May 9, 2022
Session: QCD&EW I

Optimal Transport for Jet Physics

Speaker: Tianji Cai

Conference: Phenomenology 2022 Symposium (University of Pittsburgh)

Based on "**Which metric on the space of collider events?**" [2111.03670]
"**Linearized Optimal Transport for Collider Events**" [2008.08604]
w/ Junyi Cheng, Nathaniel Craig (P.I.) & Katy Craig,
"**The Linearized Hellinger-Kantorovich Distance**" [2102.08807]
w/ J. Cheng, B. Schmitzer, M. Thorpe

Department of Physics

UC **SANTA BARBARA**

Contents

- **Introduction:**

  Why OT & What is OT, OT as the Metric, EMD & Its Generalization

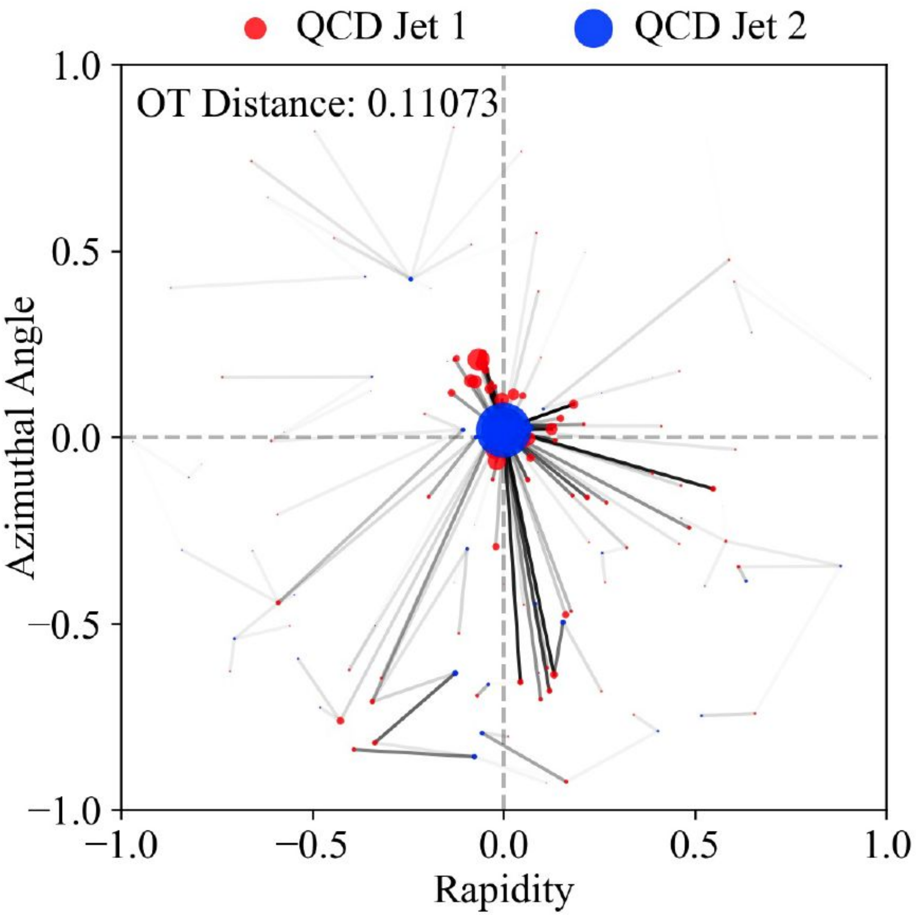
- **Theory of Optimal transport:**

  Balanced OT, Unbalanced OT,

  Practical Limitation,

  Linearized Optimal Transport (LOT)

- **LOT for Jet Tagging**
- **Summary**

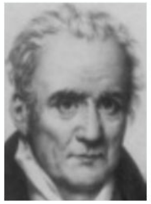


1. Introduction: Why Optimal Transport & What is OT?

Goal: Want a way to quantify the **distance** between collider events/jets.

Optimal Transport is a well-developed mathematical theory defining a family of metrics between two distributions.

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

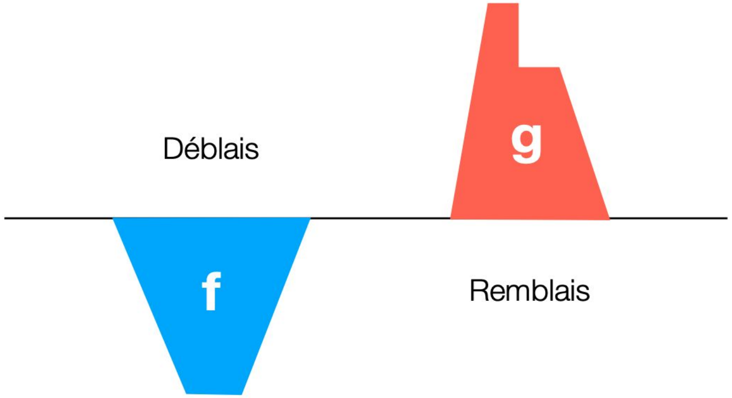
2000: Felix Otto, Cedric Villani,
Generalization of an inequality by Talagrand, as a consequence of the logarithmic Sobolev inequality

2010: Cedric Villani wins Fields medal

2018: Alessio Figalli wins Fields medal

Fundamental problem of **optimal transport:**

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



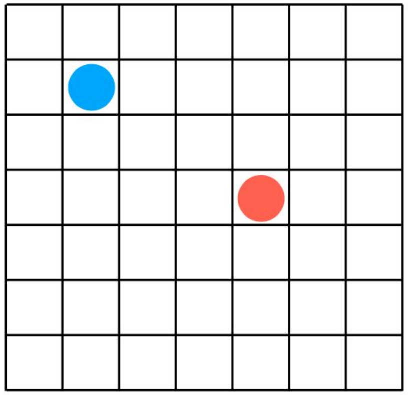
In other words, how can we optimally transport *f* to *g*?

1. Introduction: Why OT as the Metric?

Consider two particles with unit energy.

Image-based approach

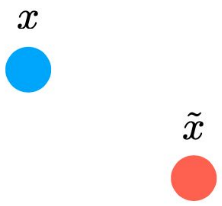
Bin on N-bin grid, represent energy distribution by vectors in **R**^{N}, compute Euclidean distance between vectors



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

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!

1. Introduction: EMD & Its Generalization

EMD Definition for Jets:

f$_{ij}$: the amount of energy moved from particle i to particle j.

theta$_{ij}$: ground distance between particles i and j

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

Standard EMD

E: Event E with total energy E
E': Event E' with total energy E'
E = E'

Conditions:

E$_i$: Energy of particle i in event E
E'$_j$: Energy of particle j in event E'

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

1. Introduction: EMD & Its Generalization

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Standard EMD

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

One Possible Generalization when E ≠ E'

Same as Standard EMD

Extra piece to account for the unequal total energy

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

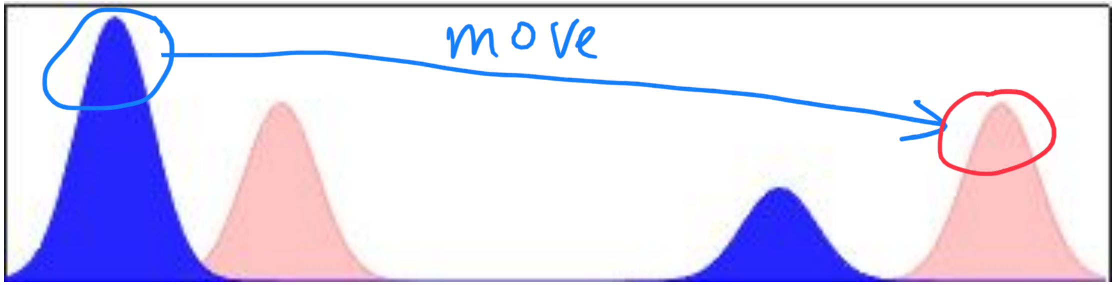
$$\tilde{\Gamma}_{\leqslant(\mathcal{E},\mathcal{E}')} := \left\{ f_{ij} : f_{ij} \geqslant 0, \sum_j f_{ij} \leqslant E_i, \sum_i f_{ij} \leqslant E'_j, \sum_{ij} f_{ij} = \min\left(\sum_i E_i, \sum_j E'_j \right) \right\}. \tag{1.3}$$

P. Komiske, E. Metodiev, J. Thaler [1902.02346]

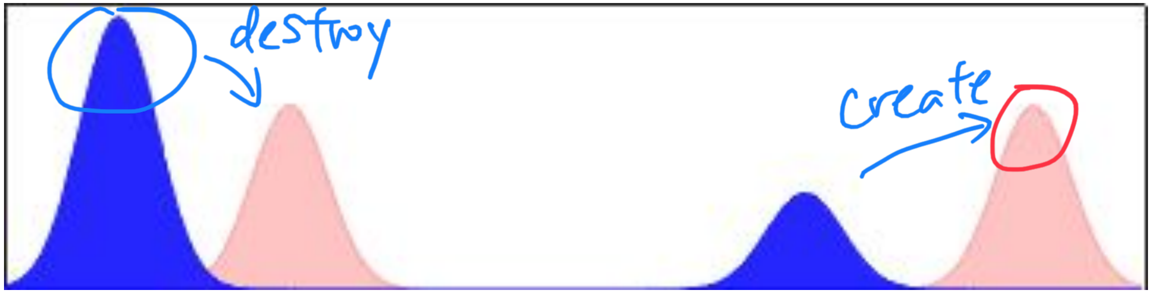
Different conditions for the unbalanced case

2. Theory of Optimal Transport

Balanced OT: Mass can only be transported, not created or destroyed.
=> Total mass has to be equal.



