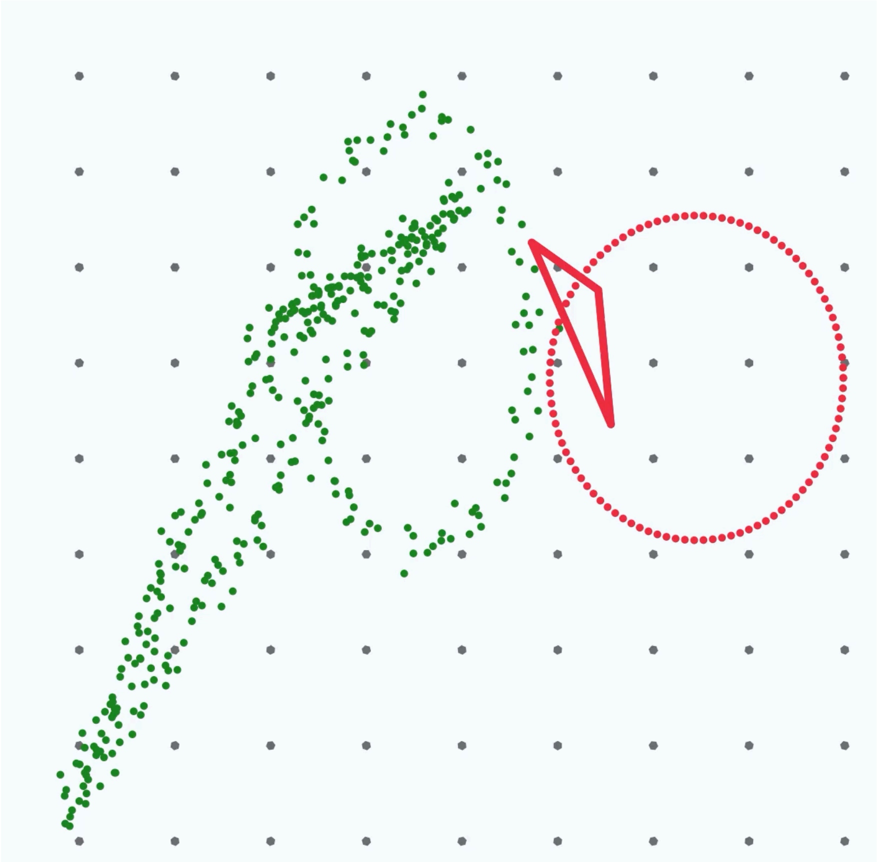
Neural Estimation of Energy Mover's Distance

NEEMo

Ouail Kitouni

Fitting Arbitrary Geometries



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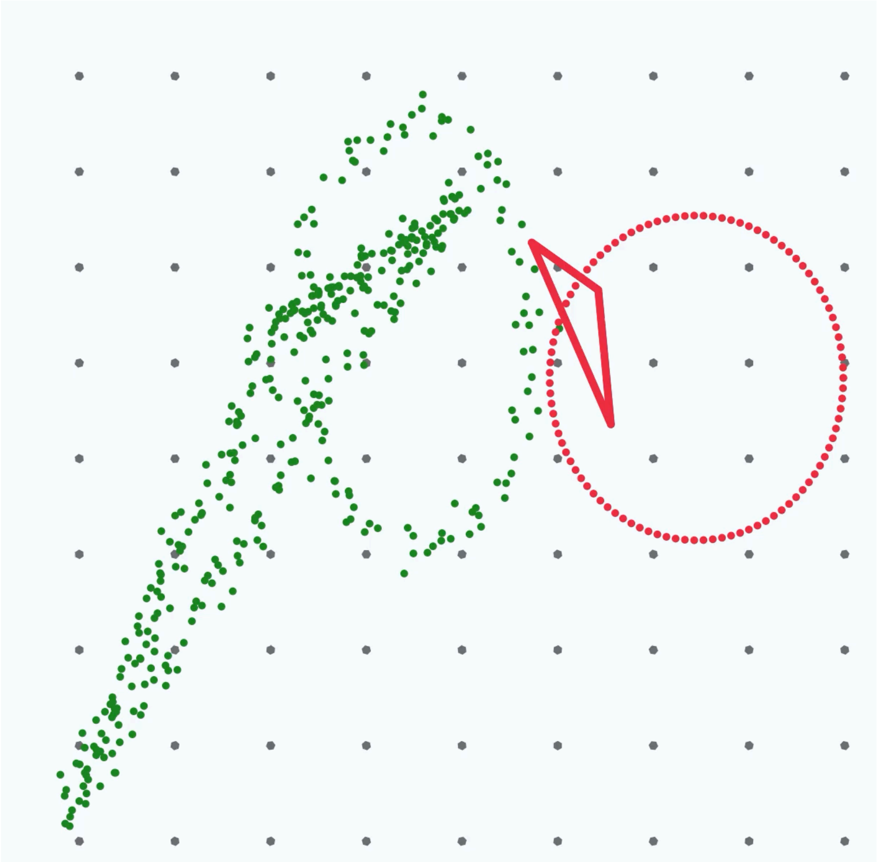

Robust and Provably Monotonic Networks

Ouail Kitouni[*], Niklas Nolte[*], Mike Williams
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Laboratory for Nuclear Science, MIT

Finding NEEMo: Geometric Fitting using Neural Estimation of the Energy Mover's Distance

