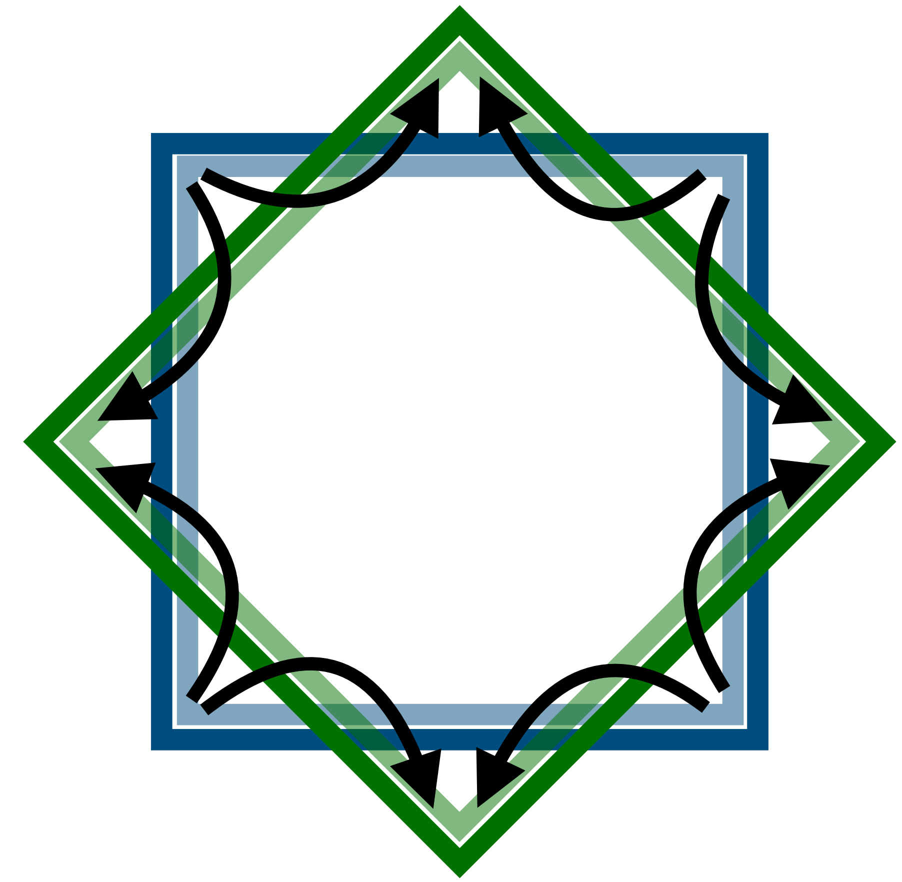


Optimal transport in high-energy physics

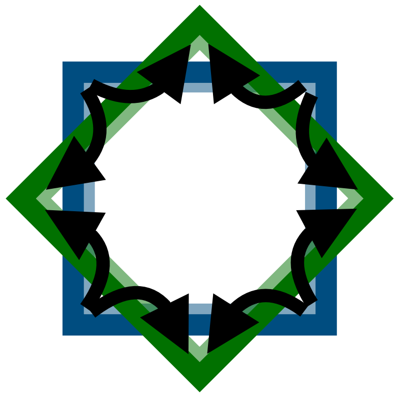
April 25, 2023

Tudor Manole
Carnegie Mellon University

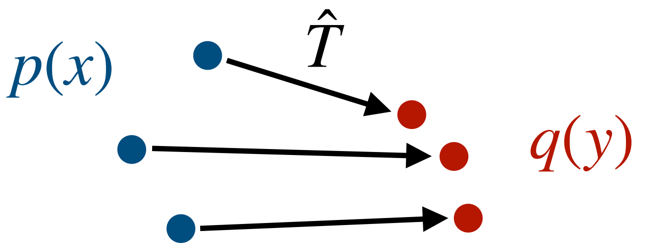
Philipp Windischhofer
University of Chicago

What can you expect?

A *(very)* brief introduction
to the world of optimal transport

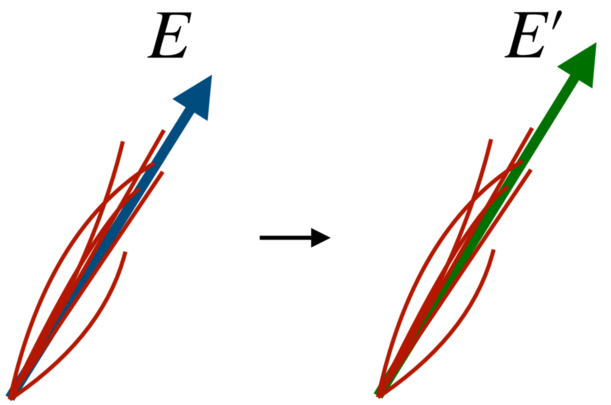


A glimpse at how to solve
optimal transport problems



(Potential) applications in
particle physics

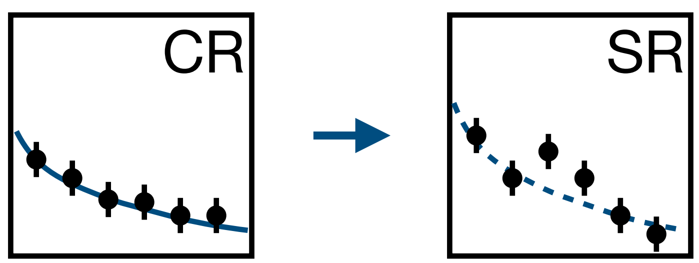
From the perspective of a
statistician *(Tudor)* and a physicist *(Philipp)*



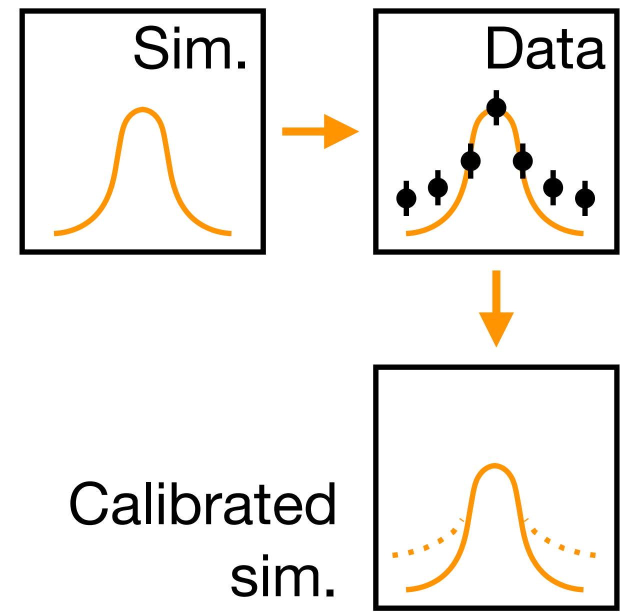
We'll be brief; let's keep the details for the discussion afterwards

Why should you care?

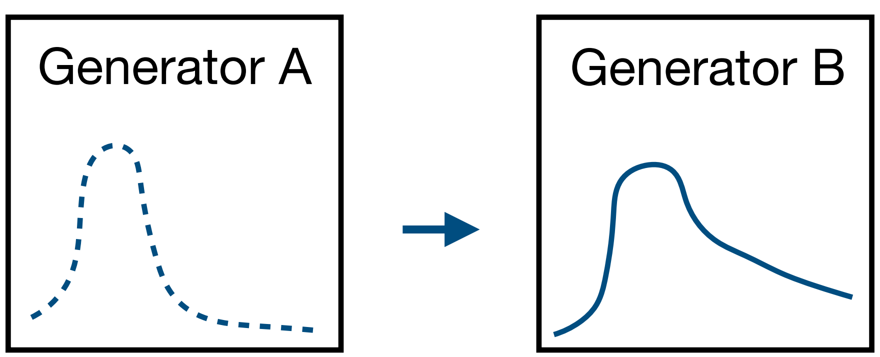
In particle physics, we manipulate (probability) **distributions on a daily basis …**



Extrapolation across phase space
(e.g. control region → signal region)

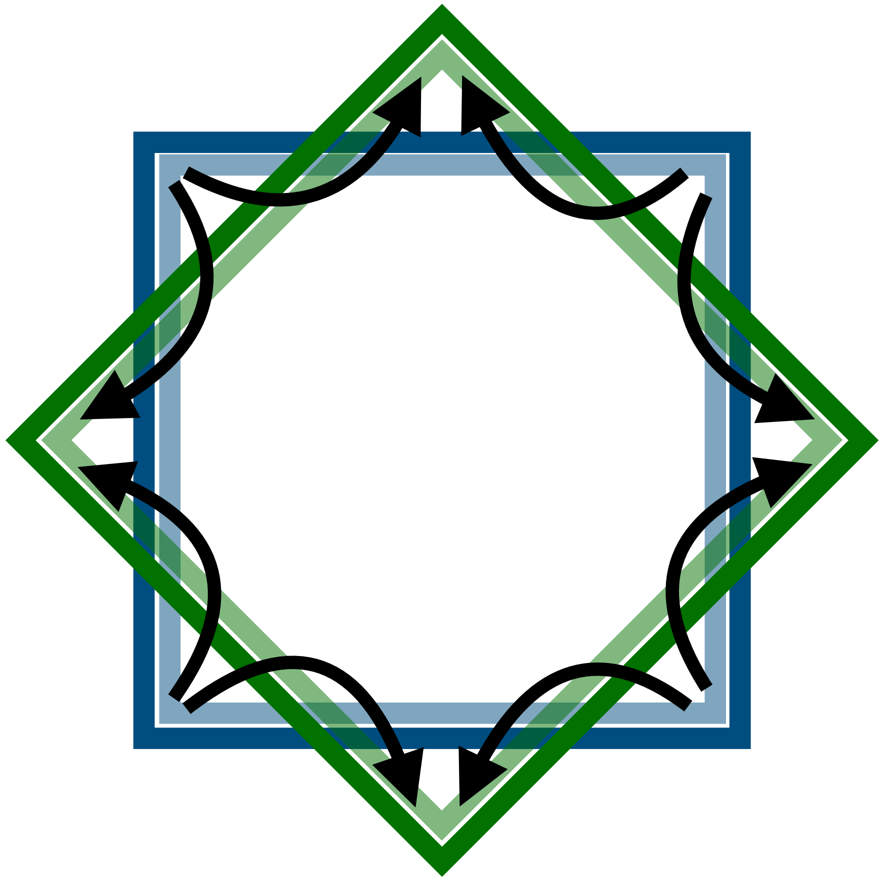


Calibration of simulation
(e.g. Monte Carlo prediction against data side bands)



Template morphing
(e.g. 2-point systematics)

… **optimal transport** provides **useful tools** *(and a unifying perspective)* for many of these!



The theory of optimal transport

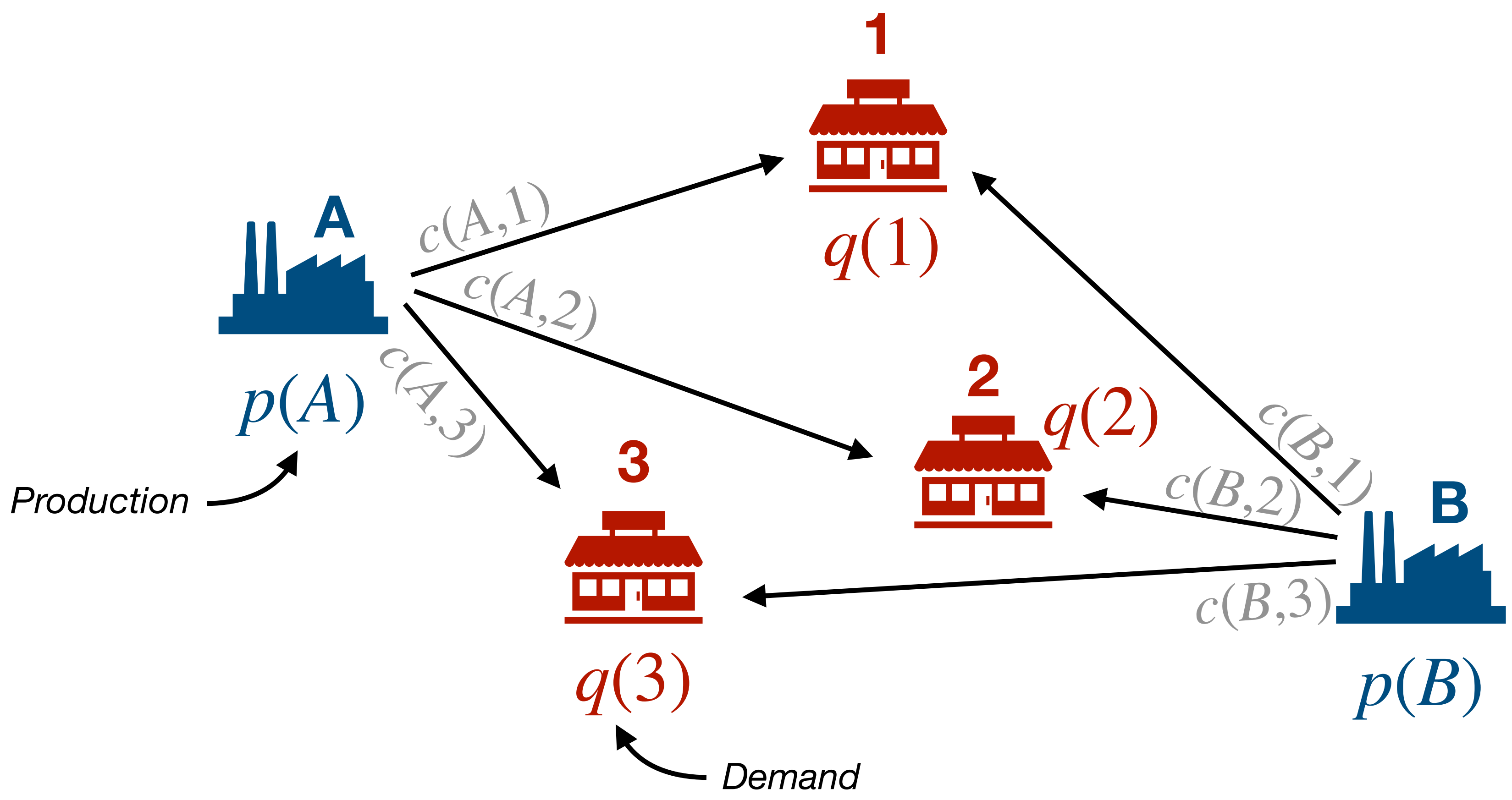
What is optimal transport?

The answer to a logistics problem!

"How to transport commodities from N ***factories*** *to M* ***stores*** *…*

… in the presence of a ***transportation cost*** *$c(a, i)$ between factory a and store i …*

… so that the total cost is minimized?



Incredibly rich mathematical problem with more than 200 years of literature

(Some of it very high-profile, Fields medal-winning work!)

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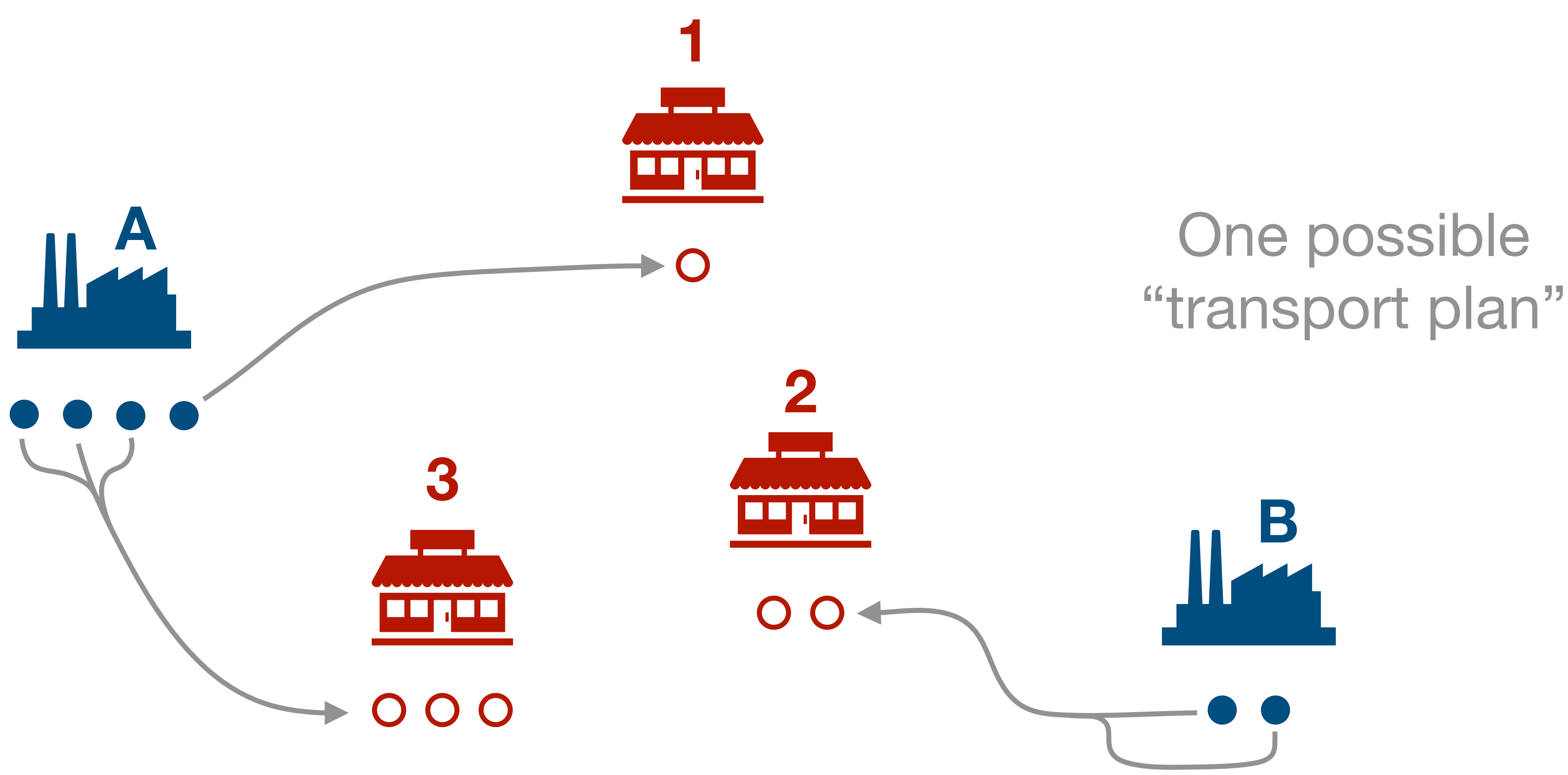