Unbalanced OT: Mass can be transported, created and destroyed.
=> Total mass can be unequal.



Credit: L. Chizat, G. Peyré, B. Schmitzer, F-X. Vialard on G. Peyré's Github.

2. Theory of OT: Balanced & Unbalanced

p-Wasserstein Distance

p=1: EMD
p=2: Monge-Kantorovich Distance (W_2); has a (weak) Riemannian structure, thus can be linearized.

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

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

2. Theory of OT: Balanced & Unbalanced

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

Hellinger-Kantorovich (HK) Distance:

The unbalanced generalization for W_2 distance; also enjoys a Riemannian structure.

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

ζ=0: No source => W_2 Distance
ζ≠0: With source => HK Distance

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

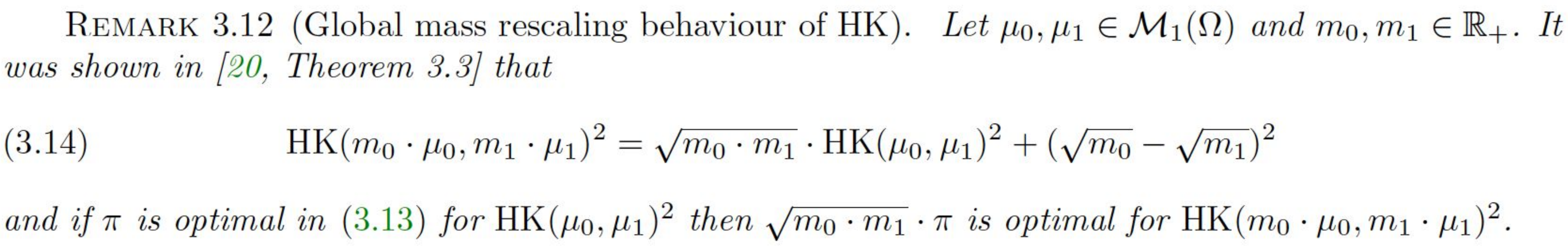
$$\mathrm{HK}(\mu_0,\mu_1)^2 := \inf\left\{J_{\mathrm{HK}}(\rho,\omega,\zeta) \mid (\rho,\omega,\zeta)\in\mathcal{CES}(\mu_0,\mu_1)\right\}.$$

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

$\boxed{\mathrm{HK}_\kappa(\mu_0,\mu_1)/\kappa \rightarrow \text{Hellinger distance (\textasciitilde Euclidean)}}$

$\boxed{\mathrm{HK}_\kappa(\mu_0,\mu_1) \rightarrow \mathrm{W}_2(\mu_0,\mu_1)}$

HK Distance: Unnormalized vs. Normalized Measures



REMARK 3.12 (Global mass rescaling behaviour of HK). *Let $\mu_0, \mu_1 \in \mathcal{M}_1(\Omega)$ and $m_0, m_1 \in \mathbb{R}_+$. It was shown in [20, Theorem 3.3] that*

$$\mathrm{HK}(m_0 \cdot \mu_0, m_1 \cdot \mu_1)^2 = \sqrt{m_0 \cdot m_1} \cdot \mathrm{HK}(\mu_0, \mu_1)^2 + (\sqrt{m_0} - \sqrt{m_1})^2 \tag{3.14}$$

and if π is optimal in (3.13) *for* $\mathrm{HK}(\mu_0, \mu_1)^2$ *then* $\sqrt{m_0 \cdot m_1} \cdot \pi$ *is optimal for* $\mathrm{HK}(m_0 \cdot \mu_0, m_1 \cdot \mu_1)^2$.

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.

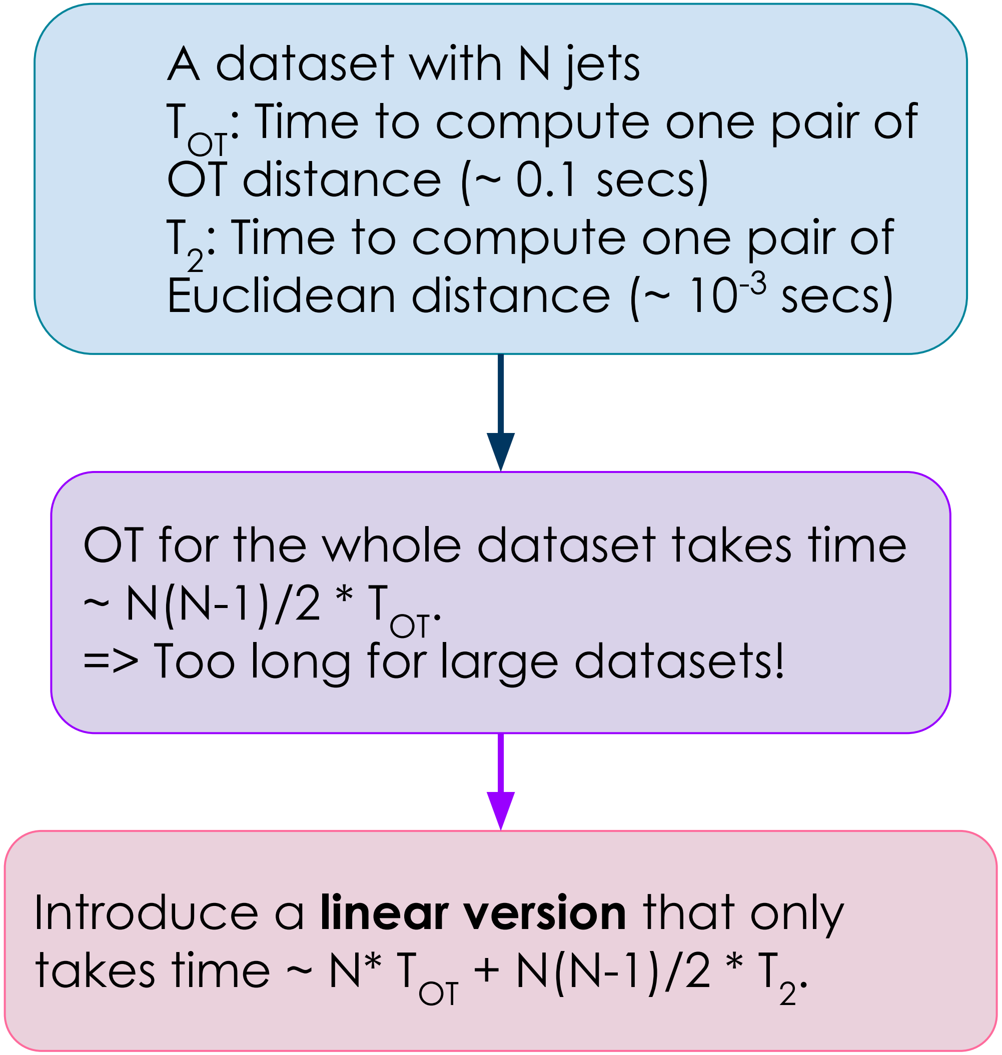
In analysis, **first normalize** all samples before computing HK, then recover the total mass difference via Eq 3.14.

Three Approaches to use OT:

1. **Normalize, then balanced W_2**
2. **Normalize, then unbalanced HK**
3. **Unbalanced HK directly**

T. Cai, J. Cheng, B. Schmitzer, M. Thorpe
[2102.08807]

2. Theory of OT: Practical Limitation of Exact OT



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

OT for the whole dataset takes time ~ $N(N-1)/2 * T_{OT}$.
=> Too long for large datasets!

