A Primer on Optimal Transport

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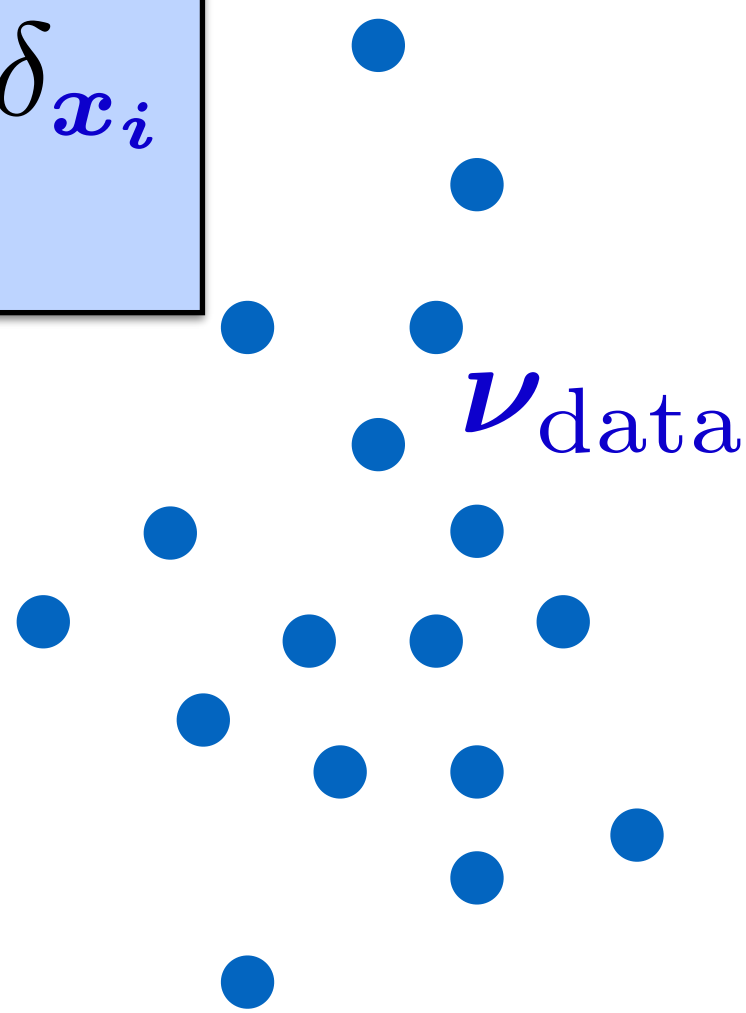
book with Gabriel Peyré

https://optimaltransport.github.io/

A Motivating Example

We collect data

$$\boldsymbol{\nu}_{\text{data}} = \frac{1}{N}\sum_{i=1}^{N}\delta_{\boldsymbol{x}_i}$$



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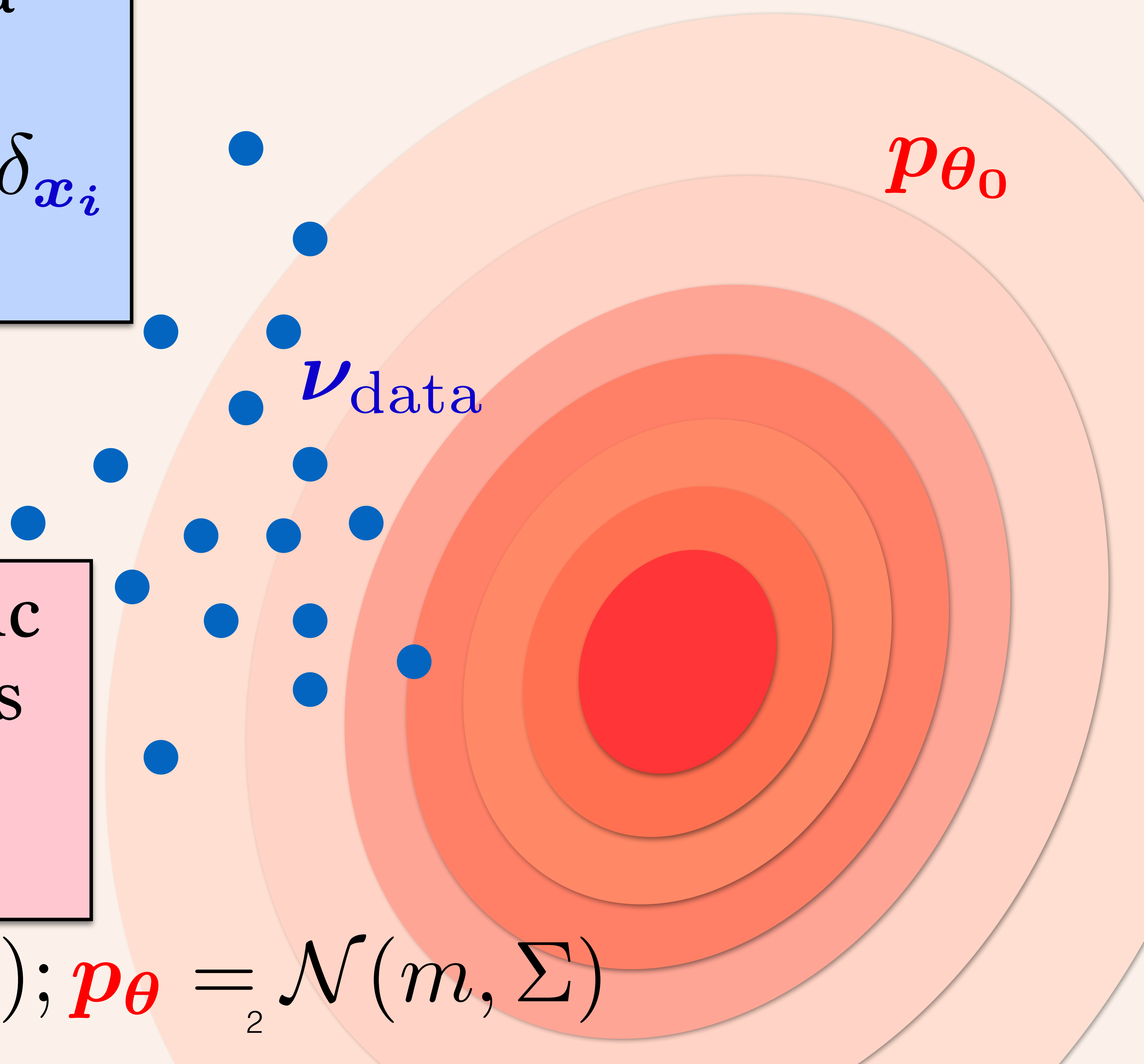
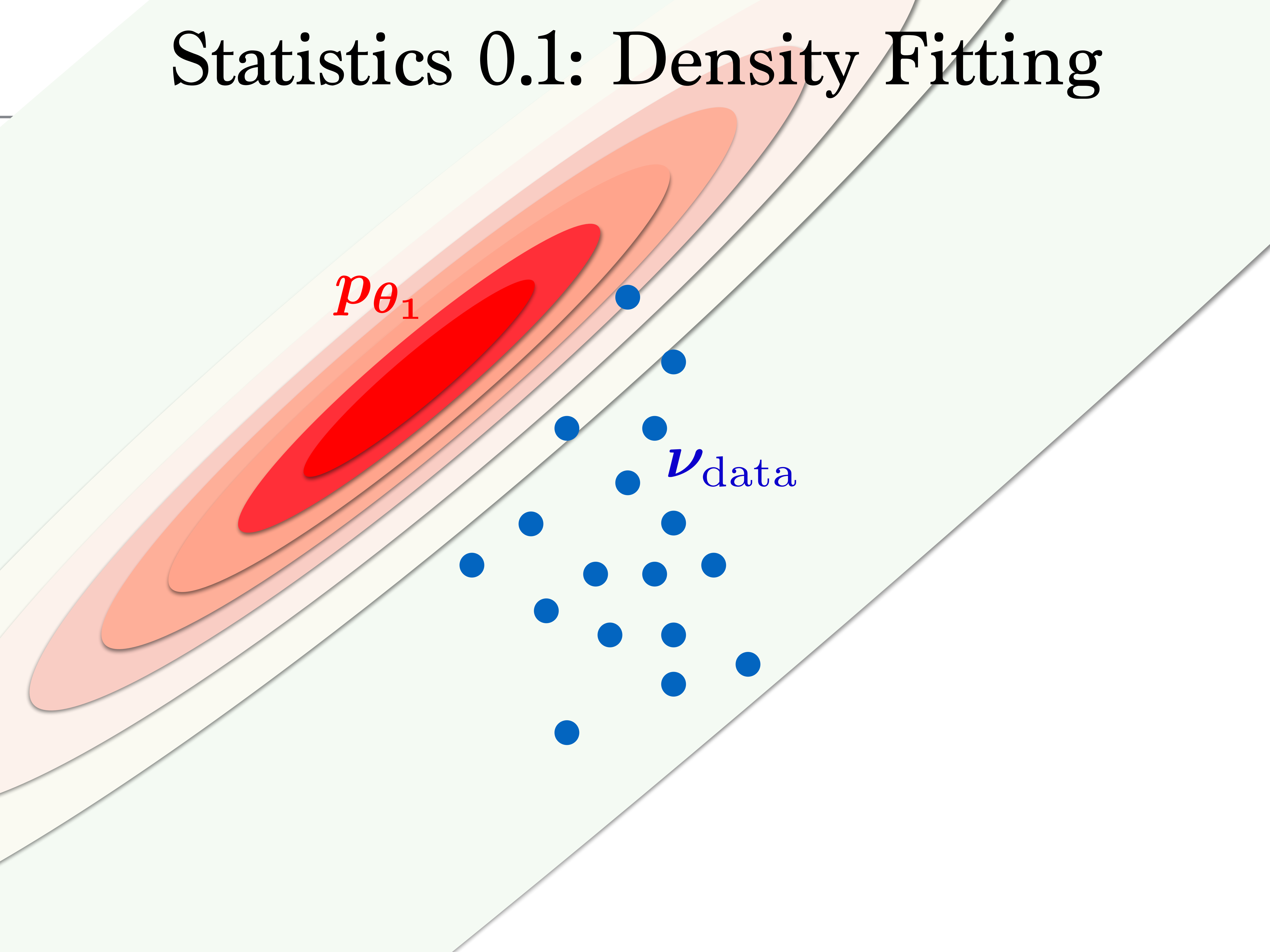


We fit a parametric family of densities

$$\{\boldsymbol{p_\theta}, \boldsymbol{\theta} \in \boldsymbol{\Theta}\}$$

$$e.g.\ \boldsymbol{\theta} = (m, \Sigma); \boldsymbol{p_\theta} = \mathcal{N}(m, \Sigma)$$

Statistics 0.1: Density Fitting



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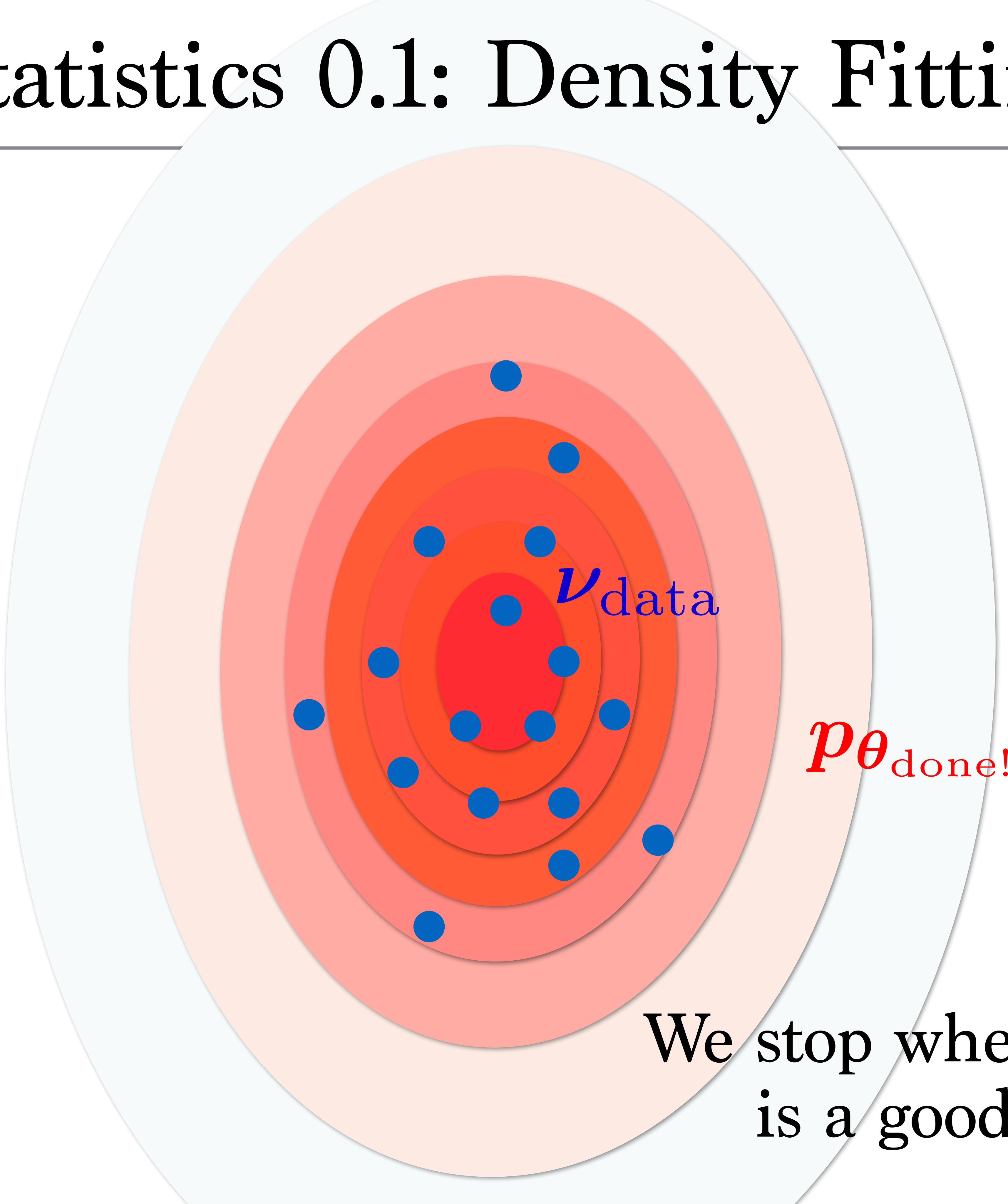
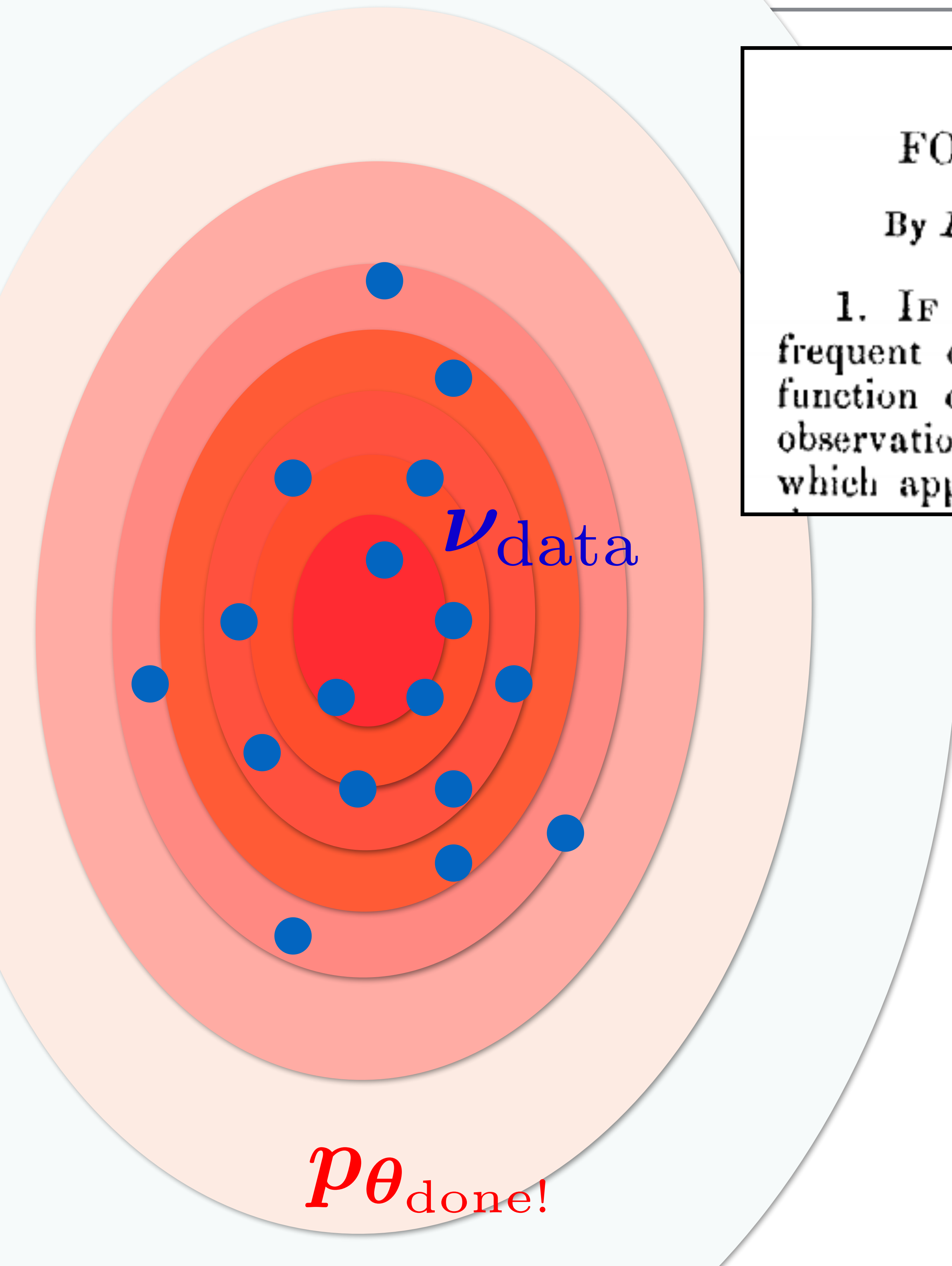


We stop when there is a good fit.

Maximum Likelihood Estimation



ON AN ABSOLUTE CRITERION FOR FITTING FREQUENCY CURVES.

By *R. A. Fisher*, Gonville and Caius College, Cambridge.

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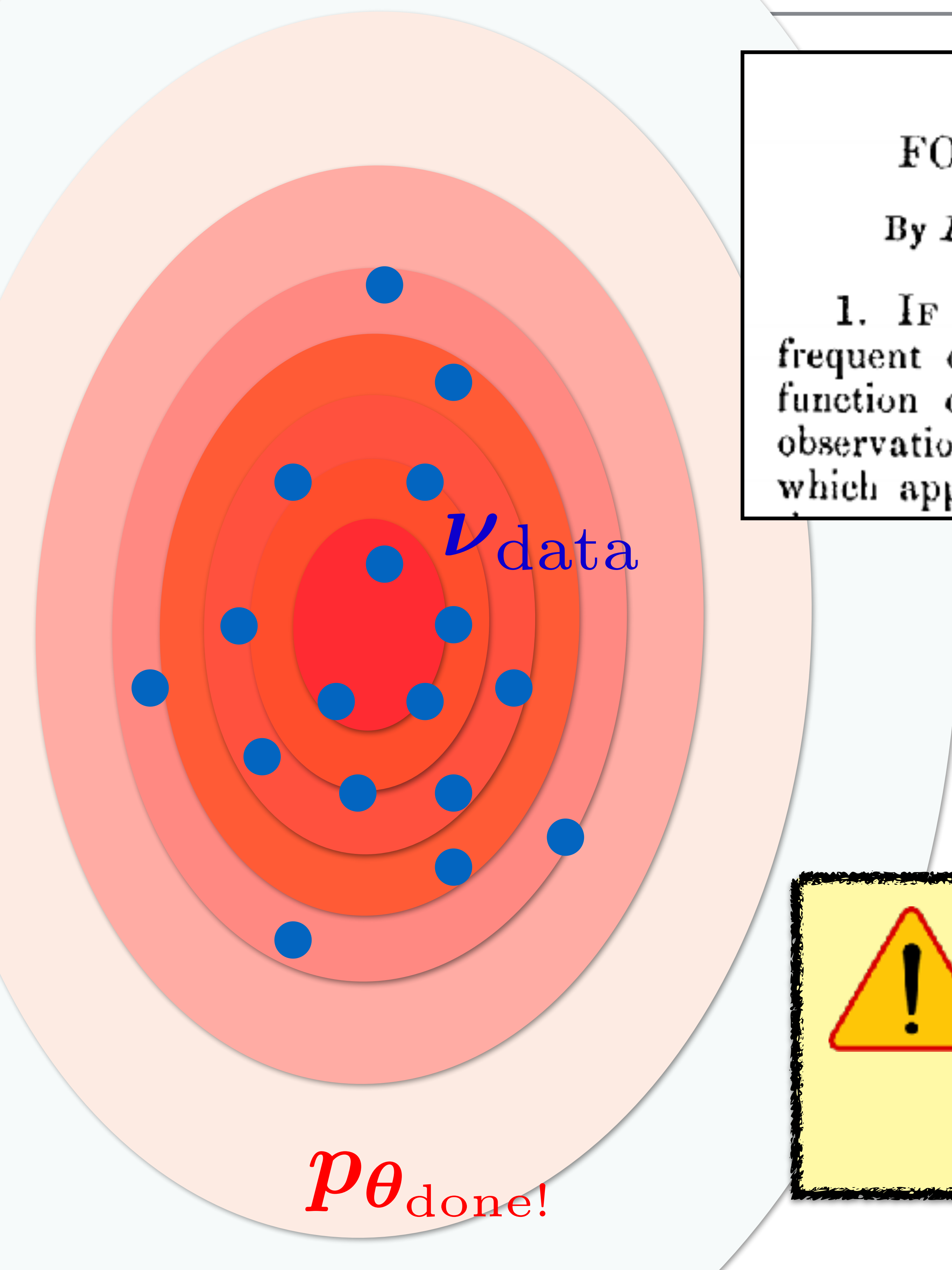

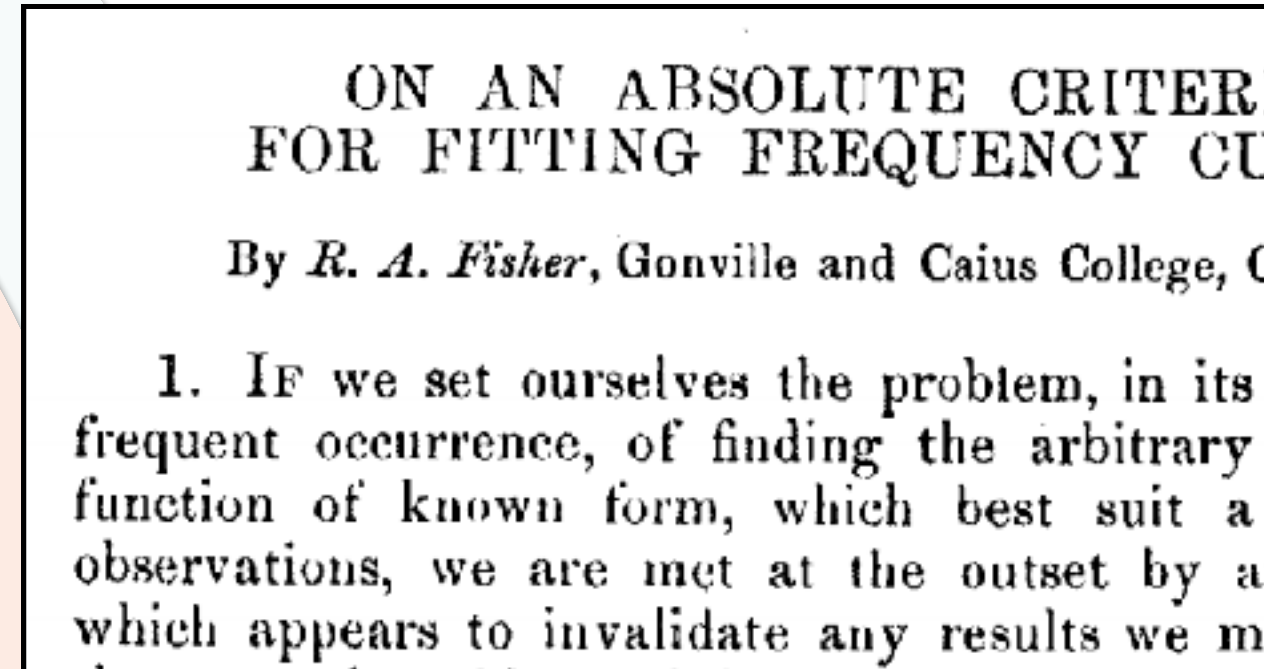
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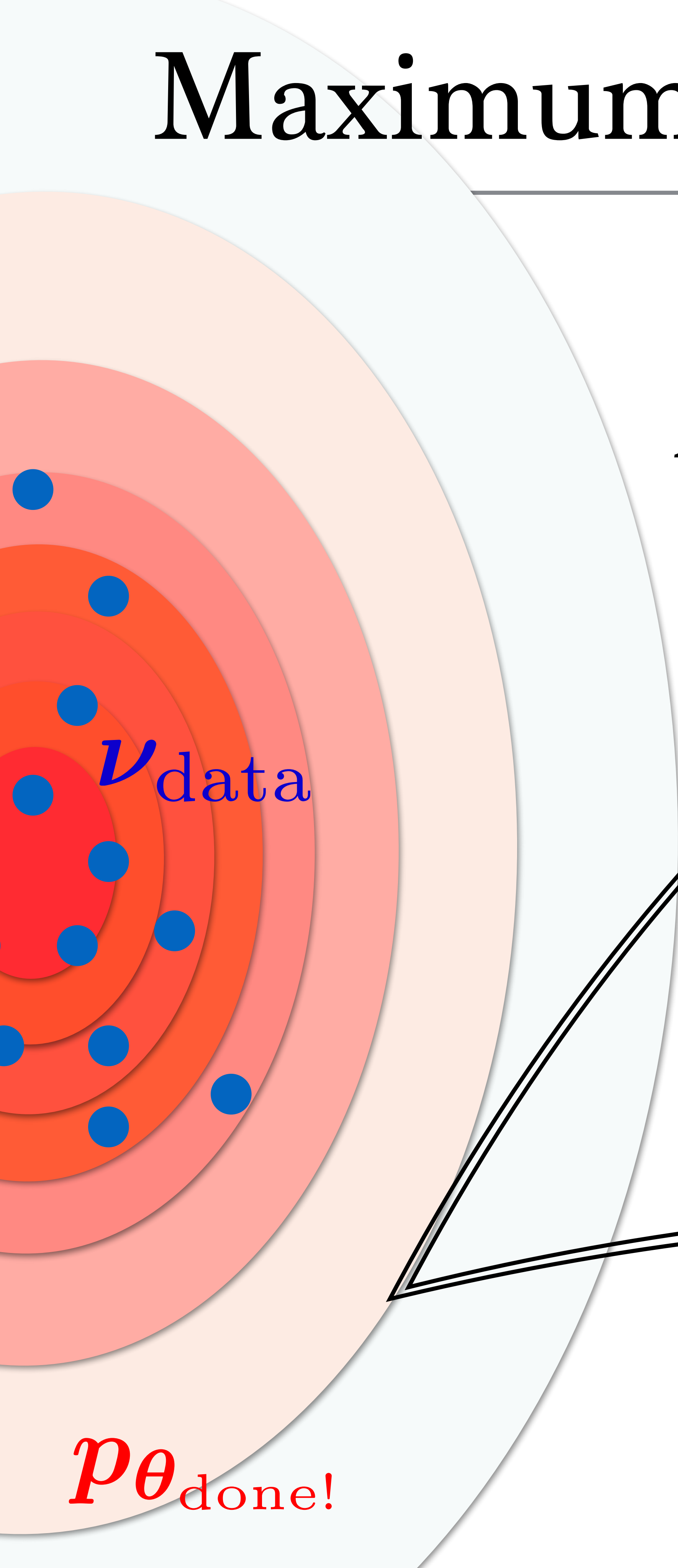
$$\max_{\boldsymbol{\theta} \in \Theta} \frac{1}{N} \sum_{i=1}^{N} \log p_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

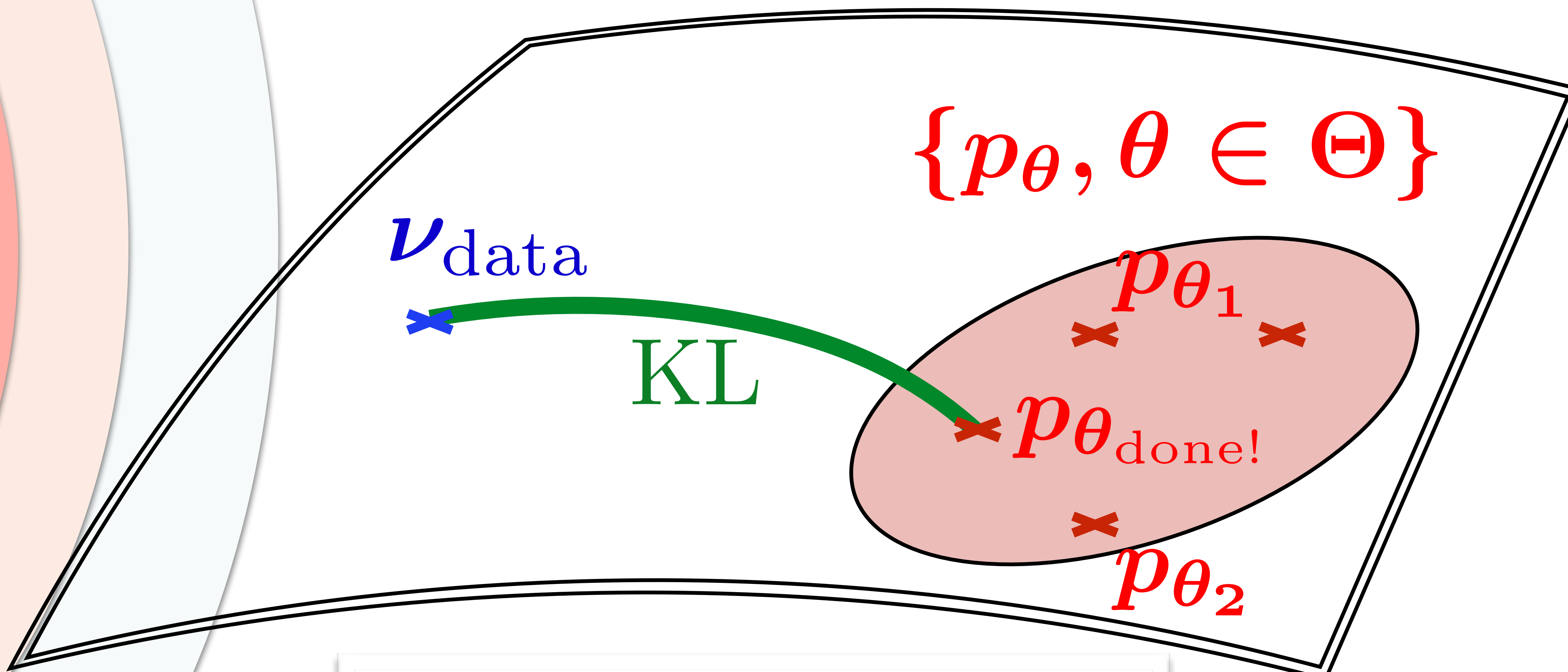
$$\log 0 = -\infty$$

$p_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$ **must** be > 0

Maximum Likelihood Estimation



Equivalent to a KL projection in the space of probability measures



$$\min_{\theta \in \Theta} \mathrm{KL}(\nu_{\text{data}} \| p_\theta)$$

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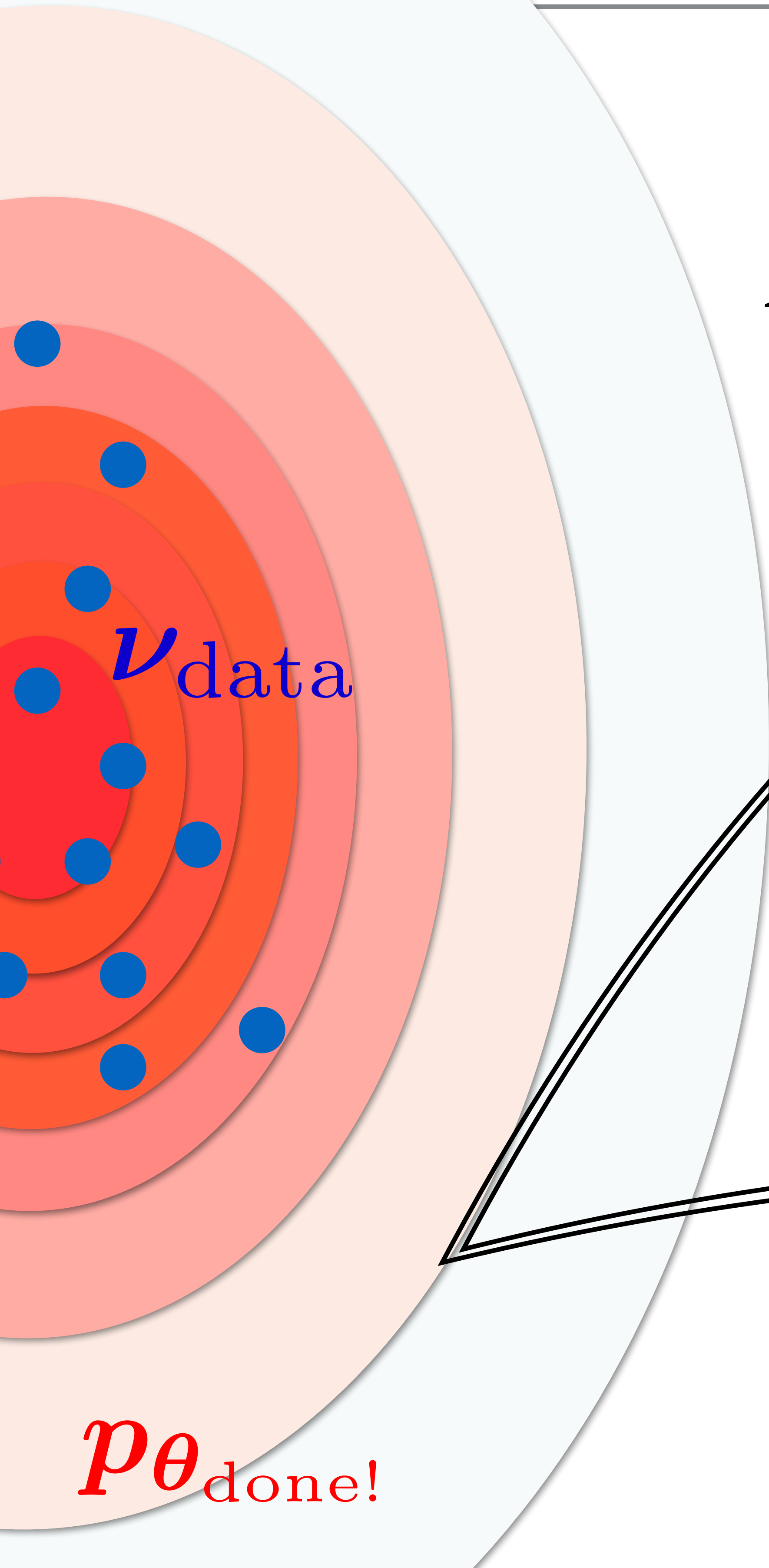

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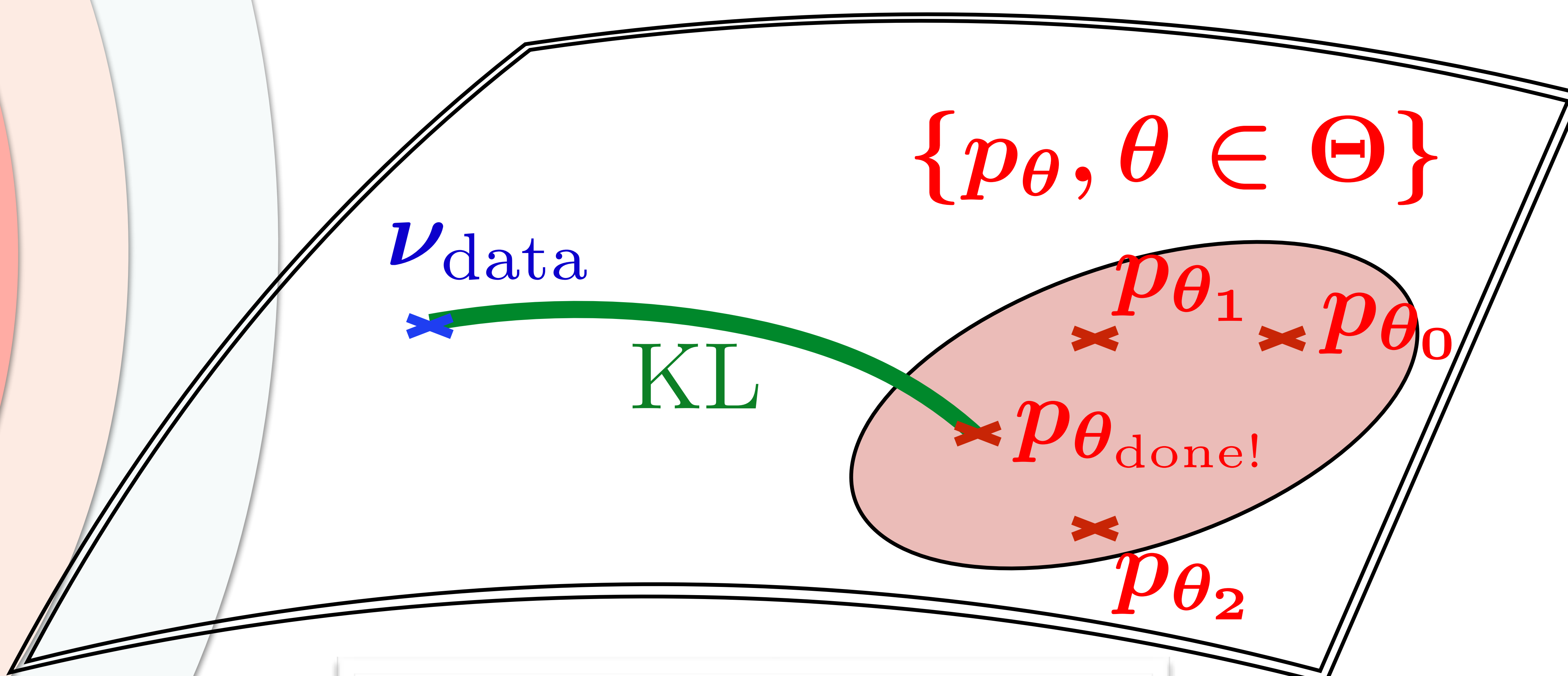
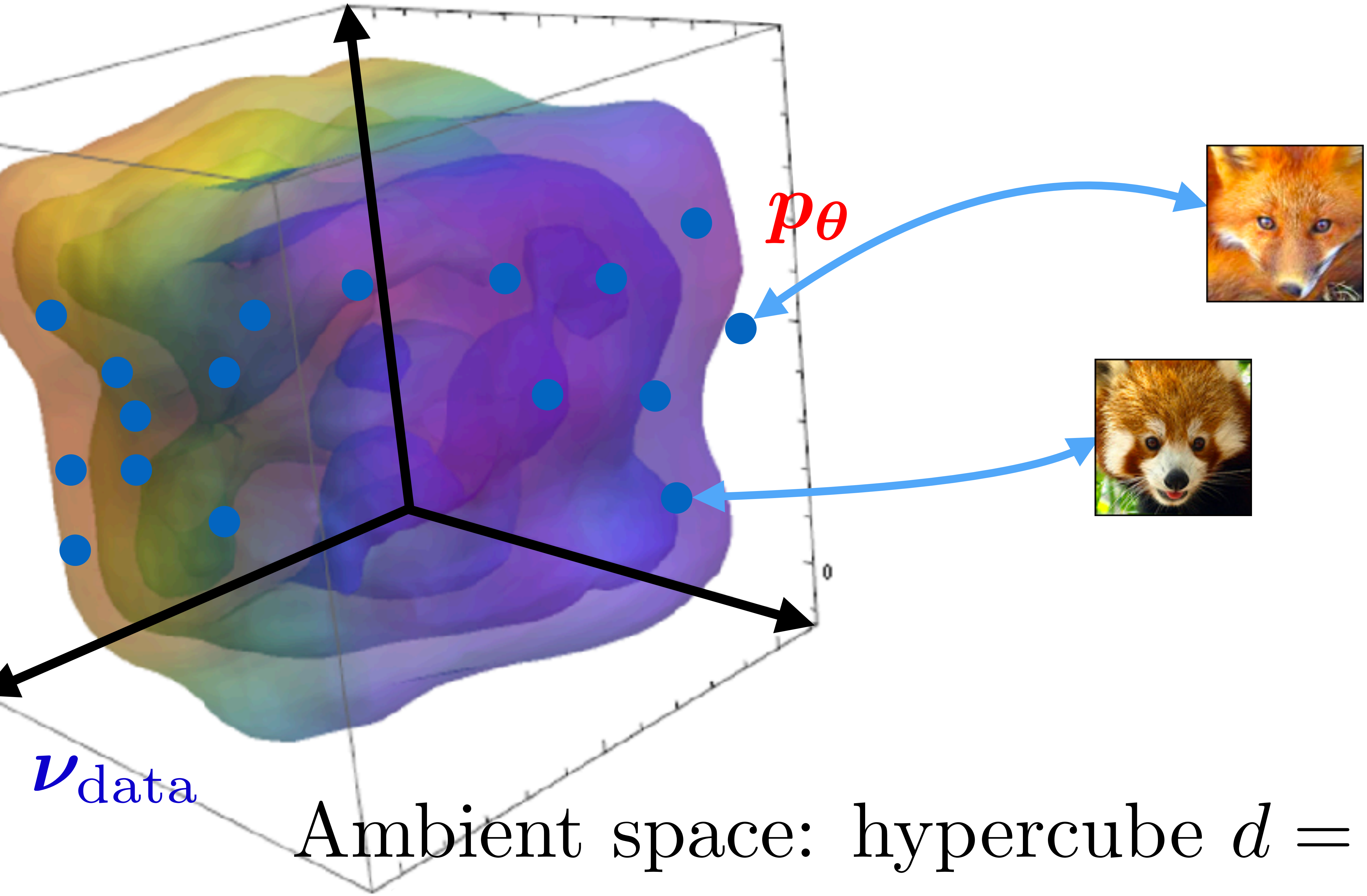


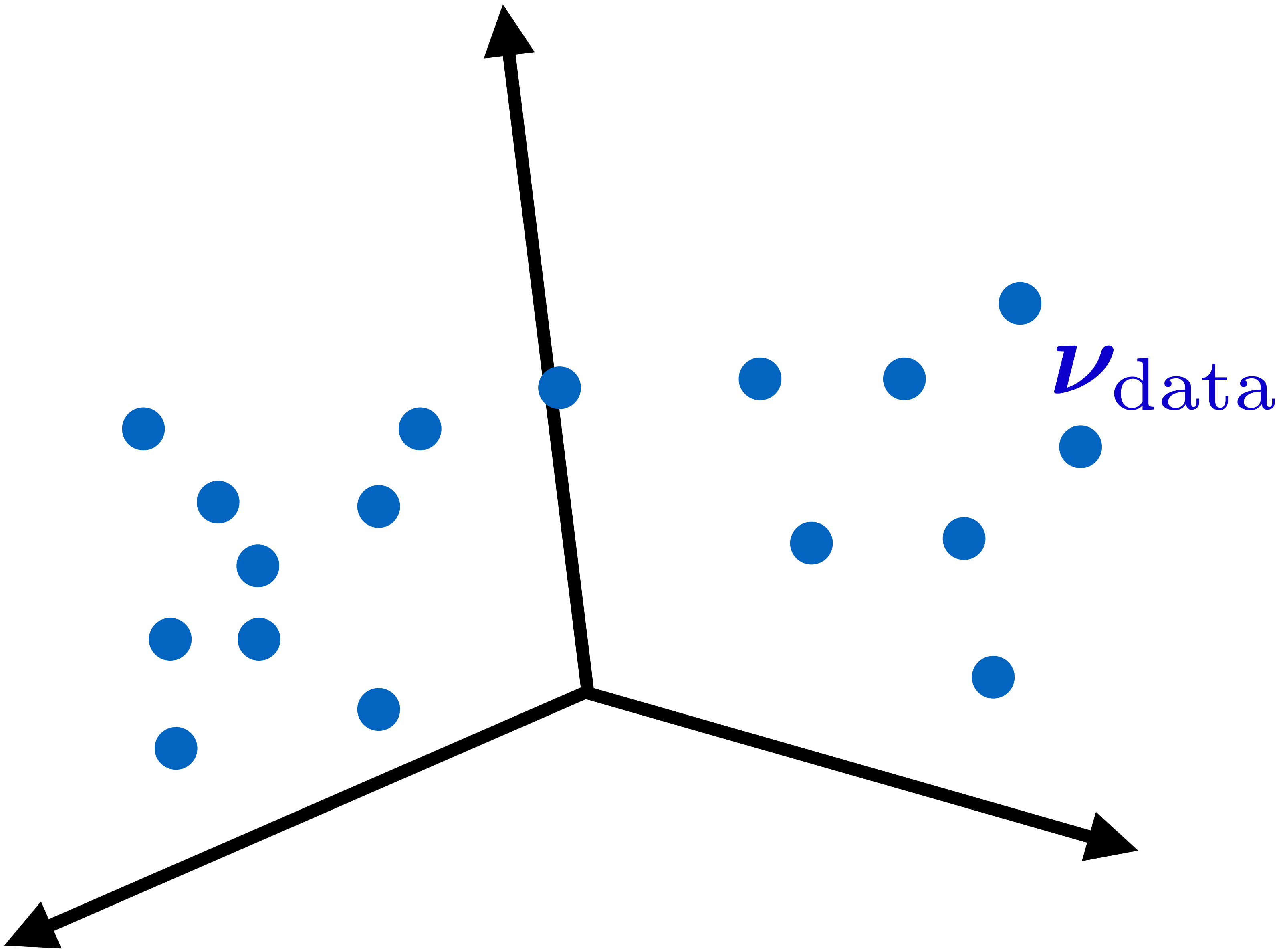
$$\min_{\boldsymbol{\theta} \in \Theta} \mathrm{KL}(\boldsymbol{\nu}_{\mathrm{data}} \| \boldsymbol{p}_{\boldsymbol{\theta}})$$

In higher dimensional spaces...



Ambient space: hypercube $d = 30.000$

Generative Models



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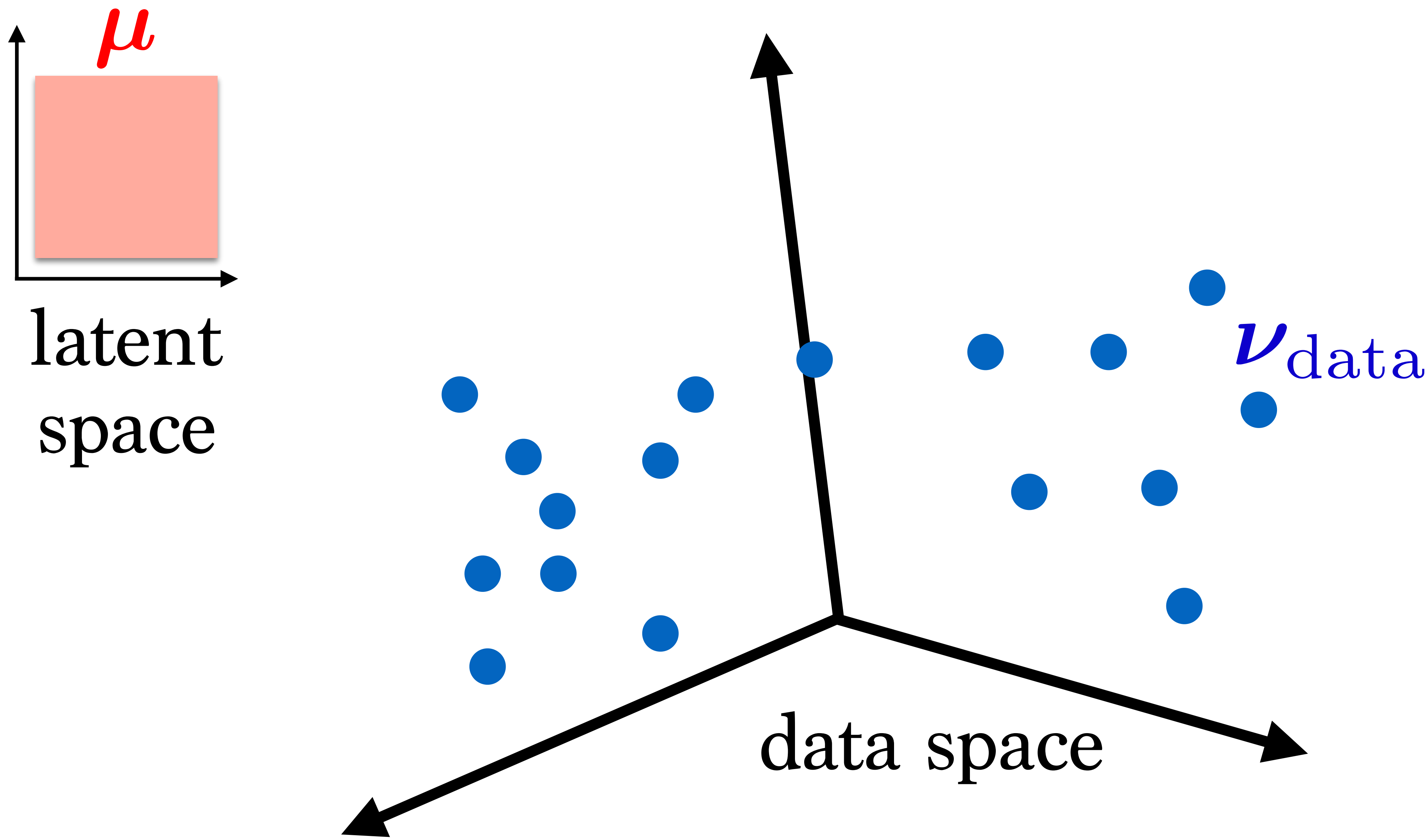

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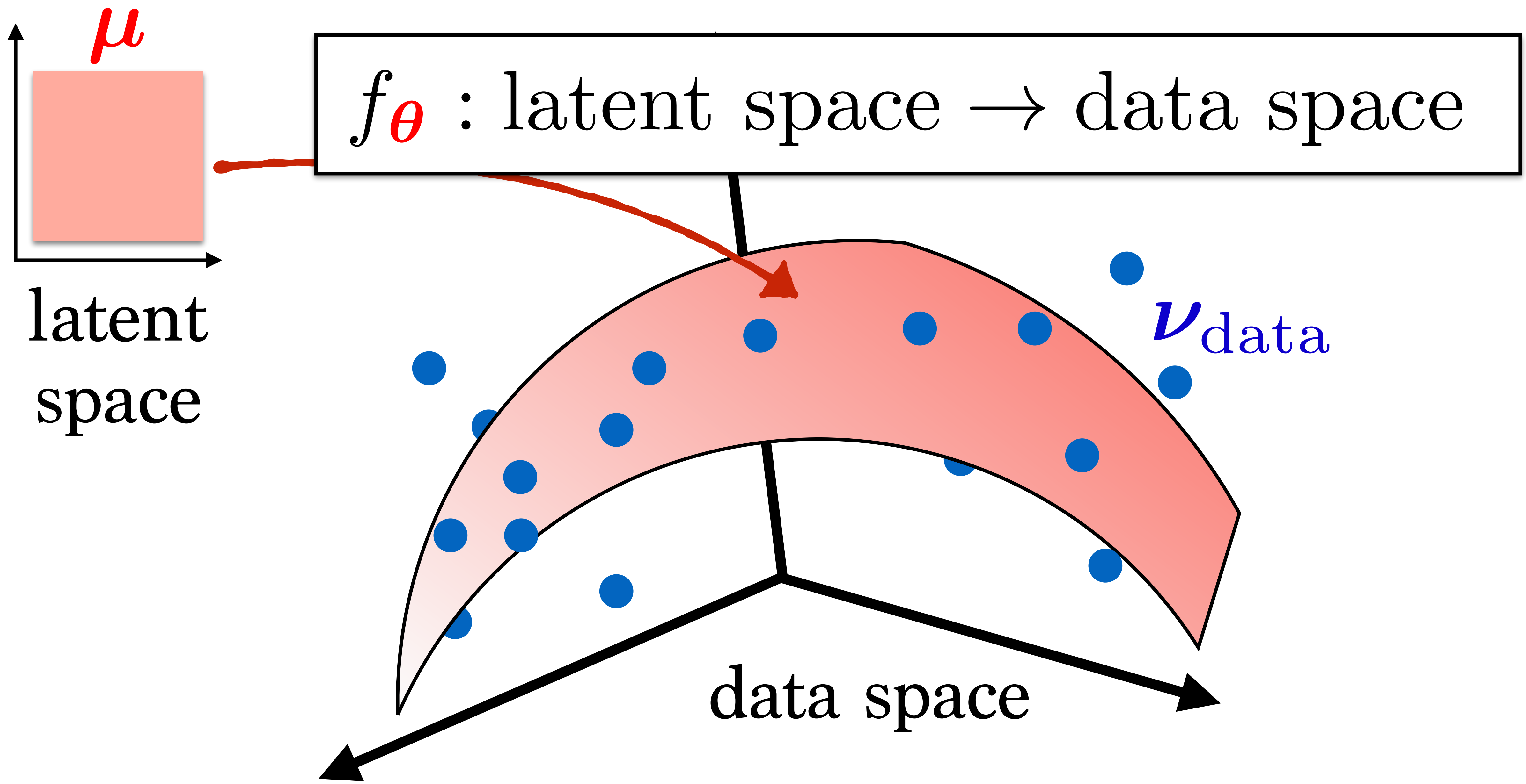

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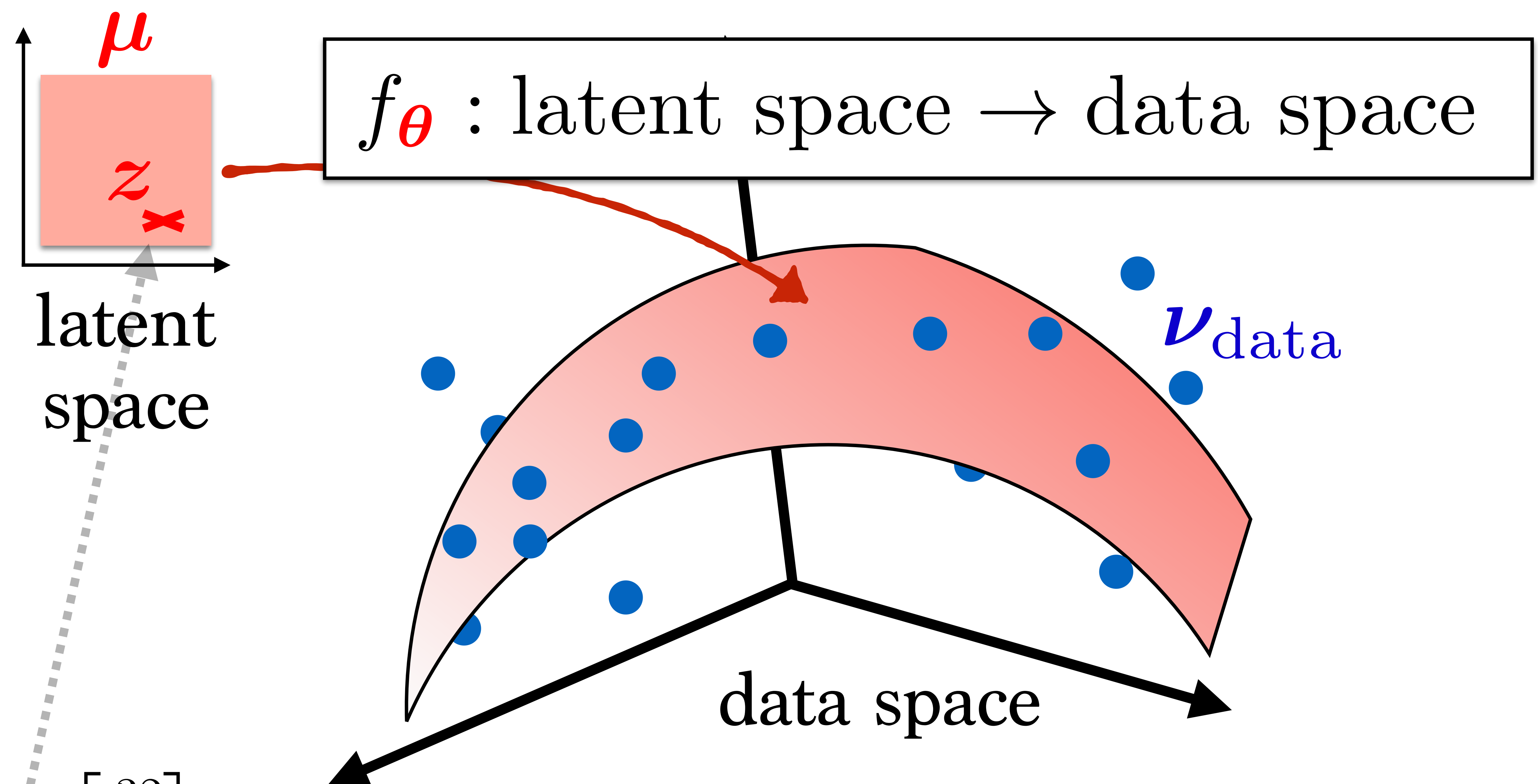
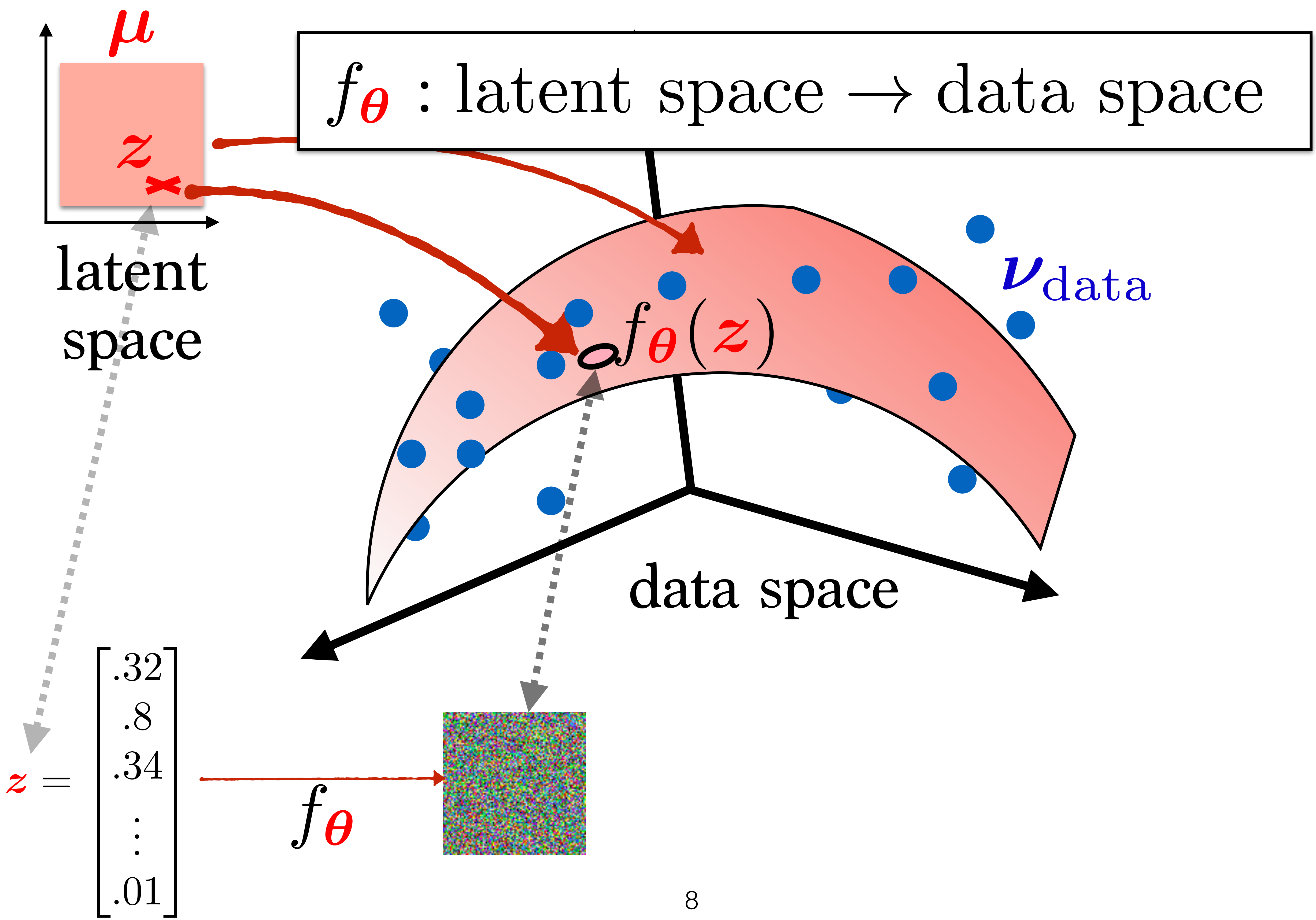


$$z = \begin{bmatrix} .32 \\ .8 \\ .34 \\ \vdots \\ .01 \end{bmatrix}$$

Generative Models



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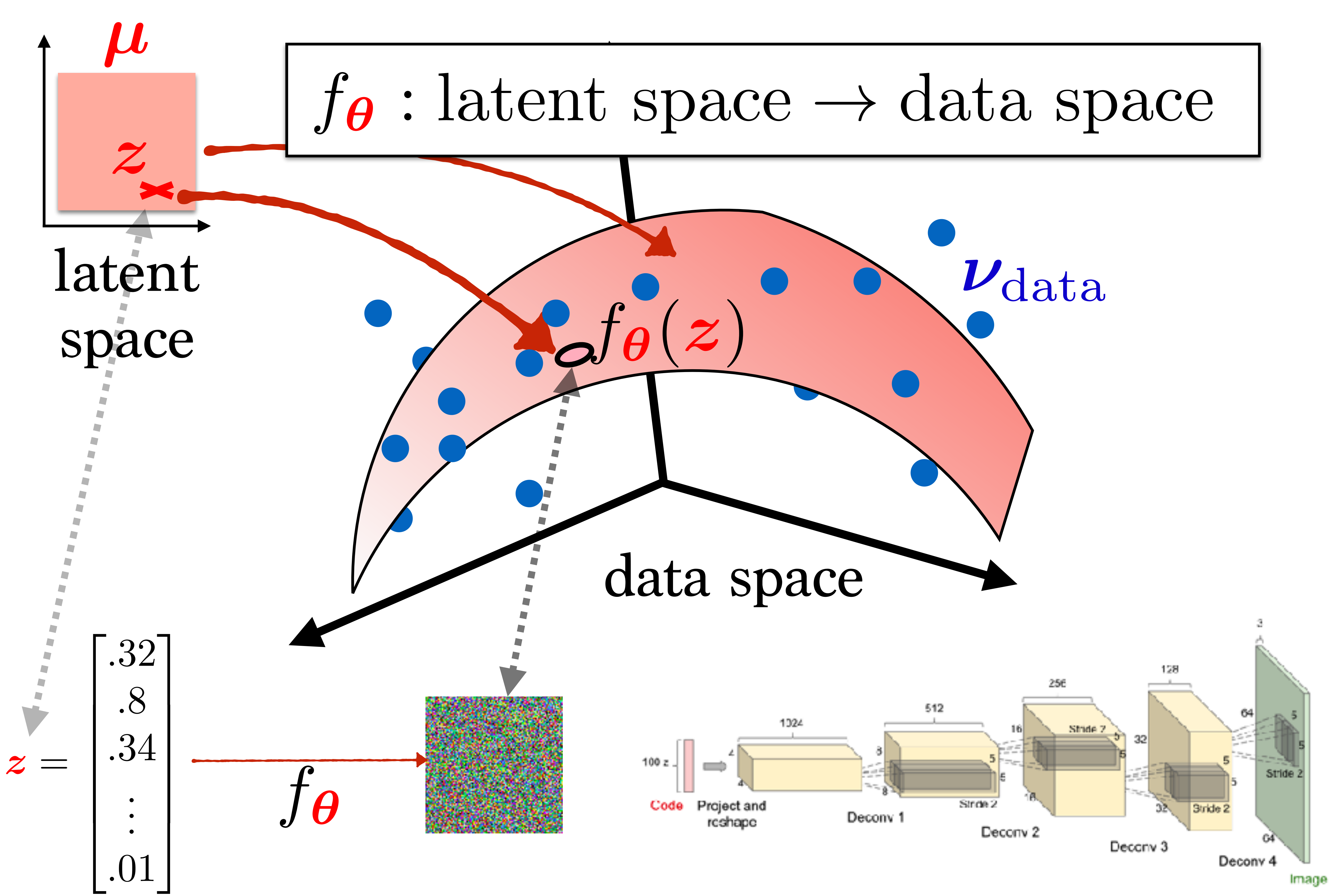

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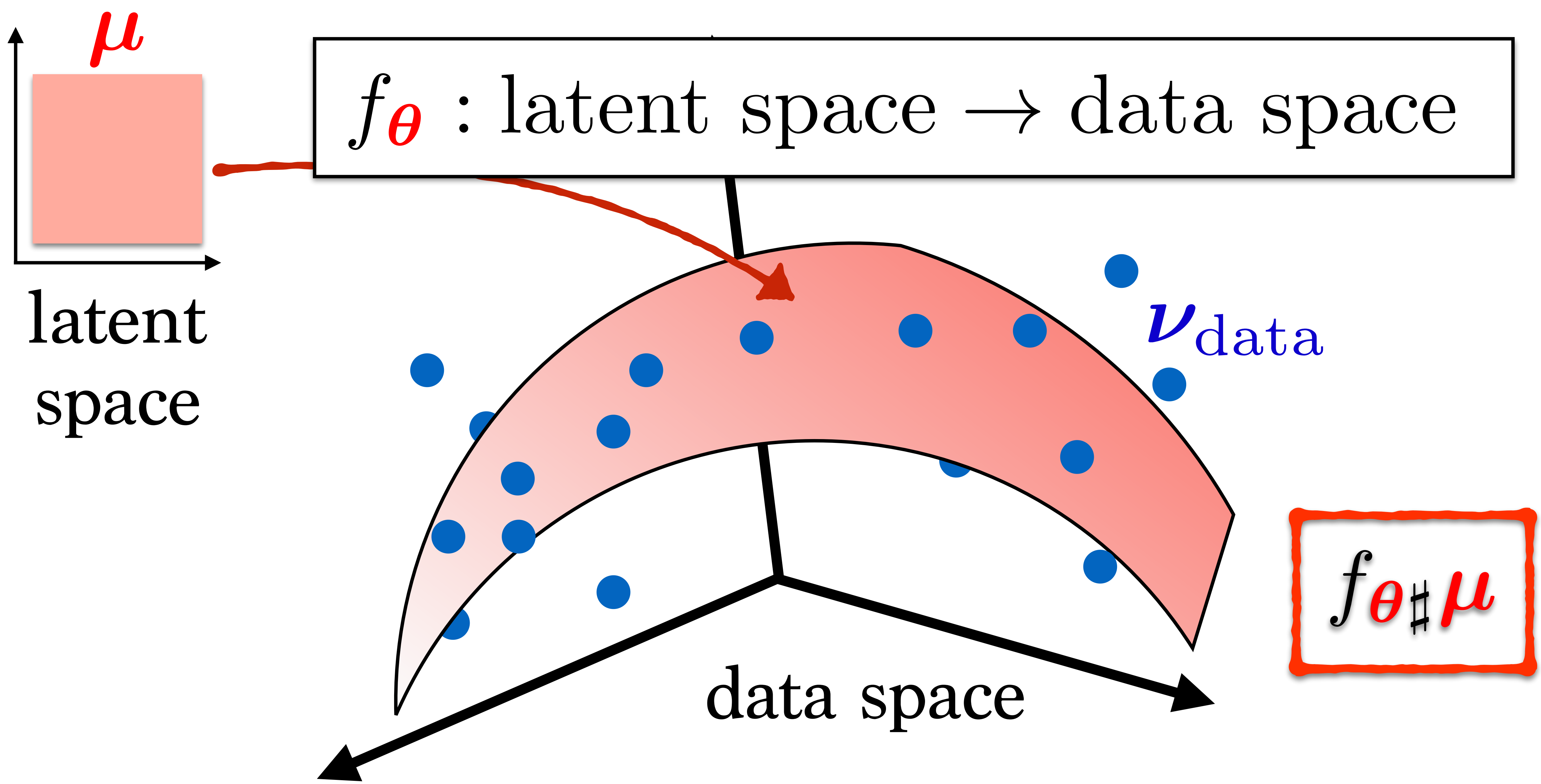

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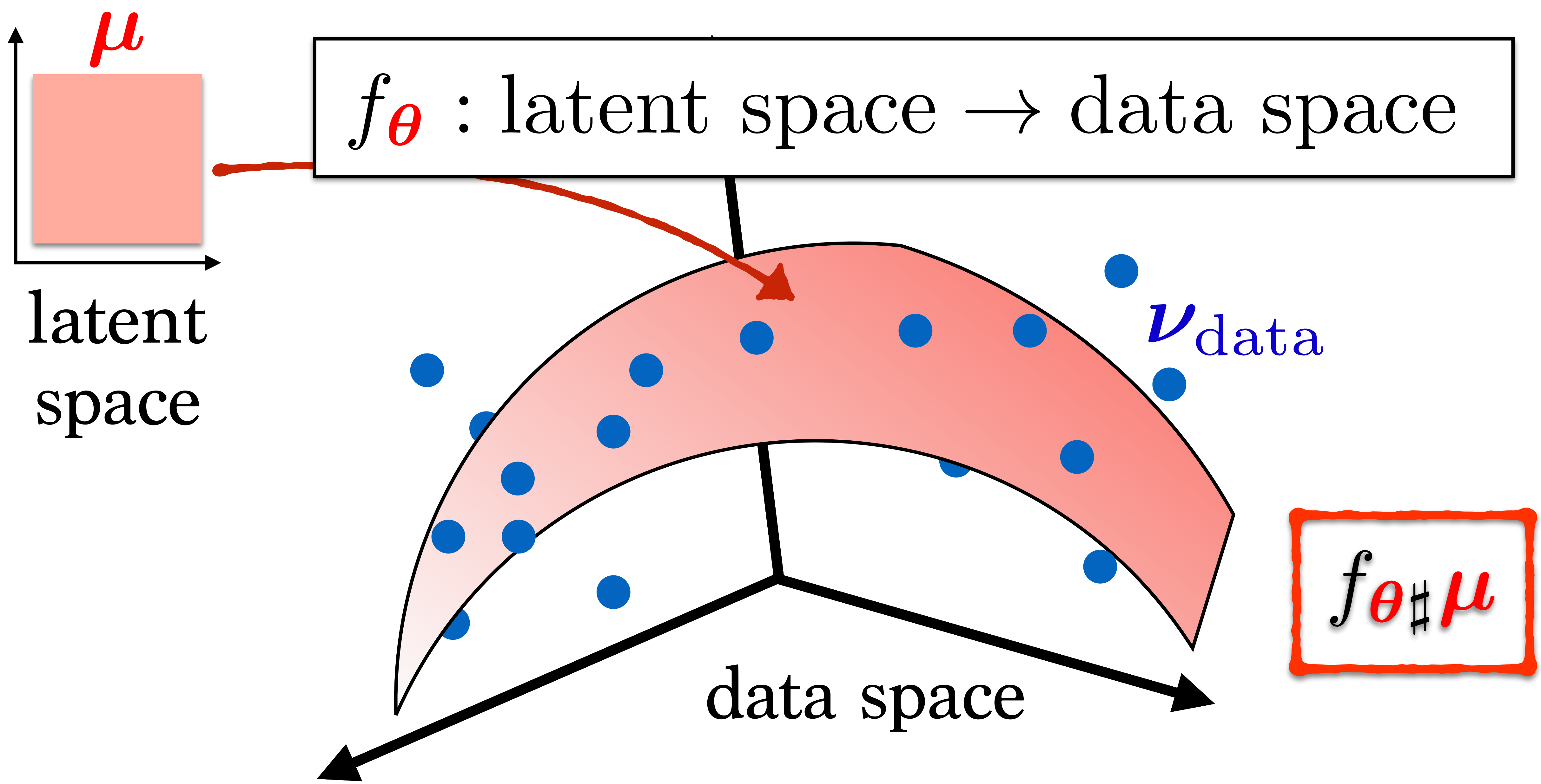
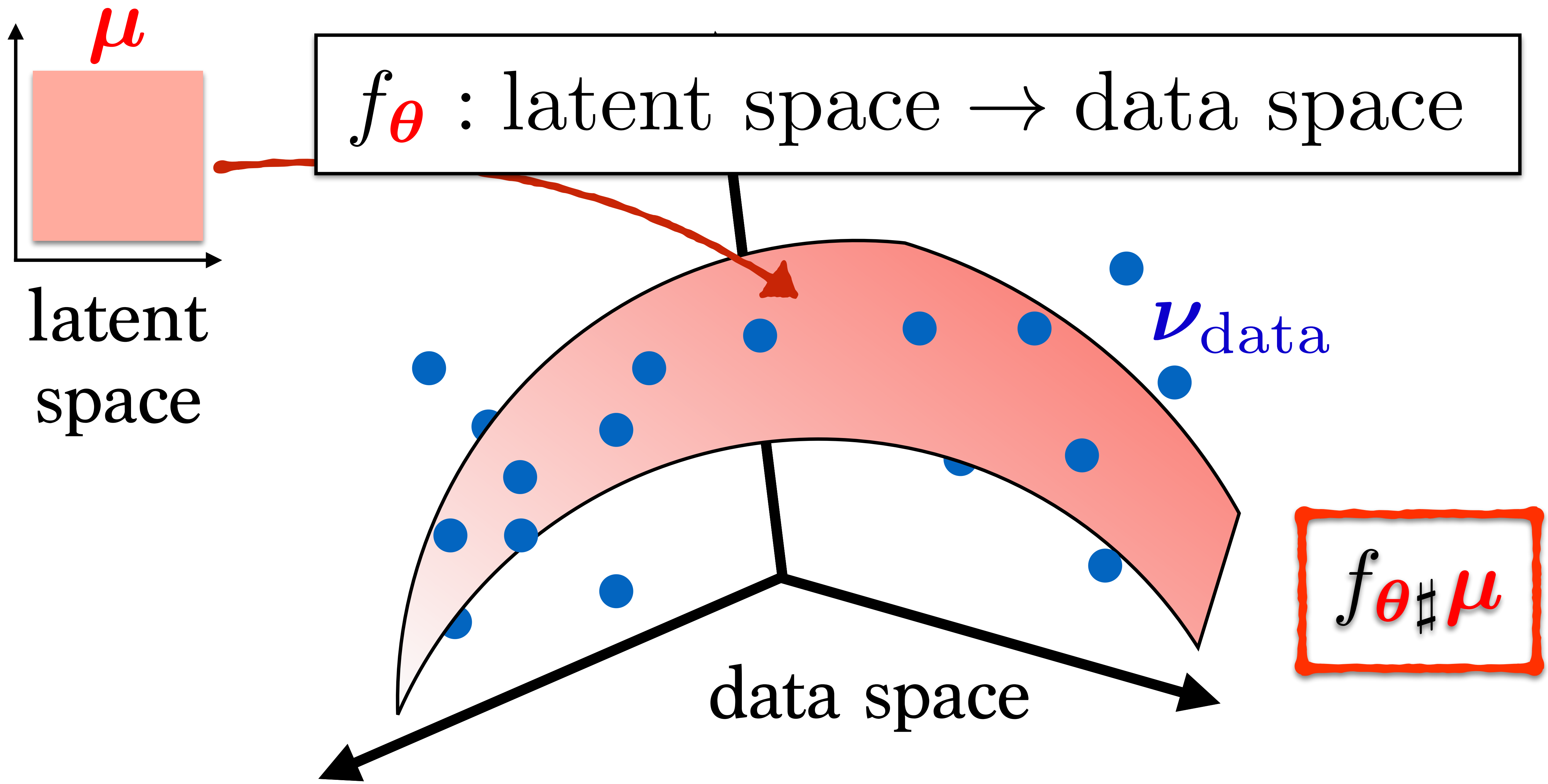


$$\text{Goal: find } \theta \text{ such that } f_{\theta\sharp}\mu \text{ fits } \nu_{\text{data}}$$