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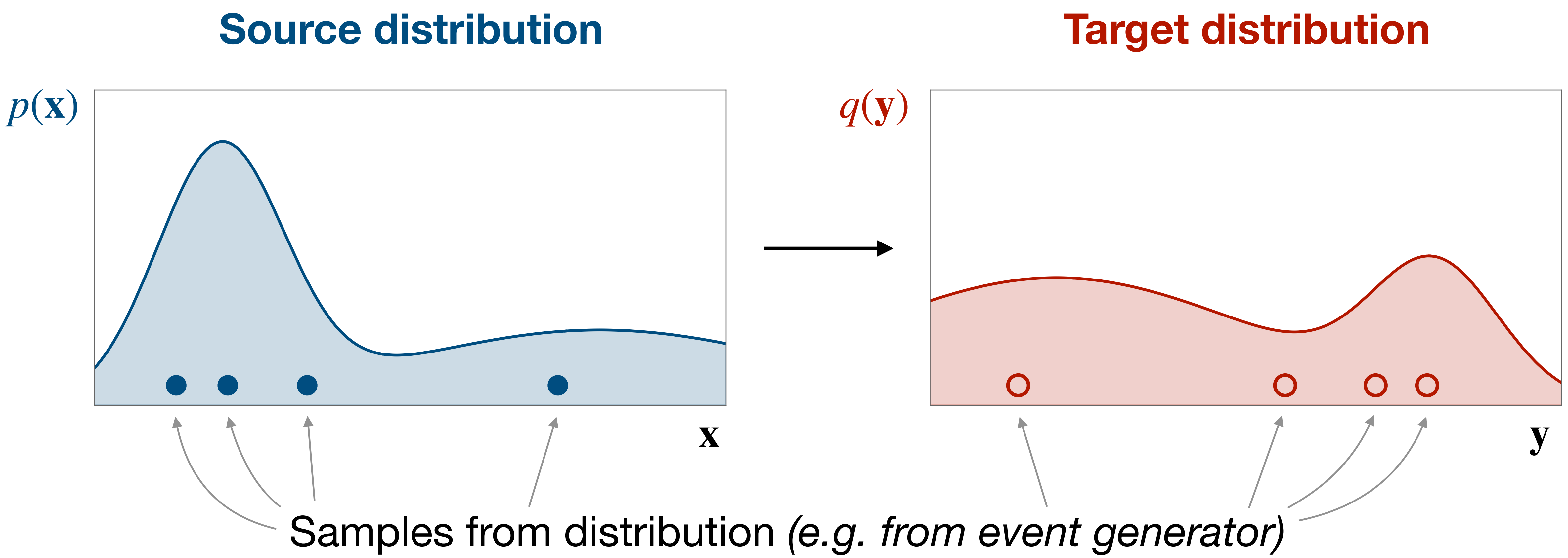
Optimal transport, for a particle physicist



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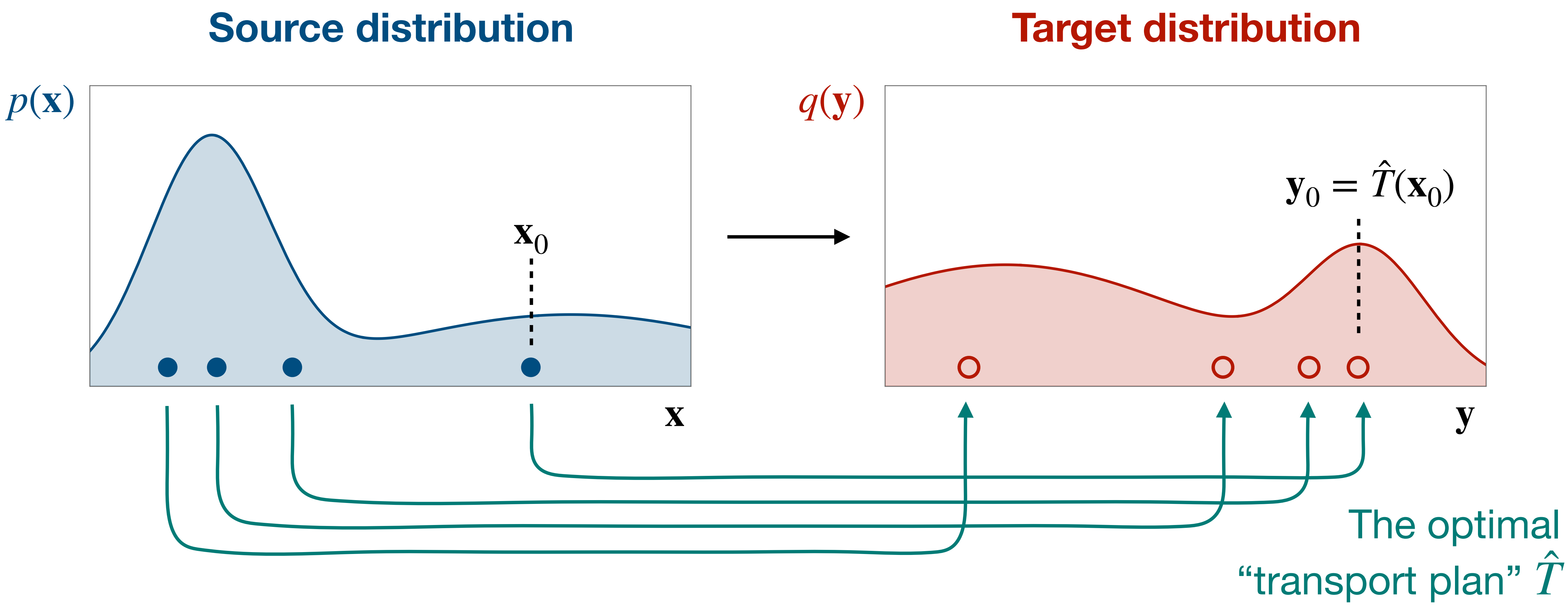


"Monge optimal transport problem":

Construct a (continuous) function $\hat{T}$ that maps $p(\mathbf{x})$ into $q(\mathbf{y})$ in an optimal way by "moving" the samples:

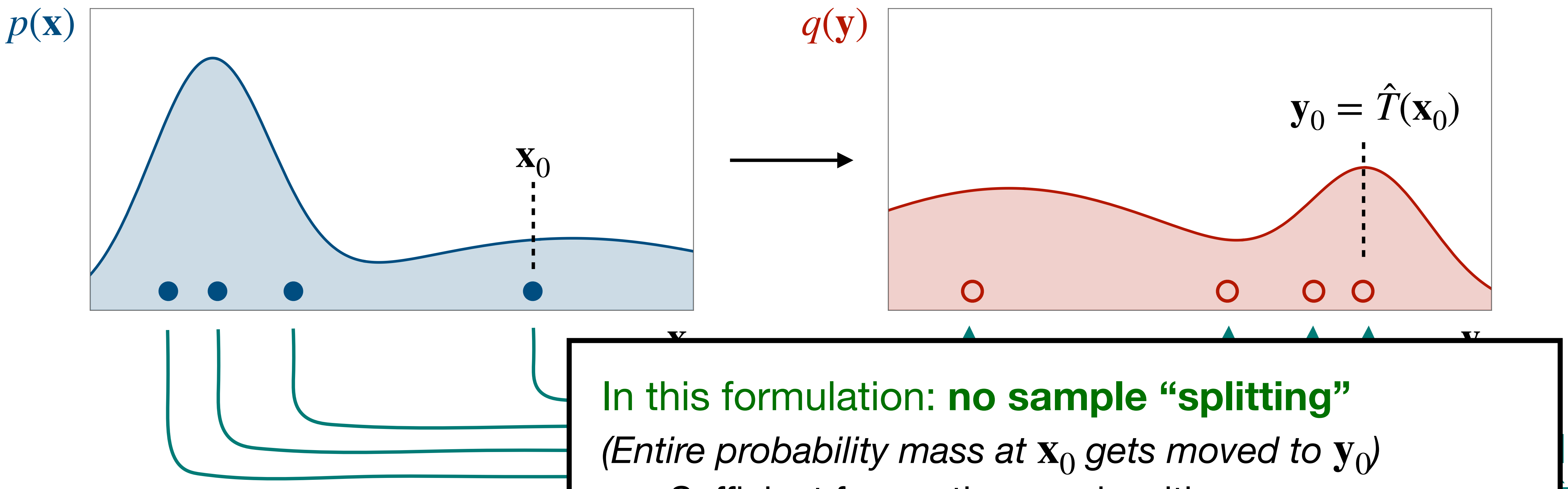
$$\mathbf{x} \mapsto \mathbf{y} = \hat{T}(\mathbf{x})$$

Transport cost $c(\mathbf{x}, \mathbf{y})$ for moving sample from $\mathbf{x}$ to $\mathbf{y}$

Such that $q(\mathbf{y}) = p(\mathbf{x}) \, (\nabla_{\mathbf{x}} \hat{T})^{-1}$ and $\hat{T} = \arg\min_T \int dx \; p(x) \; c(x, T(x))$

Optimal transport, for a particle physicist

Source distribution **Target distribution**

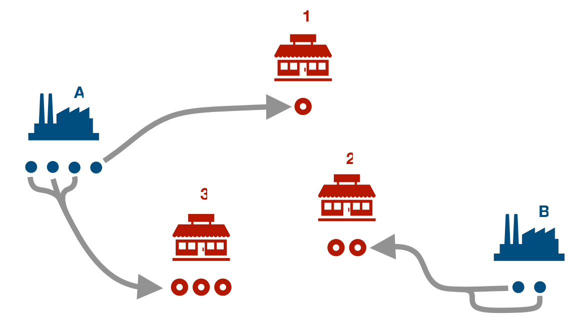


In this formulation: **no sample “splitting”**

(Entire probability mass at $\mathbf{x}_0$ gets moved to $\mathbf{y}_0$)

→ Sufficient for continuous densities

“Kantorovich problem” →



“Monge optimal transport pro

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Optimal transport, for a particle physicist

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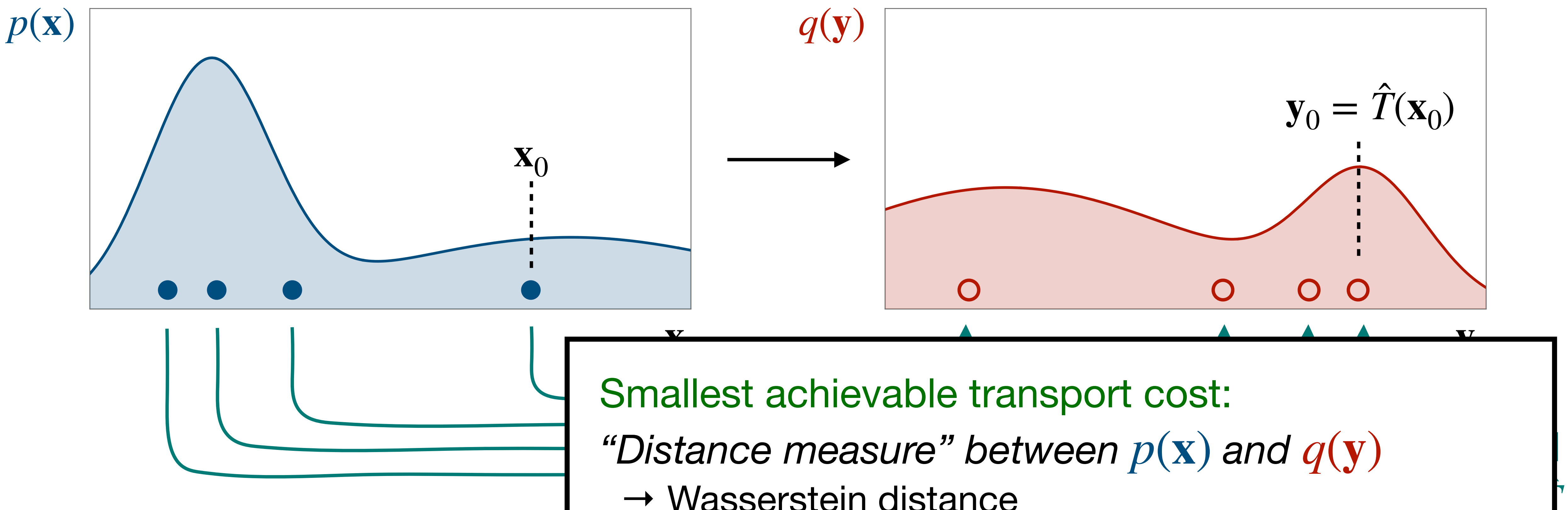

Smallest achievable transport cost:

“Distance measure” between $p(\mathbf{x})$ *and* $q(\mathbf{y})$

→ Wasserstein distance

$$W = \min_T \int dx\ p(x)\ c(x,\ T(x))$$

“Monge optimal transport pro

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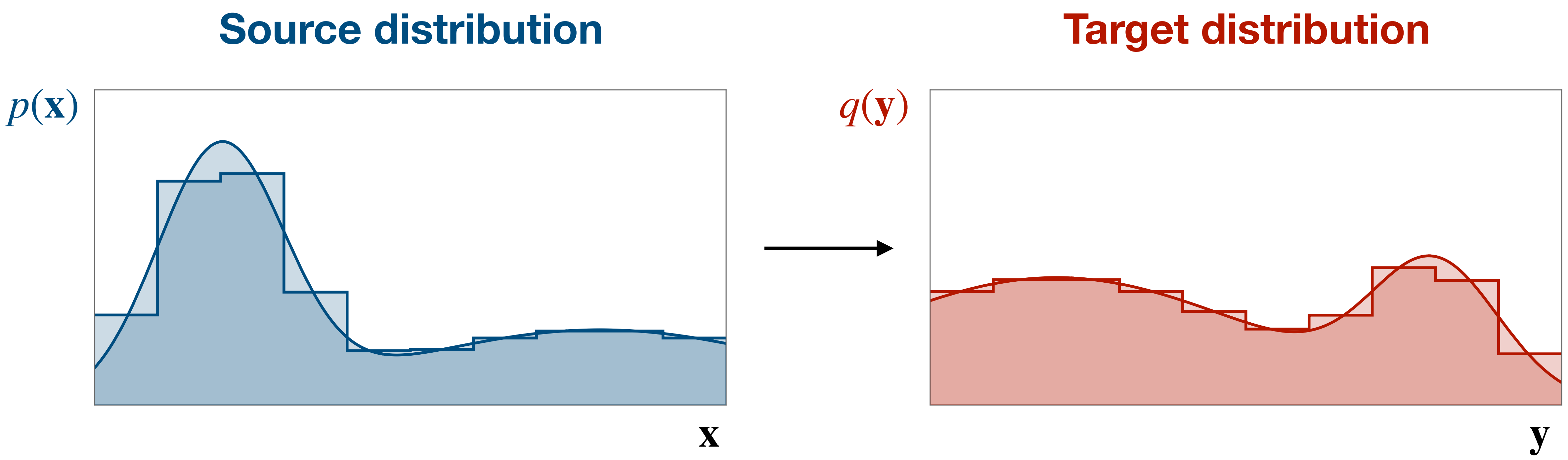
Optimal transport, for a particle physicist



Operatively, this procedure gives the same results as

→ Binning $\mathbf{x}$ and $\mathbf{y}$

→ Reweighting bin contents for $\mathbf{x}$ by the density ratio $q(\mathbf{y})/p(\mathbf{x})$

… but is also **well-behaved** where the density ratio gets very large

(Empty bins when densities don't have common support)

→ *Important for applications (see later)*

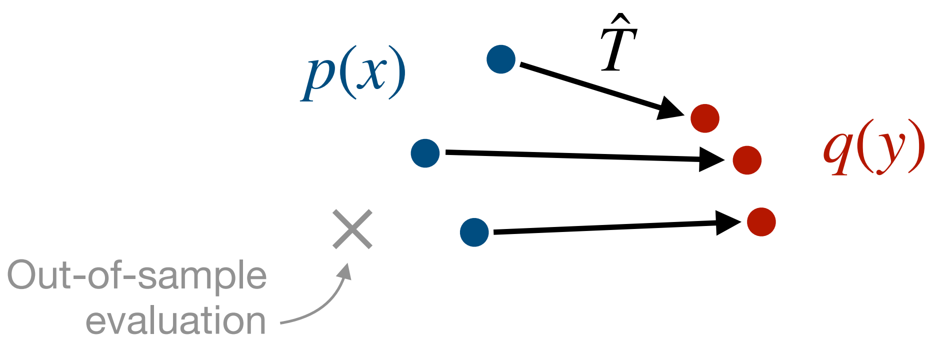
How to do optimal transport?

In general, the Monge problem is very difficult to solve!

$$q(\mathbf{y}) = p(\mathbf{x})\,(\nabla_{\mathbf{x}}\hat{T})^{-1} \qquad \hat{T} = \arg\min_{T} \int dx\; p(x)\; c(x, T(x))$$

(Highly nonlinear constraint!)

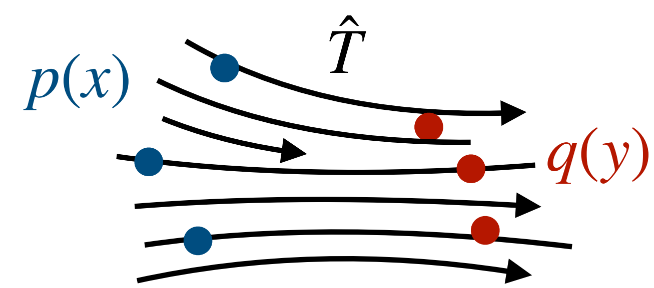
Two main classes of algorithms:



"Discrete" optimal transport

Transport empirical distributions by pairing up samples ~ $\mathcal{O}(N^2)$

Need to interpolate transport map to unseen samples



"Continuous" optimal transport

Use samples to construct continuous transport function

Need to make assumptions on underlying densities

The role of the transport cost

The character of the solution $\hat{T}$ to the Monge problem depends strongly on the cost function $c(x, y)$

Many useful cost functions are *(strictly)* convex!

E.g. $c(x, y) = |x - y|^p$ for $p > 1$

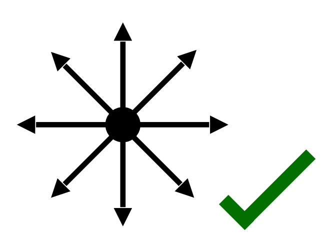
In this case: the optimal transport function is <u>unique</u> and the gradient of a potential!

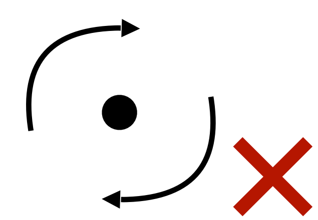
$$\hat{T}(x) = x + \nabla g(x)$$

"Transport potential"

Optimal transport ⇔ Electrostatics

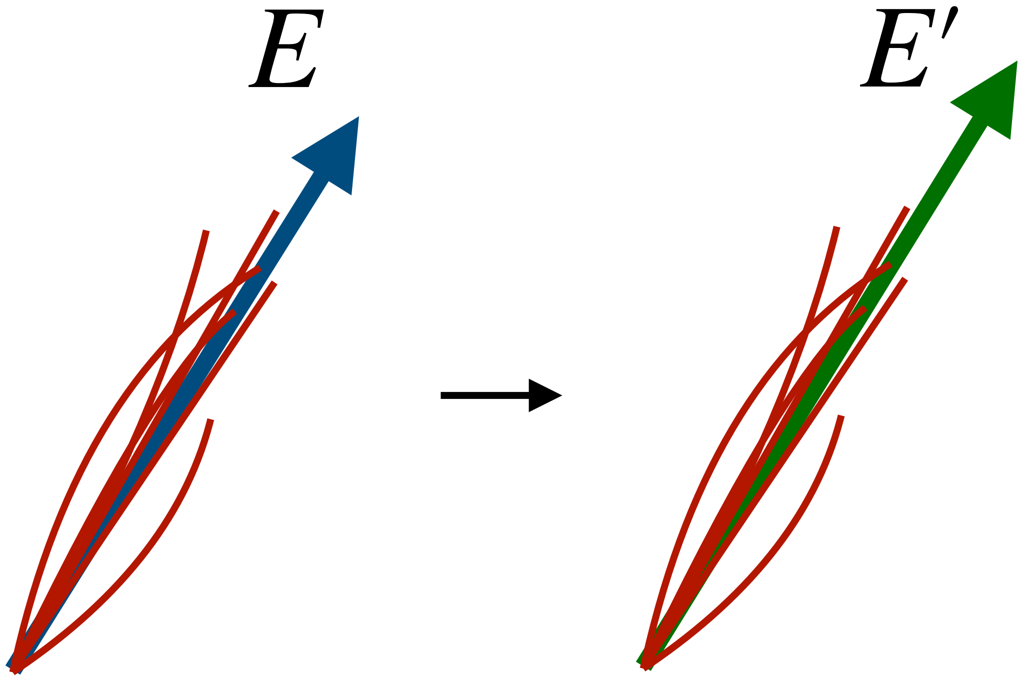
The transport vector field $\hat{T}$ has zero curl!





"Don't ship your stuff in circles."