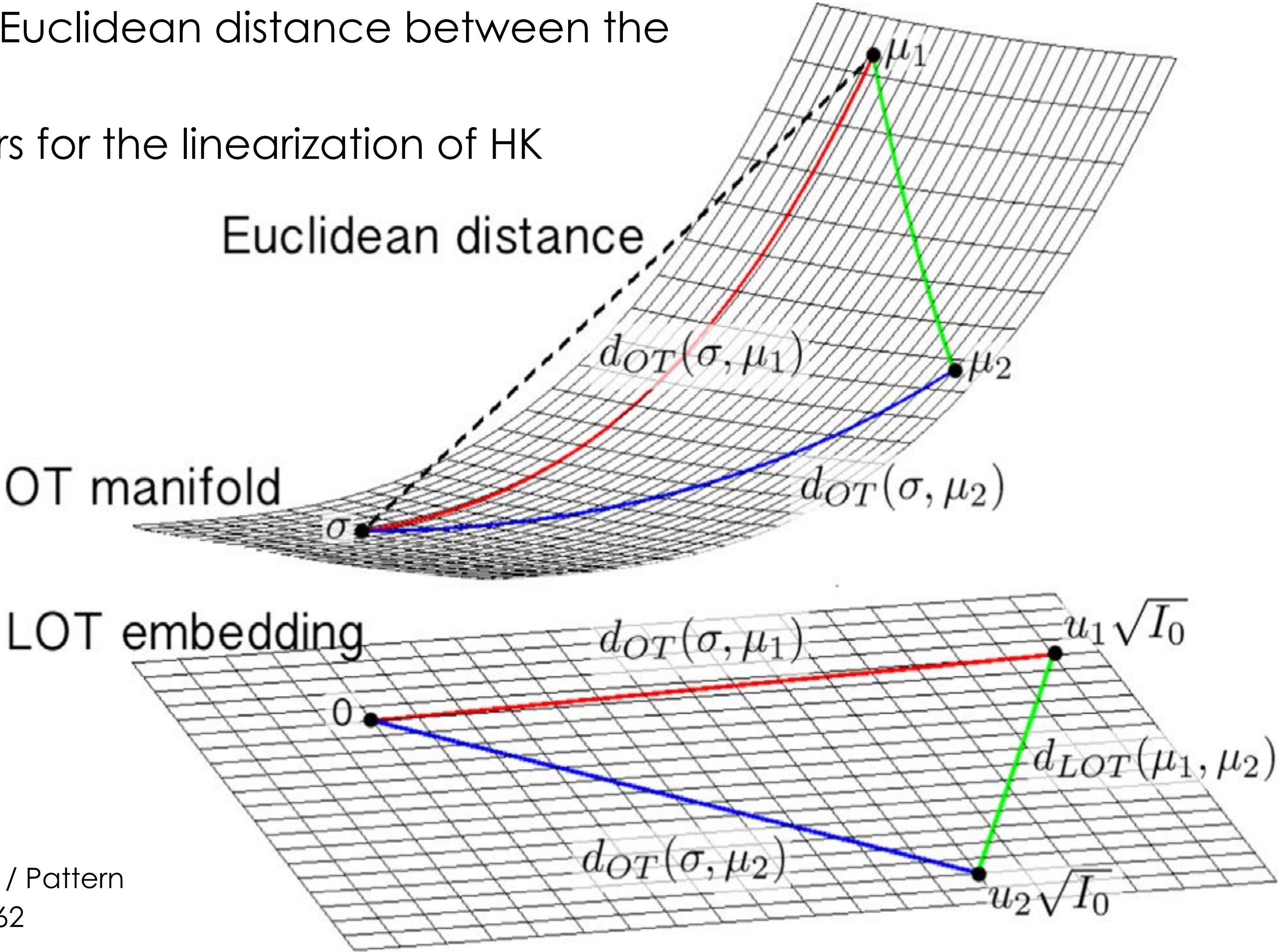
Introduce a **linear version** that only takes time ~ $N^* T_{OT} + N(N-1)/2 * T_2$.

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

Linearized Optimal Transport!

2. Theory of OT: Linearized Optimal Transport

- Project onto 2-Wasserstein tangent plane at a chosen reference event.
- Compute the Euclidean distance between the projections.
- Refer to papers for the linearization of HK distances.

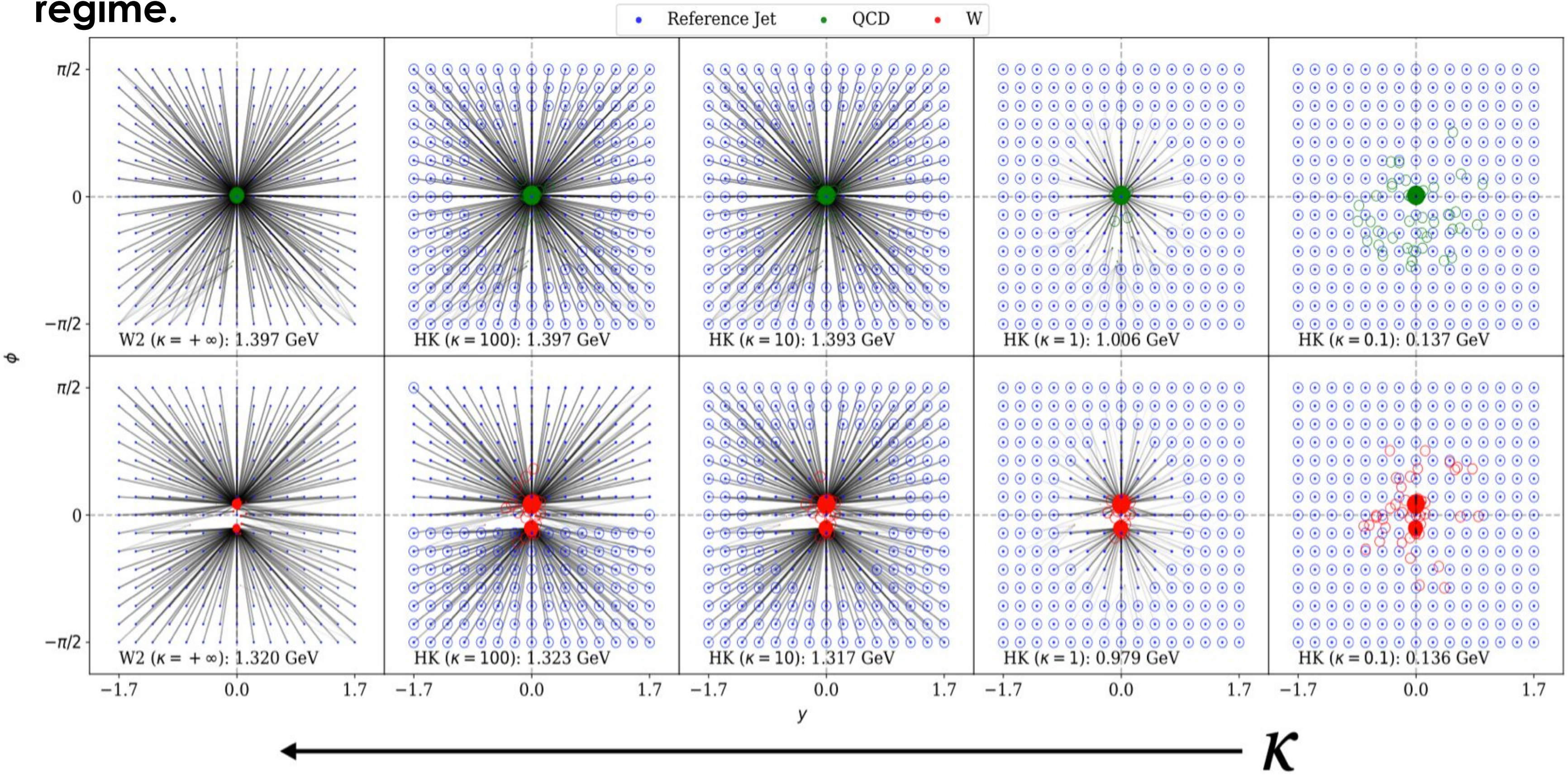


Source: Fig 1, S. Kolouri et al. / Pattern Recognition 51 (2016) 453–462

3. LOT for Jet Tagging: OT Plots

Optimal transports between the 15*15 uniform reference measure (blue) and a typical QCD jet (green), or a W jet (red), using W_2 and HK with κ = **100, 10, 1, 0.1**.