Generative Models



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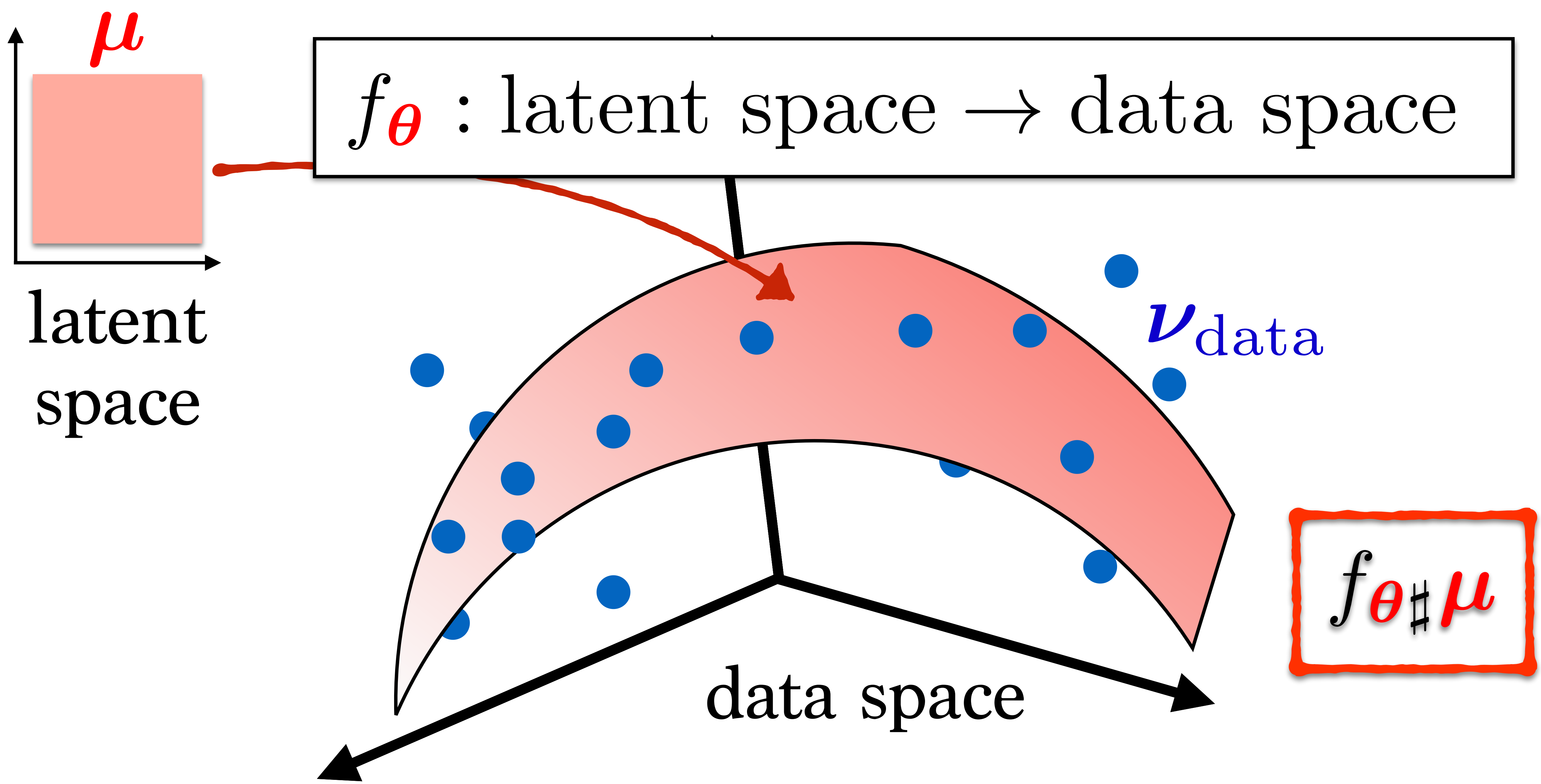
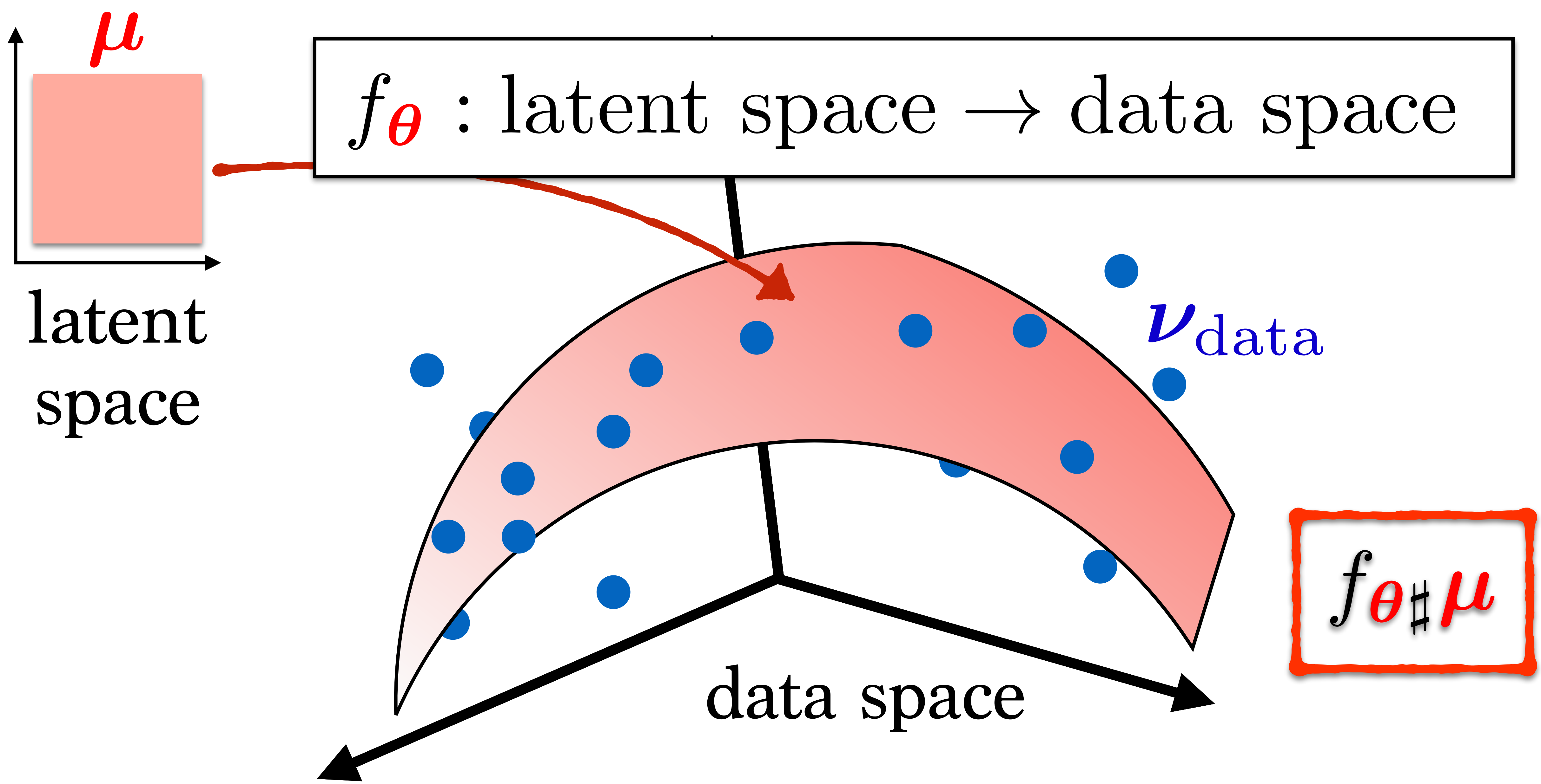


MLE

$$\max_{\theta\in\Theta} \frac{1}{N}\sum_{i=1}^{N} \log p_\theta(x_i) \quad = \quad \min_{\theta\in\Theta} \mathrm{KL}(\nu_{\text{data}} \| p_\theta)$$

Generative Models



~~MLE~~

$$\max_{\theta\in\Theta} \frac{1}{N}\sum_{i=1}^{N} \log f_{\theta\sharp}\mu(x_i) \qquad \min_{\theta\in\Theta} \mathrm{KL}(\nu_{\text{data}} \| f_{\theta\sharp}\mu)$$

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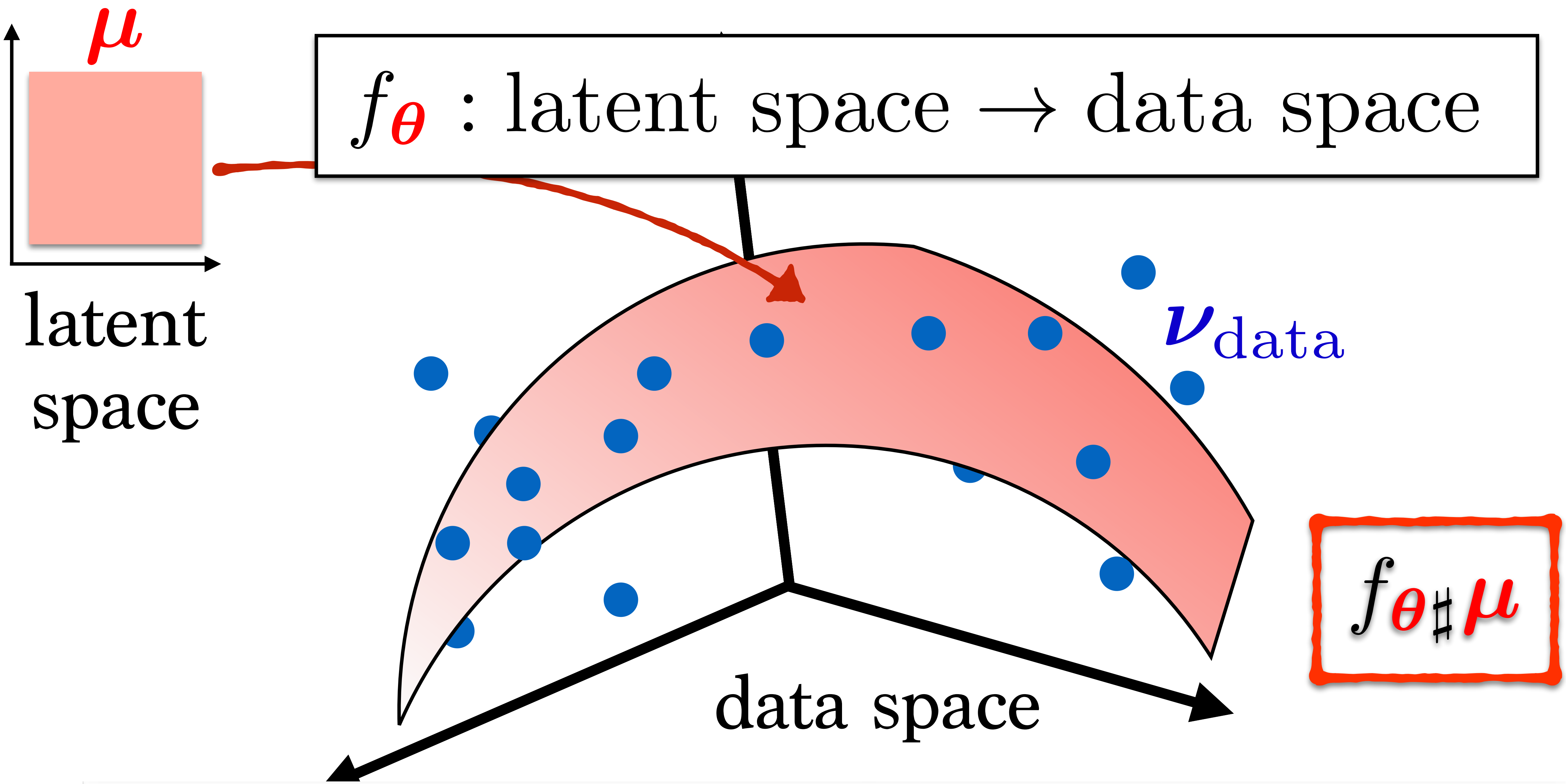
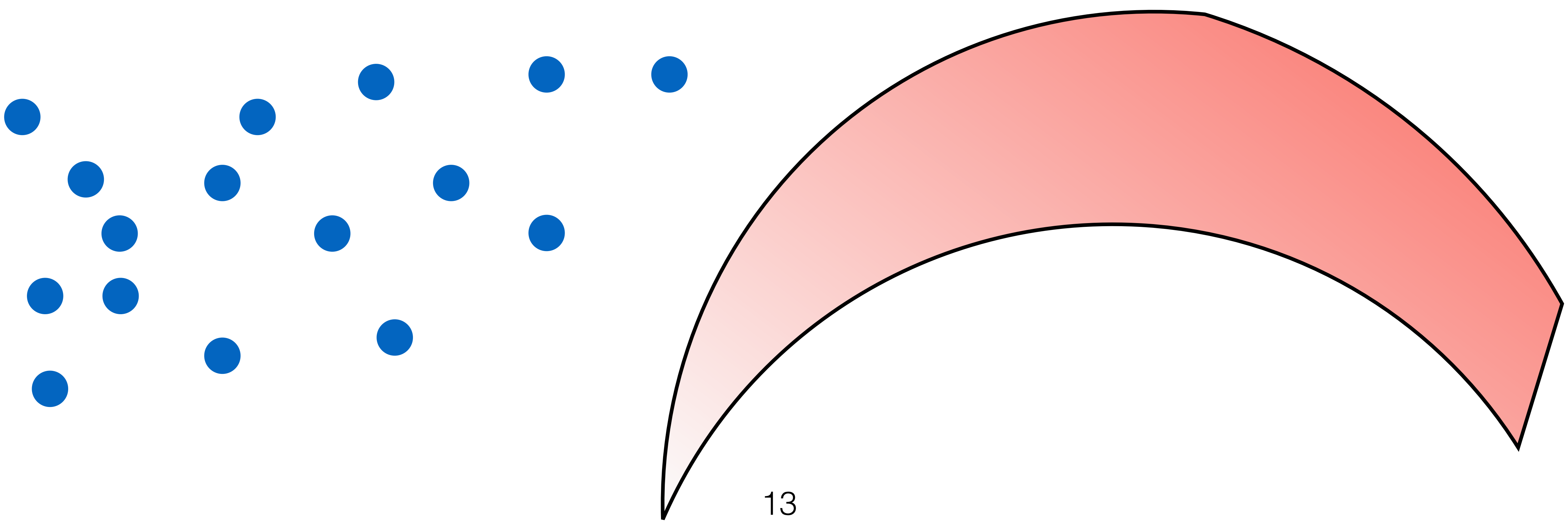


Need a more flexible **discrepancy function** to compare ν_{data} and $f_{\theta\sharp}\mu$

Workarounds?

- Formulation as **adversarial problem** **[GPM...'14]**

$$\min_{\boldsymbol{\theta}\in\Theta}\ \max_{\text{classifiers } \boldsymbol{g}}\ \text{Accuracy}_{\boldsymbol{g}}\left(\left(\boldsymbol{f}_{\boldsymbol{\theta}\sharp}\boldsymbol{\mu},+1\right),\left(\boldsymbol{\nu}_{\text{data}},-1\right)\right)$$



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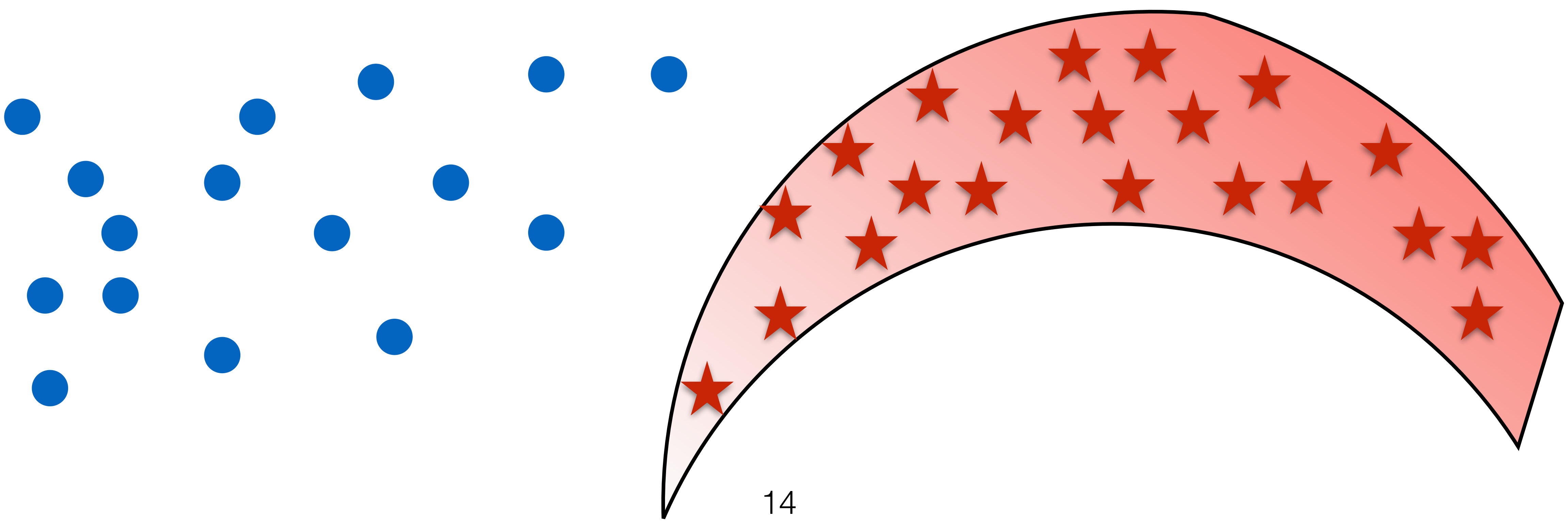

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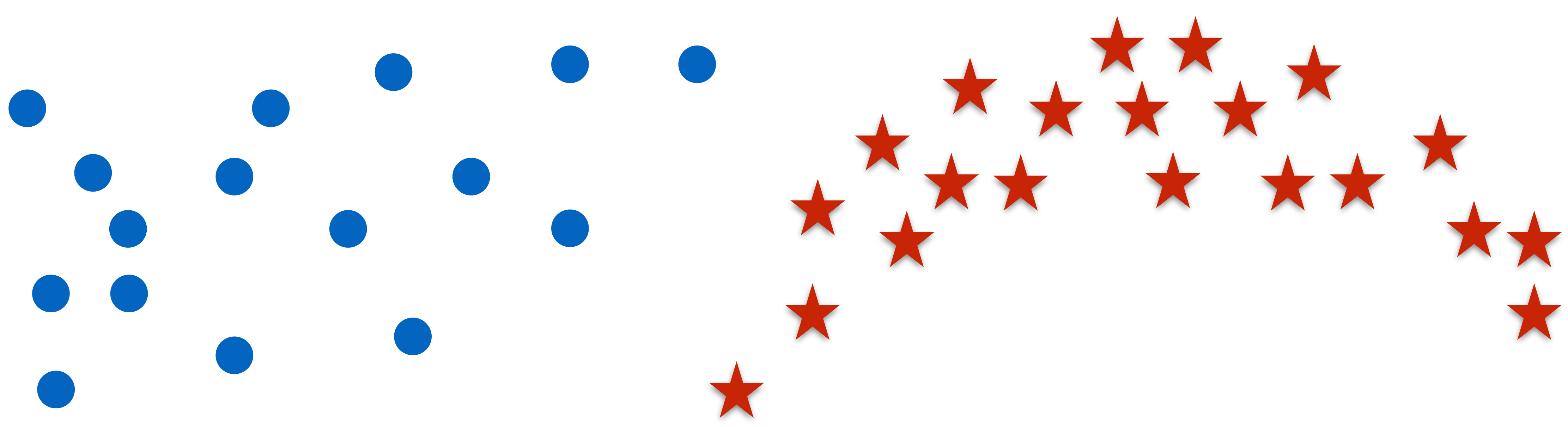

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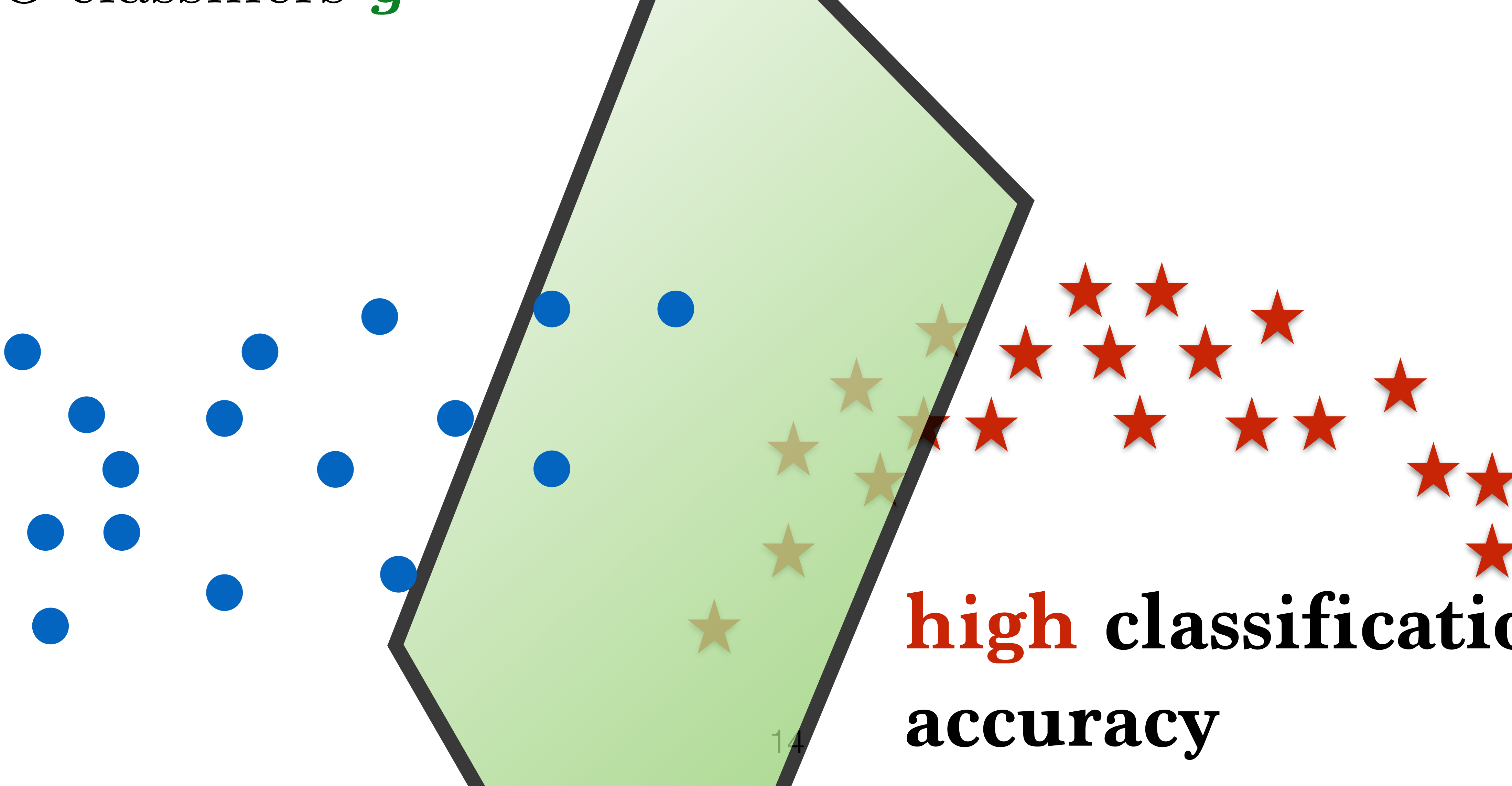

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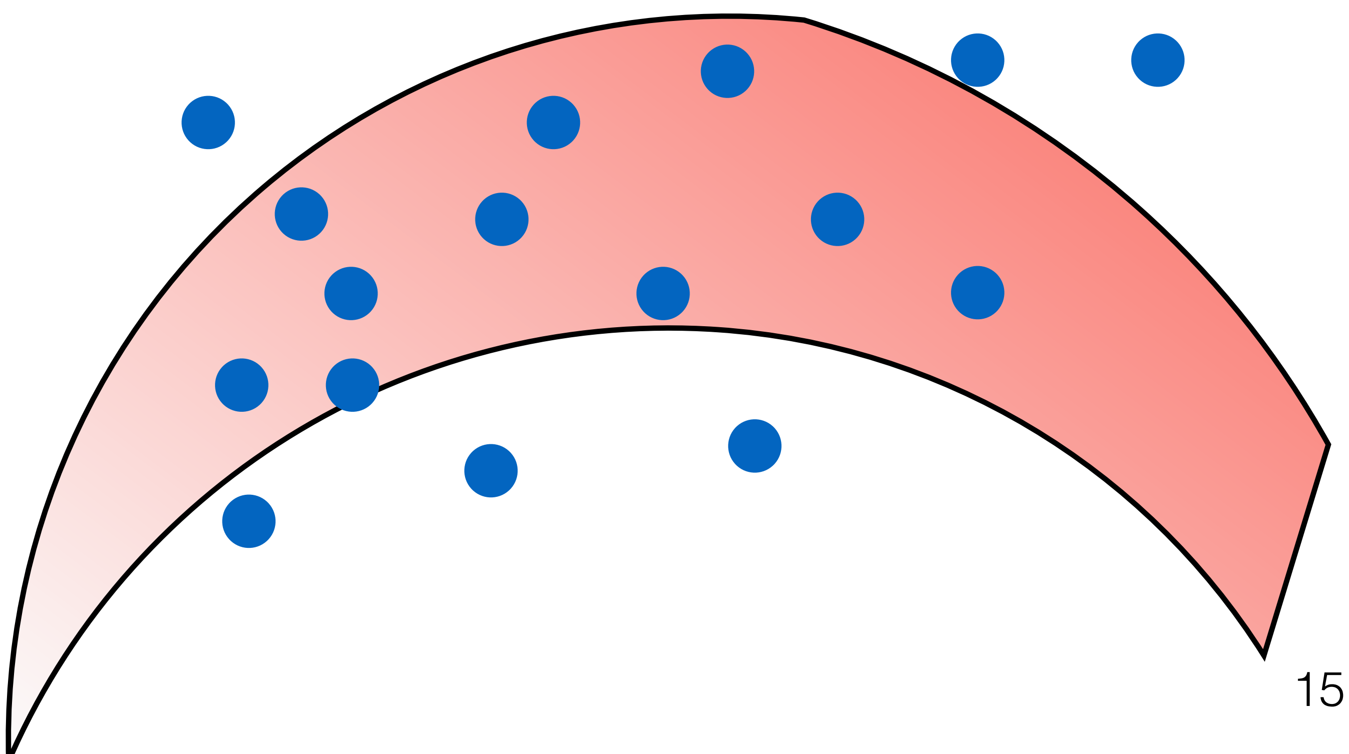

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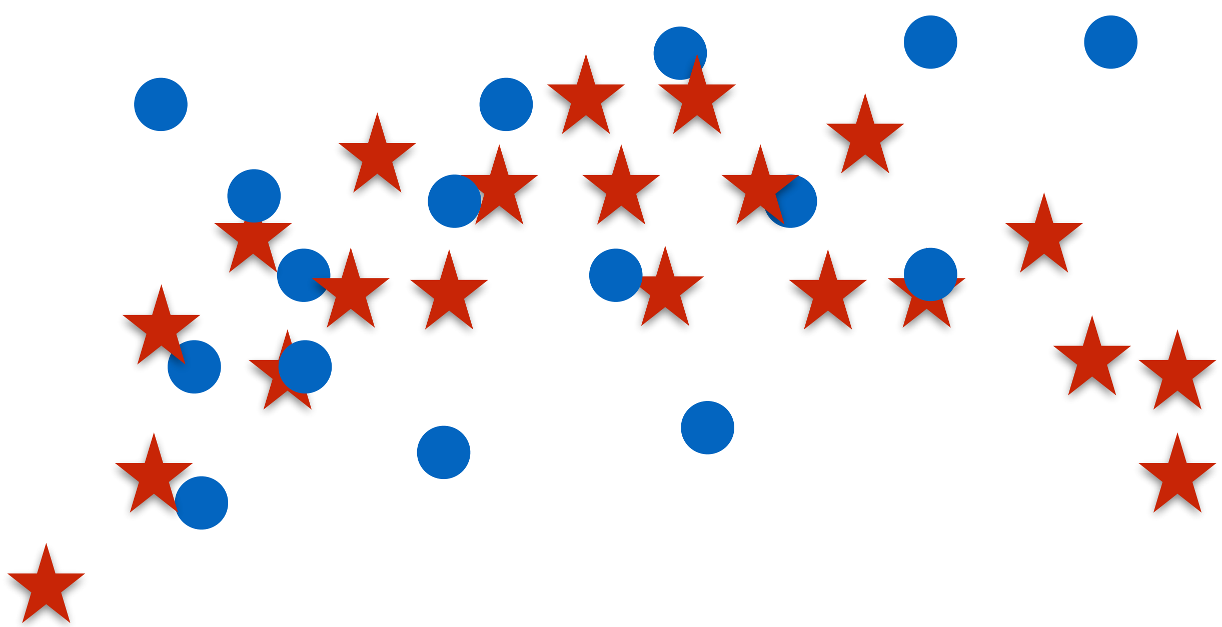

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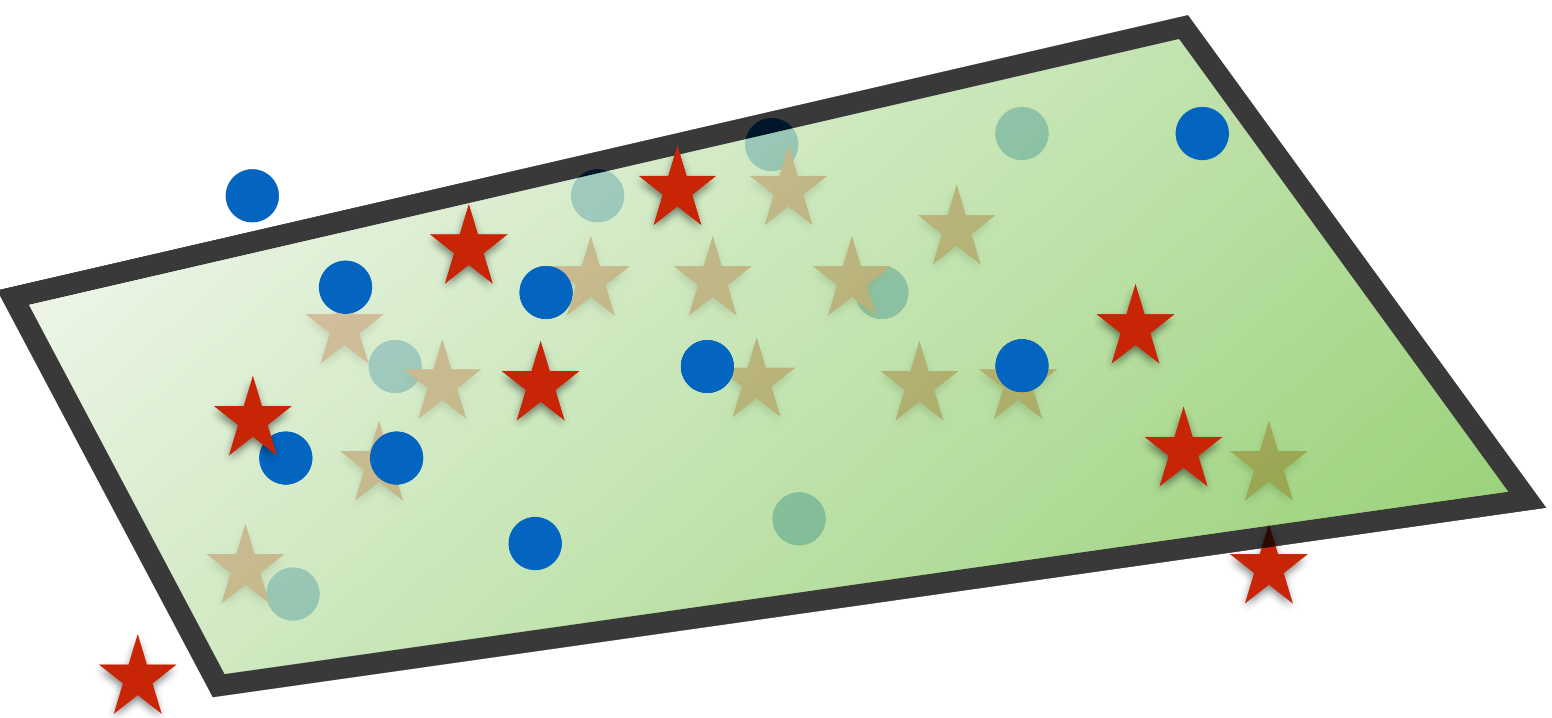
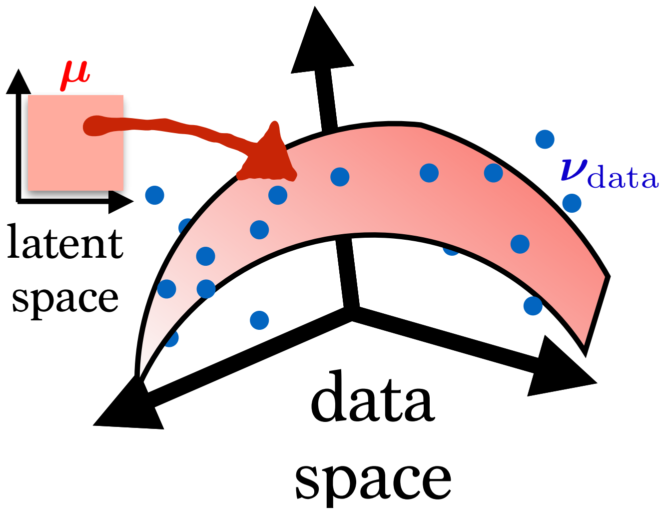


low classification accuracy…
is the goal.

Another idea?



- Use a **metric** $\boldsymbol{\Delta}$ for probability measures, that can handle measures with non-overlapping supports:

$$\min_{\boldsymbol{\theta}\in\Theta} \boldsymbol{\Delta}(\boldsymbol{\nu}_{\text{data}}, \boldsymbol{p_\theta}), \quad \textbf{not} \min_{\boldsymbol{\theta}\in\Theta} \mathrm{KL}(\boldsymbol{\nu}_{\text{data}} \| \boldsymbol{p_\theta})$$

Minimum △ Estimation

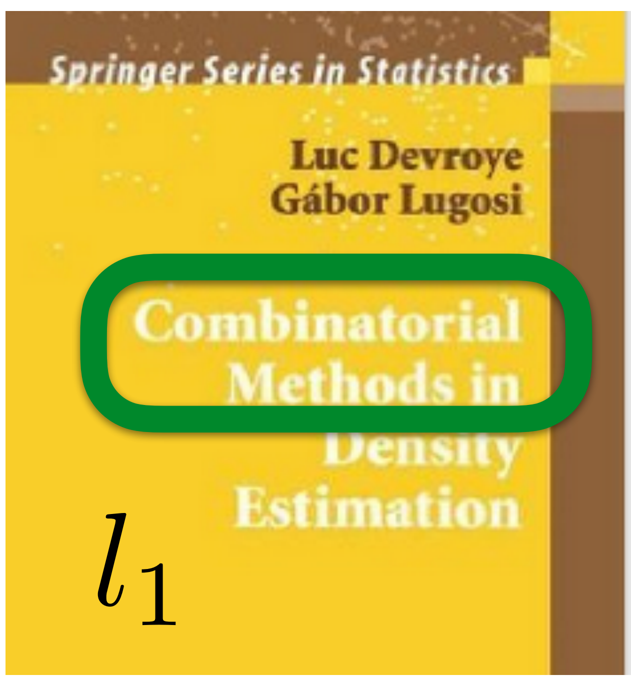
The Annals of Statistics
1980, Vol. 8, No. 3, 457–487

MINIMUM CHI-SQUARE, NOT MAXIMUM LIKELIHOOD!

BY JOSEPH BERKSON
Mayo Clinic, Rochester, Minnesota

ELSEVIER Computational Statistics & Data Analysis 29 (1998) 81–103

COMPUTATIONAL STATISTICS & DATA ANALYSIS



l_1

Minimum Hellinger distance estimation for Poisson mixtures

Dimitris Karlis, Evdokia Xekalaki*
Department of Statistics, Athens University of Economics and Business, 76 Patission Str., 104 34 Athens, Greece

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Statistics & Probability Letters 76 (2006) 1298–1302

STATISTICS & PROBABILITY LETTERS
www.elsevier.com/locate/stapro

On minimum Kantorovich distance estimators

Federico Bassetti[a], Antonella Bodini[b], Eugenio Regazzini[a,*]

△ Generative Model Estimation

Generative Moment Matching Networks

Yujia Li[1] YUJIALI@CS.TORONTO.EDU
Kevin Swersky[1] KSWERSKY@CS.TORONTO.EDU
Richard Zemel[1,2] ZEMEL@CS.TORONTO.EDU
[1]Department of Computer Science, University of Toronto, Toronto, ON, CANADA
[2]Canadian Institute for Advanced Research, Toronto, ON, CANADA

Training generative neural networks via Maximum Mean Discrepancy optimization

Gintare Karolina Dziugaite University of Cambridge
Daniel M. Roy University of Toronto
Zoubin Ghahramani University of Cambridge

MMD GAN: Towards Deeper Understanding of Moment Matching Network

Chun-Liang Li[1,*] **Wei-Cheng Chang**[1,*] **Yu Cheng**[2] **Yiming Yang**[1] **Barnabás Póczos**[1]
[1] Carnegie Mellon University, [2]IBM Research
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Wasserstein Training of Restricted Boltzmann Machines

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Klaus-Robert Müller* Technische Universität Berlin klaus-robert.mueller@tu-berlin.de
Marco Cuturi CREST, ENSAE, Université Paris-Saclay marco.cuturi@ensae.fr

Inference in generative models using the Wasserstein distance

Espen Bernton, Mathieu Gerber, Pierre E. Jacob, Christian P. Robert

Wasserstein GAN

Martin Arjovsky[1], Soumith Chintala[2], and Léon Bottou[1,2]
[1]Courant Institute of Mathematical Sciences
[2]Facebook AI Research

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Learning Generative Models with Sinkhorn Divergences

Aude Genevay CEREMADE, Université Paris-Dauphine
Gabriel Peyré CNRS and DMA, École Normale Supérieure
Marco Cuturi ENSAE CREST Université Paris-Saclay

Improving GANs Using Optimal Transport

Tim Salimans* OpenAI tim@openai.com
Han Zhang† Rutgers University han.zhang@cs.rutgers.edu
Alec Radford OpenAI alec@openai.com
Dimitris Metaxas Rutgers University dnm@cs.rutgers.edu

Minimum Kantorovich Estimation

- Use optimal transport theory, namely *Wasserstein distances* to define discrepancy Δ .

$$\min_{\boldsymbol{\theta}\in\Theta} W(\boldsymbol{\nu}_{\text{data}}, f_{\boldsymbol{\theta}\sharp}\boldsymbol{\mu})$$

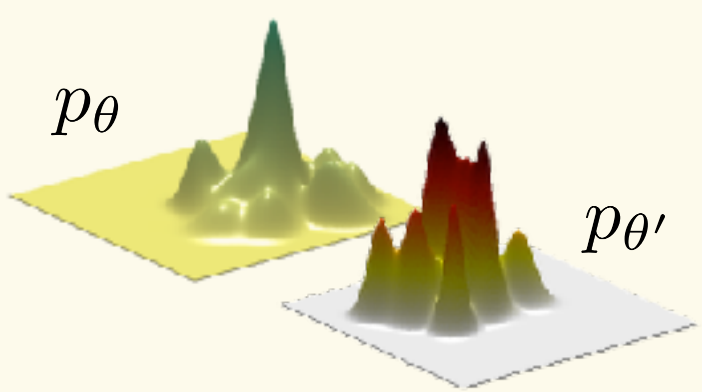
- Optimal transport? fertile field in mathematics.

Monge Kantorovich Koopmans Dantzig Brenier Gangbo Otto McCann Villani Figalli

Nobel'75 Fields'10 Fields'18

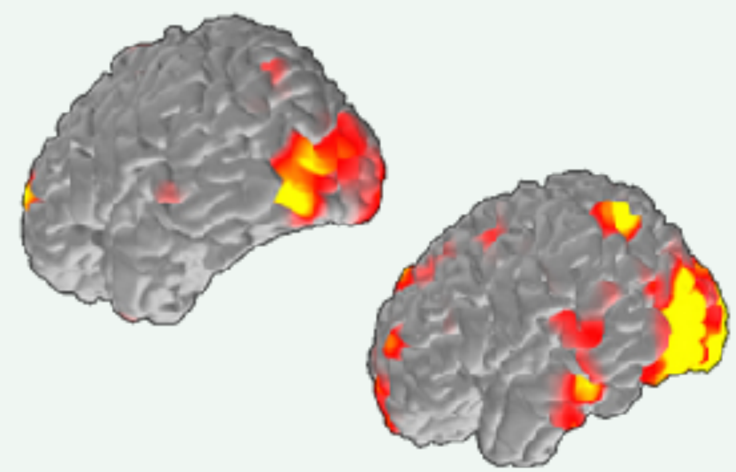
What is Optimal Transport?

The natural geometry for probability measures



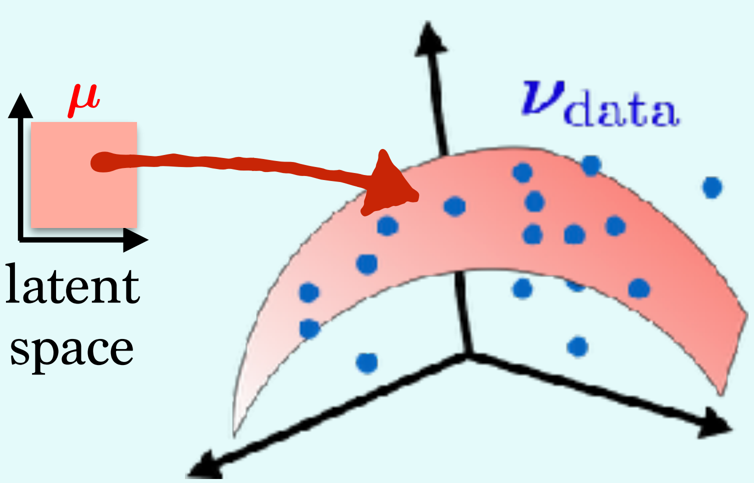
Statistical Models

Bags of features



Brain Activation Maps

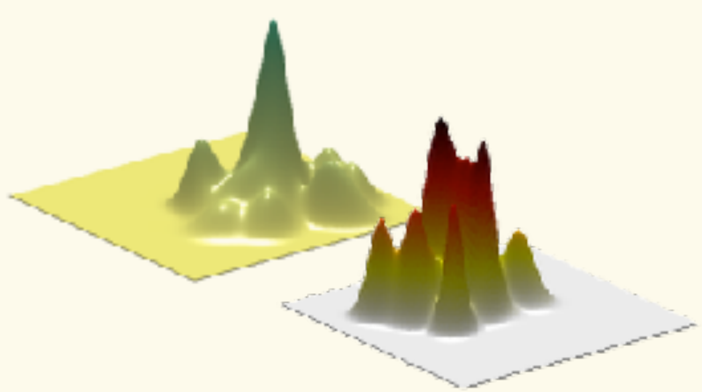
Generative Models vs. data



Color Histograms

What is Optimal Transport?

The natural geometry for probability measures supported on a metric space.



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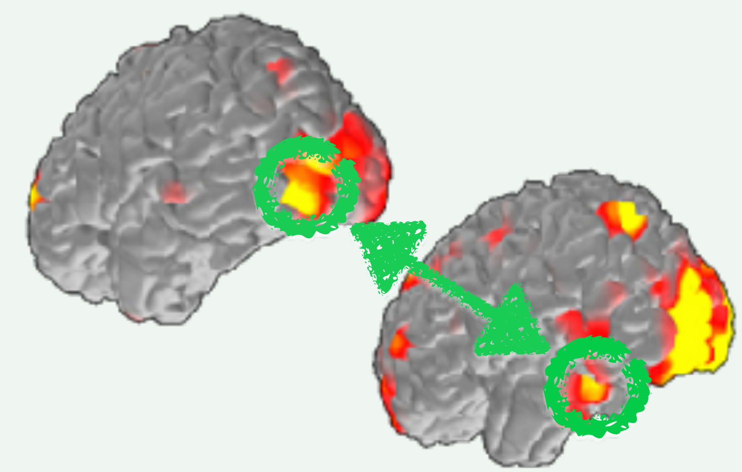

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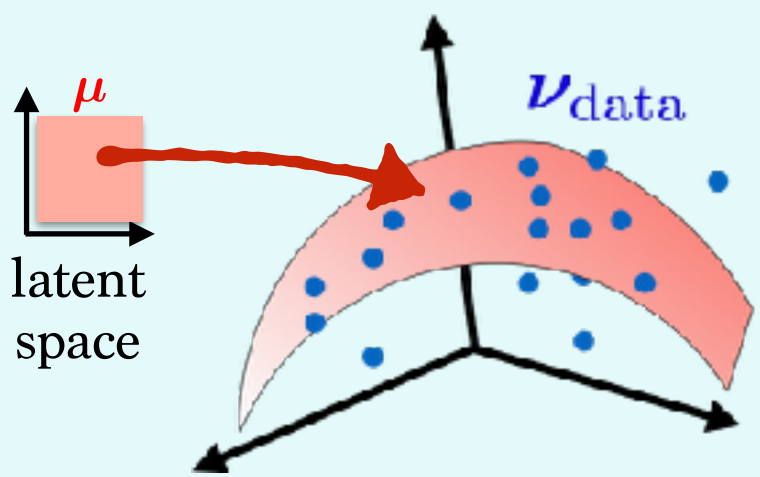

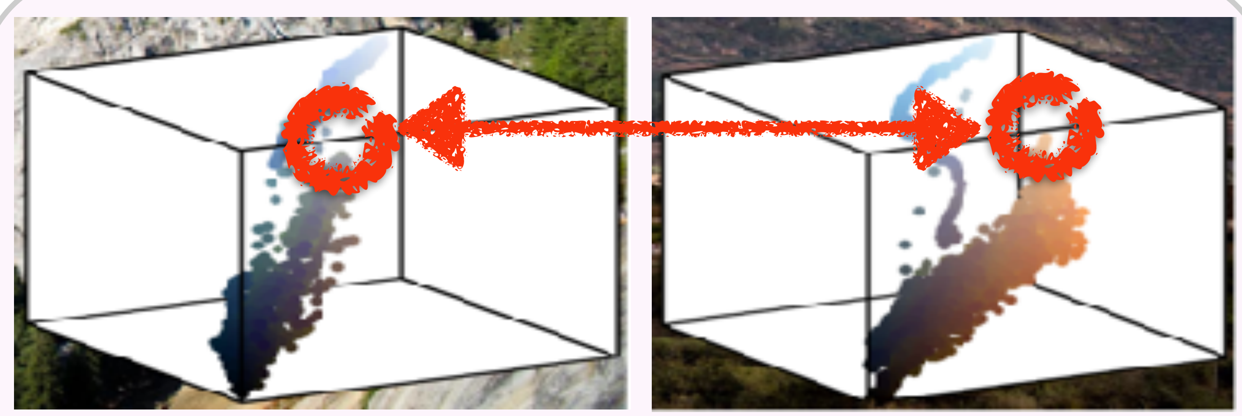

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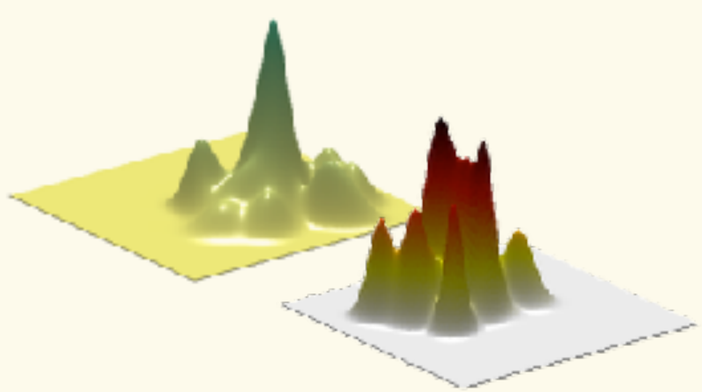

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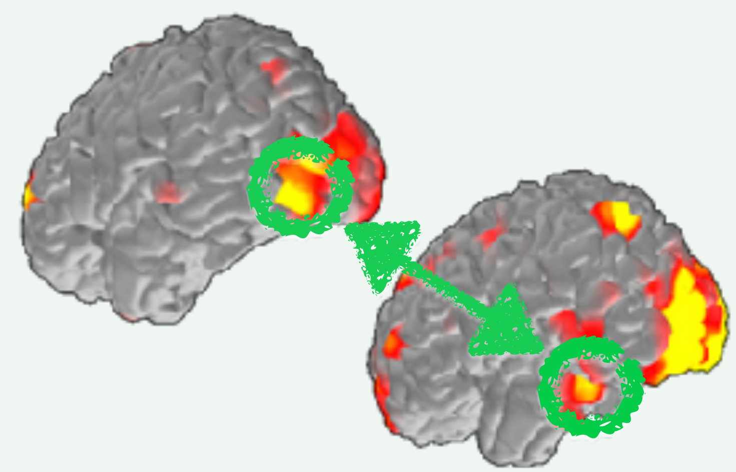
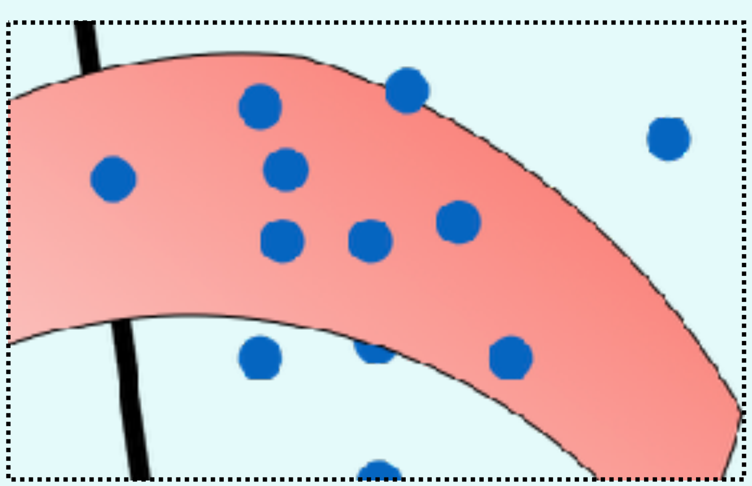
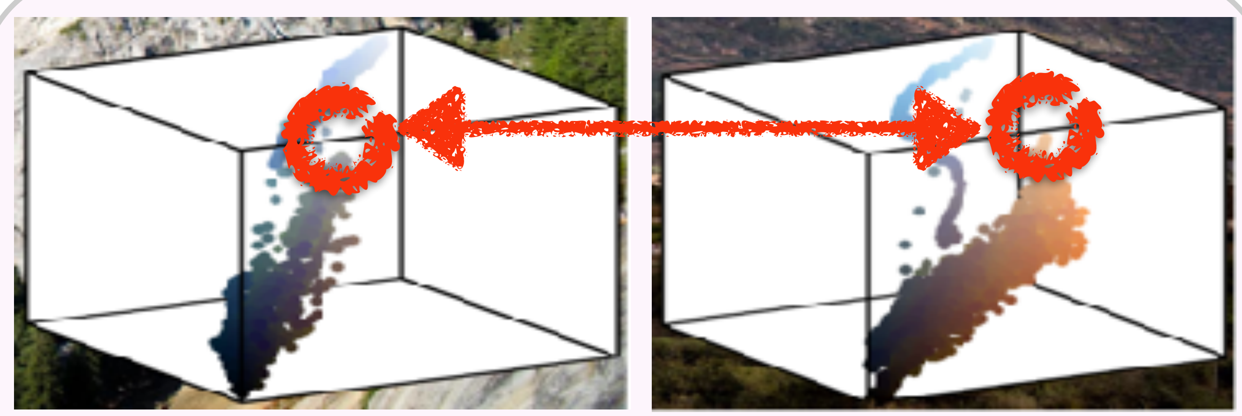


Brain Activation Maps

Generative Models vs. Data

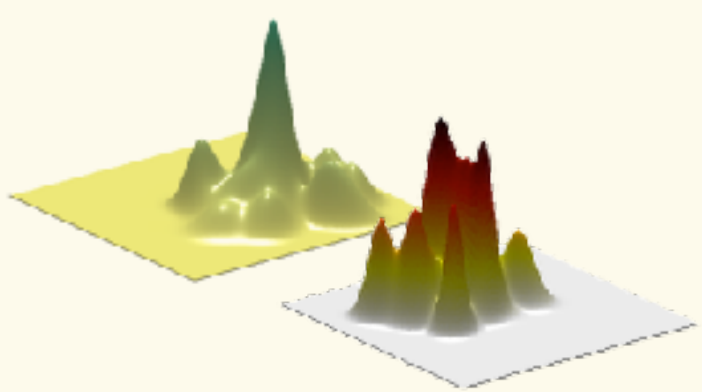




Color Histograms

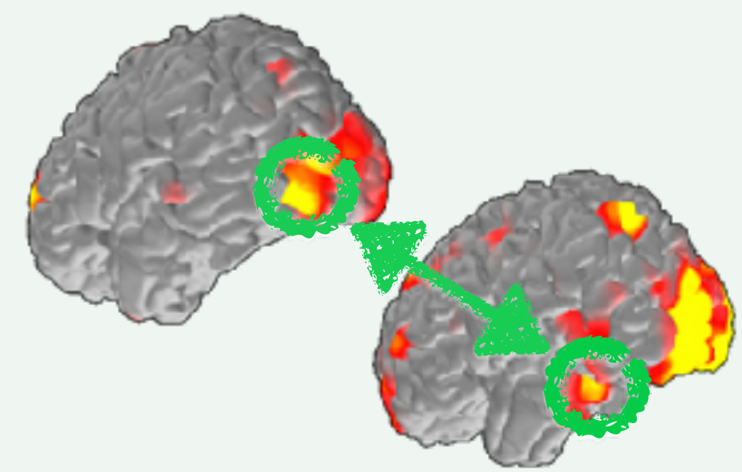
What is Optimal Transport?

The natural geometry for probability measures supported on a metric space.



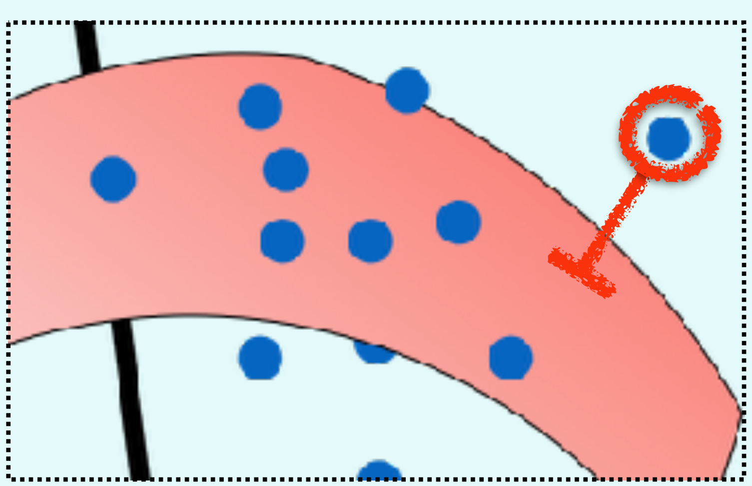
Statistical Models

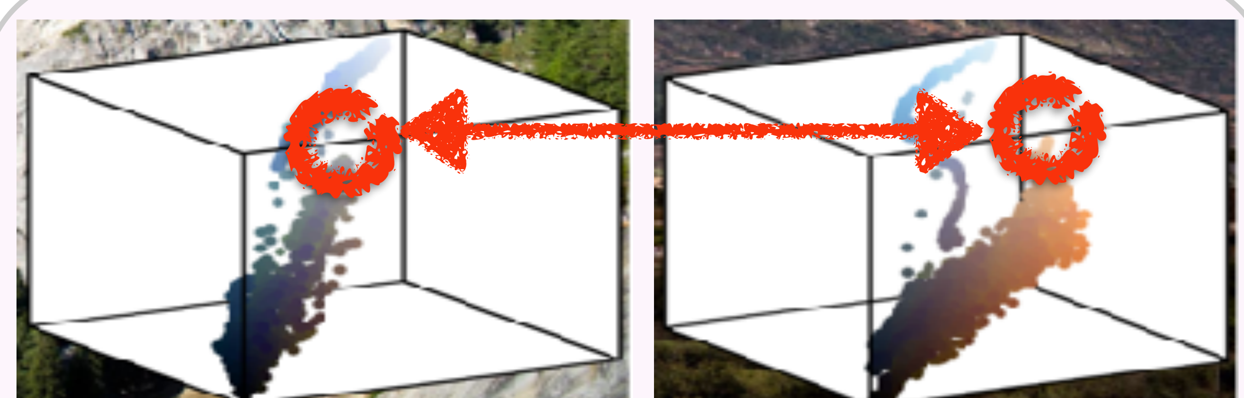
Bags of Features



Brain Activation Maps

Generative Models vs. Data





Color Histograms

Short Course Outline

1. Introduction to optimal transport
2. Optimal transport algorithms
3. Some Applications

Introduction to OT

- Two examples: moving earth & soldiers
- Monge problem, Kantorovich problem
- OT as geometry, OT as a loss function

Origins: Monge Problem (1781)

MÉMOIRE

SUR LA

THÉORIE DES DÉBLAIS ET DES REMBLAIS.

Par M. MONGE.

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.

Origins: Monge Problem (1781)

MÉMOIRES DE L'ACADÉMIE ROYALE

MÉMOIRE

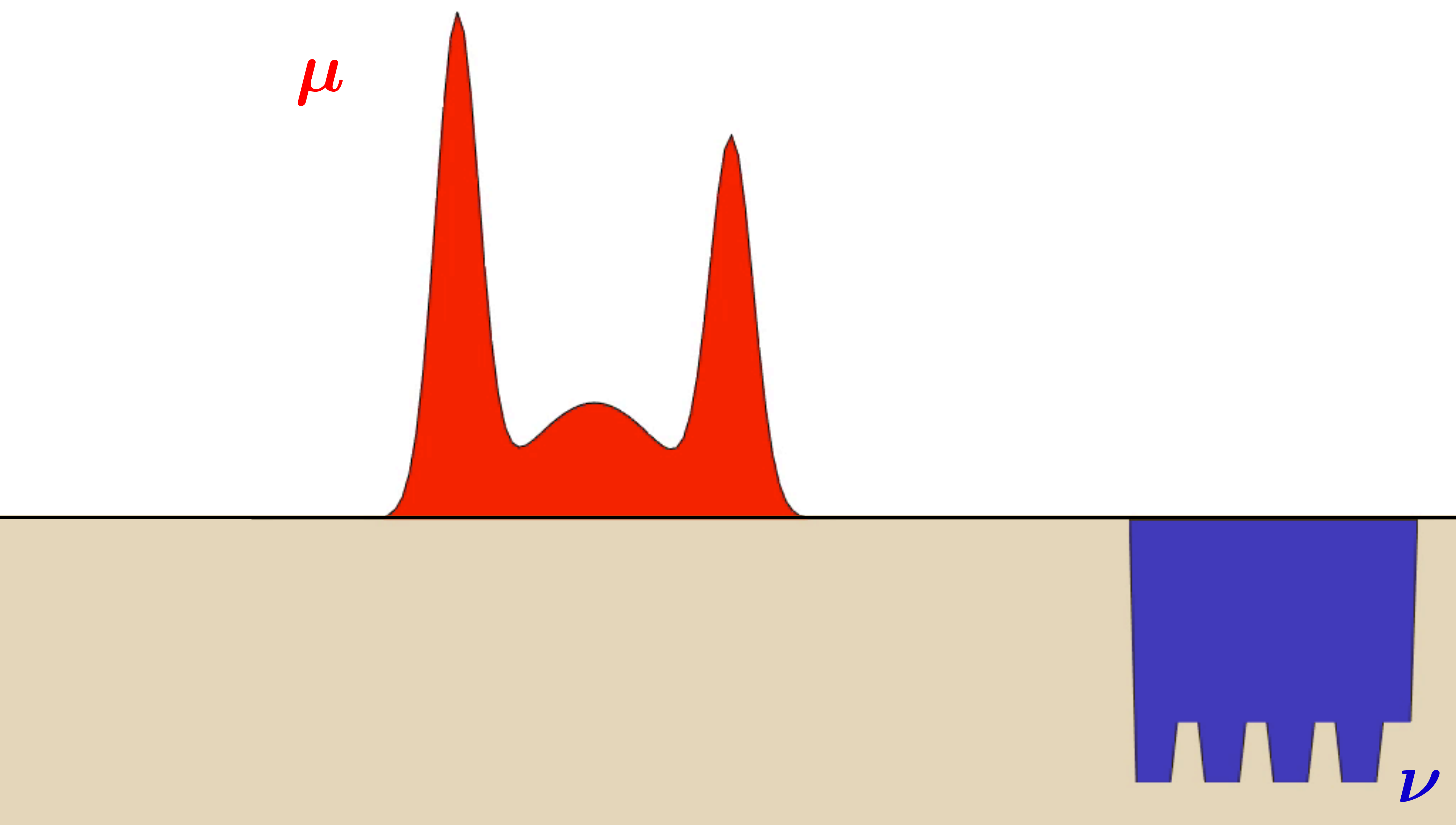
SUR LA

THÉORIE DES DÉBLAIS ET DES REMBLAIS.

When one has to bring earth from one place to another…

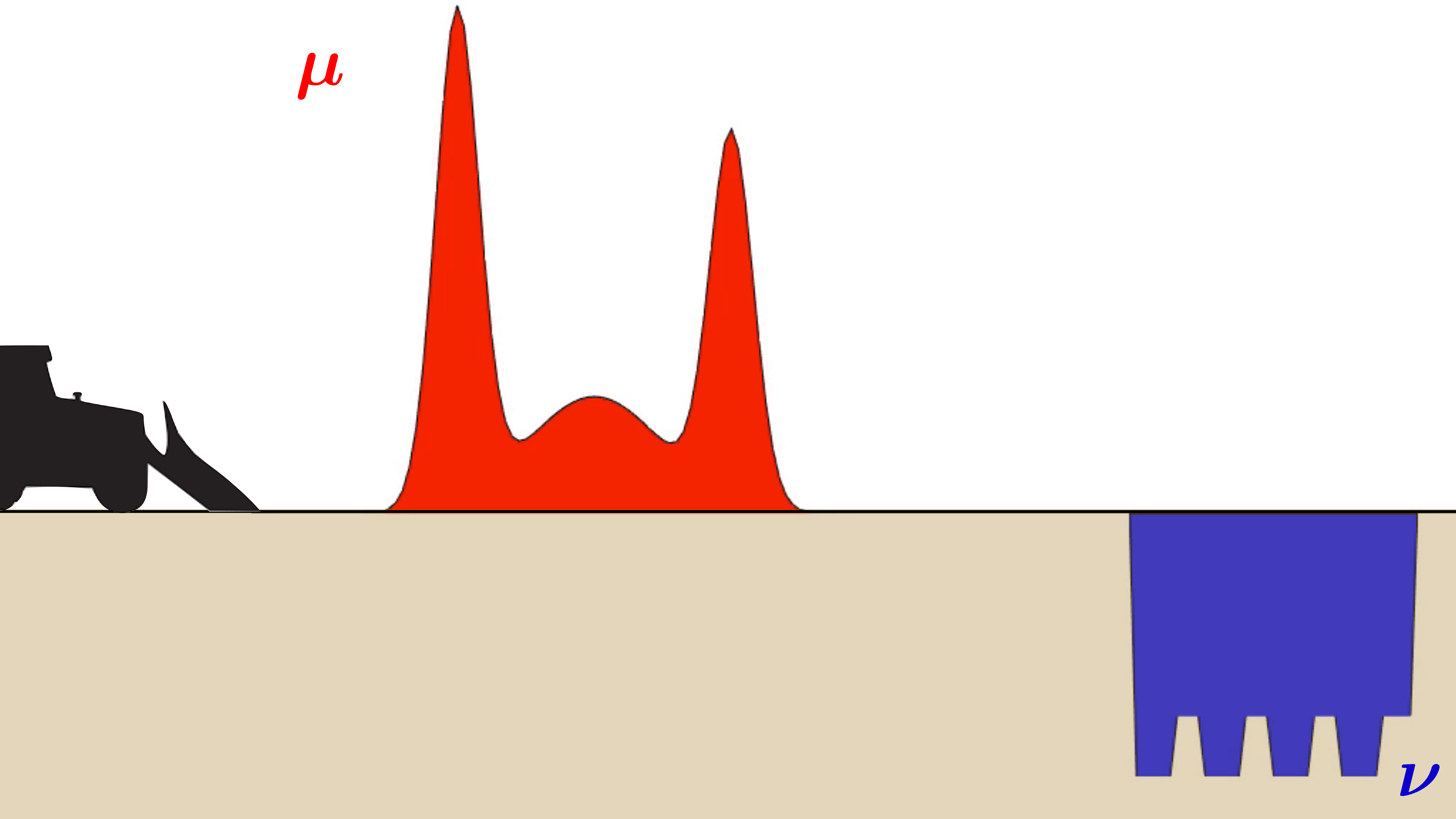
LORSQU'ON doit tranſporter des terres d'un lieu dans un autre, on a coutume de donner le nom de *Déblai* au volume des terres que l'on doit tranſporter, & le nom de *Remblai* à l'eſpace qu'elles doivent occuper après le tranſport.

Origins: Monge Problem



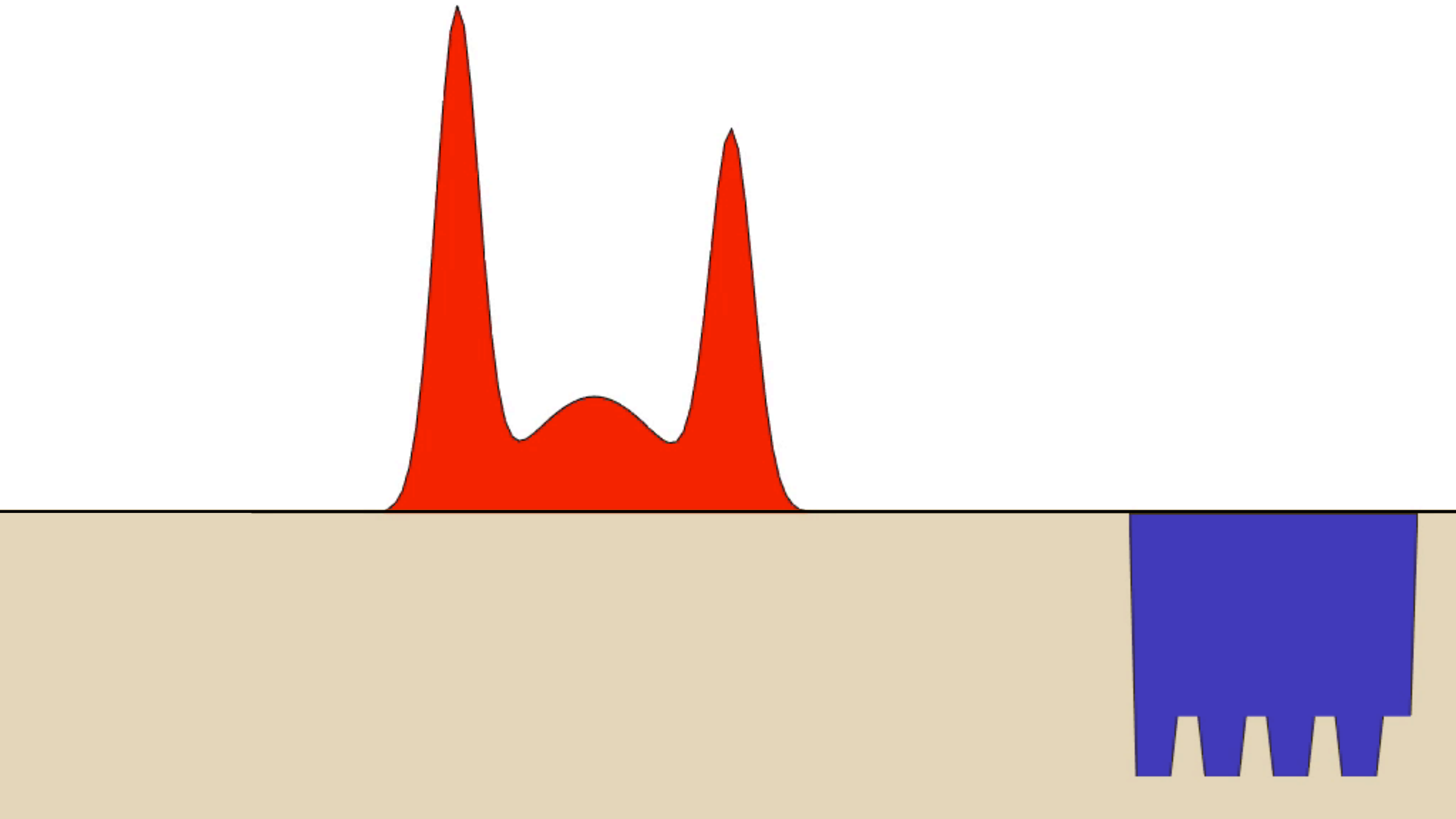
Origins: Monge Problem

In the 21st Century...



