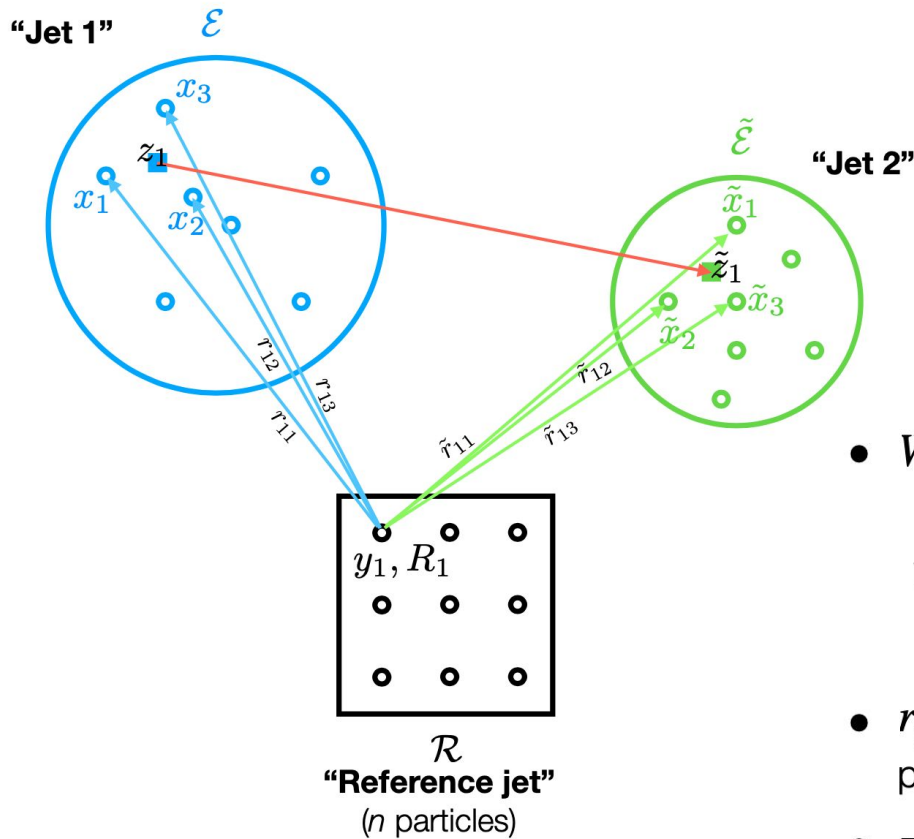
THANKS!

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Backup



Procedure to Linearize the W_2 Distance

- $W_2(\mathcal{E}, \tilde{\mathcal{E}})$: **2-Wasserstein distance**

$$W_2(\mathcal{E}, \tilde{\mathcal{E}}) = \min_{r_{ij} \in \Gamma(\mathcal{E}, \tilde{\mathcal{E}})} \left(\sum_{ij} r_{ij} \|x_i - \tilde{x}_j\|^2 \right)^{1/2}$$

- r_{ij} : **transport plan** (minimizer of W_2) from i th particle in reference to j th particle in event.
- z_i : **barycenter** (avg. of locations to which i th particle is sent, weighted by transport plan)

$$z_i = \frac{1}{R_i} \sum_j r_{ij} x_j$$

Map from \mathcal{E} to a vector in \mathbb{R}^{2n}

Can think of LOT as an approximation to W_2 distance, but also converges to a true metric $W_{2,\mathcal{R}}(\mathcal{E}, \tilde{\mathcal{E}})$ in its own right in continuum limit of reference \mathcal{R} ; this metric bounded as

$$W_2(\mathcal{E}, \tilde{\mathcal{E}}) \leq W_{2,\mathcal{R}}(\mathcal{E}, \tilde{\mathcal{E}}) \leq C W_2(\mathcal{E}, \tilde{\mathcal{E}})^{2/15}$$

- $LOT_{r,\tilde{r}}(\mathcal{E}, \tilde{\mathcal{E}})$: LOT approximation of the 2-Wasserstein distance between events $\mathcal{E}, \tilde{\mathcal{E}}$

$$LOT_{r,\tilde{r}}(\mathcal{E}, \tilde{\mathcal{E}}) = \left(\sum_i R_i \|z_i - \tilde{z}_i\|^2 \right)^{1/2}$$

Linearizing the HK distances is similar, but more complicated.

Source Distribution:

$$\mu_0 = u_0 \cdot \sigma + \mu_0^\perp$$

Two Distributions have different total mass.

Target Distribution:

$$\mu_1 = u_1 \cdot T_\# \sigma + \mu_1^\perp$$

μ_1^\perp : Mass of particles that are created from nothing.

Spatial movement of mass particles:

$$v_t := \frac{d\omega_t}{d\rho_t}$$

Change of mass of moving particles and of those that disappear entirely at $t=1$:

$$v_0(x) = \begin{cases} \frac{T(x)-x}{\|T(x)-x\|} \cdot \sqrt{\frac{u_1(T(x))}{u_0(x)}} \cdot \sin(\|T(x)-x\|) & \sigma\text{-a.e.}, \\ 0 & \mu_0^\perp\text{-a.e.}, \end{cases}$$

$$\alpha_0(x) = \begin{cases} 2 \left(\sqrt{\frac{u_1(T(x))}{u_0(x)}} \cdot \cos(\|T(x)-x\|) - 1 \right) & \sigma\text{-a.e.}, \\ -2 & \mu_0^\perp\text{-a.e.} \end{cases}$$

$$\alpha_t := \frac{d\tilde{\zeta}_t}{d\rho_t} - 2(1-t) \frac{d\mu_0^\perp}{d\rho_t}$$

$$\text{HK}(\mu_0, \mu_1)^2 = \int_{\Omega} [\|v_0\|^2 + \frac{1}{4}(\alpha_0)^2] d\mu_0 + \|\mu_1^\perp\|.$$

The tangent space now consists of a velocity field and a mass growth field.

For detailed descriptions, please refer to our math [paper](#).