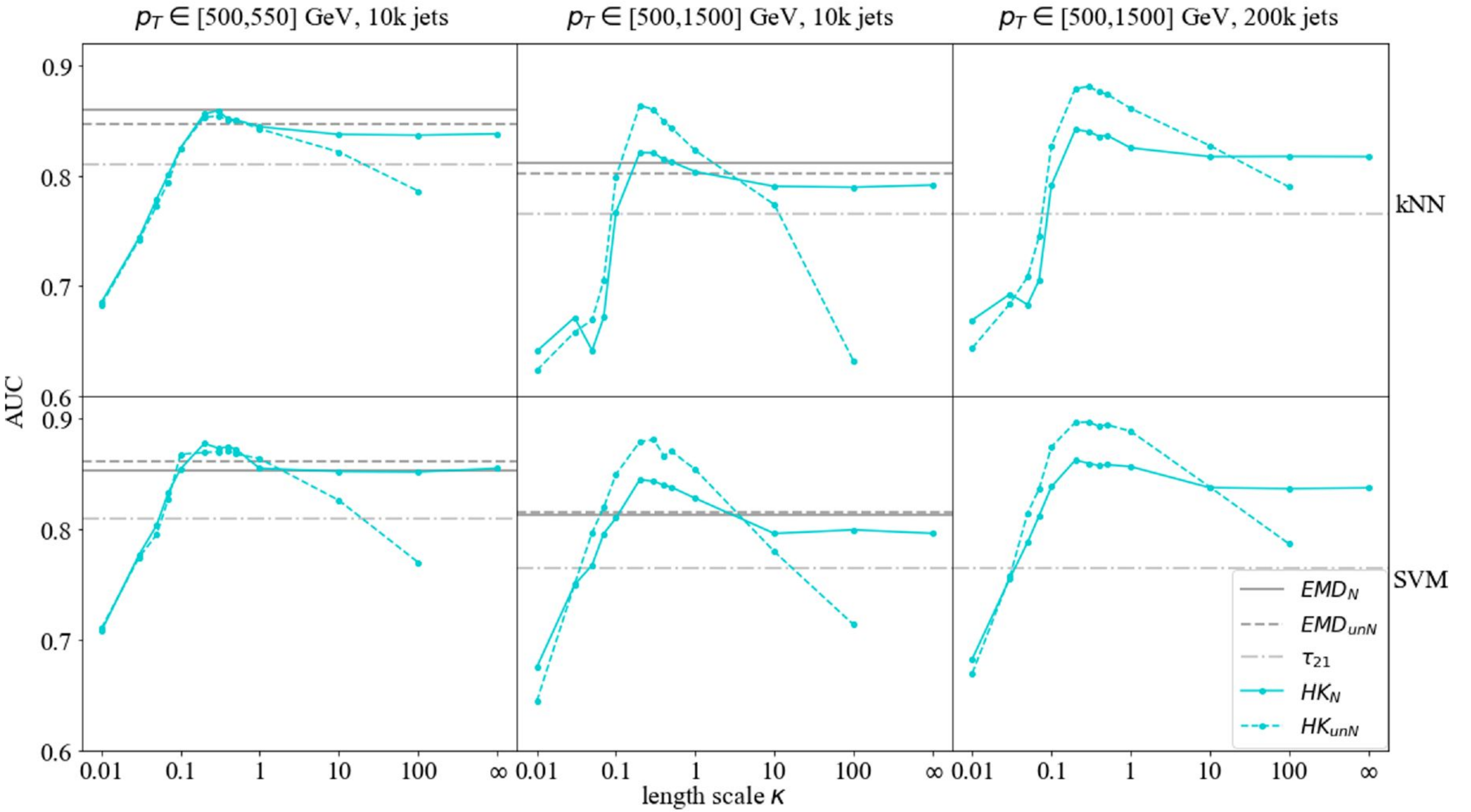
The total OT distances between the jets are similar for κ = +∞, 100, 10, the transport regime.



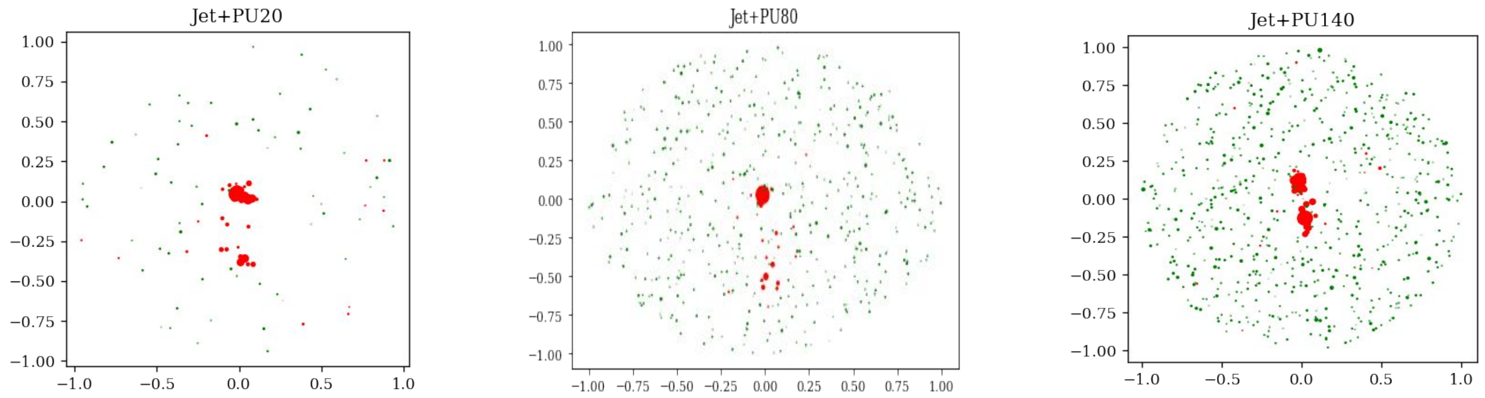
$\kappa = \infty$: original W_2 distance

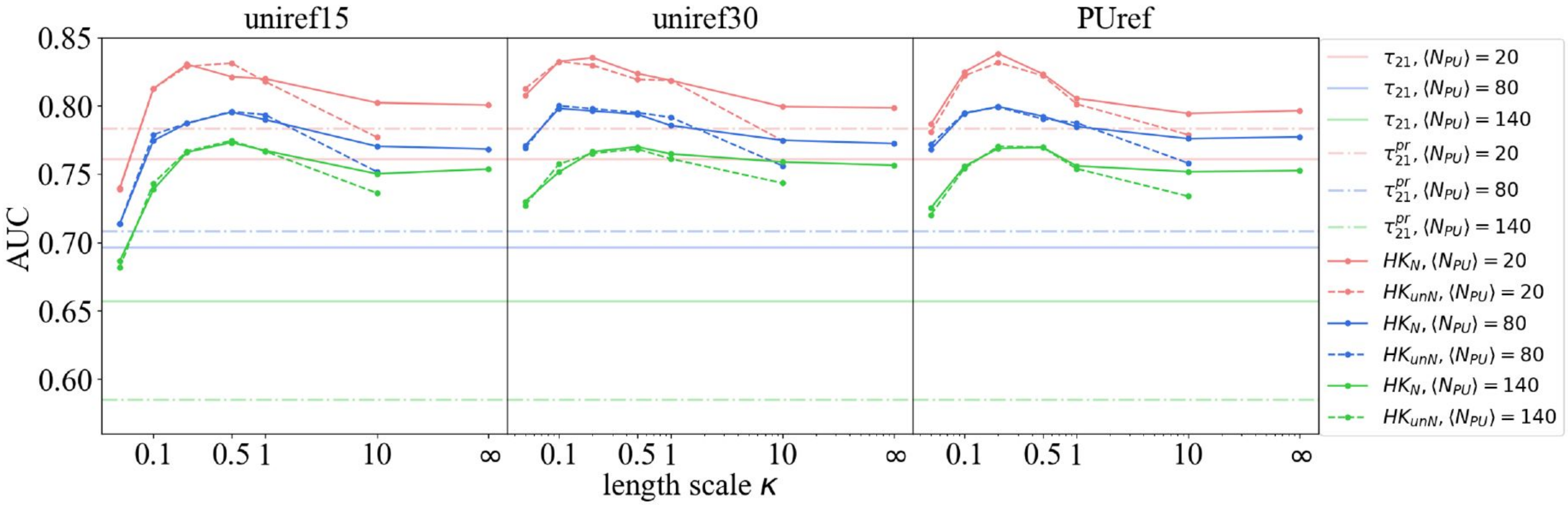
$\kappa = 0$: image difference

3. LOT for Jet Tagging: W v.s. QCD task using Linearized W_2 and HK distances with various κ



3. Pileup Effect: Is OT relatively insensitive to Pileup?





LOT-W$_2$ and LOT-HK on 10k WQCD jets with different PUs (Poisson distributions with mean N$_{PU}$ = **20, 80, 140**) compared with τ_{21} on pruned jets in the same dataset.

4. Summary

- Optimal transport provides a natural metric on the space of collider events with ideal properties.
- Useful for geometrization of LHC data, event classification, unifying description of collider observables...
- … and now computable on your laptop using Linearized Optimal Transport.

Thank you!