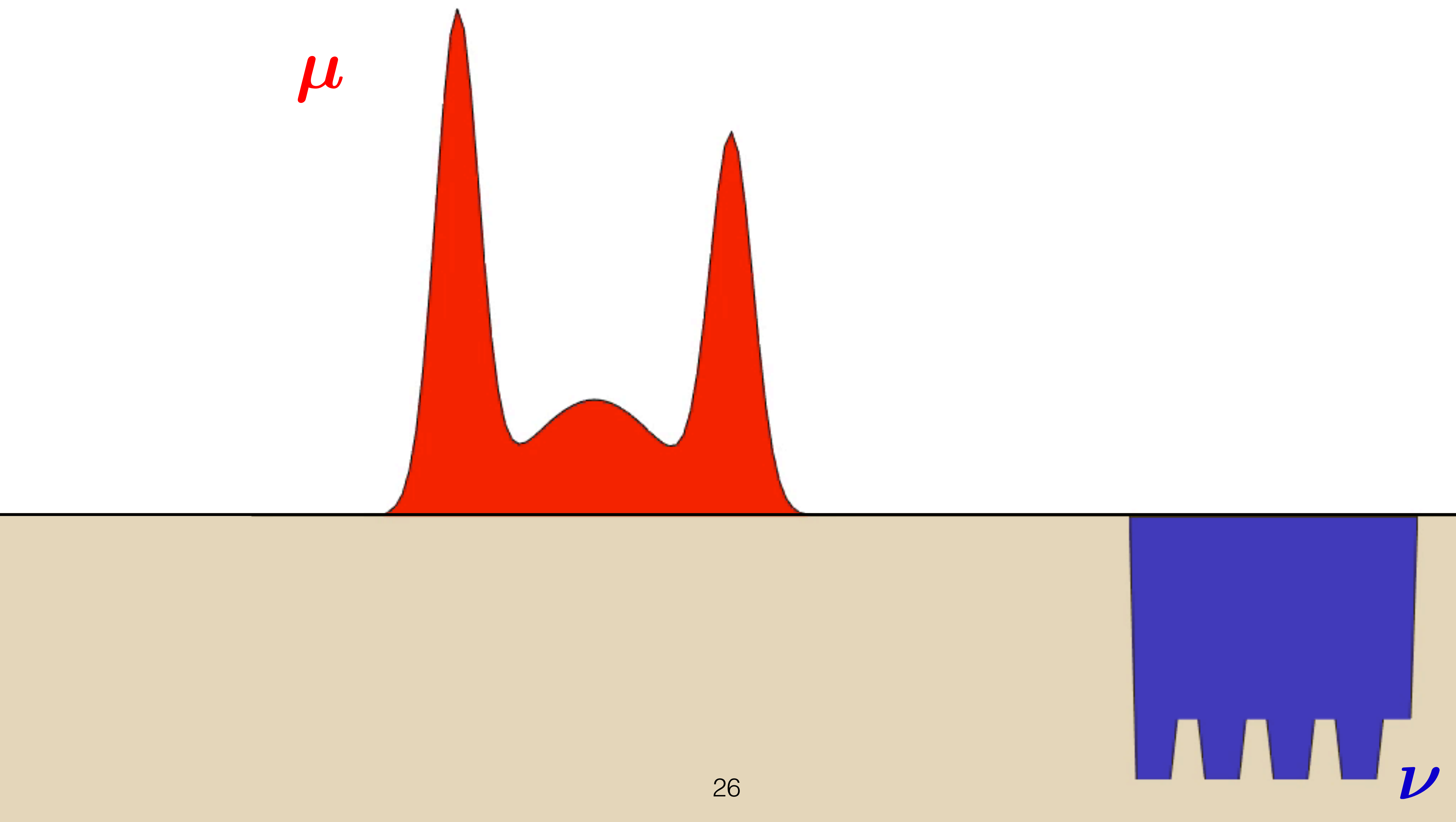
Origins: Monge Problem

In the 21st Century...



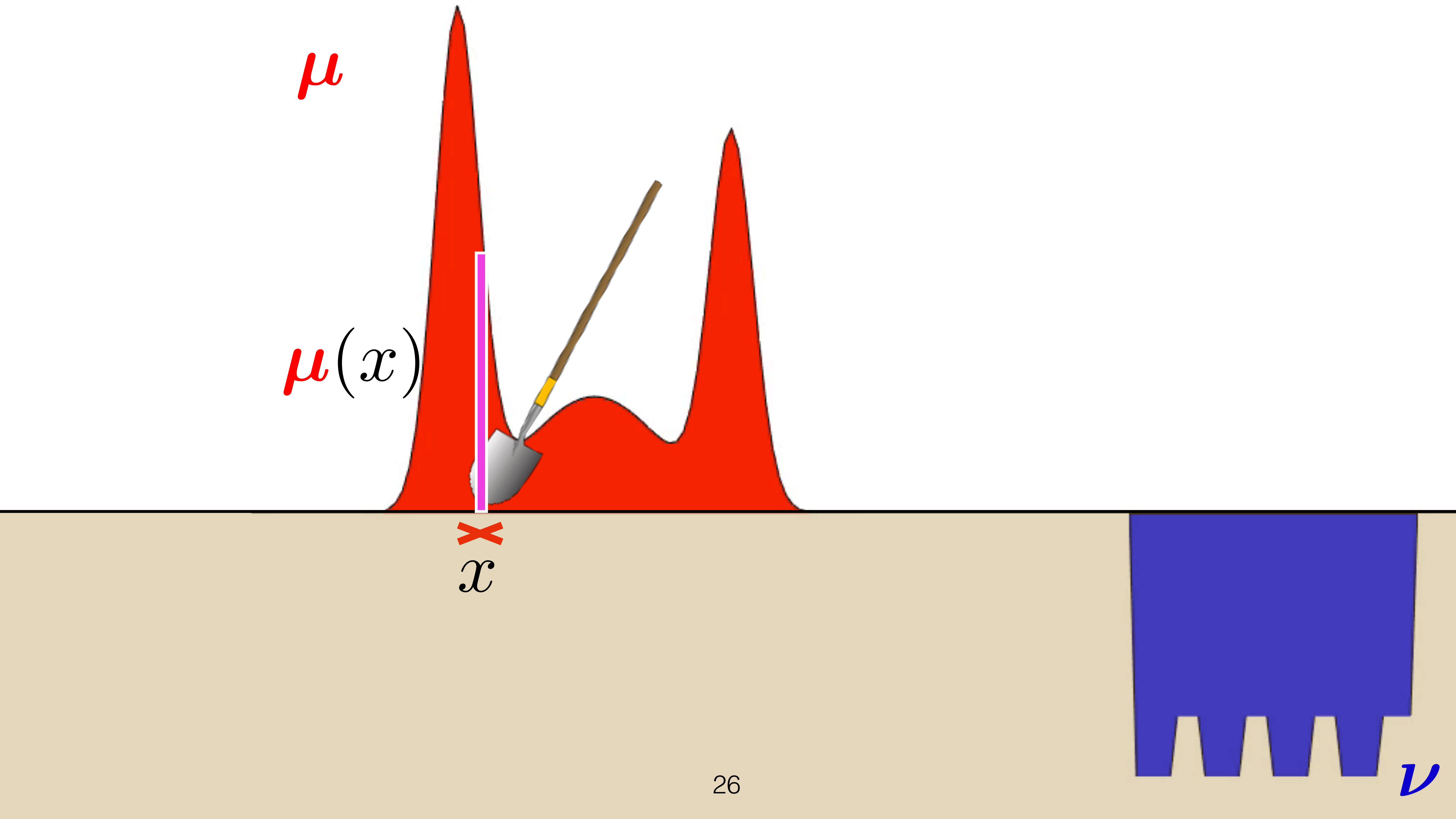
Origins: Monge's Problem

In 1781 however…



Origins: Monge's Problem

In 1781 however...



Origins: Monge's Problem

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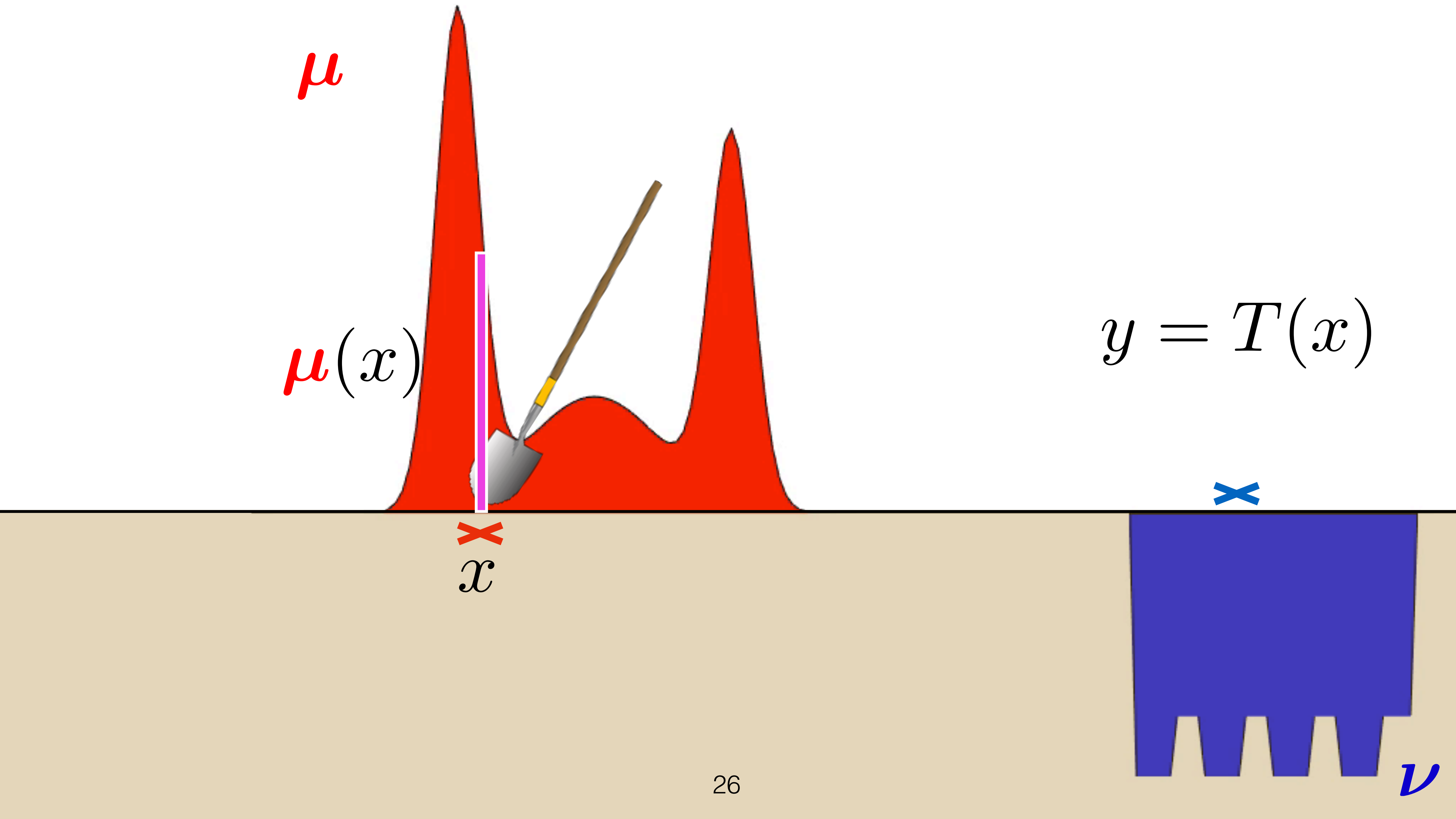

Origins: Monge's Problem

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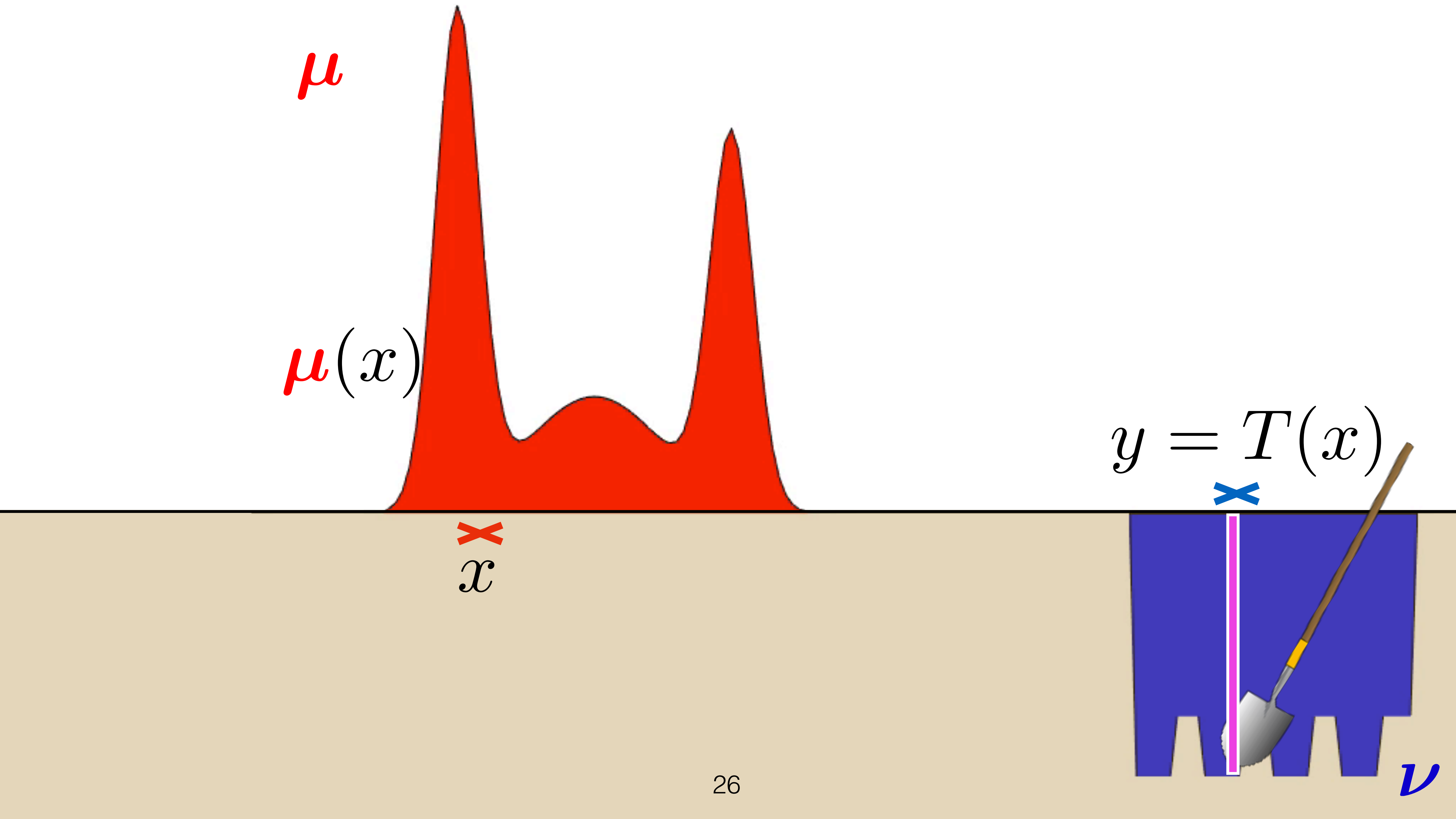
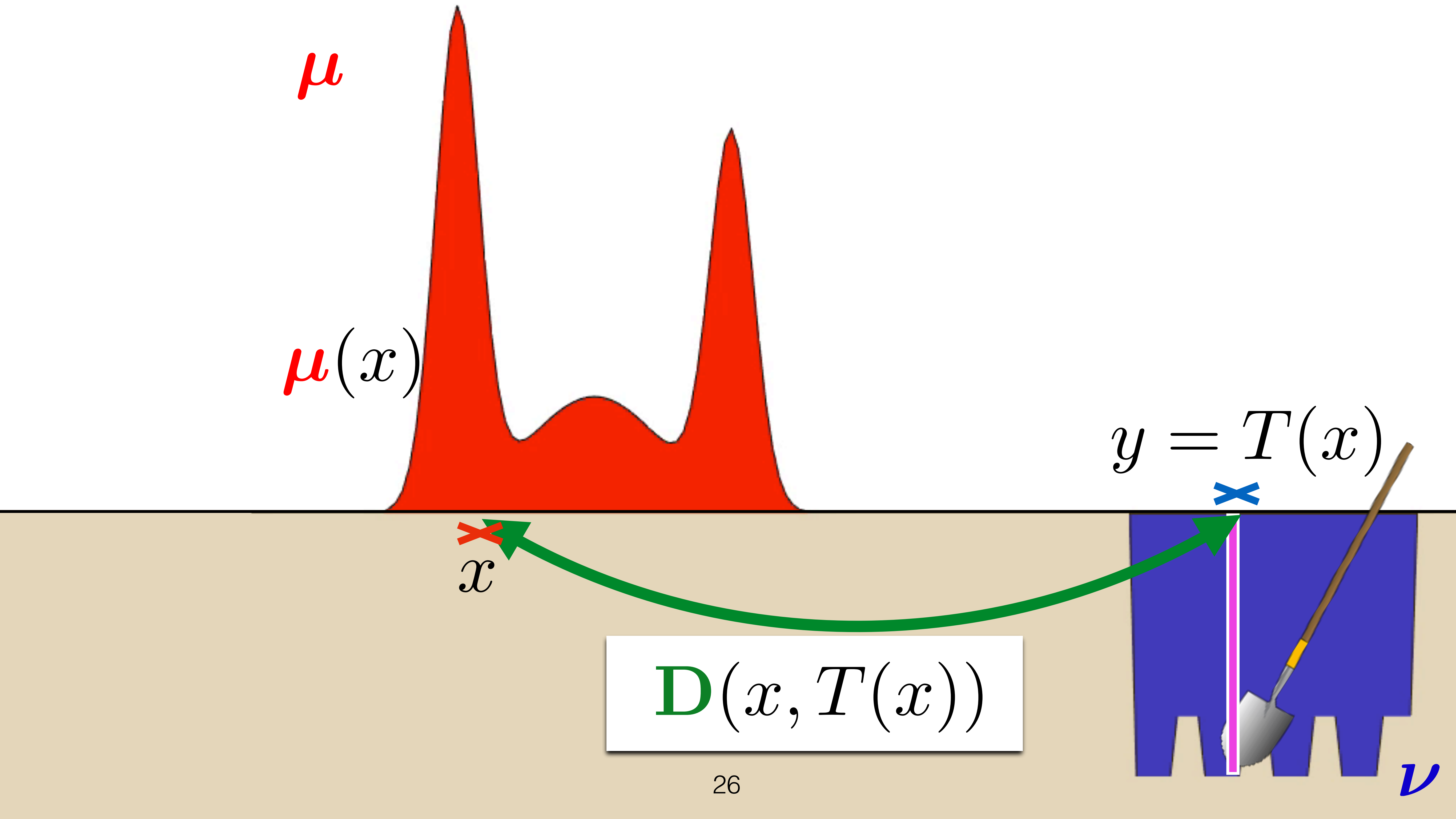


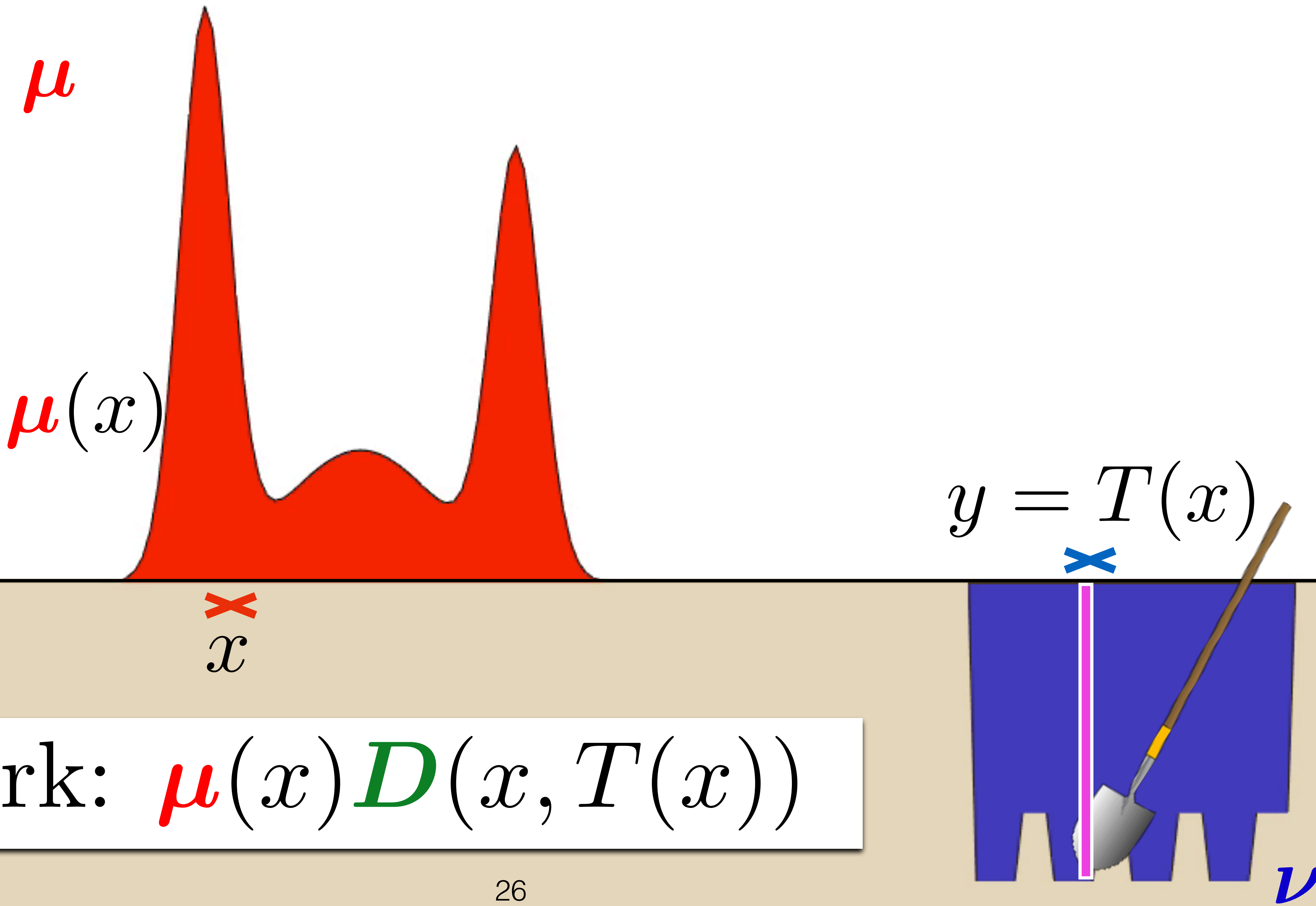
Origins: Monge's Problem

In 1781 however...



Origins: Monge's Problem

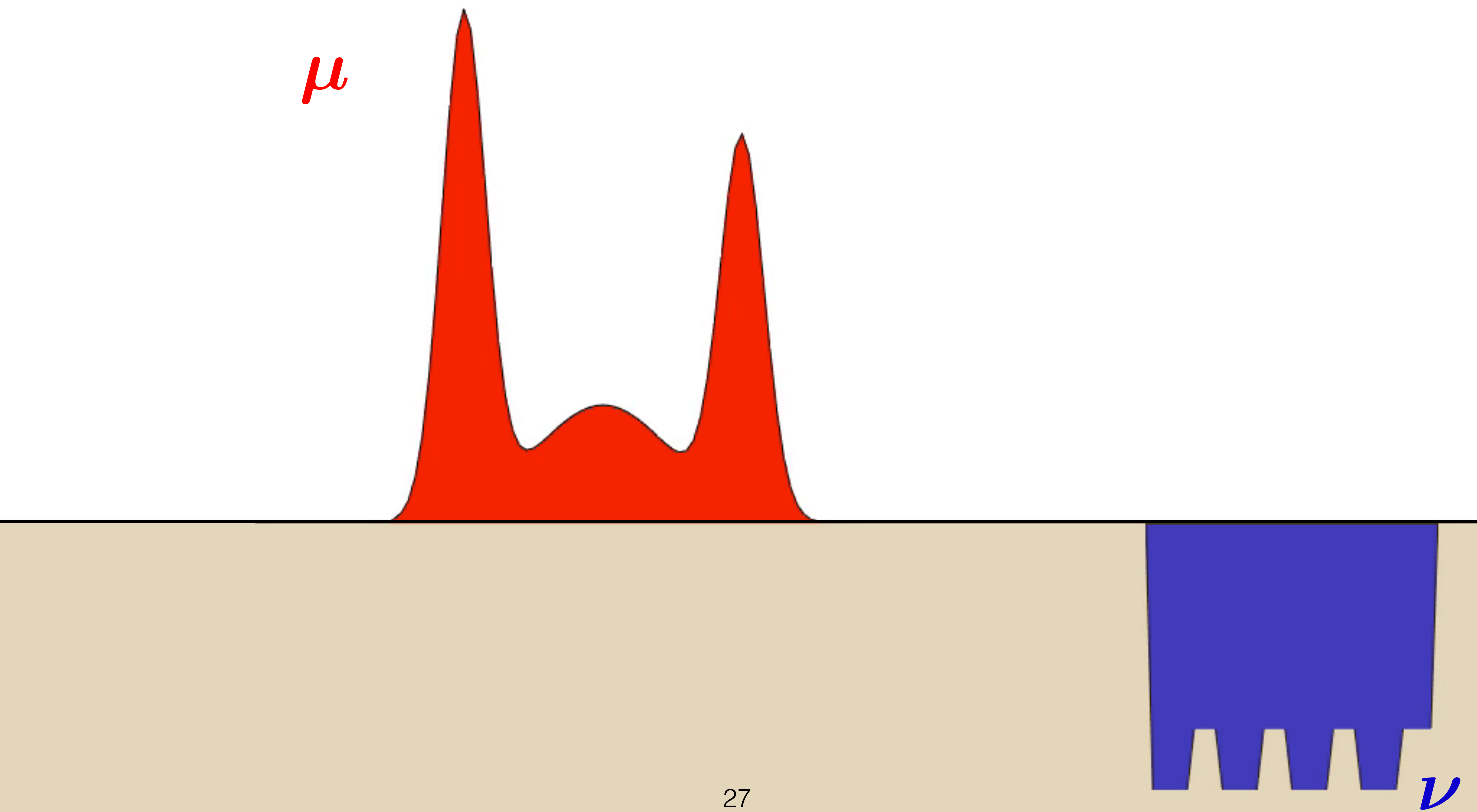
In 1781 however...



work: $\mu(x)D(x,T(x))$

Origins: Monge's Problem

T must map red to blue.



Origins: Monge's Problem

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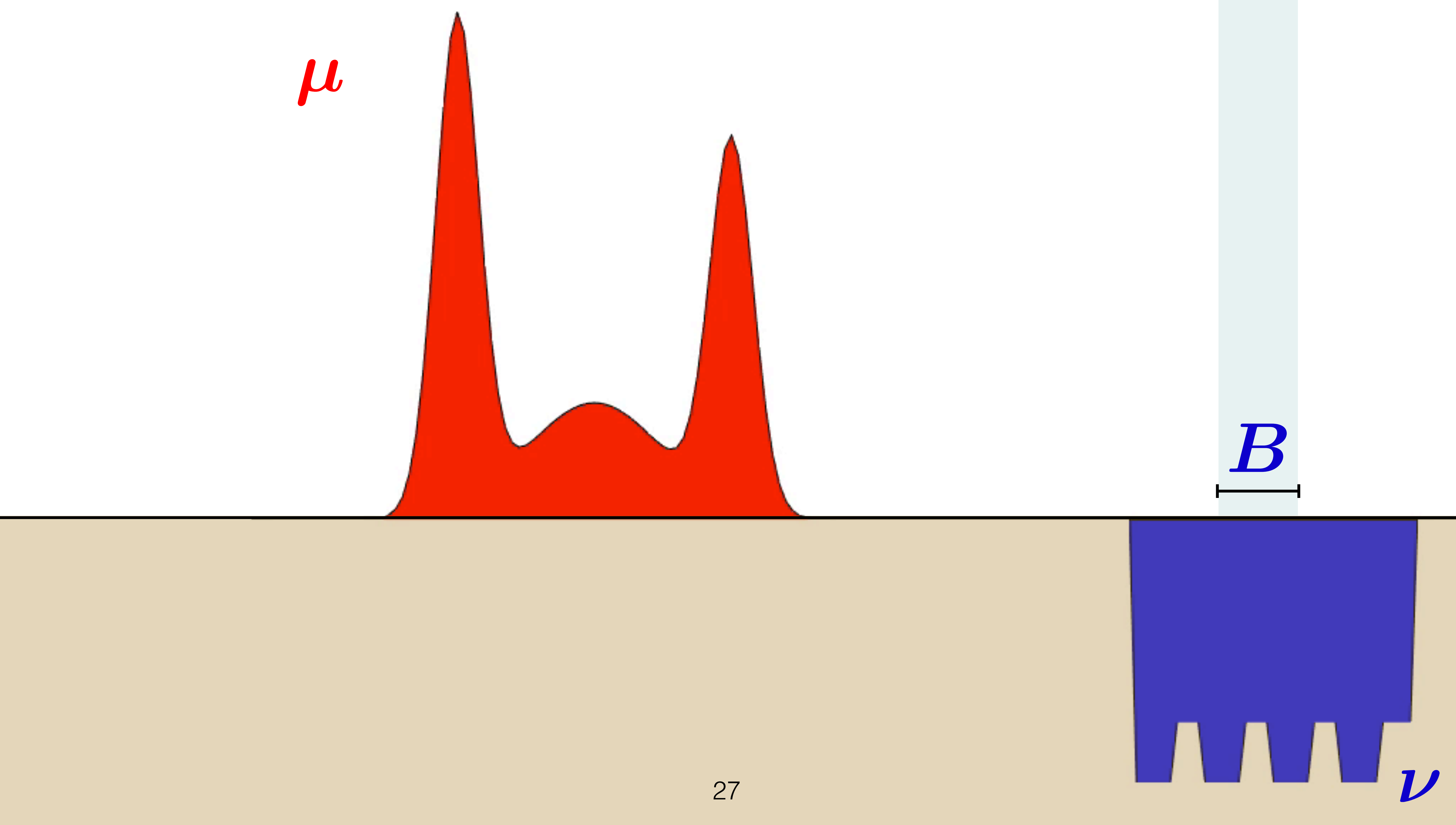

Origins: Monge's Problem

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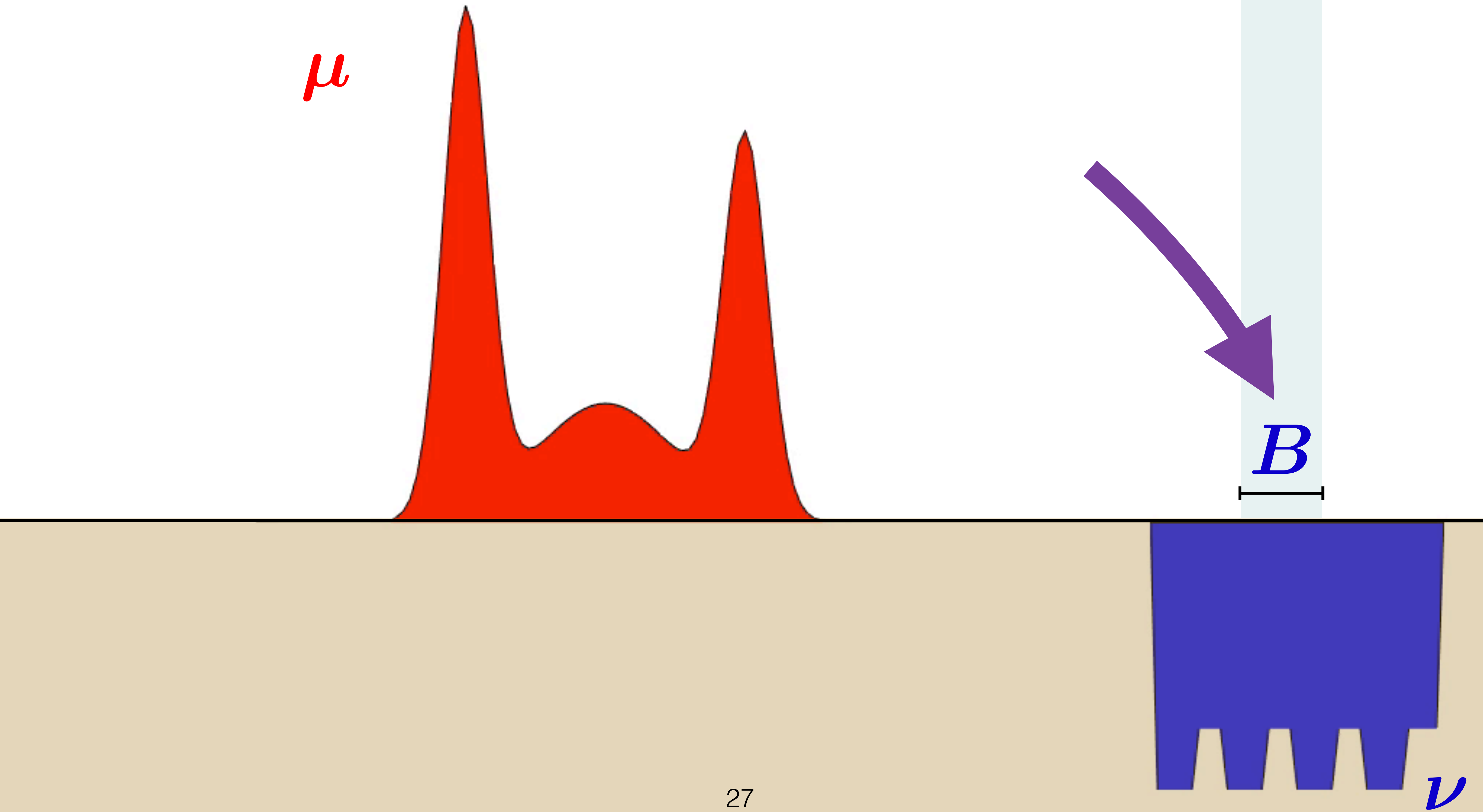

Origins: Monge's Problem

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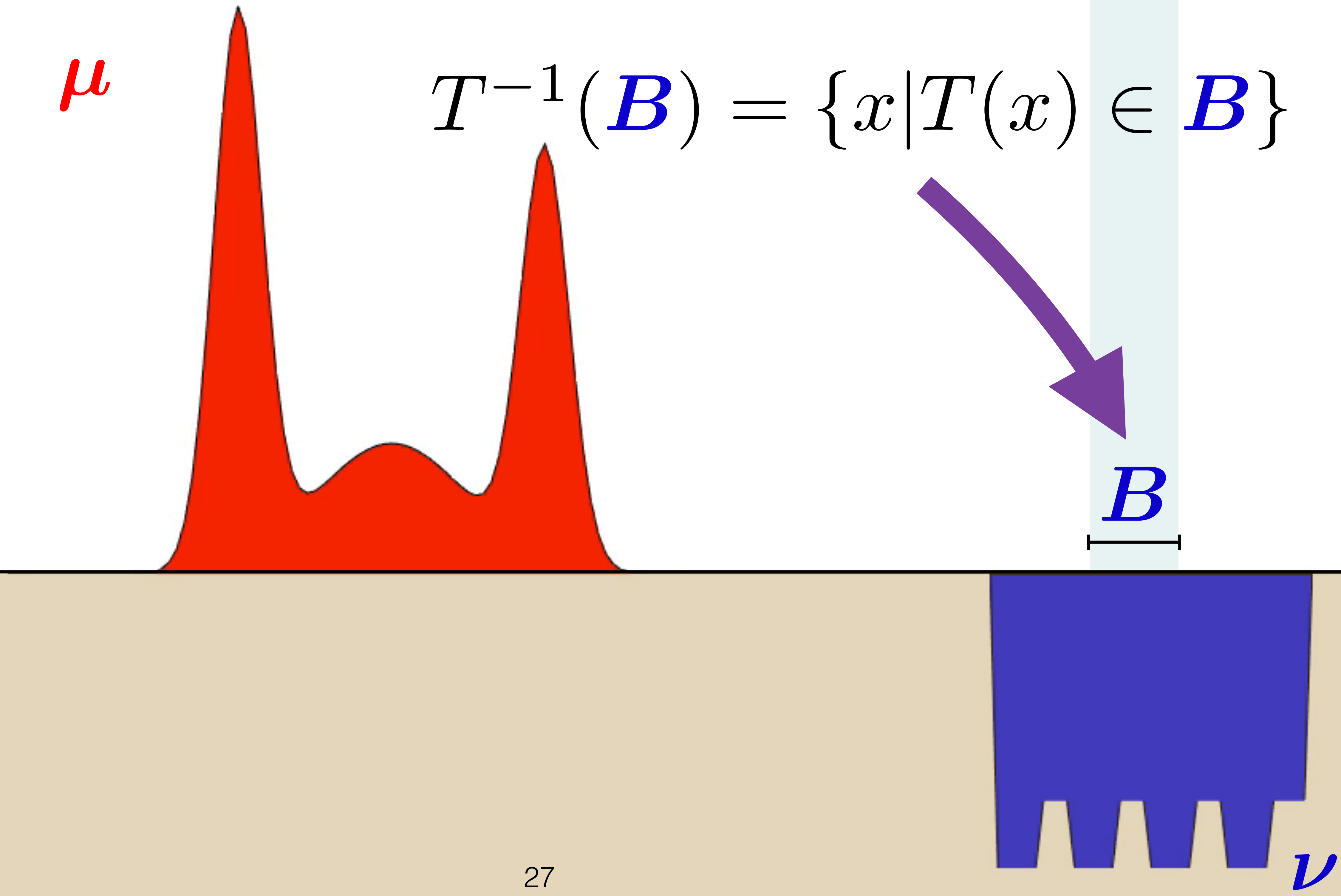
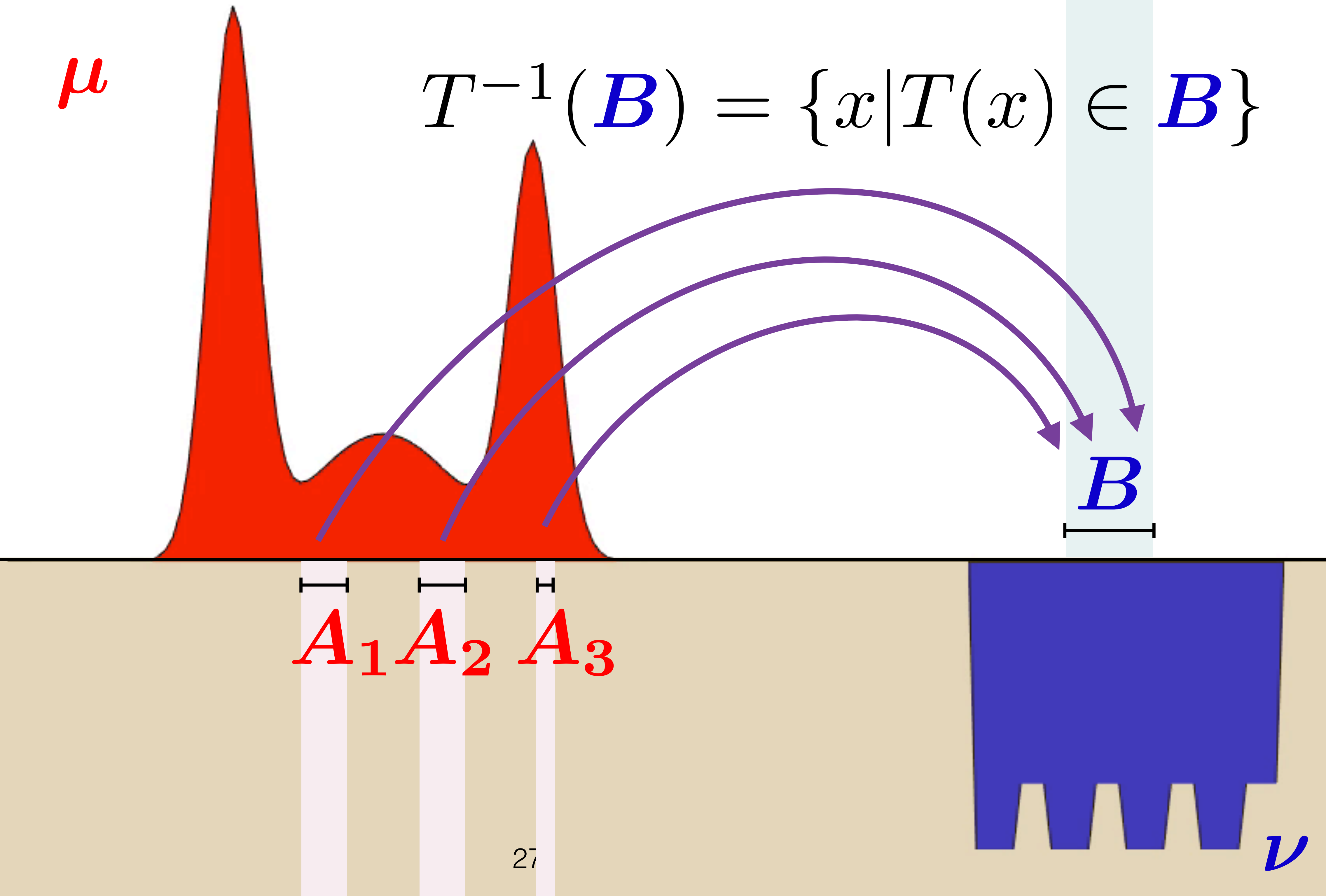


Origins: Monge's Problem

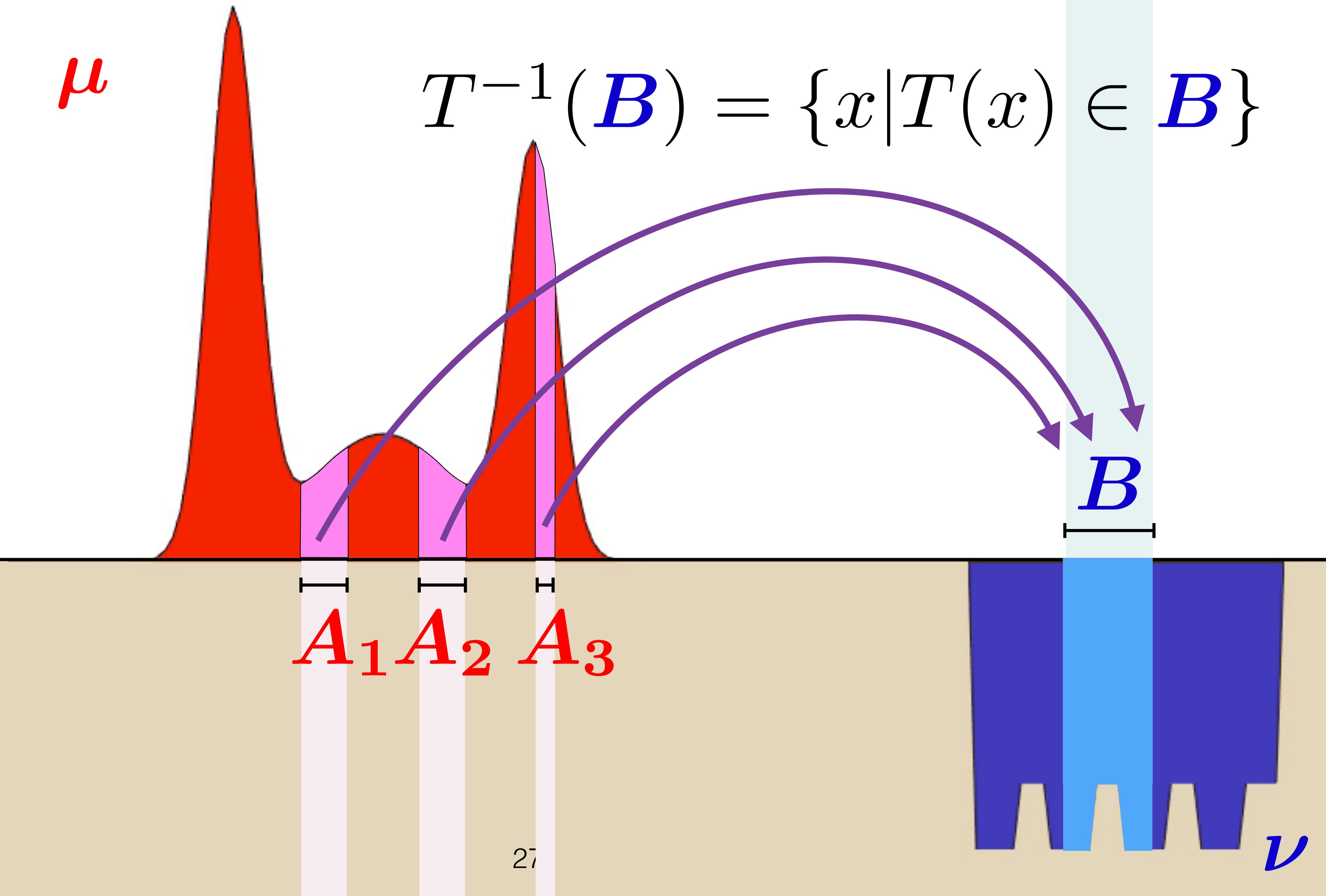
T must map red to blue.

$$T^{-1}(\boldsymbol{B}) = \{x | T(x) \in \boldsymbol{B}\}$$



Origins: Monge's Problem

T must map red to blue.



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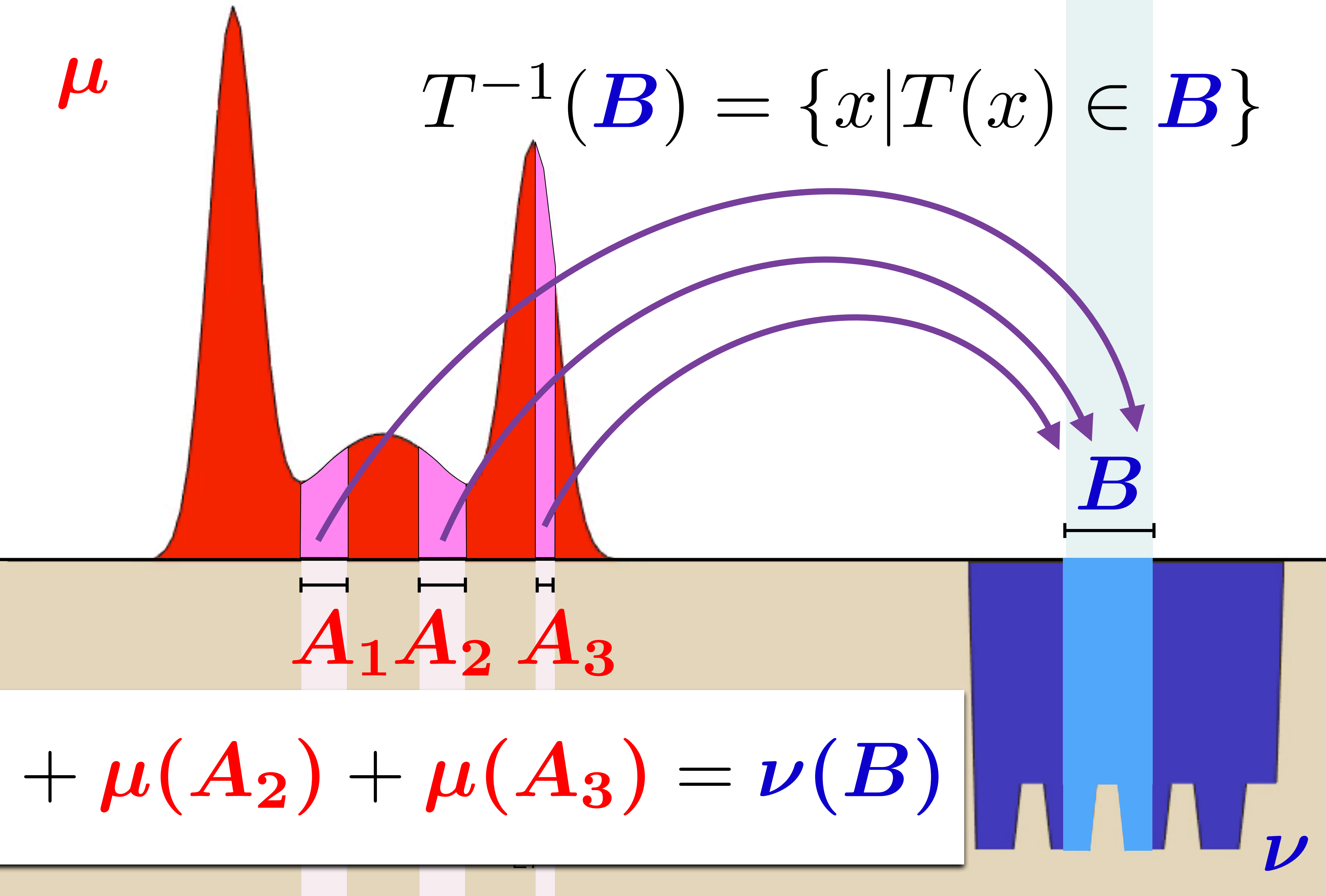
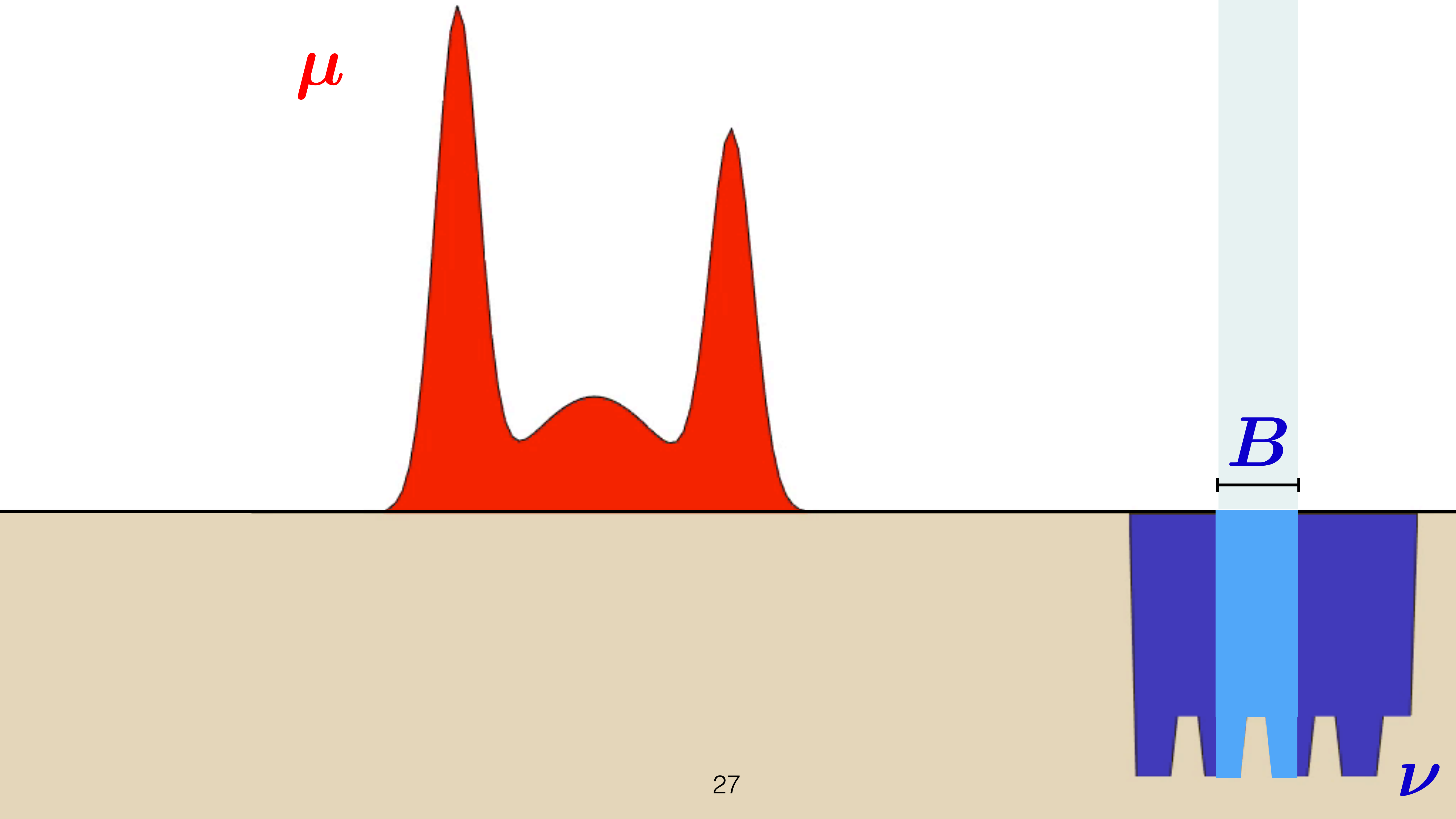


$$\boldsymbol{\mu}(\boldsymbol{A_1}) + \boldsymbol{\mu}(\boldsymbol{A_2}) + \boldsymbol{\mu}(\boldsymbol{A_3}) = \boldsymbol{\nu}(\boldsymbol{B})$$

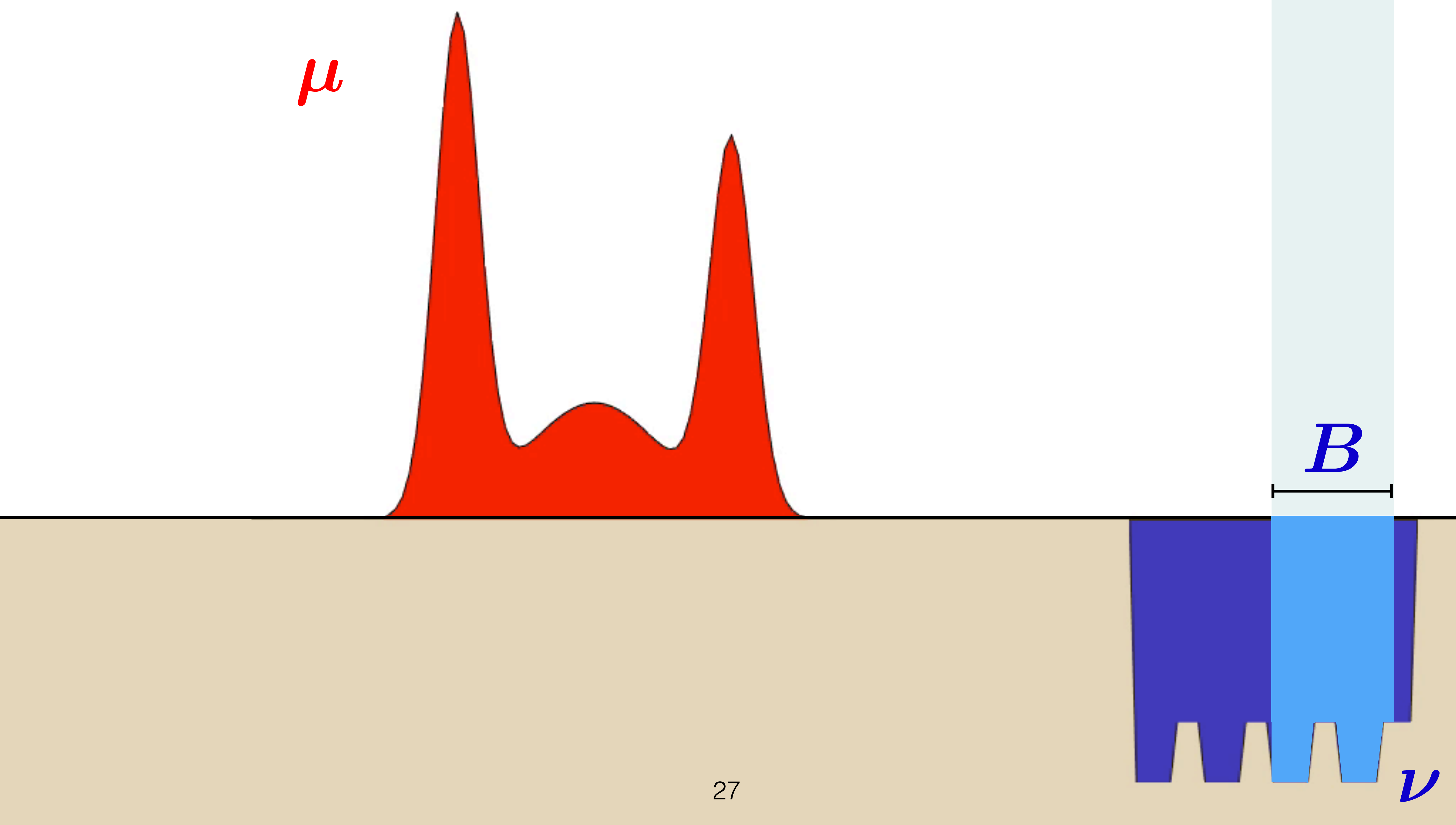
Origins: Monge's Problem

T must map red to blue.



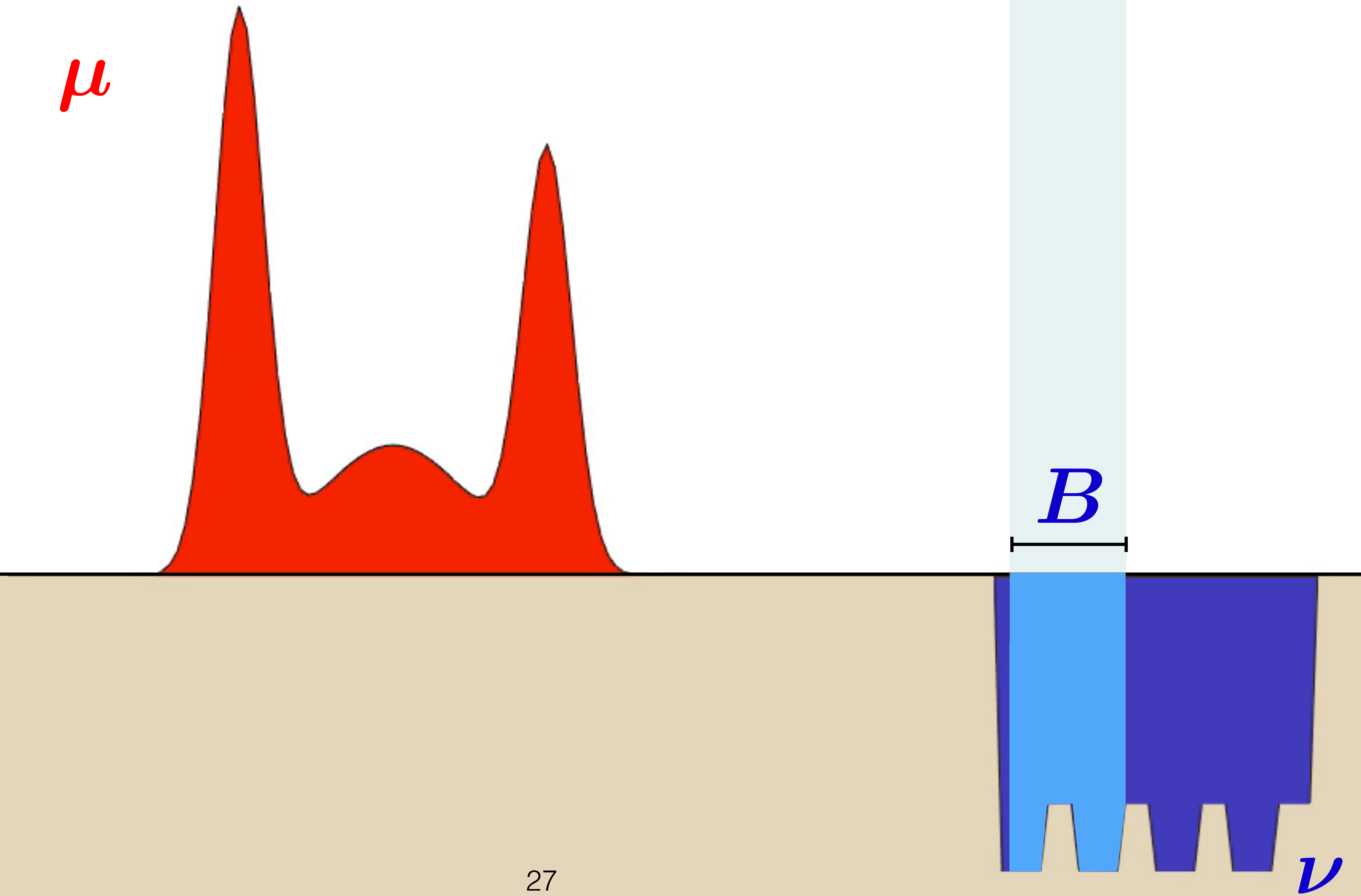
Origins: Monge's Problem

T must map red to blue.



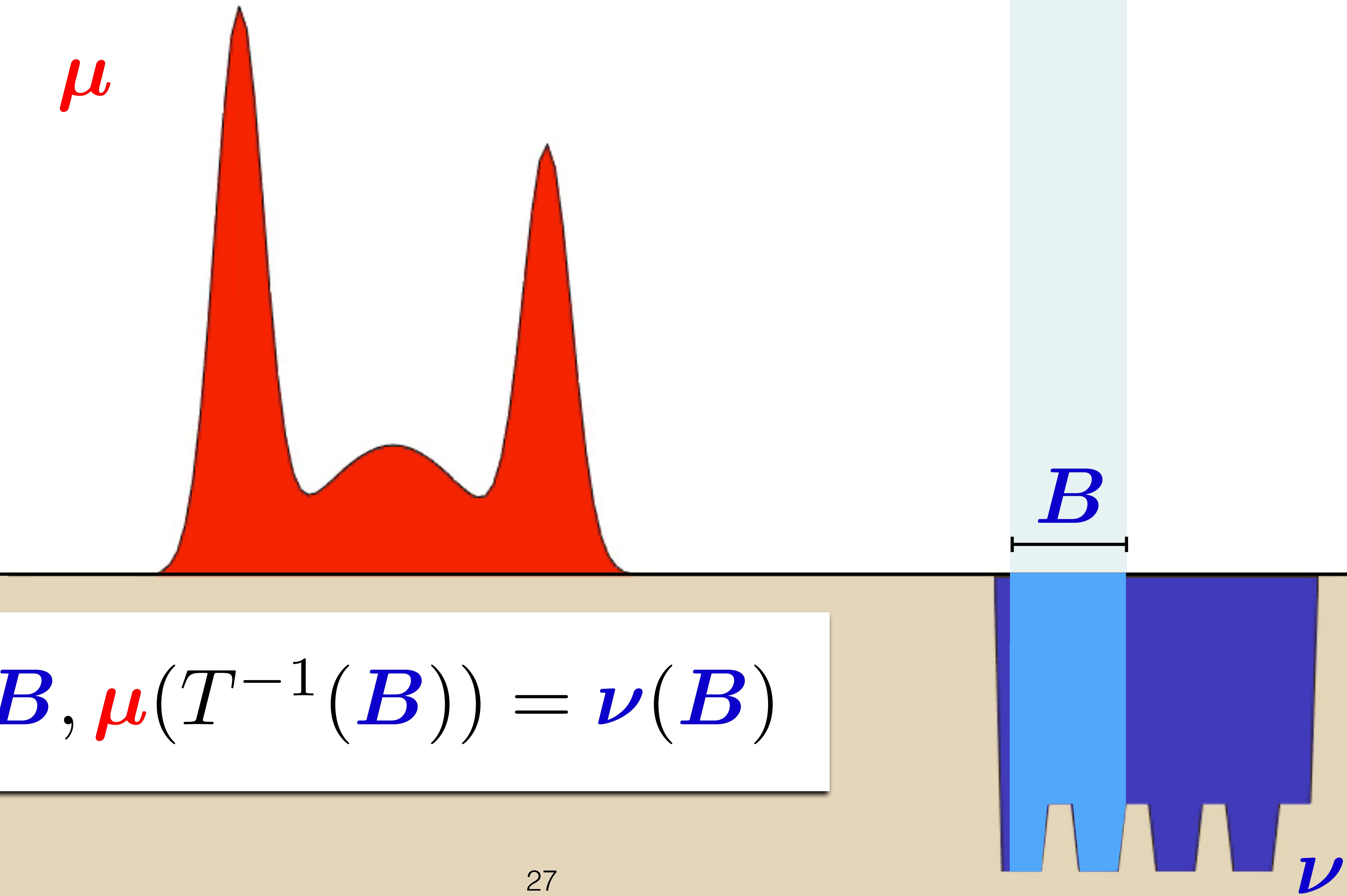
Origins: Monge's Proble

T must map red to blue.



Origins: Monge's Proble

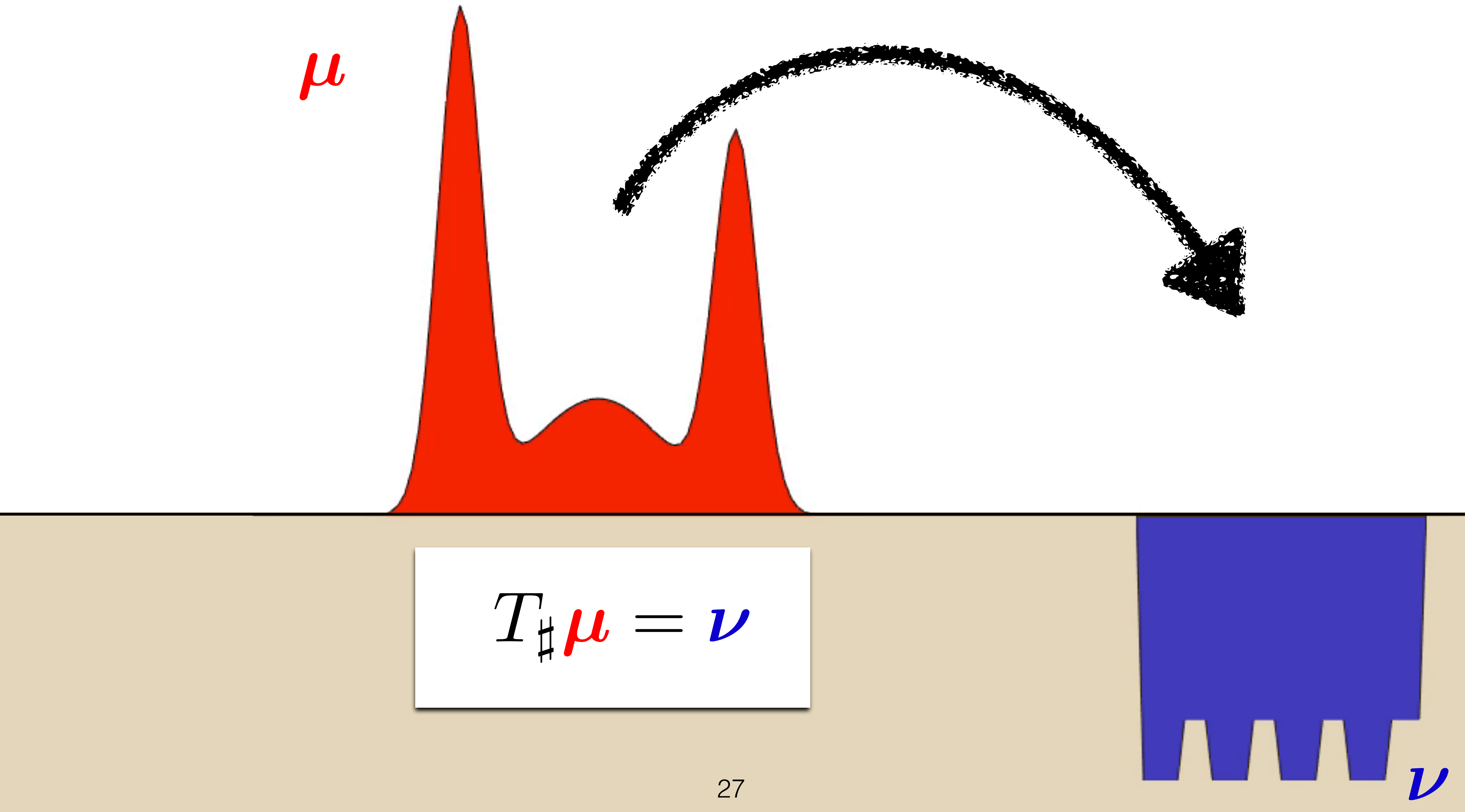
T must map red to blue.



$$\forall B, \mu(T^{-1}(B)) = \nu(B)$$

Origins: Monge's Problem

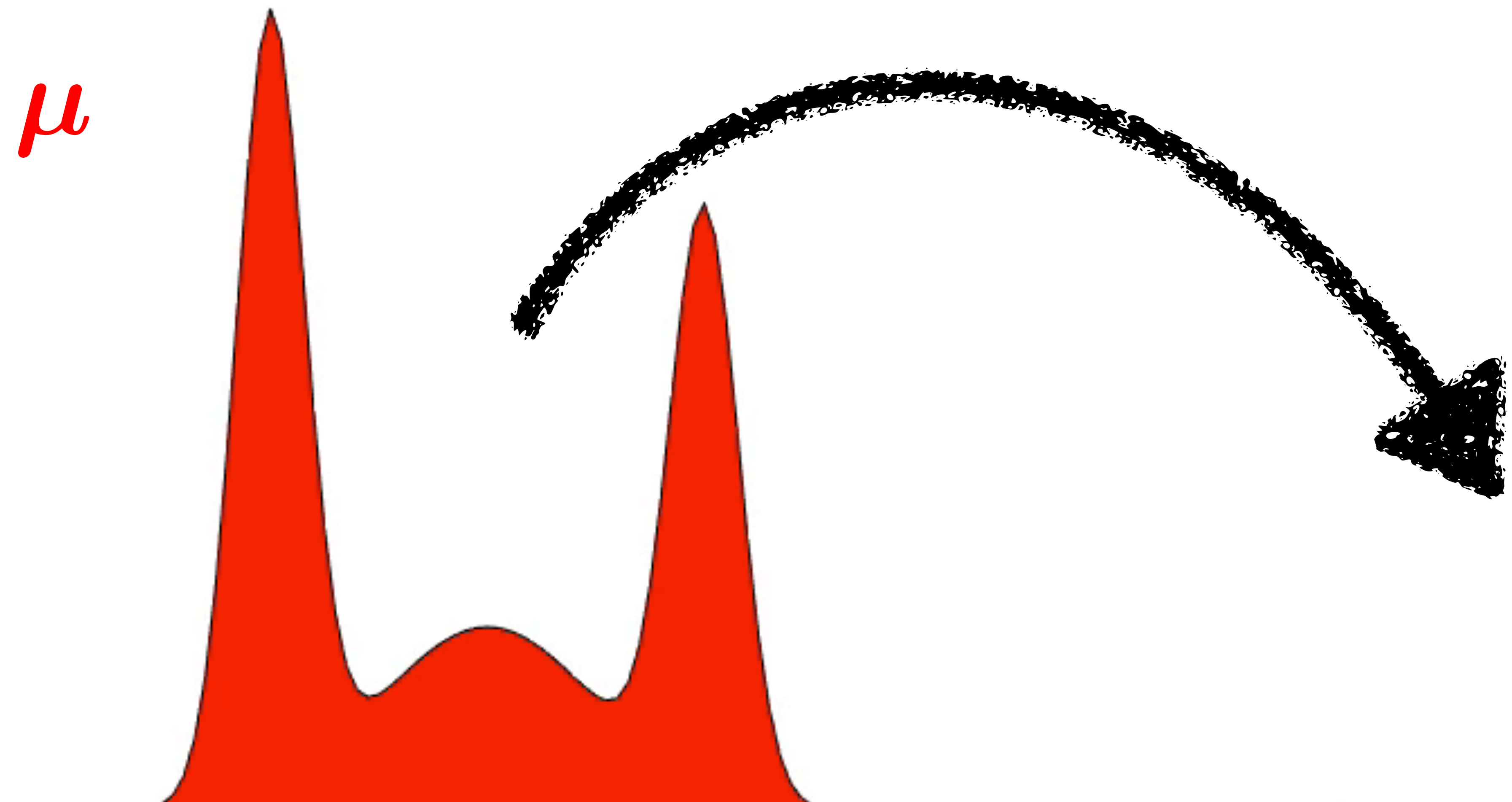
T must **push-forward** *the red measure towards the blue*



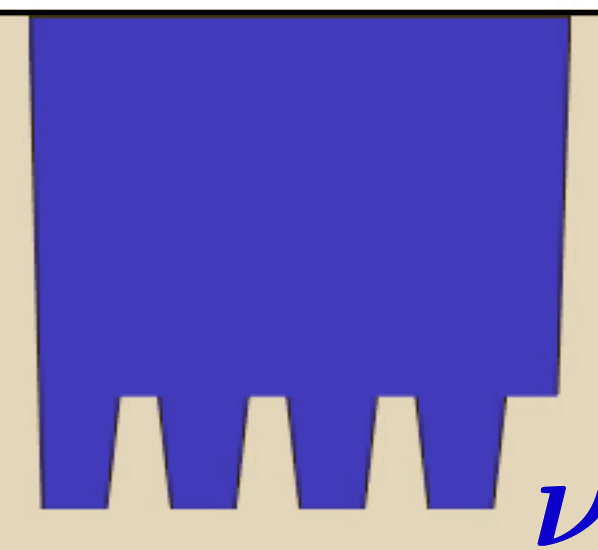
$$T_\sharp \mu = \nu$$

Origins: Monge's Problem

T must **push-forward** *the red measure towards the blue*



$$\text{What } T \text{ s.t. } T_\sharp \boldsymbol{\mu} = \boldsymbol{\nu}$$
$$\text{minimizes } \int \boldsymbol{D}(x, T(x))\boldsymbol{\mu}(dx)?$$

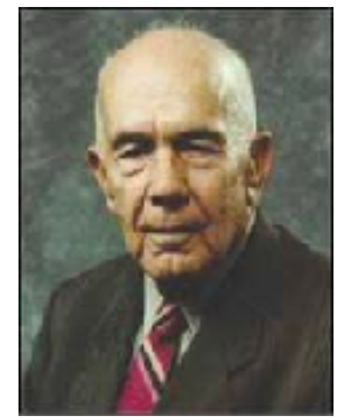


Kantorovich Problem

Kantorovich

Tolstoi

1930



Hitchcock

1939

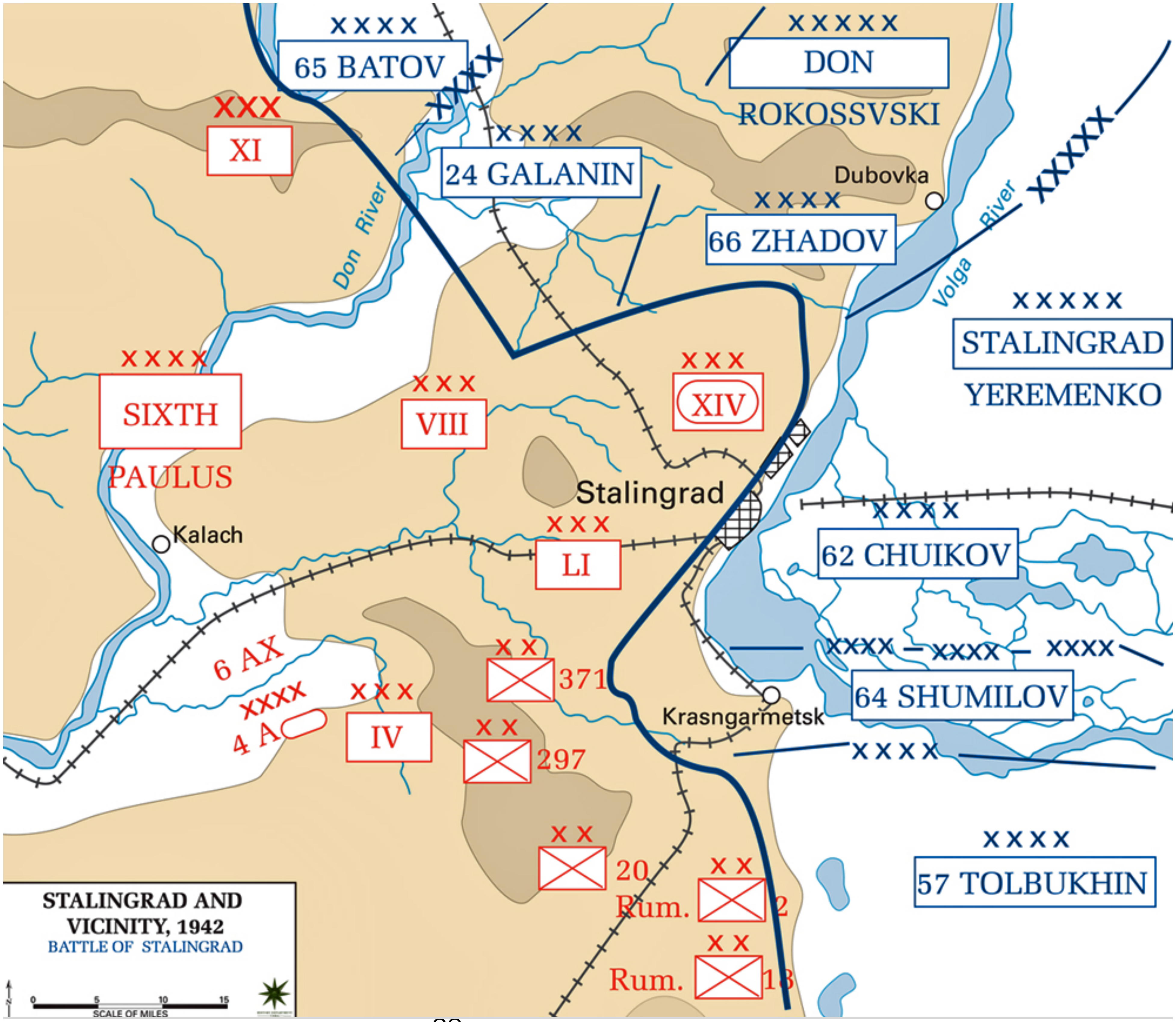
THE DISTRIBUTION OF A PRODUCT FROM SEVERAL SOURCES TO NUMEROUS LOCALITIES

By Frank L. Hitchcock

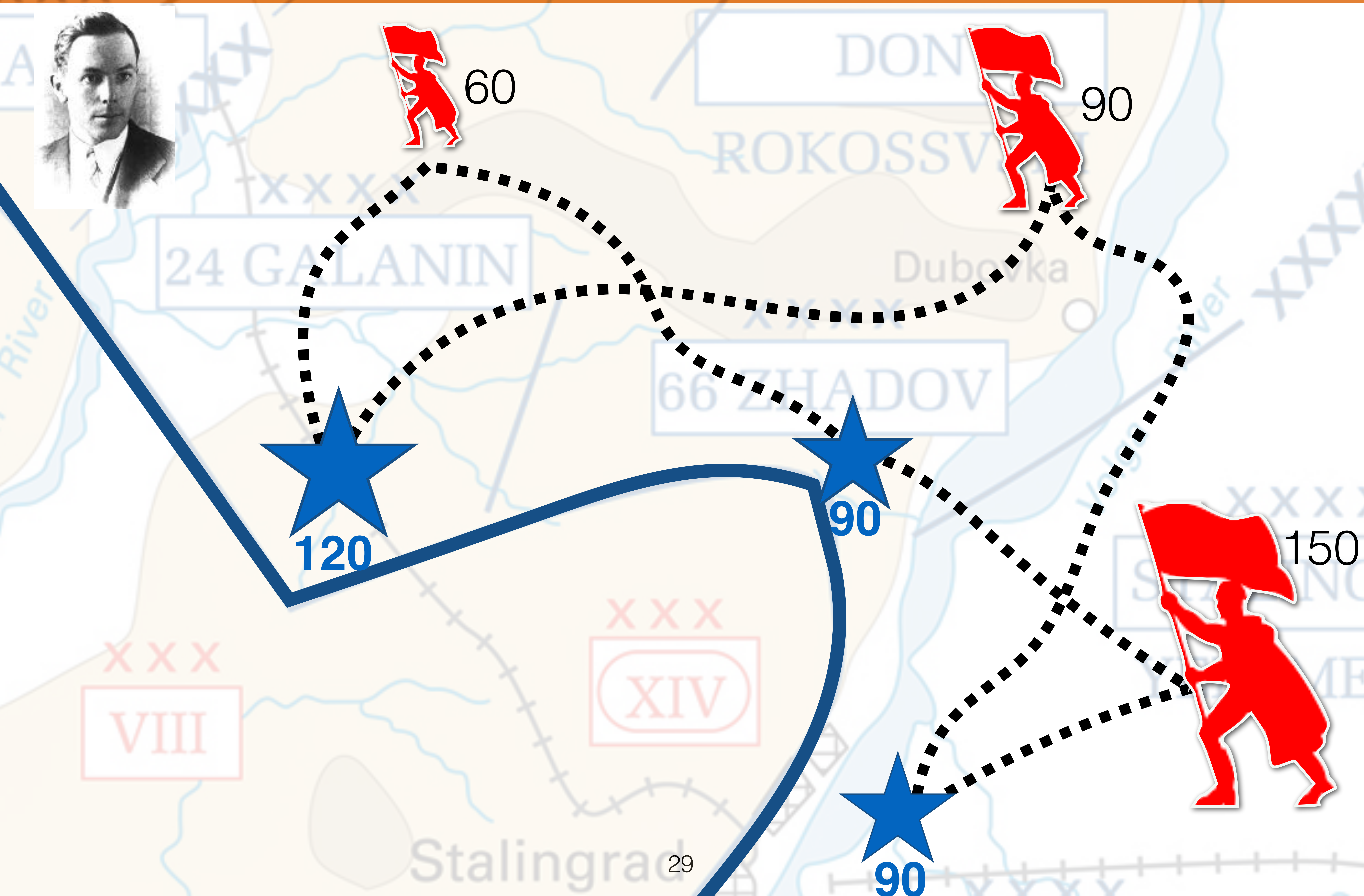
1. Statement of the problem. When several factories supply a product to a number of cities we desire the least costly manner of distribution. Due to freight rates and other matters the cost of a ton of product to a particular city will vary according to which factory supplies it, and will also vary from city to city.