→ More information on other cases in backup



(Potential) Applications in high-energy physics

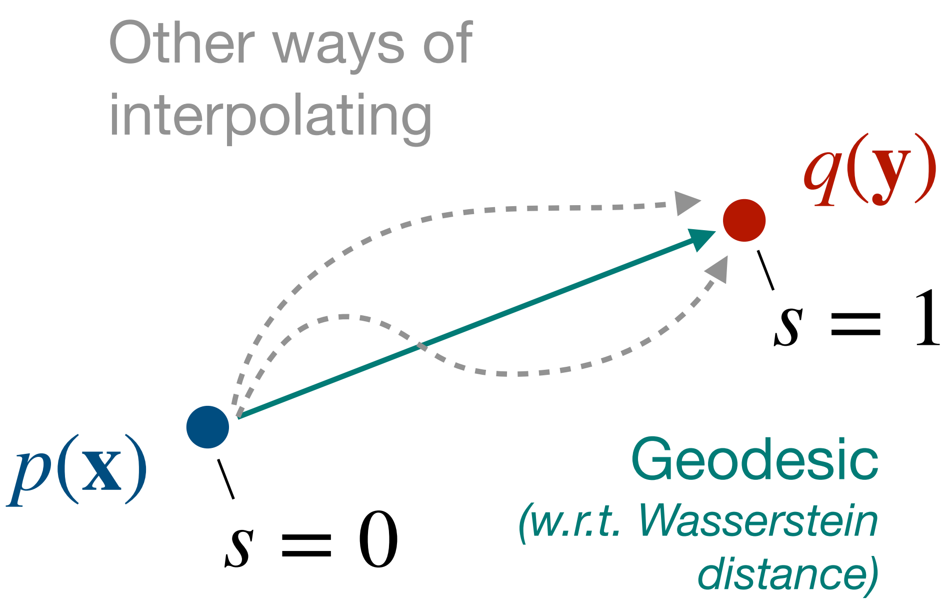
Template morphing

Optimal transport solution maps $p(\mathbf{x})$ into $q(\mathbf{y})$

$$\mathbf{x} \mapsto \mathbf{y} = \hat{T}(x) = x + \nabla g(x)$$

Can interpolate between p and q: just move each sample by a **fraction of the full gradient**

$$\hat{T}_s(x) = x + s\nabla g(x), \quad 0 \le s \le 1$$



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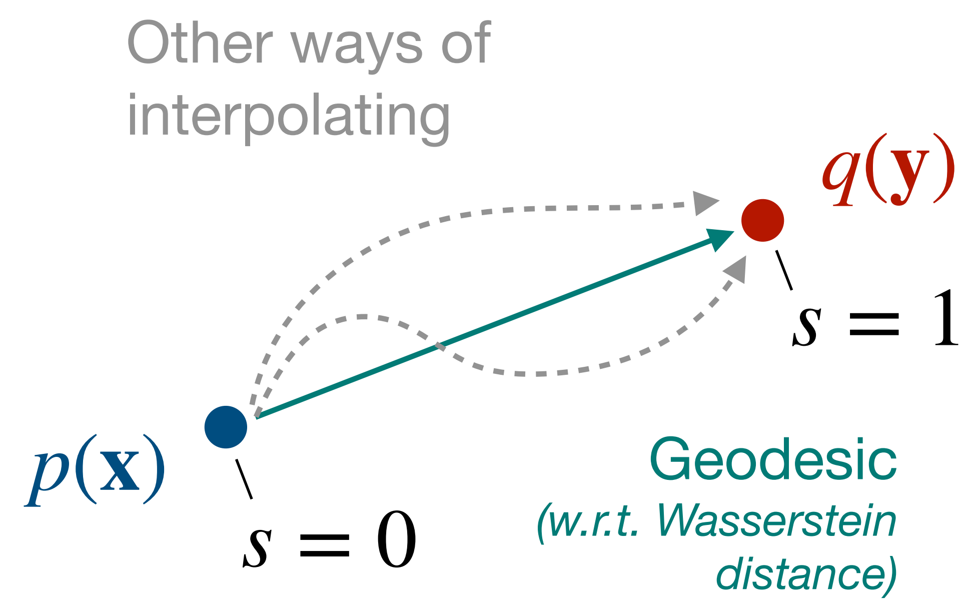
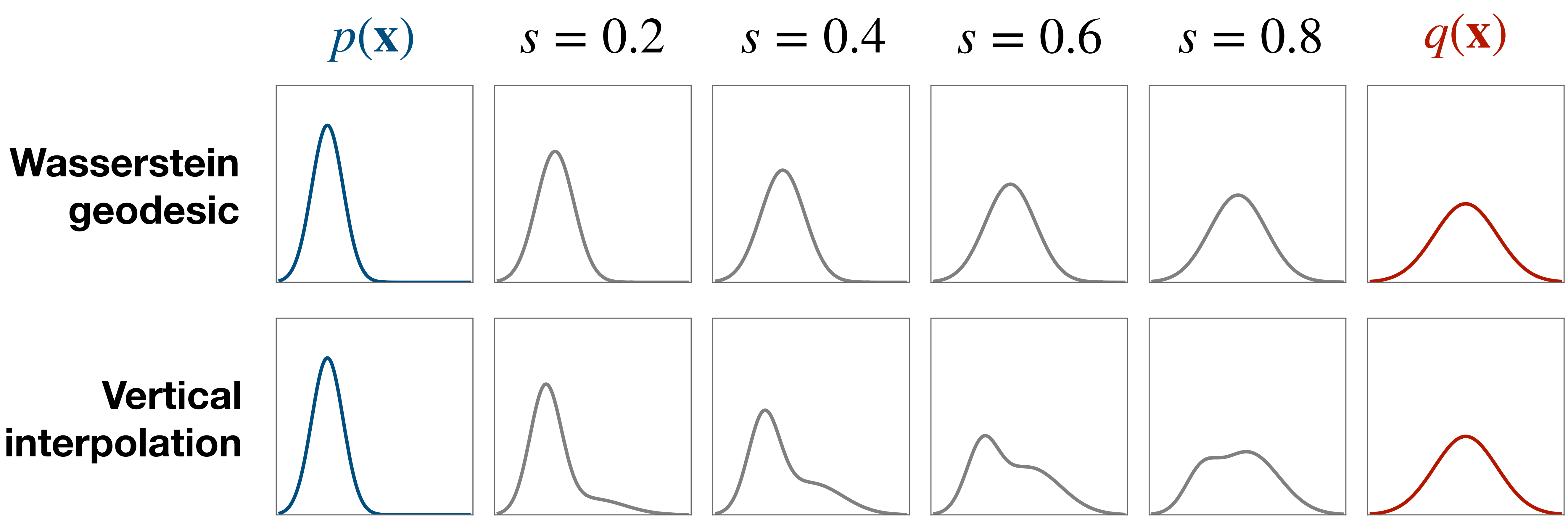
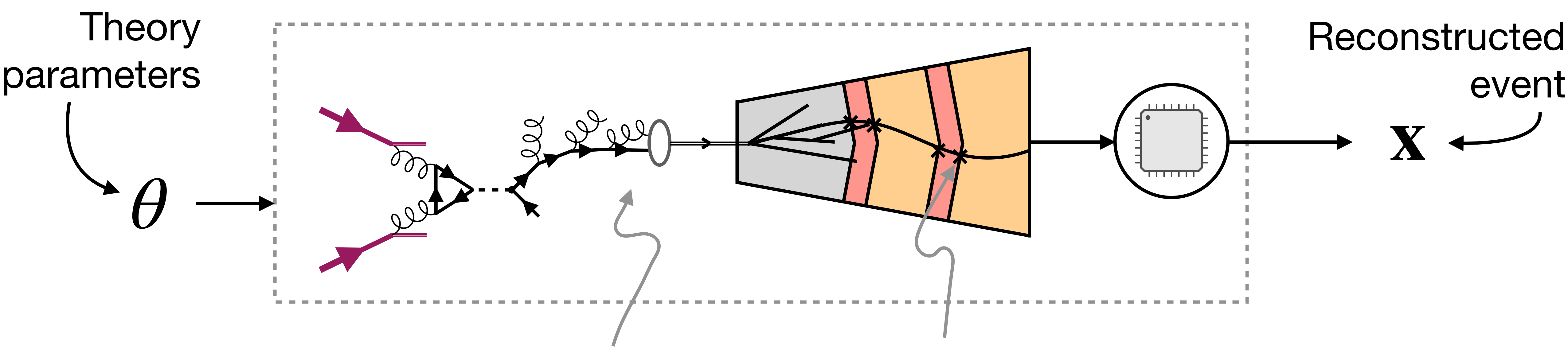




Calibrating simulations

Our field has spent several decades building extremely precise simulations …

*… they **encode** a lot of **domain knowledge**, but they are not perfect!*



Nonperturbative dynamics:
Phenomenological models
instead of rigorous calculations

Interaction with detector:
"All cables correctly included"?

Often impossible / impractical to correct the simulation model

Instead: *calibrate the simulator output*

Calibrating simulations

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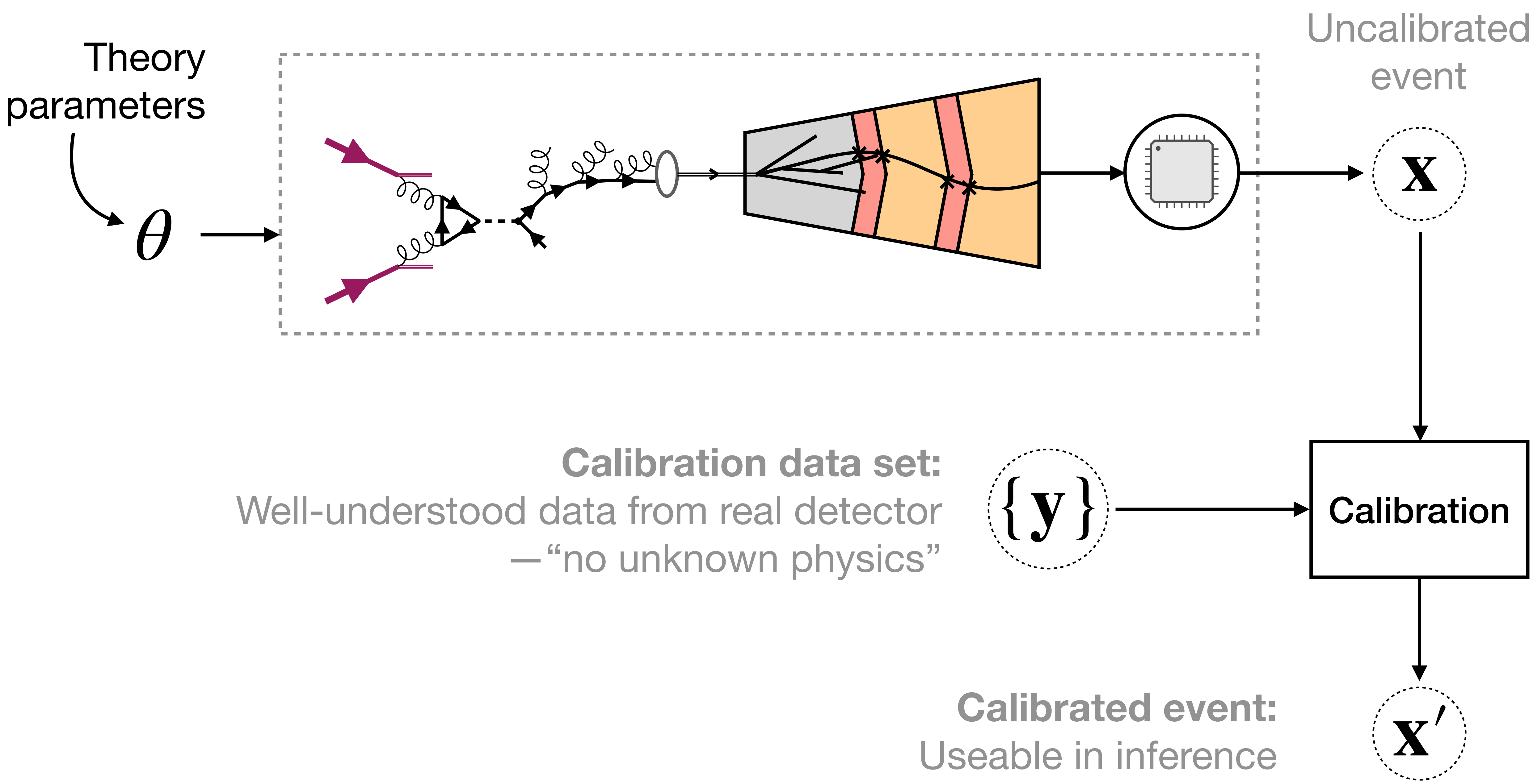

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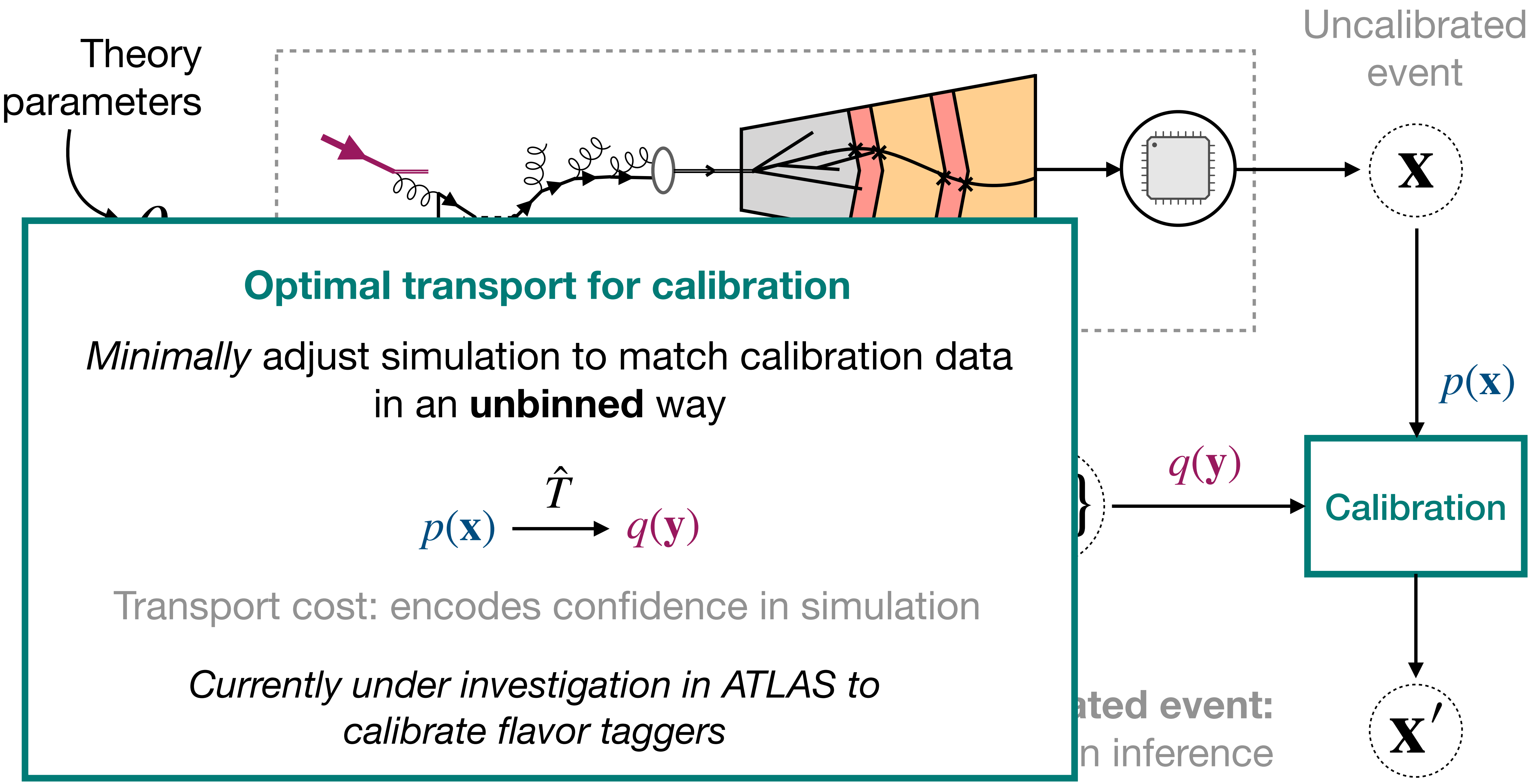


Optimal transport for calibration

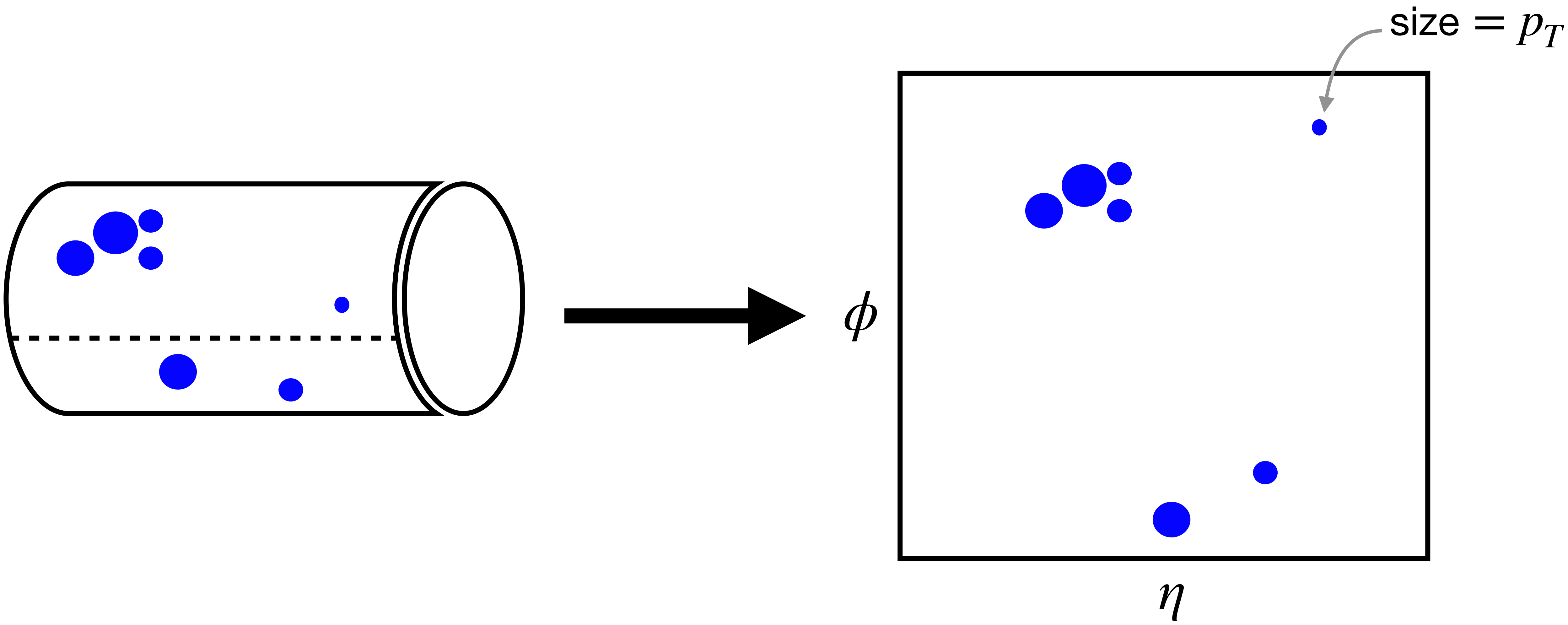
Minimally adjust simulation to match calibration data in an **unbinned** way

$$p(\mathbf{x}) \xrightarrow{\hat{T}} q(\mathbf{y})$$

Transport cost: encodes confidence in simulation

Currently under investigation in ATLAS to calibrate flavor taggers

Comparing collider events (Komiske et al. 2019)