Backup Slides

Balanced OT

p-Wasserstein Distance

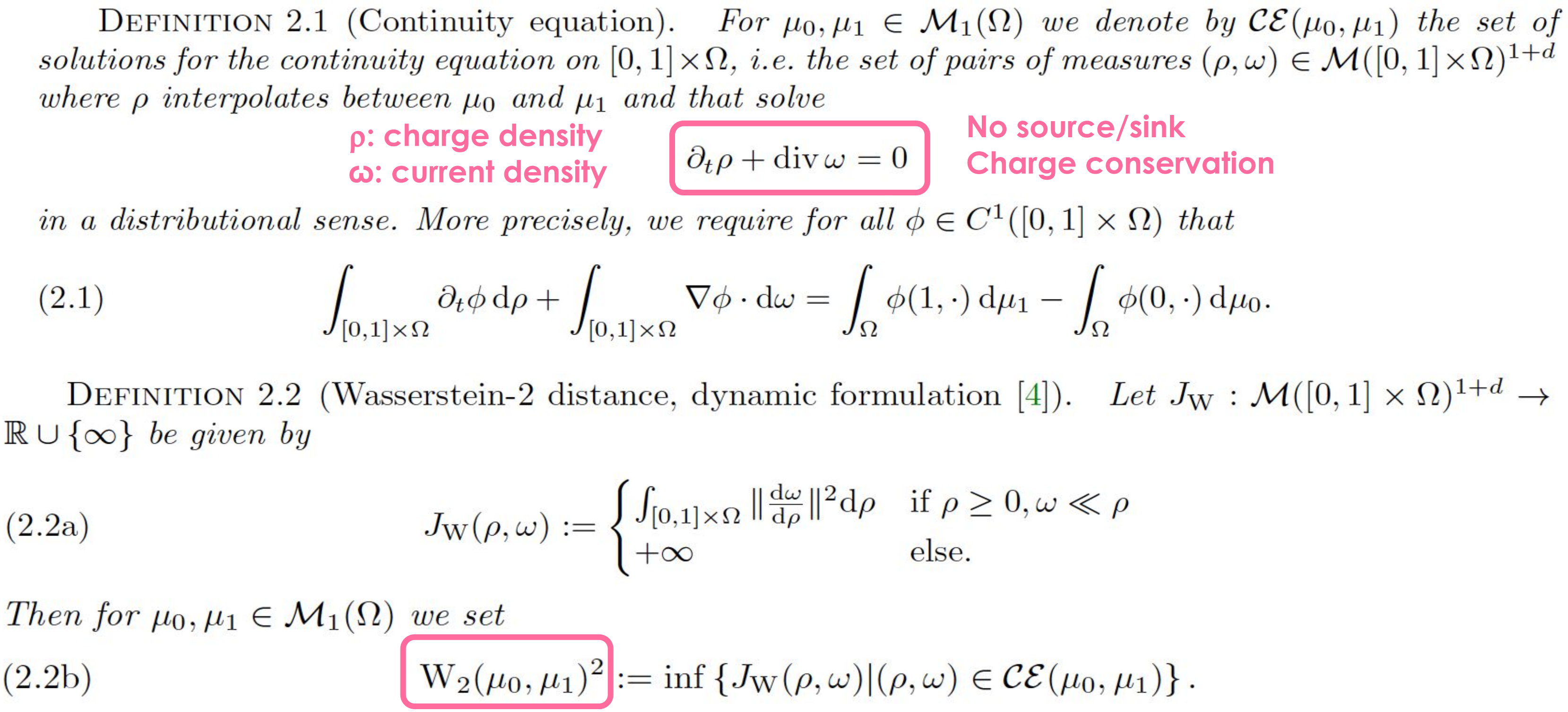
p=1: EMD
p=2: Monge-Kantorovich Distance (W_2); has a (weak) Riemannian structure, thus can be linearized.

Kantorovich formulation (static):

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

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

Benamou-Brenier formulation (dynamic):



Definition 2.1 (Continuity equation). *For $\mu_0, \mu_1 \in \mathcal{M}_1(\Omega)$ we denote by $\mathcal{CE}(\mu_0,\mu_1)$ the set of solutions for the continuity equation on $[0,1]\times\Omega$, i.e. the set of pairs of measures $(\rho,\omega) \in \mathcal{M}([0,1]\times\Omega)^{1+d}$ where ρ interpolates between μ_0 and μ_1 and that solve*

ρ: charge density
ω: current density

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

No source/sink
Charge conservation

in a distributional sense. More precisely, we require for all $\phi \in C^1([0,1]\times\Omega)$ that

$$\int_{[0,1]\times\Omega} \partial_t \phi \, \mathrm{d}\rho + \int_{[0,1]\times\Omega} \nabla\phi \cdot \mathrm{d}\omega = \int_\Omega \phi(1,\cdot)\,\mathrm{d}\mu_1 - \int_\Omega \phi(0,\cdot)\,\mathrm{d}\mu_0. \tag{2.1}$$

Definition 2.2 (Wasserstein-2 distance, dynamic formulation [4]). *Let $J_W : \mathcal{M}([0,1]\times\Omega)^{1+d} \to \mathbb{R}\cup\{\infty\}$ be given by*

$$J_W(\rho,\omega) := \begin{cases} \int_{[0,1]\times\Omega} \|\frac{\mathrm{d}\omega}{\mathrm{d}\rho}\|^2 \mathrm{d}\rho & \text{if } \rho \geq 0, \omega \ll \rho \\ +\infty & \text{else.} \end{cases} \tag{2.2a}$$

Then for $\mu_0, \mu_1 \in \mathcal{M}_1(\Omega)$ we set

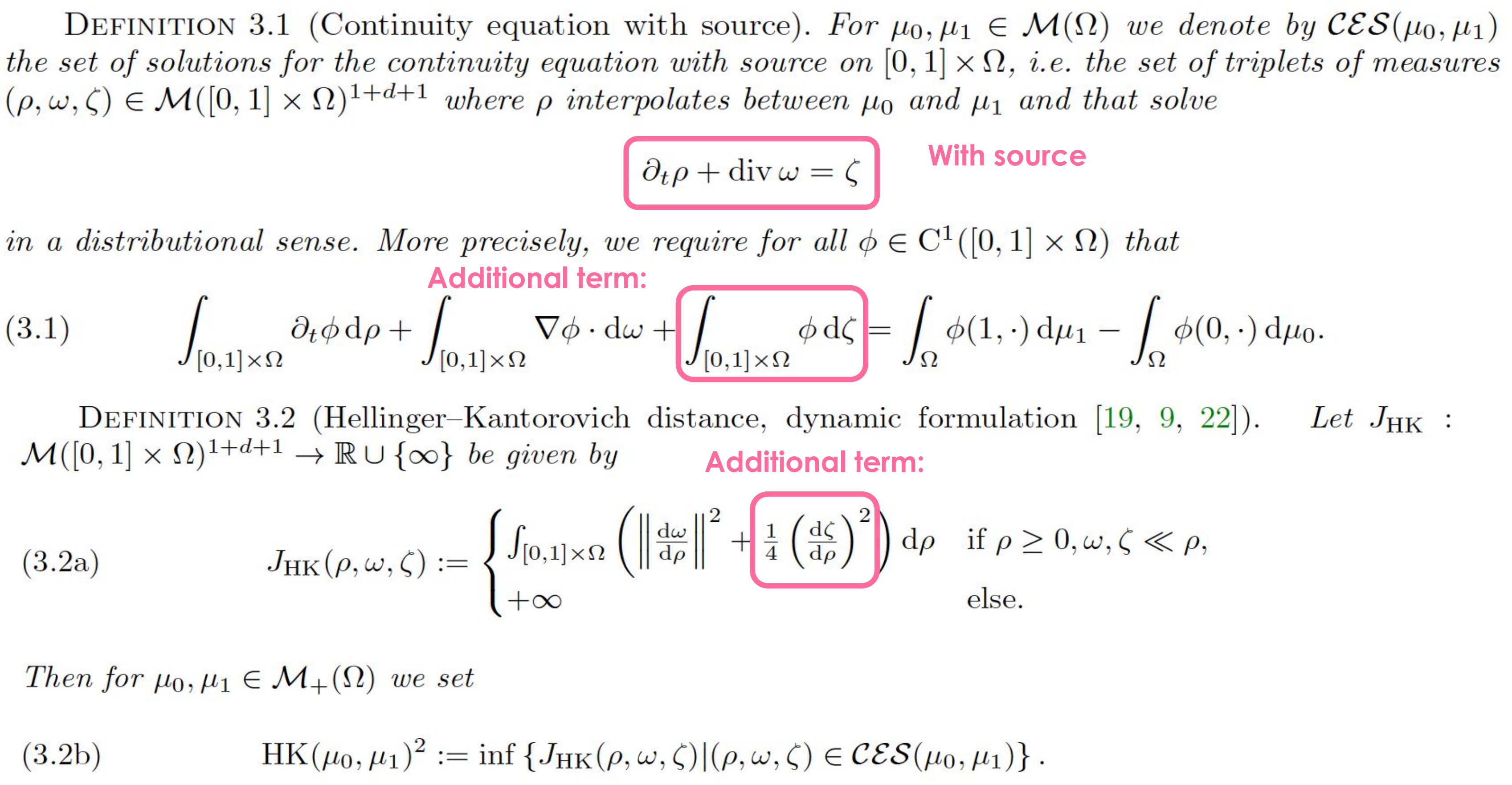
$$\boxed{W_2(\mu_0,\mu_1)^2} := \inf\{J_W(\rho,\omega) | (\rho,\omega) \in \mathcal{CE}(\mu_0,\mu_1)\}. \tag{2.2b}$$

Unbalanced OT

Hellinger-Kantorovich (HK) Distance:

The unbalanced generalization for W$_2$ distance; also enjoys a (weak) Riemannian structure, thus can be linearized.