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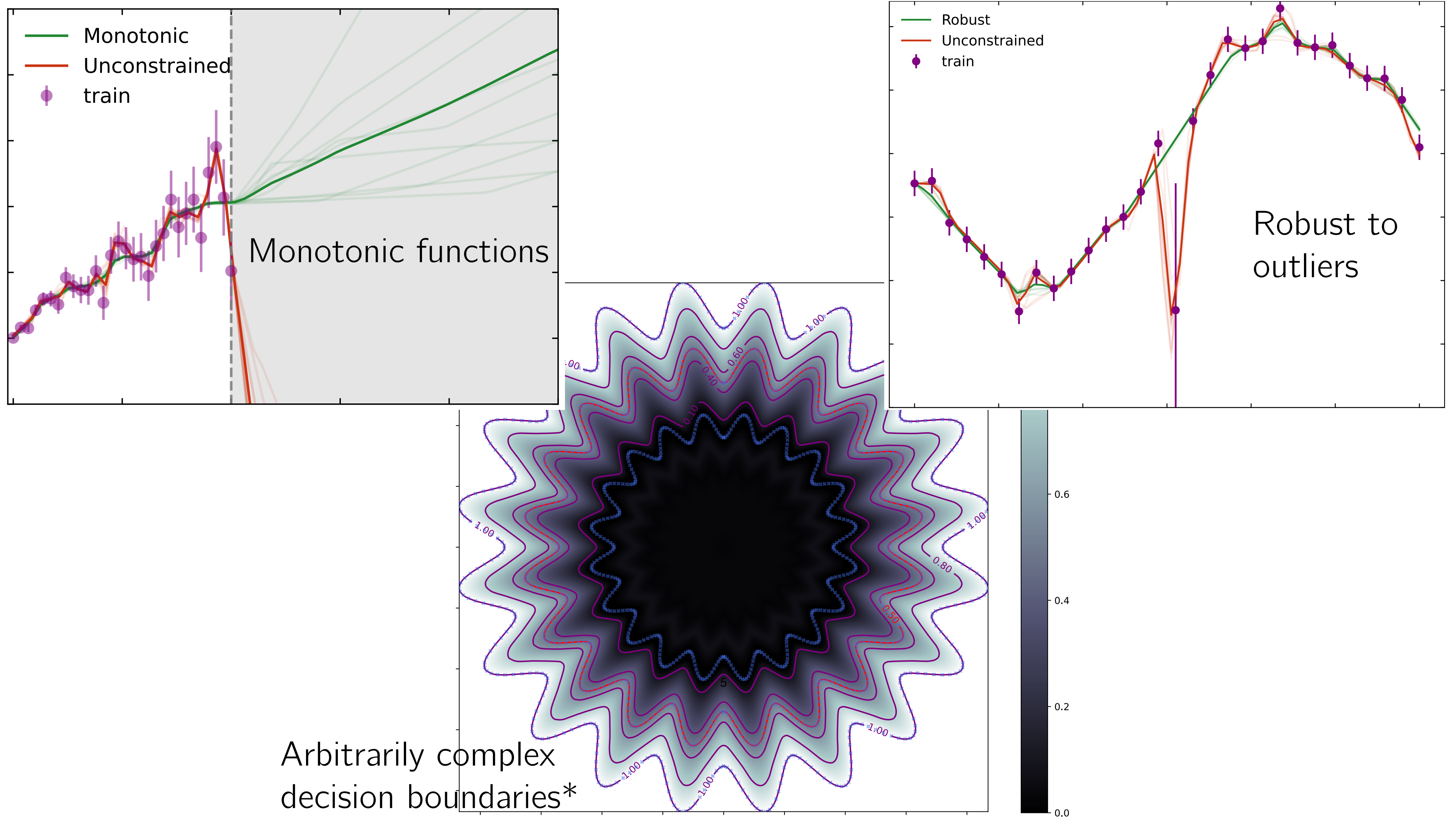
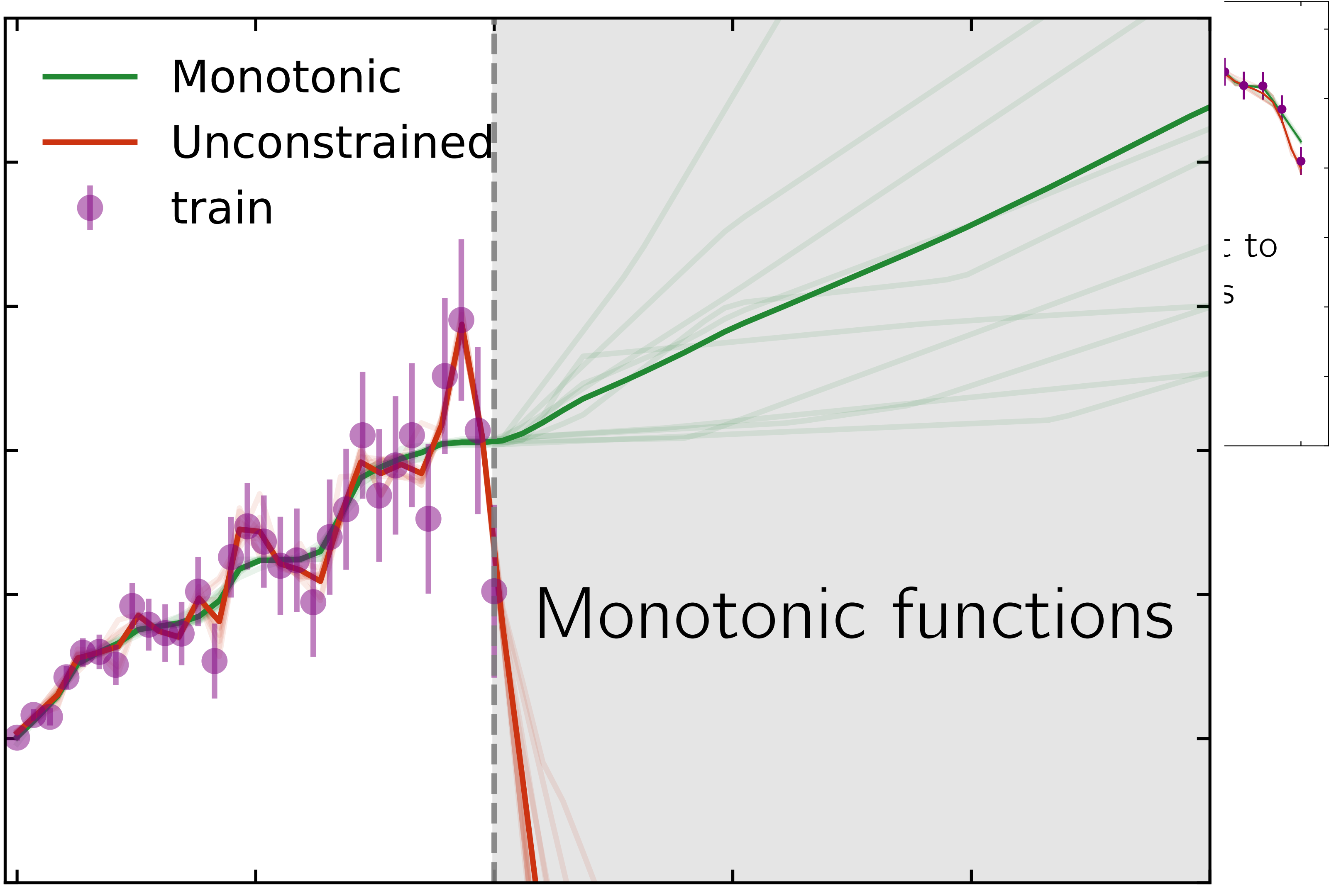
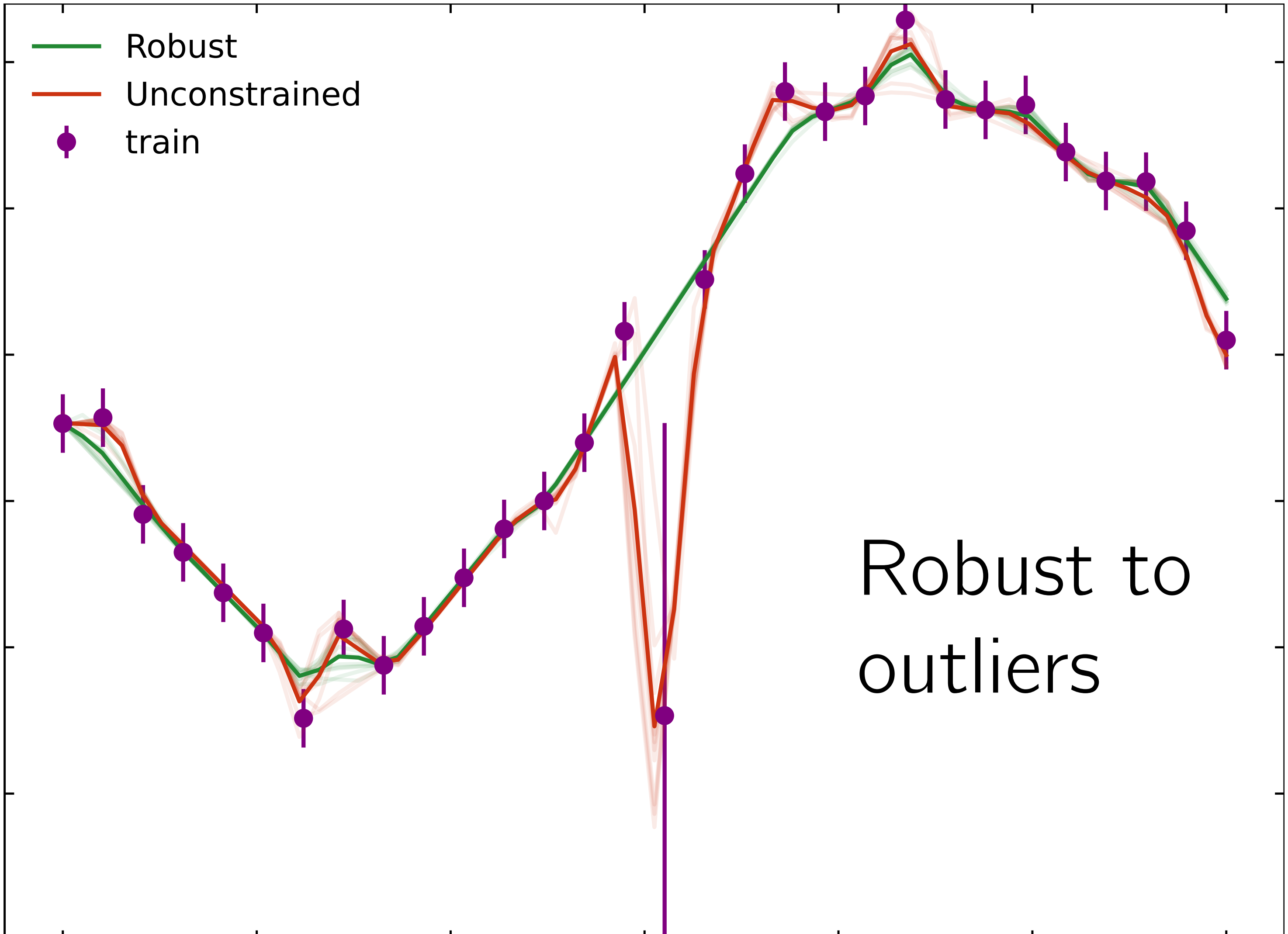
Part 1
Lipschitz
Networks


Monotonic
Unconstrained
train
Monotonic functions
Robust
Unconstrained
train
Robust to outliers
Arbitrarily complex decision boundaries*
1.00
0.60
0.40
0.10
0.80
0.50
0.6
0.4
0.2
0.0



Monotonic
Unconstrained
train
Monotonic functions


Robust
Unconstrained
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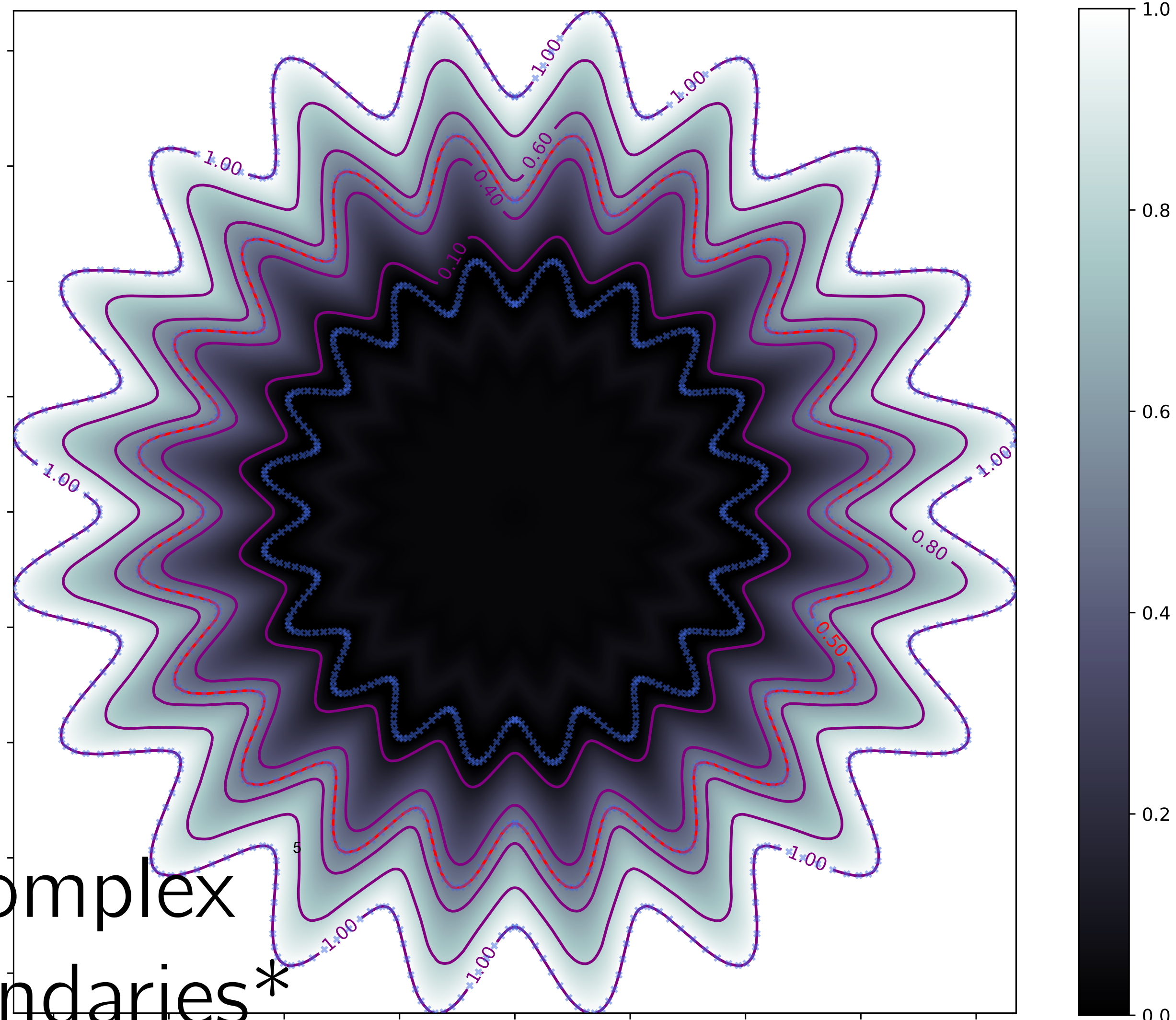
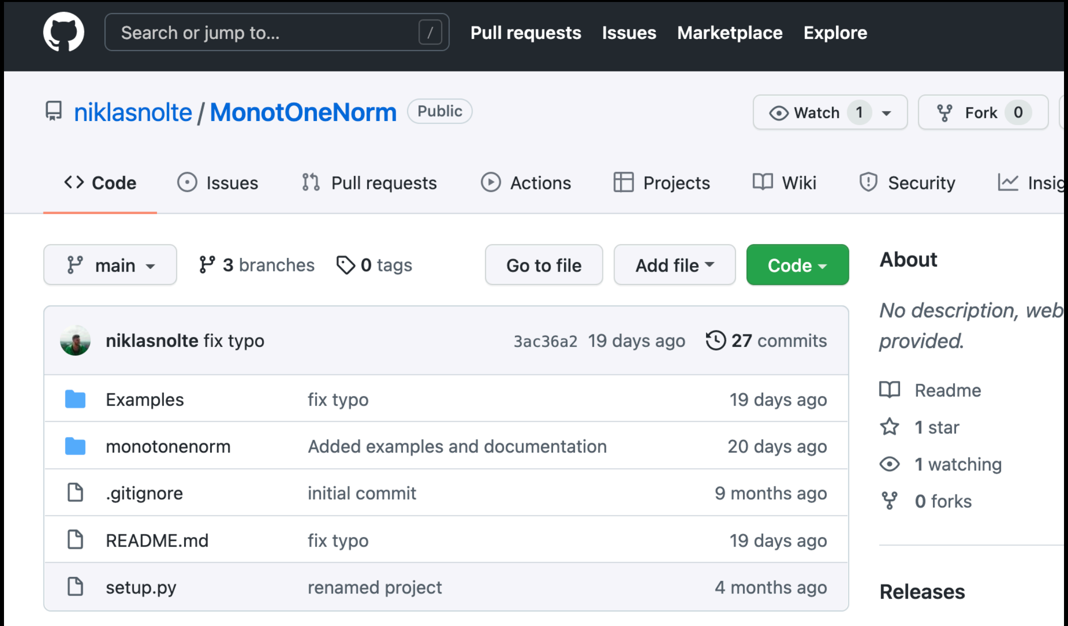