1941

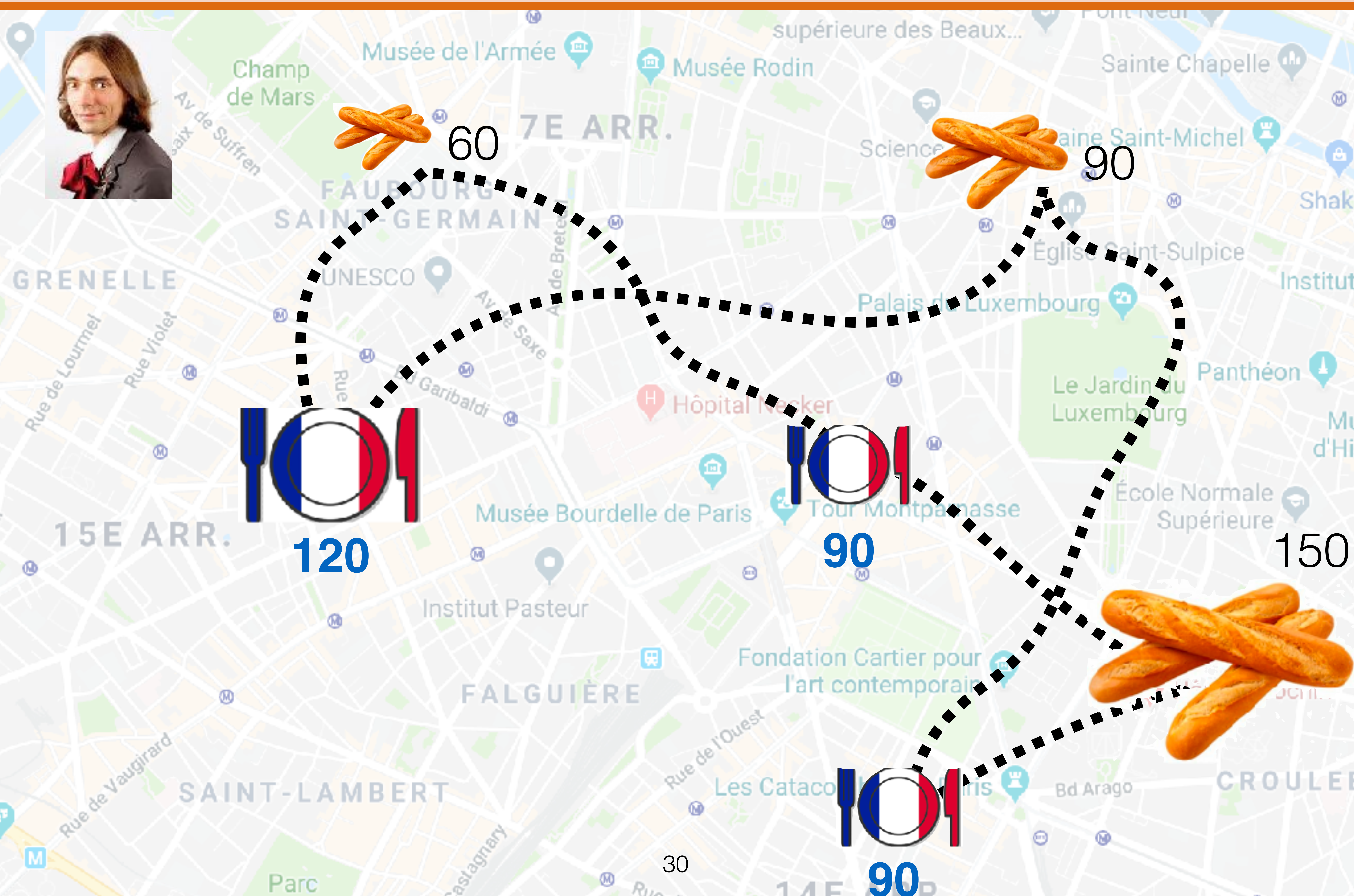
Kantorovich Problem



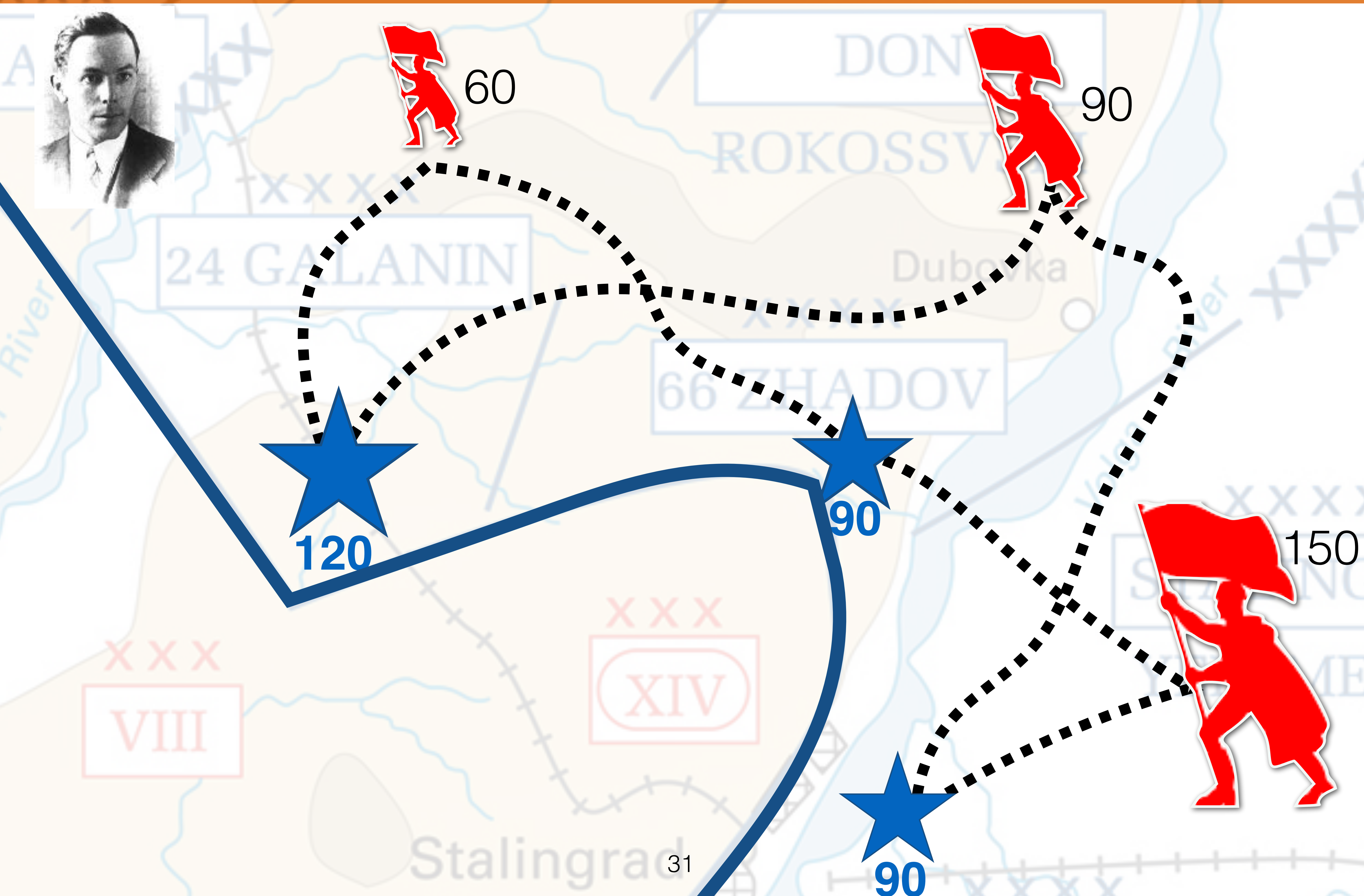
Kantorovich Problem



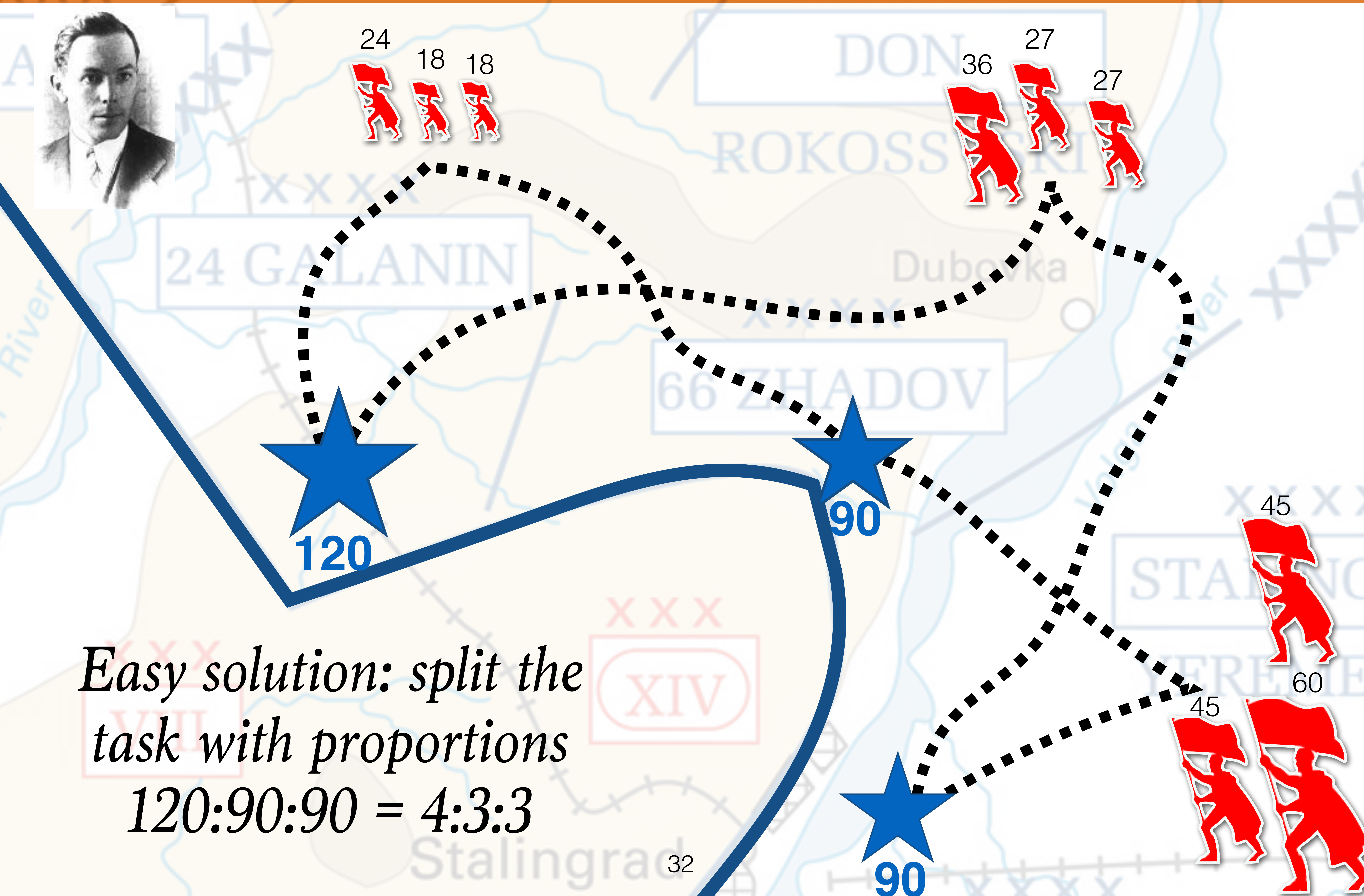
Kantorovich Problem *à la française*



Kantorovich Problem

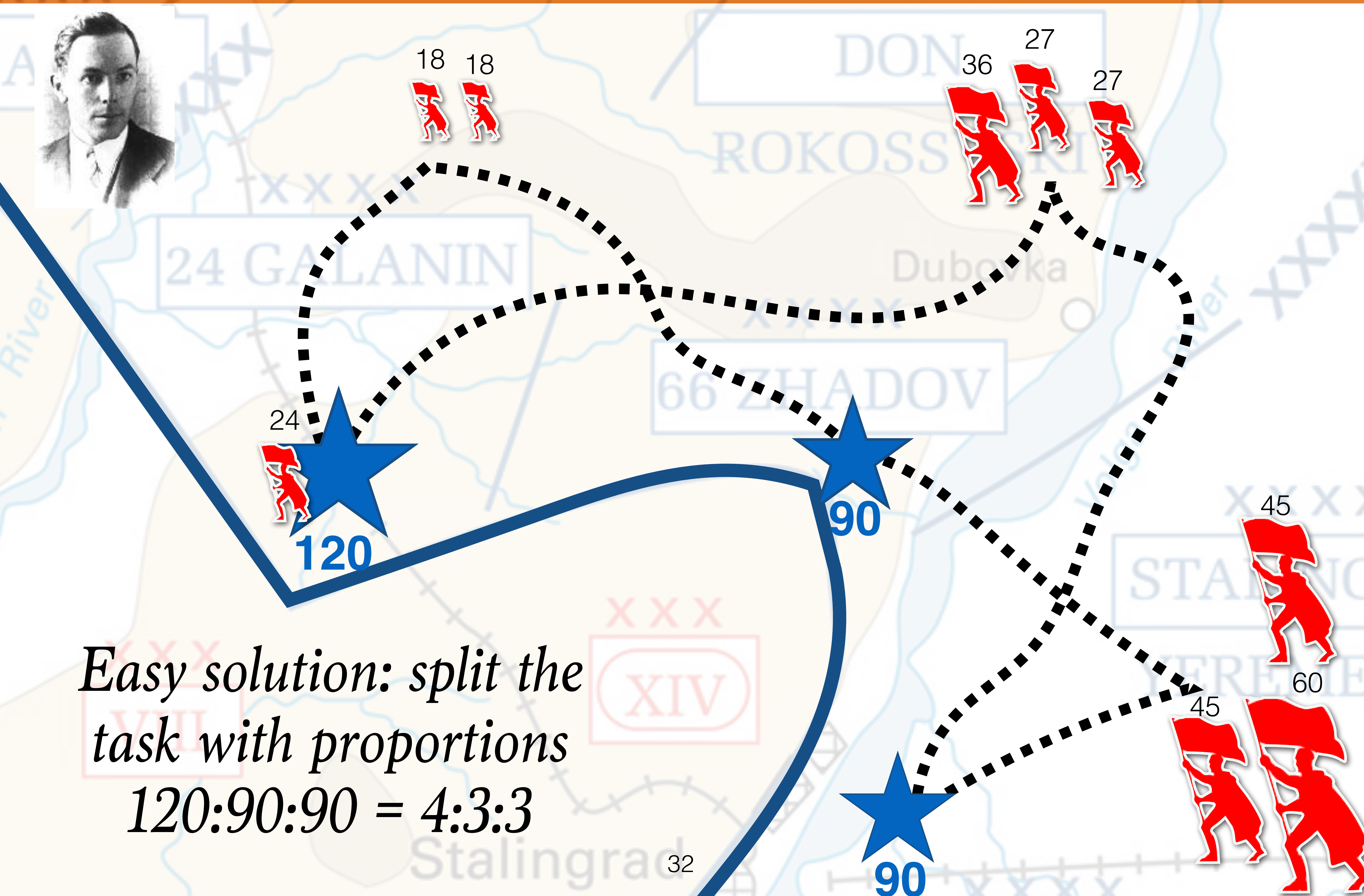


Kantorovich Problem



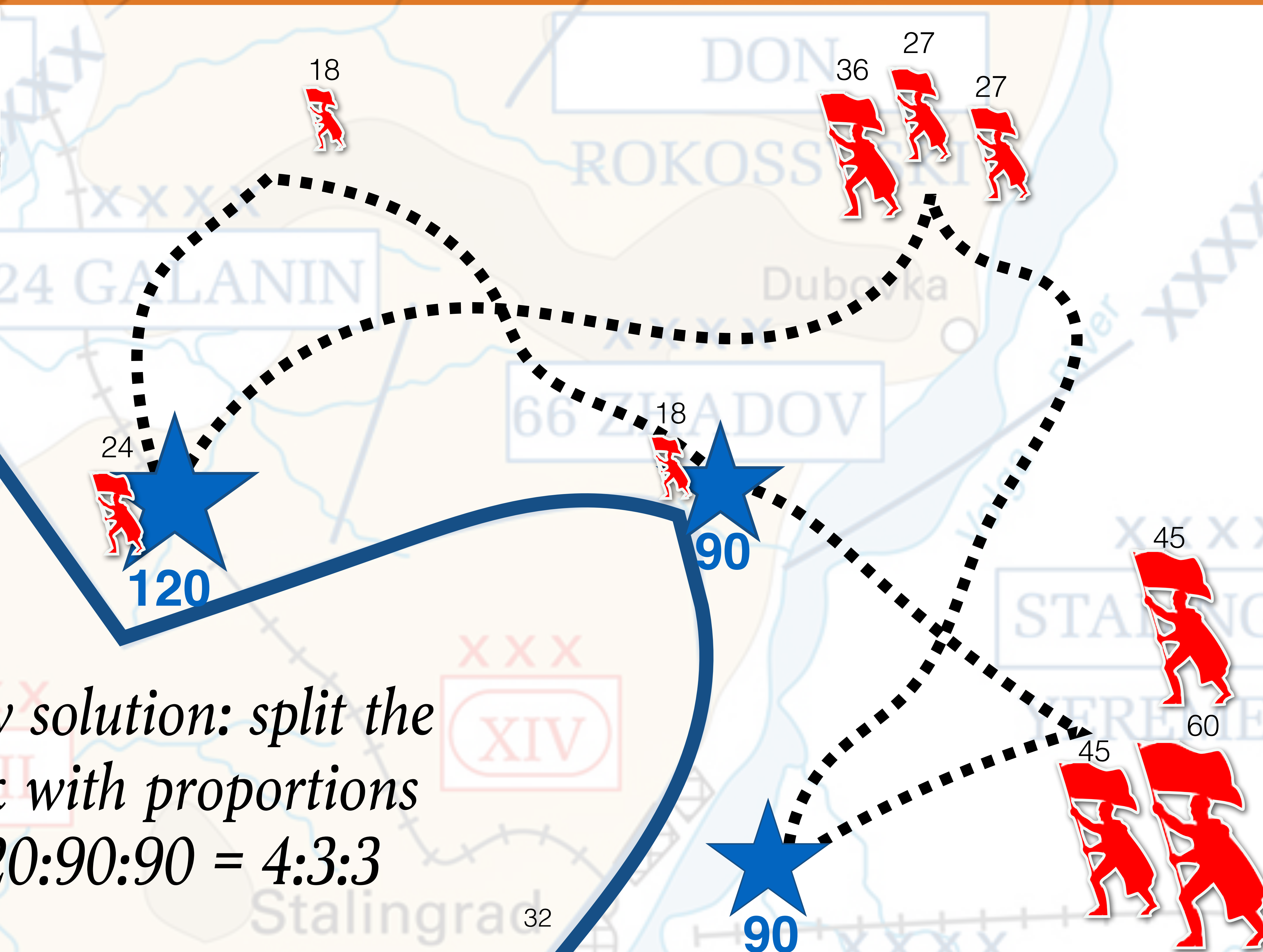
Easy solution: split the task with proportions 120:90:90 = 4:3:3

Kantorovich Problem



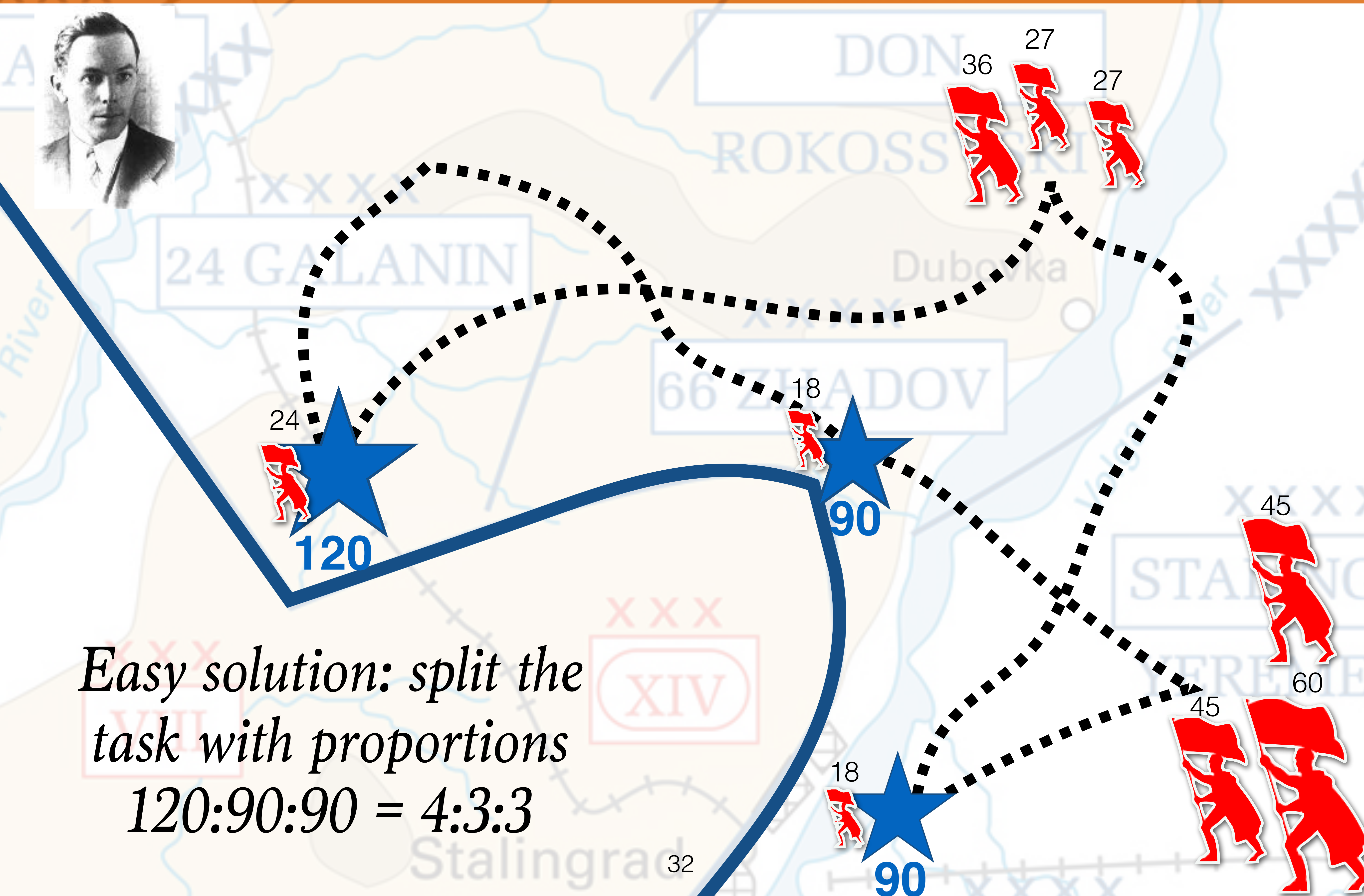
Easy solution: split the task with proportions 120:90:90 = 4:3:3

Kantorovich Problem



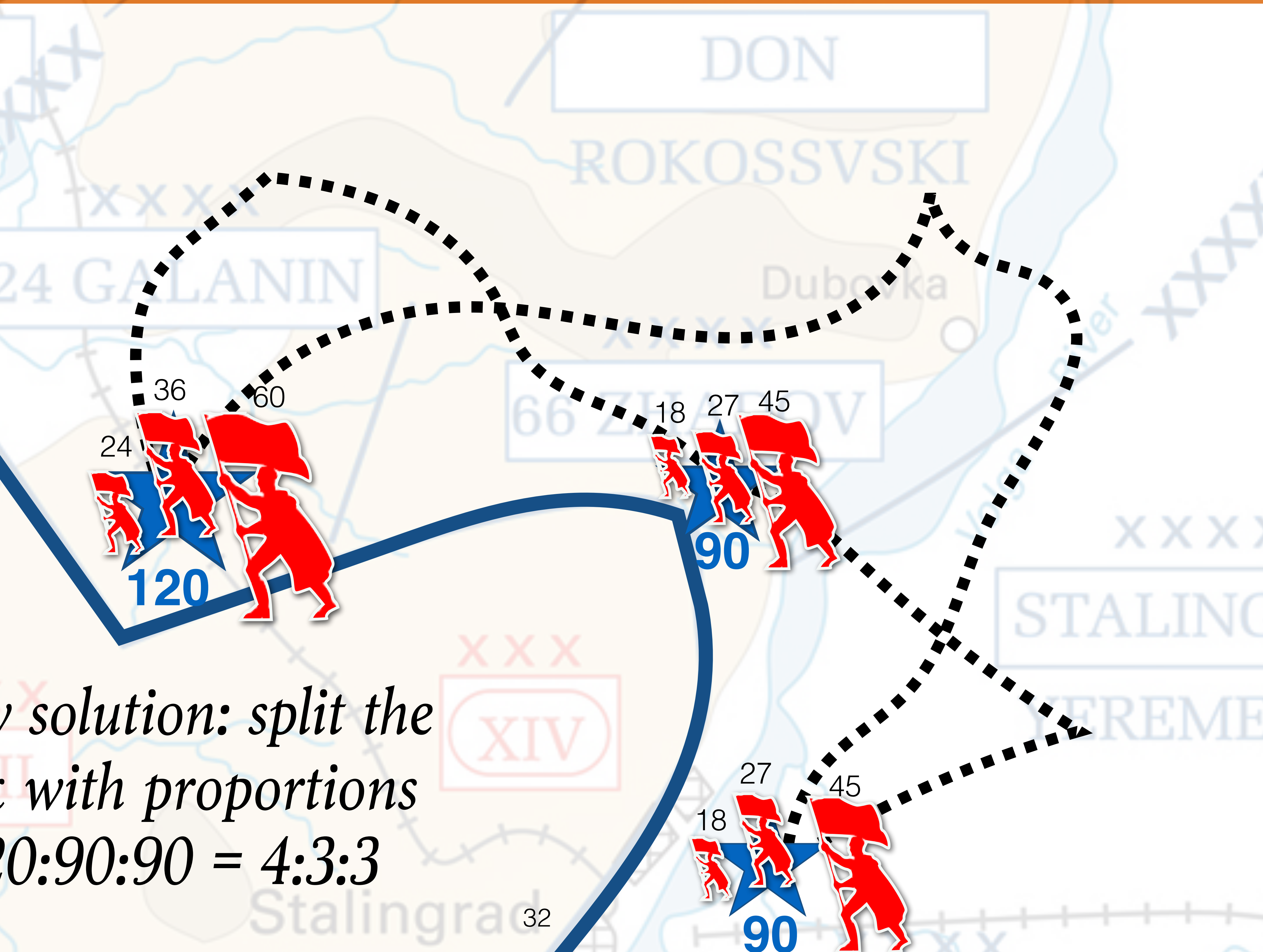
Easy solution: split the task with proportions 120:90:90 = 4:3:3

Kantorovich Problem



Easy solution: split the task with proportions 120:90:90 = 4:3:3

Kantorovich Problem



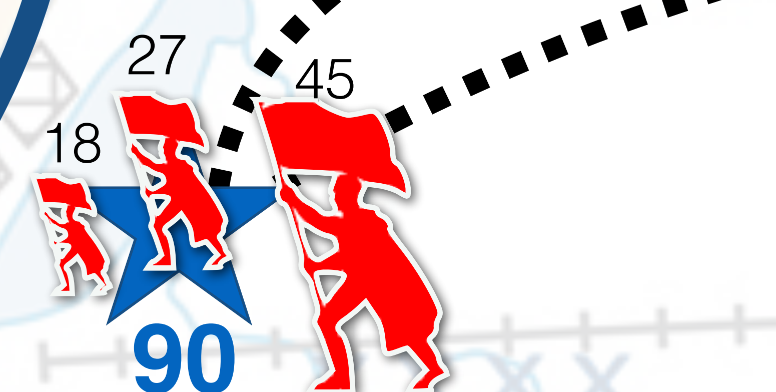
Easy solution: split the task with proportions 120:90:90 = 4:3:3

Kantorovich Problem

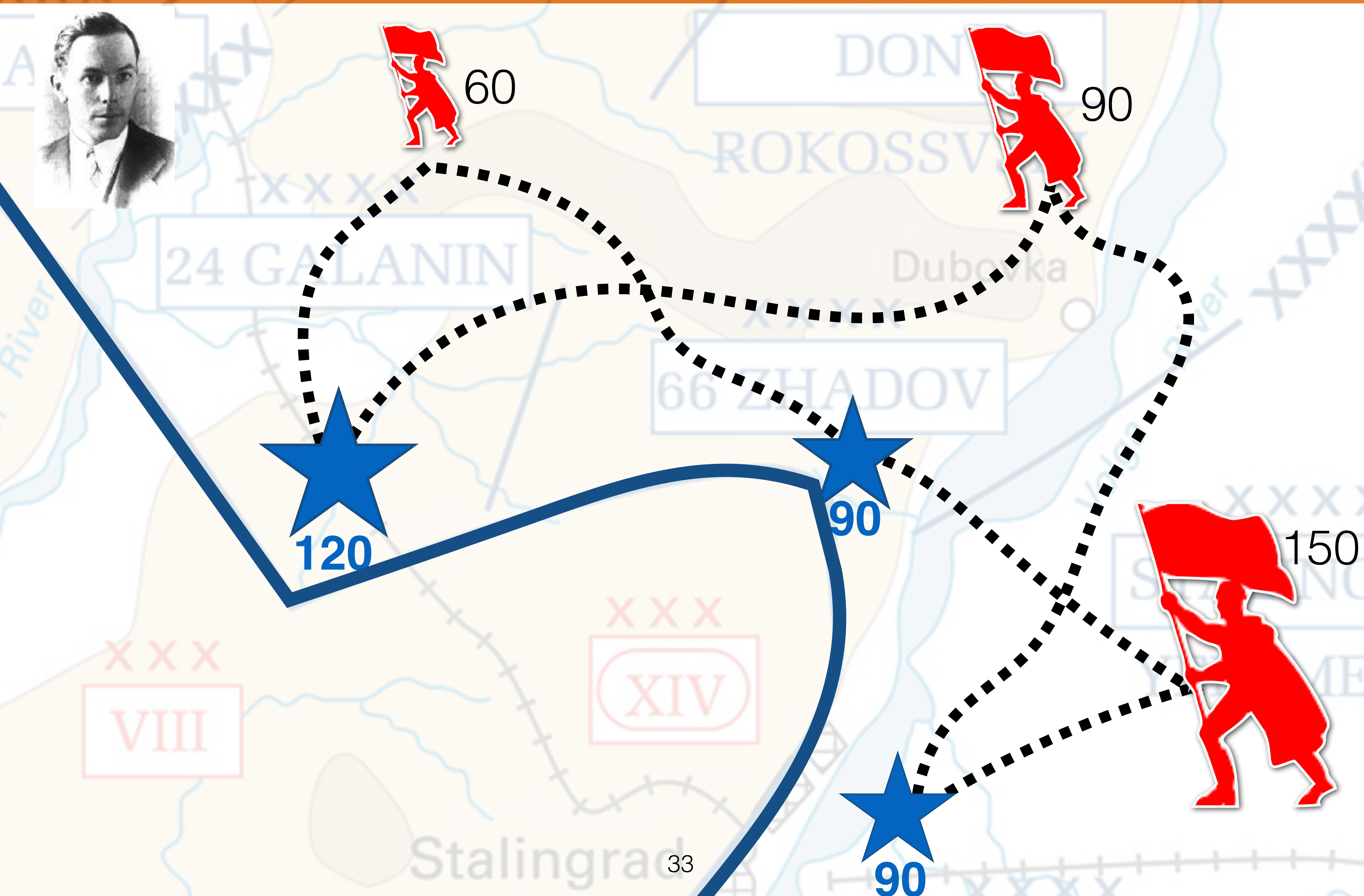
Naive approach results in many displacements...

Can we find a cheaper alternative?

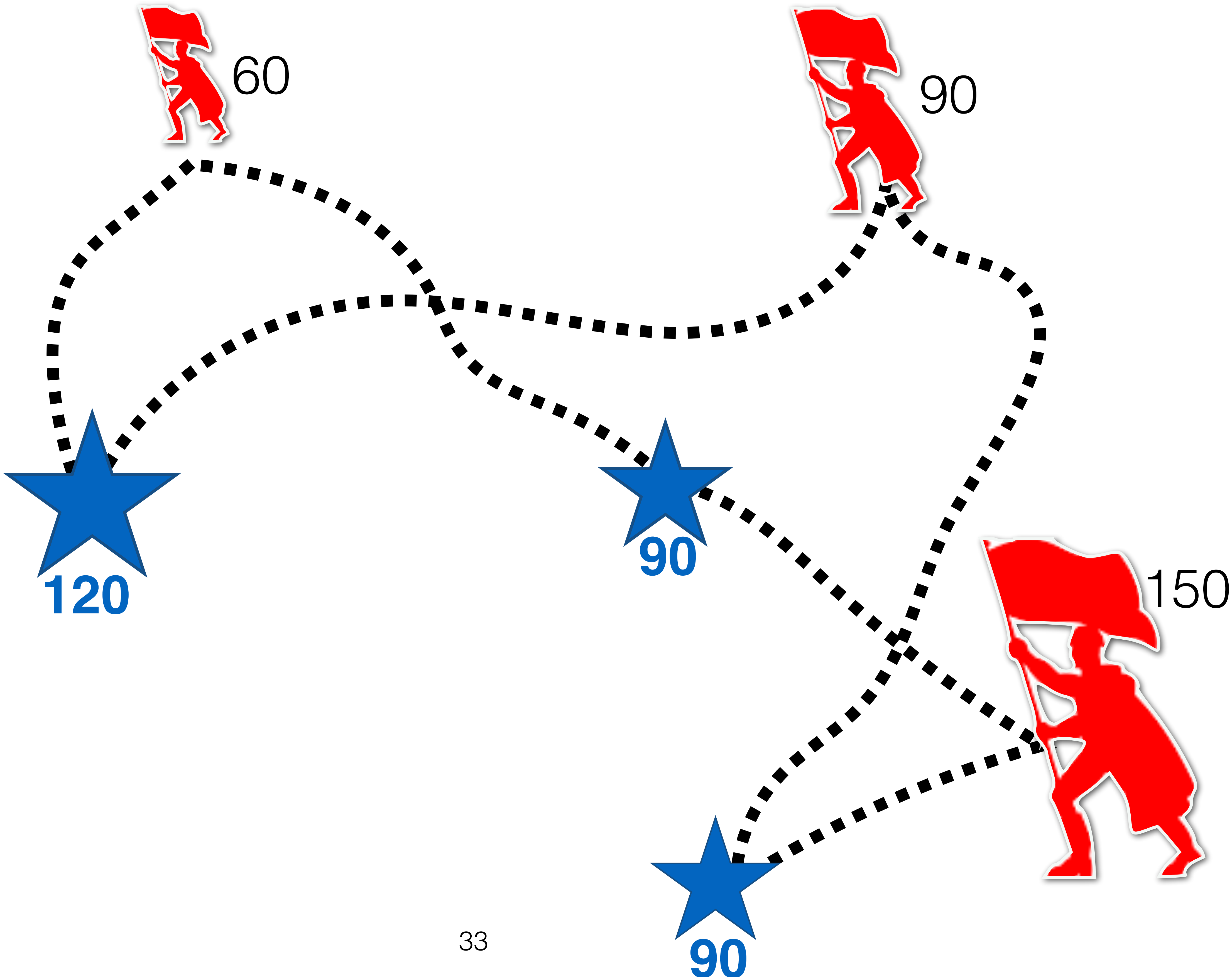
Easy solution: split the task with proportions 120:90:90 = 4:3:3



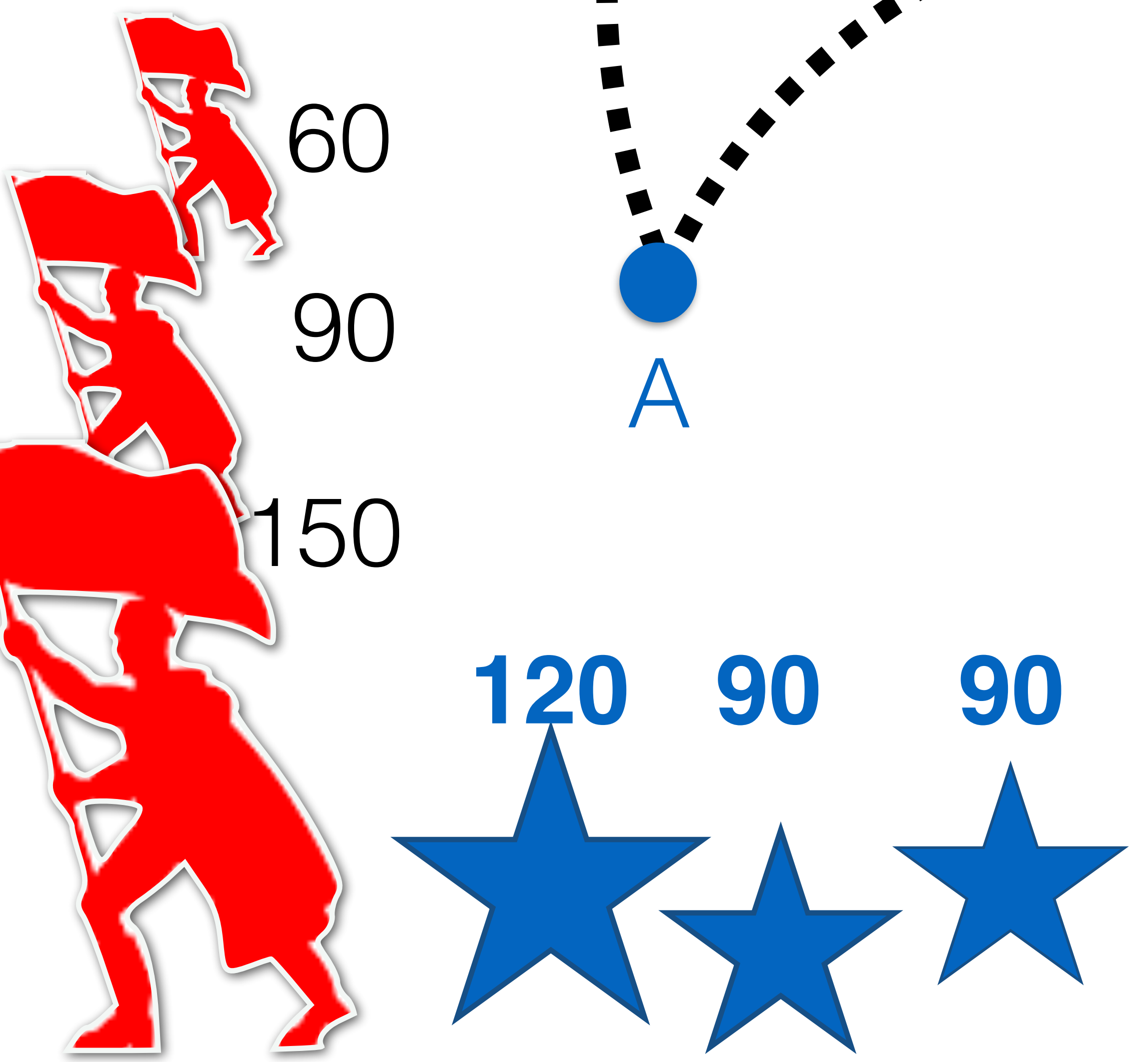
Kantorovich Problem

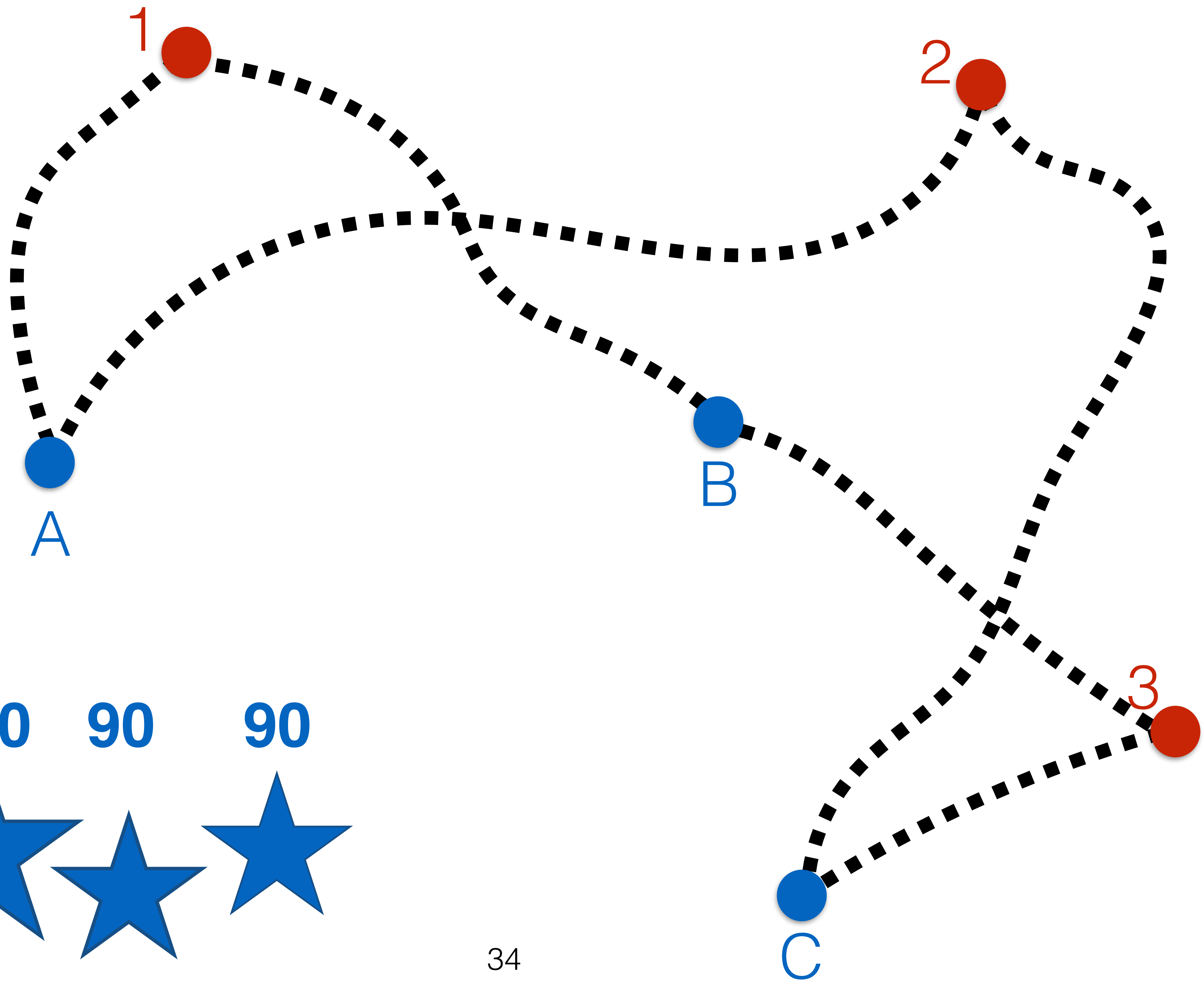


Kantorovich Problem

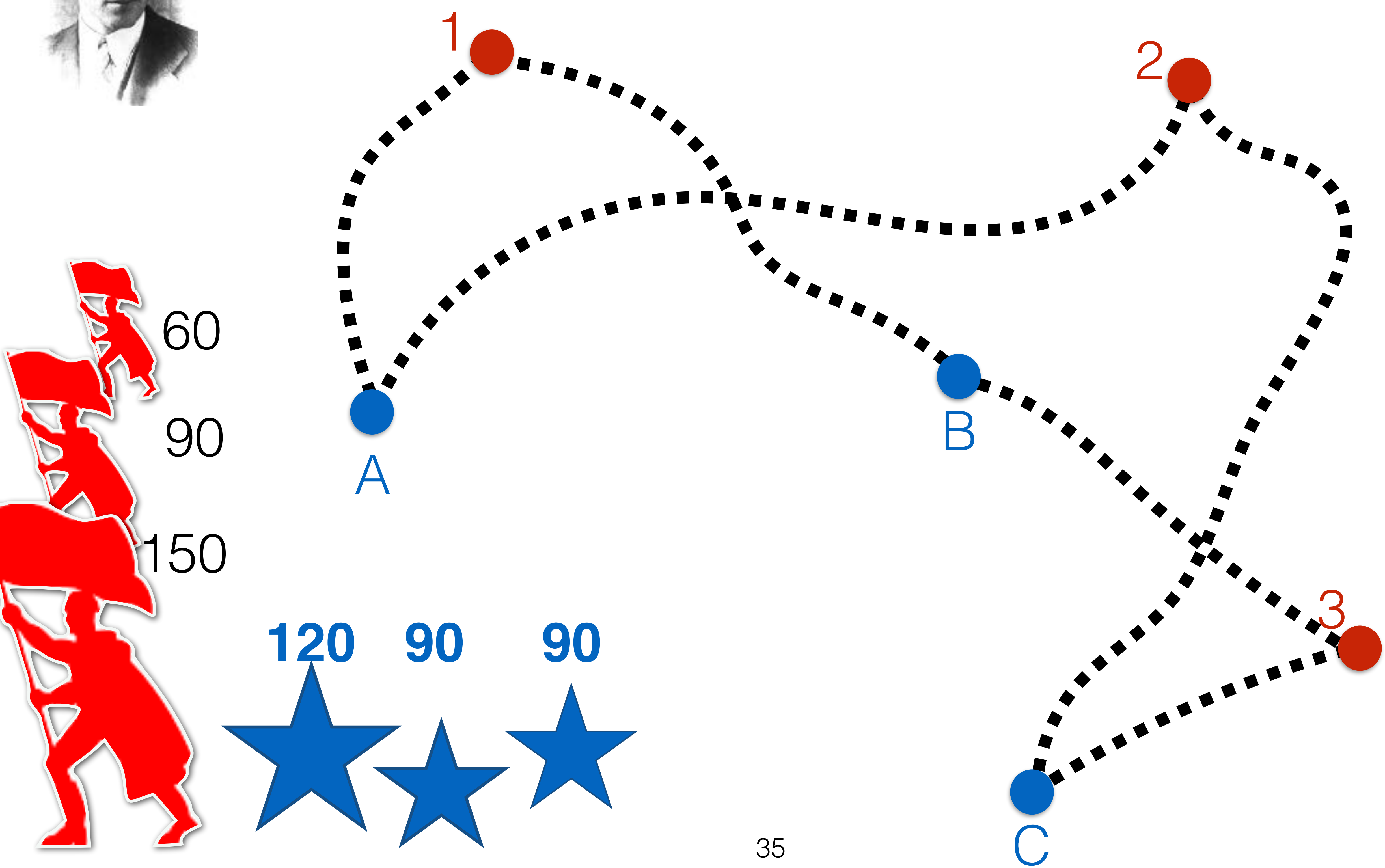


Kantorovich Problem





Kantorovich Problem



Kantorovich Problem

60	?	?	?
90	?	?	?
150	?	?	?
	120	90	90

1	d_{1A}	d_{1B}	d_{1C}
2	d_{2A}	d_{2B}	d_{2C}
3	d_{3A}	d_{3B}	d_{3C}
	A	B	C

Kantorovich Problem

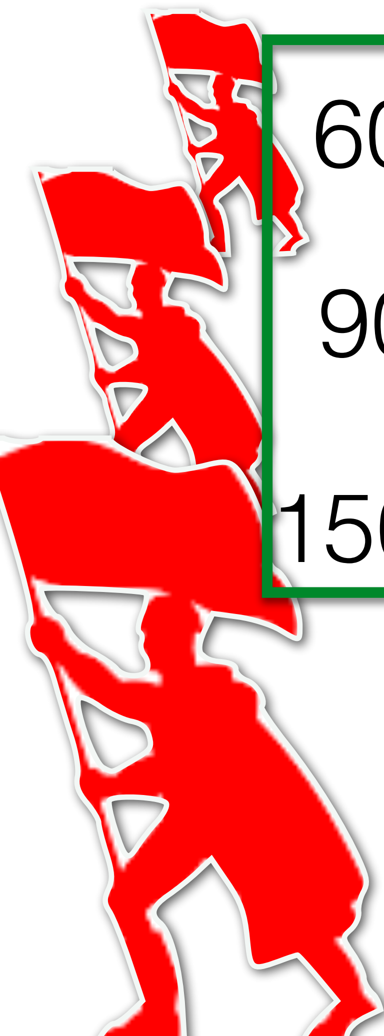
Transportation matrix			
60	?	?	?
90	?	?	?
150	?	?	?
	120	90	90

Distance matrix			
1	d_{1A}	d_{1B}	d_{1C}
2	d_{2A}	d_{2B}	d_{2C}
3	d_{3A}	d_{3B}	d_{3C}
	A	B	C

Kantorovich Problem

The problem is entirely described by **counts** *and a* **cost/distance matrix**

Transportation matrix



60	?	?	?
90	?	?	?
150	?	?	?
	120	90	90

Distance matrix

	A	B	C
1	d_{1A}	d_{1B}	d_{1C}
2	d_{2A}	d_{2B}	d_{2C}
3	d_{3A}	d_{3B}	d_{3C}

Kantorovich Problem

Transportation matrix

60	?	?	?
90	?	?	?
150	?	?	?
	120	**90**	**90**

Distance matrix

1	$d_{\mathbf{1}\mathrm{A}}$	$d_{\mathbf{1}\mathrm{B}}$	$d_{\mathbf{1}\mathrm{C}}$
2	$d_{\mathbf{2}\mathrm{A}}$	$d_{\mathbf{2}\mathrm{B}}$	$d_{\mathbf{2}\mathrm{C}}$
3	$d_{\mathbf{3}\mathrm{A}}$	$d_{\mathbf{3}\mathrm{B}}$	$d_{\mathbf{3}\mathrm{C}}$
	A	B	C

Kantorovich Problem

Transportation matrix

$$\begin{array}{c|c|c|c|}
60 & p_{\mathbf{1}\mathrm{A}} & p_{\mathbf{1}\mathrm{B}} & p_{\mathbf{1}\mathrm{C}} \\
90 & p_{\mathbf{2}\mathrm{A}} & p_{\mathbf{2}\mathrm{B}} & p_{\mathbf{2}\mathrm{C}} \\
150 & p_{\mathbf{3}\mathrm{A}} & p_{\mathbf{3}\mathrm{B}} & p_{\mathbf{3}\mathrm{C}} \\
 & \mathbf{120} & \mathbf{90} & \mathbf{90}
\end{array}$$

Distance matrix

$$\begin{array}{c|c|c|c|}
1 & d_{\mathbf{1}\mathrm{A}} & d_{\mathbf{1}\mathrm{B}} & d_{\mathbf{1}\mathrm{C}} \\
2 & d_{\mathbf{2}\mathrm{A}} & d_{\mathbf{2}\mathrm{B}} & d_{\mathbf{2}\mathrm{C}} \\
3 & d_{\mathbf{3}\mathrm{A}} & d_{\mathbf{3}\mathrm{B}} & d_{\mathbf{3}\mathrm{C}} \\
 & \mathrm{A} & \mathrm{B} & \mathrm{C}
\end{array}$$

Kantorovich Problem

Transportation matrix

$$\begin{array}{c|c|c|c|}
\hline
a_1 & p_{1A} & p_{1B} & p_{1C} \\
\hline
a_2 & p_{2A} & p_{2B} & p_{2C} \\
\hline
a_3 & p_{3A} & p_{3B} & p_{3C} \\
\hline
\multicolumn{1}{c}{} & \multicolumn{1}{c}{b_A} & \multicolumn{1}{c}{b_B} & \multicolumn{1}{c}{b_C}
\end{array}$$

Distance matrix

$$\begin{array}{c|c|c|c|}
\hline
1 & d_{1A} & d_{1B} & d_{1C} \\
\hline
2 & d_{2A} & d_{2B} & d_{2C} \\
\hline
3 & d_{3A} & d_{3B} & d_{3C} \\
\hline
\multicolumn{1}{c}{} & \multicolumn{1}{c}{A} & \multicolumn{1}{c}{B} & \multicolumn{1}{c}{C}
\end{array}$$

Kantorovich Problem

Transportation matrix

$$\begin{array}{c|c|c|c|}
a_1 & p_{1A} & p_{1B} & p_{1C} \\
a_2 & p_{2A} & p_{2B} & p_{2C} \\
a_3 & p_{3A} & p_{3B} & p_{3C} \\
 & b_A & b_B & b_C
\end{array}$$

Distance matrix

$$\begin{array}{c|c|c|c|}
1 & d_{1A} & d_{1B} & d_{1C} \\
2 & d_{2A} & d_{2B} & d_{2C} \\
3 & d_{3A} & d_{3B} & d_{3C} \\
 & \mathrm{A} & \mathrm{B} & \mathrm{C}
\end{array}$$

Constraints

$$\forall i \in \{1,2,3\}, \sum_{j \in \{A,B,C\}} p_{ij} = a_i$$

$$\forall j \in \{A,B,C\}, \sum_{i \in \{1,2,3\}} p_{ij} = b_j$$

$$p_{ij} \geq 0$$

Kantorovich Problem

Transportation matrix

a_1	$p_{1\mathrm{A}}$	$p_{1\mathrm{B}}$	$p_{1\mathrm{C}}$
a_2	$p_{2\mathrm{A}}$	$p_{2\mathrm{B}}$	$p_{2\mathrm{C}}$
a_3	$p_{3\mathrm{A}}$	$p_{3\mathrm{B}}$	$p_{3\mathrm{C}}$
	b_{A}	b_{B}	b_{C}

Distance matrix

1	$d_{1\mathrm{A}}$	$d_{1\mathrm{B}}$	$d_{1\mathrm{C}}$
2	$d_{2\mathrm{A}}$	$d_{2\mathrm{B}}$	$d_{2\mathrm{C}}$
3	$d_{3\mathrm{A}}$	$d_{3\mathrm{B}}$	$d_{3\mathrm{C}}$
	A	B	C

Constraints

$$\forall i \in \{1,2,3\}, \quad \sum_{j \in \{\mathrm{A},\mathrm{B},\mathrm{C}\}} p_{ij} = a_i$$

$$\forall j \in \{\mathrm{A},\mathrm{B},\mathrm{C}\}, \quad \sum_{i \in \{1,2,3\}} p_{ij} = b_j$$

$$p_{ij} \geq 0$$

Cost function

$$C(\boldsymbol{P}) = \sum_{j \in \{\mathrm{A},\mathrm{B},\mathrm{C}\}} \sum_{i \in \{1,2,3\}} p_{ij} d_{ij}$$

Kantorovich Problem

Transportation matrix

$$\begin{array}{c|c|c|c|}
\cline{2-4}
a_1 & p_{1A} & p_{1B} & p_{1C} \\
\cline{2-4}
a_2 & p_{2A} & p_{2B} & p_{2C} \\
\cline{2-4}
a_3 & p_{3A} & p_{3B} & p_{3C} \\
\cline{2-4}
\multicolumn{1}{c}{} & \multicolumn{1}{c}{b_A} & \multicolumn{1}{c}{b_B} & \multicolumn{1}{c}{b_C}
\end{array}$$

Distance matrix

$$\begin{array}{c|c|c|c|}
\cline{2-4}
1 & d_{1A} & d_{1B} & d_{1C} \\
\cline{2-4}
2 & d_{2A} & d_{2B} & d_{2C} \\
\cline{2-4}
3 & d_{3A} & d_{3B} & d_{3C} \\
\cline{2-4}
\multicolumn{1}{c}{} & \multicolumn{1}{c}{\text{A}} & \multicolumn{1}{c}{\text{B}} & \multicolumn{1}{c}{\text{C}}
\end{array}$$

Constraints

$$\forall i \in \{1,2,3\}, \quad \sum_{j \in \{A,B,C\}} p_{ij} = a_i$$

$$\forall j \in \{A,B,C\}, \quad \sum_{i \in \{1,2,3\}} p_{ij} = b_j$$

$$p_{ij} \geq 0$$

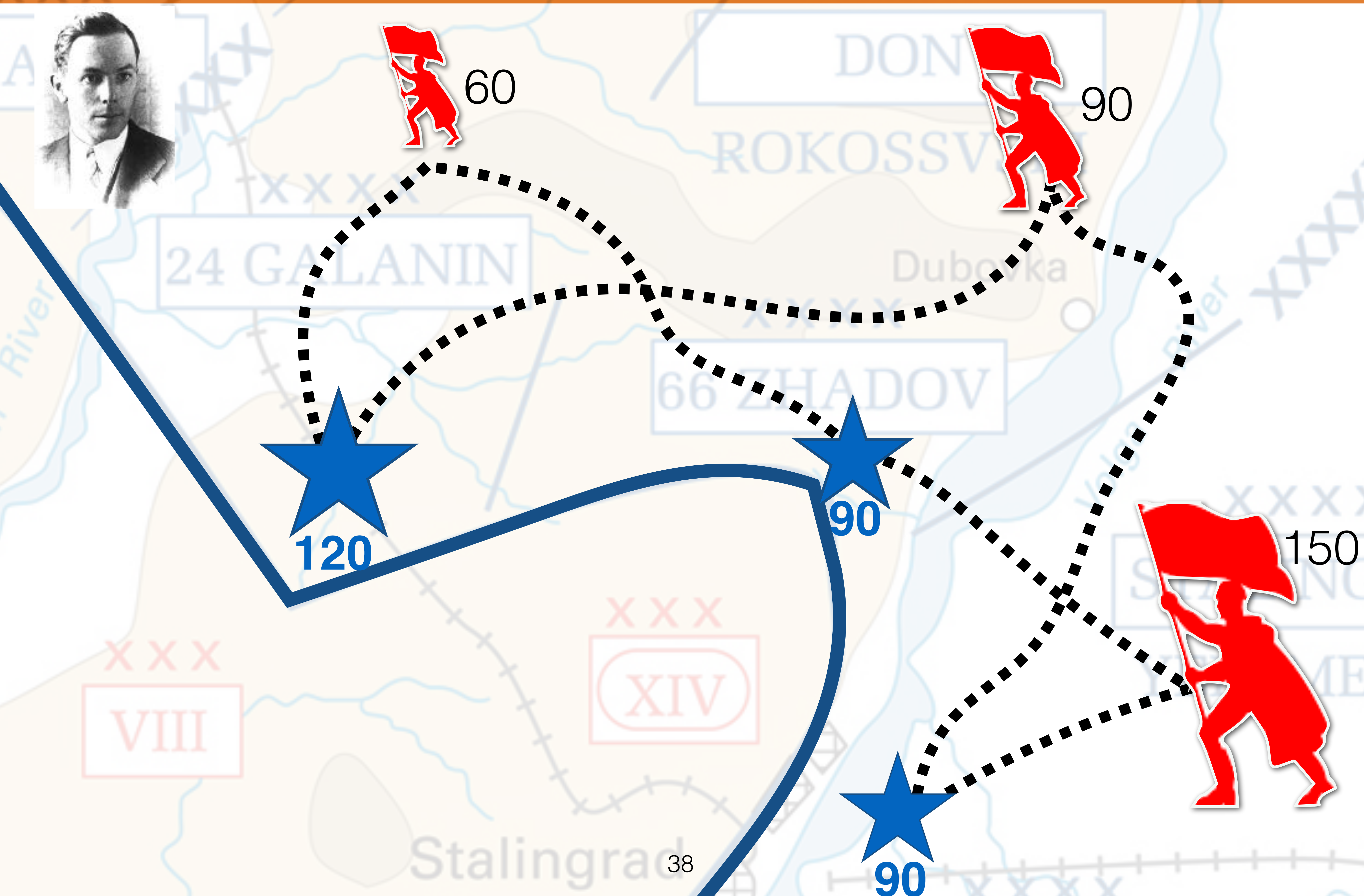
Cost function

$$C(P) = \sum_{j \in \{A,B,C\}} \sum_{i \in \{1,2,3\}} p_{ij} d_{ij}$$

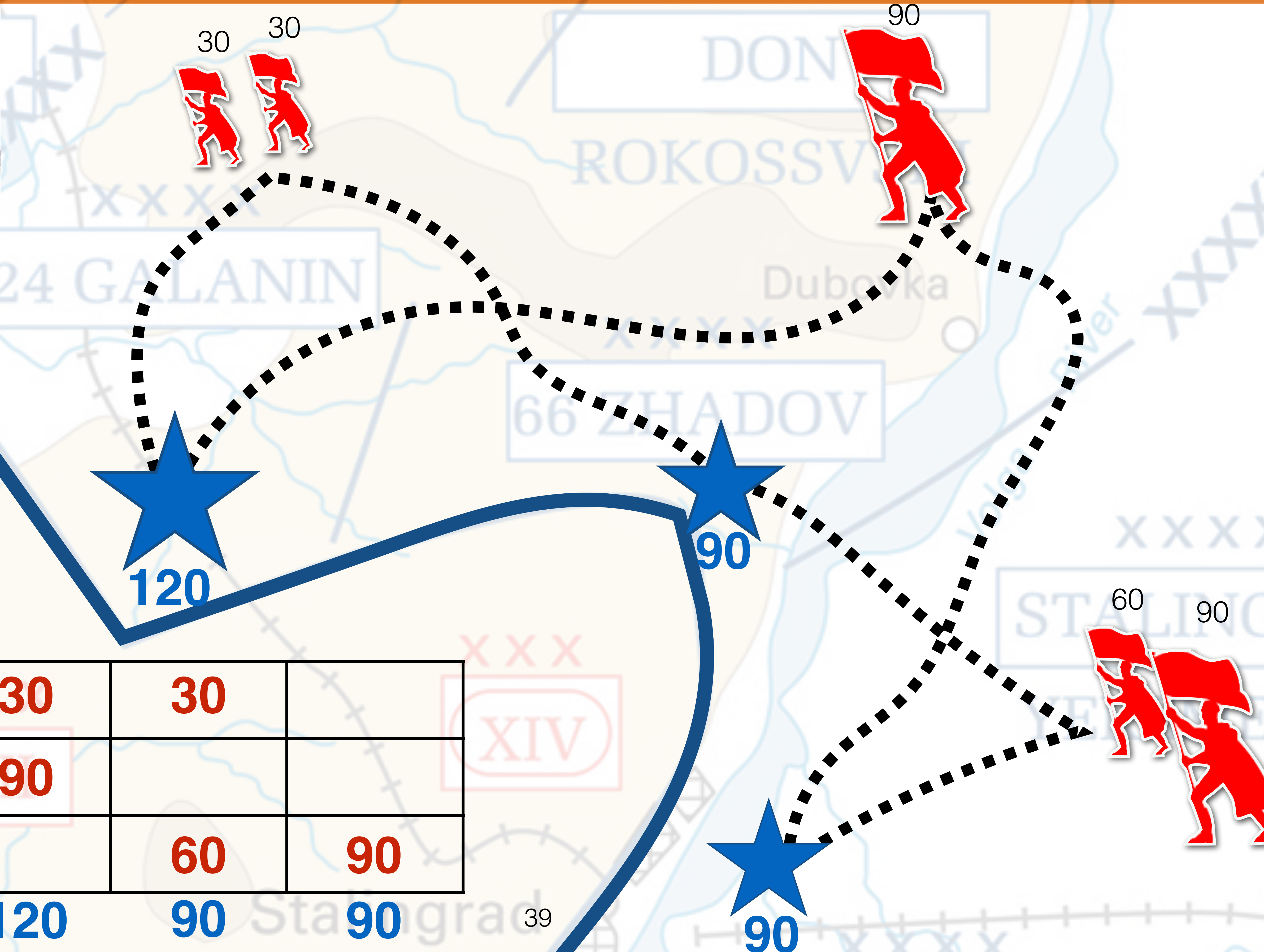
Problem

$$\min_{\text{all valid } P} C(P)$$

Kantorovich Problem

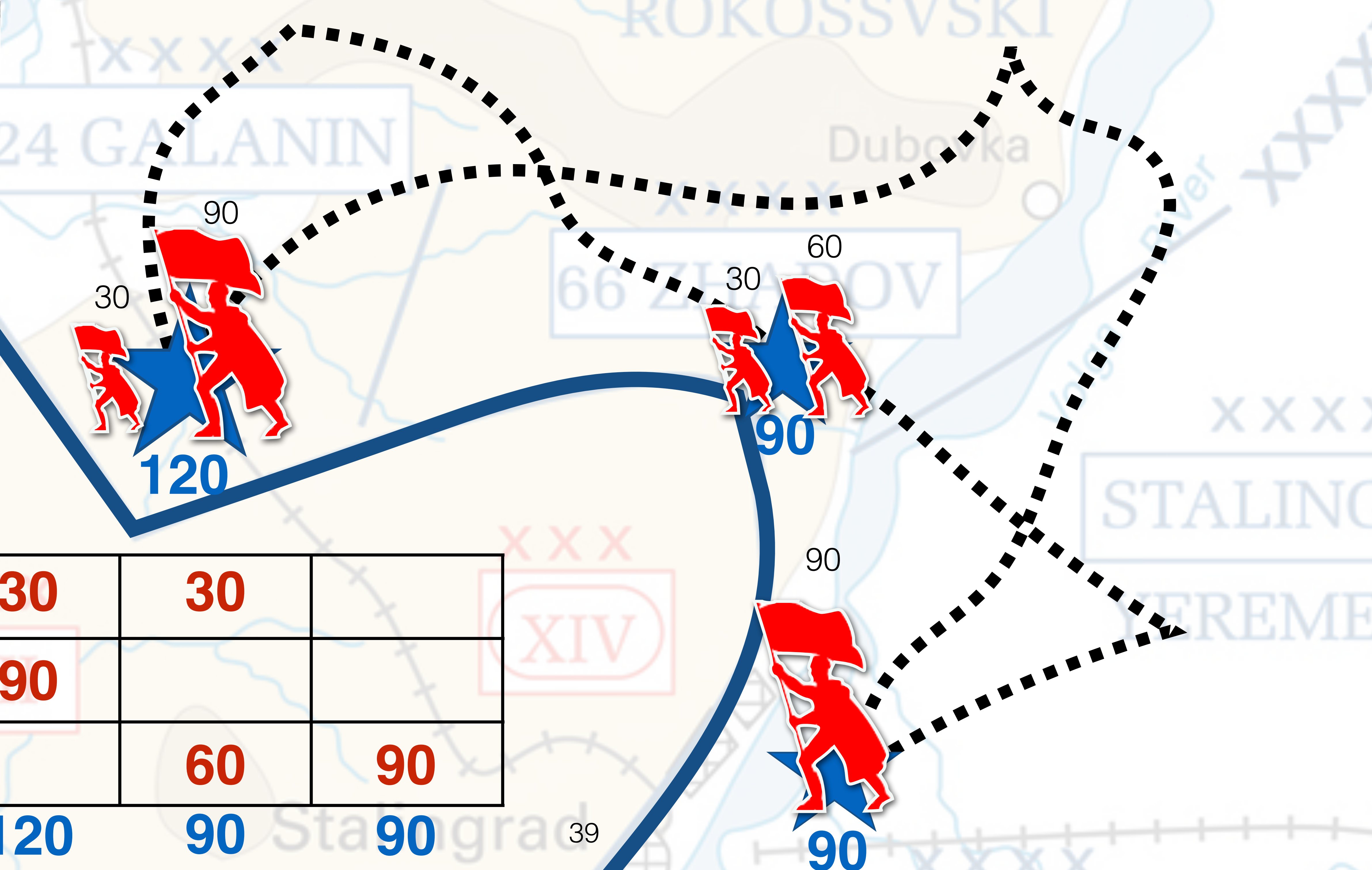


Kantorovich Problem



60	30	30	
90	90		
150		60	90
	120	90	90

Kantorovich Problem



60	30	30	
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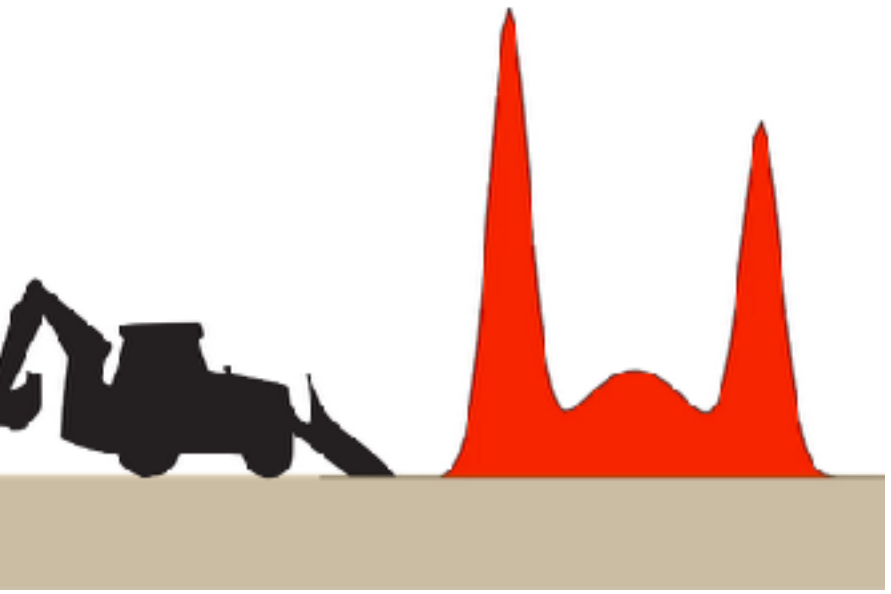
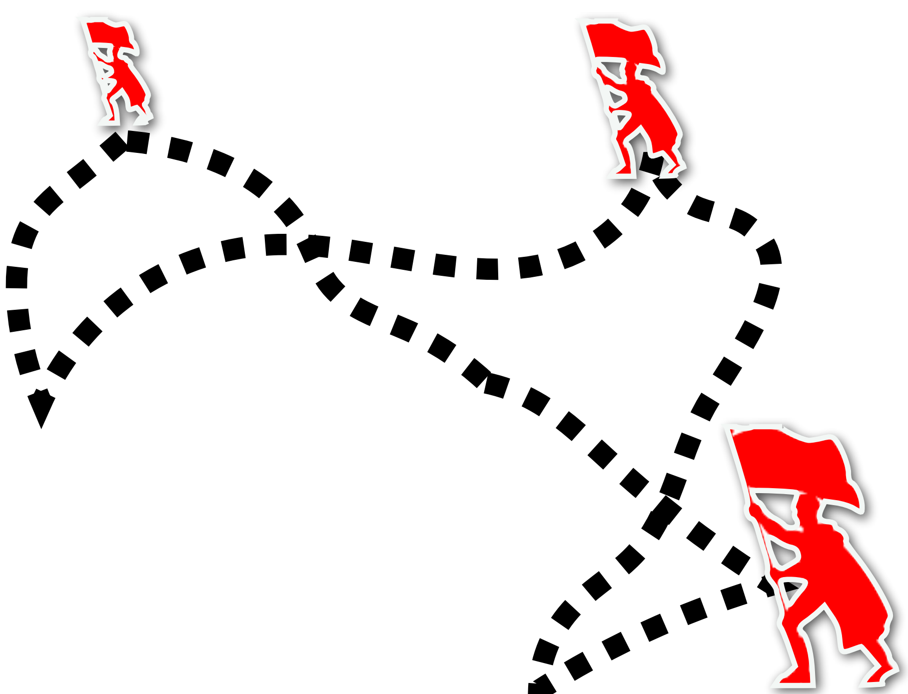
150		60	90
	120	90	90