Benamou-Brenier-type formulation (dynamic):



Definition 3.1 (Continuity equation with source). *For $\mu_0, \mu_1 \in \mathcal{M}(\Omega)$ we denote by $\mathcal{CES}(\mu_0, \mu_1)$ the set of solutions for the continuity equation with source on $[0,1] \times \Omega$, i.e. the set of triplets of measures $(\rho, \omega, \zeta) \in \mathcal{M}([0,1] \times \Omega)^{1+d+1}$ where ρ interpolates between μ_0 and μ_1 and that solve*

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

With source

in a distributional sense. More precisely, we require for all $\phi \in \mathrm{C}^1([0,1] \times \Omega)$ that

Additional term:

$$\int_{[0,1]\times\Omega} \partial_t \phi \, \mathrm{d}\rho + \int_{[0,1]\times\Omega} \nabla \phi \cdot \mathrm{d}\omega + \boxed{\int_{[0,1]\times\Omega} \phi \, \mathrm{d}\zeta} = \int_\Omega \phi(1, \cdot) \, \mathrm{d}\mu_1 - \int_\Omega \phi(0, \cdot) \, \mathrm{d}\mu_0. \tag{3.1}$$

Definition 3.2 (Hellinger–Kantorovich distance, dynamic formulation [19, 9, 22]). *Let $J_{\mathrm{HK}} : \mathcal{M}([0,1] \times \Omega)^{1+d+1} \to \mathbb{R} \cup \{\infty\}$ be given by*

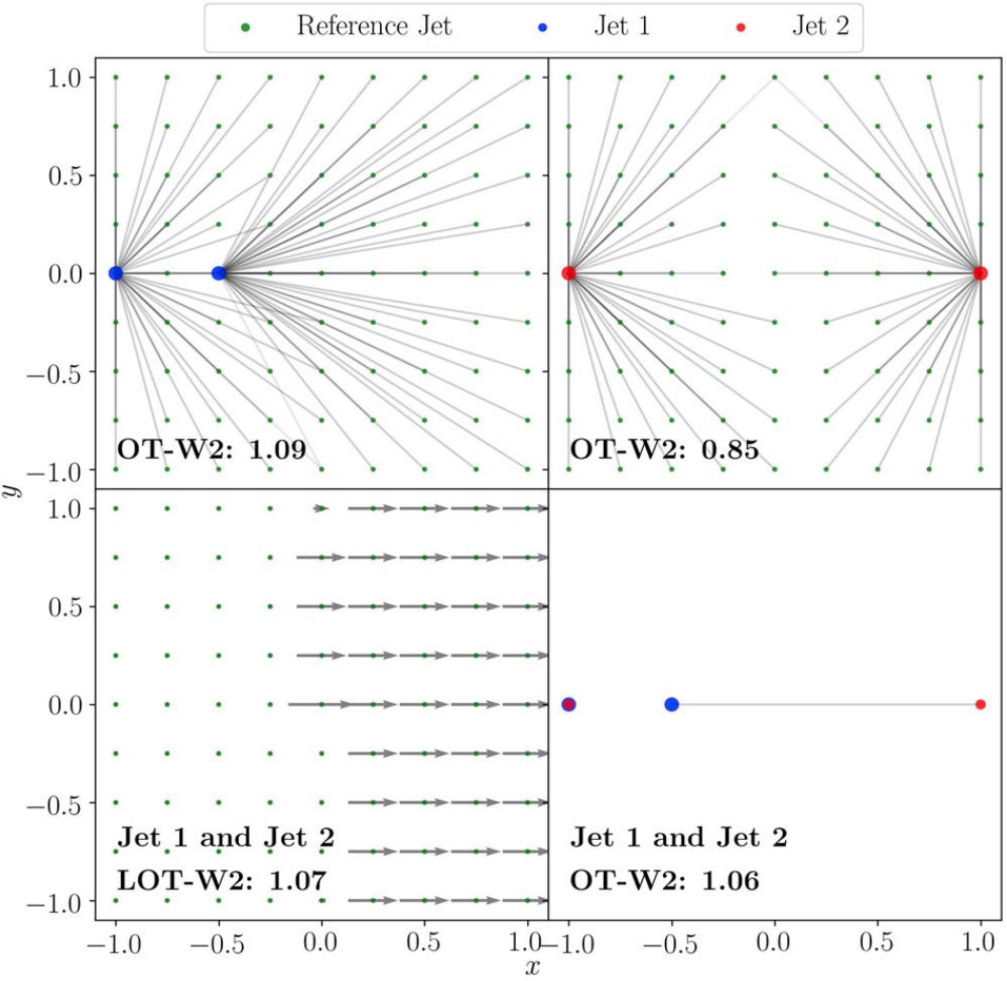
Additional term:

$$J_{\mathrm{HK}}(\rho, \omega, \zeta) := \begin{cases} \int_{[0,1]\times\Omega} \left(\left\| \frac{\mathrm{d}\omega}{\mathrm{d}\rho} \right\|^2 + \boxed{\frac{1}{4} \left(\frac{\mathrm{d}\zeta}{\mathrm{d}\rho} \right)^2} \right) \mathrm{d}\rho & \text{if } \rho \geq 0, \omega, \zeta \ll \rho, \\ +\infty & \text{else.} \end{cases} \tag{3.2a}$$

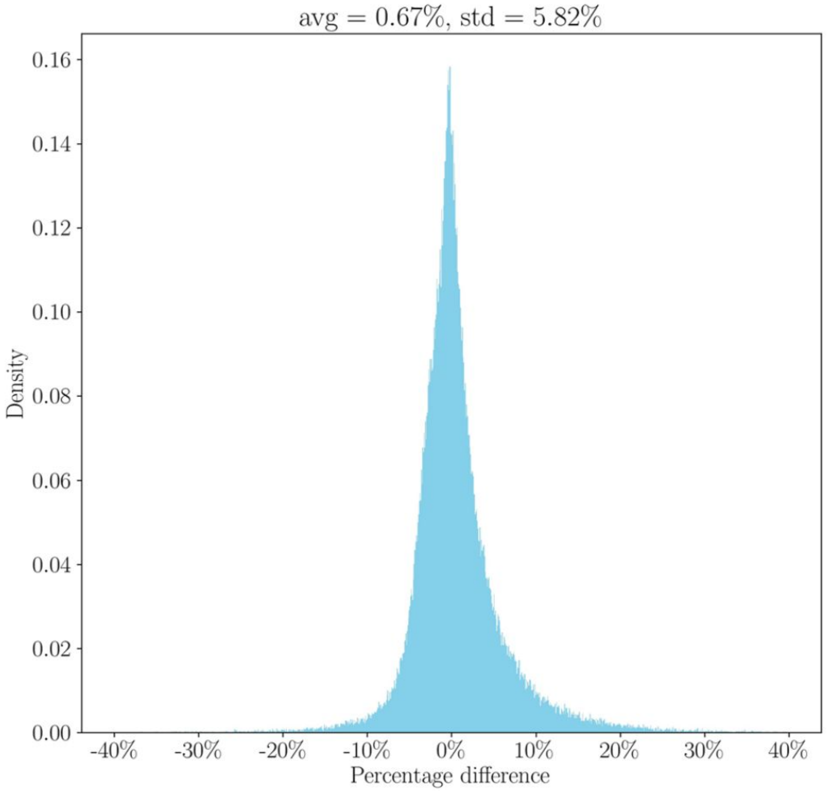
Then for $\mu_0, \mu_1 \in \mathcal{M}_+(\Omega)$ we set

$$\mathrm{HK}(\mu_0, \mu_1)^2 := \inf \left\{ J_{\mathrm{HK}}(\rho, \omega, \zeta) \middle| (\rho, \omega, \zeta) \in \mathcal{CES}(\mu_0, \mu_1) \right\}. \tag{3.2b}$$

Linearized Optimal Transport for W_2



Difference between LOT-W_2 and W_2 distances for 500 W and QCD jets.



LOT for W_2: Computation

Ref Jet: $\sigma = \sum_{k=1}^{N_\sigma} q_k \delta_{z_k}$

Jet 1: $\mu = \sum_{i=1}^{N_\mu} m_i \delta_{x_i}$

Jet 2: $\nu = \sum_{j=1}^{N_\nu} p_j \delta_{x_j}$

Normalize jet p_T to 1.

Compute OT plans f and g with respect to the ref jet where the **ground metric** is the Euclidean distance squared in the y-phi plane.

Compute Barycenters:

$$\bar{x}_k = \frac{1}{q_k} \sum_{i=1}^{N_\mu} f_{k,i} x_i \quad \text{and} \quad \bar{y}_k = \frac{1}{q_k} \sum_{j=1}^{N_\nu} g_{k,j} y_j$$

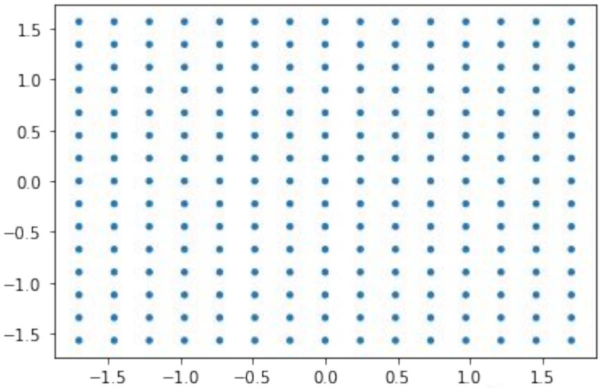
LOT distance between Jet 1 and 2:

$$\boxed{d_{aLOT,\sigma}(\mu,\nu)^2 = \min_{\substack{f \in \Pi_{OT}(\sigma,\mu) \\ g \in \Pi_{OT}(\sigma,\nu)}} \sum_{k=1}^{N_\sigma} q_k |\bar{x}_k - \bar{y}_k|^2}$$

Linear Coord for Jets: $\boxed{\mathbf{x}_n = \left(\sqrt{q_1} a_n^1 \cdots \sqrt{q_{N_\sigma}} a_n^{N_\sigma}\right)^T}$

Where a's are the barycenters of the jet.