Arbitrarily complex decision boundaries*

MontoneNorm



https://github.com/niklasnolte/MonotOneNorm

pip install monotonenorm
conda install monotonenorm -c okitouni

How does it work?

Robustness: Definition (more formally)

Small changes in the input should not lead to large changes in the output:

$$|f(x+\epsilon) - f(x)| \leq \lambda\epsilon \qquad \forall \epsilon > 0$$

Thus we would like our Neural Network to represent a Lipschitz continuous function.

Robustness: Definition (more formally)

Robustness is achieved by constraining the operator 1-norm of the weight matrices of each layer such that

$$\prod_{l=0}^{L} \|W^l\|_1 \leq \lambda$$

where λ is Lipschitz constant of the resulting network with respect to the ∞-norm.
Universal Lipschitz-λ function approximation requires activations with gradient 1 almost everywhere.
→ **GroupSort***: reorders inputs

*Sorting out Lipschitz function approximation [https://arxiv.org/abs/1811.05381]

Monotonicity using weight norm

g(x) is a λ-Lipschitz neural network. Adding the following residual connection

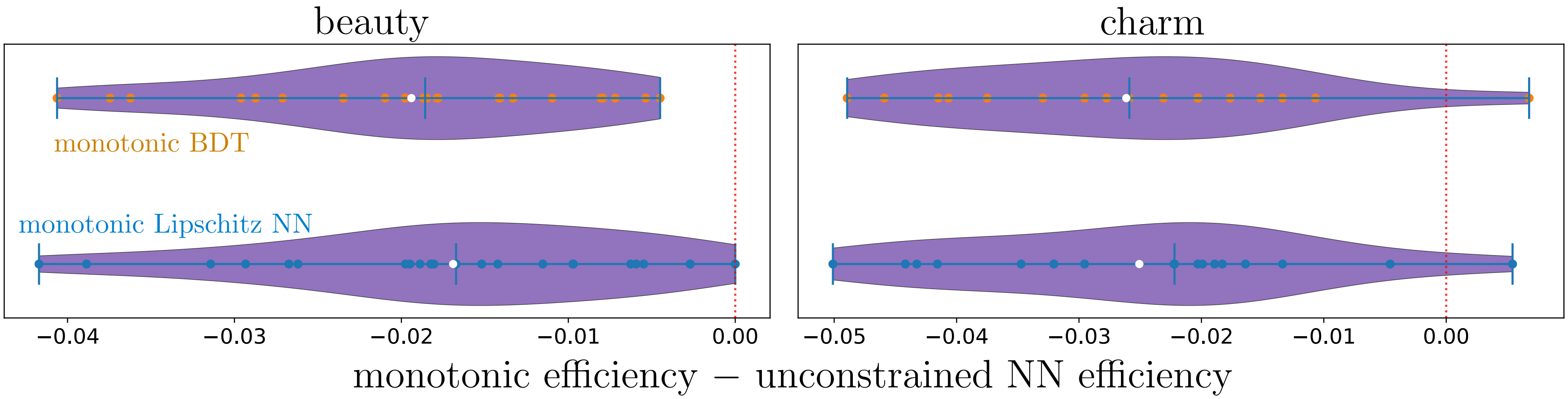
$$f(\mathbf{x}) = g(\mathbf{x}) + \lambda \sum_{i \in I} x_i$$

makes output monotonic since

$$\frac{\partial f}{\partial x_i} = \frac{\partial g}{\partial x_i} g(\mathbf{x}) + \lambda \geq 0 \quad \forall i \in I$$

Monotonic Lipschitz Networks LHCb RUN 3 trigger

This architecture is being used in the LHCb heavy-flavor RUN 3trigger.



Part 2
Neural **E**stimation of **E**nergy **Mo**ver's distance

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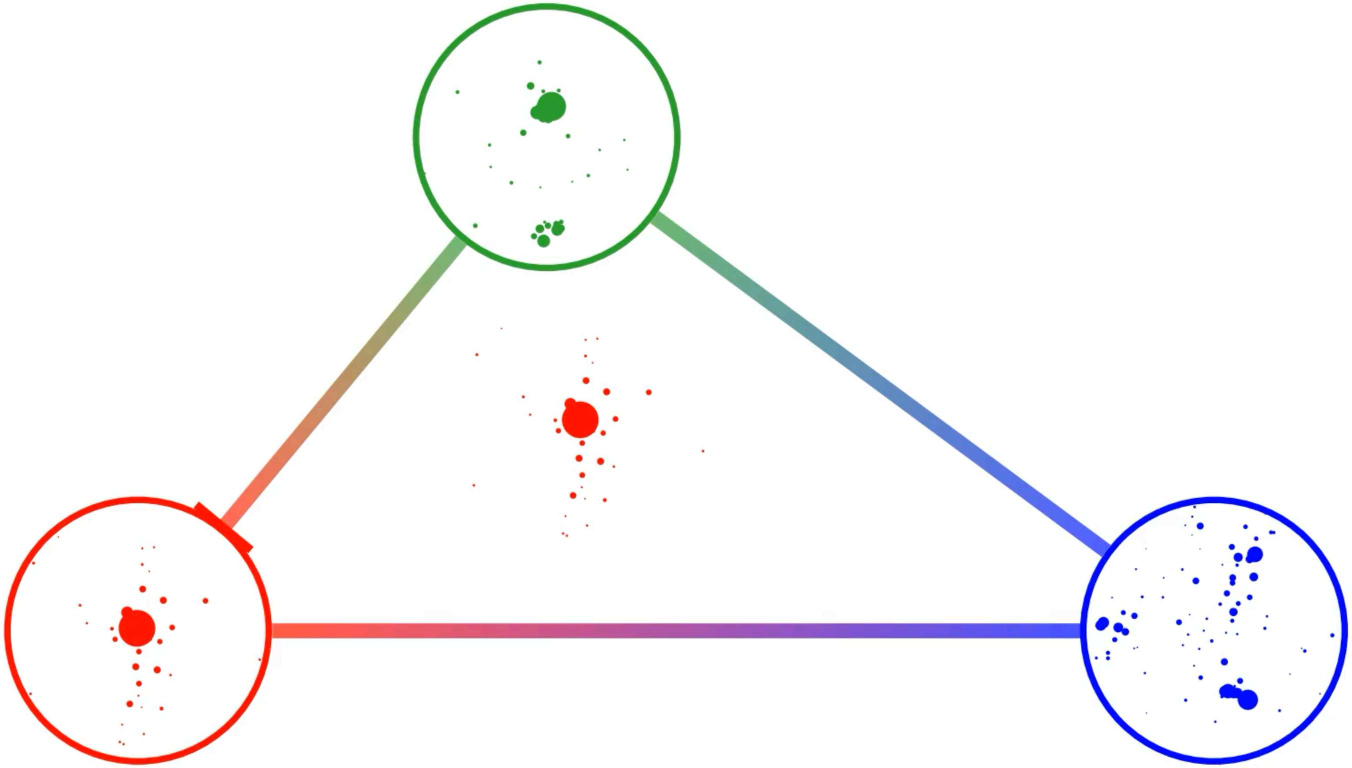
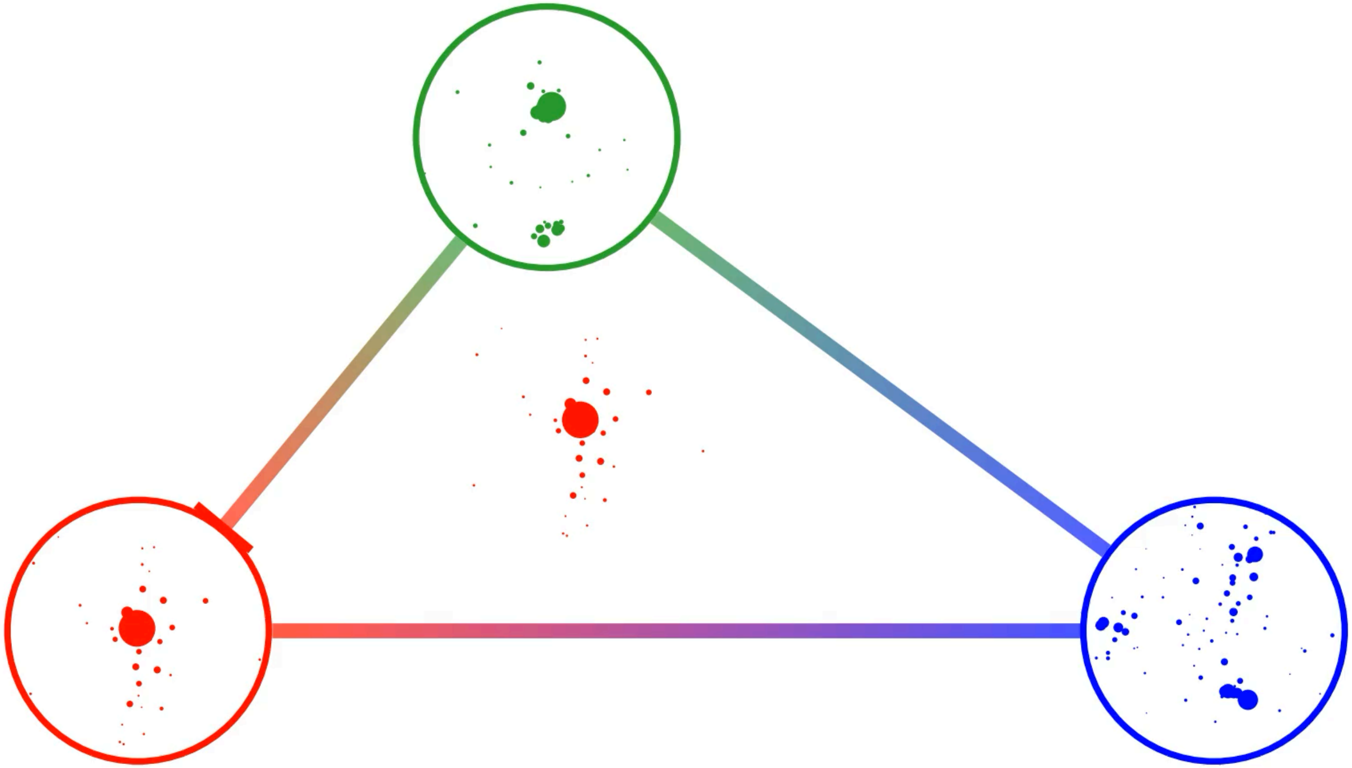
Optimal Transport - Energy Mover's Distance