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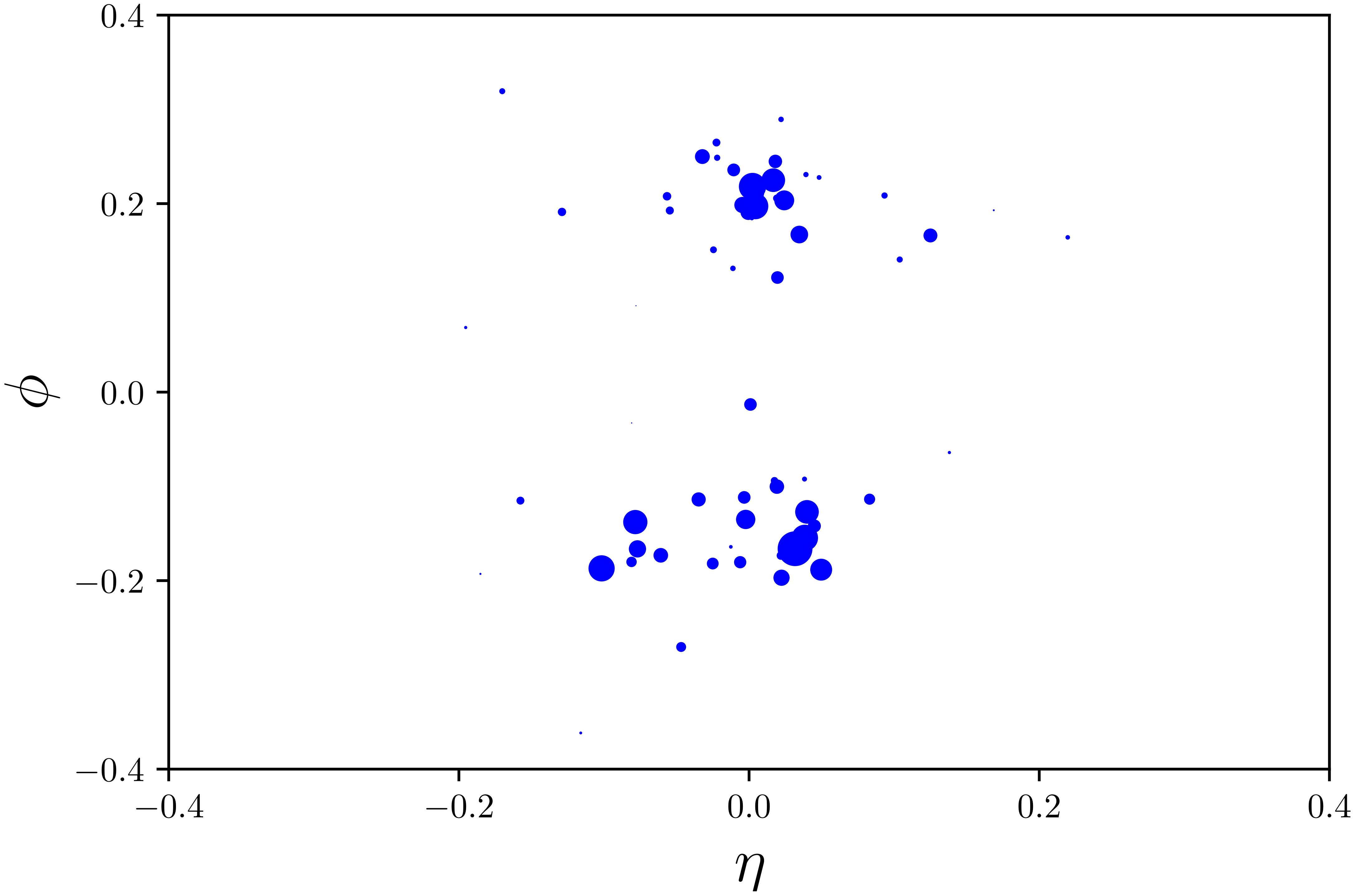

Generated with the Energyflow package based on CMS open data.

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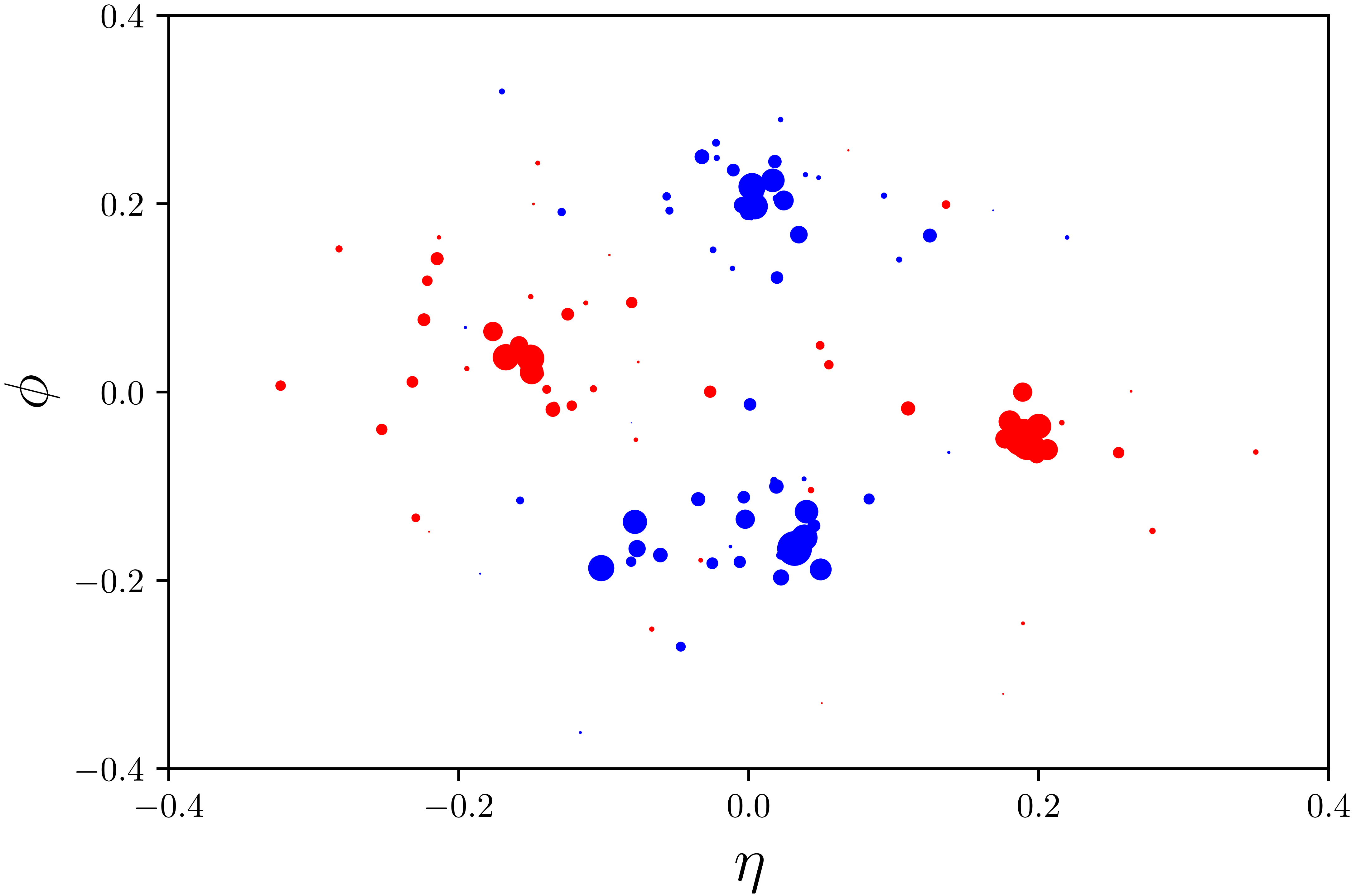

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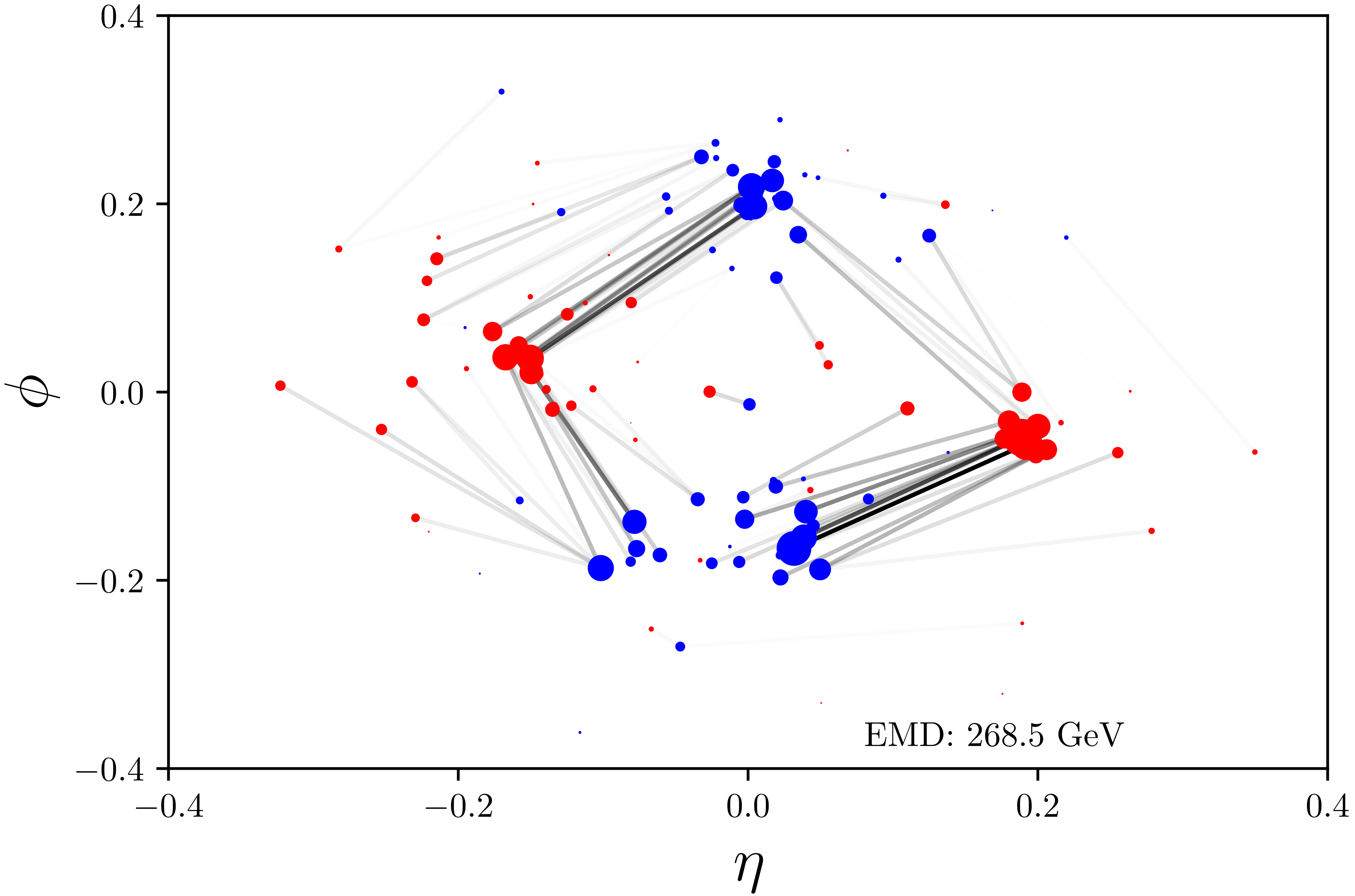

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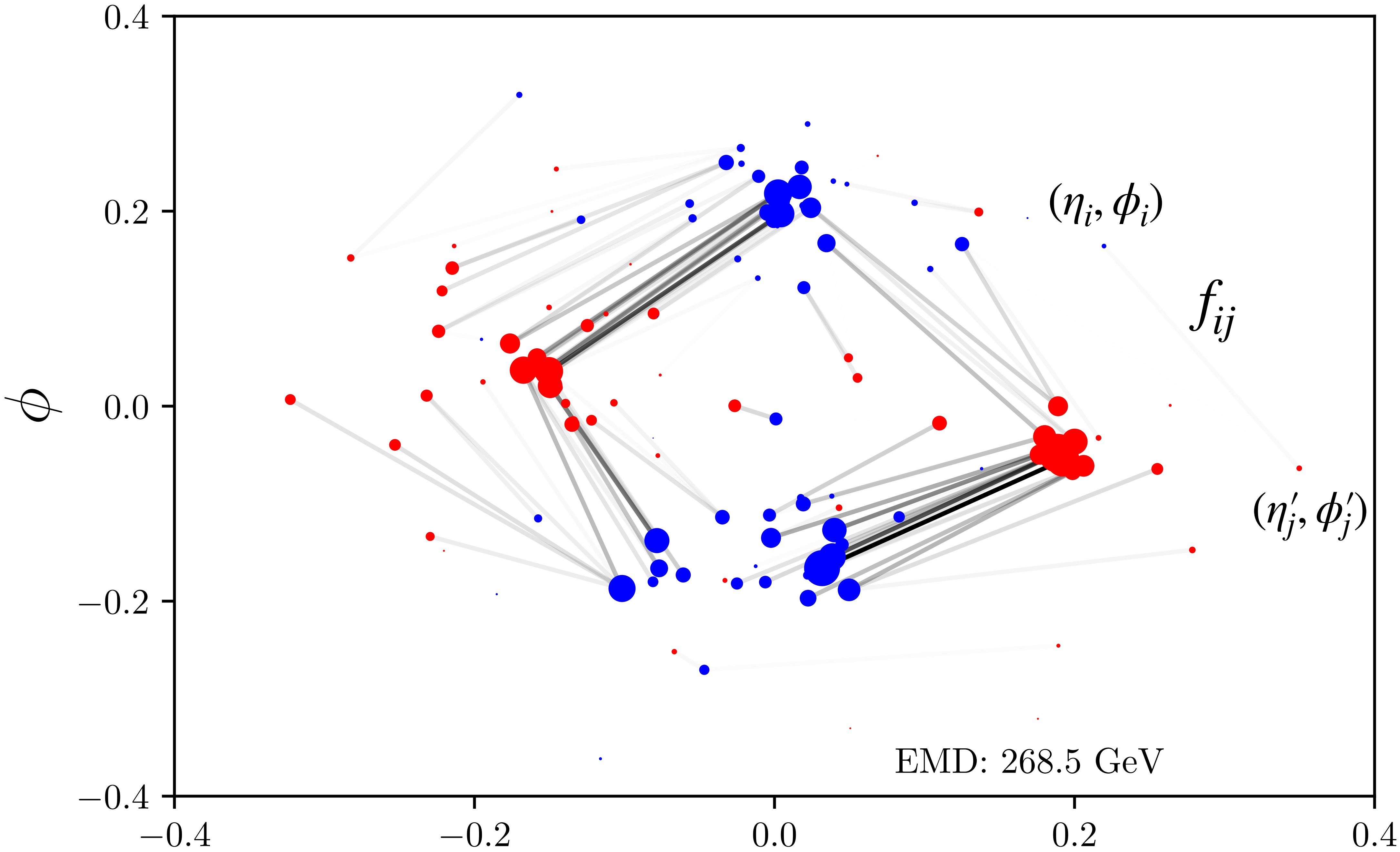


$$\textbf{EMD}(\mathcal{E}, \mathcal{E}') = \sum_{i,j} f_{ij} \|(\eta_i, \phi_i) - (\eta'_j, \phi'_j)\| + |s_T - s'_T|$$

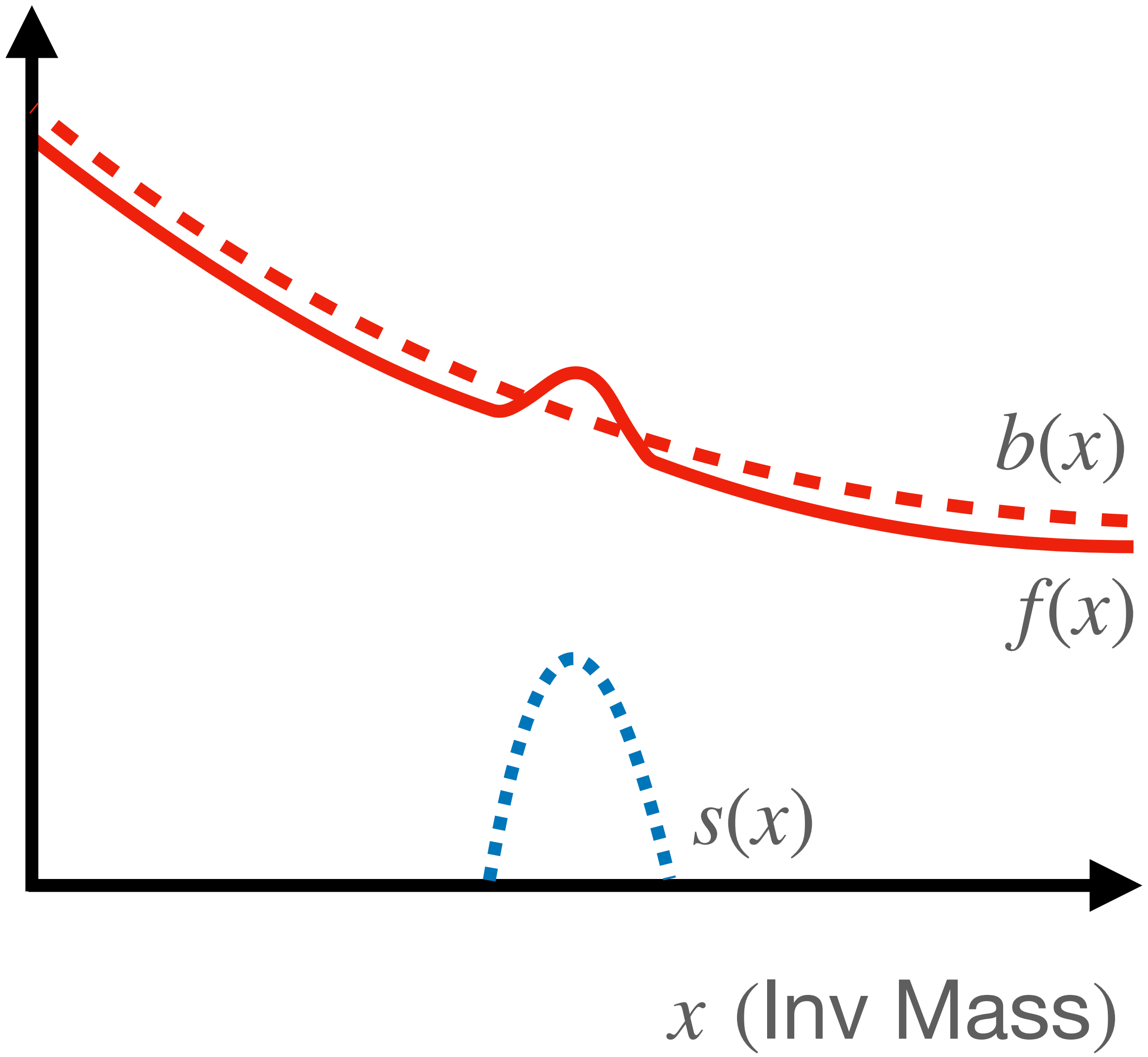
Data-driven background estimation

$$X_1, \ldots, X_n \sim f(x) = \epsilon \cdot s(x) + (1 - \epsilon) \cdot b(x)$$

s: Known signal density

b: **Unknown** background density

ϵ: Proportion of signal



Goal: Test the hypotheses

$$H_0 : \epsilon = 0, \quad H_1 : \epsilon > 0.$$

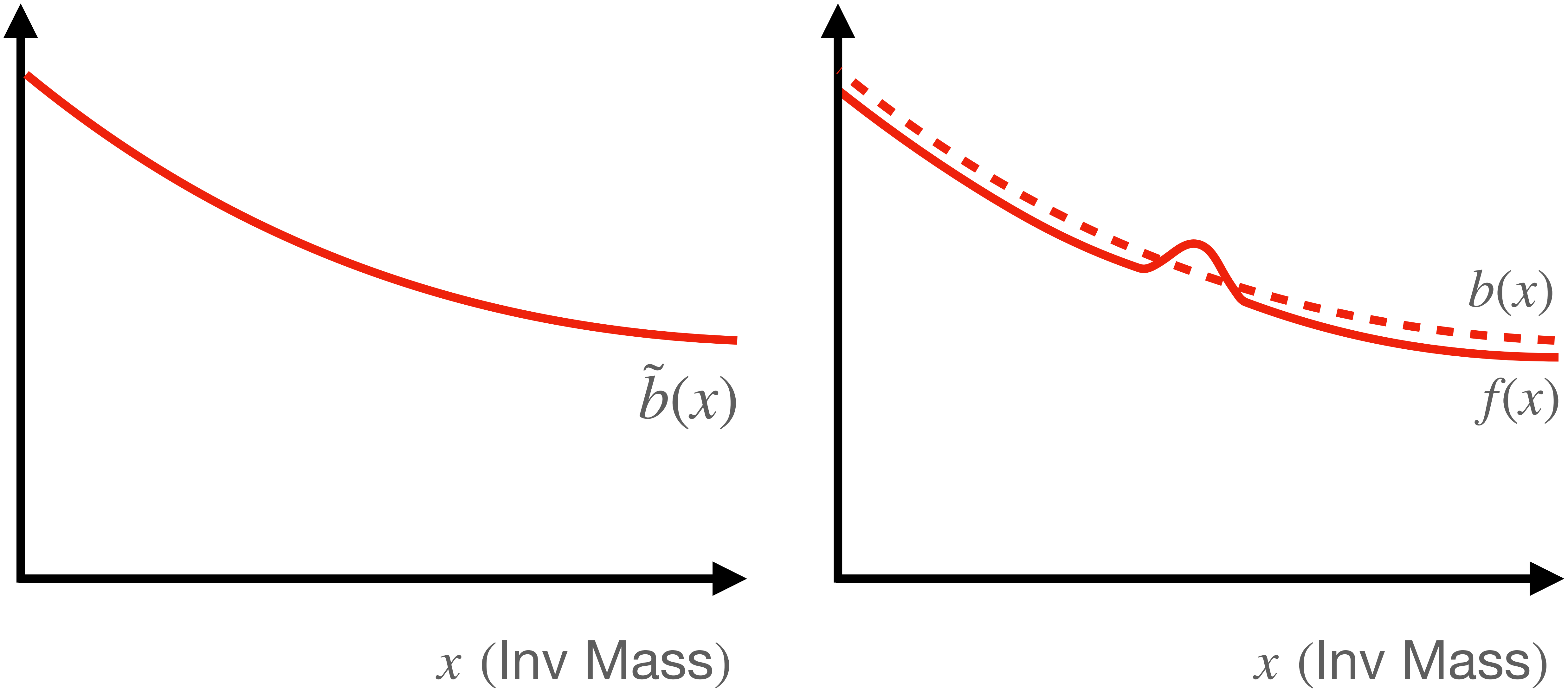
Problem: b is unknown.