Our Default Uniform Ref Jet:
225 (15*15) constituent particles
Jet pt = 525 GeV
|y| <= 1.7
|phi| <= pi/2



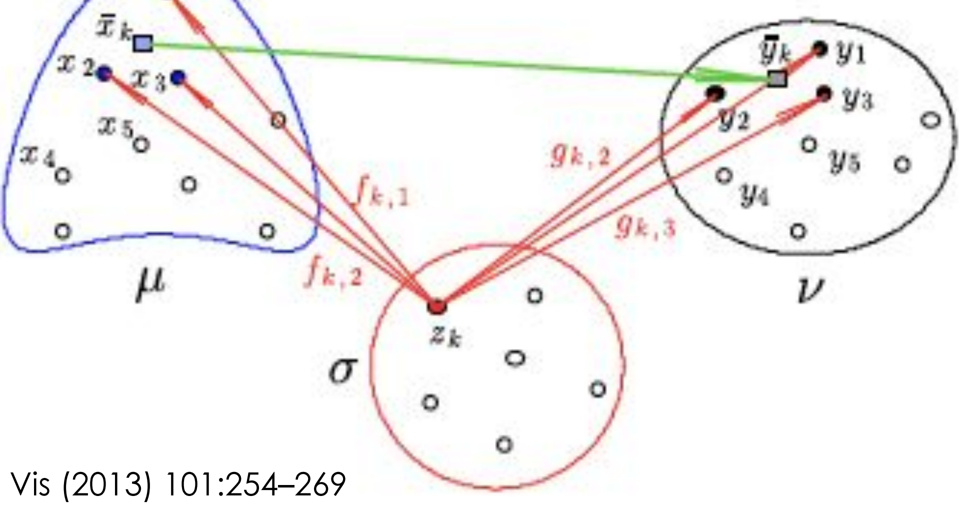


Fig 5, Wei Wang et al. / Int J Comput Vis (2013) 101:254–269

Jet Tagging: Procedure

- **Goal:**
  - Study the performance of **LOT-W_2** distance paired with various ML models on a number of different jet tagging tasks.
  - Study the effect of the length scale **κ in [0.01, 100]** of **LOT-HK** distances on the tagging task of W and QCD discrimination.

- **Tagging Tasks:**
  - W v.s. QCD jets (primary)
  - t v.s. QCD, t v.s. W
  - Higgs v.s. QCD, Higgs v.s. W

$$q\bar{q} \rightarrow Z(\rightarrow \nu\bar{\nu}) + H(\rightarrow b\bar{b})$$

  - BSM v.s. QCD, BSM v.s. W

"BSM": Color sextet scalar

$$q\bar{q} \rightarrow \phi\bar{\phi}$$

$$\phi \rightarrow qq$$

$$m_\phi = 100\,\mathrm{GeV}$$

$$\Gamma_\phi = 2\,\mathrm{GeV}$$

- **Data Generation:**
  - **MadGraph** 2.6.7: pp collisions at **$\sqrt{s}$ = 14 TeV**
  - **Pythia** 8.243: Hadronization, multiparton interactions on with default tuning and showering parameters. No detector simulation.
  - **FastJet** 3.3.2: **anti-kt (R=1.0)**. Up to three jets with **p_T in 500-550 GeV** and **$|y|$<1.7** are kept.

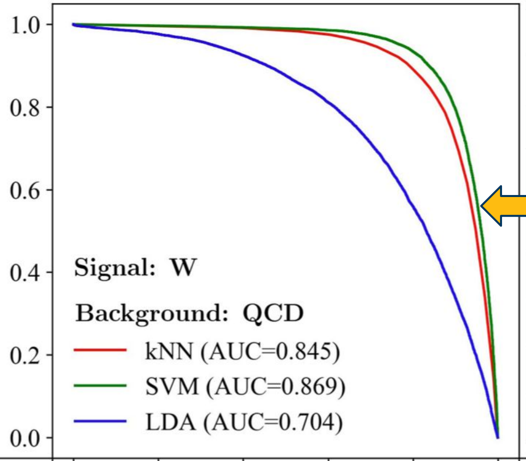
- **Jet Preprocessing:**
  - Centering the jet axis
  - Rotation: vertically align the principal component of the constituent p_T in the y-phi plane.

- **LOT Computation:** with a uniform ref jet of 15*15 particles

- **ML Models:**
  - **LDA:** Supervised Classification & Visualization
  - **kNN:** Supervised Classification
    - k in [10, 1000], increment 10
  - **SVM:** Supervised Classification
    - C, γ in [10^{-5}, 10^{5}], increment 10

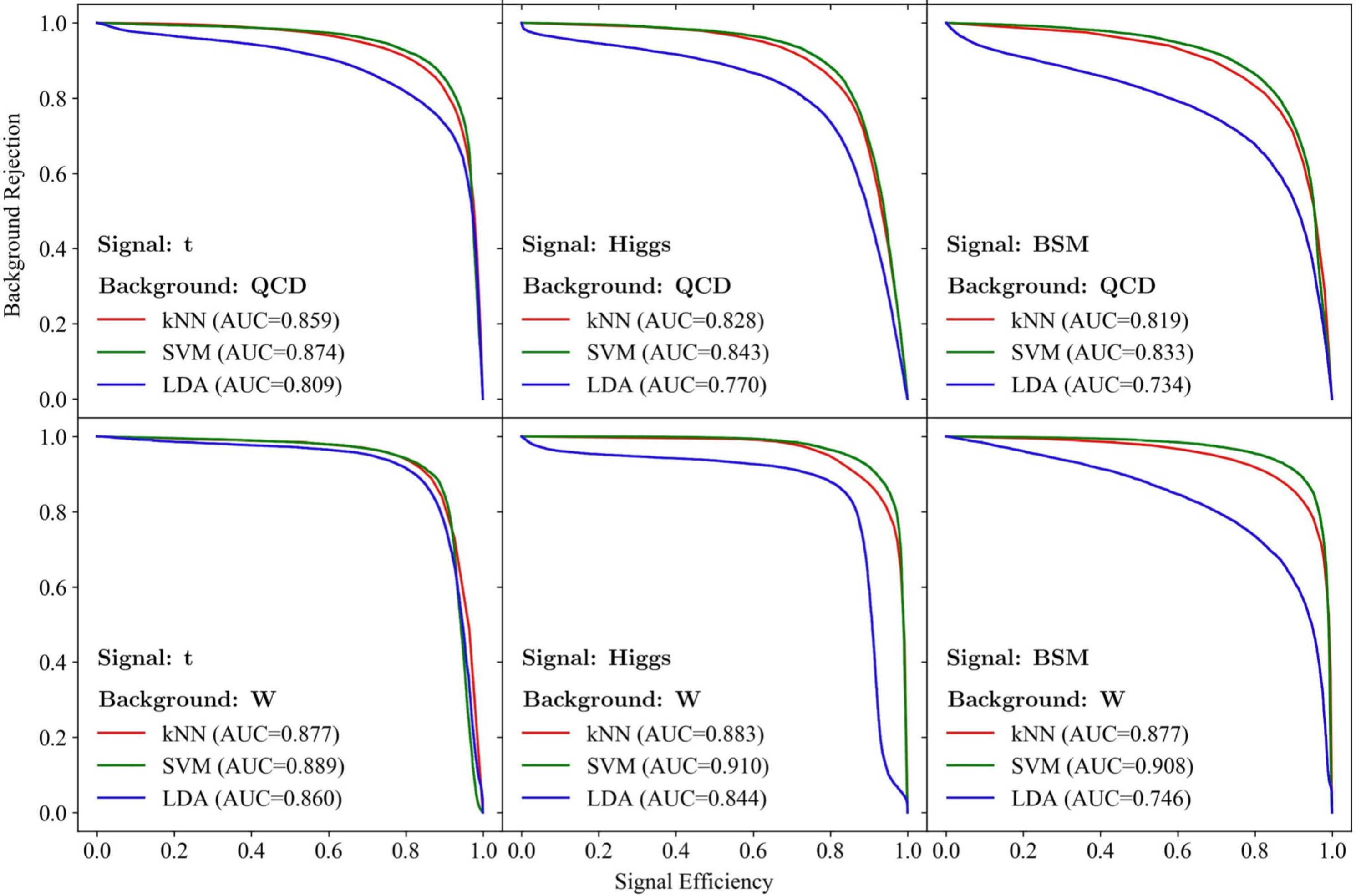
Full datasets: 140k jets in total for each task (balanced). **Sample datasets: 10k** jets for each task (balanced). Used to pick hyper-parameters of ML models for LOT-W_2, but as the full datasets for LOT-HK.