The Metric Space of Collider Events [arxiv.org/abs/1902.02346]

Optimal Transport - Energy Mover's Distance



The Metric Space of Collider Events [arxiv.org/abs/1902.02346]

Earth Mover's Distance

The primal formulation of the EMD is an optimization over joint probability distributions

$$\mathrm{EMD}(\mathbb{P}, \mathbb{Q}) = \inf_{\gamma \in \Pi(\mathbb{P}, \mathbb{Q})} \mathbb{E}_{(x,y) \sim \gamma} \left[||x - y||_2 \right],$$

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Event 1

Earth Mover's Distance

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Event 1

Event 2

Earth Mover's Distance

The primal formulation of the EMD is an optimization over joint probability distributions

$$\mathrm{EMD}(\underbrace{\mathbb{P}}_{\text{Event 1}}, \underbrace{\mathbb{Q}}_{\text{Event 2}}) = \inf_{\gamma \in \Pi(\mathbb{P},\mathbb{Q})} \mathbb{E}_{(x,y)\sim \underbrace{\gamma}_{\text{Energies}}} \left[||x - y||_2 \right],$$

Earth Mover's Distance

The primal formulation of the EMD is an optimization over joint probability distributions

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Event 1

Event 2

Energies

Spatial Coordinates

Kantorovich-Rubinstein - Dual Formulation

The dual formulation is an optimization over 1-Lipschitz continuous functions

$$\mathrm{EMD}(\mathbb{P}, \mathbb{Q}) = \sup_{||f||_L \leq 1} \mathbb{E}_{x \sim \mathbb{P}}\left[f(x)\right] - \mathbb{E}_{x \sim \mathbb{Q}}\left[f(x)\right],$$

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Kantorovich potential

NEEMo Algorithm

Parametrized shape:

θ

Target Distribution

$\mathbb{Q} = \{e^i, \mathbf{x}^i\}_{i=1}^n$

Forward pass $\longrightarrow$

Backward pass $\dashrightarrow$

NEEMo Algorithm

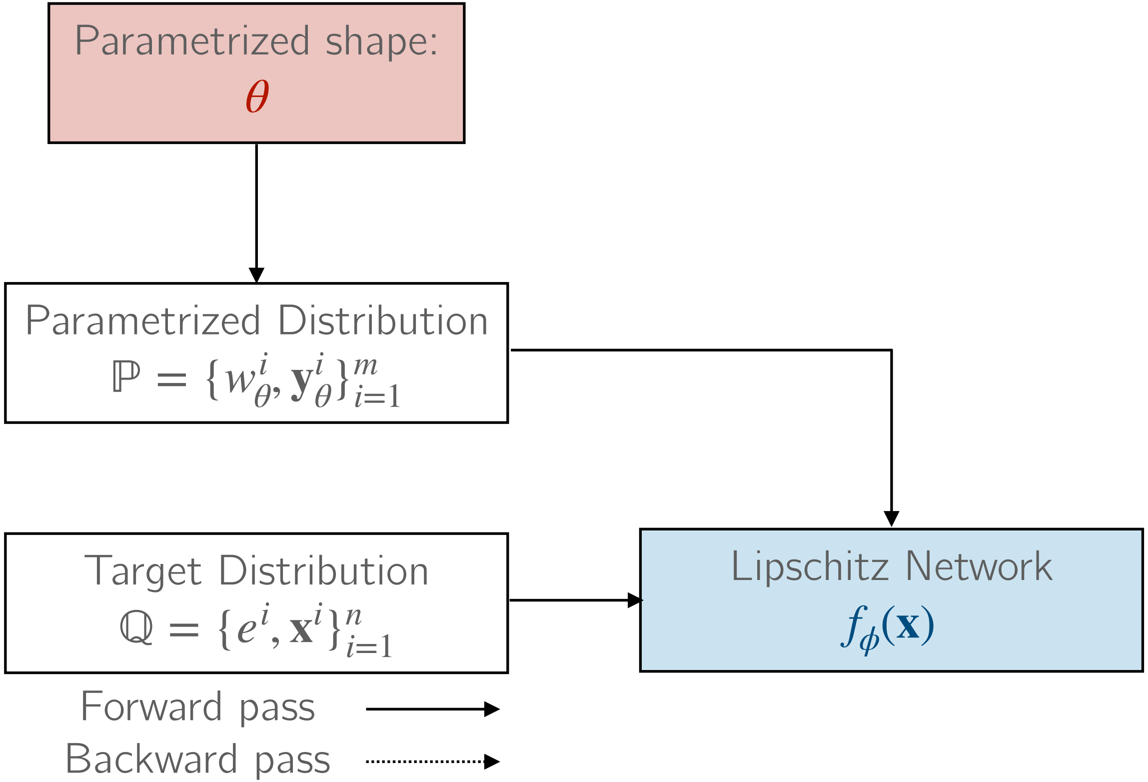
Parametrized shape:
θ

Parametrized Distribution
$\mathbb{P} = \{w_\theta^i, \mathbf{y}_\theta^i\}_{i=1}^m$