- Example: HH→4b search

Data-driven background estimation

$$X_1, \ldots, X_n \sim f(x) = \epsilon \cdot s(x) + (1-\epsilon) \cdot b(x)$$

Assume we also have**:** $Y_1, \ldots, Y_m \sim \tilde{b}(x) \approx b(x)$



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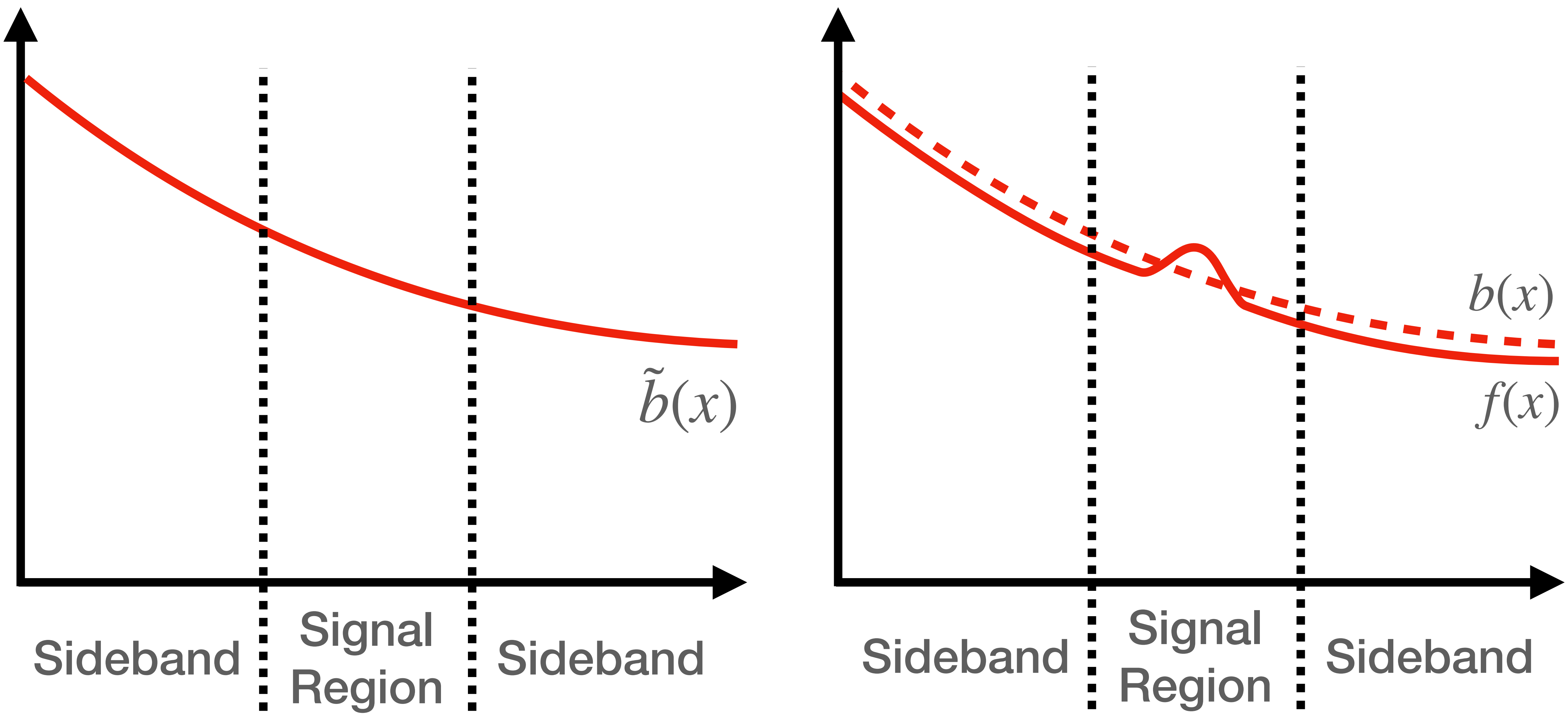
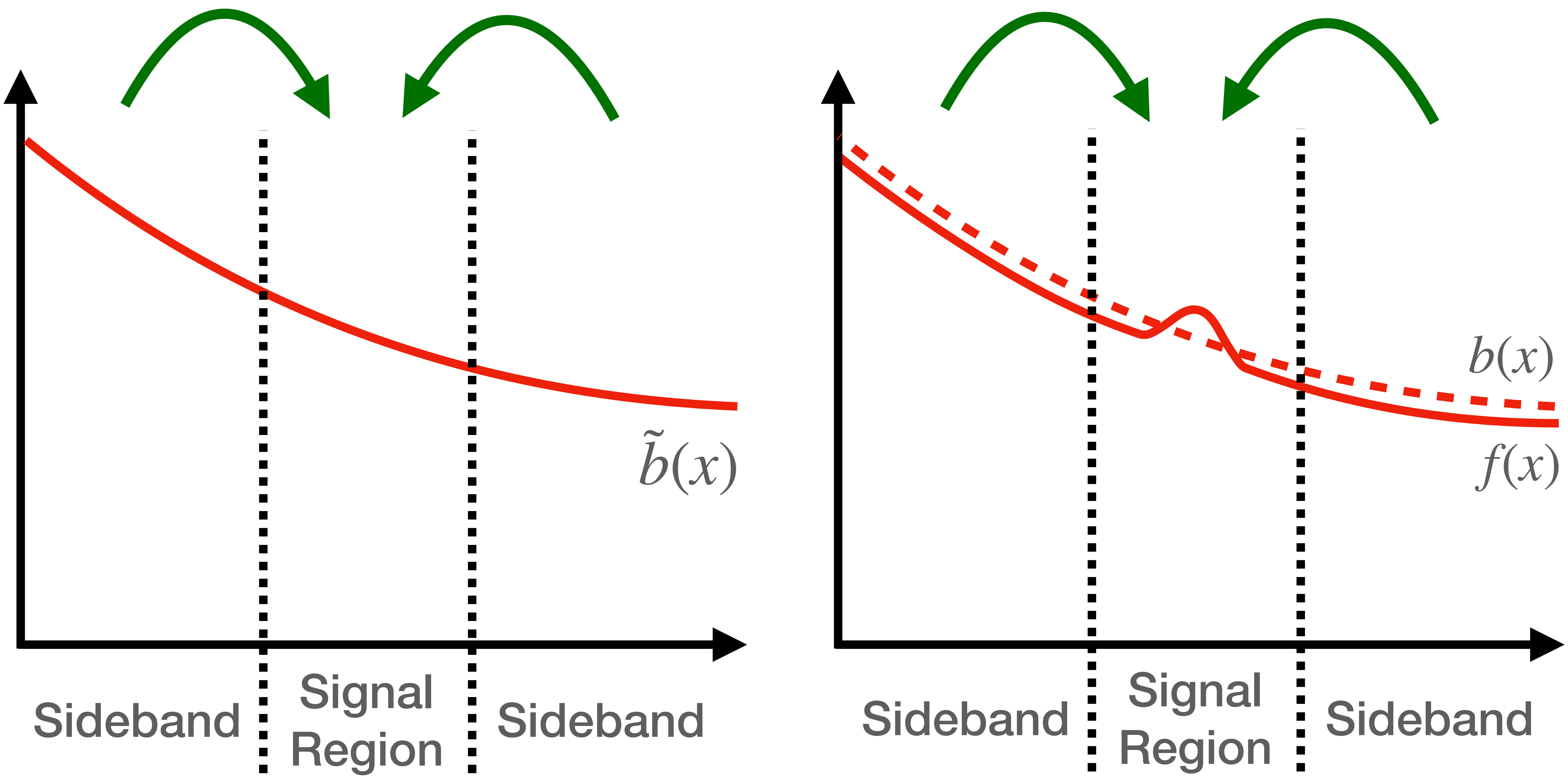


Data-driven background estimation

Step 1: Fit OT map $\hat{T}$ from Sideband to Signal Region of $\tilde{b}$

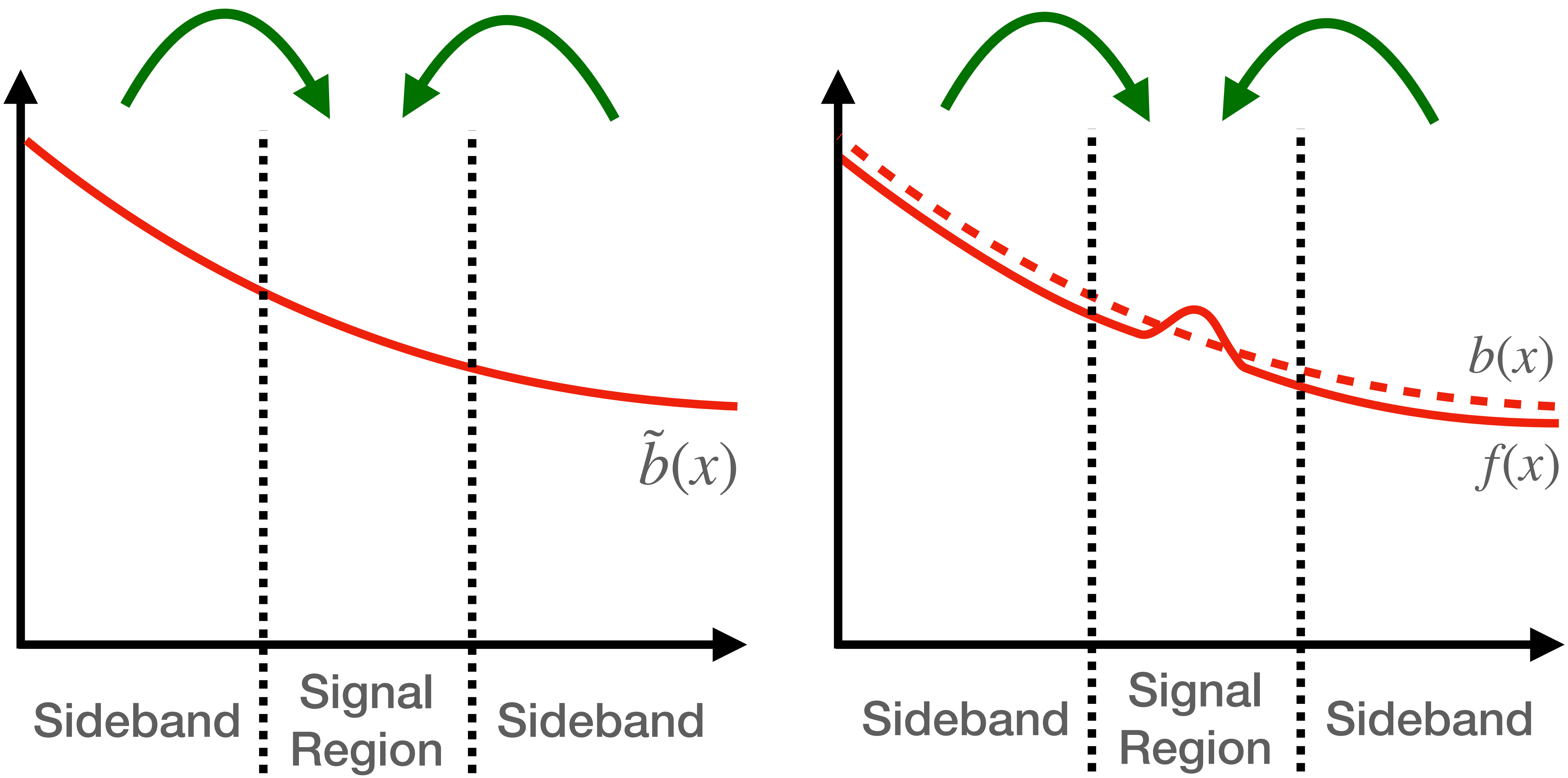
Step 2: Evaluate on Sideband of b (distinct extrapolation from ABCD method!)



Data-driven background estimation

Hierarchical Optimal Transport:

The ground cost is itself the EMD between collider events!



Optimal transport for domain adaptation

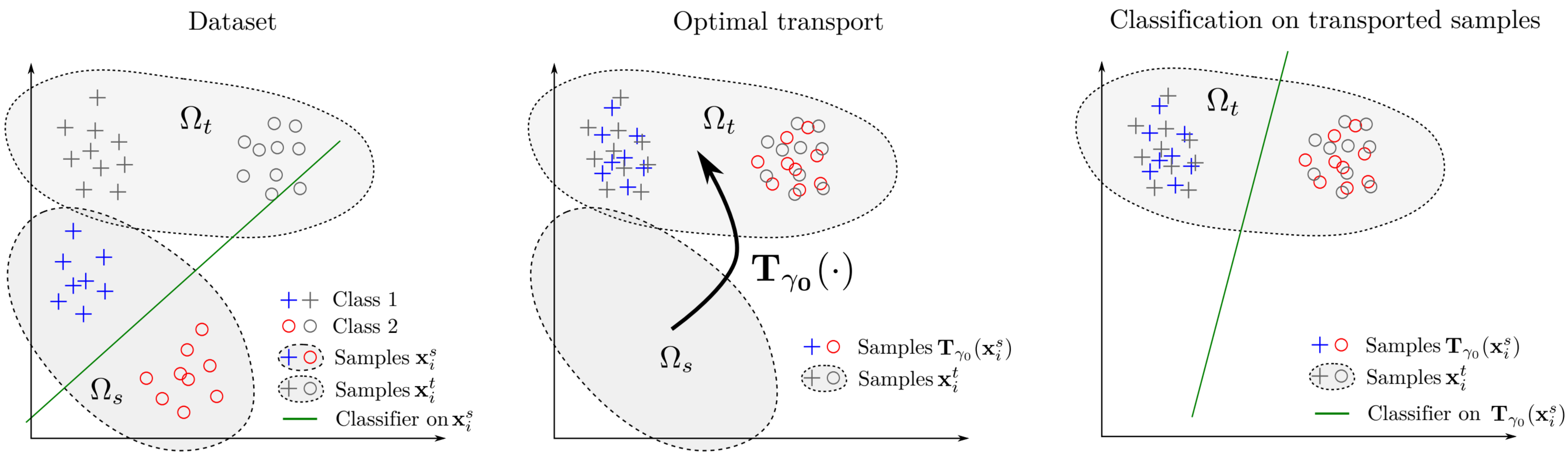
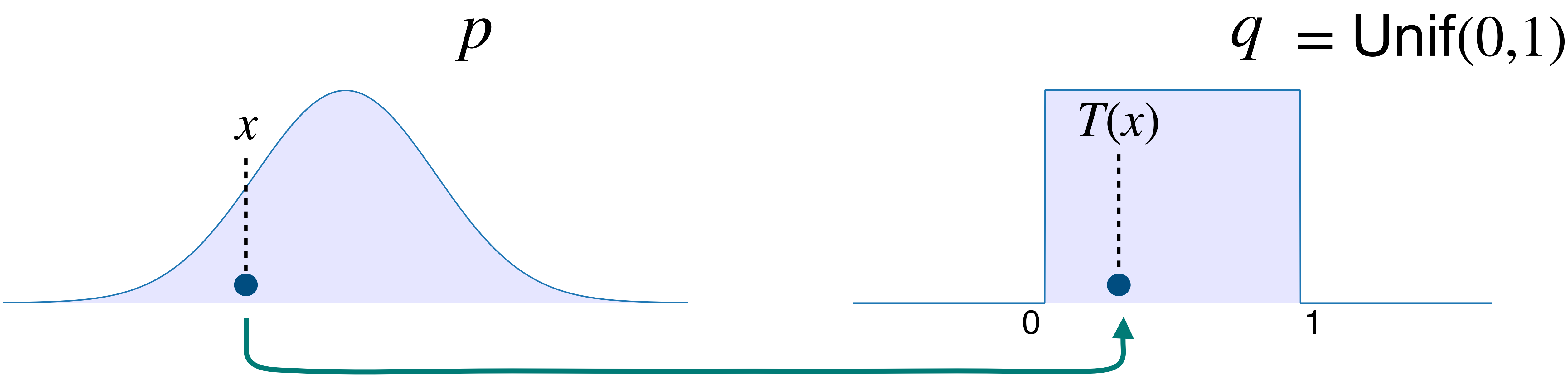


Image Credit: Courty et al (2016)

Multivariate C.D.F.s and quantiles

(Consider $c = \|\cdot\|^2$)



$T(x) = \int_{\infty}^{x} p(y)dy$ (T is the C.D.F. of p)!