Mathematical Formalism

These problems involve discrete and continuous **probability measures** on a geometric space Ω

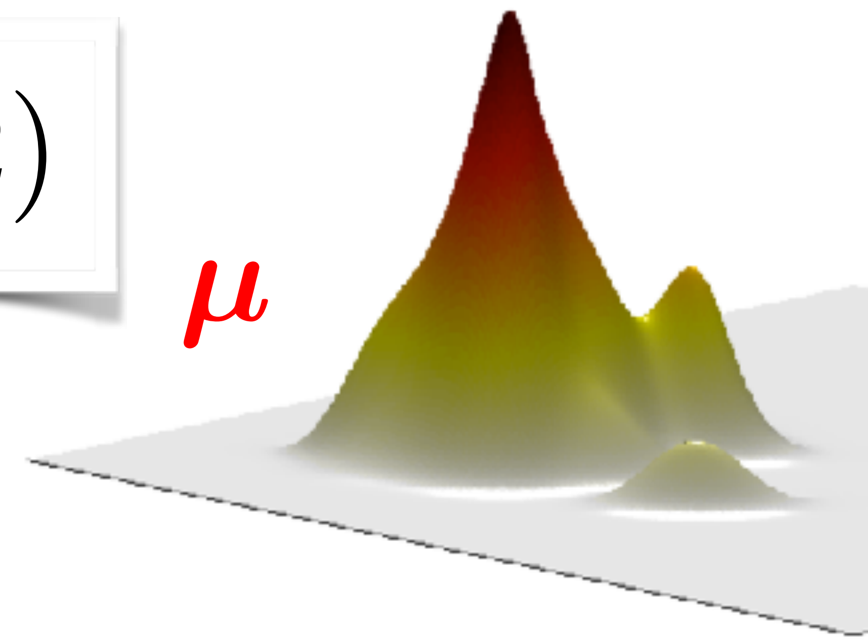




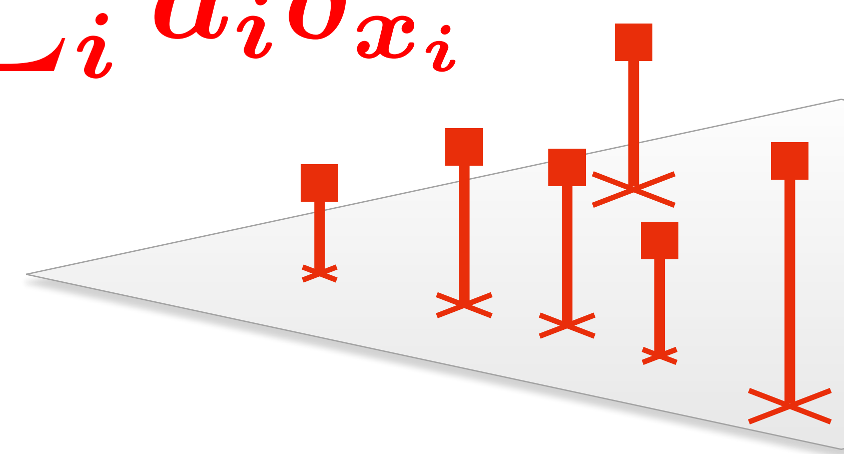
$\longmapsto$

$\mathcal{P}(\Omega)$

$\boldsymbol{\mu}$



$\sum_i a_i \delta_{x_i}$

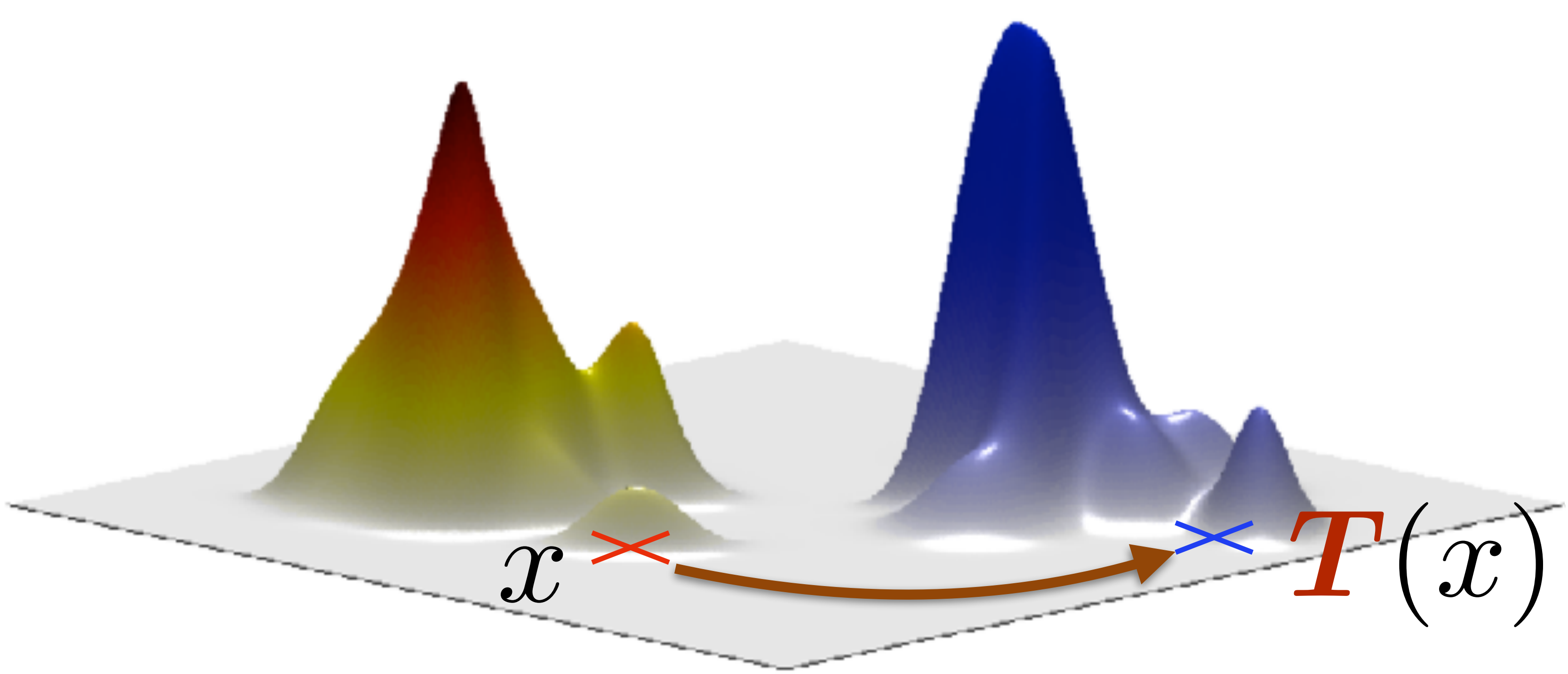


Monge Problem

Ω a measurable space, $\boldsymbol{c} : \Omega \times \Omega \to \mathbb{R}$.
$\boldsymbol{\mu}, \boldsymbol{\nu}$ two probability measures in $\mathcal{P}(\Omega)$.

[Monge'81] problem: find a map $\boldsymbol{T} : \Omega \to \Omega$

$$\inf_{\boldsymbol{T}_\sharp \boldsymbol{\mu} = \boldsymbol{\nu}} \int_\Omega \boldsymbol{c}(x, \boldsymbol{T}(x)) \boldsymbol{\mu}(dx)$$



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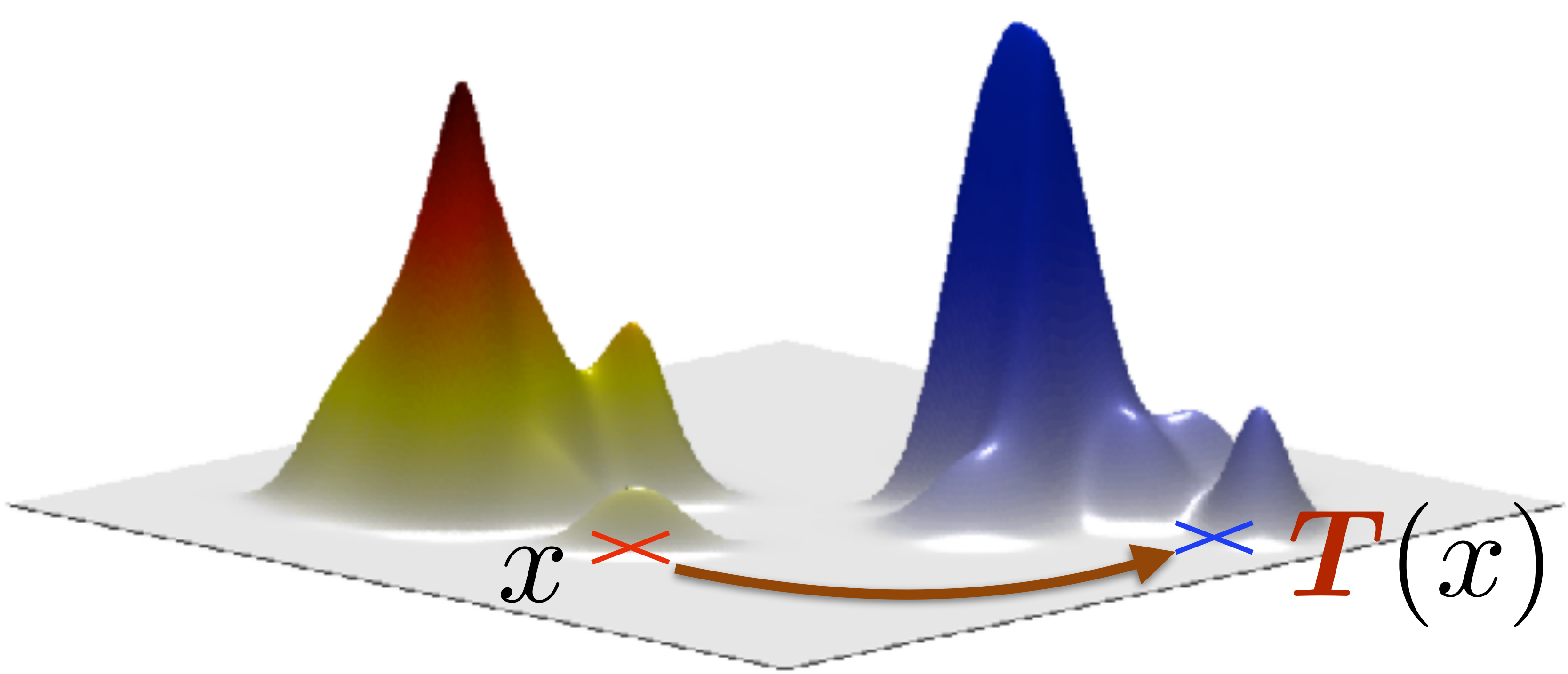
[Brenier'87] If $\Omega = \mathbb{R}^d$, $\boldsymbol{c} = \|\cdot - \cdot\|^2$,
$\boldsymbol{\mu}, \boldsymbol{\nu}$ a.c., then $\boldsymbol{T} = \nabla \boldsymbol{u}$, $\boldsymbol{u}$ **convex**.



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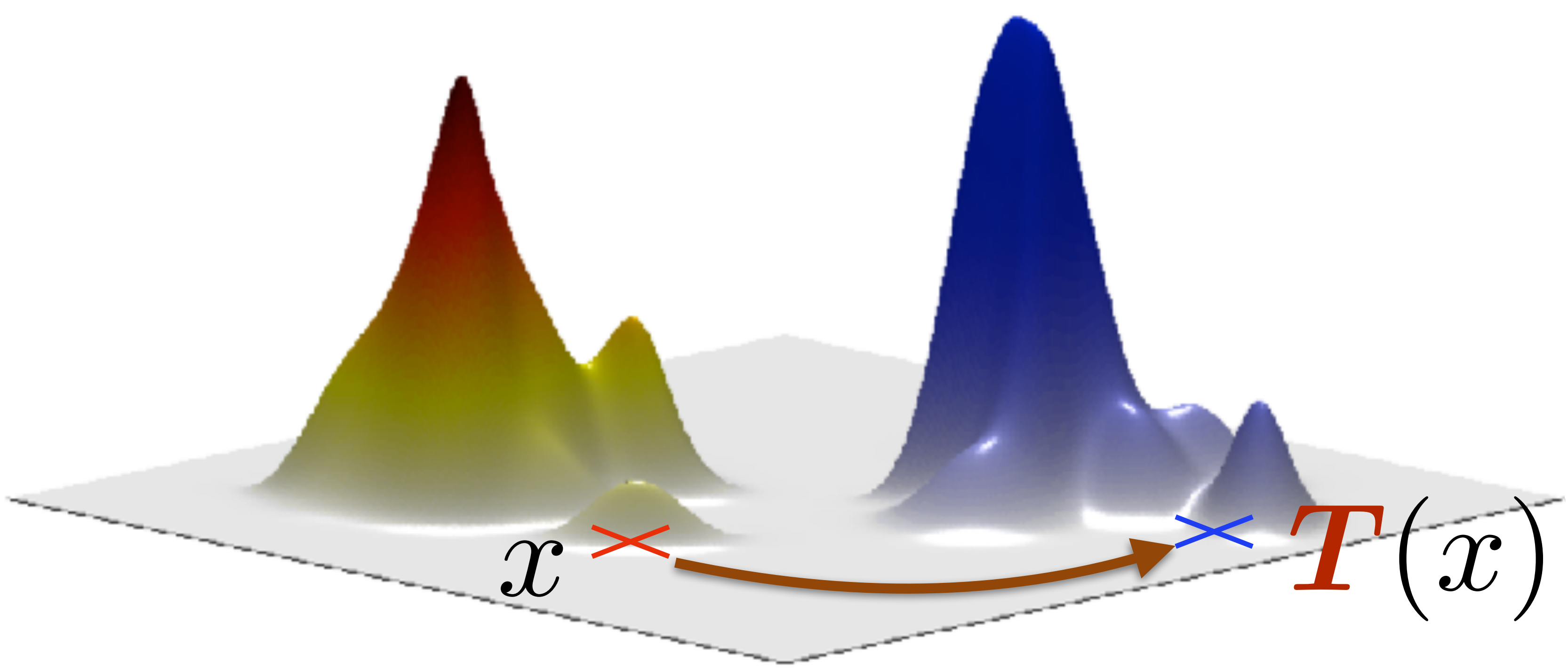

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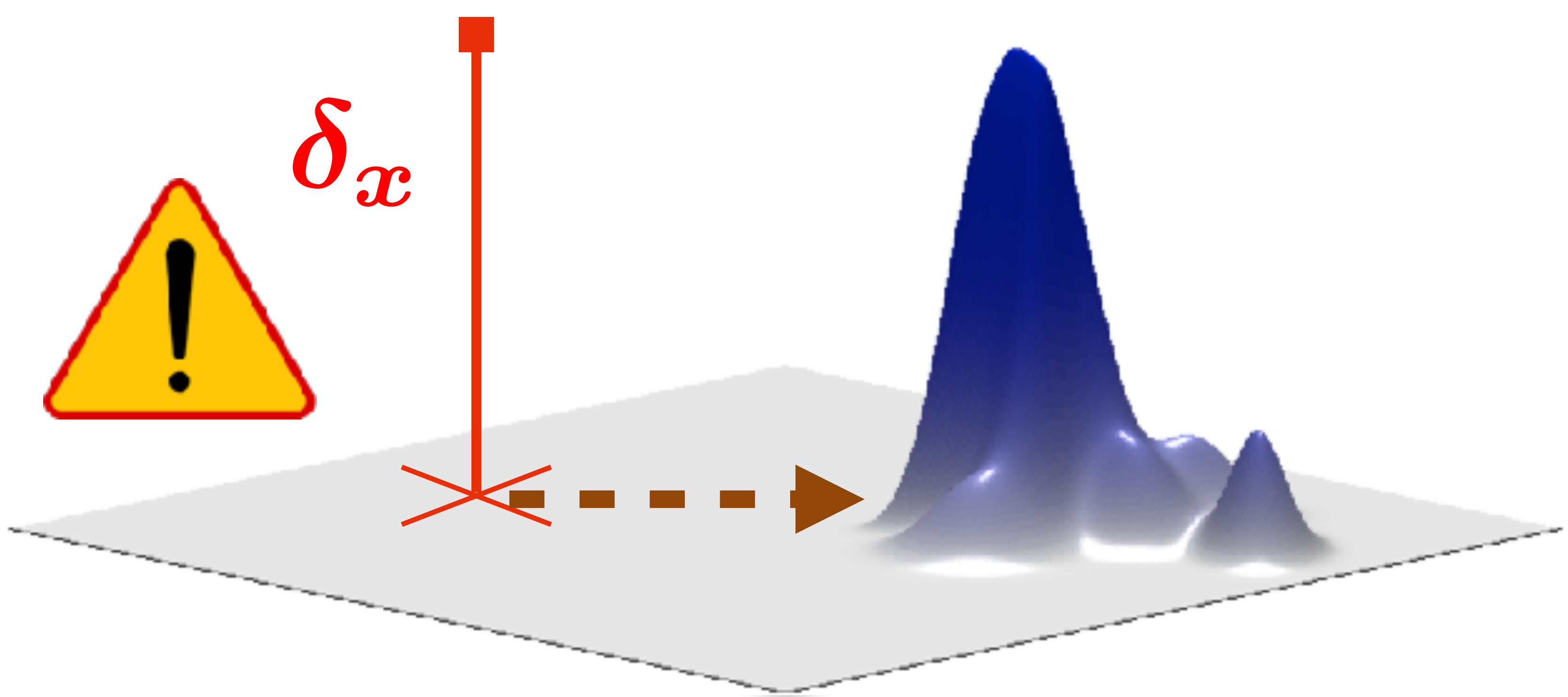
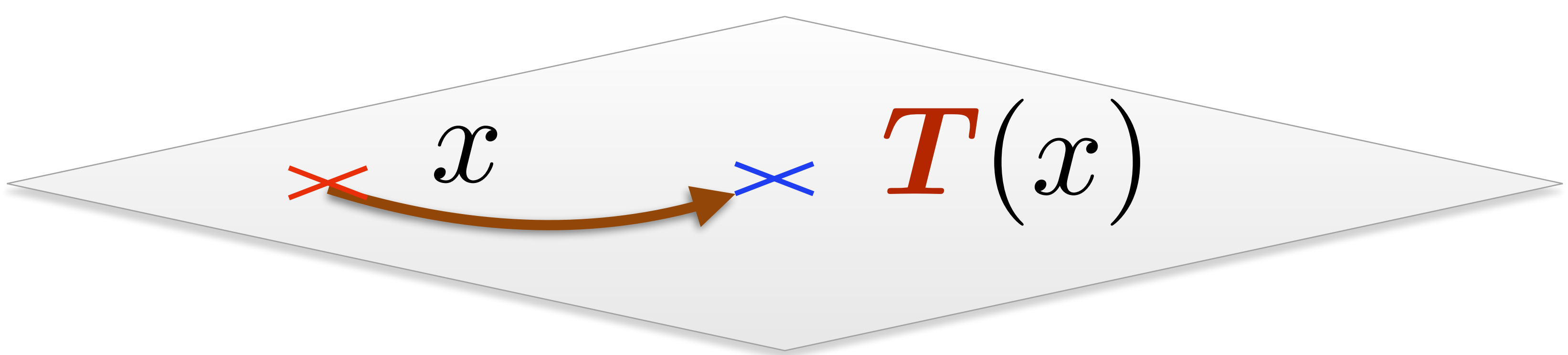


Kantorovich Relaxation

Instead of maps $\boldsymbol{T} : \Omega \rightarrow \Omega$,

consider probabilistic maps,

i.e. **couplings** $\boldsymbol{P} \in \mathcal{P}(\Omega \times \Omega)$:



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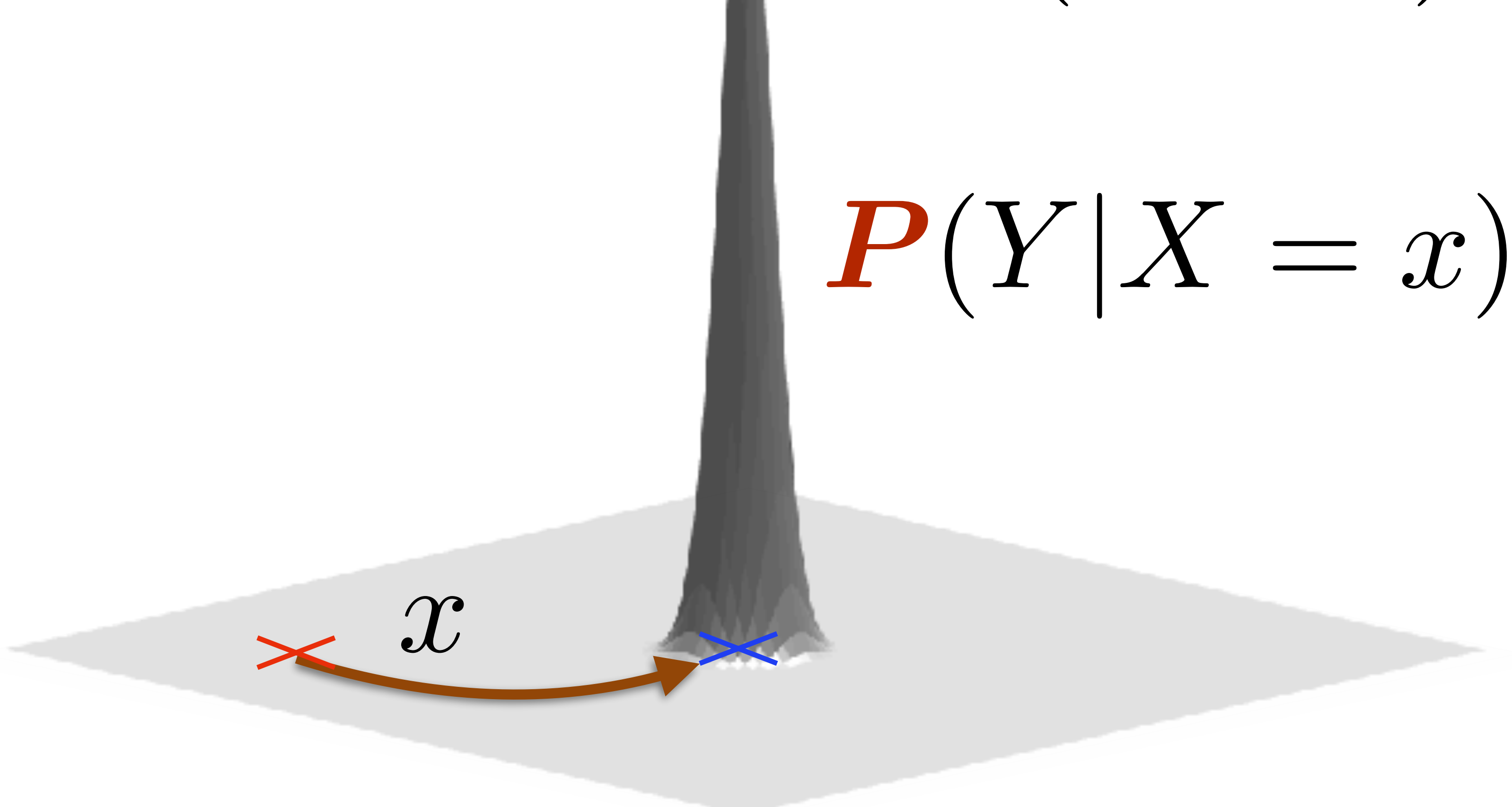

$$\boldsymbol{P}(Y|X = x)$$

Kantorovich Relaxation

Instead of maps $\boldsymbol{T} : \Omega \to \Omega$,

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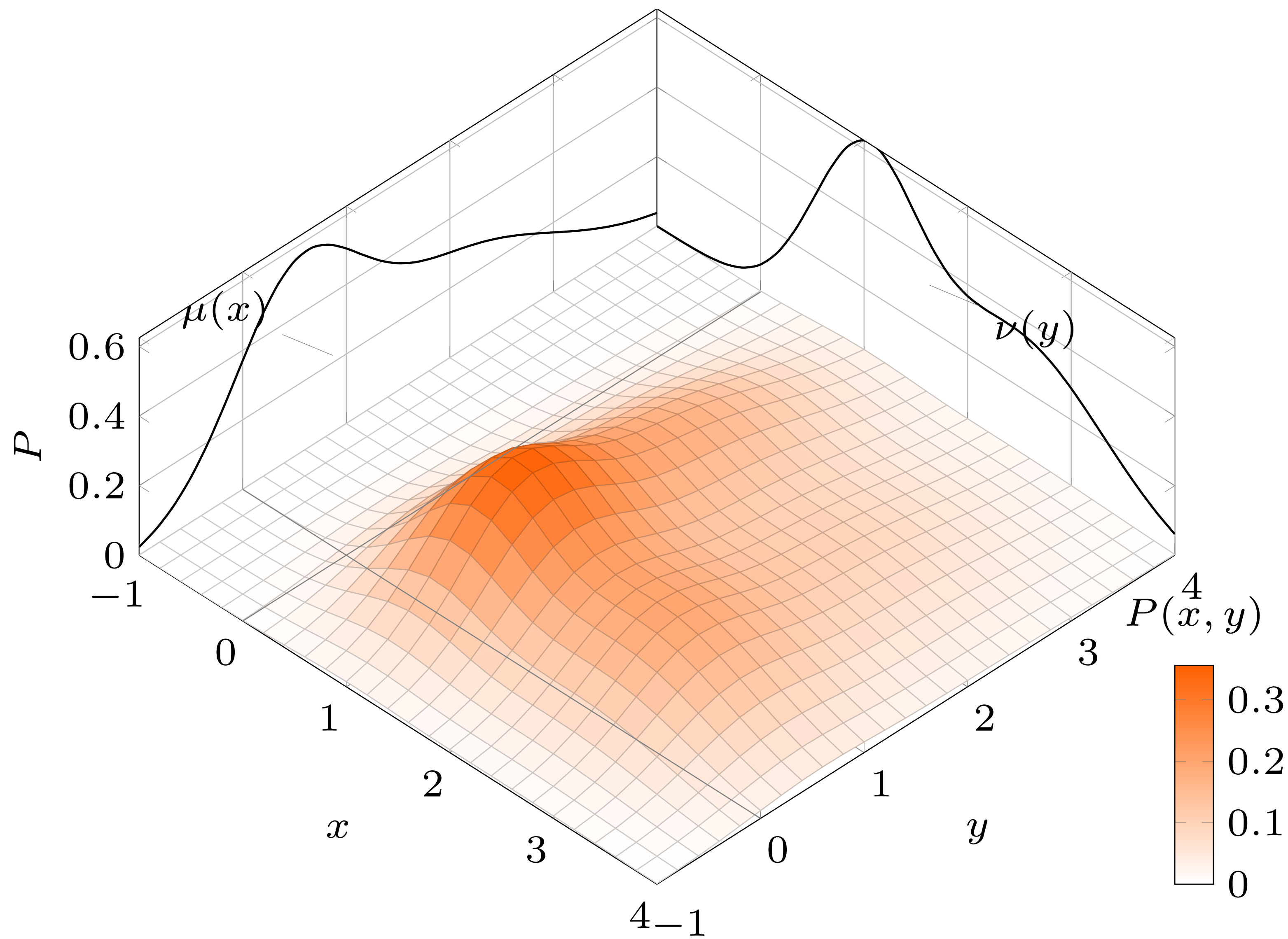
i.e. **couplings** $\boldsymbol{P} \in \mathcal{P}(\Omega \times \Omega)$:

$$\Pi(\boldsymbol{\mu}, \boldsymbol{\nu}) \stackrel{\text{def}}{=} \{\boldsymbol{P} \in \mathcal{P}(\Omega \times \Omega) | \forall \boldsymbol{A}, \boldsymbol{B} \subset \Omega,$$
$$\boldsymbol{P}(\boldsymbol{A} \times \Omega) = \boldsymbol{\mu}(\boldsymbol{A}),$$
$$\boldsymbol{P}(\Omega \times \boldsymbol{B}) = \boldsymbol{\nu}(\boldsymbol{B})\}$$

Kantorovich Relaxation

$$\Pi(\mu, \nu) \stackrel{\text{def}}{=} \{ P \in \mathcal{P}(\Omega \times \Omega) | \forall A, B \subset \Omega, \; P(A \times \Omega) = \mu(A), P(\Omega \times B) = \nu(B) \}$$



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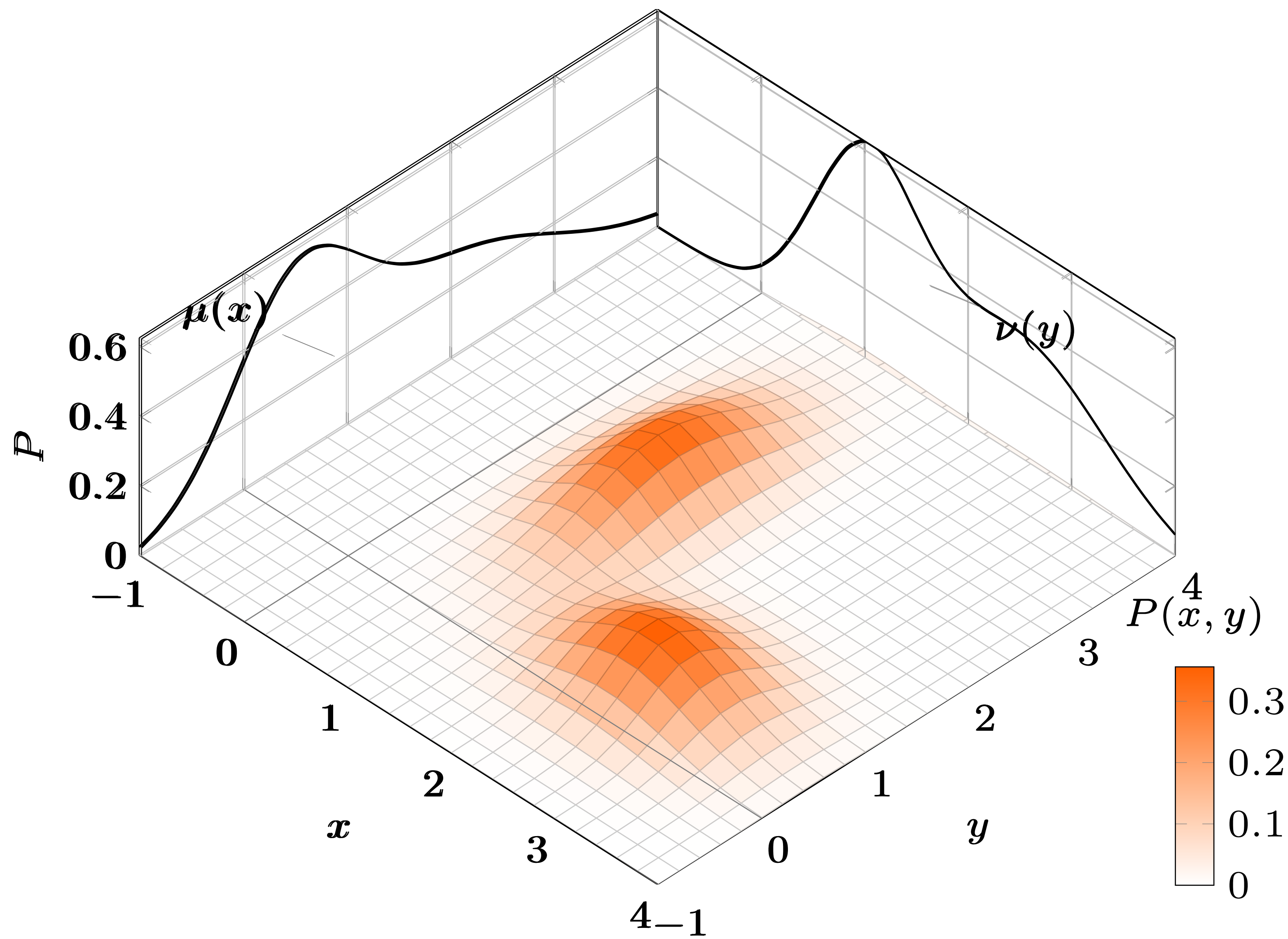

Kantorovich Problem

$$\inf_{\boldsymbol{T}_\sharp \boldsymbol{\mu} = \boldsymbol{\nu}} \int_\Omega \boldsymbol{c}(x, \boldsymbol{T}(x)) \boldsymbol{\mu}(dx)$$

MONGE

Def. Given $\boldsymbol{\mu}, \boldsymbol{\nu}$ in $\mathcal{P}(\Omega)$; a cost function $\boldsymbol{c}$ on $\Omega \times \Omega$, the Kantorovich problem is

$$\inf_{\boldsymbol{P} \in \Pi(\boldsymbol{\mu}, \boldsymbol{\nu})} \iint \boldsymbol{c}(x, y) \boldsymbol{P}(dx, dy).$$

PRIMAL

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PRIMAL

$$\sup_{\substack{\boldsymbol{\varphi} \in L_1(\boldsymbol{\mu}), \boldsymbol{\psi} \in L_1(\boldsymbol{\nu}) \\ \boldsymbol{\varphi}(x) + \boldsymbol{\psi}(y) \leq \boldsymbol{c}(x, y)}} \int \boldsymbol{\varphi} d\boldsymbol{\mu} + \int \boldsymbol{\psi} d\boldsymbol{\nu}.$$

DUAL

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Def. Given $\boldsymbol{\mu}, \boldsymbol{\nu}$ in $\mathcal{P}(\Omega)$; a cost function $\boldsymbol{c}$ on $\Omega \times \Omega$, the Kantorovich problem is

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PRIMAL

For two real-valued functions $\boldsymbol{\varphi}, \boldsymbol{\psi}$ on Ω,

$$(\boldsymbol{\varphi} \oplus \boldsymbol{\psi})(x, y) \stackrel{\text{def}}{=} \boldsymbol{\varphi}(x) + \boldsymbol{\psi}(y)$$

Kantorovich Problem

Def. Given $\boldsymbol{\mu}, \boldsymbol{\nu}$ in $\mathcal{P}(\Omega)$; a cost function $\boldsymbol{c}$ on $\Omega \times \Omega$, the Kantorovich problem is

$$\inf_{\boldsymbol{P} \in \Pi(\boldsymbol{\mu}, \boldsymbol{\nu})} \iint \boldsymbol{c}(x, y) \boldsymbol{P}(dx, dy).$$

PRIMAL

$$\sup_{\substack{\boldsymbol{\varphi} \in L_1(\boldsymbol{\mu}), \boldsymbol{\psi} \in L_1(\boldsymbol{\nu}) \\ \boldsymbol{\varphi} \oplus \boldsymbol{\psi} \leq \boldsymbol{c}}} \int \boldsymbol{\varphi} d\boldsymbol{\mu} + \int \boldsymbol{\psi} d\boldsymbol{\nu}.$$

DUAL

Deriving Kantorovich Duality

$$\iota_{\Pi}(\boldsymbol{P}) = \sup_{\boldsymbol{\varphi},\boldsymbol{\psi}} \left[\int \boldsymbol{\varphi} d\boldsymbol{\mu} + \int \boldsymbol{\psi} d\boldsymbol{\nu} - \iint \boldsymbol{\varphi} \oplus \boldsymbol{\psi} d\boldsymbol{P} \right]$$

$$= \begin{cases} 0 & \text{if } \boldsymbol{P} \in \Pi(\boldsymbol{\mu}, \boldsymbol{\nu}), \\ +\infty & \text{otherwise.} \end{cases}$$

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$$\inf_{\boldsymbol{P} \in \Pi(\boldsymbol{\mu},\boldsymbol{\nu})} \iint \boldsymbol{c}\, d\boldsymbol{P}$$

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$$\inf_{\cancel{\boldsymbol{P} \in \Pi(\boldsymbol{\mu},\boldsymbol{\nu})}} \iint \boldsymbol{c}\, d\boldsymbol{P}$$

$$\inf_{\boldsymbol{P} \in \mathcal{P}_+(\Omega^2)} \iint \boldsymbol{c}\, d\boldsymbol{P} + \boxed{\iota_\Pi(\boldsymbol{P})}$$

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$$\boxed{\inf_{\boldsymbol{P} \in \mathcal{P}_+(\Omega^2)} \iint \boldsymbol{c}\, d\boldsymbol{P} + \iota_\Pi(\boldsymbol{P})}$$

Deriving Kantorovich Duality

$$\inf_{P \in \mathcal{P}_+(\Omega^2)} \iint c \, dP + \iota_\Pi(P)$$

$$\inf_{P \in \mathcal{P}_+(\Omega^2)} \iint c \, dP + \sup_{\varphi, \psi} \int \varphi d\mu + \int \psi d\nu - \iint \varphi \oplus \psi dP$$

Deriving Kantorovich Duality

$$\boxed{\inf_{\boldsymbol{P}\in\mathcal{P}_+(\Omega^2)} \iint \boldsymbol{c}\, d\boldsymbol{P} + \iota_\Pi(\boldsymbol{P})}$$

$$\inf_{\boldsymbol{P}\in\mathcal{P}_+(\Omega^2)} \sup_{\boldsymbol{\varphi},\boldsymbol{\psi}} \iint \boldsymbol{c}\, d\boldsymbol{P} + \int \boldsymbol{\varphi} d\boldsymbol{\mu} + \int \boldsymbol{\psi} d\boldsymbol{\nu} - \iint \boldsymbol{\varphi} \oplus \boldsymbol{\psi} d\boldsymbol{P}$$

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Deriving Kantorovich Duality

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$$\inf_{\boldsymbol{P} \in \mathcal{P}_+(\Omega)} \iint (\boldsymbol{c} - \boldsymbol{\varphi} \oplus \boldsymbol{\psi}) d\boldsymbol{P} = \begin{cases} 0 & \text{if } \boldsymbol{c} - \boldsymbol{\varphi} \oplus \boldsymbol{\psi} \geq 0. \\ -\infty & \text{otherwise} \end{cases}$$

Deriving Kantorovich Duality

$$\inf_{P \in \mathcal{P}_+(\Omega^2)} \iint c \, dP + \iota_\Pi(P)$$

$$\sup_{\varphi,\psi} \inf_{P \in \mathcal{P}_+(\Omega^2)} \iint (c - \varphi \oplus \psi) dP \qquad + \int \varphi d\mu + \int \psi d\nu$$

$$\inf_{P \in \mathcal{P}_+(\Omega)} \iint (c - \varphi \oplus \psi) dP = \begin{cases} 0 & \text{if } c - \varphi \oplus \psi \geq 0. \\ -\infty & \text{otherwise} \end{cases}$$

$$\sup_{\varphi \oplus \psi \leq c} \int \varphi d\mu + \int \psi d\nu.$$

DUAL

Wasserstein Distances

Let $p \geq 1$. Let $\boldsymbol{c}(x, y) := \boldsymbol{D}^p(x, y)$, a metric.

Def. The p-**Wasserstein distance** between $\boldsymbol{\mu}, \boldsymbol{\nu}$ in $\mathcal{P}(\Omega)$ is

$$W_p(\boldsymbol{\mu}, \boldsymbol{\nu}) \stackrel{\text{def}}{=} \left(\inf_{\boldsymbol{P} \in \Pi(\boldsymbol{\mu}, \boldsymbol{\nu})} \iint \boldsymbol{D}(\boldsymbol{x}, \boldsymbol{y})^p \boldsymbol{P}(dx, dy) \right)^{1/p}.$$

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Kantorovich Duality

$$W_p^p(\boldsymbol{\mu},\boldsymbol{\nu}) = \sup_{\substack{\boldsymbol{\varphi}\in L_1(\boldsymbol{\mu}),\boldsymbol{\psi}\in L_1(\boldsymbol{\nu})\\ \boldsymbol{\varphi}(x)+\boldsymbol{\psi}(y)\leq \boldsymbol{D}^p(x,y)}} \int \boldsymbol{\varphi}\, d\boldsymbol{\mu} + \int \boldsymbol{\psi}\, d\boldsymbol{\nu}.$$

DUAL

- Kantorovich Duality is **interesting** from a computational perspective: easier to store 2 functions than a whole coupling.
- D transforms: go from **two** to **one** dual potential.

D transforms

$$W_p^p(\mu, \nu) = \sup_{\substack{\varphi \in L_1(\mu), \psi \in L_1(\nu) \\ \varphi(x) + \psi(y) \leq D^p(x,y)}} \int \varphi d\mu + \int \psi d\nu.$$

DUAL

Imagine we choose a φ. Can we find a good ψ?

D transforms

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We need that ψ satisfies for *all* $\boldsymbol{x}, \boldsymbol{y}$

$$\boldsymbol{\varphi}(\boldsymbol{x}) + \psi(\boldsymbol{y}) \le \boldsymbol{D}^p(\boldsymbol{x},\boldsymbol{y})$$

D transforms

$$W_p^p(\mu,\nu) = \sup_{\substack{\varphi\in L_1(\mu),\psi\in L_1(\nu)\\ \varphi(x)+\psi(y)\leq D^p(x,y)}} \int \varphi d\mu + \int \psi d\nu.$$

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We need that ψ satisfies for *all* x, y

$$\varphi(x) + \psi(y) \leq D^p(x,y)$$

$$\psi(y) \leq D^p(x,y) - \varphi(x)$$

D transforms

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We need that ψ satisfies for *all* $\boldsymbol{x}, \boldsymbol{y}$

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$$\psi(\boldsymbol{y}) \leq \boldsymbol{D}^p(\boldsymbol{x}, \boldsymbol{y}) - \varphi(\boldsymbol{x})$$

$$\psi(\boldsymbol{y}) \leq \inf_{\boldsymbol{x}} \boldsymbol{D}^p(\boldsymbol{x}, \boldsymbol{y}) - \varphi(\boldsymbol{x})$$

D transforms

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DUAL

For given $\boldsymbol{\varphi}$, cannot get a better $\boldsymbol{\psi}$ than

$$\overline{\boldsymbol{\varphi}}(\boldsymbol{y}) \stackrel{\text{def}}{=} \inf_{\boldsymbol{x}} \boldsymbol{D}^p(\boldsymbol{x},\boldsymbol{y}) - \boldsymbol{\varphi}(\boldsymbol{x}).$$

D transforms

$$W_p^p(\boldsymbol{\mu},\boldsymbol{\nu}) = \sup_{\substack{\varphi\in L_1(\boldsymbol{\mu}),\psi\in L_1(\boldsymbol{\nu})\\ \varphi(x)+\psi(y)\leq \boldsymbol{D}^p(x,y)}} \int \varphi d\boldsymbol{\mu} + \int \psi d\boldsymbol{\nu}.$$

DUAL

For given φ, cannot get a better ψ than

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$$W_p^p(\boldsymbol{\mu},\boldsymbol{\nu}) = \sup_{\varphi} \int \varphi d\boldsymbol{\mu} + \int \overline{\varphi} d\boldsymbol{\nu}.$$

SEMI-DUAL

D transforms

$$\overline{\boldsymbol{\varphi}}(\boldsymbol{y}) \stackrel{\text{def}}{=} \inf_{\boldsymbol{x}} D^p(\boldsymbol{x}, \boldsymbol{y}) - \boldsymbol{\varphi}(\boldsymbol{x}).$$

$$\overline{\psi}(\boldsymbol{x}) = \inf_{\boldsymbol{y}} D^p(\boldsymbol{x}, \boldsymbol{y}) - \psi(\boldsymbol{y}).$$

D transforms

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$$W_p^p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \sup_{\varphi} \int \overline{\overline{\varphi}} d\boldsymbol{\mu} + \int \overline{\varphi} d\boldsymbol{\nu}.$$

D transforms

$$\overline{\varphi}(y) \stackrel{\text{def}}{=} \inf_{x} D^p(x, y) - \varphi(x).$$

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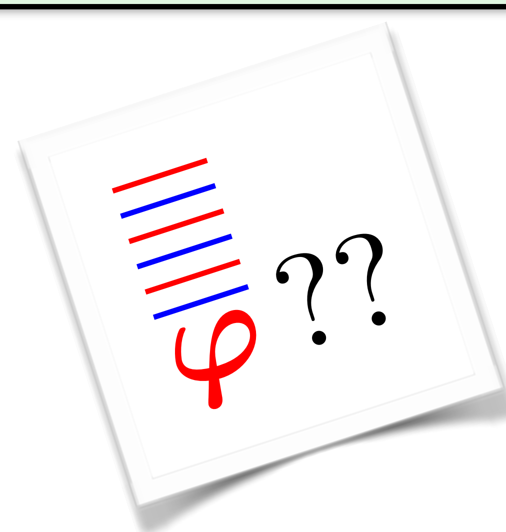

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$$\overline{\varphi}(y) \stackrel{\text{def}}{=} \inf_{x} D^p(x, y) - \varphi(x).$$

$$\overline{\psi}(x) = \inf_{y} D^p(x, y) - \psi(y).$$

$$W_p^p(\mu, \nu) = \sup_{\varphi} \int \overline{\overline{\varphi}} d\mu + \int \overline{\varphi} d\nu.$$

For all φ, we have $\overline{\overline{\overline{\varphi}}} = \overline{\varphi}$

D transforms

$$\overline{\varphi}(\boldsymbol{y}) \stackrel{\text{def}}{=} \inf_{\boldsymbol{x}} \boldsymbol{D}^p(\boldsymbol{x}, \boldsymbol{y}) - \varphi(\boldsymbol{x}).$$

$$\overline{\psi}(\boldsymbol{x}) = \inf_{\boldsymbol{y}} \boldsymbol{D}^p(\boldsymbol{x}, \boldsymbol{y}) - \psi(\boldsymbol{y}).$$

$$W_p^p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \sup_{\varphi} \int \overline{\overline{\varphi}} d\boldsymbol{\mu} + \int \overline{\varphi} d\boldsymbol{\nu}.$$

For all φ, we have $\overline{\overline{\overline{\varphi}}} = \overline{\varphi}$

φ is $\boldsymbol{D}^p$-concave if $\exists \phi : \varphi = \overline{\phi}$

φ is $\boldsymbol{D}^p$-concave $\Rightarrow \overline{\overline{\varphi}} = \varphi$

D transforms

$$\overline{\varphi}(y) \stackrel{\text{def}}{=} \inf_{x} D^p(x, y) - \varphi(x).$$

$$\overline{\psi}(x) = \inf_{y} D^p(x, y) - \psi(y).$$

$$W_p^p(\mu, \nu) = \sup_{\varphi} \int \overline{\overline{\varphi}} d\mu + \int \overline{\varphi} d\nu.$$

$$W_p^p(\mu, \nu) = \sup_{\varphi \text{ is } D^p\text{-concave}} \int \varphi d\mu + \int \overline{\varphi} d\nu.$$

D transforms, W_1

Prop. If $\boldsymbol{c} = \boldsymbol{D}$, namely $p = 1$, then φ is $\boldsymbol{D}$-concave $\Leftrightarrow \overline{\varphi} = -\varphi$, φ is 1-Lipschitz

For given $\boldsymbol{x}$, $\overline{\varphi}_{\boldsymbol{x}}(\boldsymbol{y}) \stackrel{\text{def}}{=} \boldsymbol{D}(\boldsymbol{x}, \boldsymbol{y}) - \varphi(\boldsymbol{x})$ is 1-Lipschitz.

D transforms, W_1

Prop. If $c = D$, namely $p = 1$, then φ is D-concave $\Leftrightarrow \overline{\varphi} = -\varphi$, φ is 1-Lipschitz

For given x, $\overline{\varphi}_x(y) \stackrel{\text{def}}{=} D(x, y) - \varphi(x)$ is 1-Lipschitz.

$$\overline{\varphi}_x(y) - \overline{\varphi}_x(y') = D(x, y) - D(x, y') \leq D(y, y')$$

D transforms, W_1

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D transforms, W_1

Prop. If $c = D$, namely $p = 1$, then φ is D-concave $\Leftrightarrow \overline{\varphi} = -\varphi$, φ is 1-Lipschitz

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$\Rightarrow \overline{\varphi}(y) = \inf_x \overline{\varphi}_x(y)$ is 1-Lipschitz.

$\Rightarrow \overline{\varphi}(y) - \overline{\varphi}(x) \leq D(x, y)$

D transforms, W_1

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$$\Rightarrow \overline{\varphi}(y) - \overline{\varphi}(x) \leq D(x, y)$$

$$\Rightarrow -\overline{\varphi}(x) \leq D(x, y) - \overline{\varphi}(y)$$

$$\Rightarrow -\overline{\varphi}(x) \leq \inf_y D(x, y) - \overline{\varphi}(y)$$

D transforms, W_1

Prop. If $c = D$, namely $p = 1$, then φ is D-concave $\Leftrightarrow \overline{\varphi} = -\varphi$, φ is 1-Lipschitz

For given x, $\overline{\varphi}_x(y) \stackrel{\text{def}}{=} D(x, y) - \varphi(x)$ is 1-Lipschitz.

$\Rightarrow \overline{\varphi}(y) = \inf_x \overline{\varphi}_x(y)$ is 1-Lipschitz.

$\Rightarrow \overline{\varphi}(y) - \overline{\varphi}(x) \le D(x, y)$

$\Rightarrow -\overline{\varphi}(x) \le D(x, y) - \overline{\varphi}(y)$

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$\Rightarrow -\overline{\varphi}(x) \le \inf_y D(x, y) - \overline{\varphi}(y) \le -\overline{\varphi}(x)$

D transforms, W_1

Prop. If $c = D$, namely $p = 1$, then φ is D-concave $\Leftrightarrow \overline{\varphi} = -\varphi$, φ is 1-Lipschitz

For given x, $\overline{\varphi}_x(y) \overset{\text{def}}{=} D(x, y) - \varphi(x)$ is 1-Lipschitz.

$\Rightarrow \overline{\varphi}(y) = \inf_x \overline{\varphi}_x(y)$ is 1-Lipschitz.

$\Rightarrow \overline{\varphi}(y) - \overline{\varphi}(x) \leq D(x, y)$

$\Rightarrow -\overline{\varphi}(x) \leq D(x, y) - \overline{\varphi}(y)$

$\Rightarrow -\overline{\varphi}(x) \leq \inf_y D(x, y) - \overline{\varphi}(y)$

$\Rightarrow -\overline{\varphi}(x) \leq \inf_y D(x, y) - \overline{\varphi}(y) \leq -\overline{\varphi}(x)$

$\Rightarrow -\overline{\varphi}(x) \leq \overline{\overline{\varphi}}(x) \leq -\overline{\varphi}(x)$ and $\overline{\varphi}(x) = -\varphi(x)$

D transforms, W_1

$$W_1(\mu,\nu) = \sup_{\varphi \text{ is } D\text{-concave}} \int \varphi \, d\mu + \int \overline{\varphi} \, d\nu.$$

SEMI-DUAL

Prop. If $c = D$, then
φ is D-concave $\Leftrightarrow \overline{\varphi} = -\varphi$, φ is 1-Lipschitz

$$W_1(\mu,\nu) = \sup_{\varphi \text{ 1-Lipschitz}} \int \varphi (d\mu - d\nu).$$

W1

Links between Monge & Kantorovich

Prop. For "well behaved" costs $\boldsymbol{c}$, if $\boldsymbol{\mu}$ has a density then an *optimal* Monge map $T^\star$ between $\boldsymbol{\mu}$ and $\boldsymbol{\nu}$ must exist.

Prop. In that case

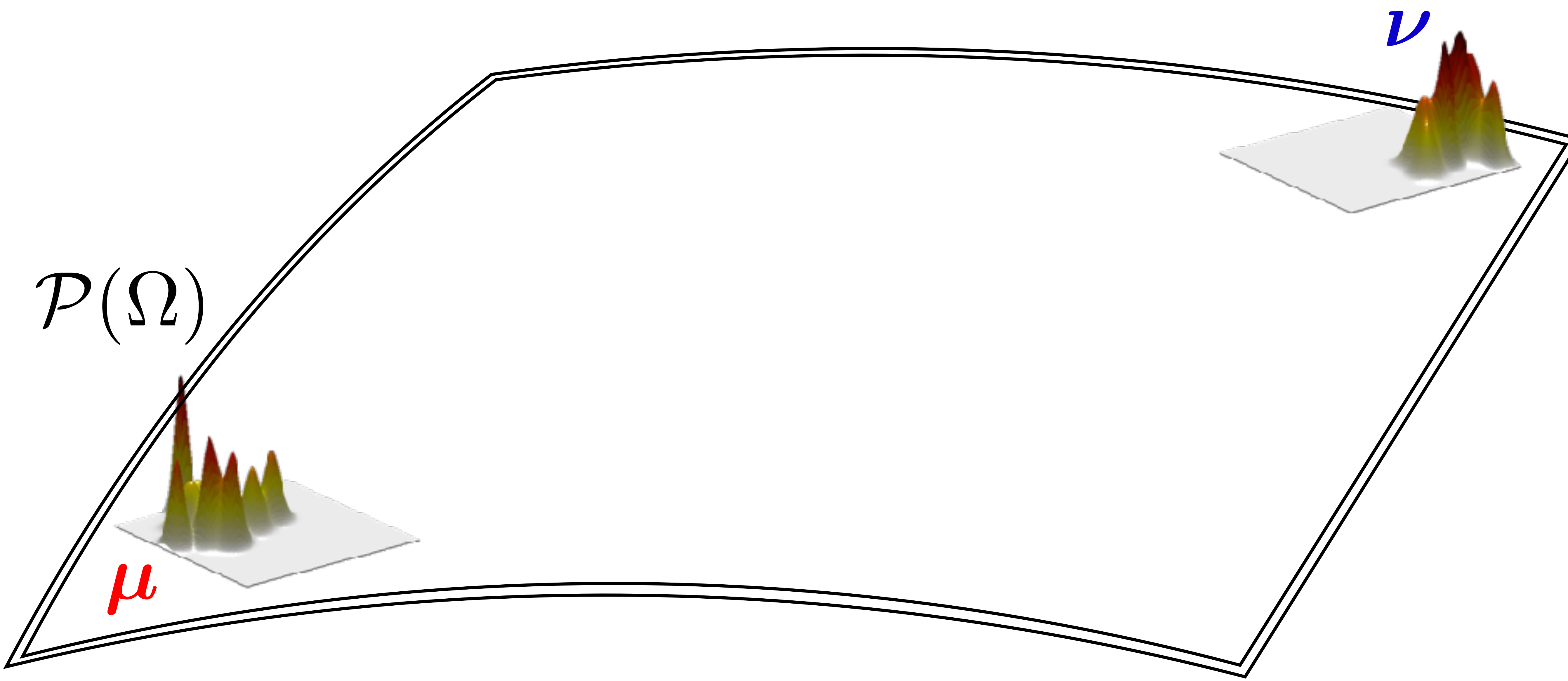
$$\boldsymbol{P}^\star := (\mathrm{Id}, T^\star)_\sharp \boldsymbol{\mu} \in \Pi(\boldsymbol{\mu}, \boldsymbol{\nu})$$

is also *optimal* for the Kantorovich problem.

[Brenier'91] [Smith&Knott'87] [McCann'01]

Optimal Transport Geometry

Very different geometry than standard information divergences (KL, Euclidean)



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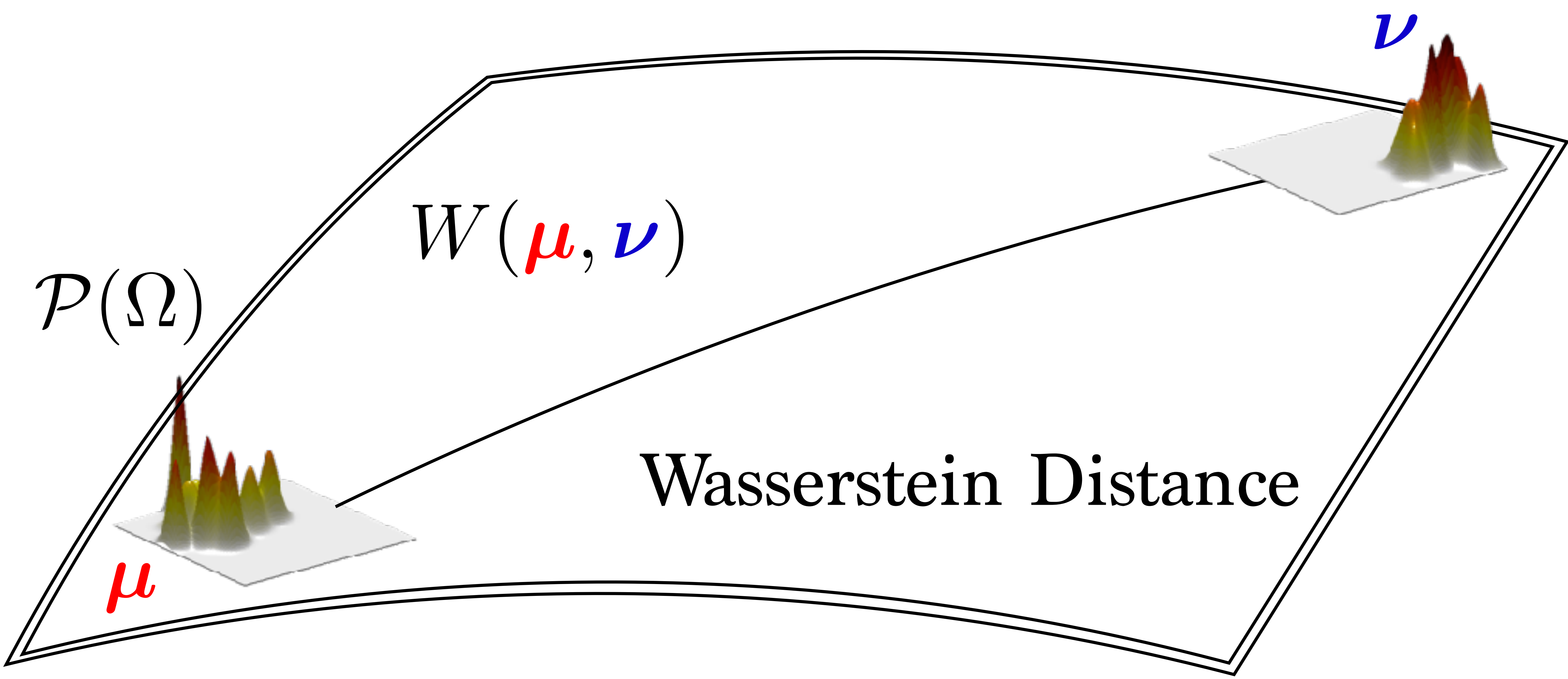

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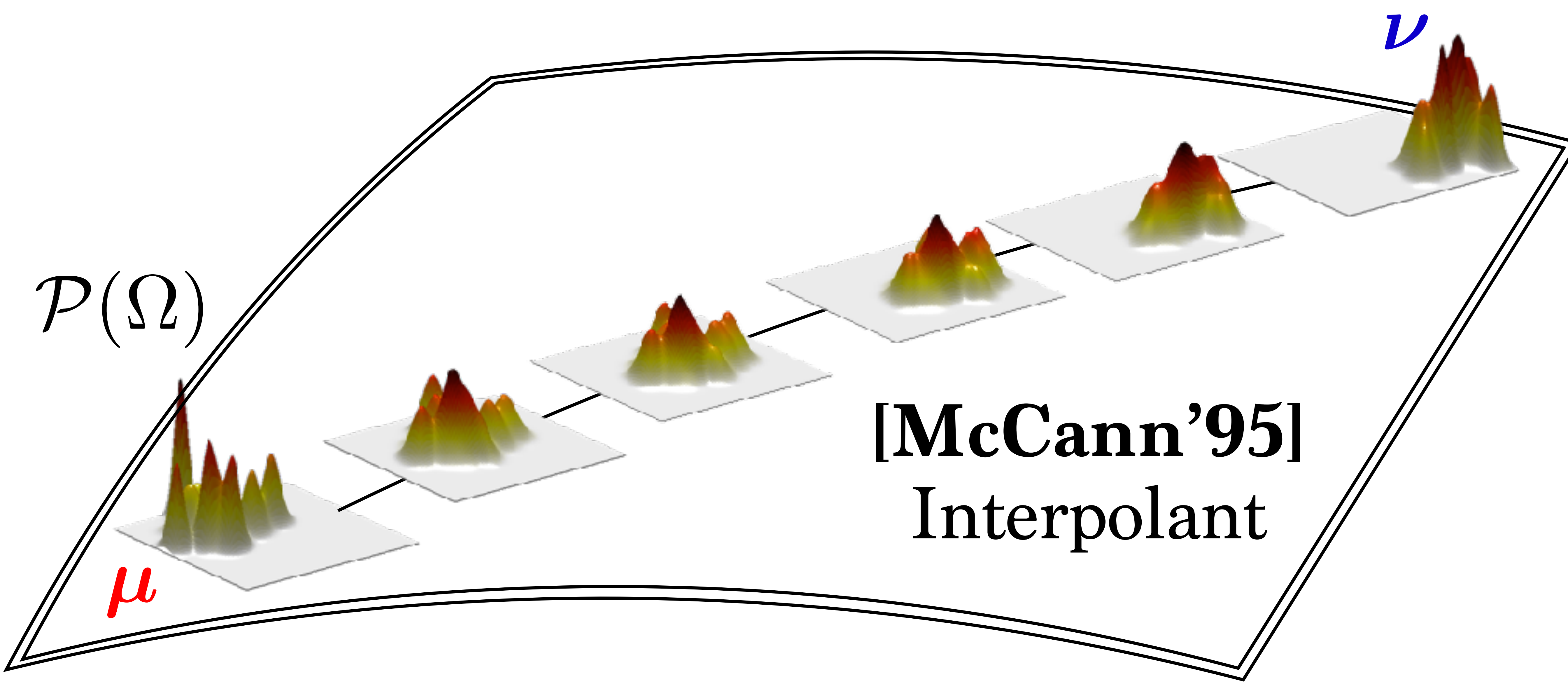

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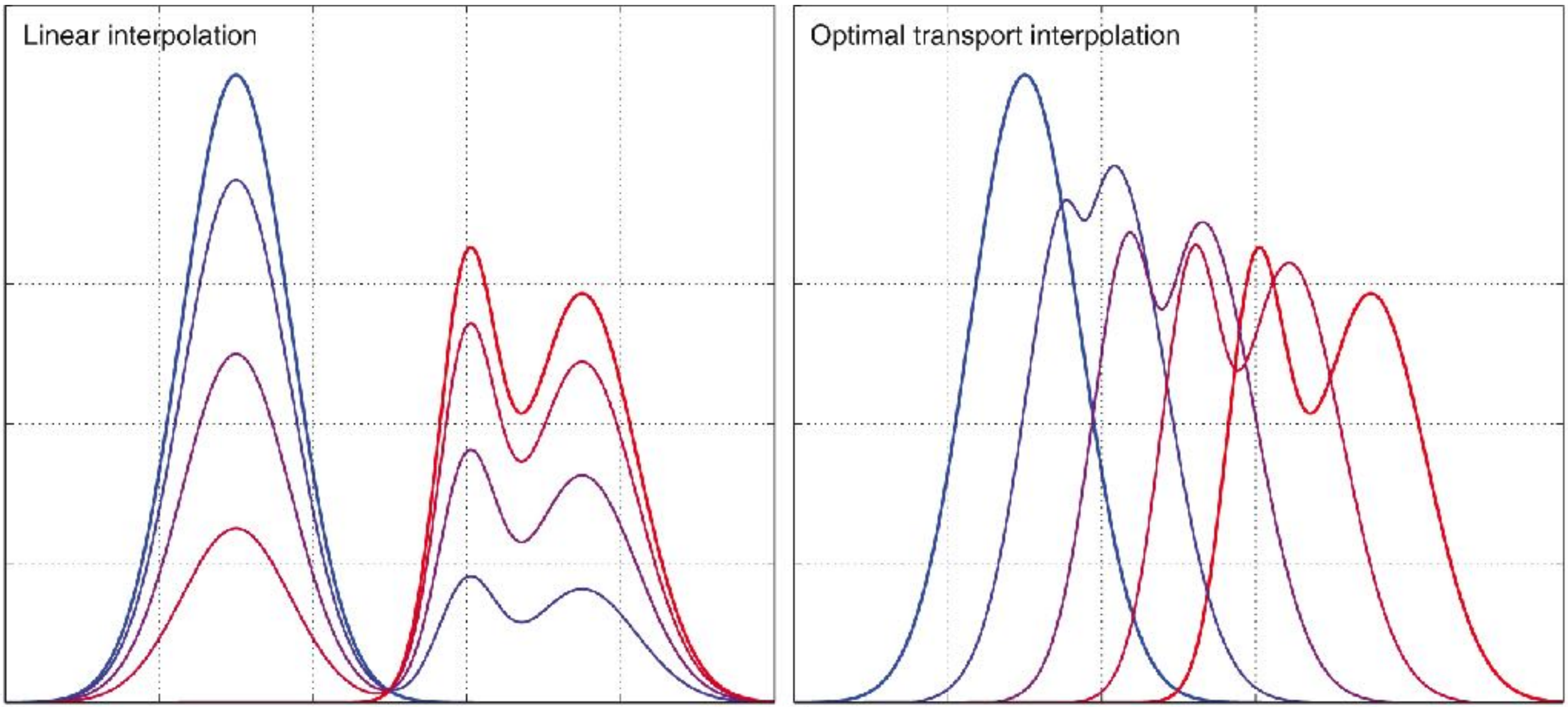

Optimal Transport Geometry

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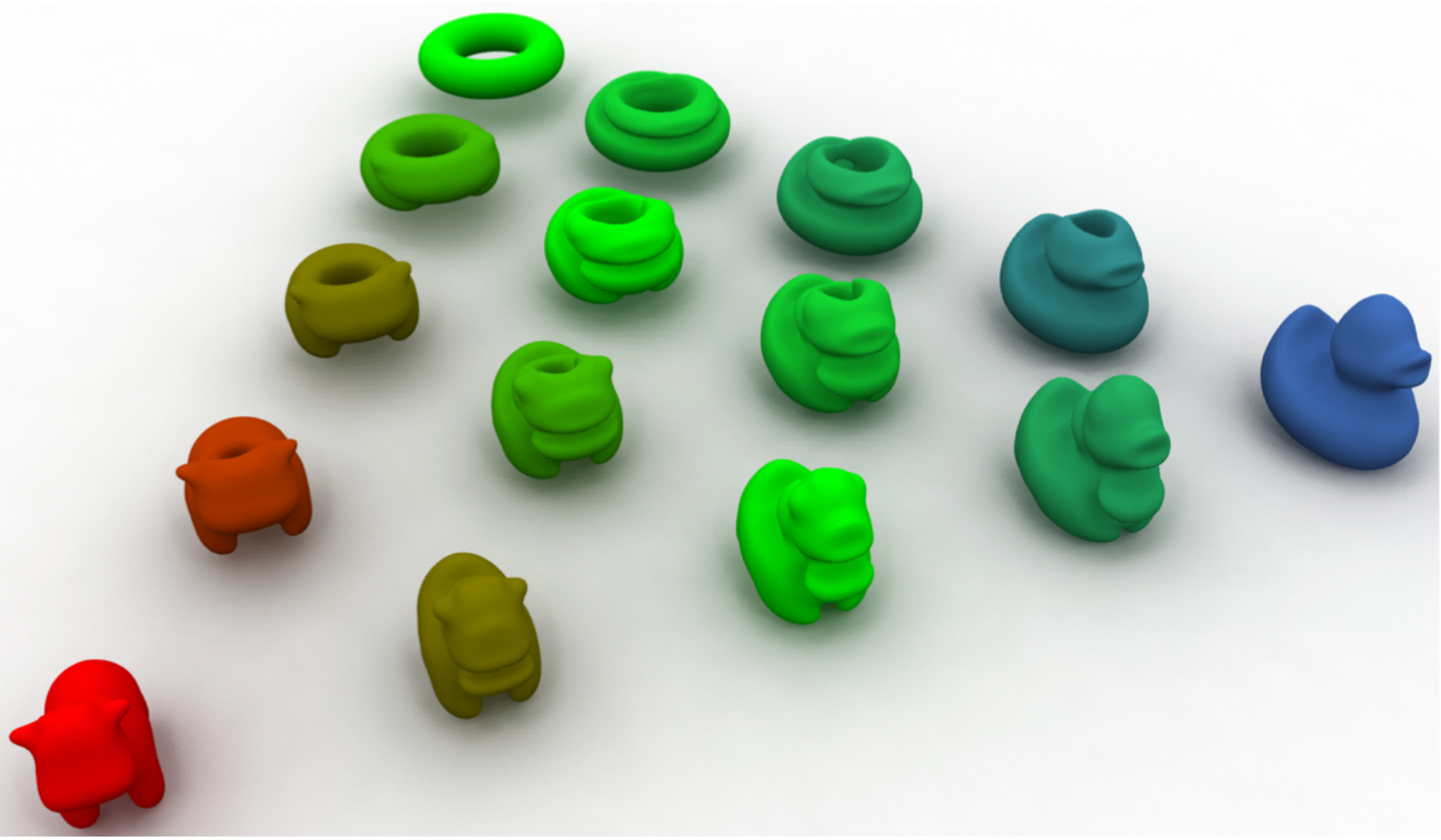
[SDPC..'15]

Optimal Transport Geometry

Very different geometry than standard information divergences (*KL*, Euclidean)



[SDPC..'15]

Optimal Transport Geometry

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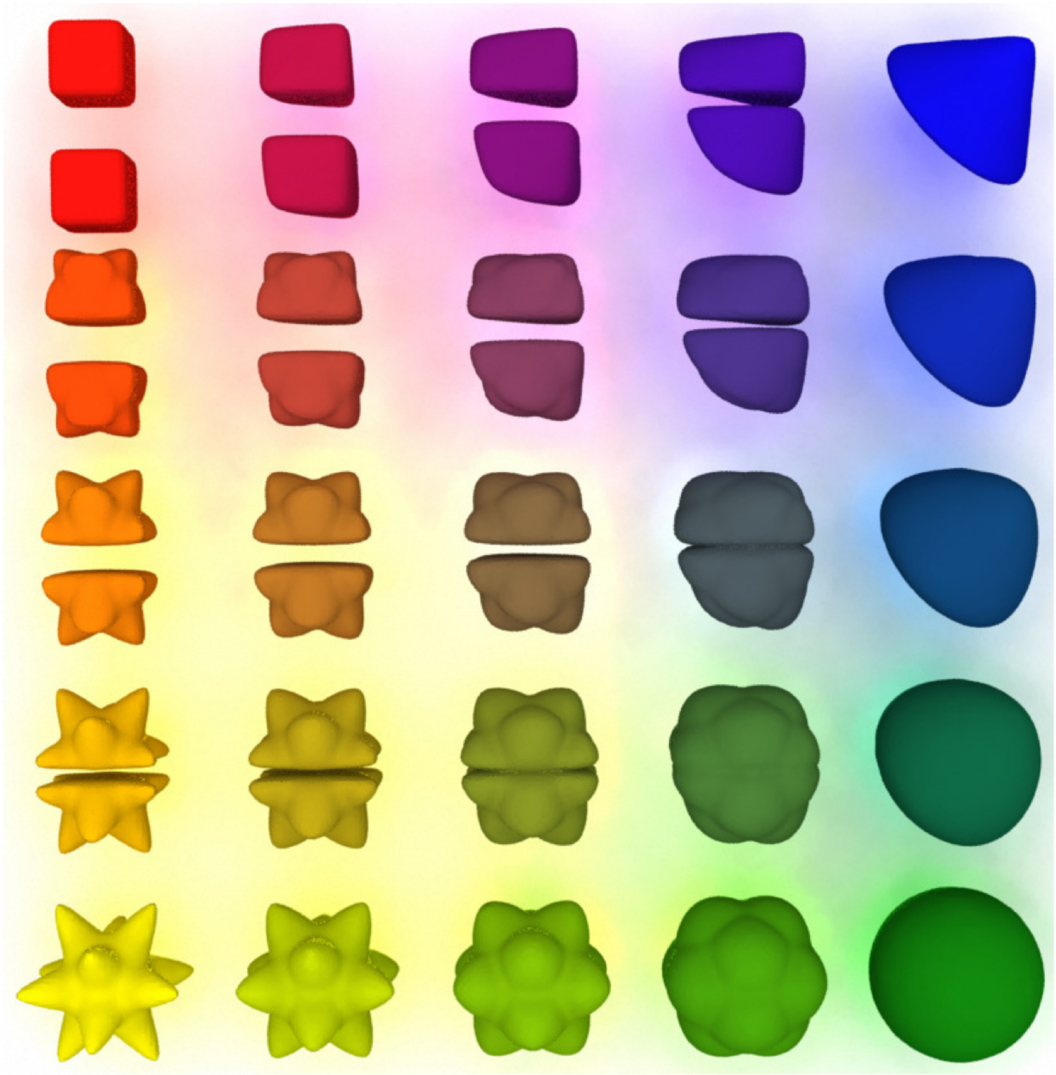


[SDPC..'15]

Computational OT

Up to 2010: OT solvers $W_p(\boldsymbol{\mu}, \boldsymbol{\nu}) = ?$

Goal now: use OT as a **loss or fidelity** term

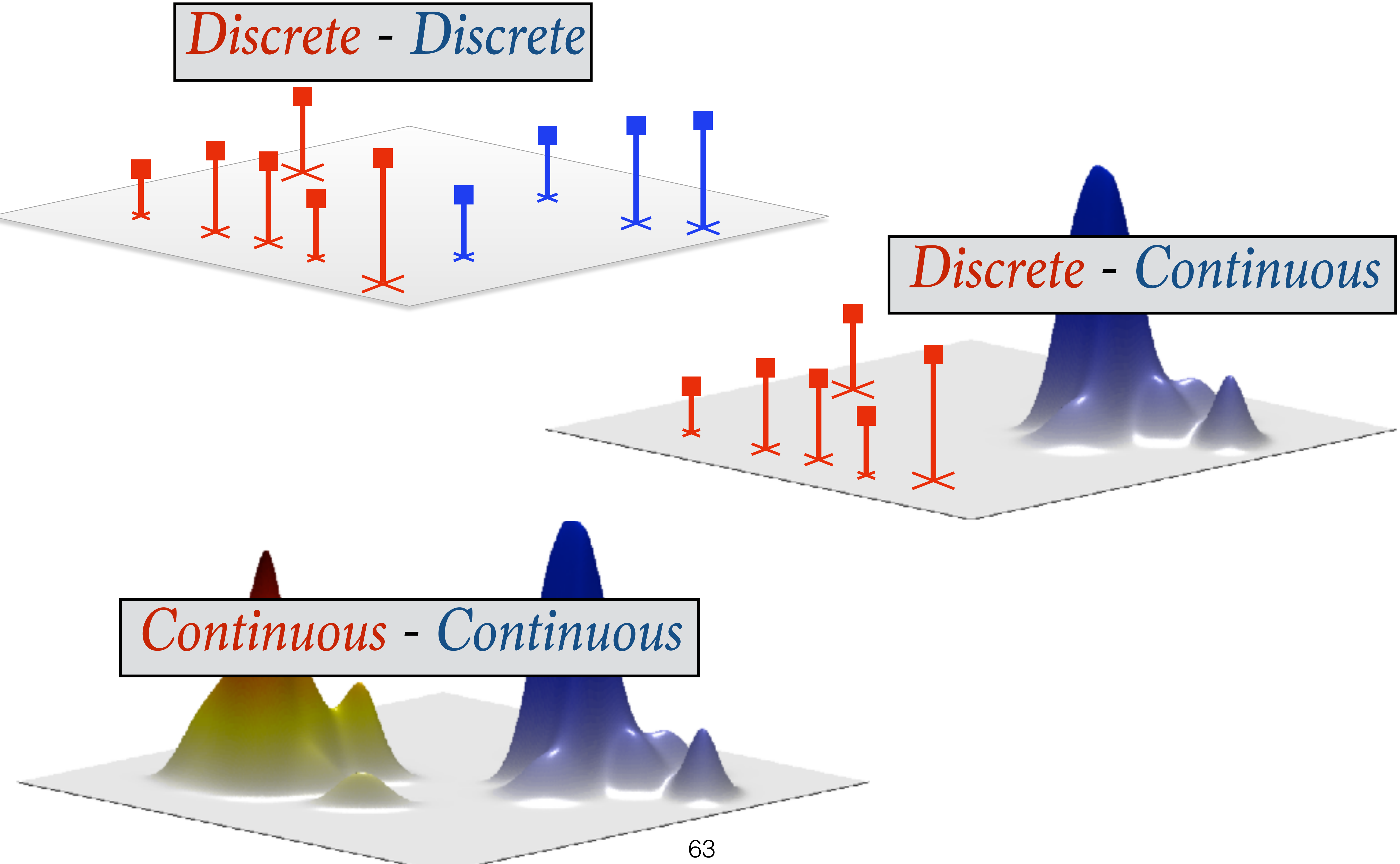
$$\underset{\boldsymbol{\mu} \in \mathcal{P}(\Omega)}{\operatorname{argmin}} \; F(W_p(\boldsymbol{\mu}, \boldsymbol{\nu_1}), W_p(\boldsymbol{\mu}, \boldsymbol{\nu_2}), \dots, \boldsymbol{\mu}) = ?$$

$$\nabla_{\boldsymbol{\mu}} W_p(\boldsymbol{\mu}, \boldsymbol{\nu_1}) = ?$$

2. How to compute OT

- Typology: discrete/continuous problems
- Easy cases, zoo of solvers
- Entropic regularization
- Differentiability of the W distance

How can we compute OT?