OT for Jet Tagging: ML with LOT-W_2 for 7 tasks



Datasets	Model	AUC
Our work	$k_{=20}$NN-LOT	0.845
	SVM-LOT	0.869
	LDA-LOT	0.704
Komiske, Metodiev, Thaler 1902.02346	$k_{=32}$NN-EMD	0.887
	$\tau_2^{\beta=1}$ / $\tau_1^{\beta=1}$	0.776
	PFN	0.919
	EFPs	0.917
	EFN	0.904

Comparison with other methods



140k jets whose p_T is in **500-550** GeV, using **15*15** uniform reference

Jet Tagging: ML with LOT-W_2 for W v.s. QCD

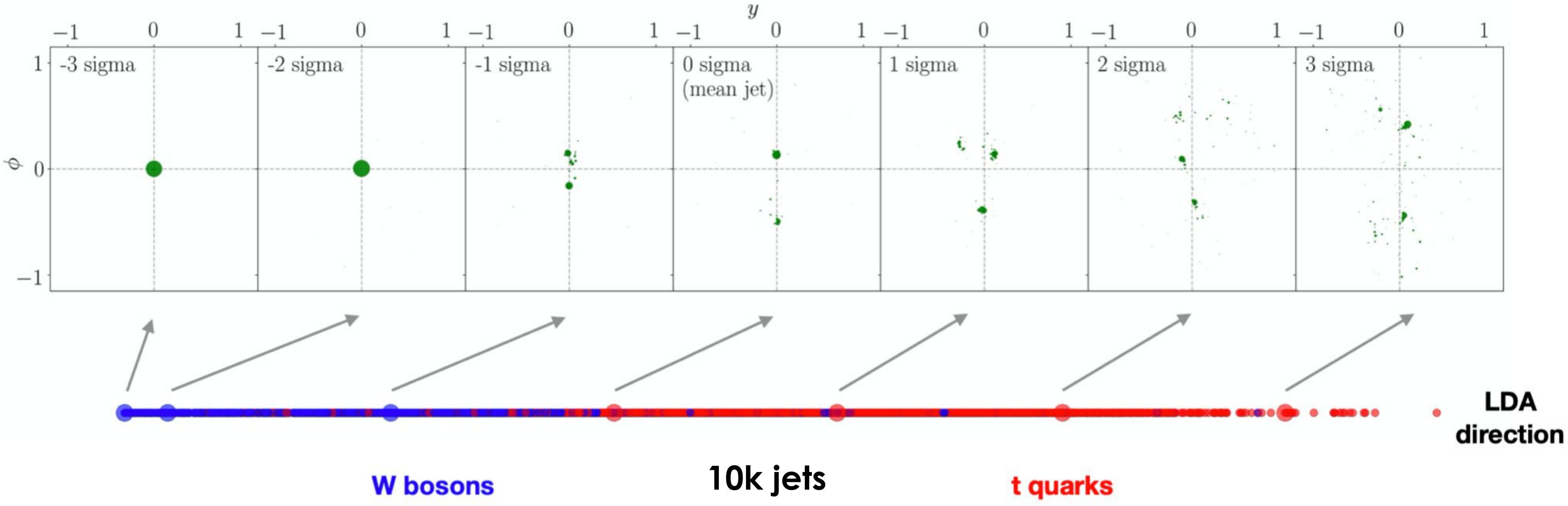
On Sample Dataset (10k jets):

Model	AUC	Best Hyper-param
kNN	0.819	k=20
SVM	0.841	C=1, gamma=100
LDA	0.690	N/A

On Full Dataset (140k jets):

Model	TPR	FPR	Approx. Run Time
kNN	0.803	0.112	4 hours
SVM	0.845	0.108	6 hours
LDA	0.716	0.308	seconds

Jet Tagging: LDA Visualization with LOT-W_2 for t v.s. W



LDA direction

W bosons

10k jets

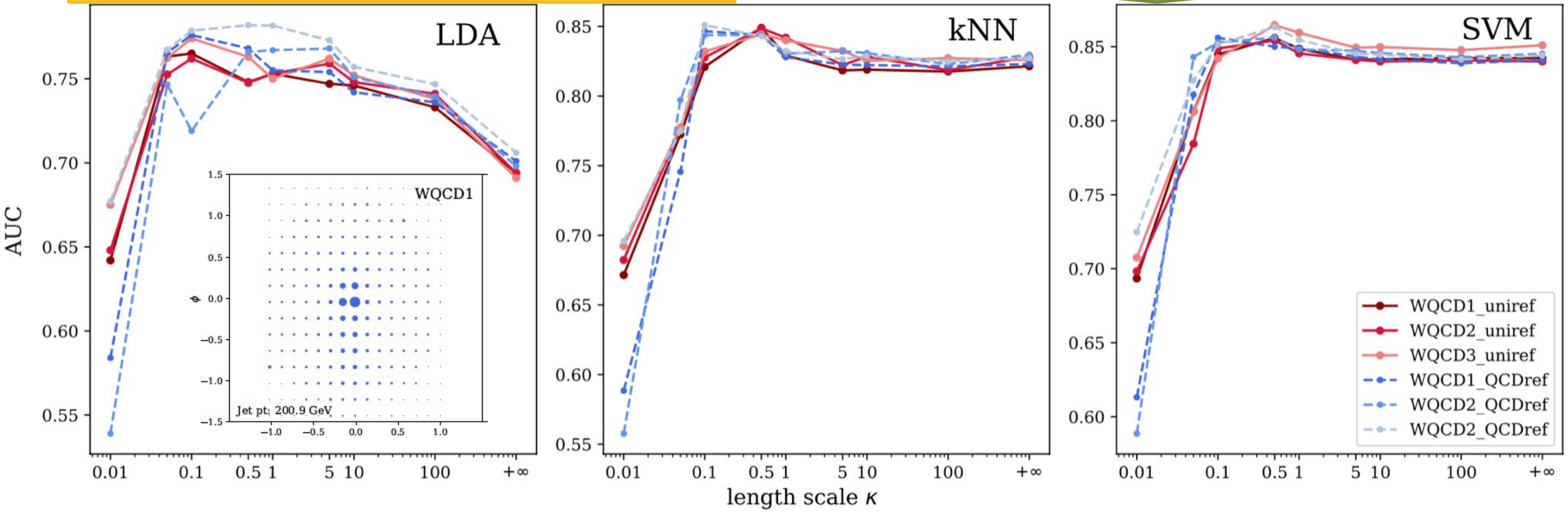
t quarks

Jet Tagging: ML with LOT-HK of various κ for W v.s. QCD

	length scale κ	$+\infty$	100	10	5	1	0.7	0.5	0.3	0.1	0.05	0.01
LDA	**AUC**	**0.694**	**0.733**	**0.746**	**0.747**	**0.752**	**0.751**	**0.748**	**0.760**	**0.765**	**0.763**	**0.642**
	TPR	0.684	0.684	0.703	0.721	0.724	0.740	0.736	0.692	0.704	0.731	0.770
	FPR	0.296	0.218	0.211	0.226	0.220	0.239	0.239	0.171	0.174	0.205	0.486
	run time	several seconds										
kNN [10, 200]	**AUC**	**0.821**	**0.818**	**0.819**	**0.818**	**0.829**	**0.841**	**0.849**	**0.847**	**0.821**	**0.772**	**0.671**
	TPR	0.771	0.763	0.768	0.763	0.760	0.791	0.798	0.809	0.821	0.783	0.733
	FPR	0.128	0.127	0.130	0.126	0.102	0.110	0.100	0.114	0.181	0.238	0.390
	hyperpar. k	30	20	30	20	10	20	10	20	10	10	30
	run time	1.5 hours										
SVM	**AUC**	**0.842**	**0.842**	**0.842**	**0.841**	**0.849**	**0.851**	**0.856**	**0.853**	**0.845**	**0.806**	**0.694**
	TPR	0.817	0.819	0.817	0.819	0.823	0.829	0.832	0.829	0.788	0.741	0.787
	FPR	0.133	0.134	0.134	0.137	0.126	0.127	0.120	0.124	0.099	0.128	0.401
	hyperpar. C	1	1	1	1	1	1	1	1	1	10	10
	hyperpar. γ	100	100	100	100	100	100	100	100	1000	1000	100000
	run time	5 hours										

Results for the WQCD1 (10k jets)dataset using the uniform reference jet

Results for three WQCD datasets using the uniform or the QCD-average reference jet


LDA
kNN
SVM
AUC
+∞
length scale κ
WQCD1
Jet pt: 200.9 GeV
φ
WQCD1_uniref
WQCD2_uniref
WQCD3_uniref
WQCD1_QCDref
WQCD2_QCDref
WQCD2_QCDref