Suggests a way to define <u>multivariate</u> C.D.F.s and quantiles

Given a reference density f and a multivariate density p:

- **The OT map from f to p is called the multivariate C.D.F. of p**
- **The OT map from p to f is called the multivariate quantile of p.**

Multivariate C.D.F.s and quantiles

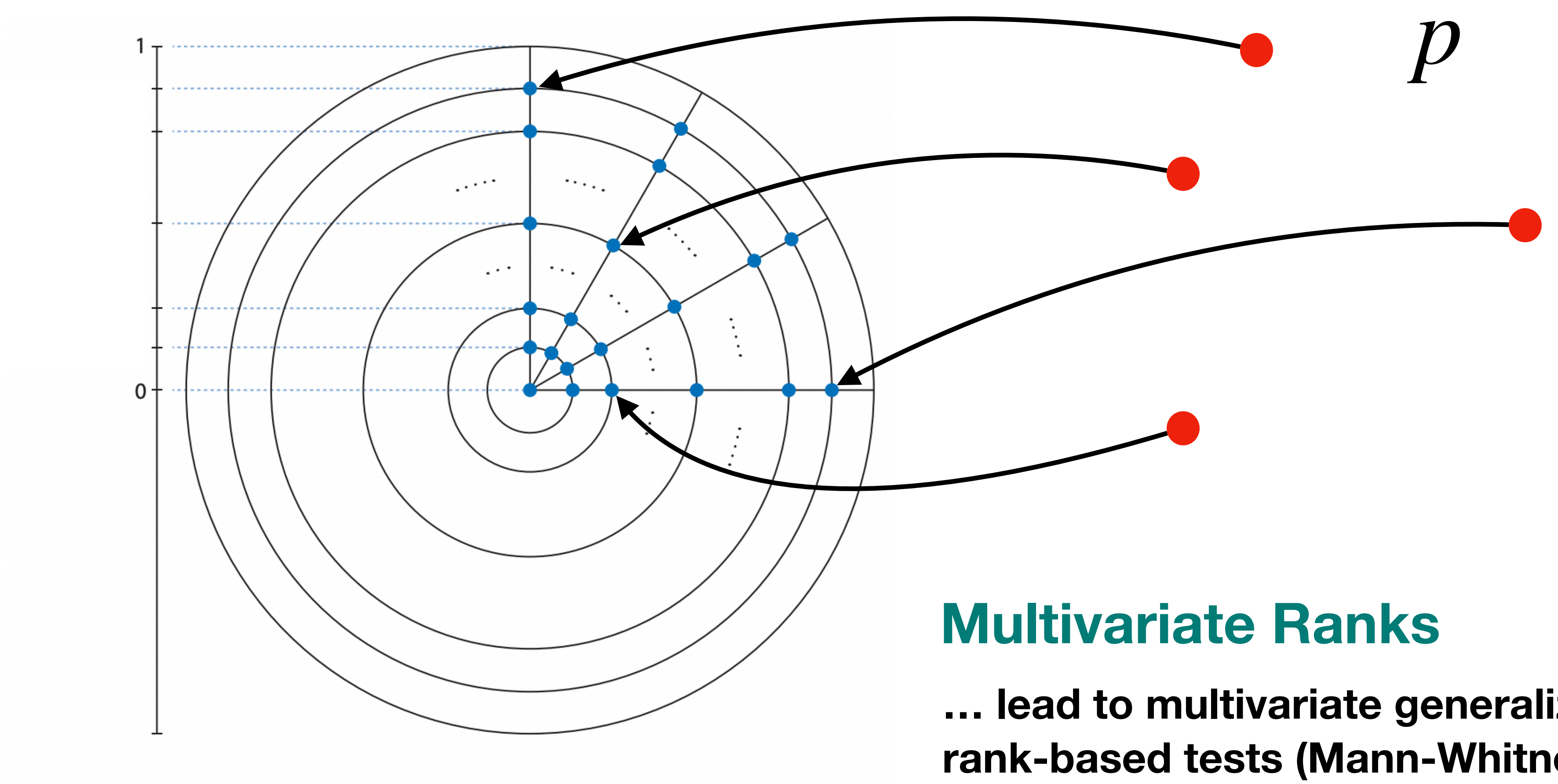


Image Credit: Hallin (2022).

Multivariate Ranks

… lead to multivariate generalizations of classical rank-based tests (Mann-Whitney test, Hoeffding's independence test, Wilcoxon's rank-sign test, etc.)

Suggests a way to define multivariate C.D.F.s and quantiles

Given a **reference density** f and a multivariate density p:

- The OT map from f to p is called the **multivariate C.D.F.** of p
- The OT map from p to f is called the **multivariate quantile** of p.

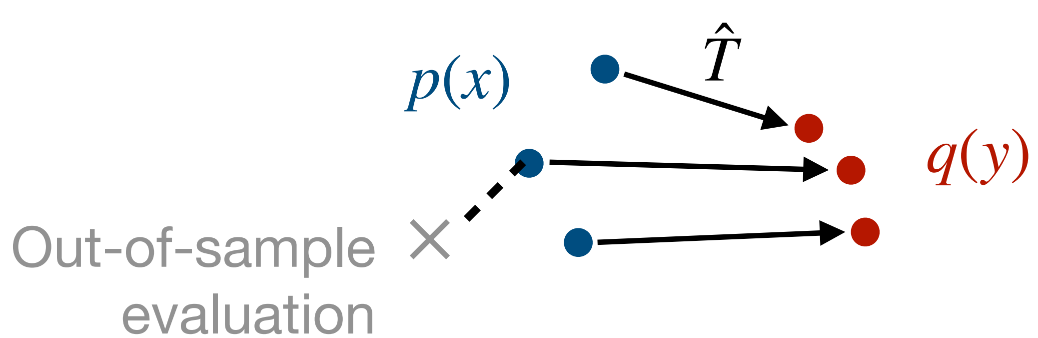
Outlook and Open Problems

Optimal transport has become popular in statistics/HEP-ex because it:

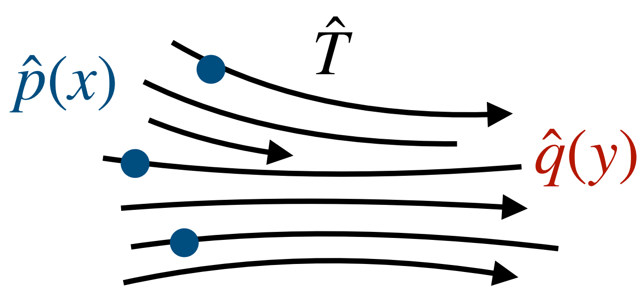
- Provides a canonical way to transport probability distributions
- Stays faithful to the underlying geometry of the space (via the choice of c).
- Yields a metric between distributions for which smoothing is not needed.
- Generalizes traditional statistical notions related to monotonicity (quantiles, CDFs, etc.).
- …

Many open problems remain!

- *Computationally and statistically efficient estimators of OT maps?*
  - “Map-then-smooth estimators”
  - “Smooth-then-map estimators”
  - Other heuristics: input convex neural networks, etc.



“Map-then-smooth”



“Smooth-then-map”

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- *Computationally and statistically efficient estimators of OT maps?*
  - "Map-then-smooth estimators"
  - "Smooth-then-map estimators"
  - Other heuristics: input convex neural networks, etc.

- *Quantifying statistical uncertainty for OT maps?*
  - For smooth-then map estimators, we recently showed that, for some $\Sigma_n(x)$,

$$\Sigma_n(x)\left(\hat{T}_n(x) - T(x)\right) \rightsquigarrow N(0, I_d)\,.$$

  - Does this hold for more practical estimators?
  - Is the bootstrap valid?

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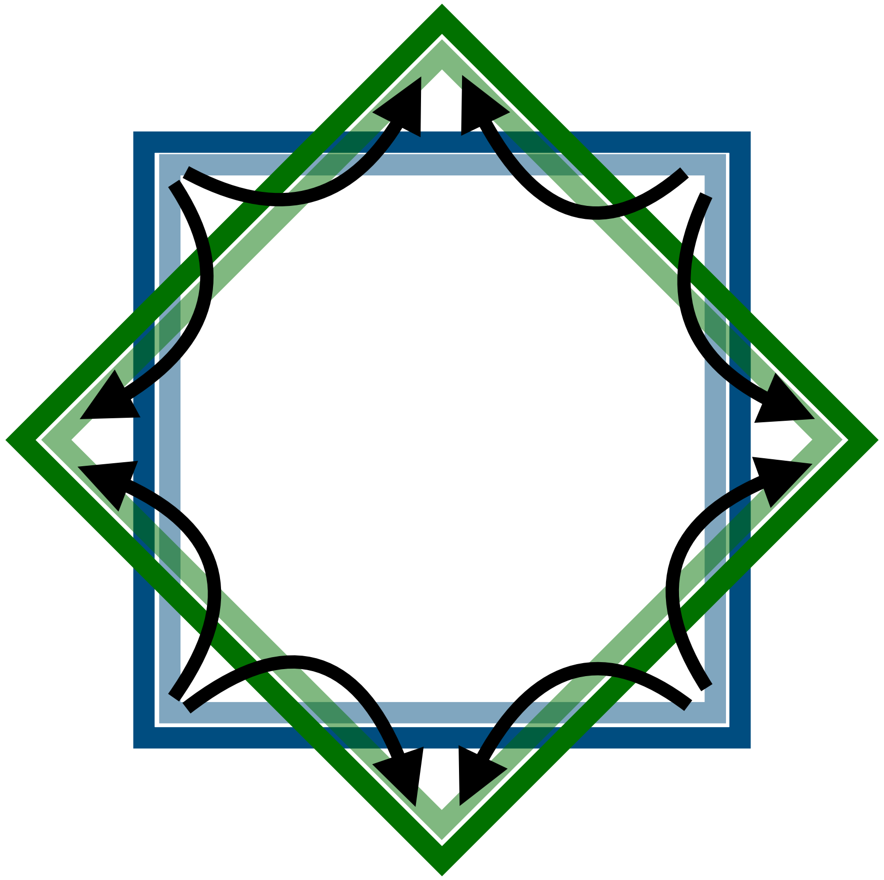


Backup

What is optimal transportation?

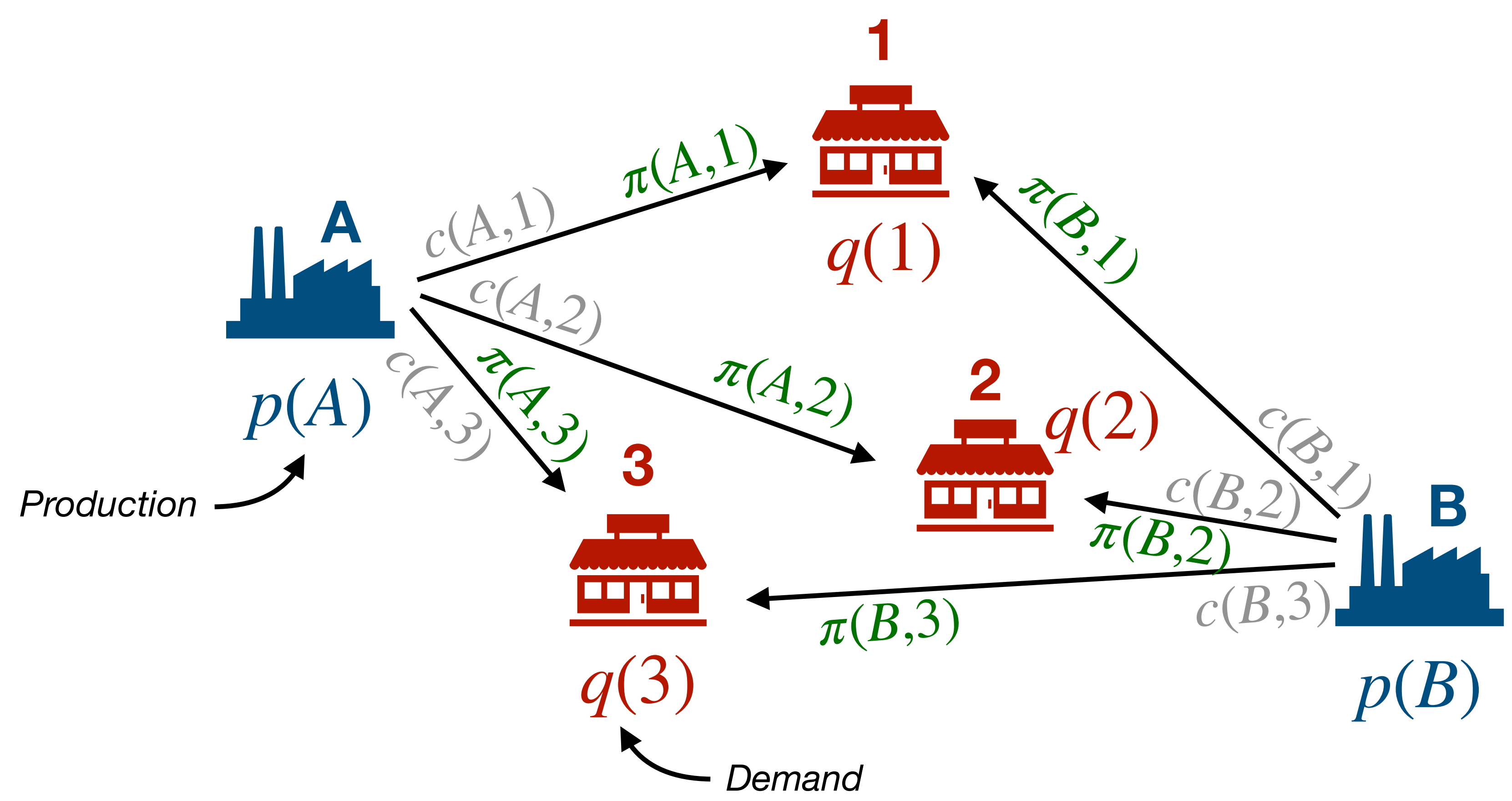
The answer to a logistics problem!

Optimal transportation plan → $\hat{\pi} = \arg\min_{\pi} \sum_a \sum_i \pi(a,i)\, c(a,i)$

Transportation cost *(per unit mass)*: $c(a,i)$

Optimization over all possible transportation plans: $\arg\min_{\pi}$

Mass transported from factory a to store i *("transportation plan")*: $\pi(a,i)$



Assume total production $p(A) + p(B)$ *equals total demand* $q(1) + q(2) + q(3)$

What is optimal transportation?

The answer to a logistics problem!

$$\hat{\pi} = \arg\min_{\pi} \sum_a \sum_i \pi(a,i)\, c(a,i)$$

Optimal transportation plan → $\hat{\pi}$

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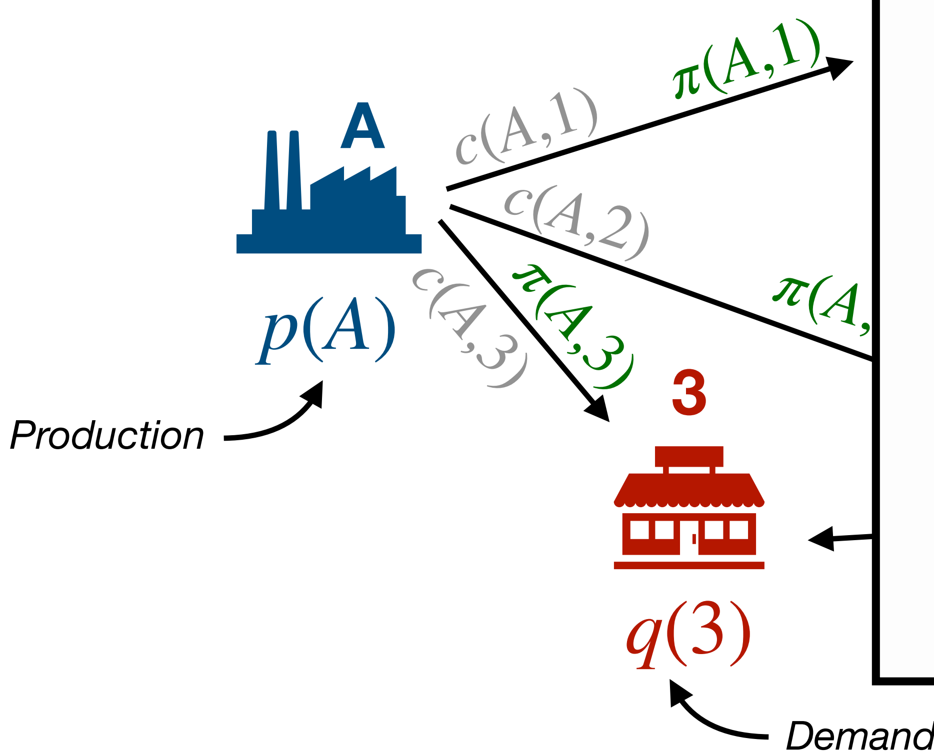


"All possible" transportation plans?

Must satisfy two conditions:

$$\sum_i \pi(a,i) = p(a) \quad \forall a$$

"Entire production is shipped"

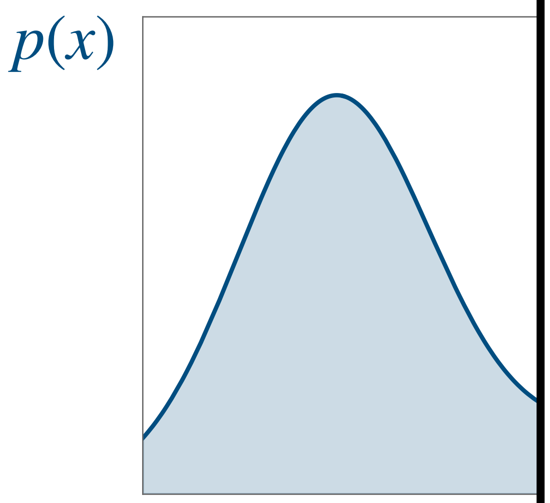
$$\sum_a \pi(a,i) = q(i) \quad \forall i$$

"Entire demand is satisfied"

Assume total production $p(A) + p(B)$ *equals total demand* $q(1) + q(2) + q(3)$

Optimal transport, now continuous

How about a continuous **distribution of production** $p(x)$ and a **continuous distribution of demand** $q(y)$?