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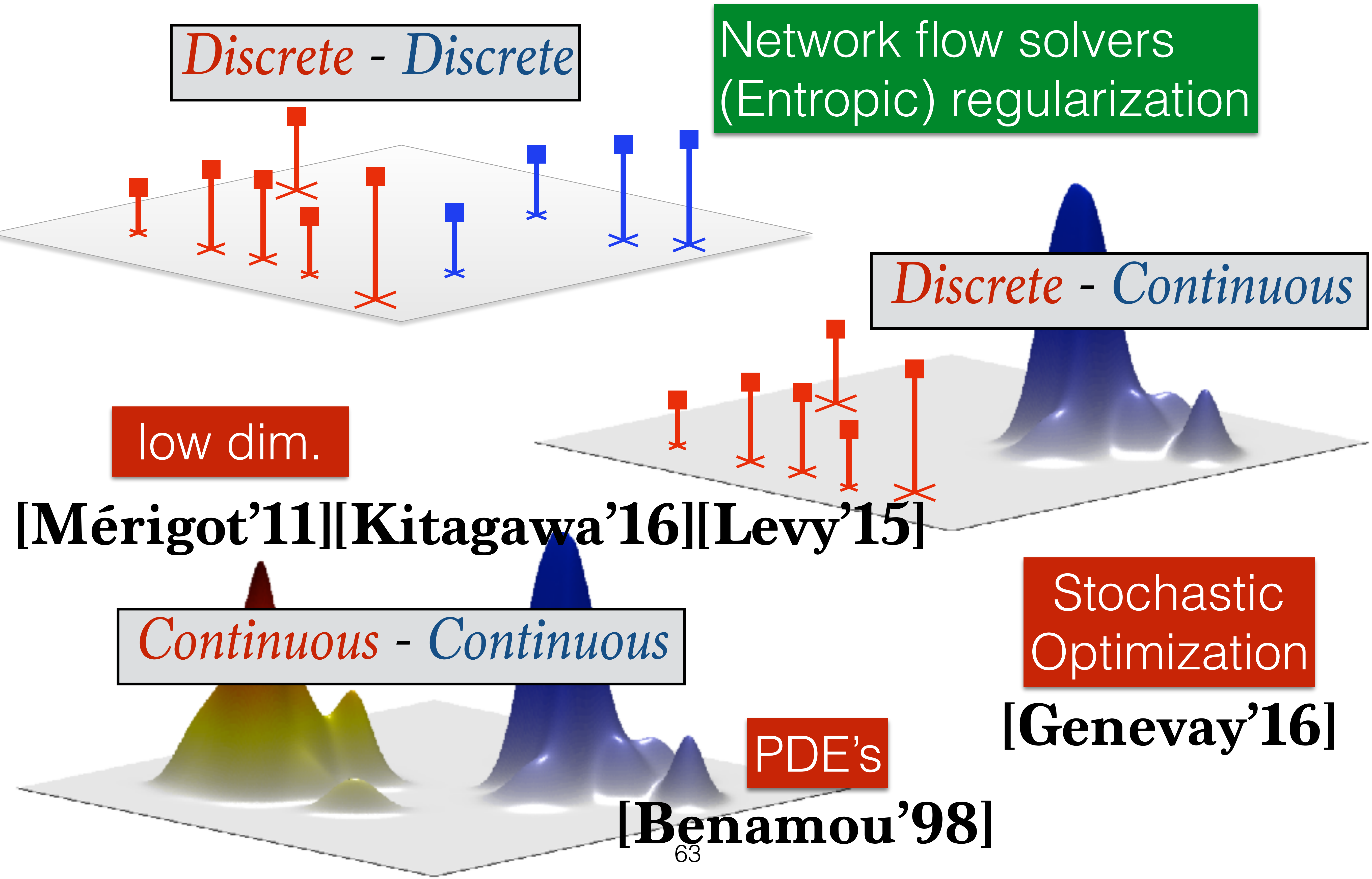

Easy (1): Univariate Measures

Remark. If $\Omega = \mathbb{R}$, $\boldsymbol{c}(x, y) = \boldsymbol{c}(|x - y|)$, $\boldsymbol{c}$ convex, $F_{\boldsymbol{\mu}}^{-1}, F_{\boldsymbol{\nu}}^{-1}$ quantile functions,

$$W(\boldsymbol{\mu}, \boldsymbol{\nu}) = \int_0^1 \boldsymbol{c}(|F_{\boldsymbol{\mu}}^{-1}(x) - F_{\boldsymbol{\nu}}^{-1}(x)|)dx$$

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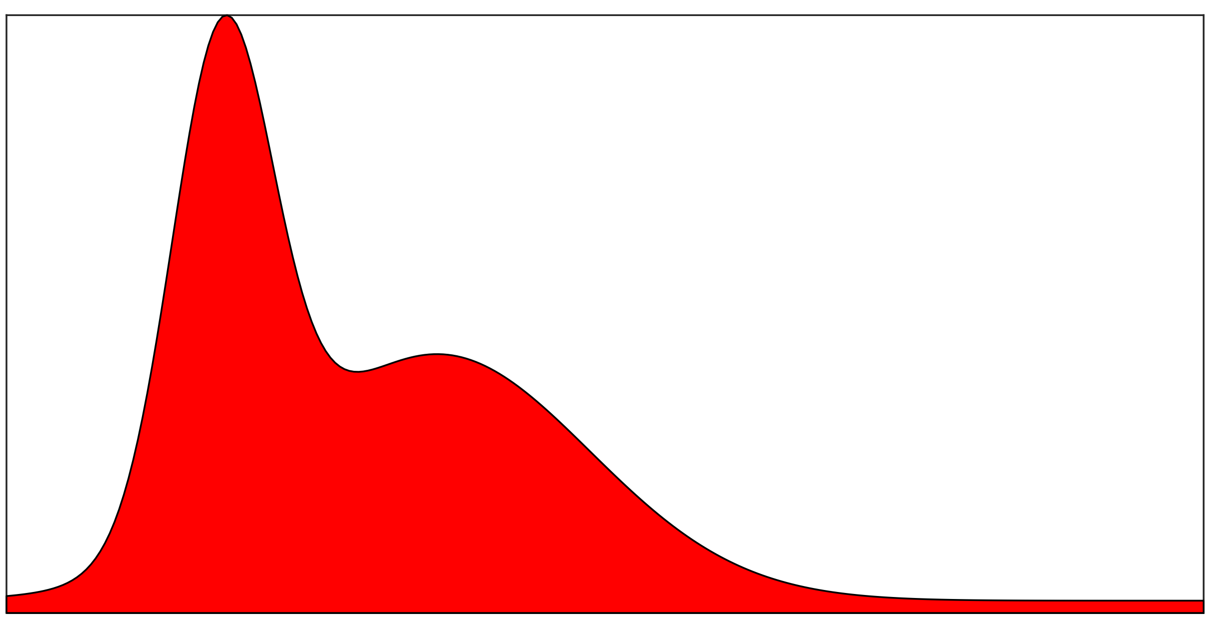
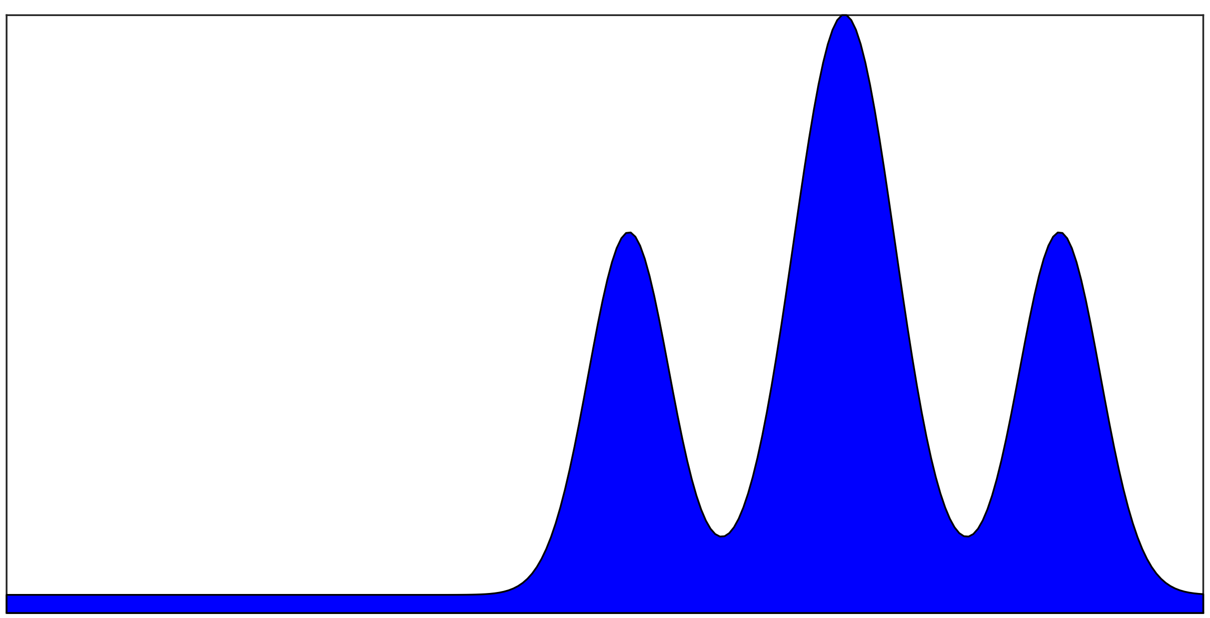


$\boldsymbol{\mu}$

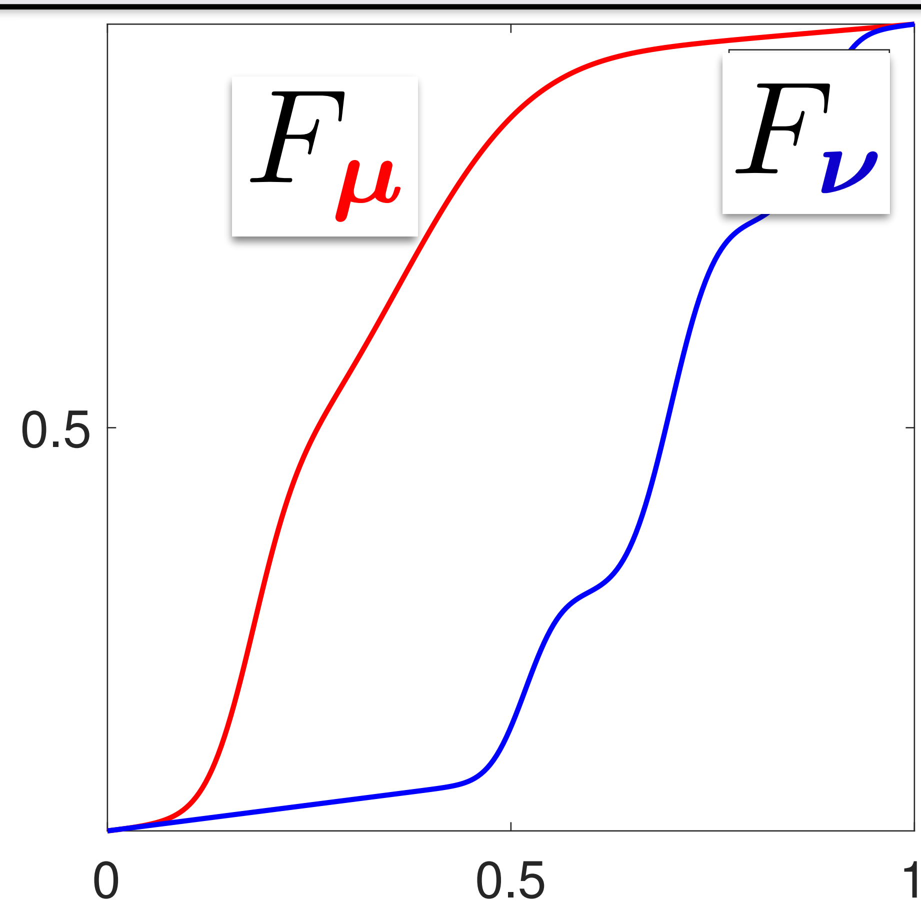


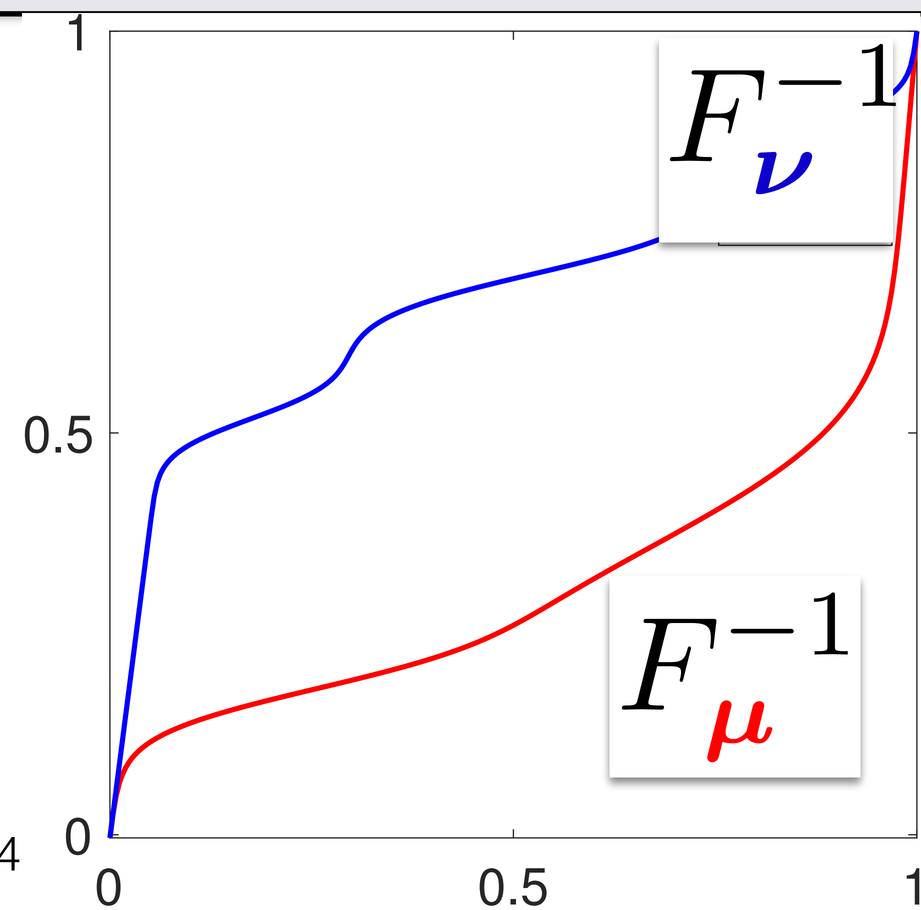
$\boldsymbol{\nu}$

Easy (1): Univariate Measures

Remark. If $\Omega = \mathbb{R}$, $c(x,y) = c(|x-y|)$, c convex, F_μ^{-1}, F_ν^{-1} quantile functions,

$$W(\mu,\nu) = \int_0^1 c(|F_\mu^{-1}(x) - F_\nu^{-1}(x)|)dx$$





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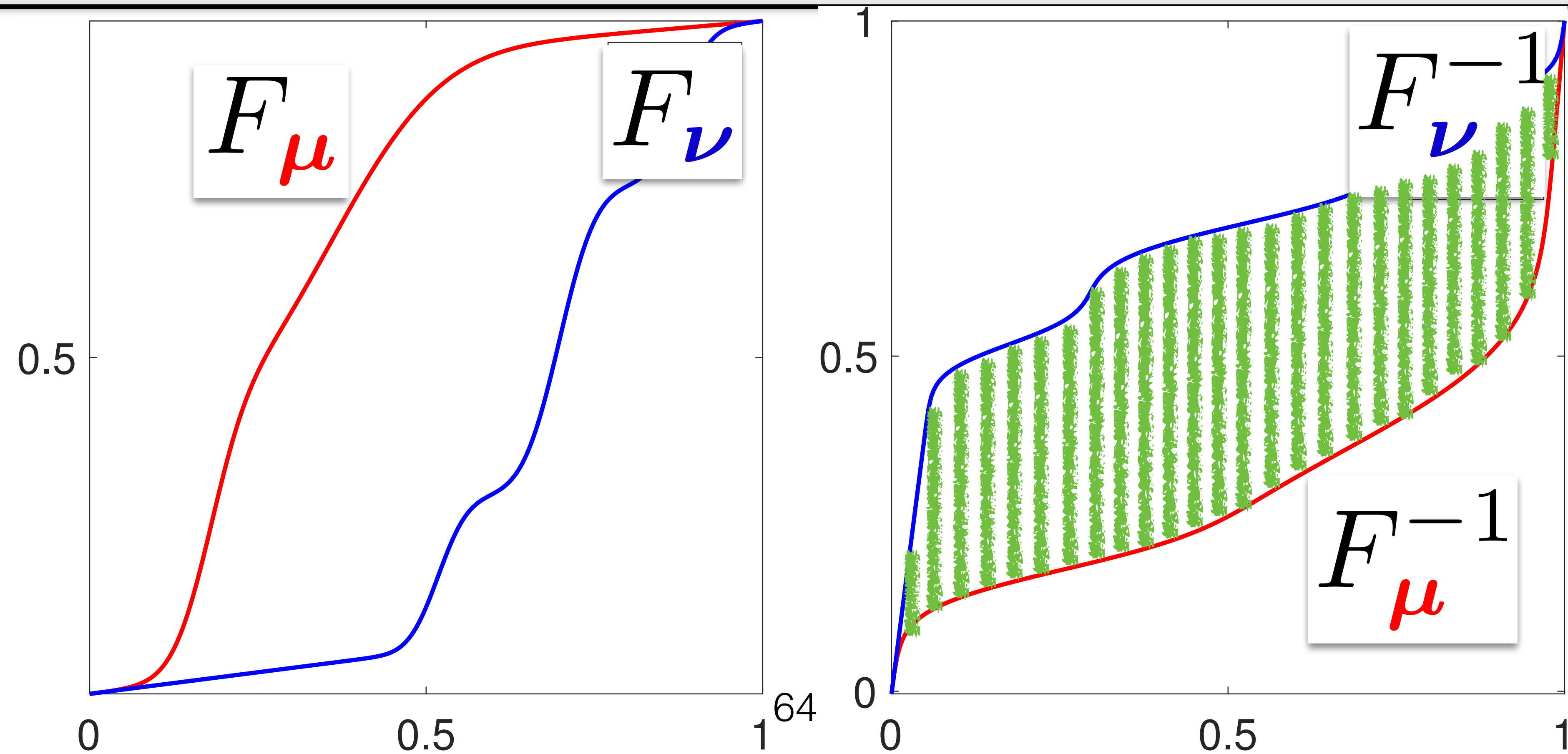

Easy (2): Gaussian Measures

Remark. If $\Omega = \mathbb{R}^d$, $\boldsymbol{c}(x,y) = \|x-y\|^2$, and $\boldsymbol{\mu} = \mathcal{N}(\mathbf{m}_{\boldsymbol{\mu}}, \boldsymbol{\Sigma}_{\boldsymbol{\mu}})$, $\boldsymbol{\nu} = \mathcal{N}(\mathbf{m}_{\boldsymbol{\nu}}, \boldsymbol{\Sigma}_{\boldsymbol{\nu}})$ then

$$W_2^2(\boldsymbol{\mu},\boldsymbol{\nu}) = \|\mathbf{m}_{\boldsymbol{\mu}} - \mathbf{m}_{\boldsymbol{\nu}}\|^2 + B(\boldsymbol{\Sigma}_{\boldsymbol{\mu}}, \boldsymbol{\Sigma}_{\boldsymbol{\nu}})^2$$

where B is the Bures metric

$$B(\boldsymbol{\Sigma}_{\boldsymbol{\mu}}, \boldsymbol{\Sigma}_{\boldsymbol{\nu}})^2 = \operatorname{trace}(\boldsymbol{\Sigma}_{\boldsymbol{\mu}} + \boldsymbol{\Sigma}_{\boldsymbol{\nu}} - 2(\boldsymbol{\Sigma}_{\boldsymbol{\mu}}^{1/2}\boldsymbol{\Sigma}_{\boldsymbol{\nu}}\boldsymbol{\Sigma}_{\boldsymbol{\mu}}^{1/2})^{1/2}).$$

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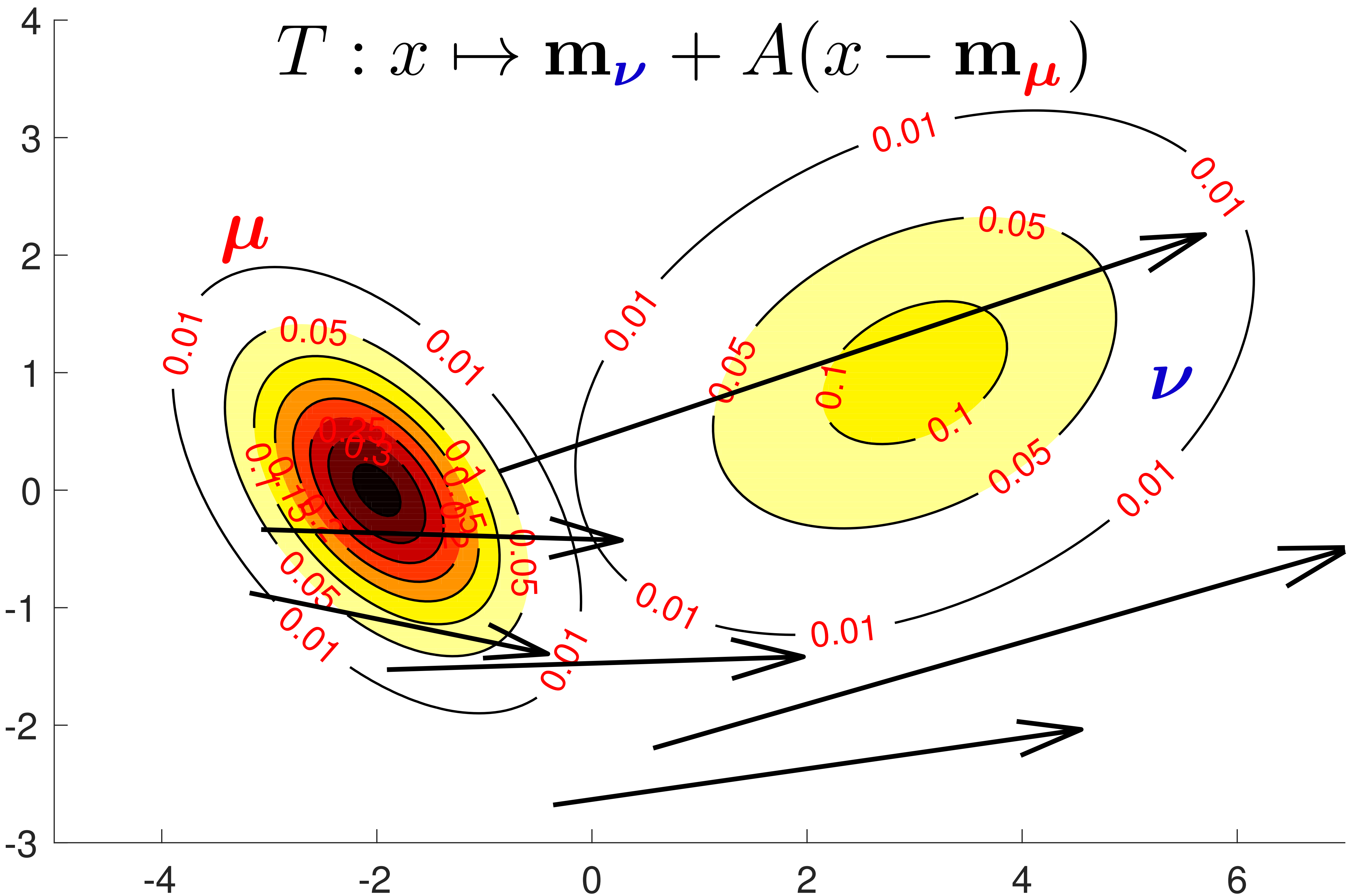
The map $T : x \mapsto \mathbf{m}_{\boldsymbol{\nu}} + A(x - \mathbf{m}_{\boldsymbol{\mu}})$ is **optimal**, where $A = \boldsymbol{\Sigma}_{\boldsymbol{\mu}}^{-\frac{1}{2}} \left(\boldsymbol{\Sigma}_{\boldsymbol{\mu}}^{\frac{1}{2}} \boldsymbol{\Sigma}_{\boldsymbol{\nu}} \boldsymbol{\Sigma}_{\boldsymbol{\mu}}^{\frac{1}{2}} \right)^{\frac{1}{2}} \boldsymbol{\Sigma}_{\boldsymbol{\mu}}^{-\frac{1}{2}}$.

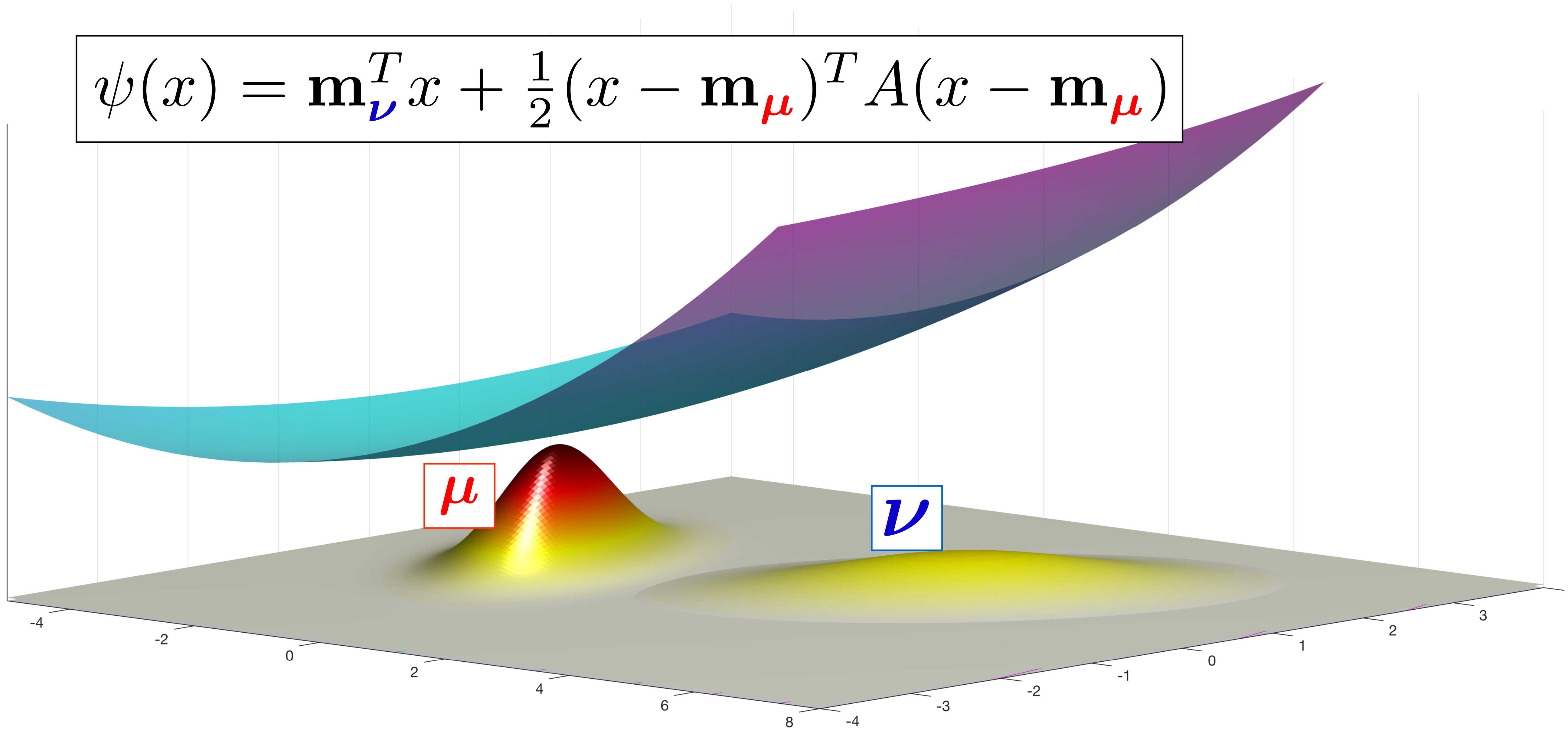
Easy (2): Gaussian Measures



Easy (2): Gaussian Measures

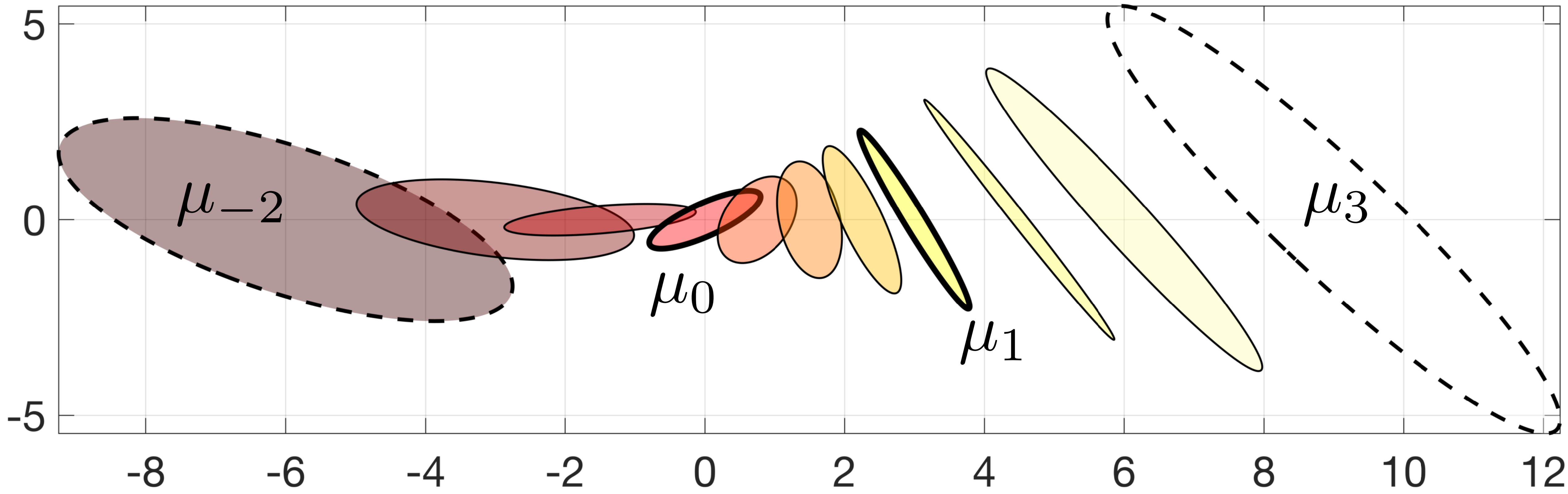
$$T = \nabla\psi : x \mapsto \mathbf{m}_{\boldsymbol{\nu}} + A(x - \mathbf{m}_{\boldsymbol{\mu}})$$

$$\boxed{\psi(x) = \mathbf{m}_{\boldsymbol{\nu}}^T x + \frac{1}{2}(x - \mathbf{m}_{\boldsymbol{\mu}})^T A(x - \mathbf{m}_{\boldsymbol{\mu}})}$$



Easy (2): Gaussian Measures

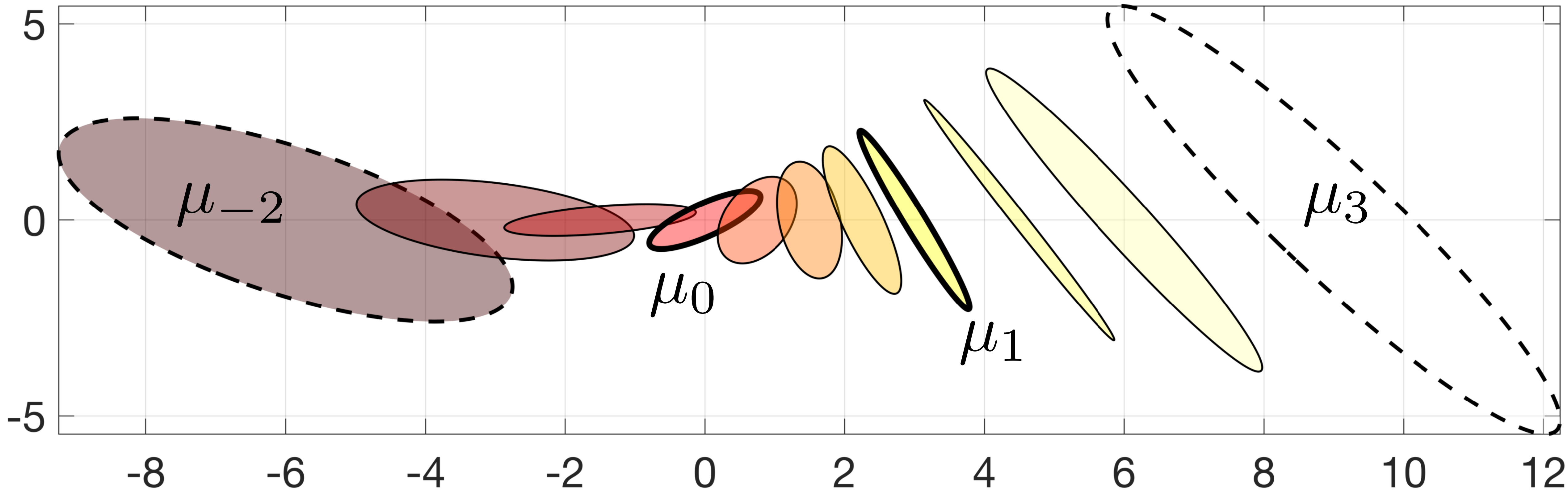
W_2 geodesic $(\mu_t)_t$ from μ_0 to μ_1 ($t \in [0,1]$) and extrapolation

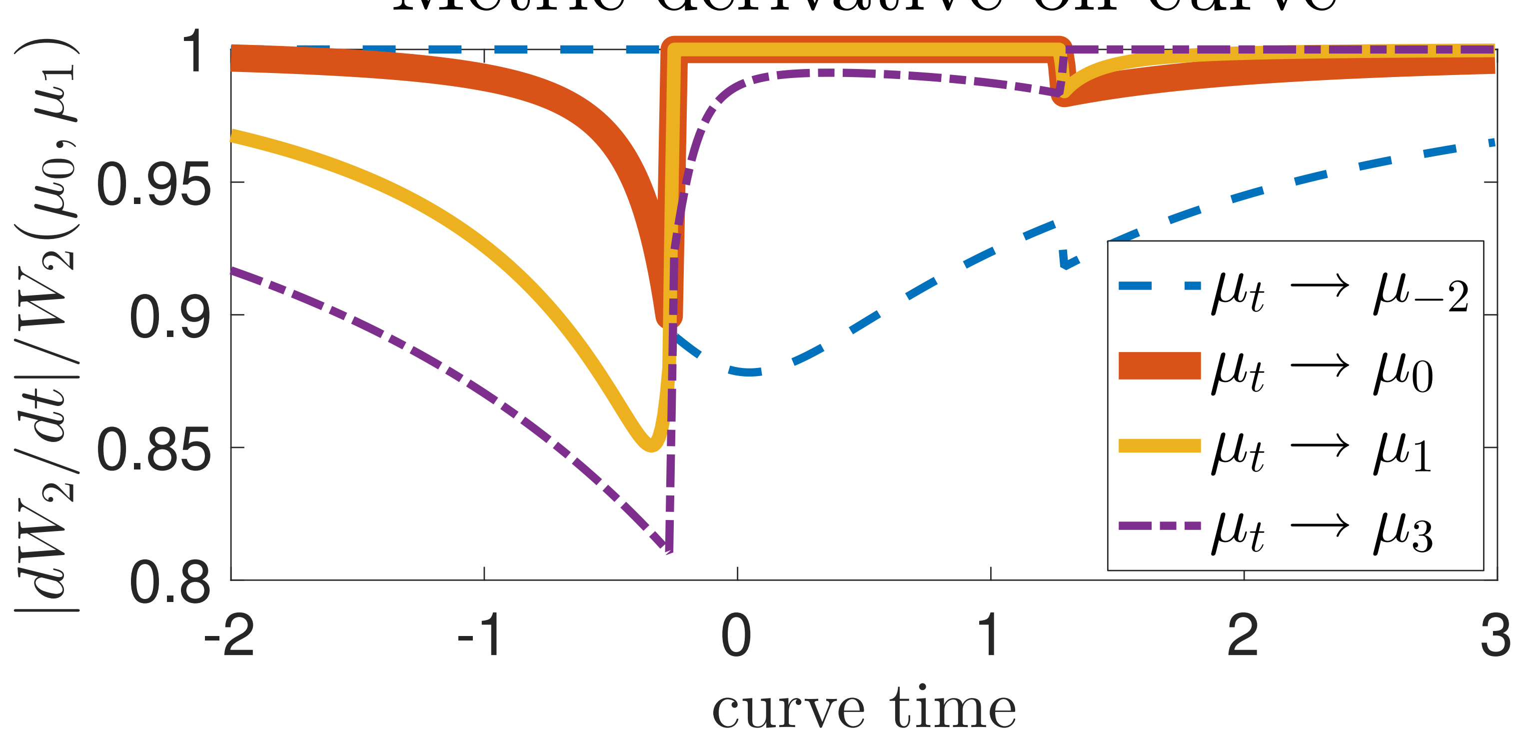


$$\Sigma_{t} = ((1-t)\,I + tA)\,\Sigma_{\mu}\,((1-t)\,I + tA)$$

Easy (2): Gaussian Measures

W_2 geodesic $(\mu_t)_t$ from μ_0 to μ_1 ($t \in [0,1]$) and extrapolation





Easy (3): Elliptical Distributions

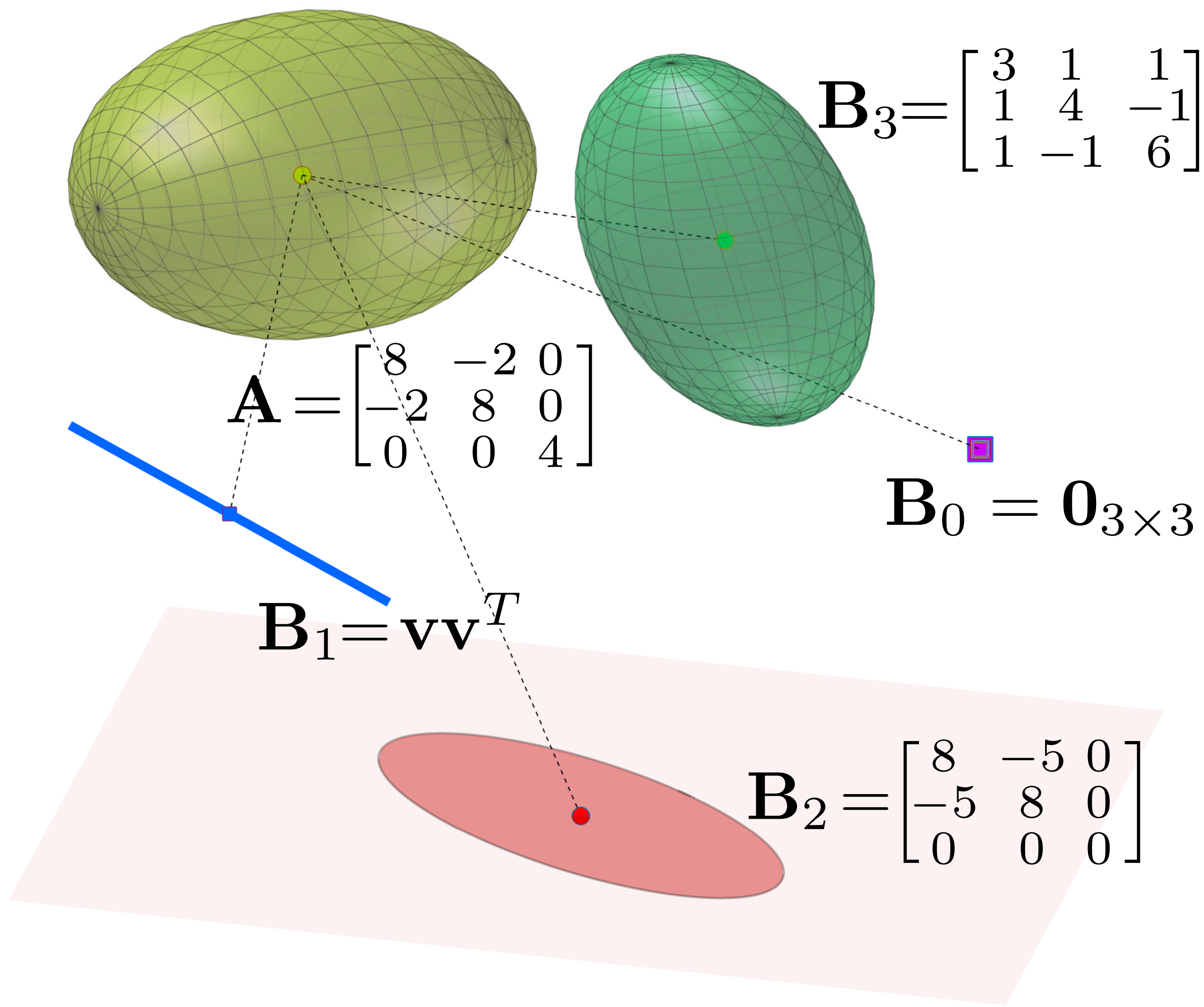
$$T = \nabla\psi : x \mapsto \mathbf{m}_{\boldsymbol{\nu}} + A(x - \mathbf{m}_{\boldsymbol{\mu}})$$

[Gelbrich'92] shows that the linear map T is also **optimal** for elliptically contoured distributions, *i.e.* distributions whose MGF are

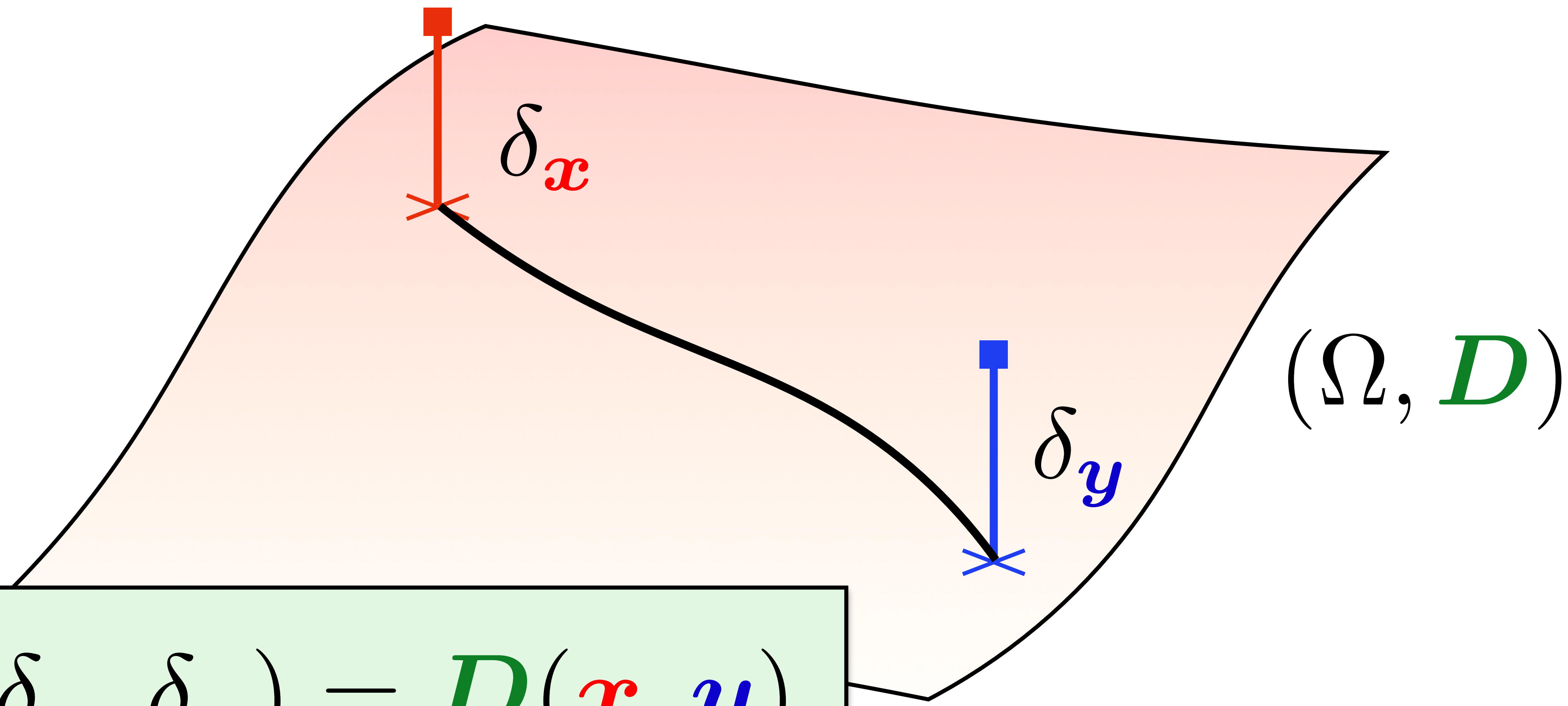
$$\boxed{\phi_X(\mathbf{t}) = \mathbb{E}\left[e^{\sqrt{-1}\mathbf{t}^T X}\right] = e^{\sqrt{-1}\mathbf{t}^T \mathbf{m}} g(\mathbf{t}^T \boldsymbol{C}\mathbf{t}) \quad g \text{ of positive type.}}$$

Same formula applies, but variance is a factor (depends on g) of **C**, hence Bures factor is scaled.

Easy (3): Uniform Ellipses



Wasserstein Between Two Diracs

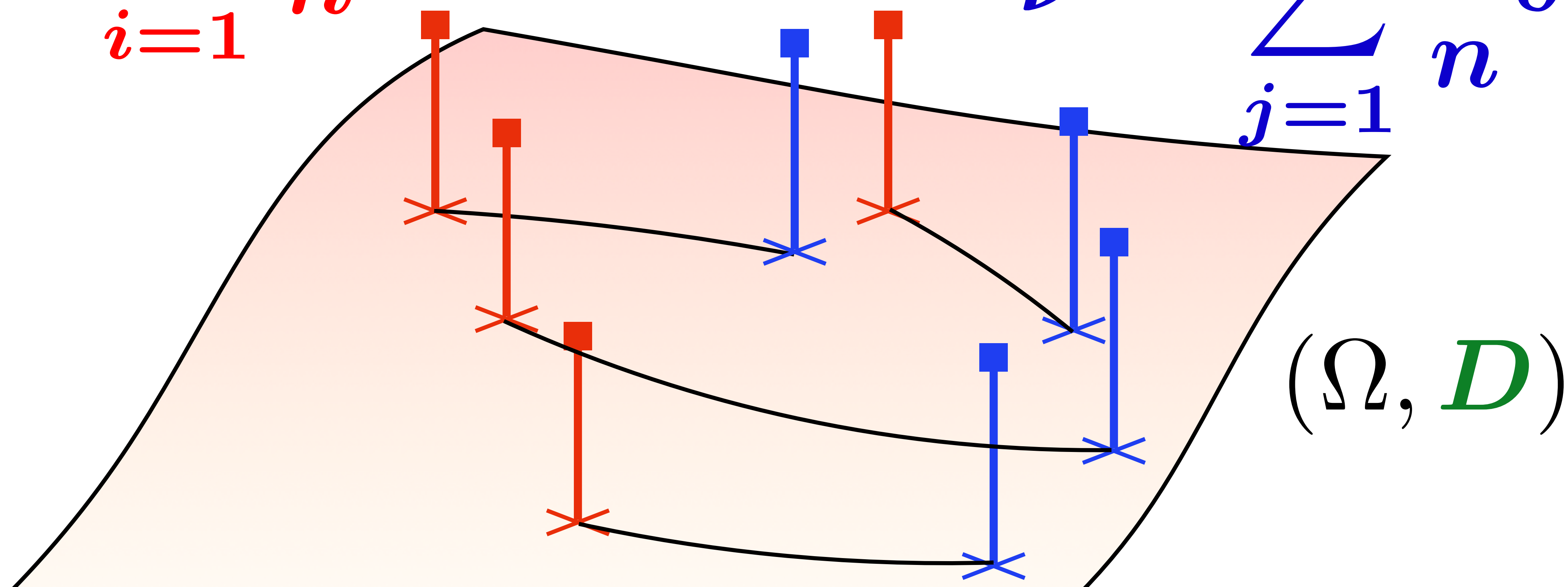


$$W_p(\delta_{\boldsymbol{x}}, \delta_{\boldsymbol{y}}) = \boldsymbol{D}(\boldsymbol{x}, \boldsymbol{y})$$

Linear Assignment $\subset$ Wasserstein

$$\boldsymbol{\mu} = \sum_{i=1}^{n} \frac{1}{n} \boldsymbol{\delta}_{\boldsymbol{x}_i}$$

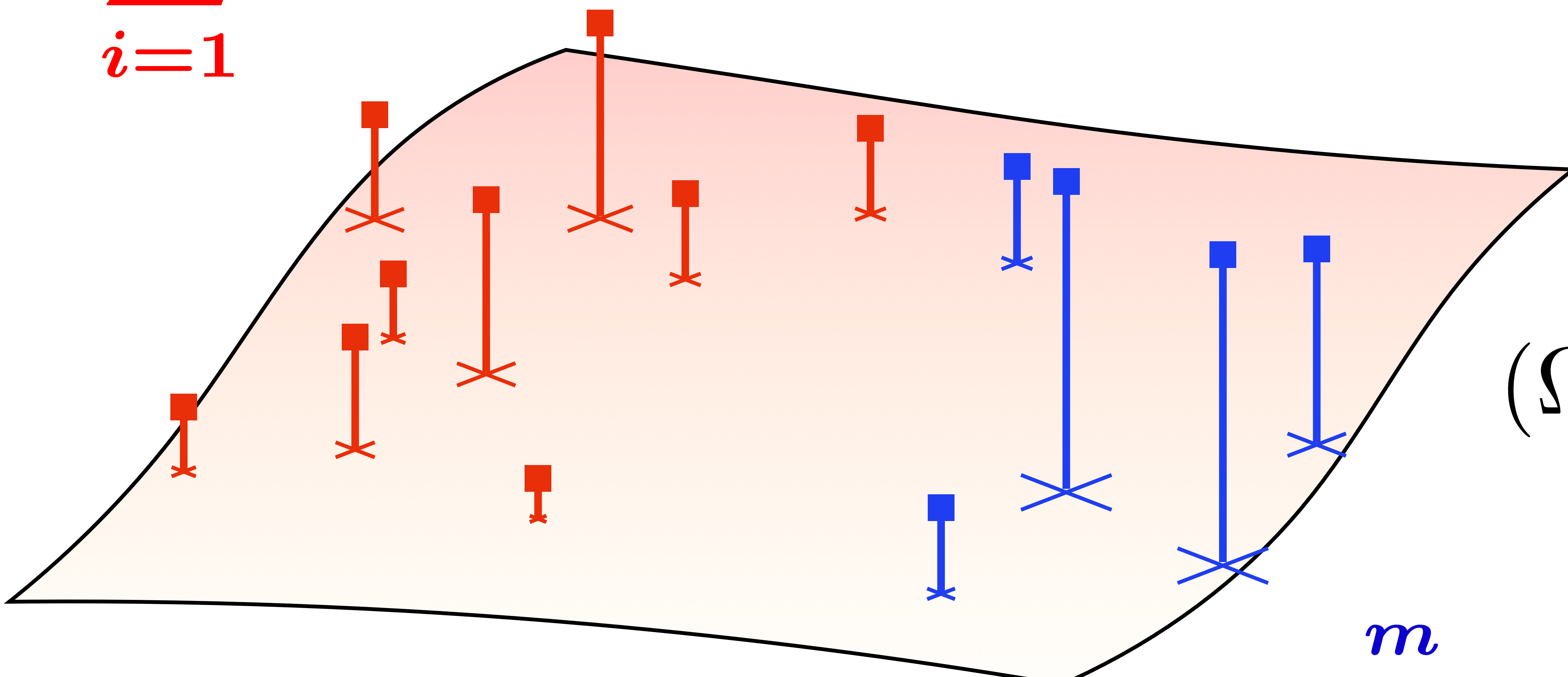
$$\boldsymbol{\nu} = \sum_{j=1}^{n} \frac{1}{n} \boldsymbol{\delta}_{\boldsymbol{y}_j}$$



$$W_p^p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \min_{\boldsymbol{\sigma} \in S_n} \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{D}(\boldsymbol{x}_i, \boldsymbol{y}_{\boldsymbol{\sigma}_i})^p$$

OT on Two Empirical Measures

$$\mu = \sum_{i=1}^{n} a_i \delta_{x_i}$$

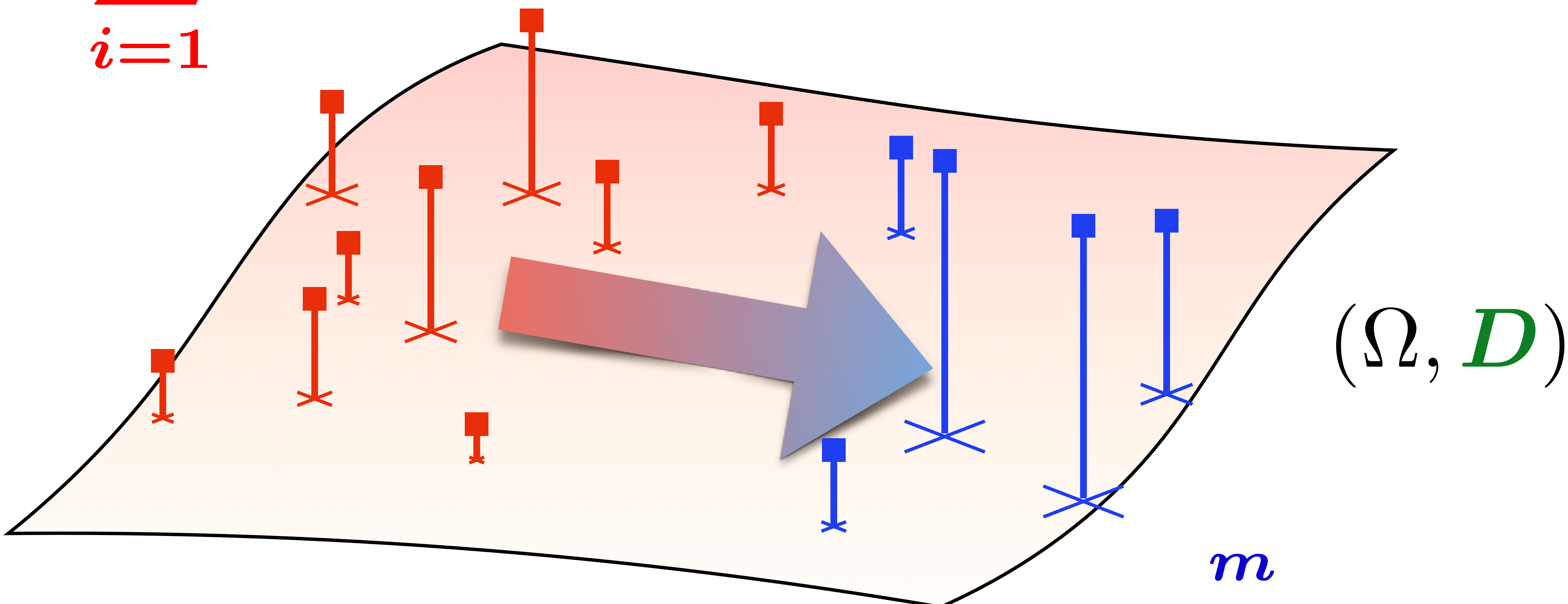


$$(\Omega, D)$$

$$\nu = \sum_{j=1}^{m} b_j \delta_{y_j}$$

OT on Two Empirical Measures

$$\mu = \sum_{i=1}^{n} a_i \delta_{x_i}$$



$$\nu = \sum_{j=1}^{m} b_j \delta_{y_j}$$

Wasserstein on Empirical Measures

Consider $\mu = \sum_{i=1}^{n} a_i \delta_{x_i}$ and $\nu = \sum_{j=1}^{m} b_j \delta_{y_j}$.

$$M_{XY} \stackrel{\text{def}}{=} [D(x_i, y_j)^p]_{ij}$$

$$U(a, b) \stackrel{\text{def}}{=} \{P \in \mathbb{R}_+^{n\times m} | P\mathbf{1}_m = a, P^T\mathbf{1}_n = b\}$$

Def. Optimal Transport Problem

$$W_p^p(\mu, \nu) = \min_{P \in U(a,b)} \langle P, M_{XY} \rangle$$

Dual Kantorovich Problem

$$W_p^p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \min_{\substack{\boldsymbol{P} \in \mathbb{R}_+^{n \times m} \\ \boldsymbol{P}\mathbf{1}_m = \boldsymbol{a}, \boldsymbol{P}^T\mathbf{1}_n = \boldsymbol{b}}} \langle \boldsymbol{P}, M_{\boldsymbol{X}\boldsymbol{Y}} \rangle$$

Dual Kantorovich Problem

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Def. Dual OT problem

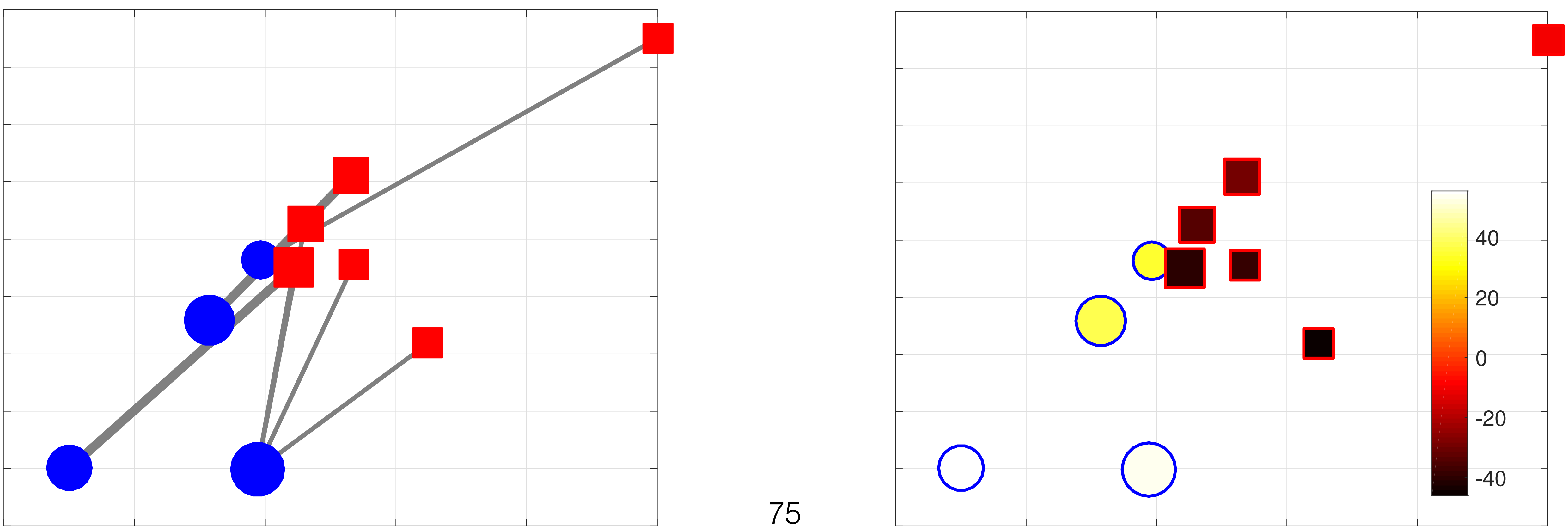
$$W_p^p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \max_{\substack{\boldsymbol{\alpha} \in \mathbb{R}^n, \boldsymbol{\beta} \in \mathbb{R}^m \\ \boldsymbol{\alpha}_i + \boldsymbol{\beta}_j \leq D(\boldsymbol{x}_i, \boldsymbol{y}_j)^p}} \alpha^T \boldsymbol{a} + \beta^T \boldsymbol{b}$$

Dual Kantorovich Problem

$$W_p^p(\boldsymbol{\mu},\boldsymbol{\nu}) = \min_{\substack{\boldsymbol{P}\in\mathbb{R}_+^{n\times m}\\ \boldsymbol{P}\mathbf{1}_m=\boldsymbol{a},\boldsymbol{P}^T\mathbf{1}_n=\boldsymbol{b}}} \langle \boldsymbol{P}, M_{\boldsymbol{XY}} \rangle$$

Def. Dual OT problem

$$W_p^p(\boldsymbol{\mu},\boldsymbol{\nu}) = \max_{\substack{\boldsymbol{\alpha}\in\mathbb{R}^n,\boldsymbol{\beta}\in\mathbb{R}^m\\ \boldsymbol{\alpha}_{\boldsymbol{i}}+\boldsymbol{\beta}_{\boldsymbol{j}}\leq D(\boldsymbol{x}_{\boldsymbol{i}},\boldsymbol{y}_{\boldsymbol{j}})^p}} \alpha^T\boldsymbol{a} + \beta^T\boldsymbol{b}$$