Target Distribution
$\mathbb{Q} = \{e^i, \mathbf{x}^i\}_{i=1}^n$

Forward pass $\longrightarrow$
Backward pass $\dashrightarrow$

NEEMo Algorithm



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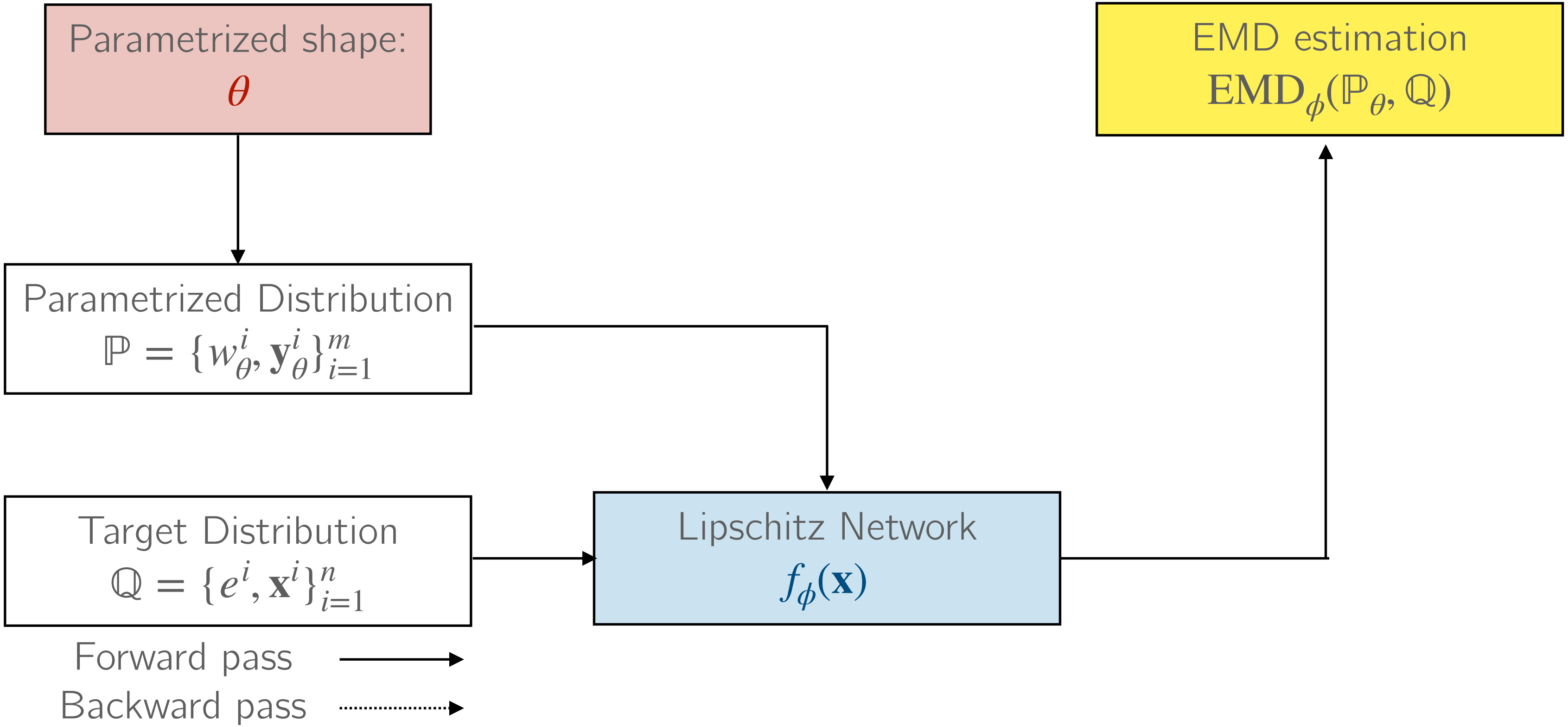

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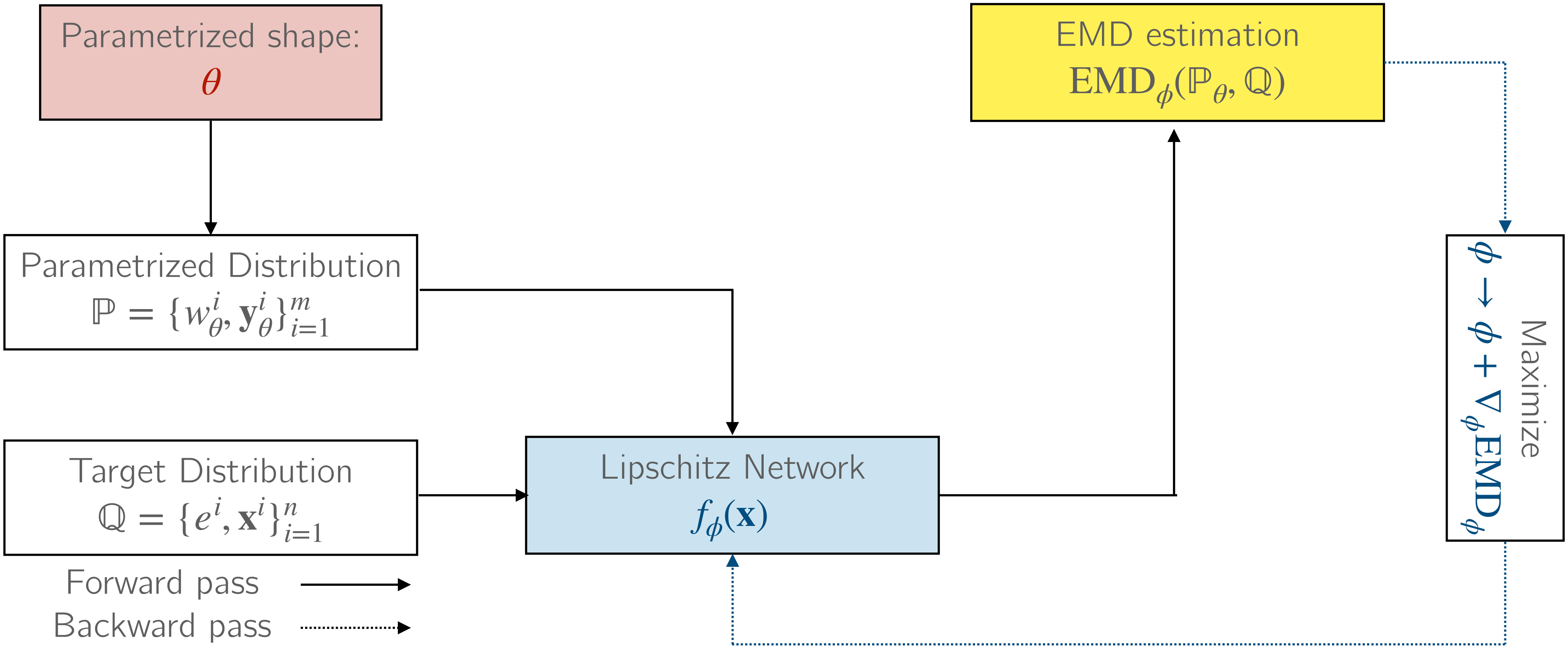

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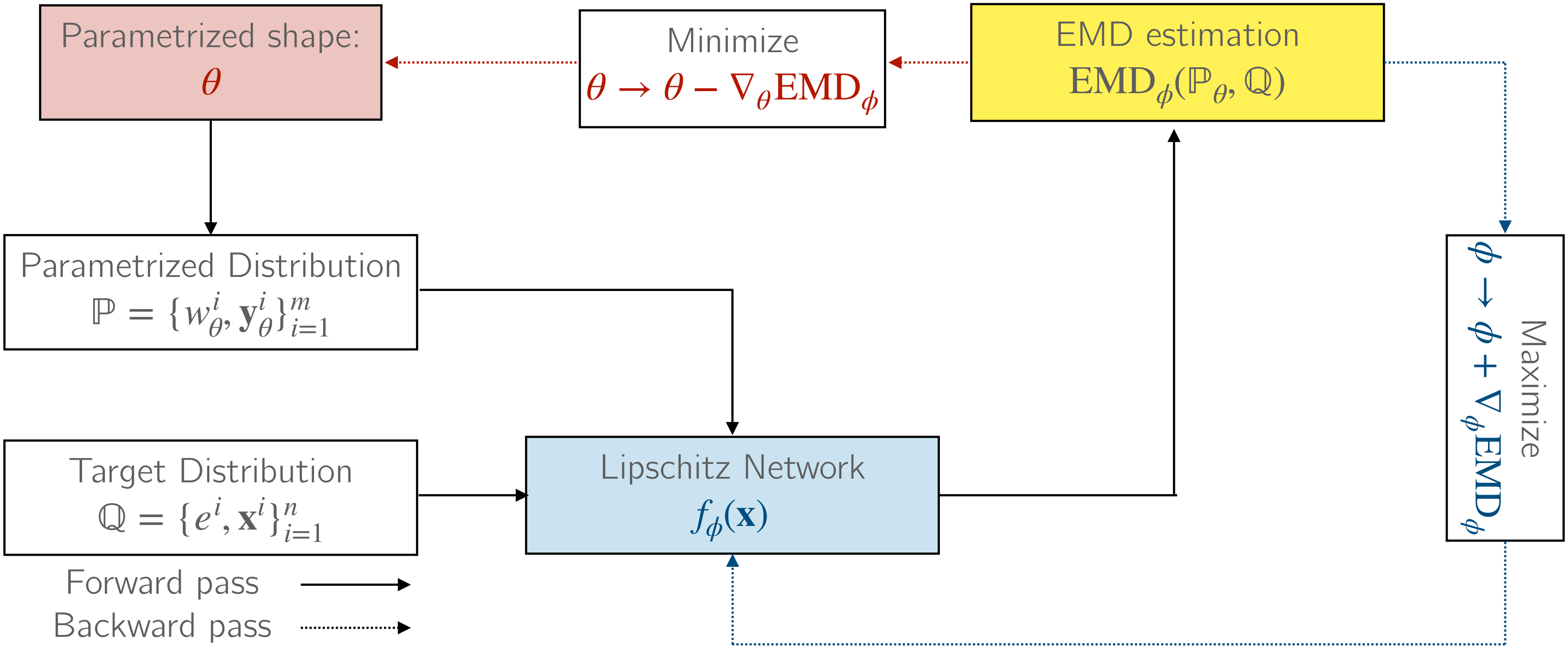

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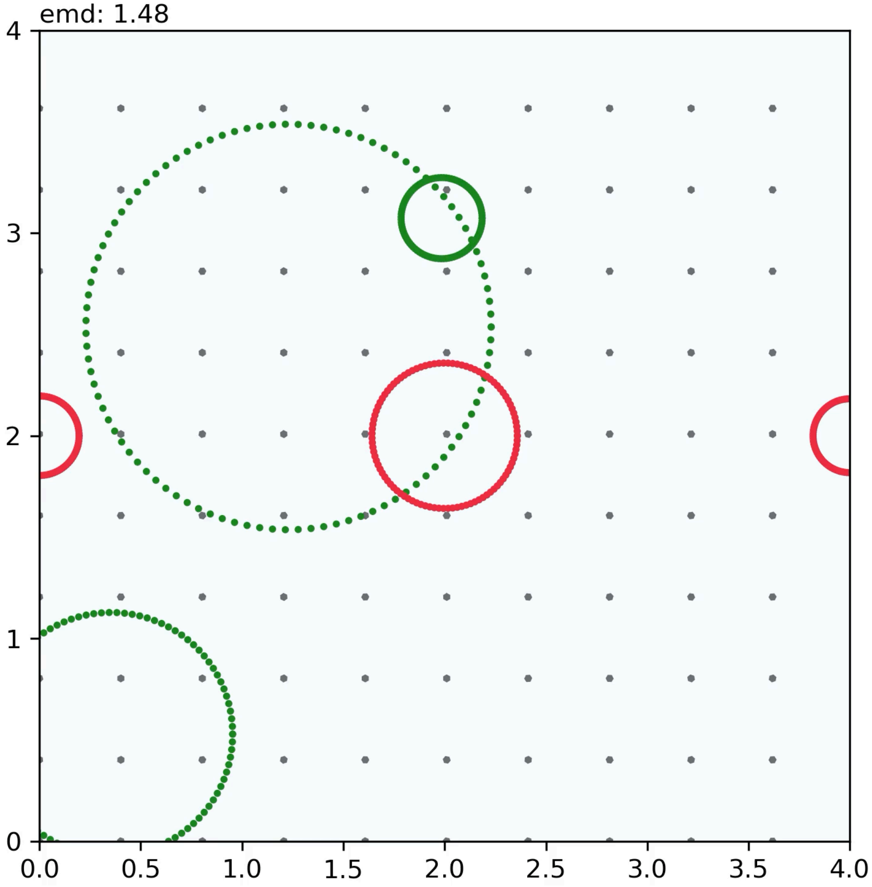