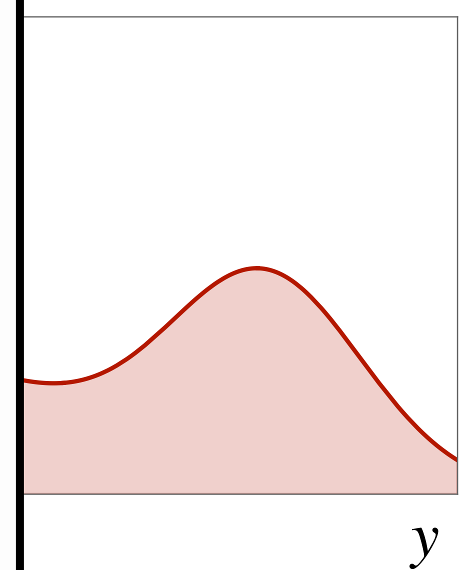
Remember: the marginals of any admissible transport plan must give the source and target distributions:

$$\int dy \;\; \pi(x,y) = p(x)$$

"Entire mass picked up"

$$\int dx \;\; \pi(x,y) = q(y)$$

"Entire mass delivered"



Cost to transport one unit of mass from x to y: $c(x,y)$

Transport plan: move an amount $\pi(x,y)$ from x to y

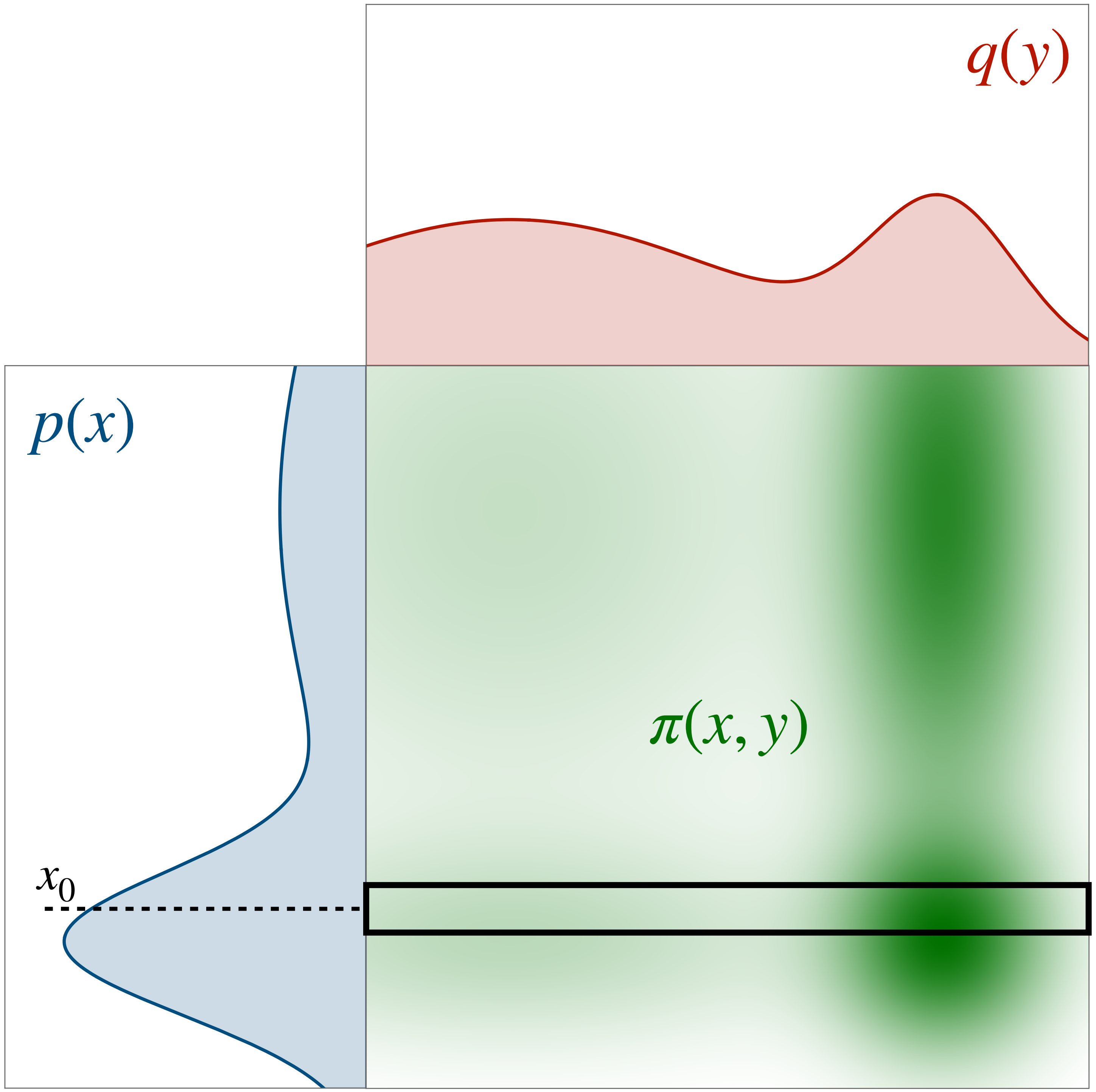
Transport plan with minimal cost:

$$\hat{\pi} = \arg\min_{\pi} \int dx\, dy \;\; \pi(x,y) \; c(x,y)$$

"Kantorovich optimal transport problem"

Optimal transport, now continuous

How about a continuous **distribution of production** $p(x)$ and a **continuous distribution of demand** $q(y)$?



$\pi(x_0, y) \sim q(y)$

It is not difficult to satisfy these constraints!

$$\pi(x, y) = p(x)\, q(y)$$

(Is admissible, but rarely minimal)

This transport plan distributes Mass from x_0 across all y

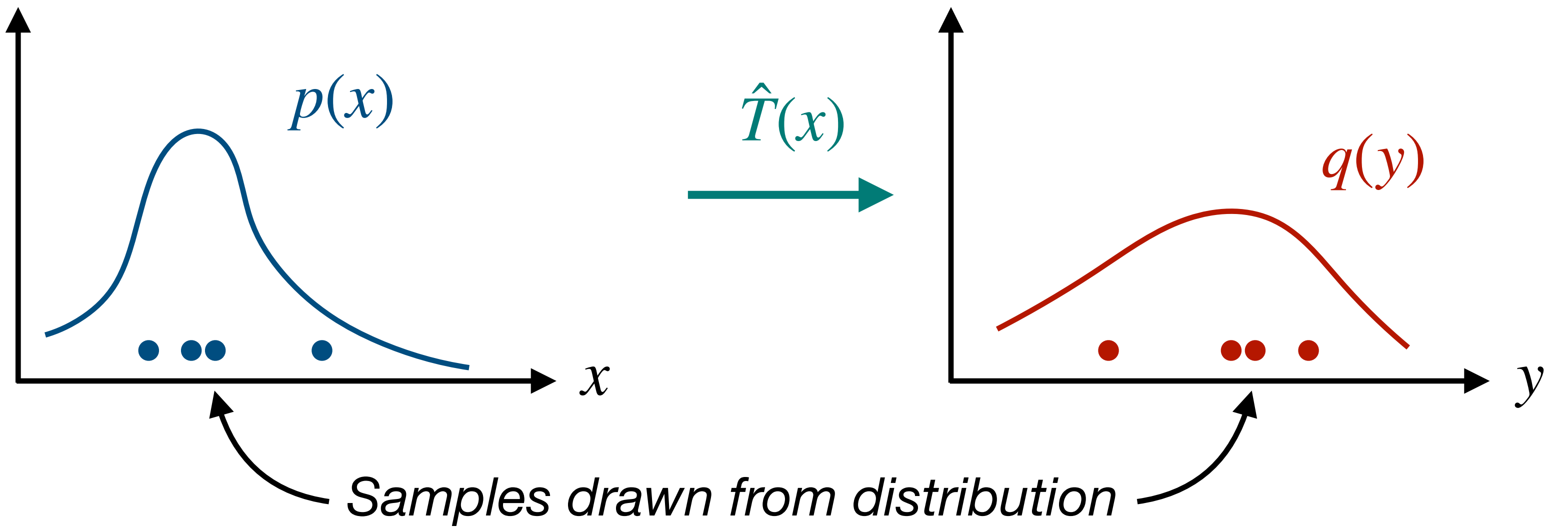
Constraints:

$$\int dy \;\; \pi(x, y) = p(x)$$

$$\int dx \;\; \pi(x, y) = q(y)$$

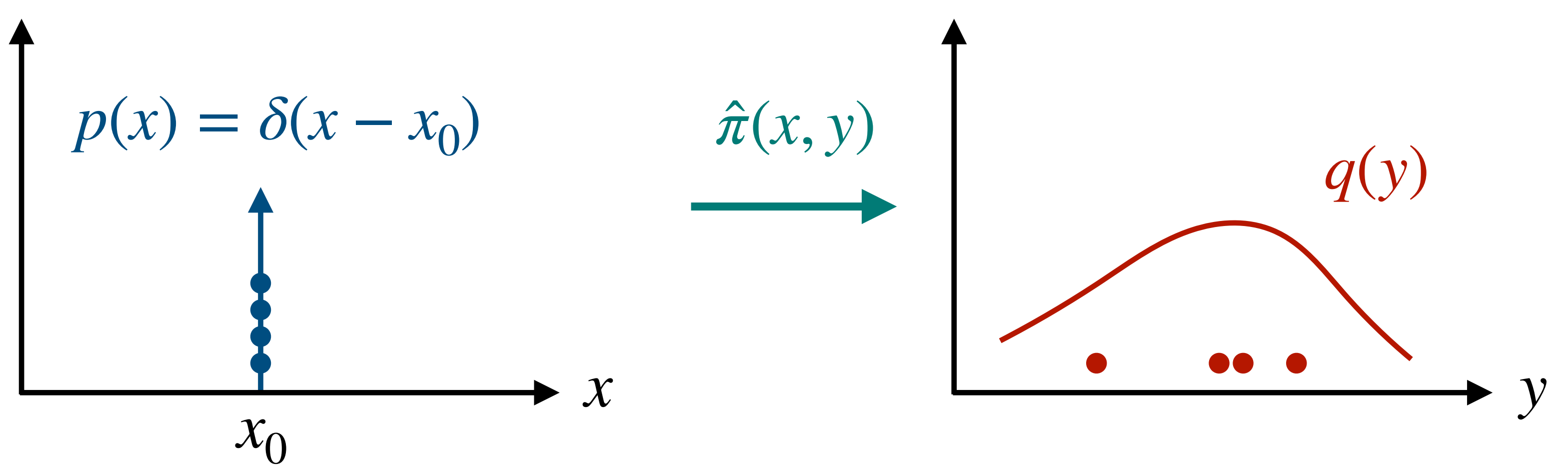
Monge vs. Kantorovich

Transport between two smooth distributions:



Deterministic transport
("reordering of samples") sufficient
→ ***Monge problem***

Transport between non-smooth and smooth distribution:



Need stochastic transport
("random smearing of samples")
→ ***Kantorovich problem***

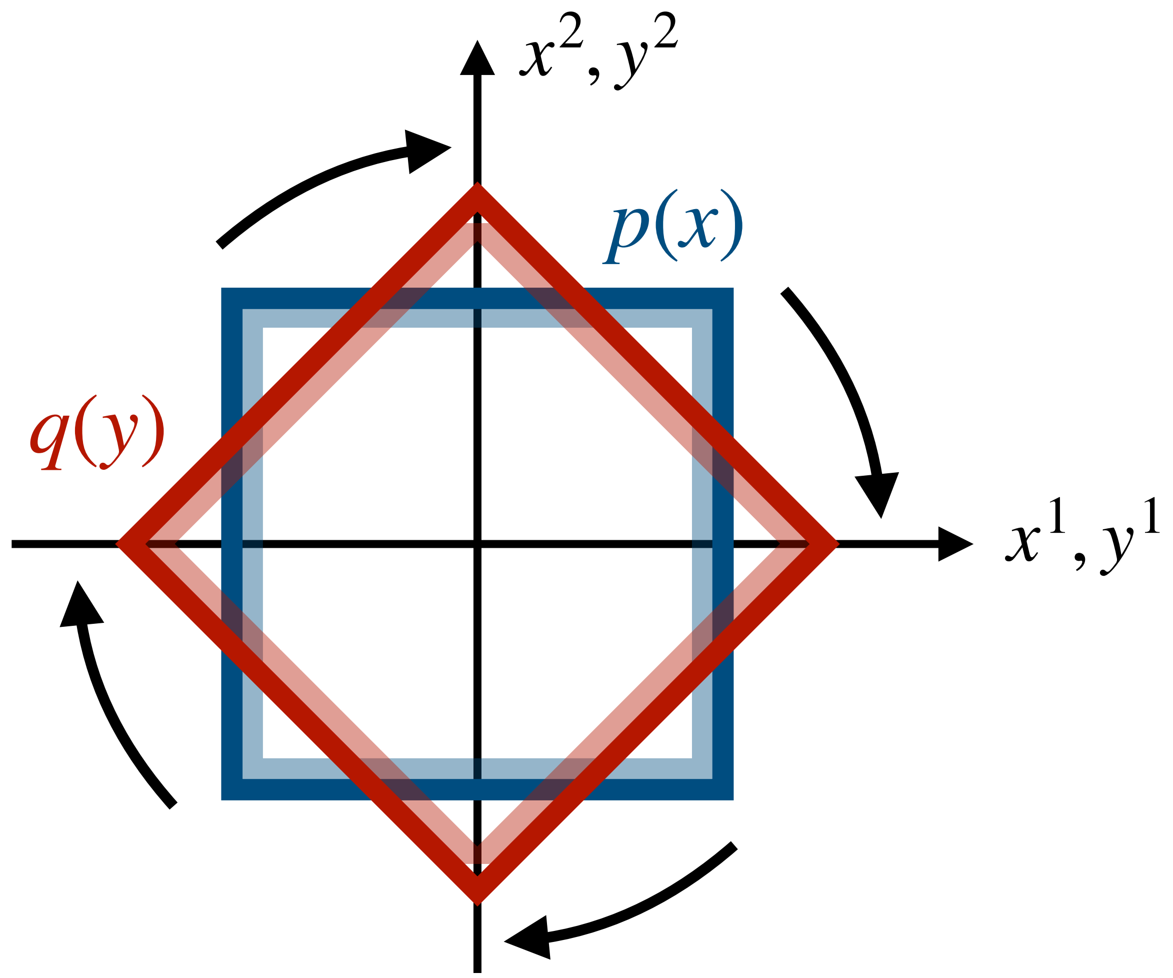
The choice of cost function

Many useful cost functions are convex!

E.g. $c(x, y) = |x - y|^p$ for $p > 1$

… let's look at a few examples!

$p = 2$, i.e. $c(x, y) = |x - y|^2$



Example:

Source distribution $p(x)$ populates inside of axis-aligned square

Target distribution $q(y)$ populates "rotated" square

But: rotation is not a gradient vector field!

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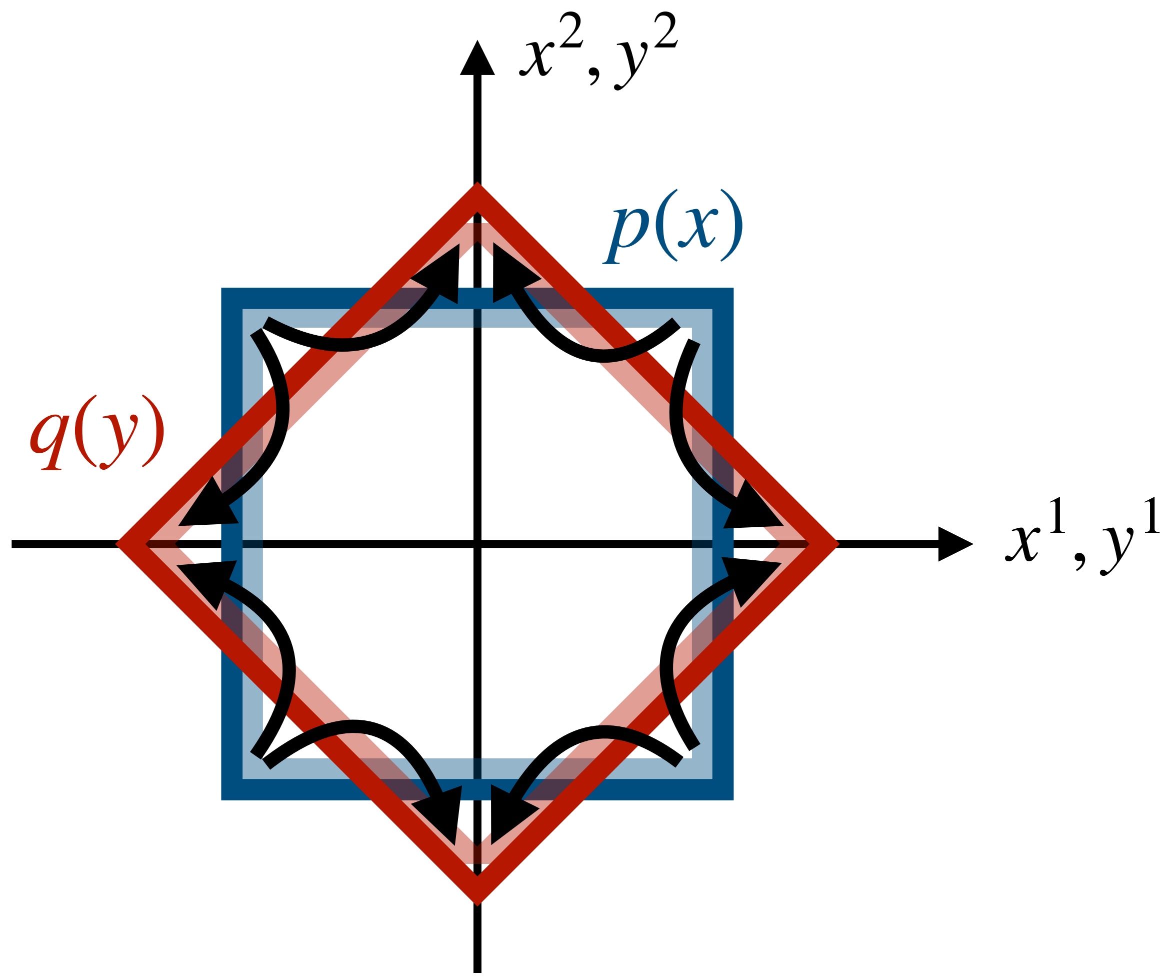

Example:

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Target distribution $q(y)$ populates "rotated" square

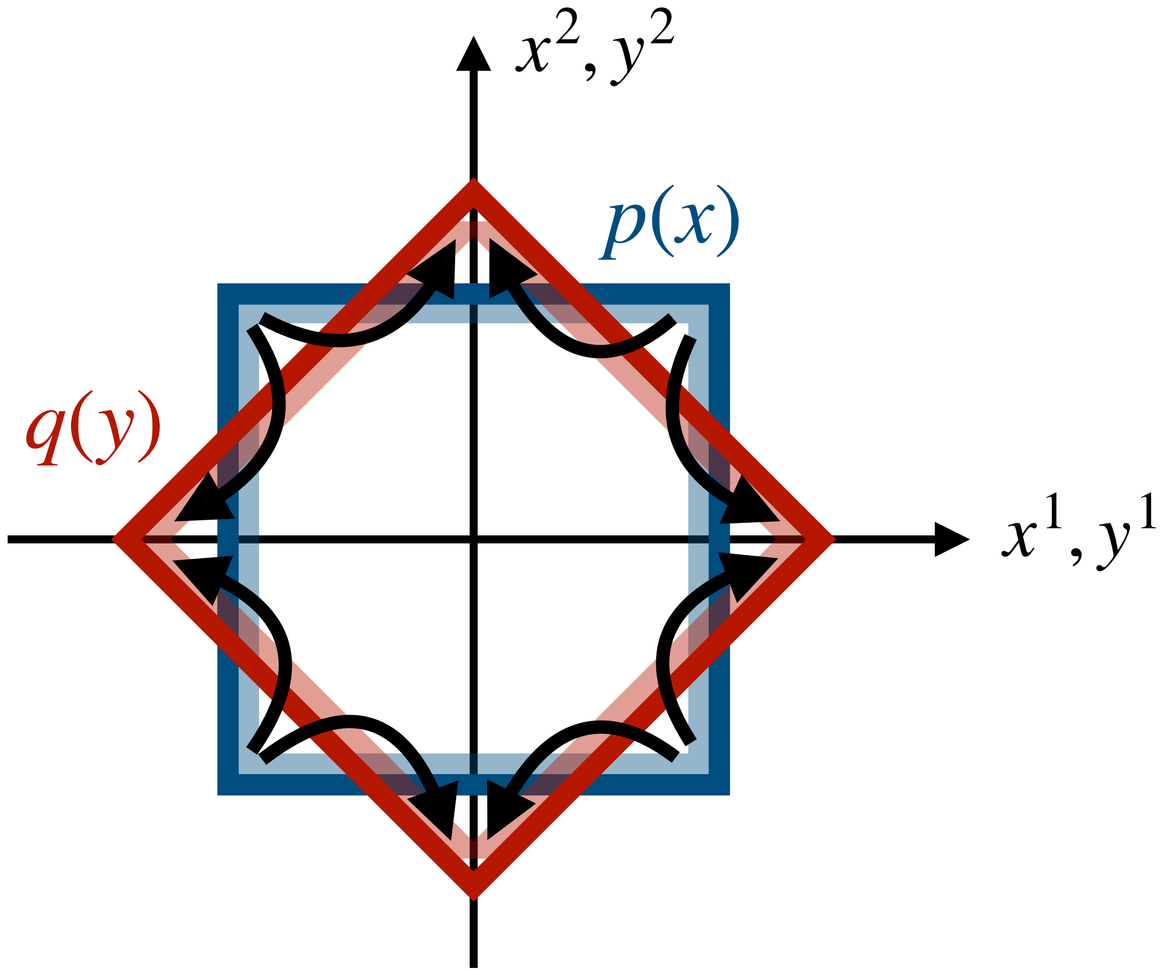
But: rotation is not a gradient vector field!