Dual Kantorovich Problem

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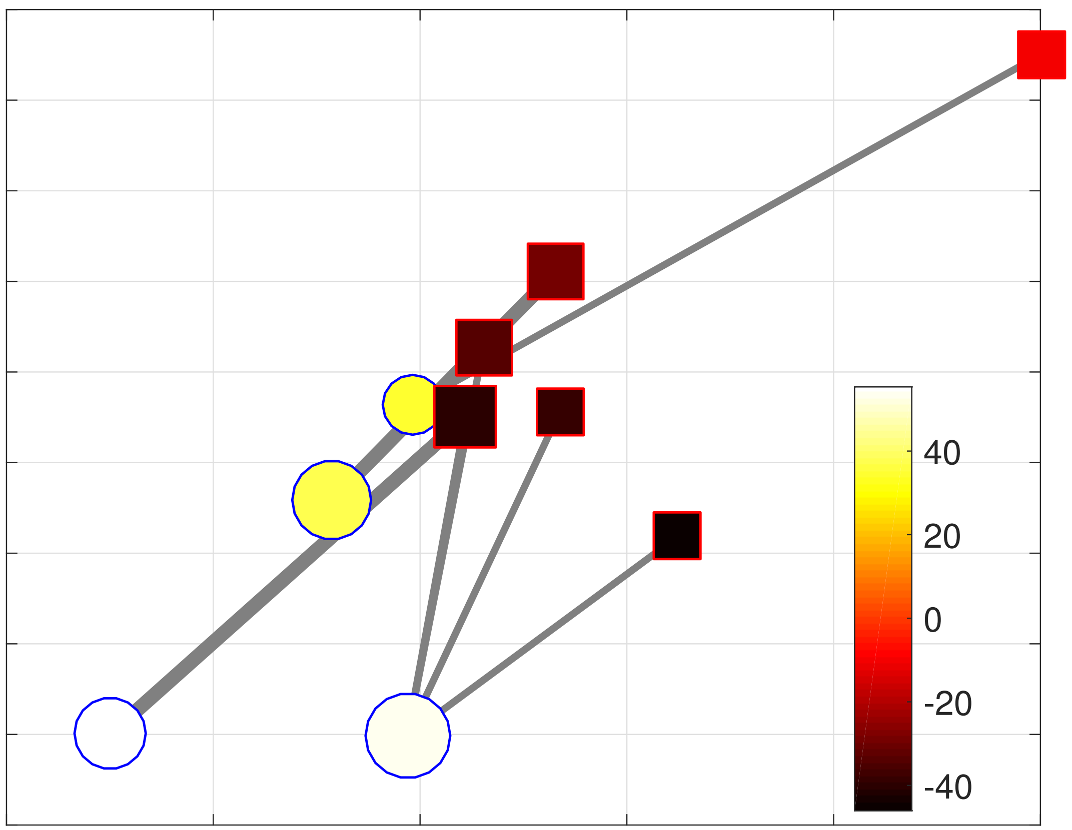
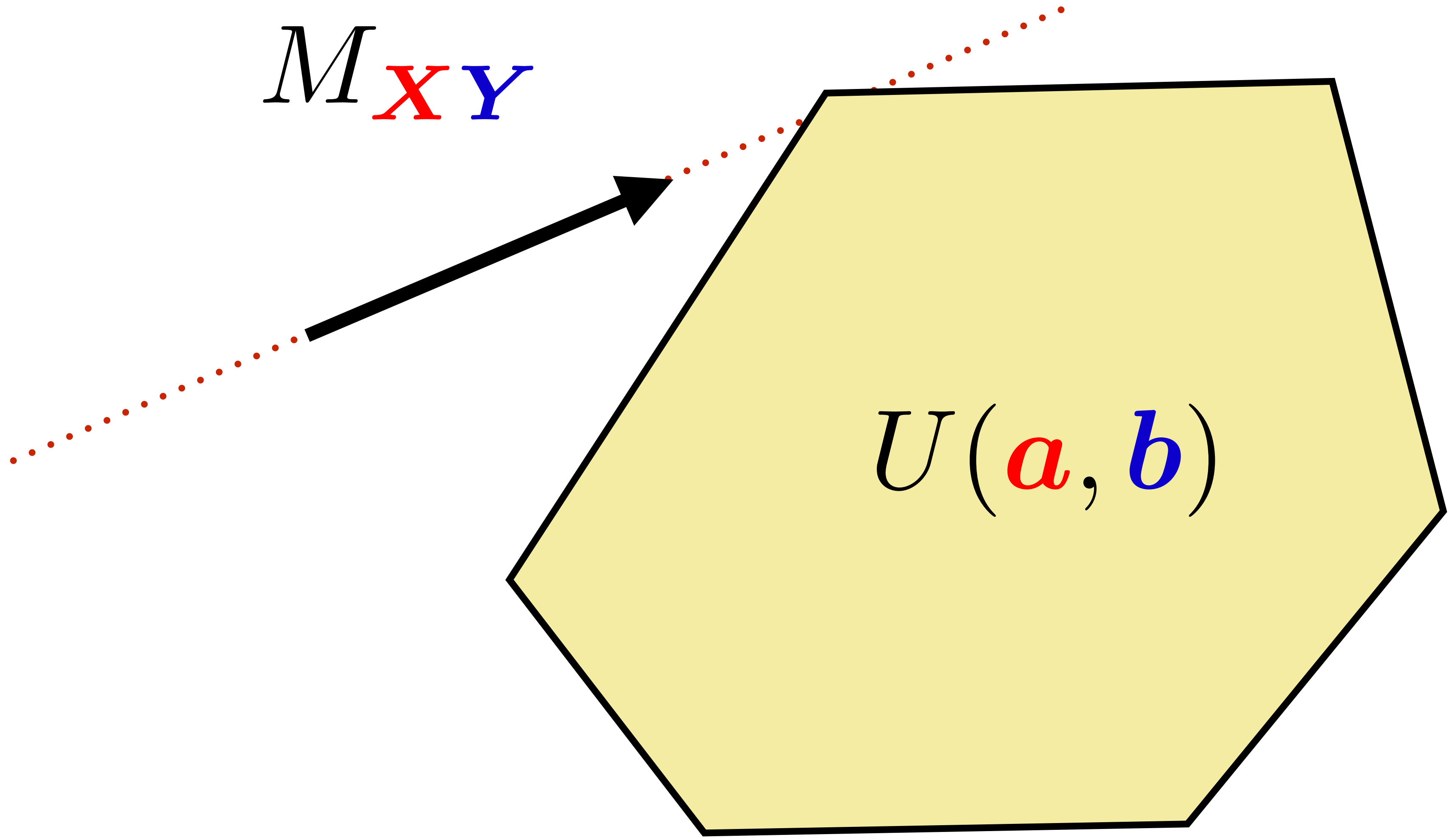
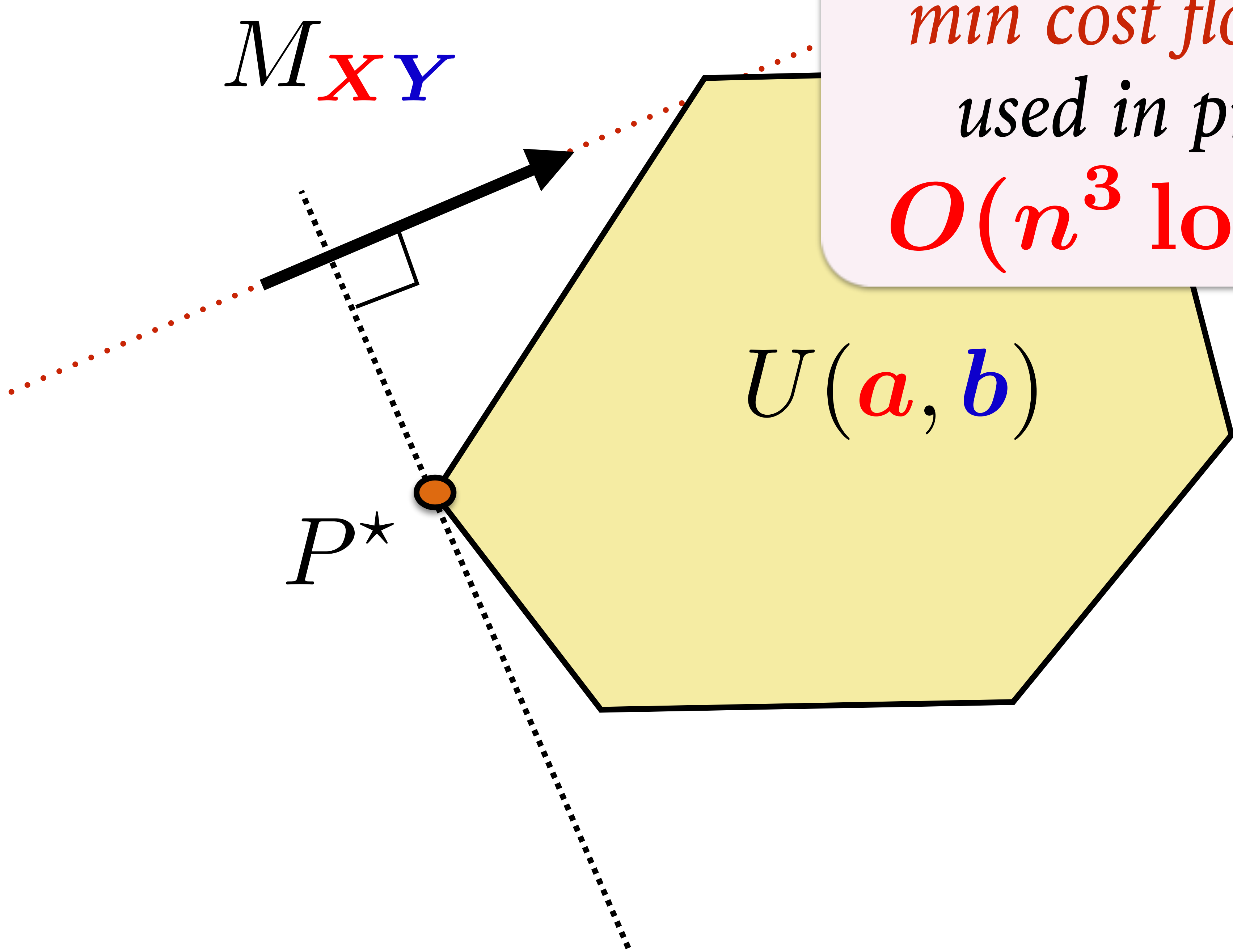
$$W_p^p(\boldsymbol{\mu},\boldsymbol{\nu}) = \max_{\substack{\boldsymbol{\alpha}\in\mathbb{R}^n,\boldsymbol{\beta}\in\mathbb{R}^m\\ \boldsymbol{\alpha}_{\boldsymbol{i}}+\boldsymbol{\beta}_{\boldsymbol{j}}\leq D(\boldsymbol{x}_{\boldsymbol{i}},\boldsymbol{y}_{\boldsymbol{j}})^p}} \alpha^T\boldsymbol{a}+\beta^T\boldsymbol{b}$$



Solving the OT Problem

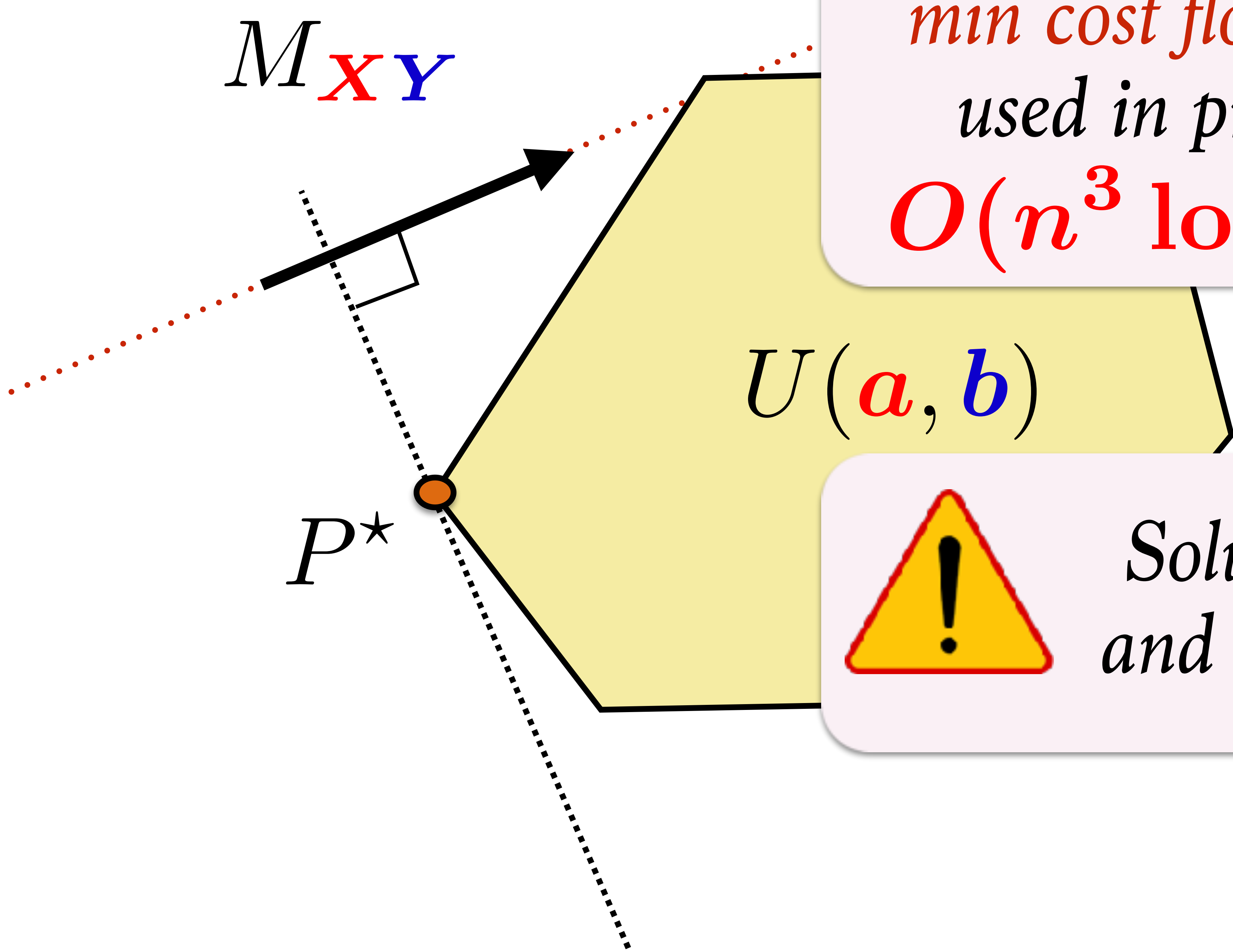


Solving the OT Problem



min cost flow solver
used in practice.
$O(n^3 \log(n))$

Solving the OT Problem



min cost flow solver *used in practice.*

$O(n^3 \log(n))$

Solution $P^\star$ *unstable and not always unique.*

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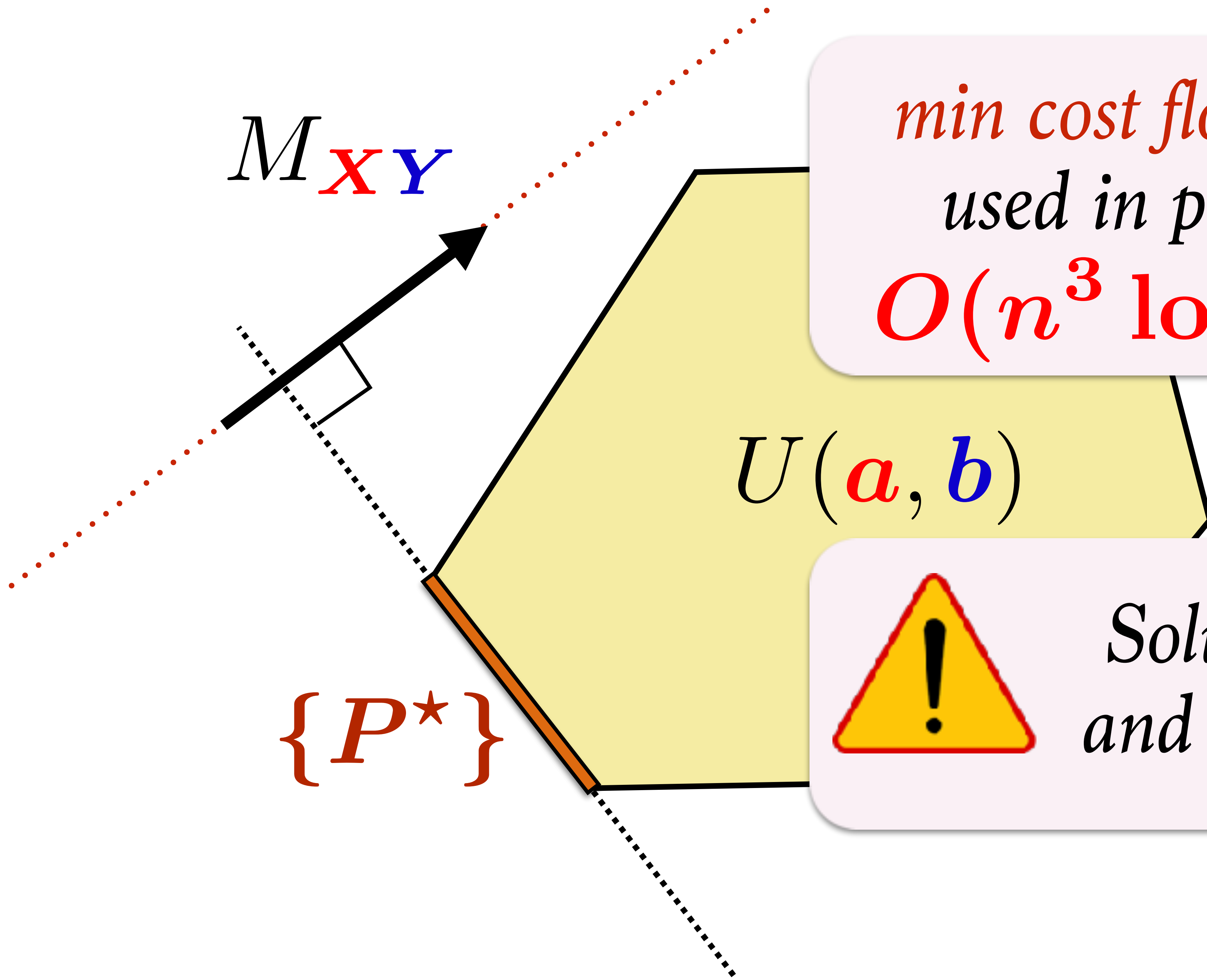

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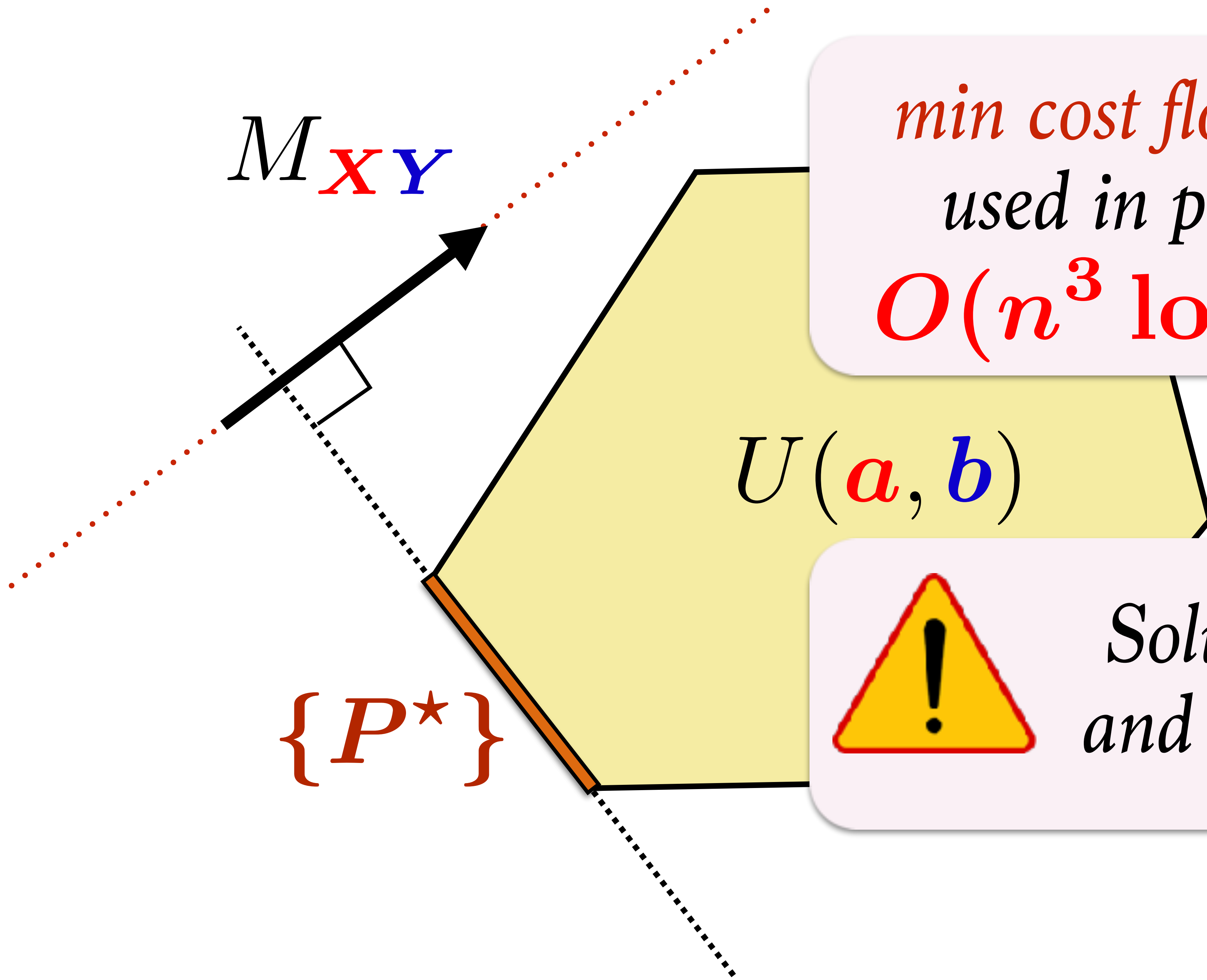

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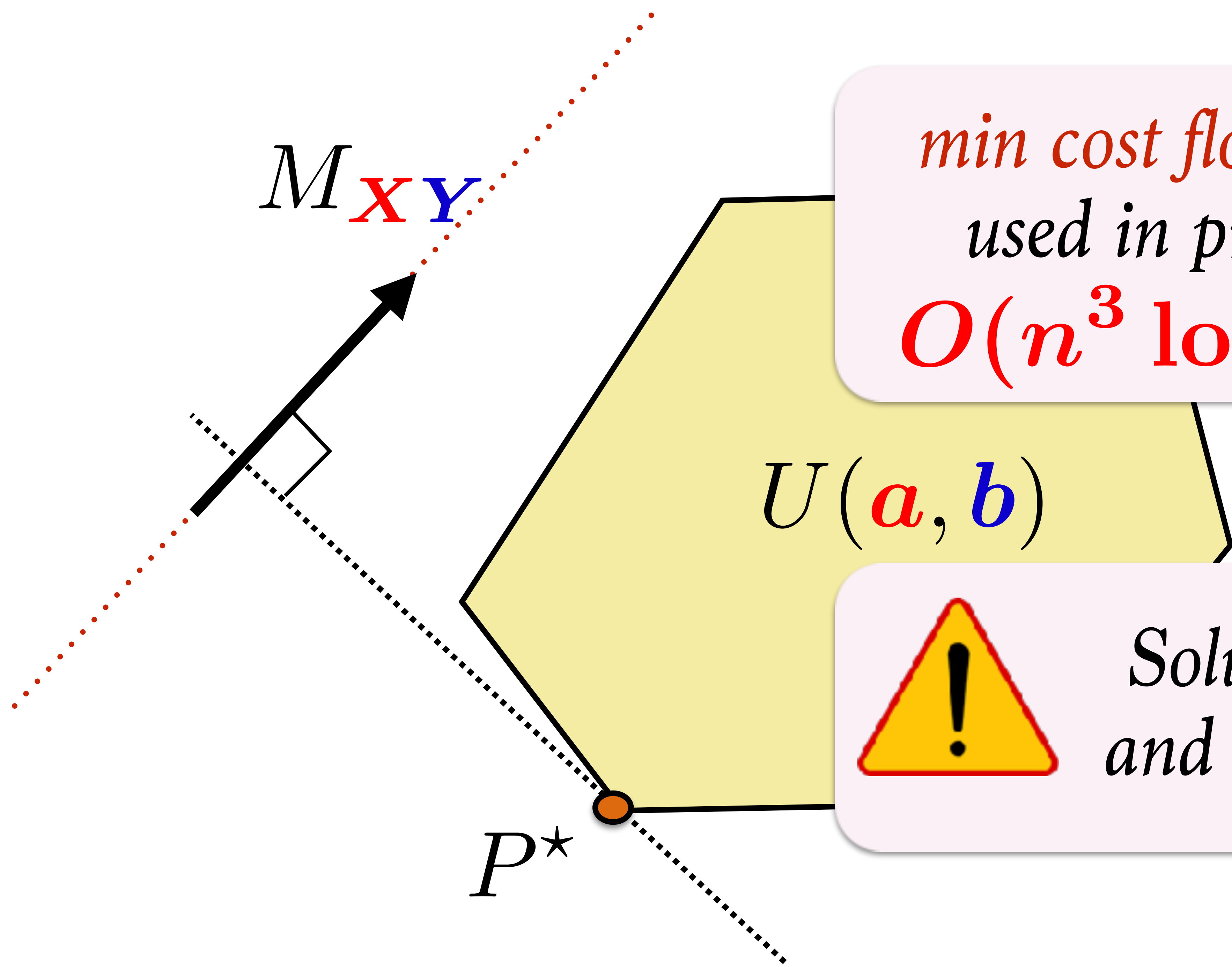

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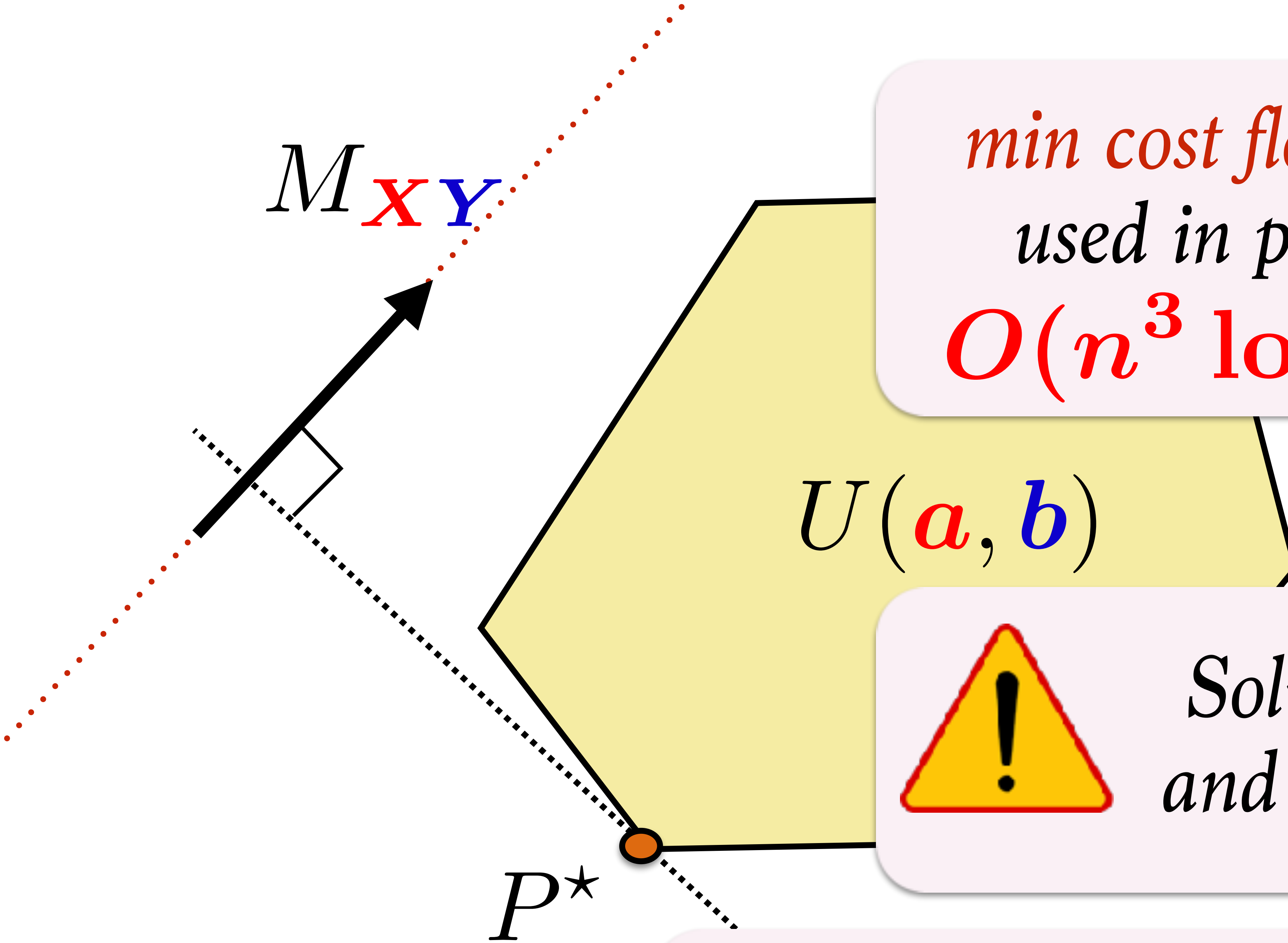

min cost flow solver *used in practice.* $O(n^3 \log(n))$

Solution $P^\star$ *unstable and not always unique.*

$W_p^p(\boldsymbol{\mu}, \boldsymbol{\nu})$ not differentiable.