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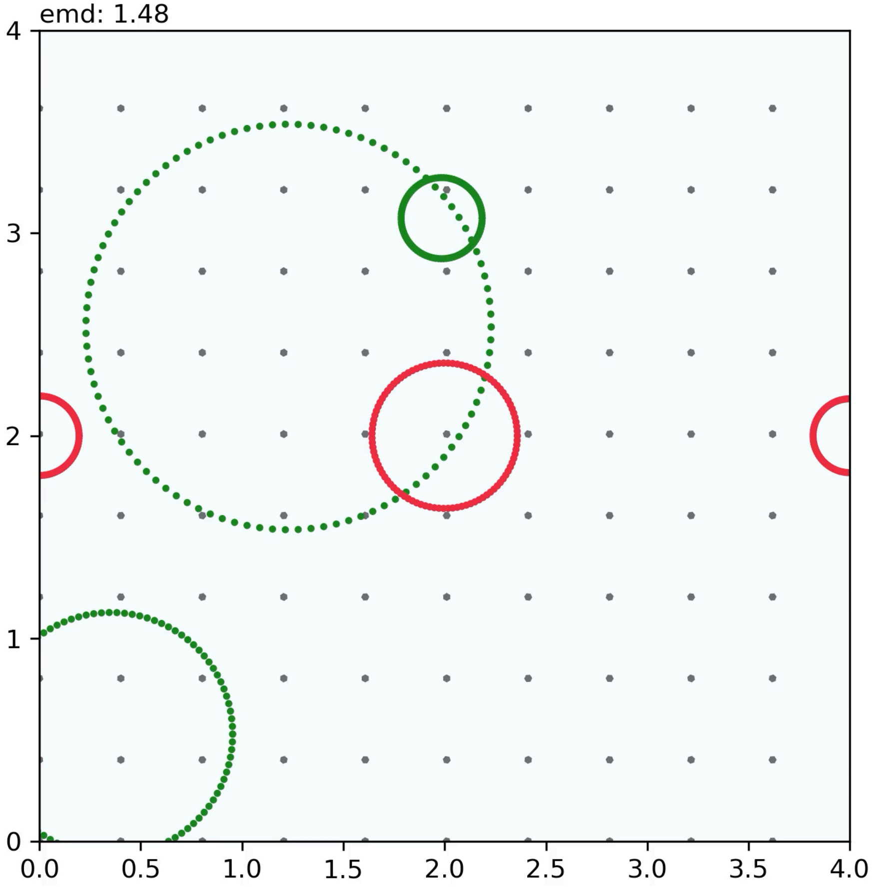
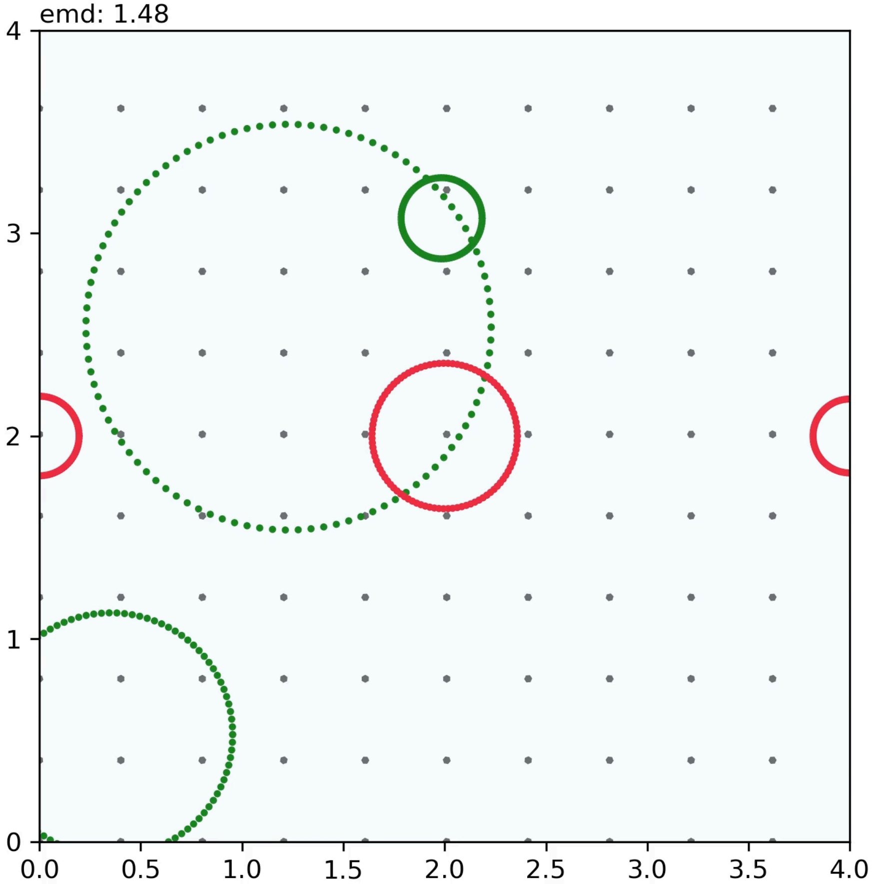


Fitting Arbitrary Geometries

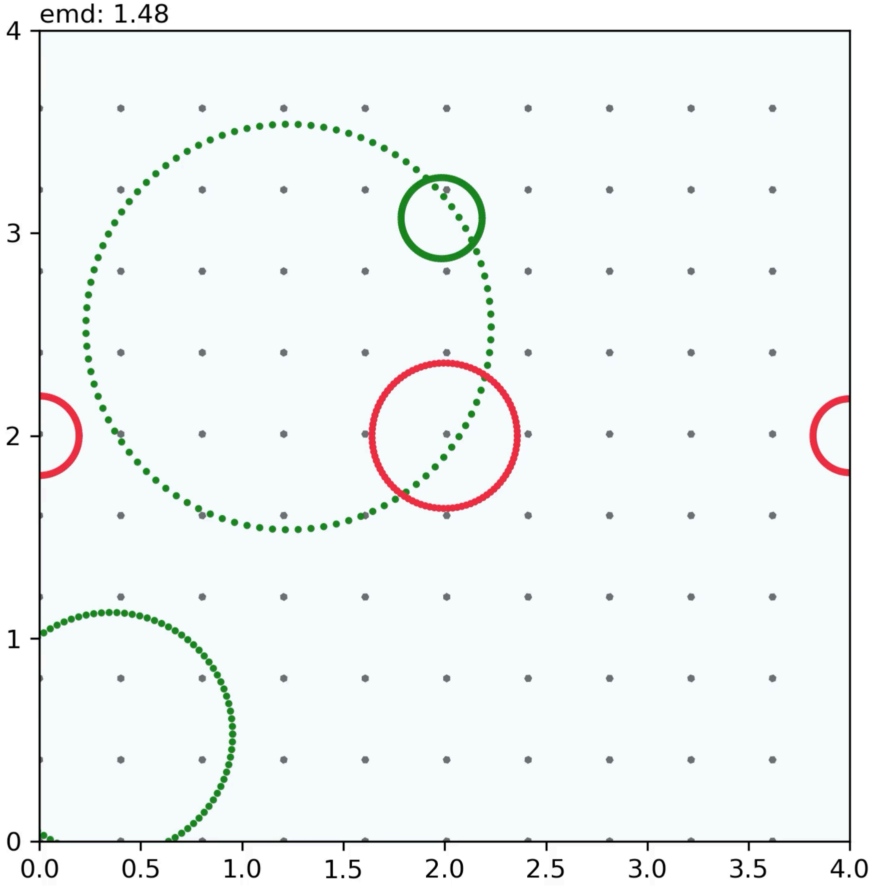
Possible use cases:



Fitting Arbitrary Geometries

Possible use cases:

- Floating term for a uniform background to mitigate pileup



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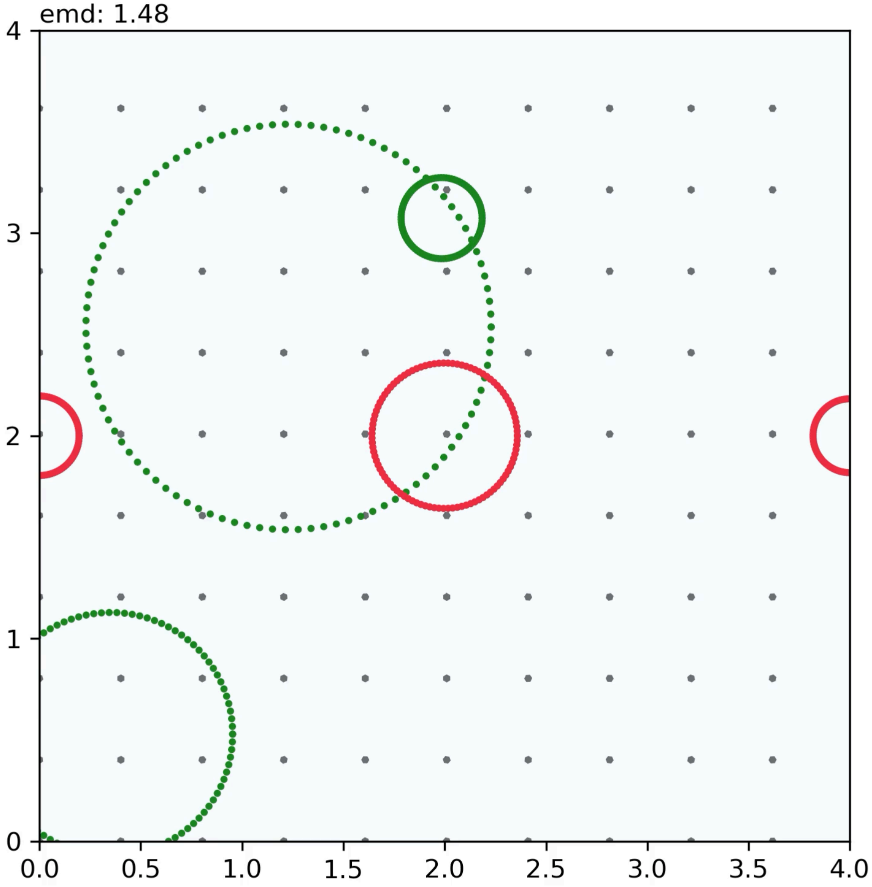
Possible use cases:

- Floating term for a uniform background to mitigate pileup
- Clustering with jet energy estimation



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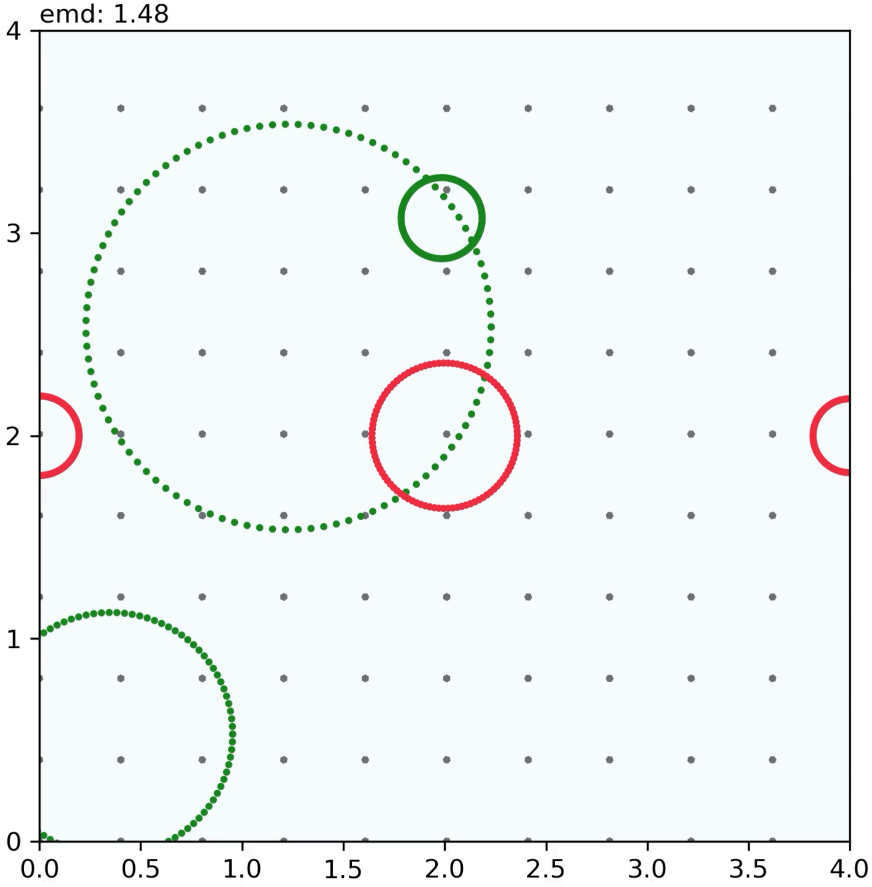
- Variable shape clusters (learned radii, ellipses, arbitrary shapes, etc.)



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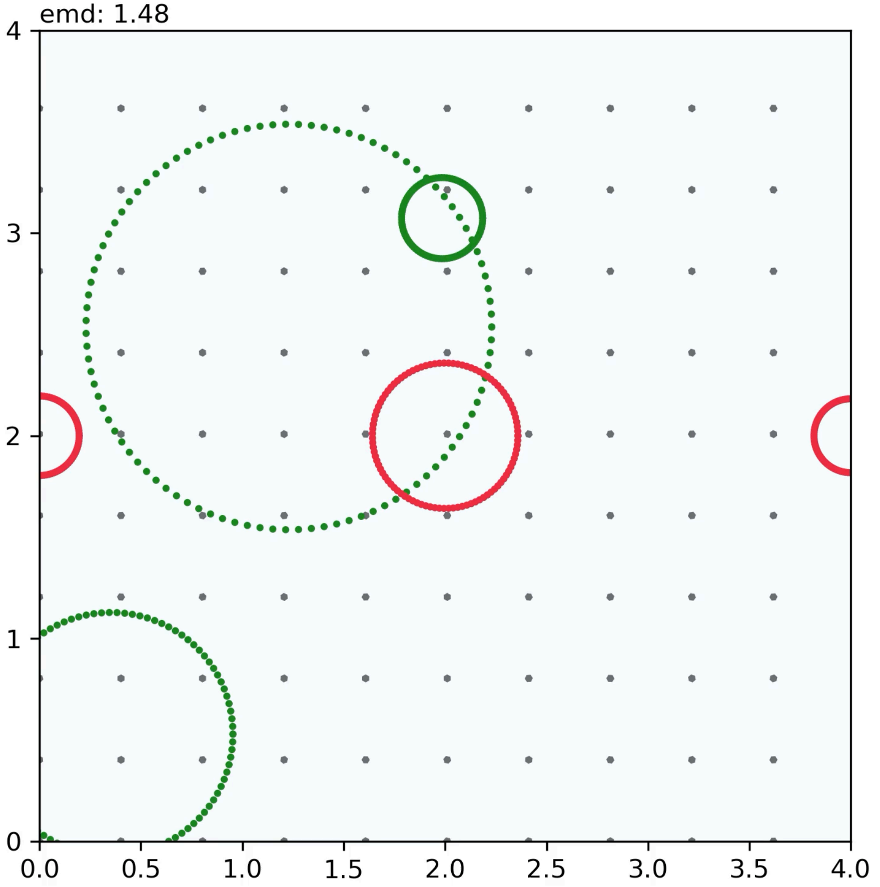
- New (and old) observables: N-subjet, N-circle, triangularness, etc.



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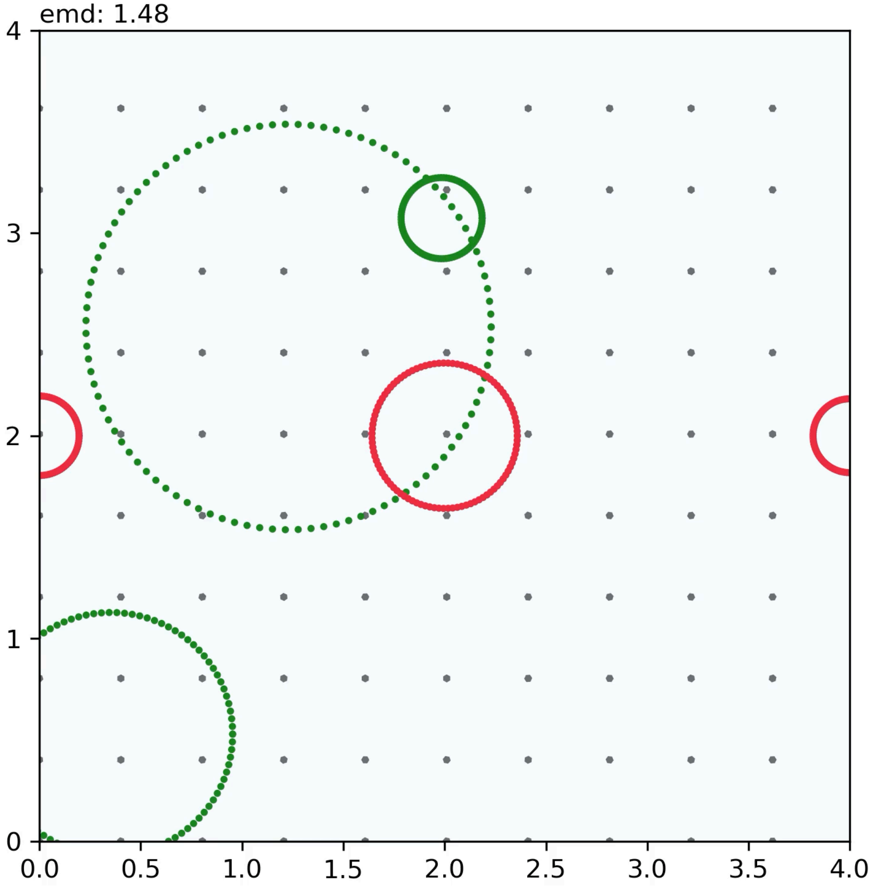
All in a unified framework given by the Energy Mover's Distance*