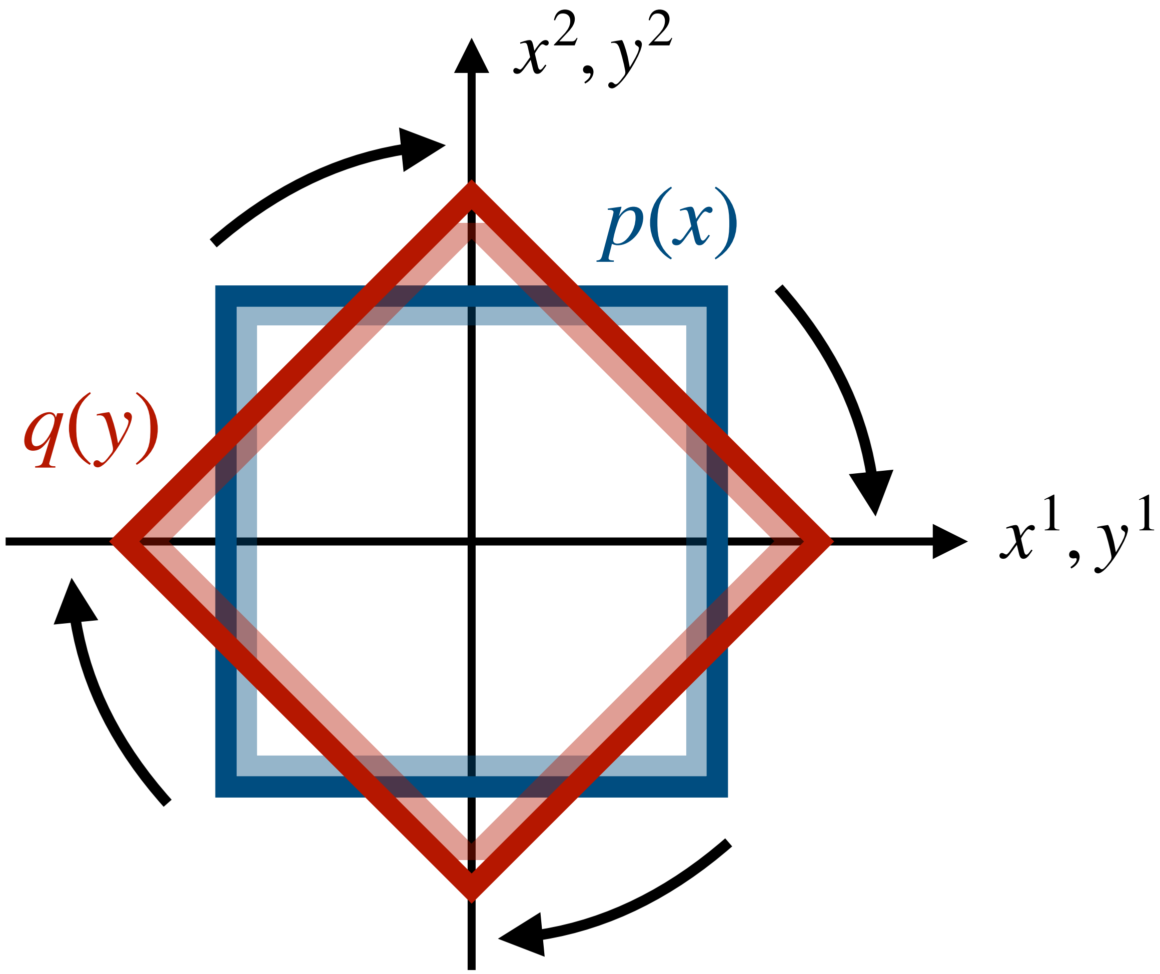
The optimal transport solution looks like this

Calibrating simulations: the right cost function

Example from before: simulation of a square, but rotation angle incorrectly modeled

Uncalibrated simulation **Calibration data**





Optimal in Euclidean plane

$$ds^2 = dr^2 + r^2 d\phi^2$$

Optimal on a cone manifold

$$ds^2 = \alpha^2 dr^2 + r^2 d\phi^2, \alpha > 1$$

Use this if rotational degree of freedom is known to be poorly modeled

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… let's look at a few examples!

$p = 2$, i.e. $c(x, y) = |x - y|^2$

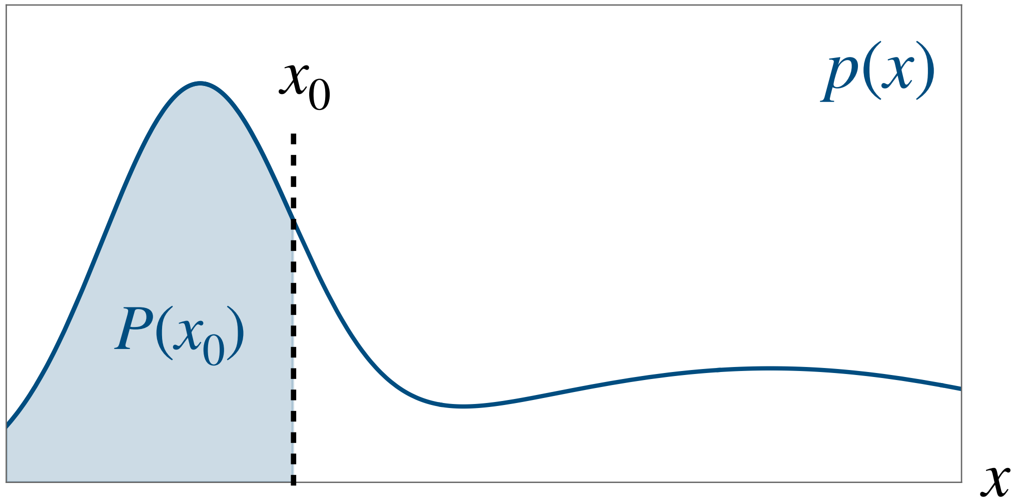
For 1-dimensional distributions:

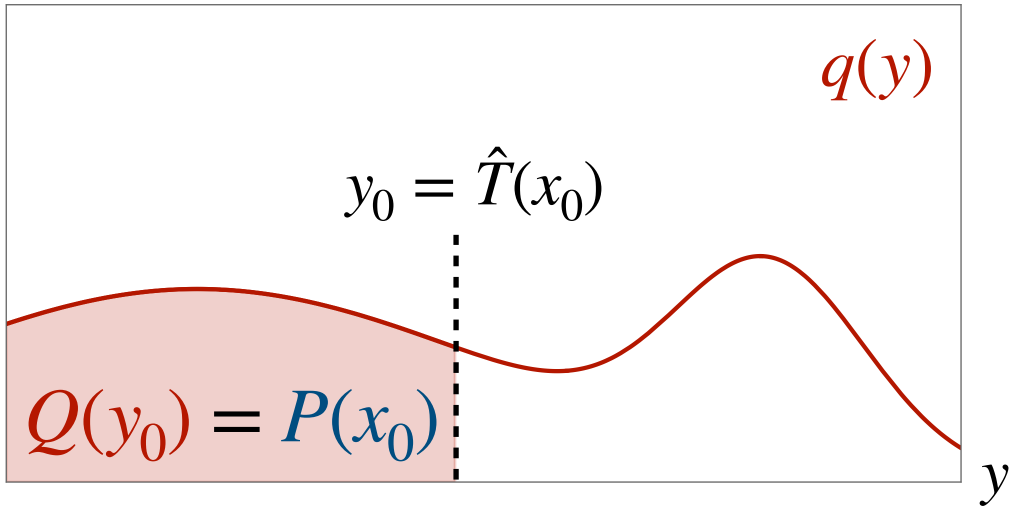
The optimal transport solution performs quantile-matching *(works for all convex cost functions!)*

$$\hat{T}(x) = Q^{-1}(P(x))$$

Cumulative distributions of $p(x)$, $q(y)$:

Generically: $F(x) = \int_0^x dx' f(x')$





The choice of cost function

Many useful cost functions are convex!

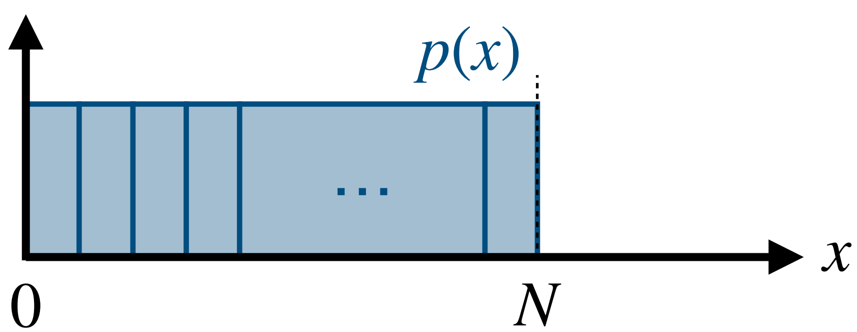
E.g. $c(x, y) = |x - y|^p$ for $p > 1$

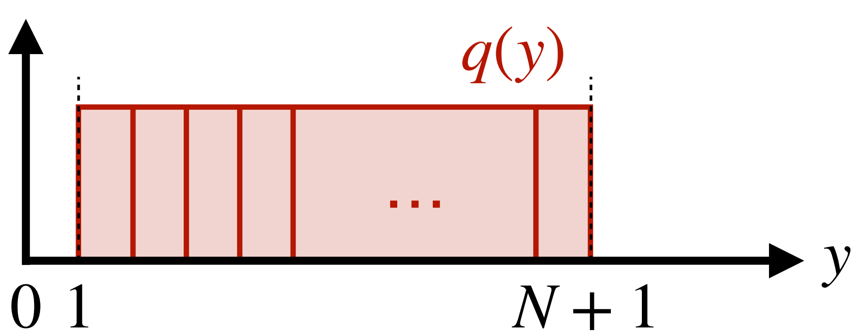
… let's look at a few examples!

$p = 1$, i.e. $c(x, y) = |x - y|$ *(Monge's original problem)*

This is a much more complicated case!

Solutions exist for smooth distributions, but no longer unique!





Example:

Uniform source and target distributions
(e.g. rows of N books, shifted by one)

The choice of cost function

Many useful cost functions are convex!

E.g. $c(x, y) = |x - y|^p$ for $p > 1$

… let's look at a few examples!

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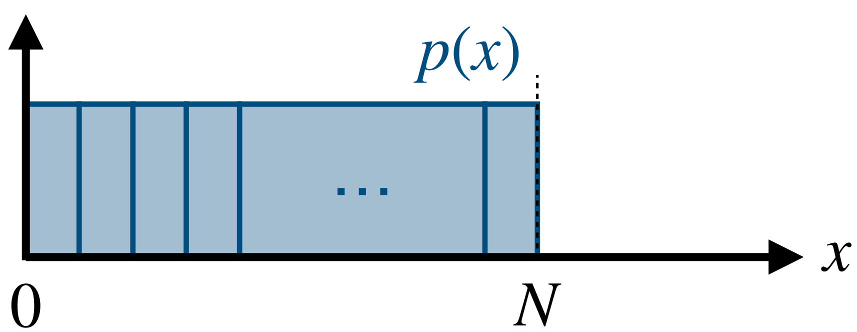
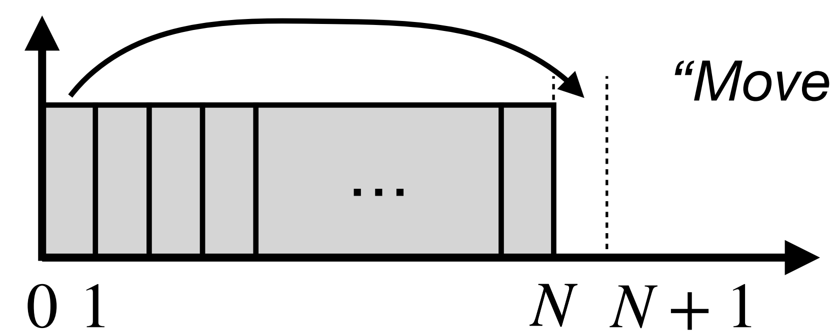
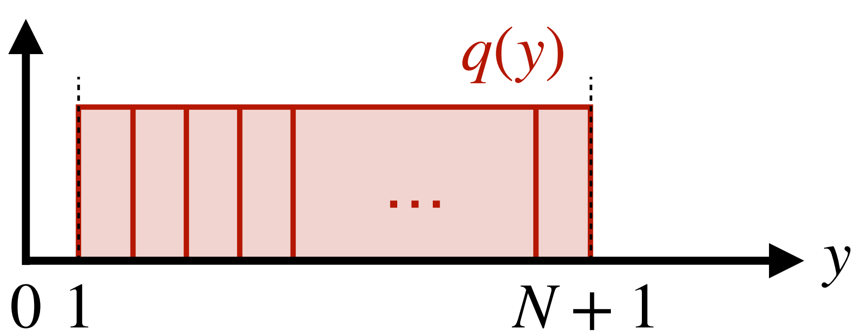
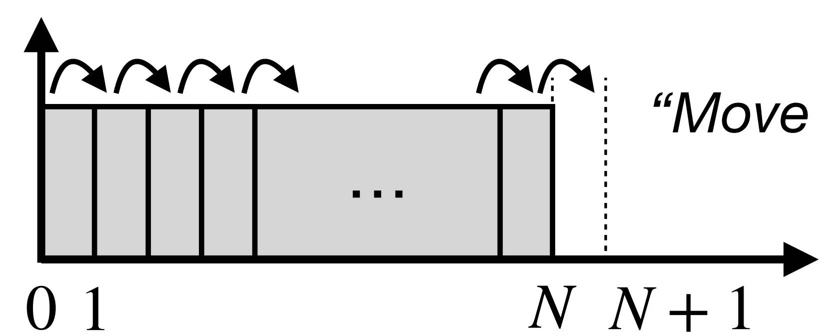




"Move 1 book by N"





"Move N books by 1"

A solution sketch

$\hat{T} = \nabla \hat{g}$

Monge problem

Nonlinear constraint

$$\hat{T} = \arg\min_T \int dx\; p(x)\; c(x, T(x))$$

$$\pi(x, y) = p(x)\,\delta[y - T(x)] \qquad q(y) = p(x)\left(\frac{dT}{dx}\right)^{-1}$$

Equivalence for smooth distributions

Kantorovich problem

Linear constraints!

$$\hat{\pi} = \arg\min_\pi \int dx\,dy\; \pi(x, y)\; c(x, y)$$

$$\int dy\; \pi(x, y) = p(x) \qquad \int dx\; \pi(x, y) = q(y)$$

Kantorovich-Rubinstein duality

Dual Kantorovich problem

Convex constraints
→ manageable!

$$\hat{f}, \hat{g} = \arg\max_{f,g} \int dy\, q(y)\, f(y) + \int dx\, p(x) g(x)$$

$$g(x) + f(y) \le c(x, y)$$

The Kantorovich-Rubinstein duality

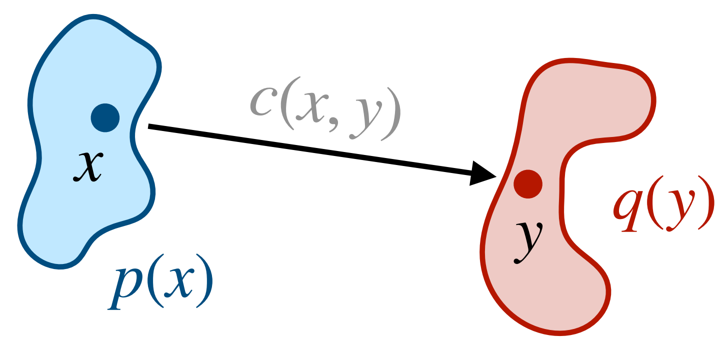
Primal problem:

$$\hat{\pi} = \arg\min_{\pi} \int dx\, dy\; \pi(x, y)\, c(x, y)$$

$$\int dy\; \pi(x, y) = p(x) \qquad \int dx\; \pi(x, y) = q(y)$$

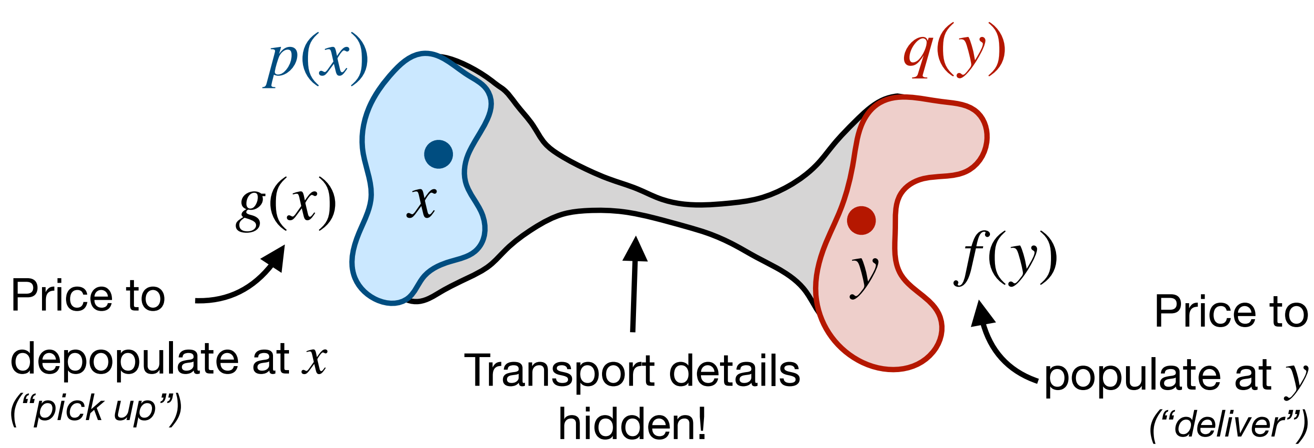
"Operative perspective":

Optimise transportation plan based on point-to-point cost $c(x, y)$



"Black-box perspective":

Optimize prices $g(x)$ and $f(y)$: maximize revenue while underbidding point-to-point transport



Dual problem:

$$\hat{f}, \hat{g} = \arg\max_{f,g} \int dy\, q(y)\, f(y) + \int dx\, p(x)\, g(x)$$

$$g(x) + f(y) \leq c(x, y)$$

The dual problem

The dual problem is (much) easier to solve numerically:

$$\hat{f}, \hat{g} = \arg\max_{f,g} \int dy\, q(y)\, f(y) + \int dx\, p(x) g(x)$$

$$g(x) + f(y) \leq c(x, y)$$

For $c(x, y) = |x - y|^2$, $\hat{f}$ and $\hat{g}$ are Legendre-conjugates!

Legendre transform in classical mechanics:

$$H(p) + L(\dot{q}) = p\dot{q}$$

Hamiltonian *Lagrangian*

$$\hat{g} = \arg\max_{g \in \text{cvx}} \int dy\, q(y)\, g^*(y) + \int dx\, p(x) g(x)$$

Legendre transform: $g^*(y) = \max_x \left[x \cdot y - g(x)\right]$

Maximise this "loss function" over all convex functions $g(x)$

Recover optimal transport function $\hat{T} = \nabla \hat{g}$

Some statistical applications of Wasserstein distances

- **Goodness-of-fit Testing:** Given $X_1, \ldots, X_n \sim p$ and known q, one can test

$$H_0 : p = q, \quad H_1 : p \neq q$$

using the test statistic $W_p(P_n, q)$, where P_n is the empirical distribution.

  - Similar ideas apply to **two-sample testing**.

- **Minimum-distance Estimation:** Given a parametric model $(p_\theta)_{\theta \in \Theta}$ and $X_1, \ldots, X_n \sim p_{\theta_0}$, construct the following estimator for θ_0:

$$\hat{\theta} = \operatorname*{argmin}_{\theta \in \Theta} W_p(P_n, p_\theta)\,.$$

Broad message: Unlike many classical metrics, the Wasserstein distance is well-defined for empirical measures, and provides a useful <u>data analytic tool</u>.

The Earth Mover's Distance a.k.a. Partial OT)

$$\mathrm{EMD}(\mathcal{E}, \mathcal{E}') = \min_{\{f_{ij} \geq 0\}} \sum_{ij} f_{ij} \frac{\theta_{ij}}{R} + \left| \sum_i E_i - \sum_j E'_j \right|,$$

$$\sum_j f_{ij} \leq E_i, \qquad \sum_i f_{ij} \leq E'_j, \qquad \sum_{ij} f_{ij} = E_{\min},$$

See Komiske et al., 2019.