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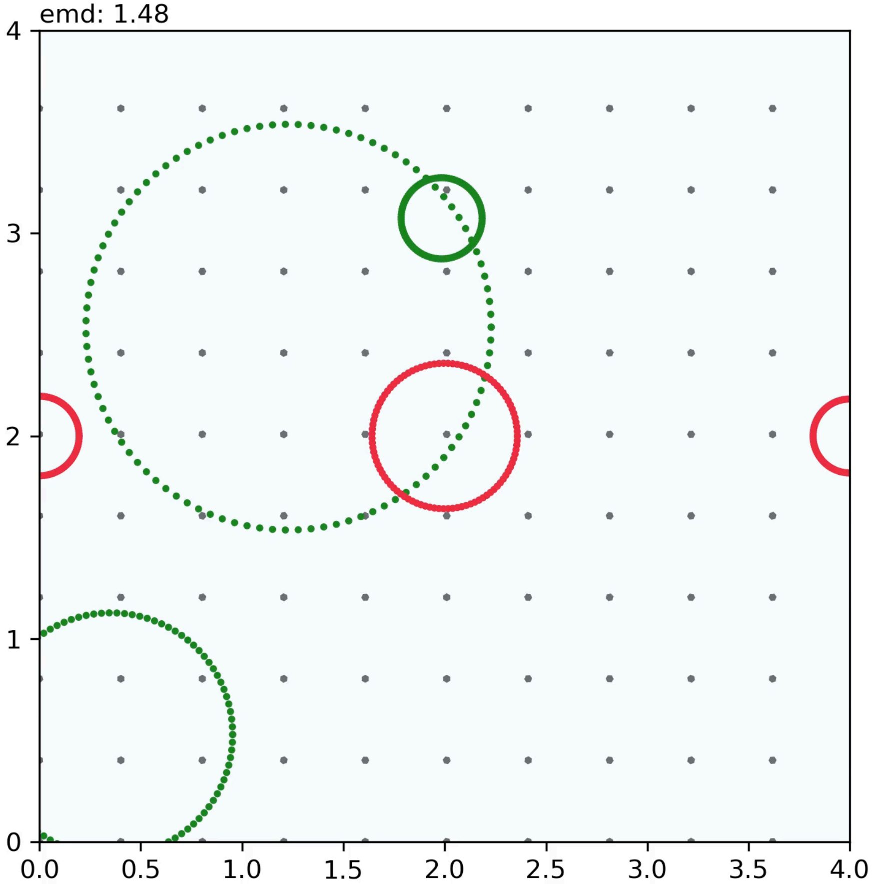
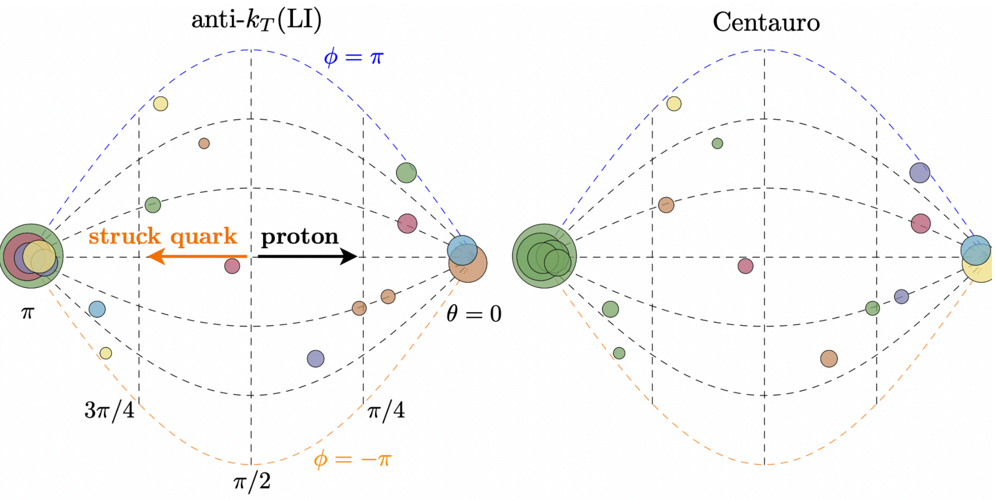


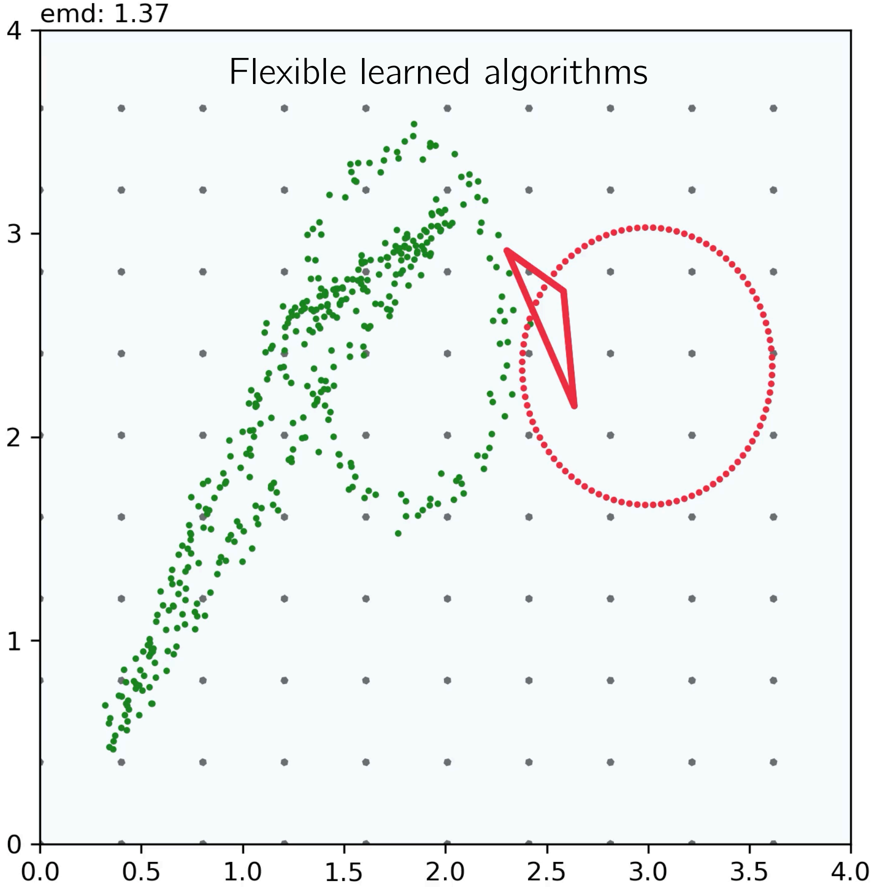
*Can You Hear the Shape of a Jet [https://indi.to/rbQ5j]

EIC - Applications

Hand-designed algorithms



Asymmetric jet clustering in deep-inelastic scattering
[arxiv.org/pdf/2006.10751.pdf]



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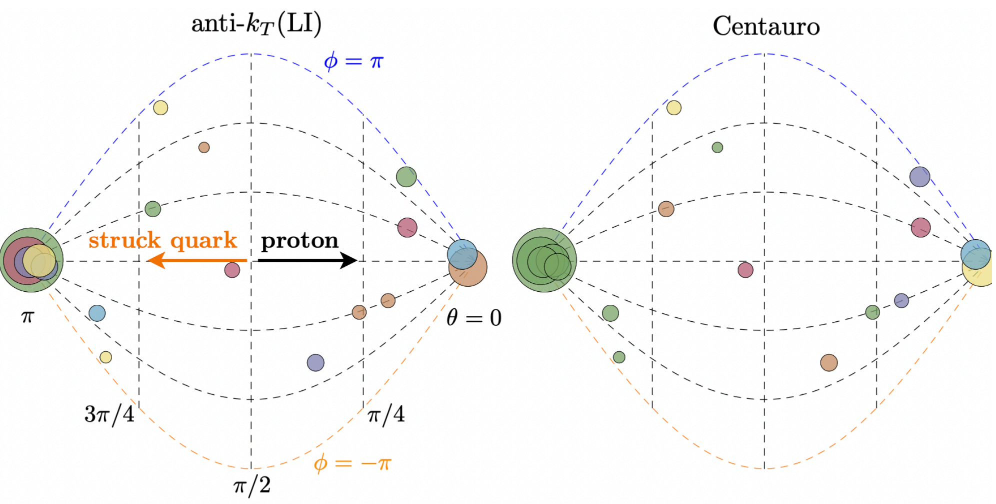

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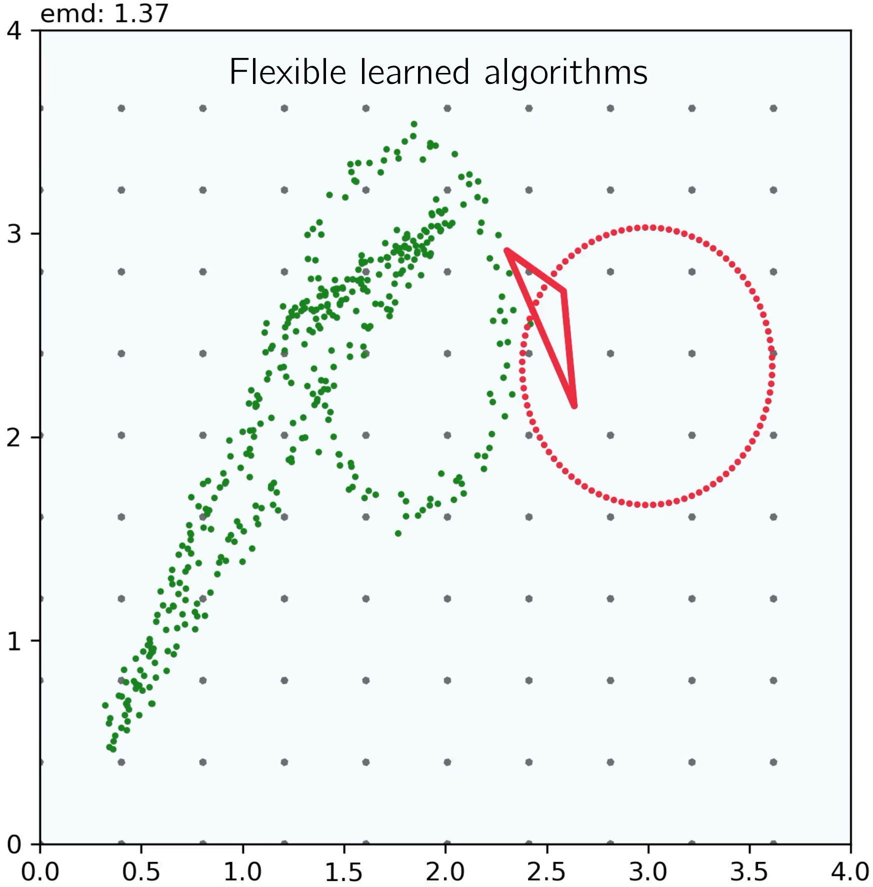
Flexible learned algorithms



Questions

https://arxiv.org/abs/2112.00038
https://arxiv.org/abs/2209.15624

NEEMo

https://github.com/okitouni/EnergyMover-Dual/tree/neurips2022

Monotonenorm

https://github.com/niklasnolte/MonotOneNorm

pip install monotonenorm

conda install monotonenorm -c okitouni