Discrete OT Problem

```c
/*
    emd.c

    Last update: 3/14/98

    An implementation of the Earth Movers Distance.
    Based of the solution for the Transportation problem as described in
    "Introduction to Mathematical Programming" by F. S. Hillier and
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    Copyright (C) 1998 Yossi Rubner
    Computer Science Department, Stanford University
    E-Mail: rubner@cs.stanford.edu   URL: http://vision.stanford.edu/~rubner
*/

/*#include <stdio.h>
#include <stdlib.h>*/
#include <math.h>

#include "emd.h"

#define DEBUG_LEVEL 0
/*
 DEBUG_LEVEL:
   0 = NO MESSAGES
   1 = PRINT THE NUMBER OF ITERATIONS AND THE FINAL RESULT
   2 = PRINT THE RESULT AFTER EVERY ITERATION
   3 = PRINT ALSO THE FLOW AFTER EVERY ITERATION
   4 = PRINT A LOT OF INFORMATION (PROBABLY USEFUL ONLY FOR THE AUTHOR)
*/


#define MAX_SIG_SIZE1  (MAX_SIG_SIZE+1)  /* FOR THE POSIBLE DUMMY FEATURE */

/* NEW TYPES DEFINITION */

/* node1_t IS USED FOR SINGLE-LINKED LISTS */
typedef struct node1_t {
  int i;
  double val;
  struct node1_t *Next;
} node1_t;

/* node1_t IS USED FOR DOUBLE-LINKED LISTS */
typedef struct node2_t {
  int i, j;
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/* GLOBAL VARIABLE DECLARATION */
static int _n1, _n2;                          /* SIGNATURES SIZES */
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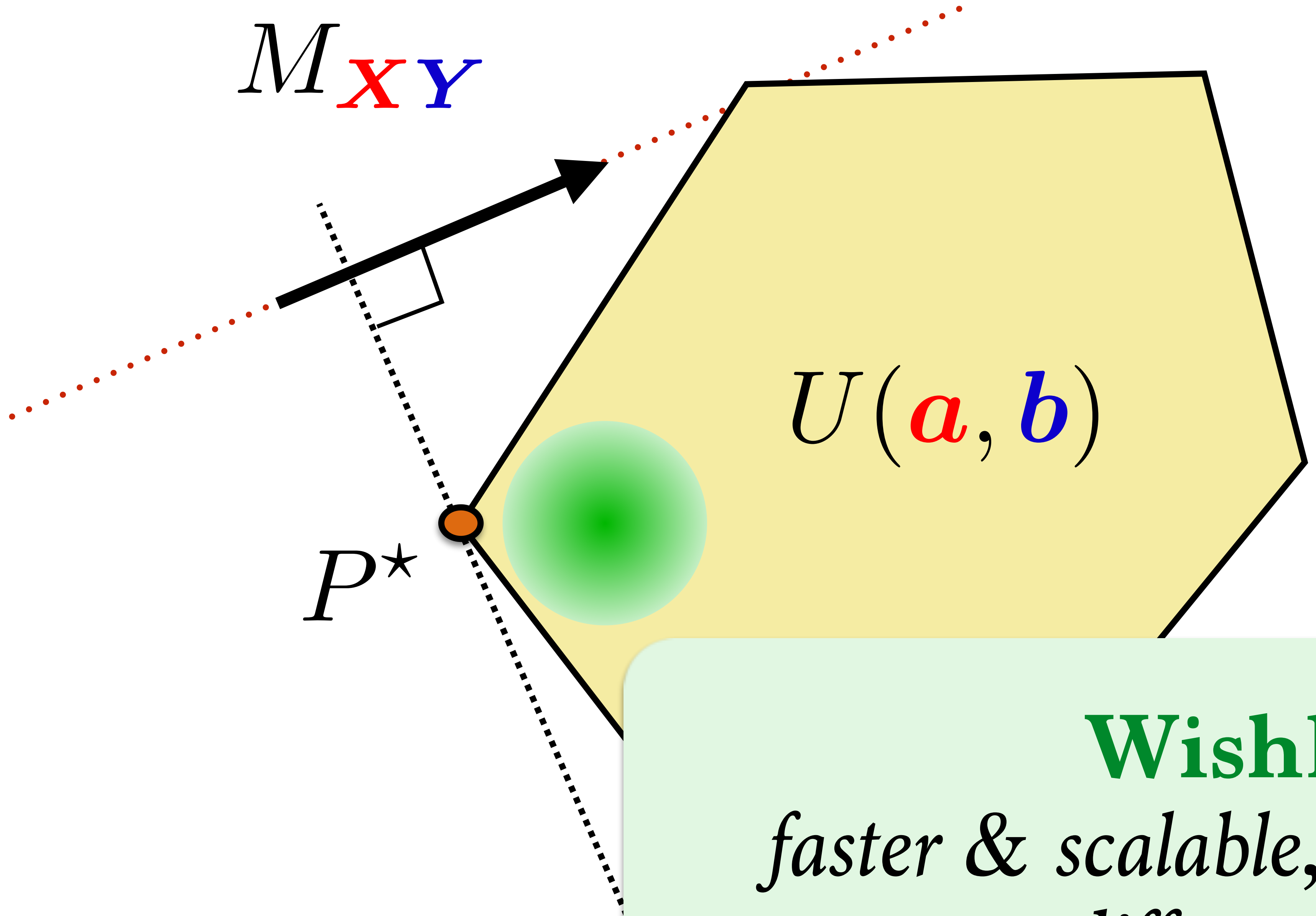
Solution: Regularization



Wishlist:
faster & *scalable*, more *stable*,
differentiable

Entropic Regularization [Wilson'62]

Def. Regularized Wasserstein, $\gamma \geq 0$

$$W_\gamma(\boldsymbol{\mu}, \boldsymbol{\nu}) \stackrel{\text{def}}{=} \min_{\boldsymbol{P} \in U(\boldsymbol{a}, \boldsymbol{b})} \langle \boldsymbol{P}, M_{\boldsymbol{XY}} \rangle - \gamma E(\boldsymbol{P})$$

$$E(P) \stackrel{\text{def}}{=} - \sum_{i,j=1}^{nm} P_{ij} (\log P_{ij} - 1)$$

Note: Unique optimal solution because of strong concavity of entropy

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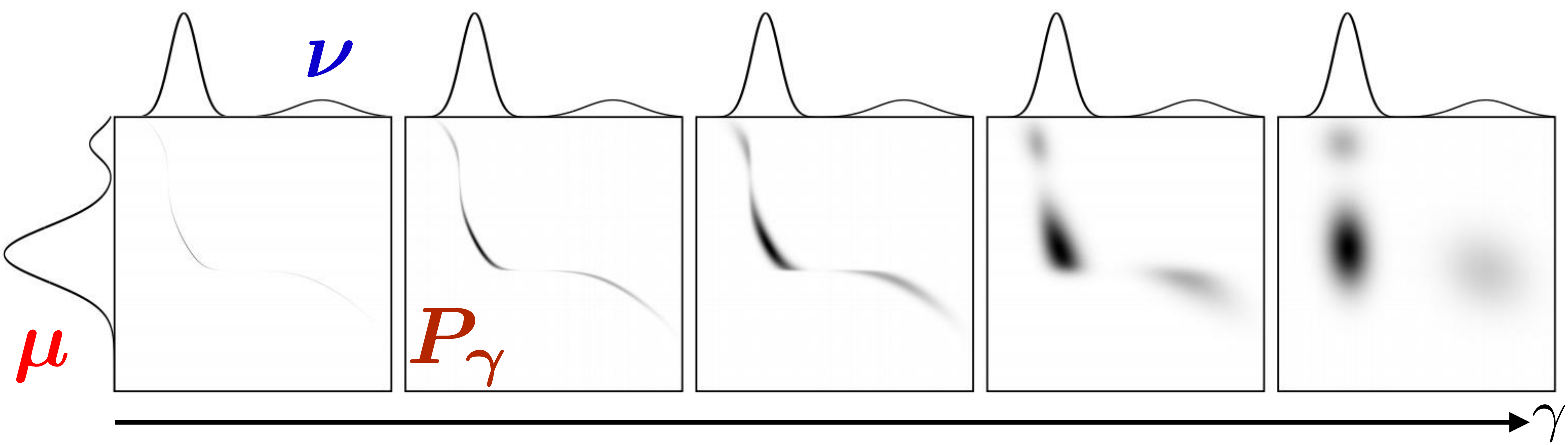

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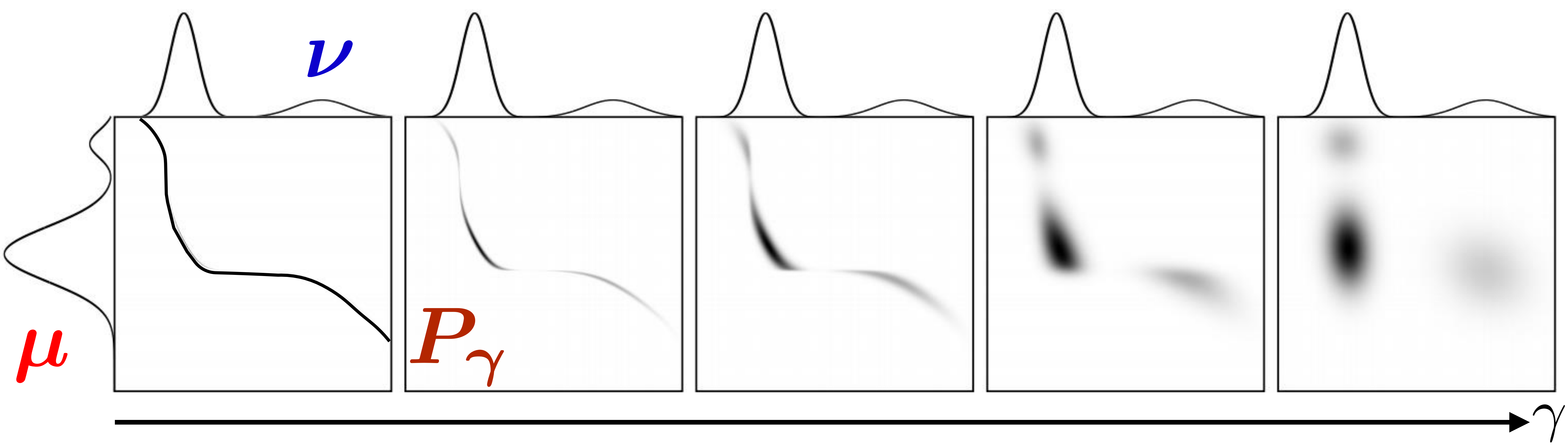

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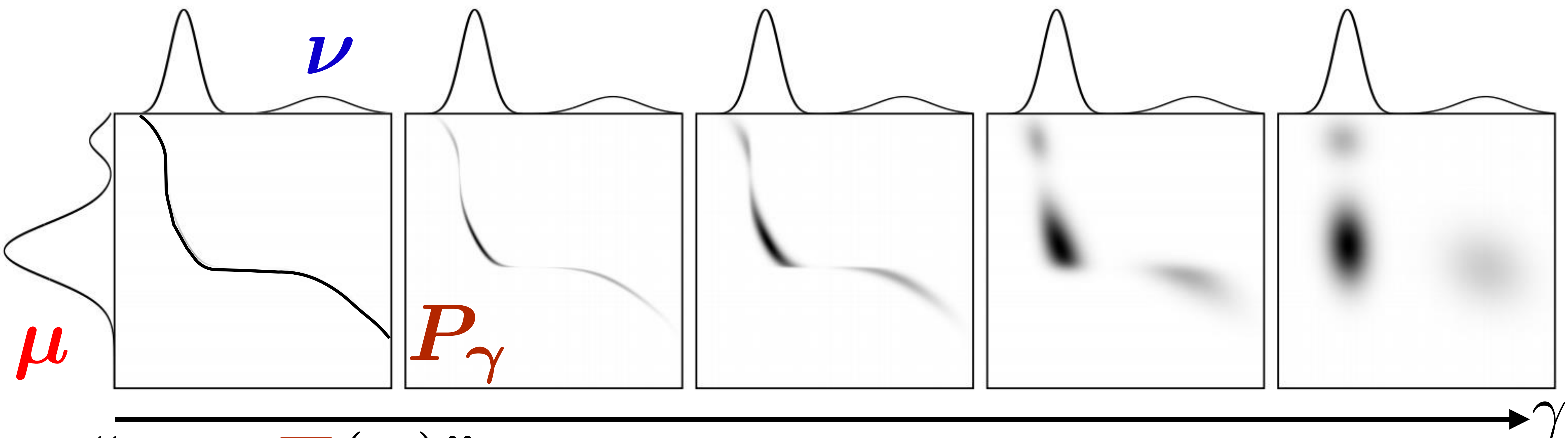

$\approx$ "$\boldsymbol{y} = \boldsymbol{T}(\boldsymbol{x})$"

Note: Unique optimal solution because of strong concavity of entropy

Fast & Scalable Algorithm

Prop. If $P_\gamma \stackrel{\text{def}}{=} \underset{\boldsymbol{P}\in U(\boldsymbol{a},\boldsymbol{b})}{\operatorname{argmin}} \langle \boldsymbol{P}, M_{\boldsymbol{XY}} \rangle - \gamma E(\boldsymbol{P})$

then $\exists! \boldsymbol{u} \in \mathbb{R}_+^n, \boldsymbol{v} \in \mathbb{R}_+^m$, such that

$$P_\gamma = \mathbf{diag}(\boldsymbol{u}) K \mathbf{diag}(\boldsymbol{v}), \quad K \stackrel{\text{def}}{=} e^{-M_{\boldsymbol{XY}}/\gamma}$$

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$$L(P,\alpha,\beta) = \sum_{ij} P_{ij} M_{ij} + \gamma P_{ij}(\log P_{ij} - 1) + \alpha^T(P\mathbf{1} - \boldsymbol{a}) + \beta^T(P^T\mathbf{1} - \boldsymbol{b})$$

$$\partial L / \partial P_{ij} = M_{ij} + \gamma \log P_{ij} + \alpha_i + \beta_j$$

$$(\boldsymbol{\partial L / \partial P_{ij}} = 0) \Rightarrow P_{ij} = \boldsymbol{e}^{\frac{\boldsymbol{\alpha_i}}{\boldsymbol{\gamma}}} \; e^{-\frac{M_{ij}}{\gamma}} \; \boldsymbol{e}^{\frac{\boldsymbol{\beta_j}}{\boldsymbol{\gamma}}} = \boldsymbol{u_i} \, K_{ij} \boldsymbol{v_j}$$

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Fast & Scalable Algorithm

Sinkhorn's Algorithm : Repeat

1. $\boldsymbol{u} = \boldsymbol{a} / K\boldsymbol{v}$
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- **[Sinkhorn'64]** proved convergence for the first time.
- **[Lorenz'89]** linear convergence, see **[Altschuler'17]**
- $O(nm)$ complexity, GPGPU parallel **[Cuturi'13]** .
- $O(n \log n)$ on gridded spaces using convolutions. **[Solomon'15]**

Fast & Scalable Algorithm

- **[Sinkhorn'64]** fixed-point iterations for $(\boldsymbol{u}, \boldsymbol{v})$

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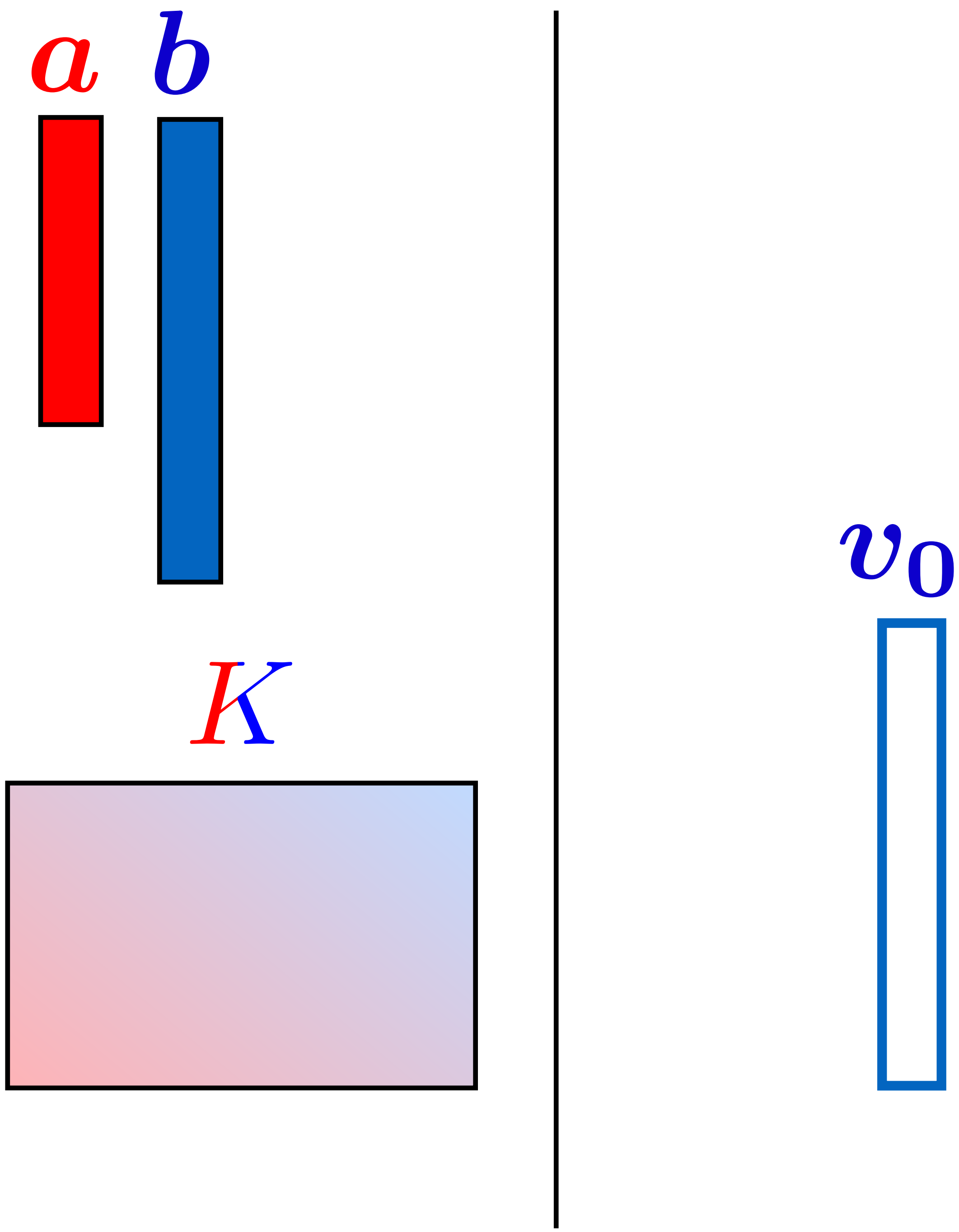

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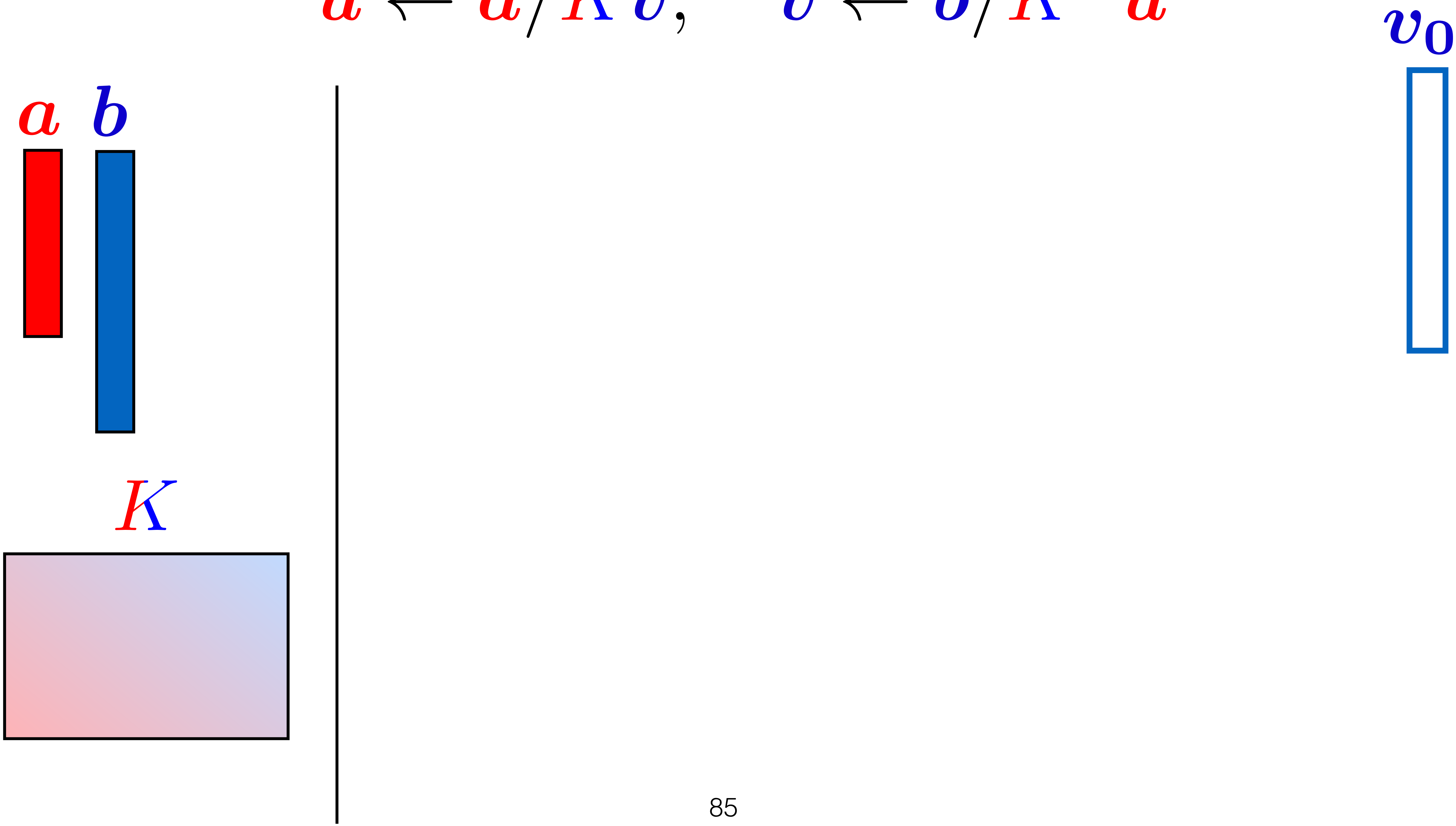

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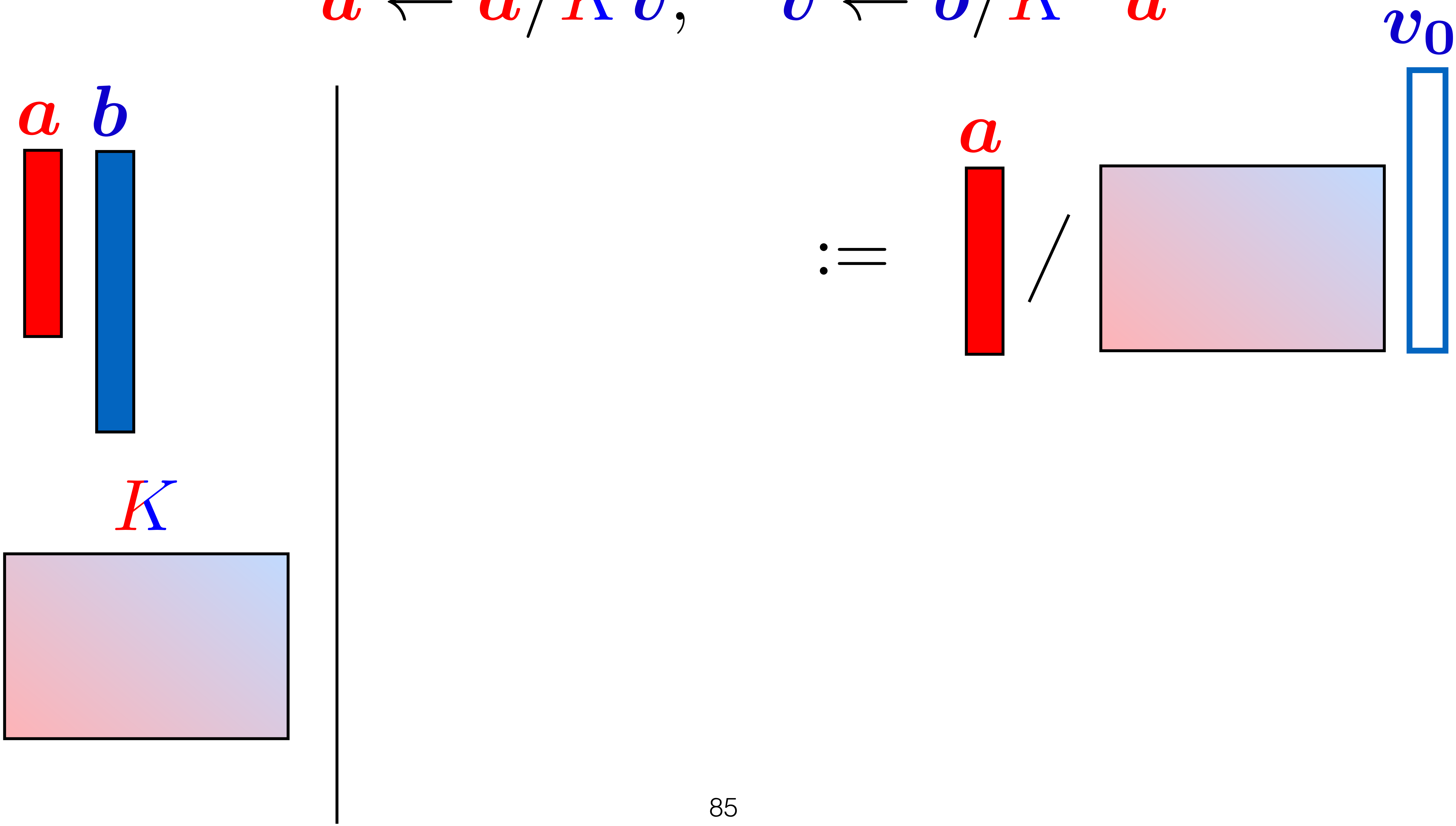

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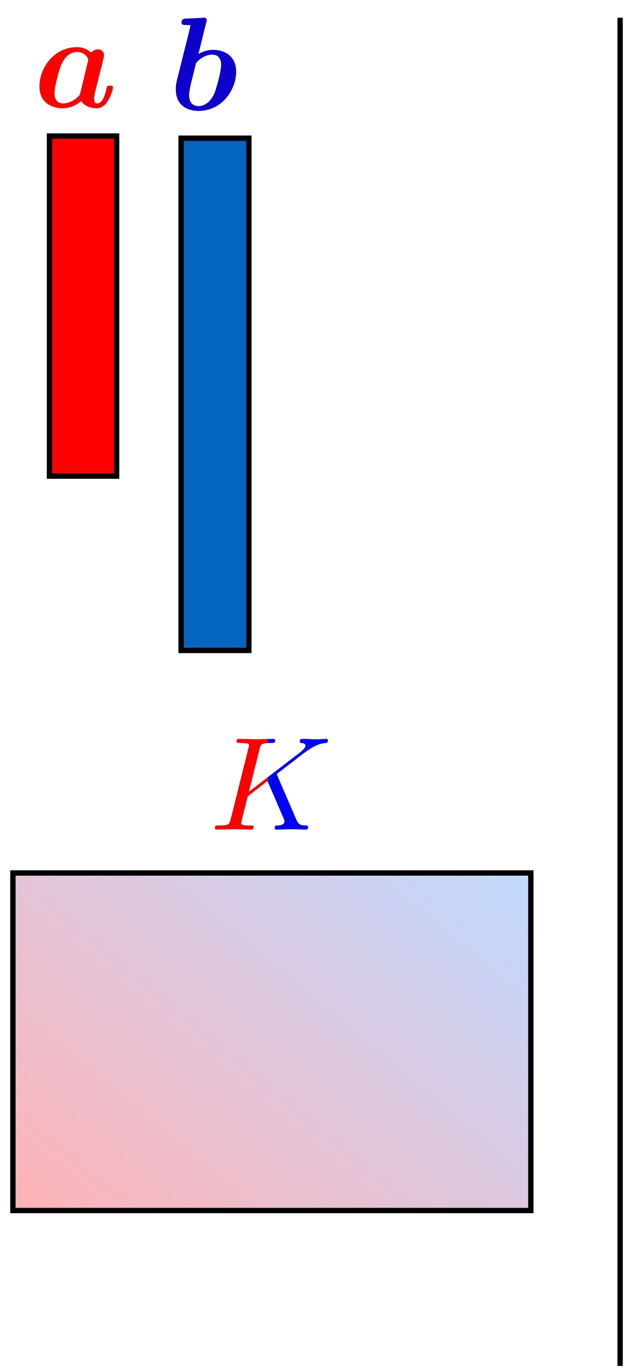

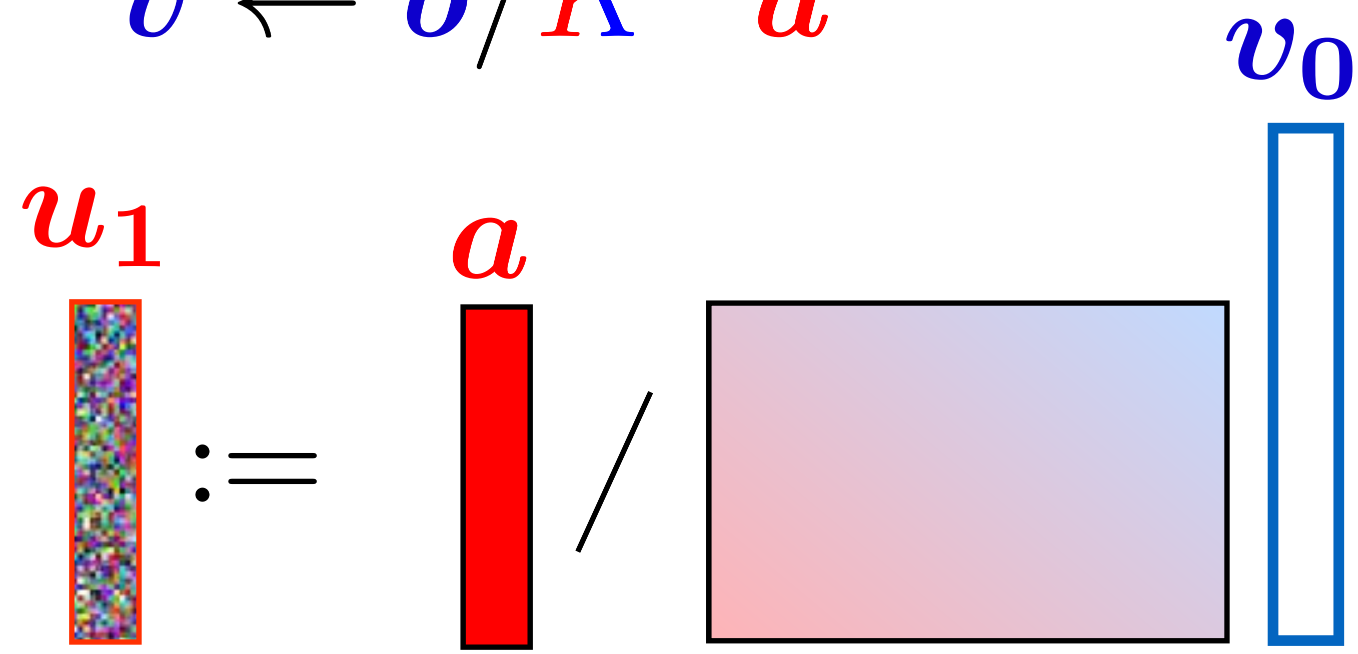

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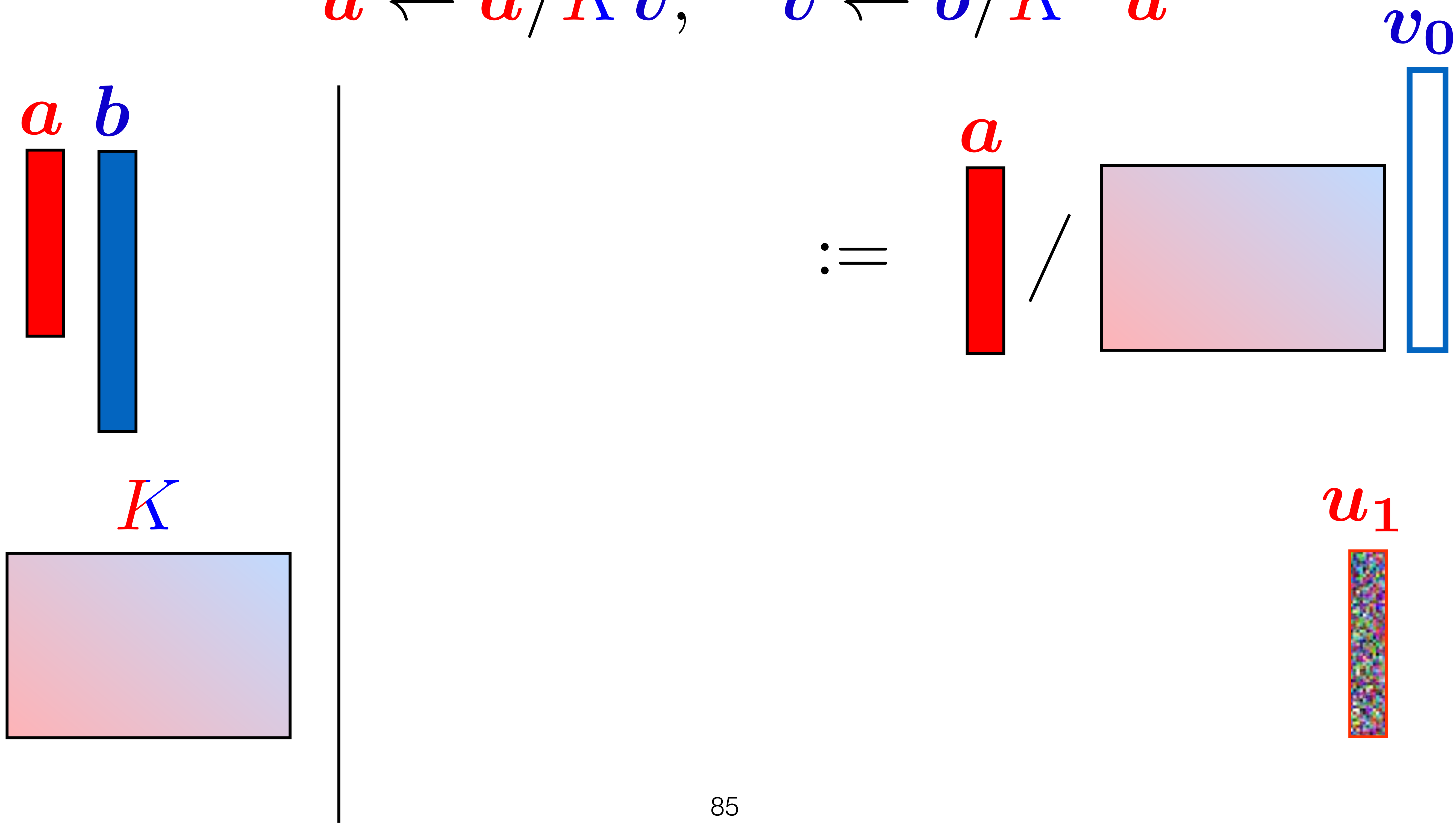

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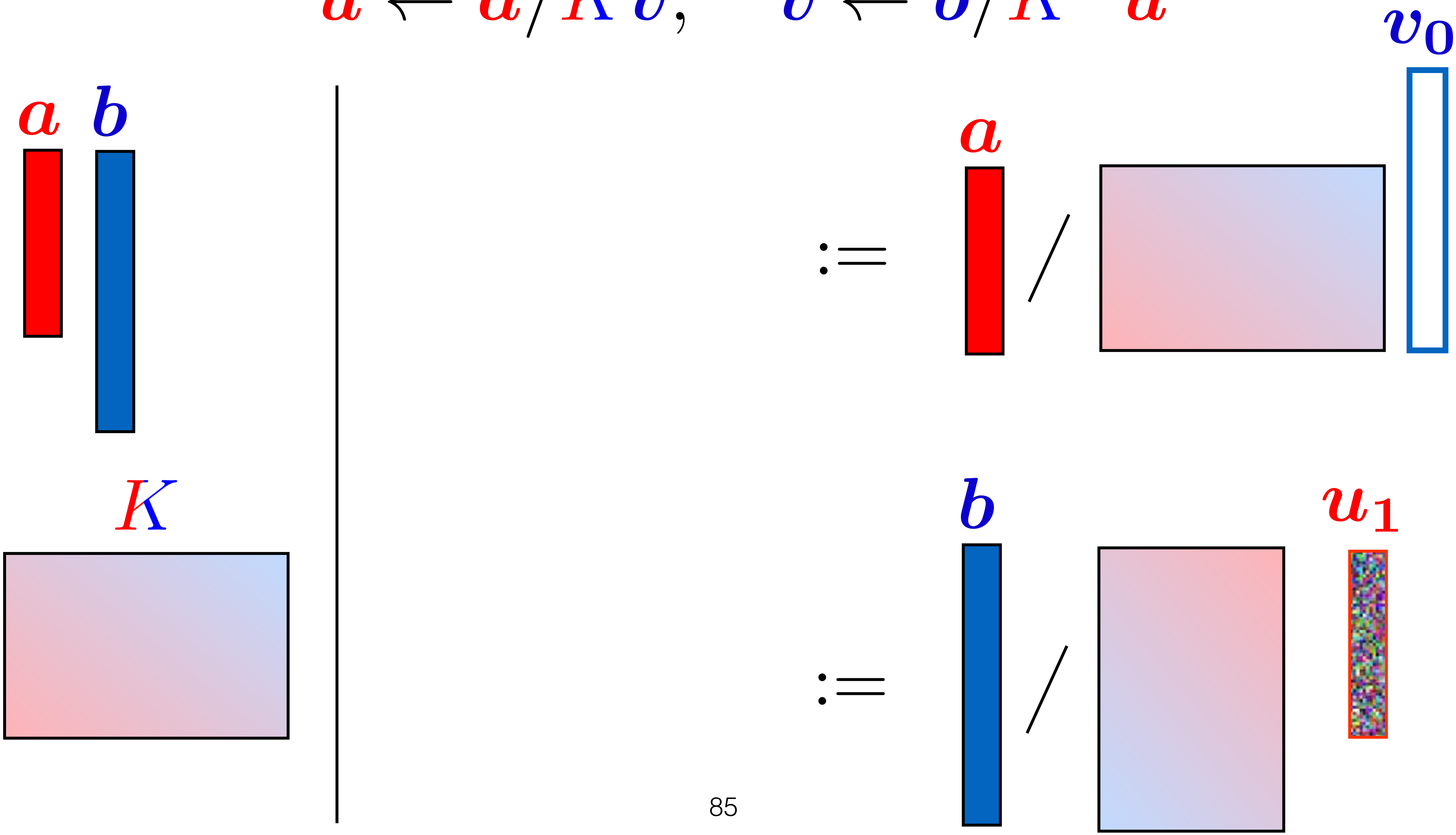

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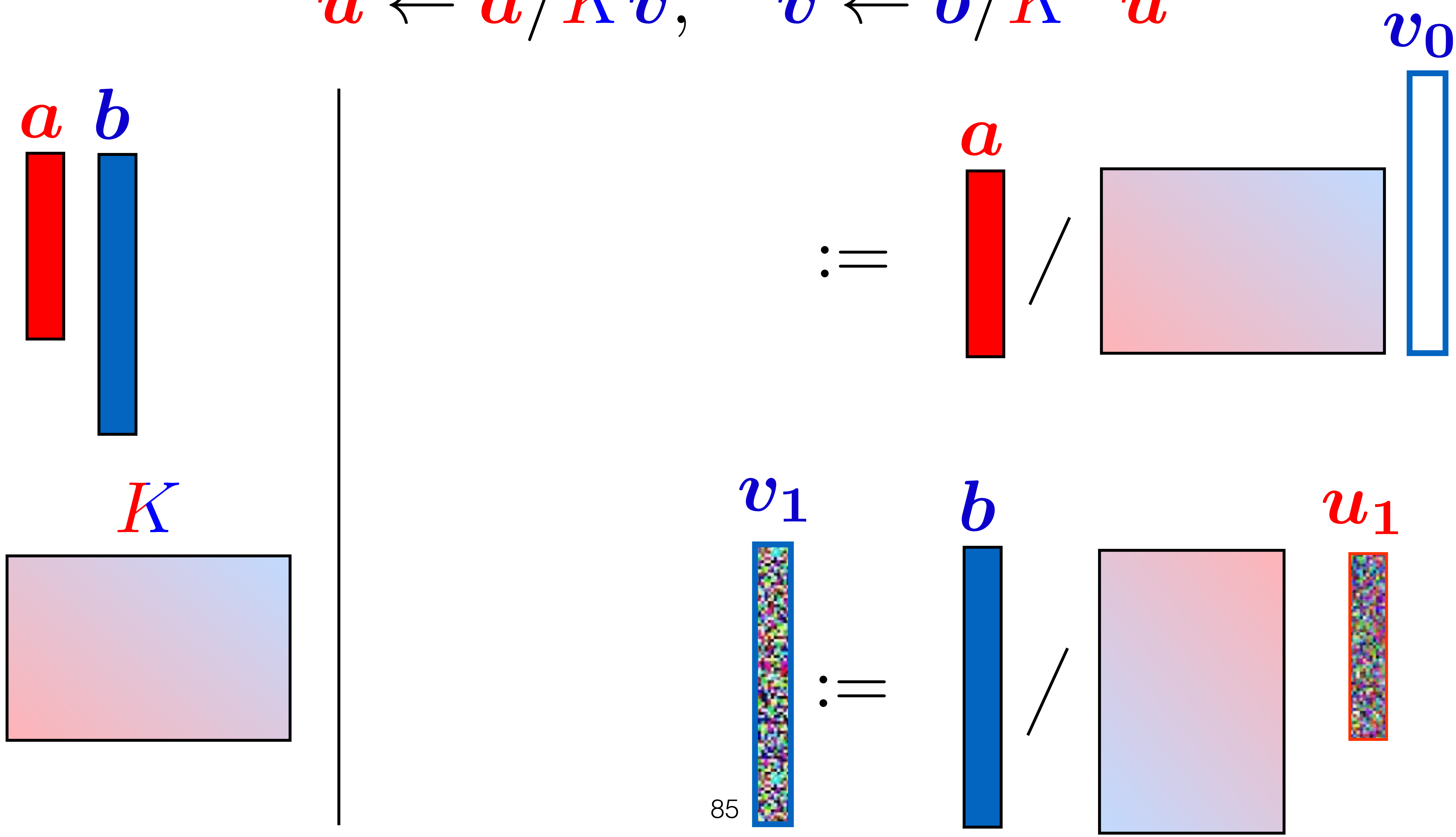

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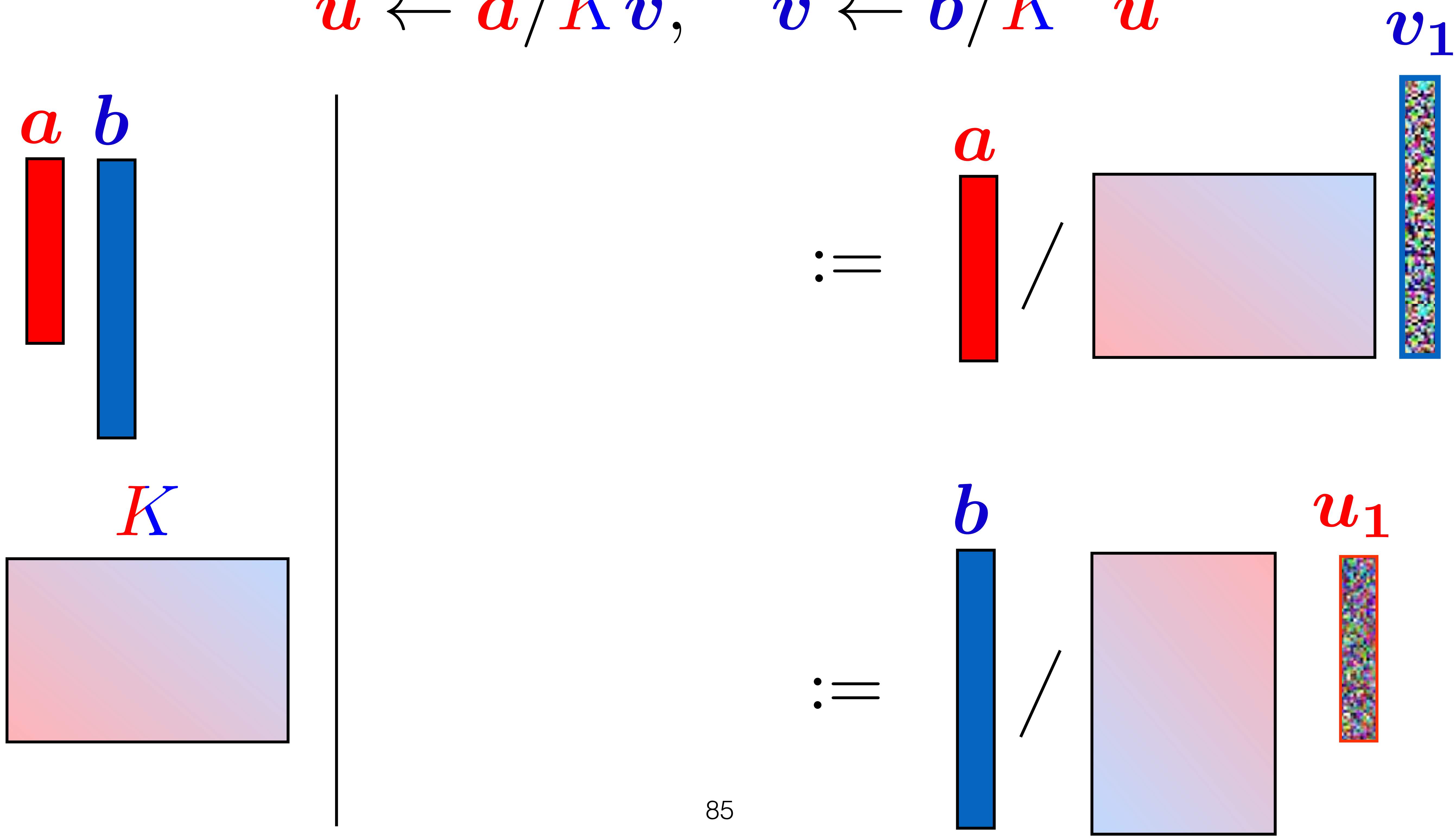

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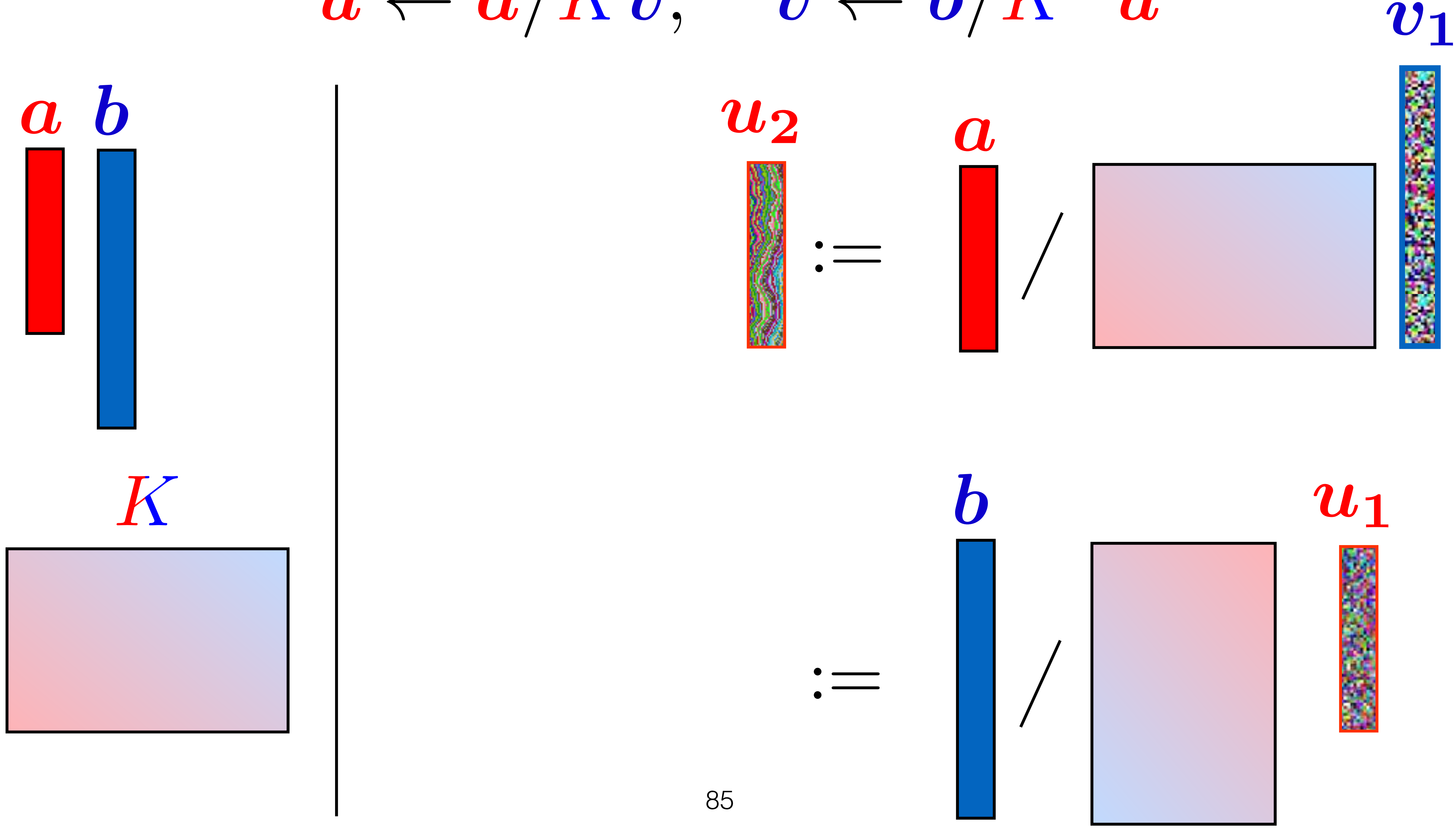

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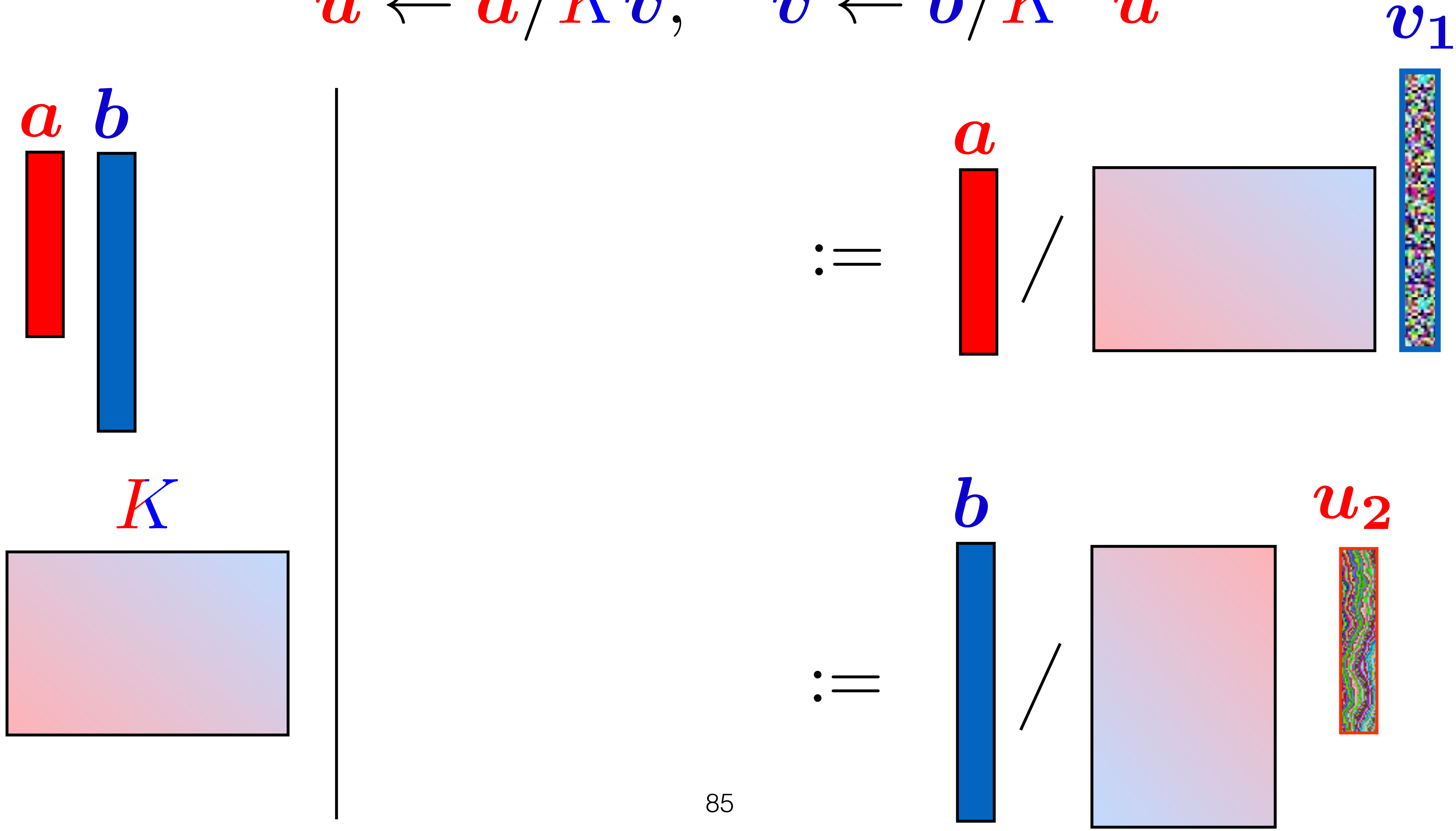

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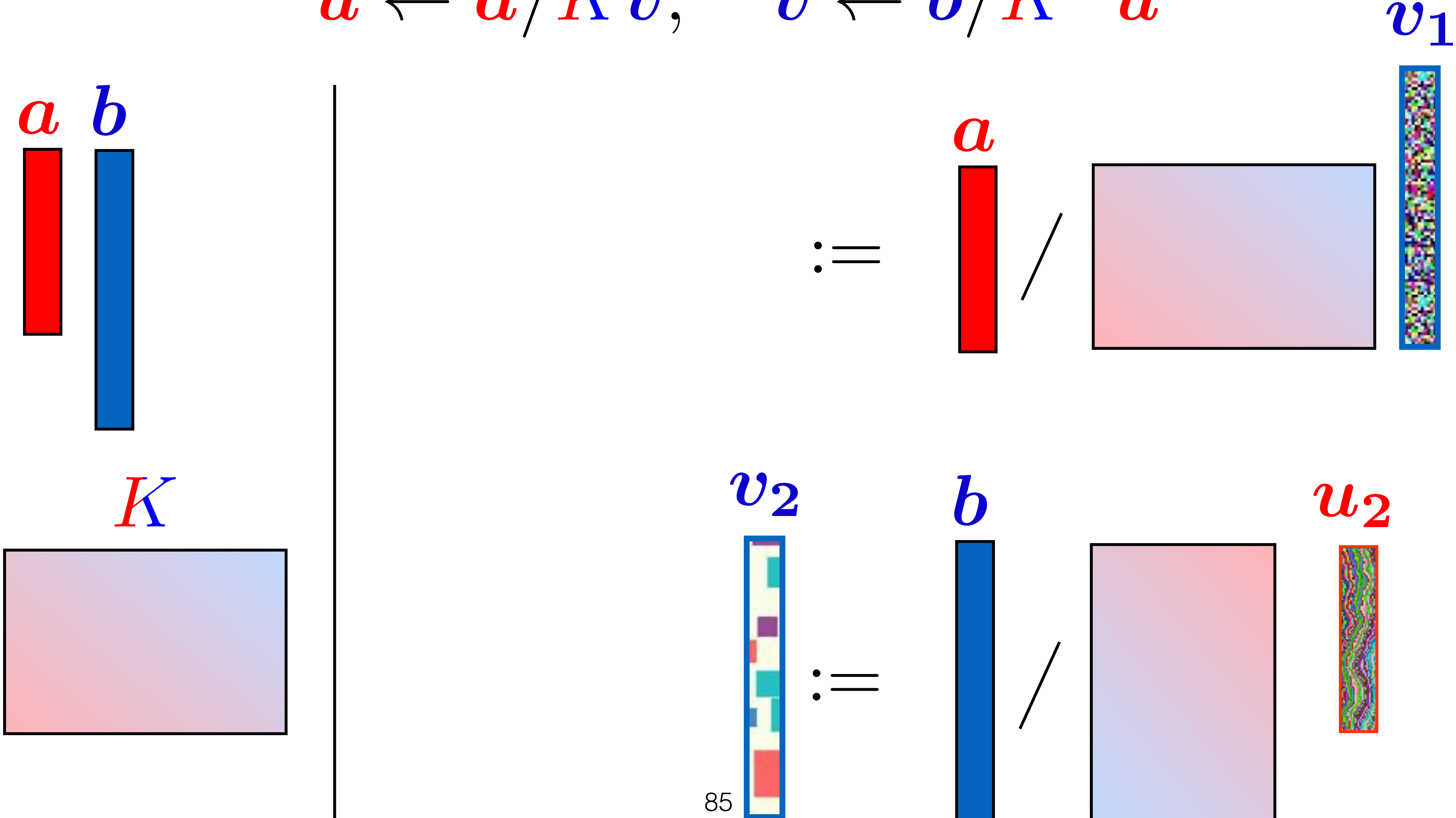

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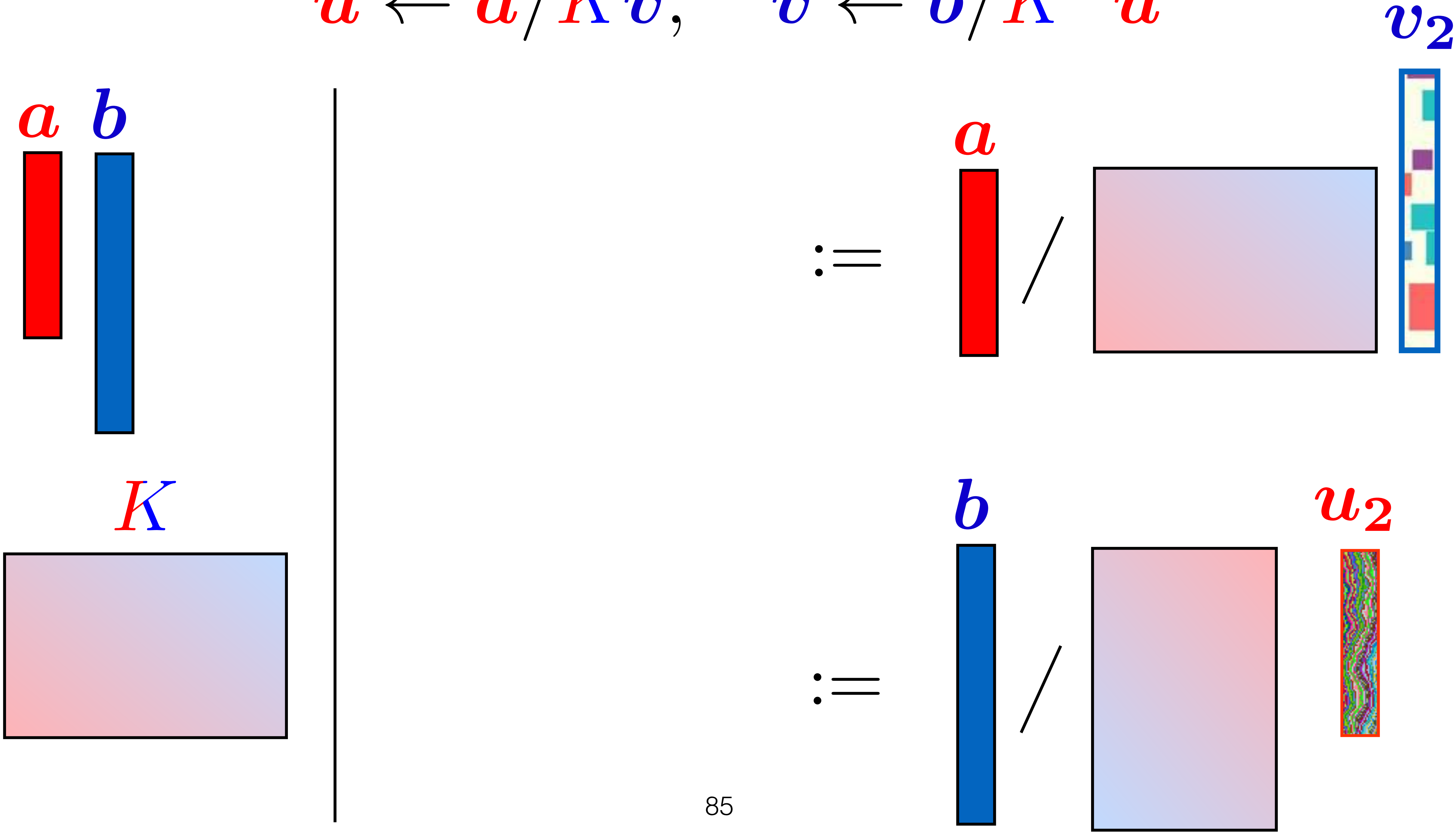

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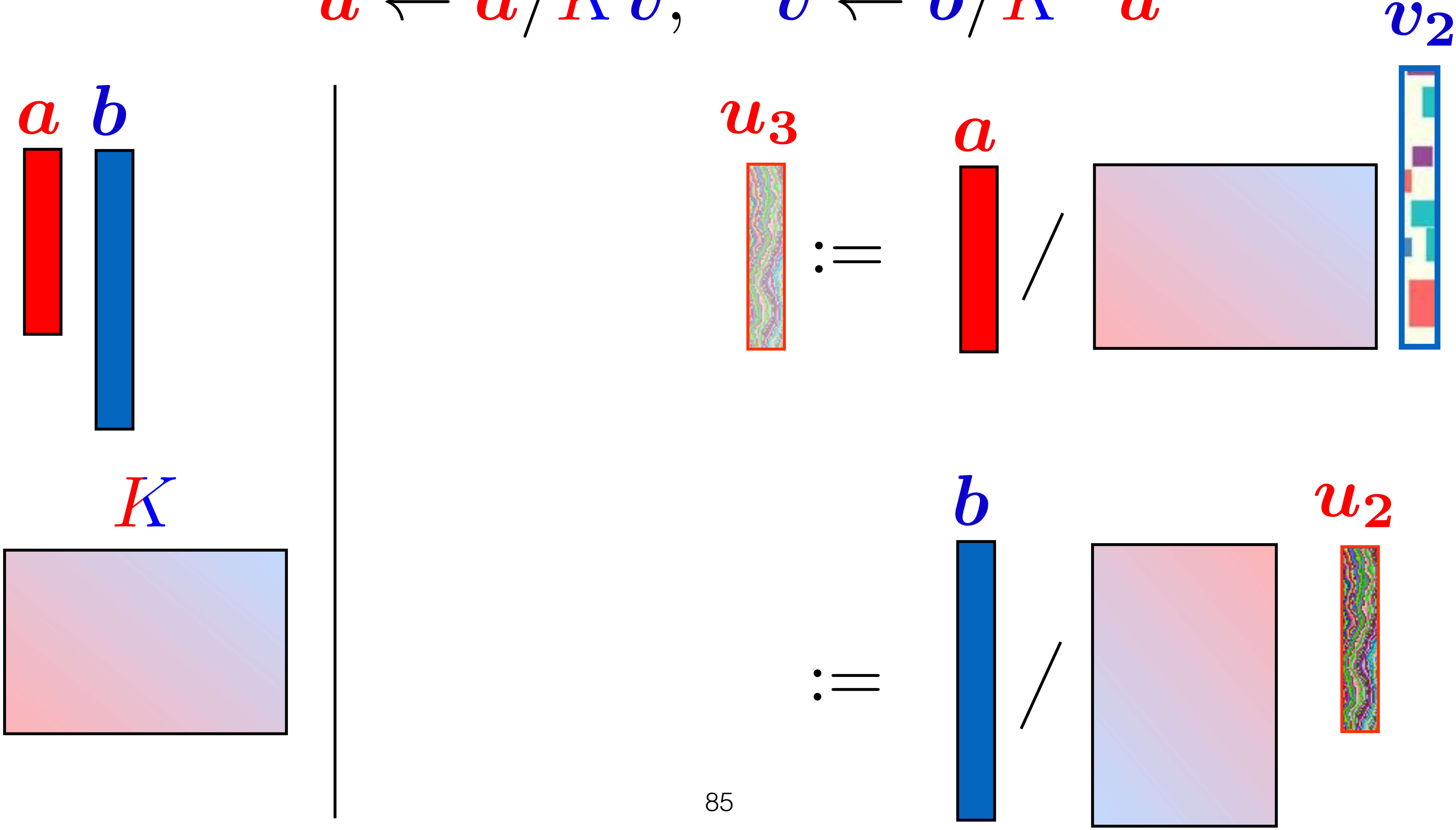
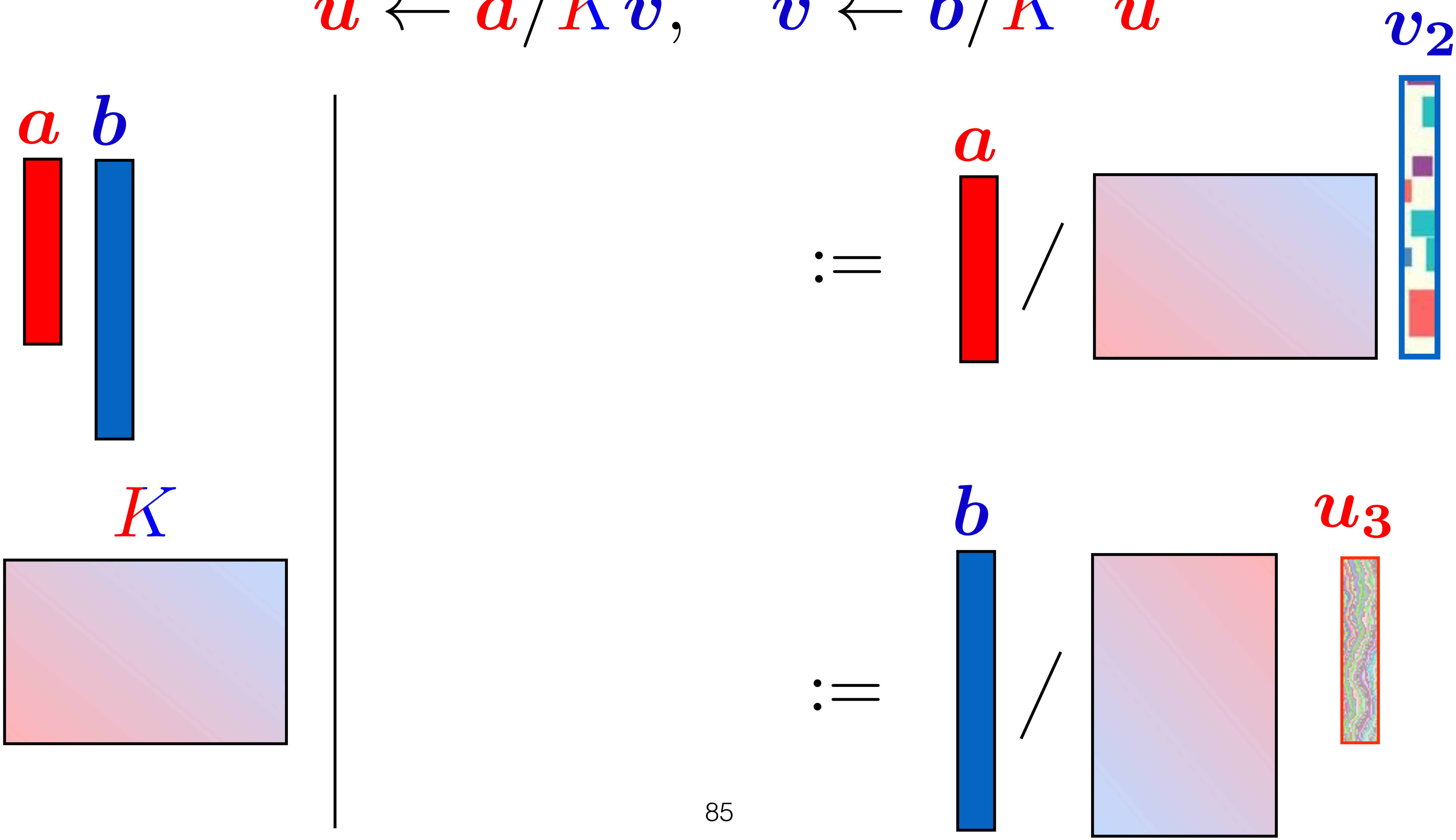


Fast & Scalable Algorithm

- **[Sinkhorn'64]** fixed-point iterations for $(\boldsymbol{u}, \boldsymbol{v})$

$$\boldsymbol{u} \leftarrow \boldsymbol{a}/K\boldsymbol{v}, \quad \boldsymbol{v} \leftarrow \boldsymbol{b}/K^T\boldsymbol{u}$$



Fast & Scalable Algorithm

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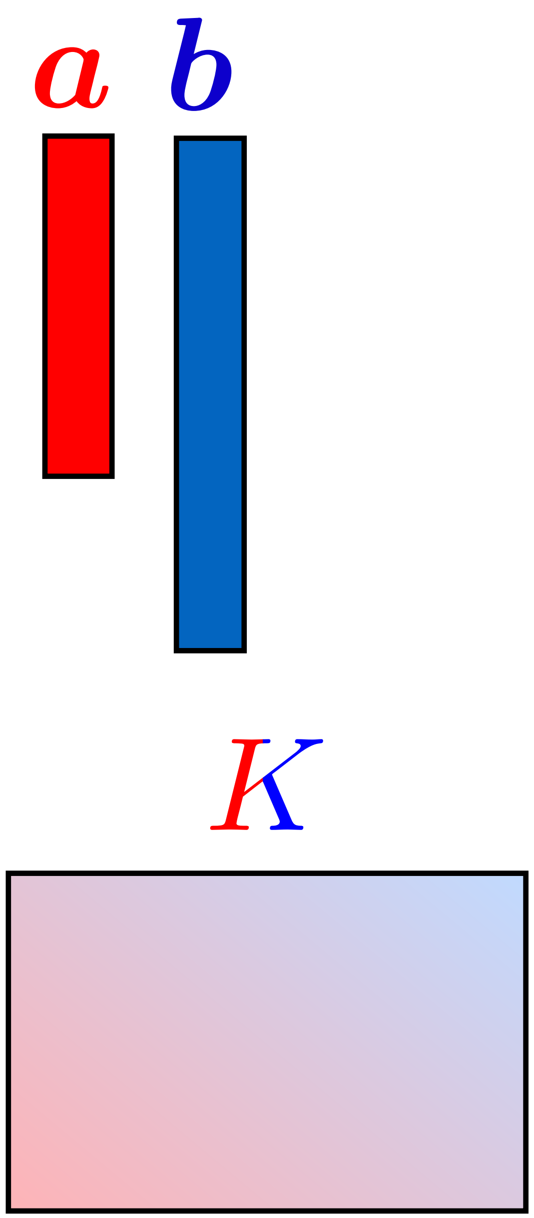
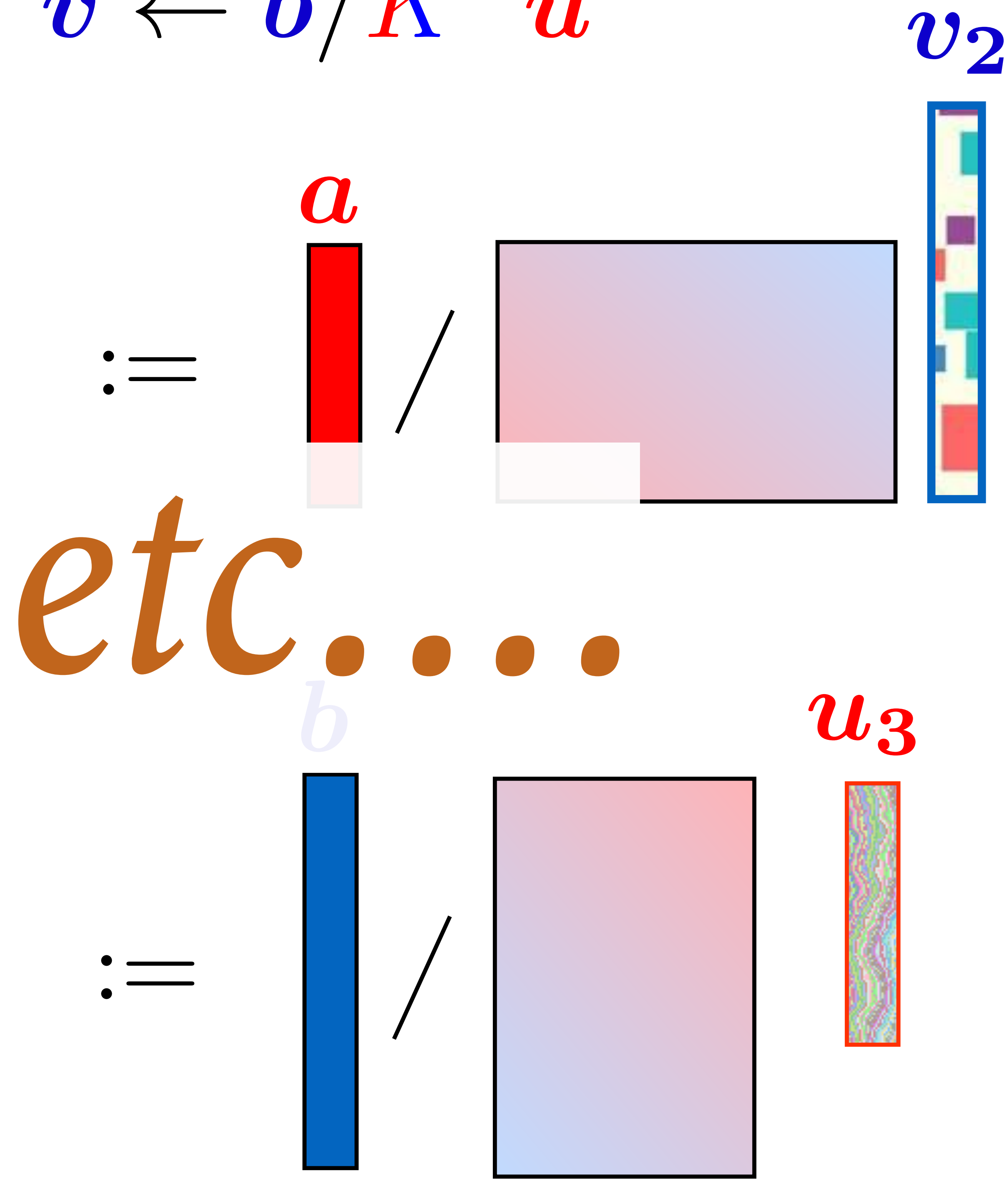
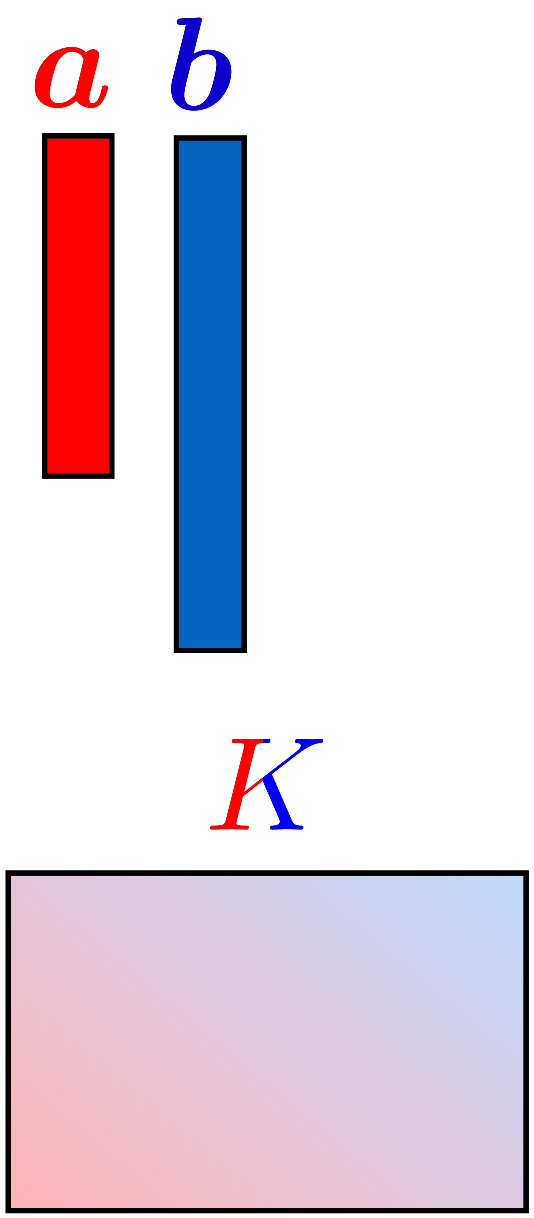
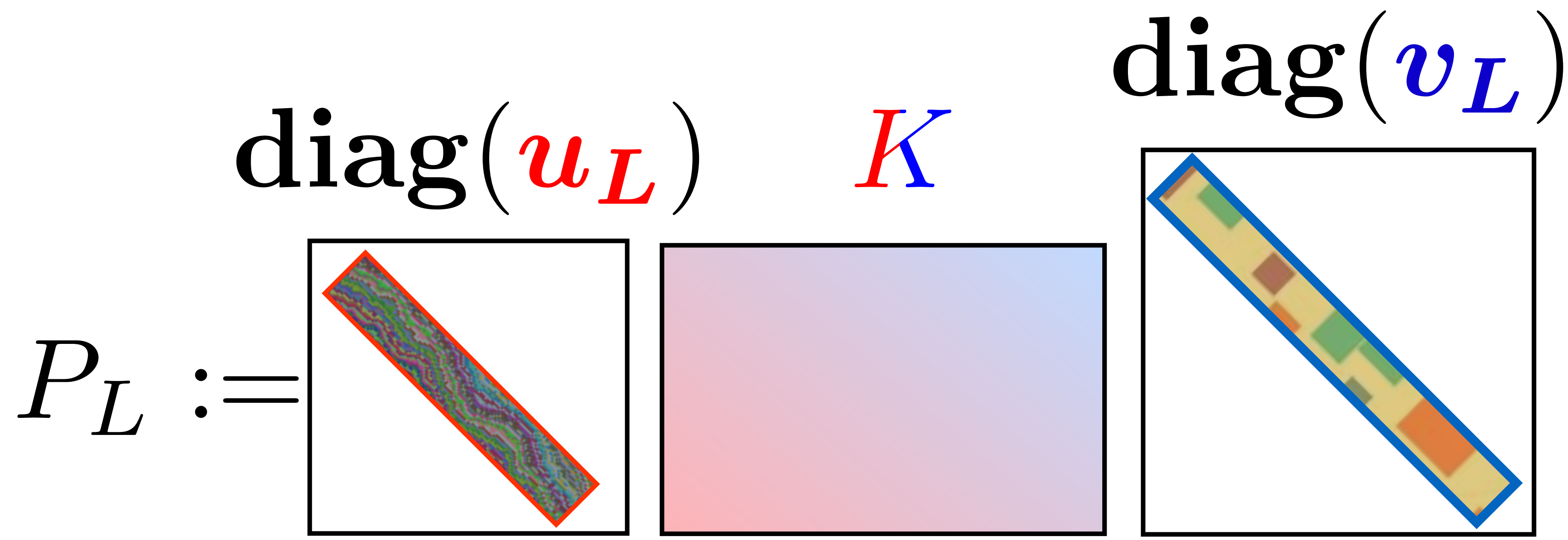




Fast & Scalable Algorithm

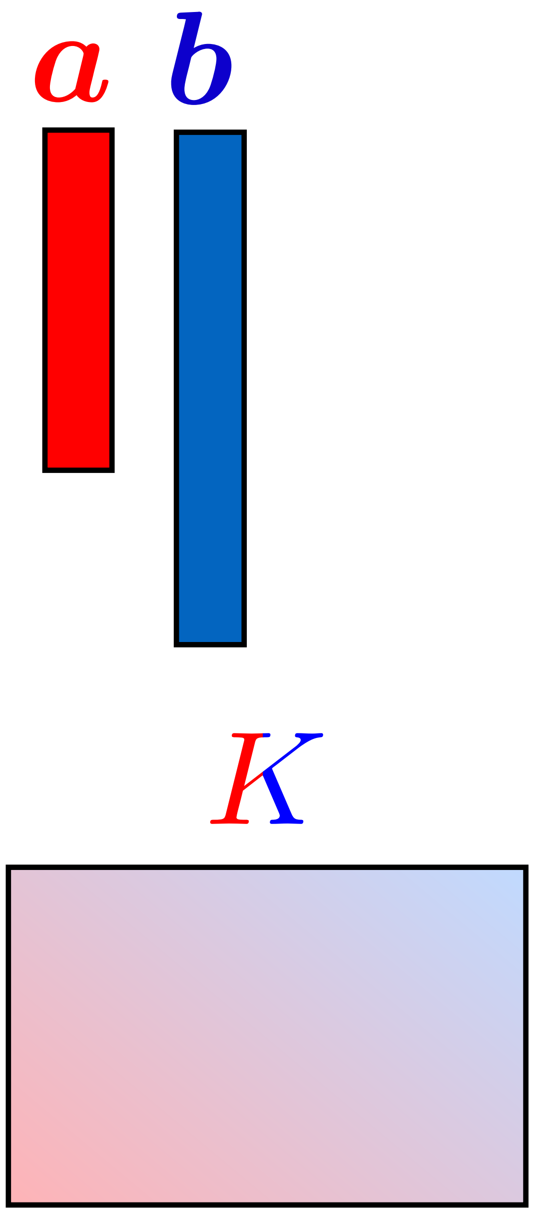
- **[Sinkhorn'64]** fixed-point iterations.



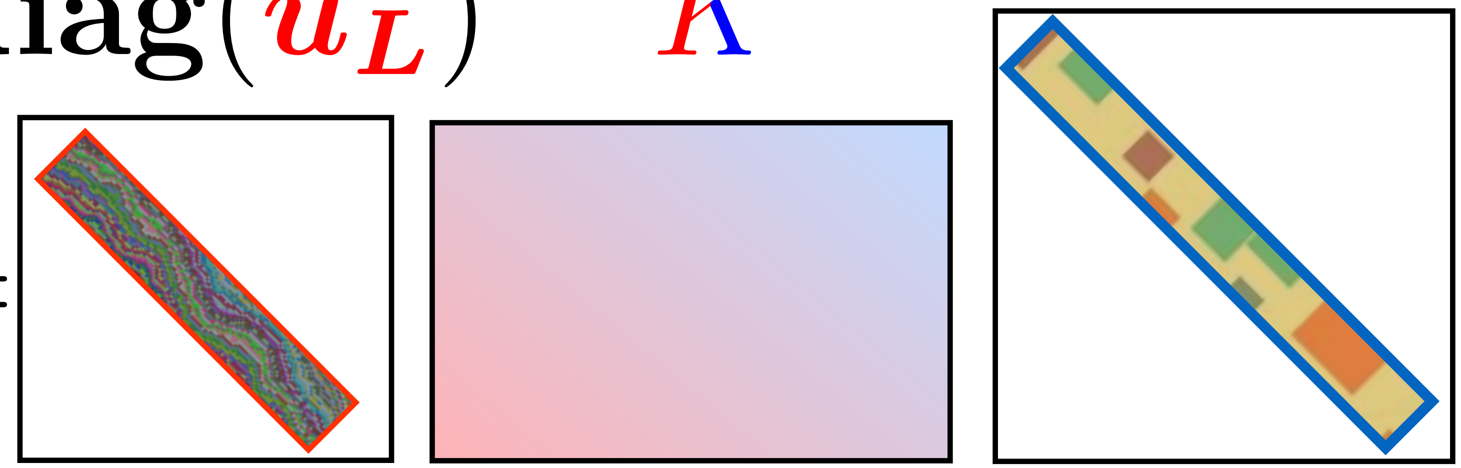


Fast & Scalable Algorithm

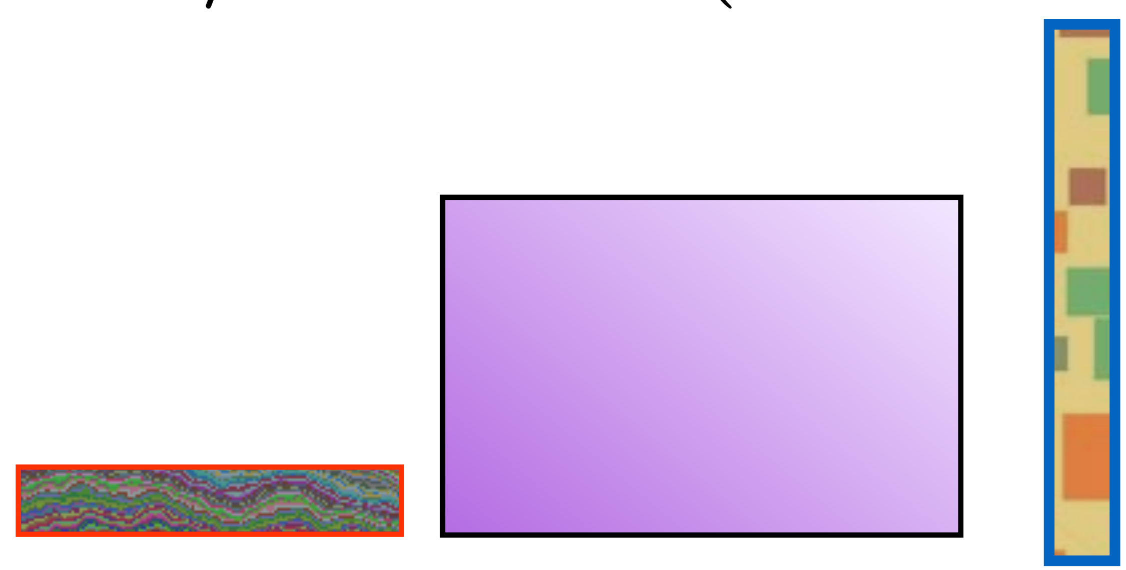
- **[Sinkhorn'64]** fixed-point iterations.



$$P_L := \mathrm{diag}(\boldsymbol{u_L})\, K\, \mathrm{diag}(\boldsymbol{v_L})$$

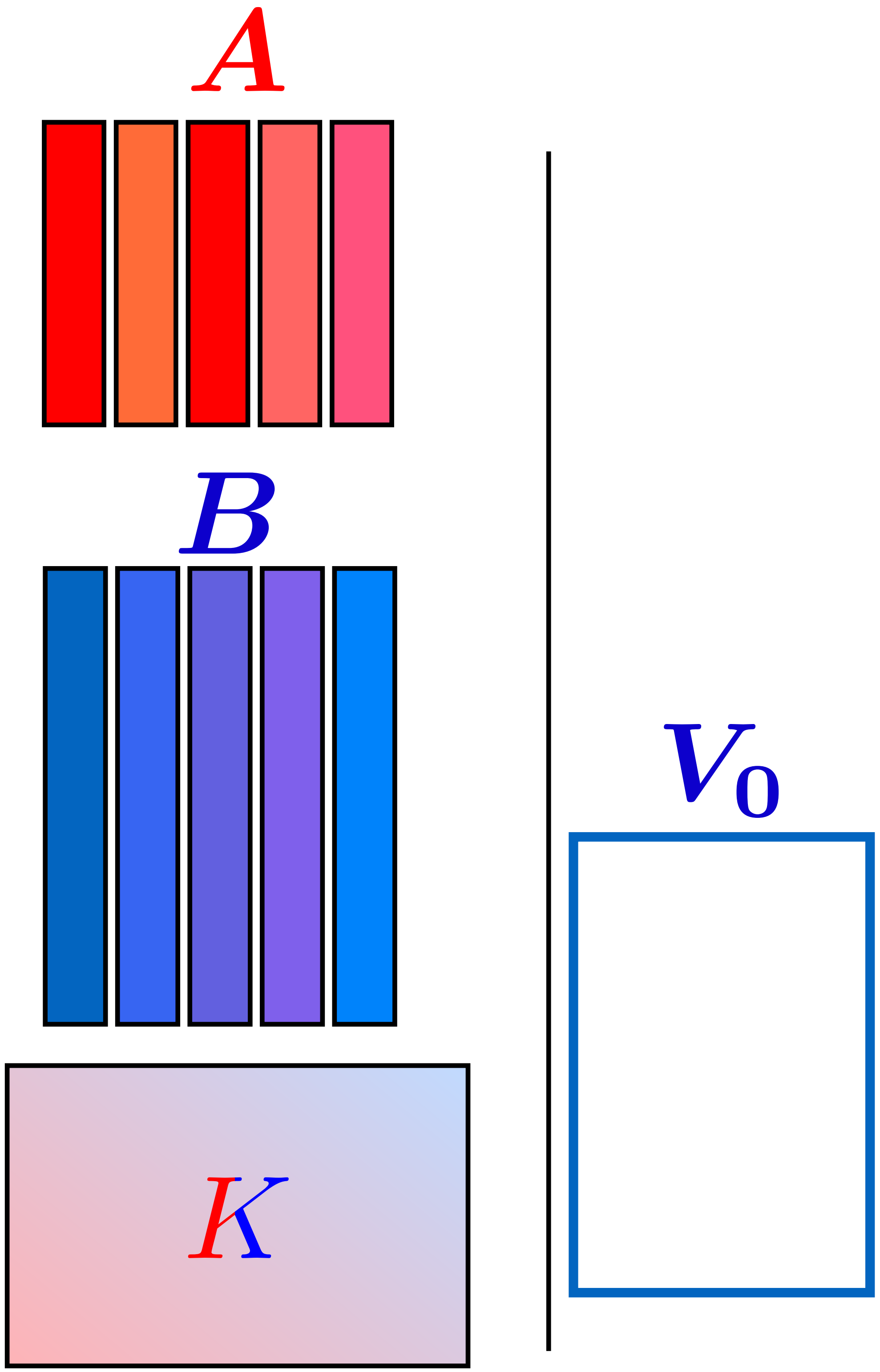


$$\langle P_L, M_{\boldsymbol{XY}} \rangle = \boldsymbol{u_L}^T (K \odot M_{\boldsymbol{XY}}) \boldsymbol{v_L}$$



Also embarrassingly parallel

- **[Sinkhorn'64]** with *matrix* fixed-point iterations



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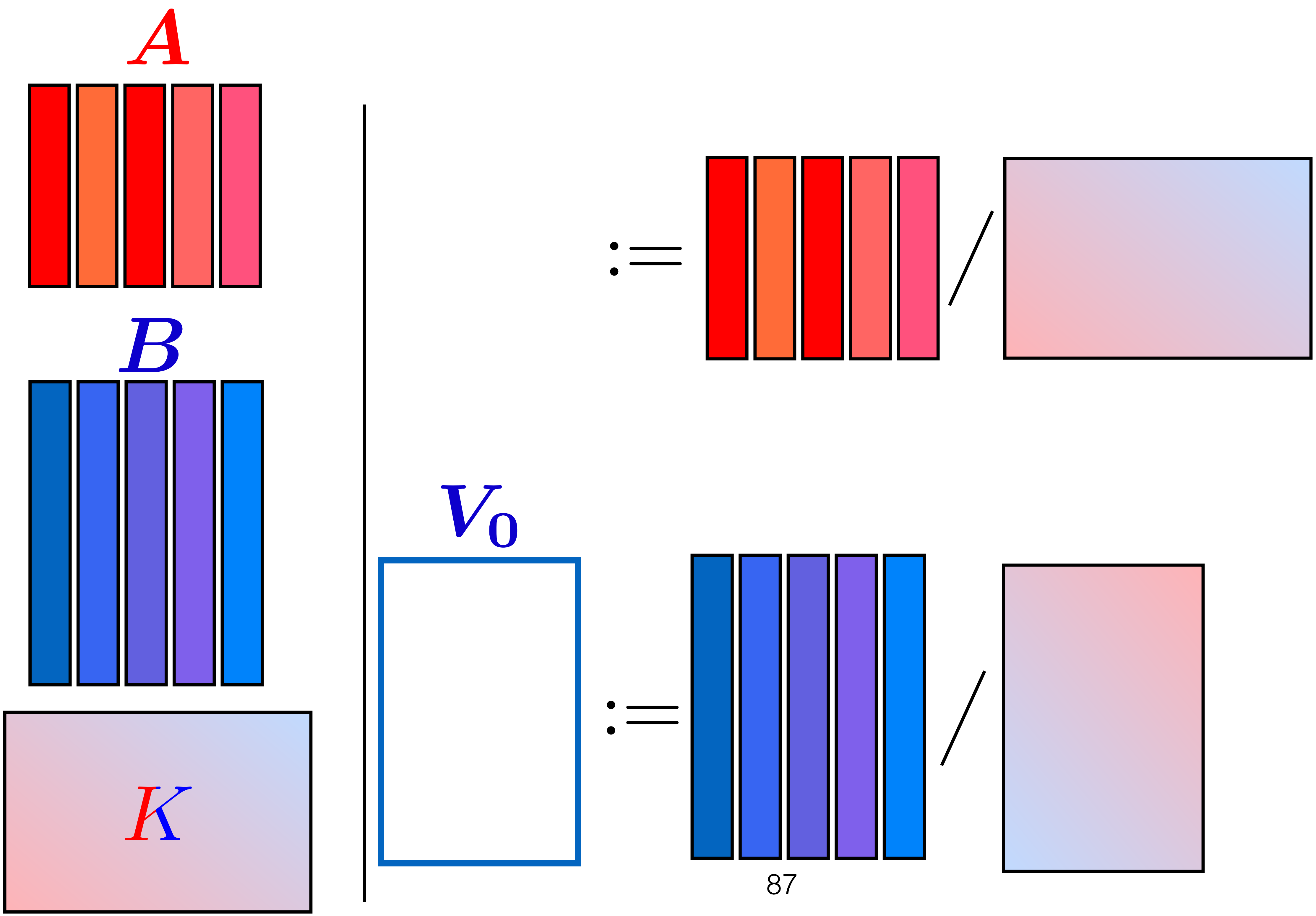

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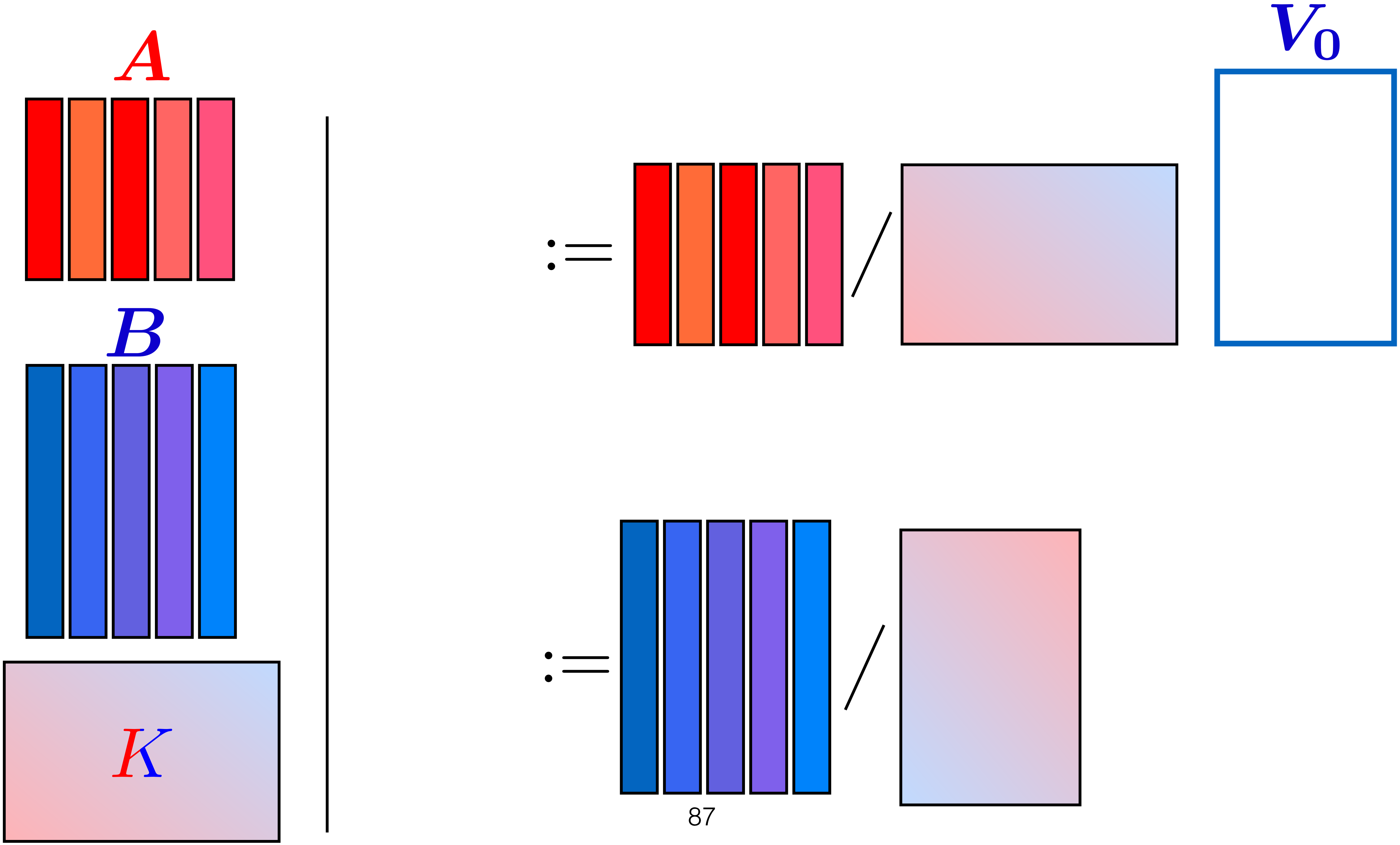

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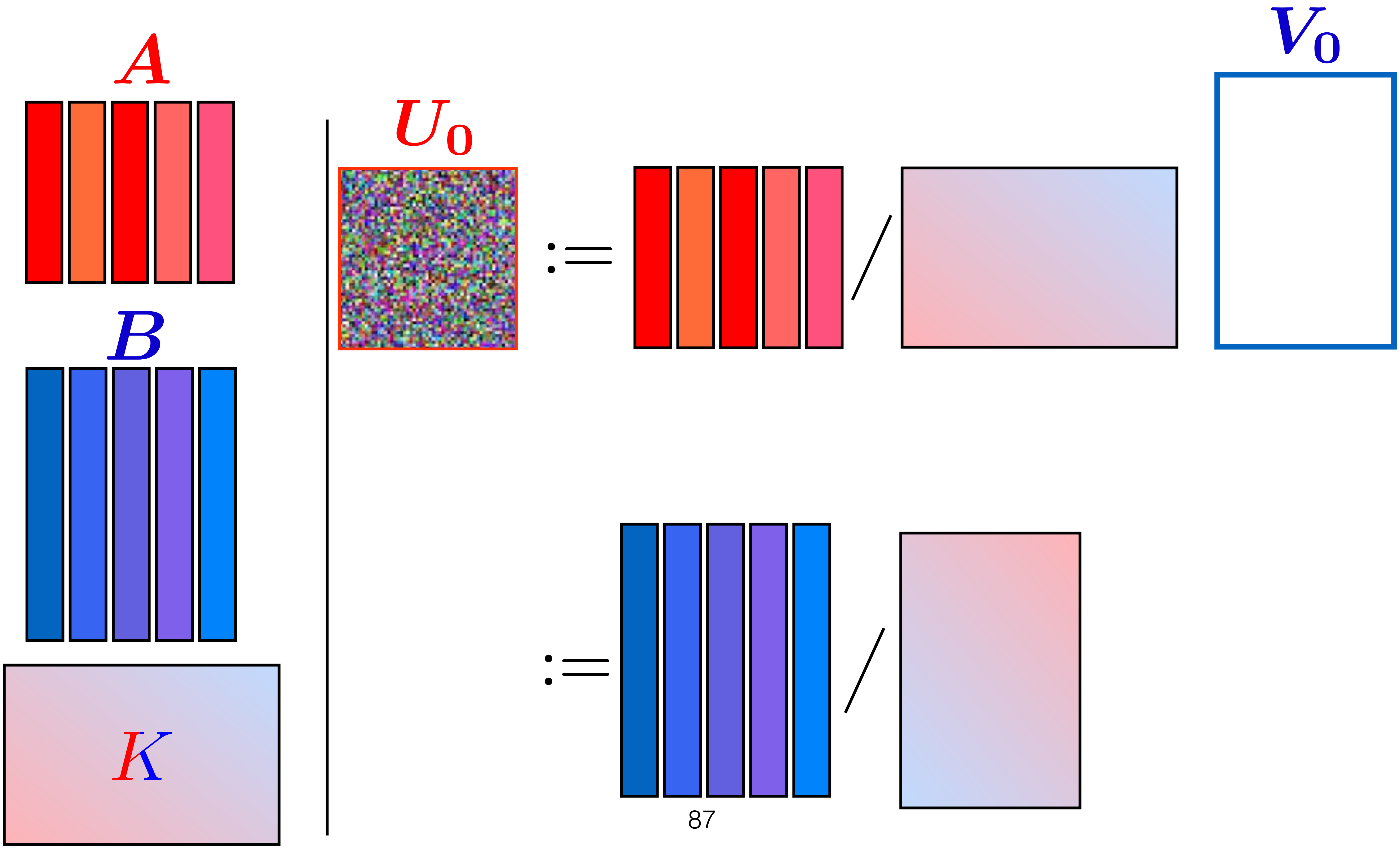

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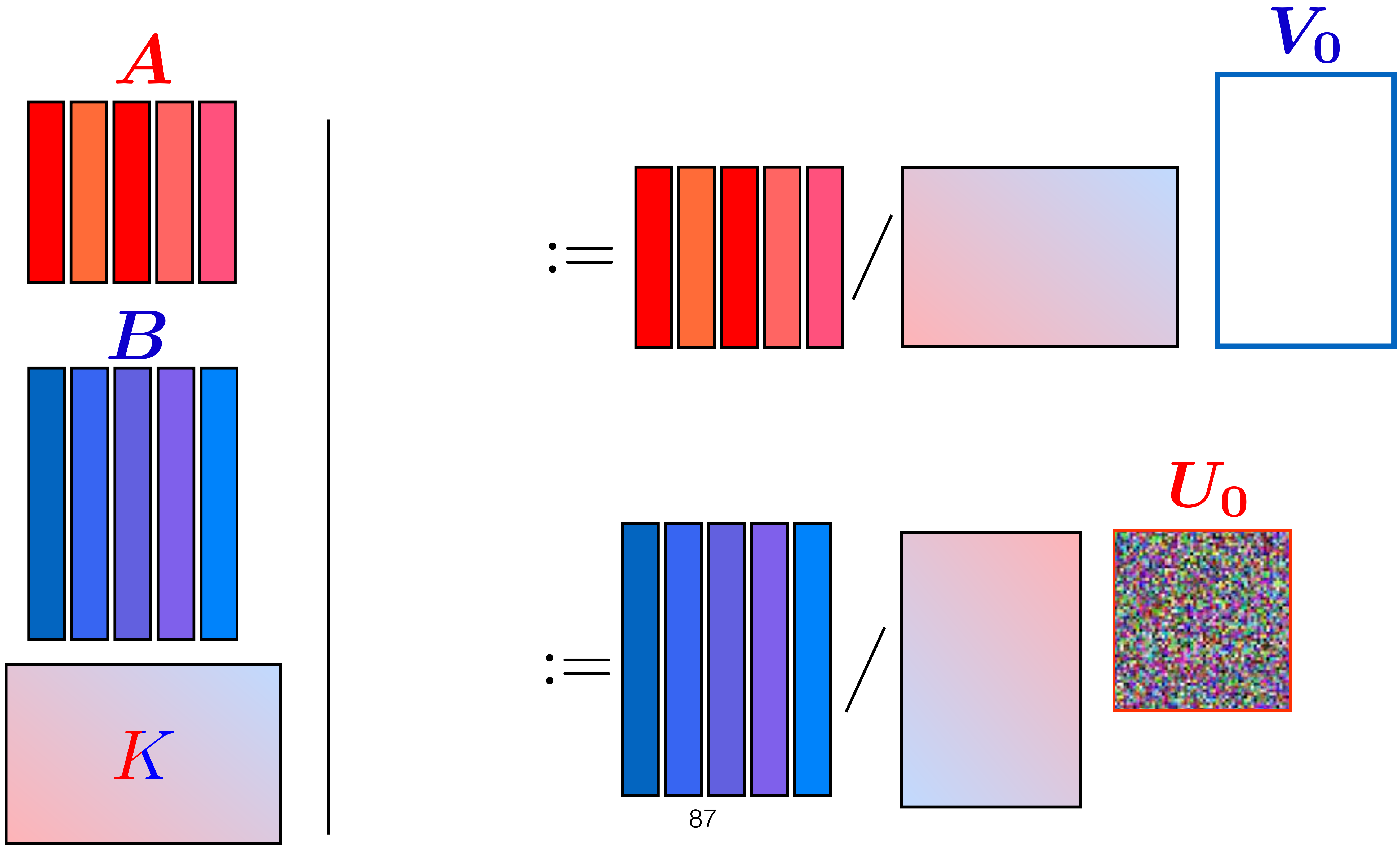

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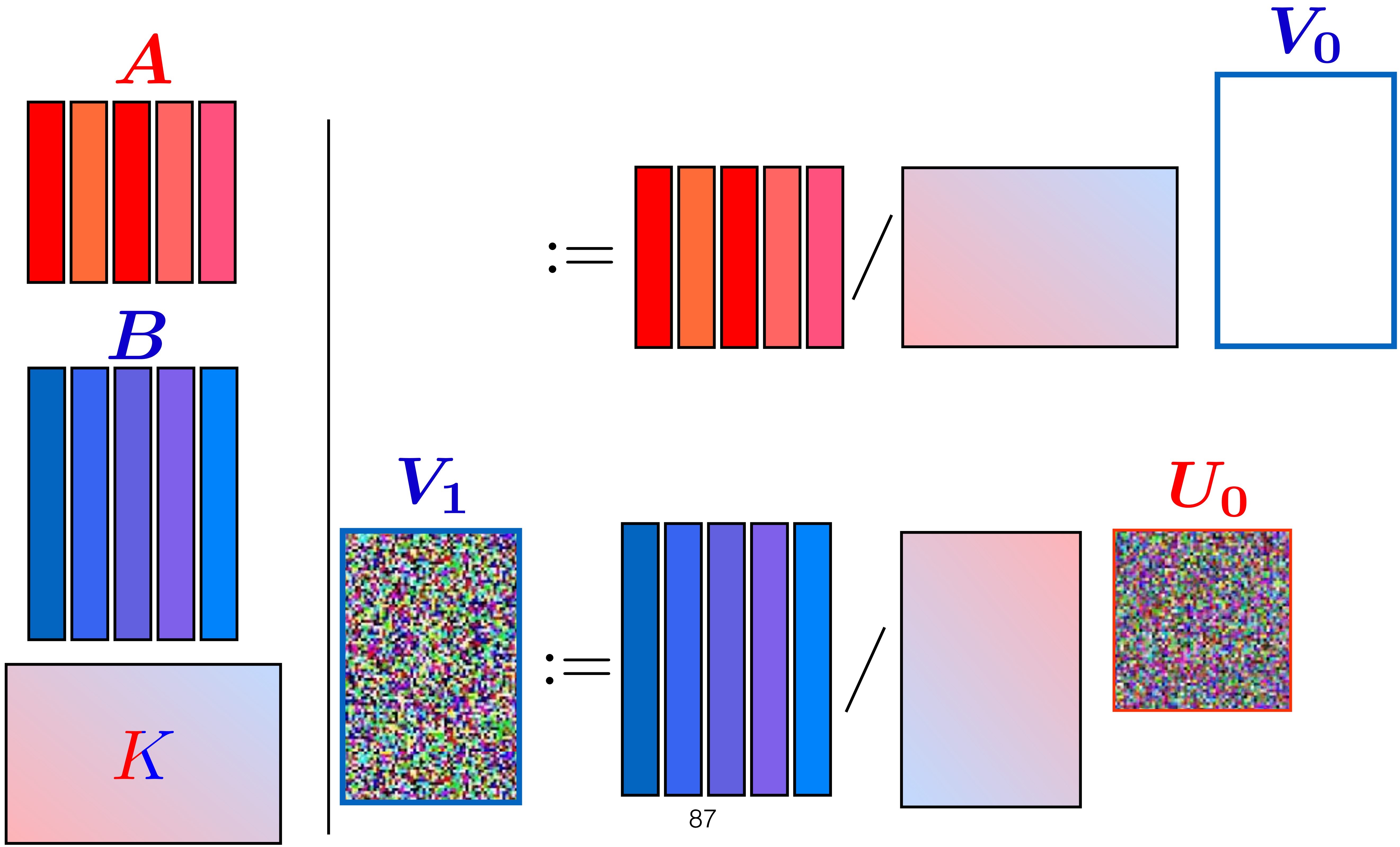

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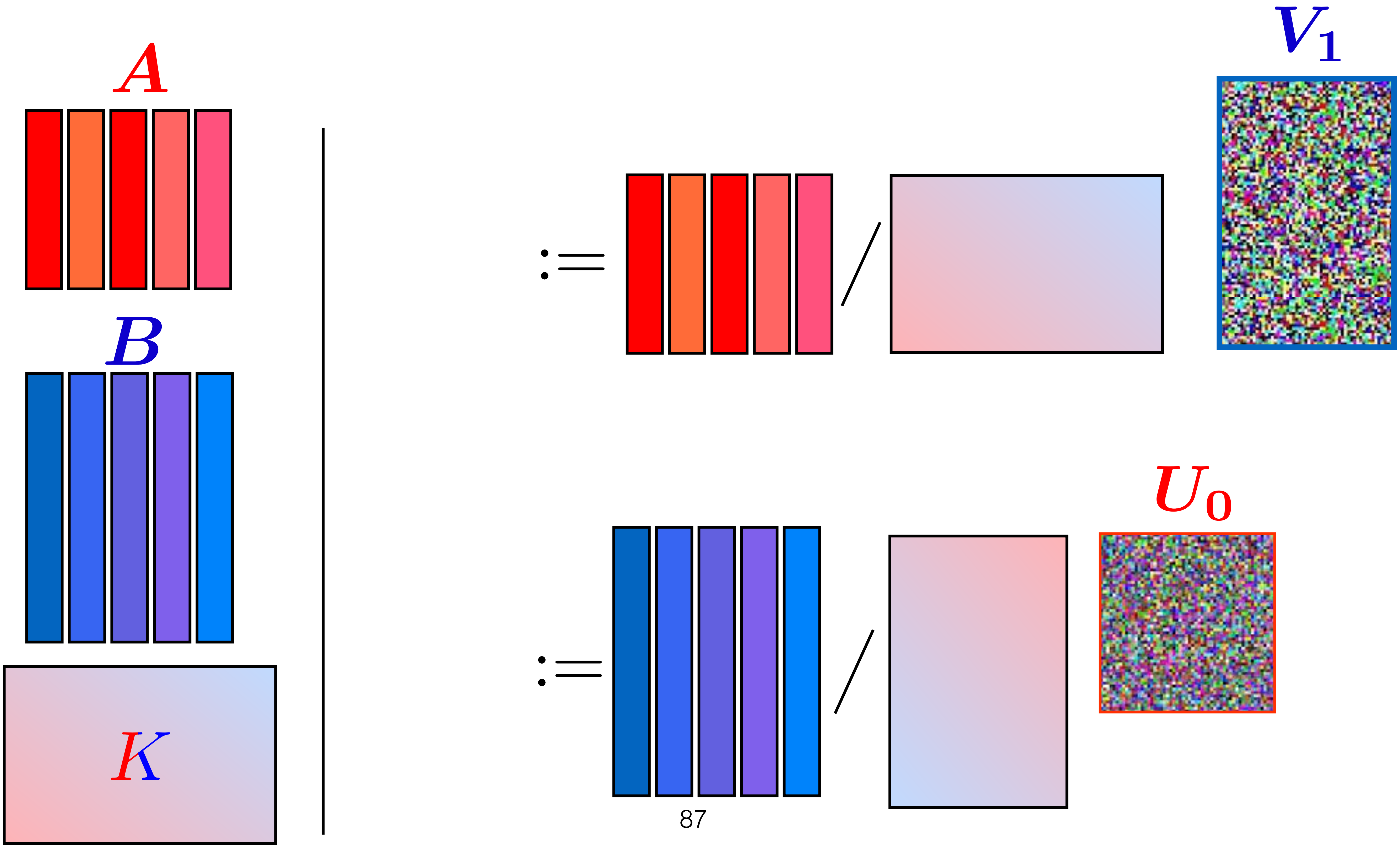

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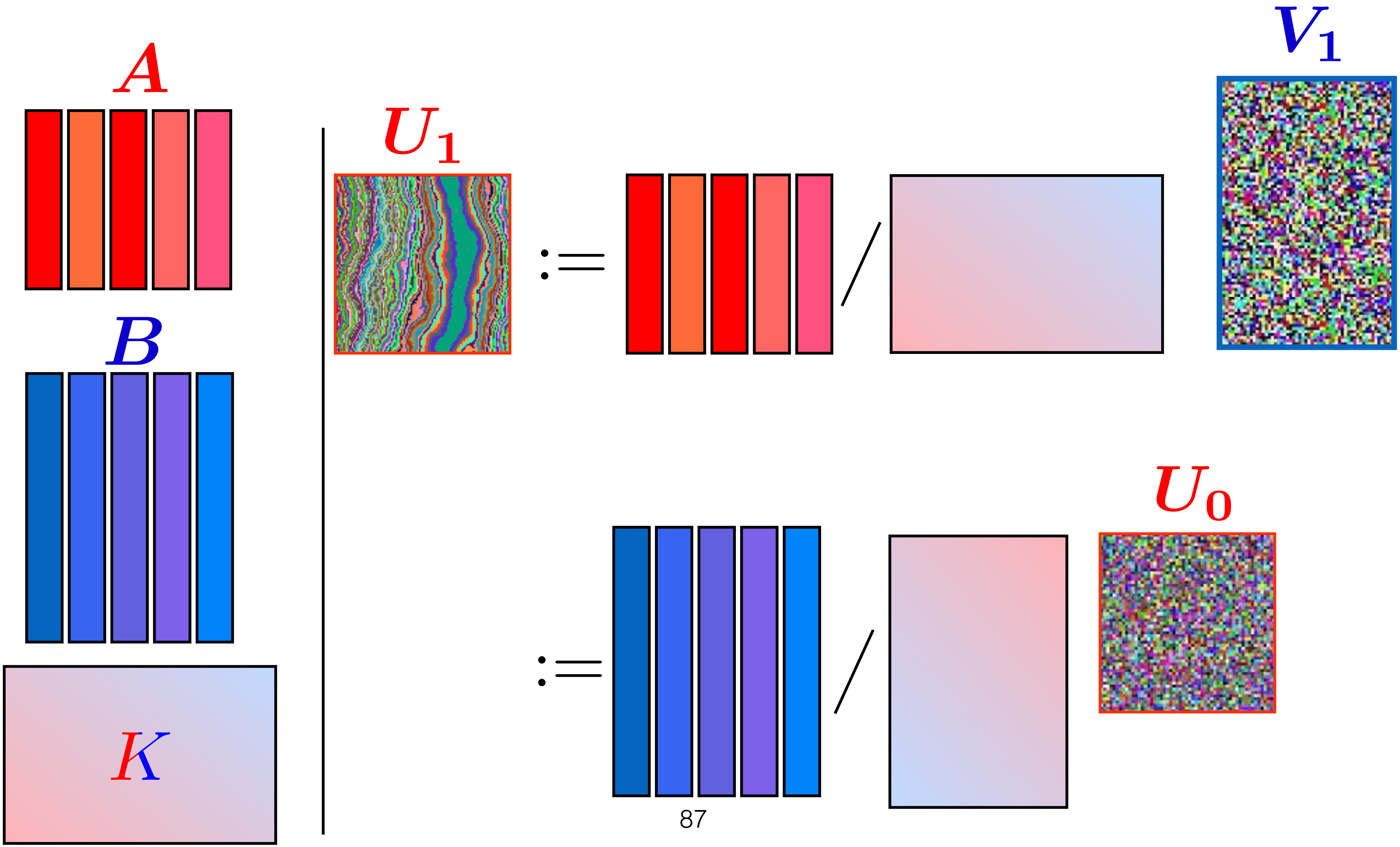

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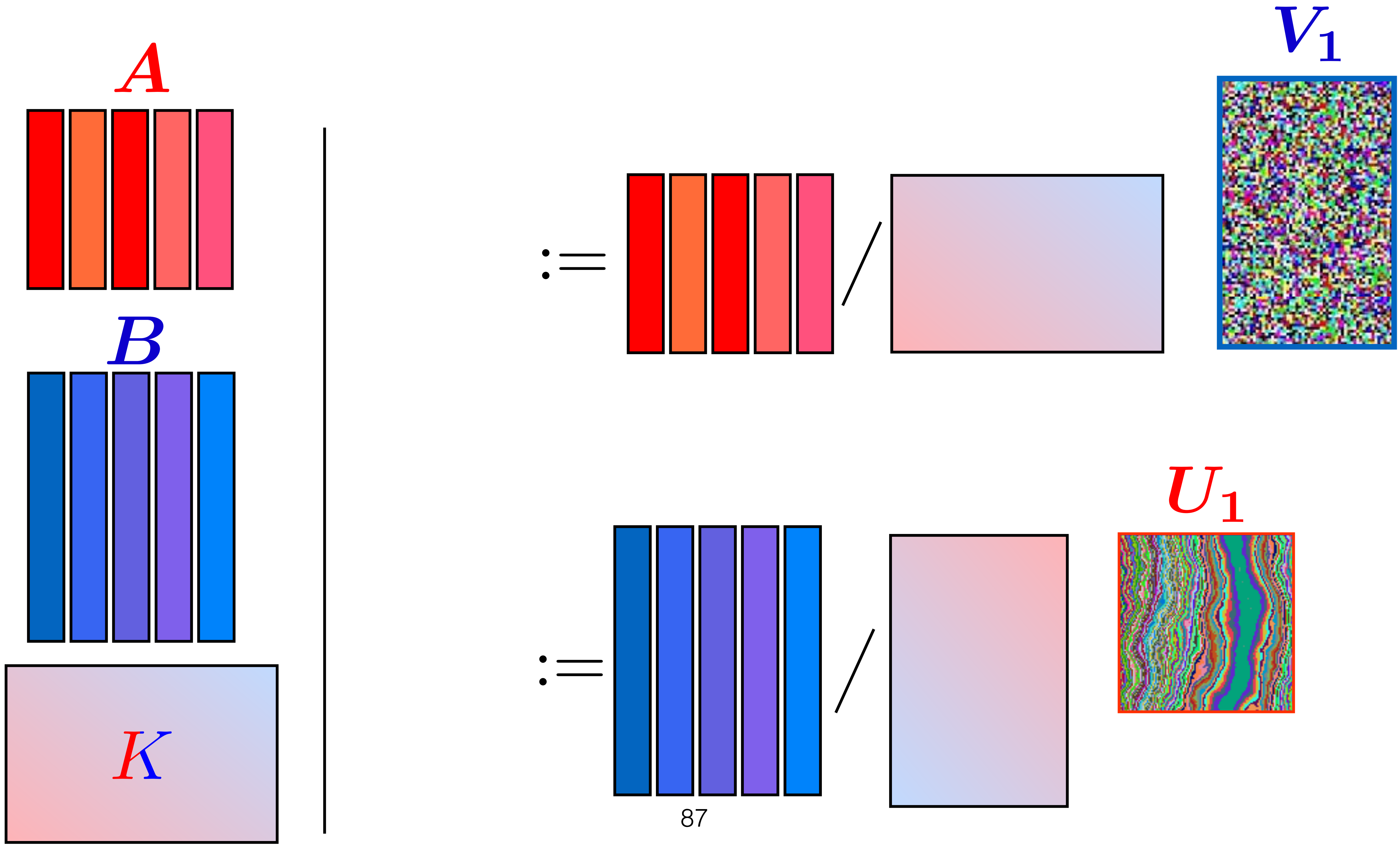

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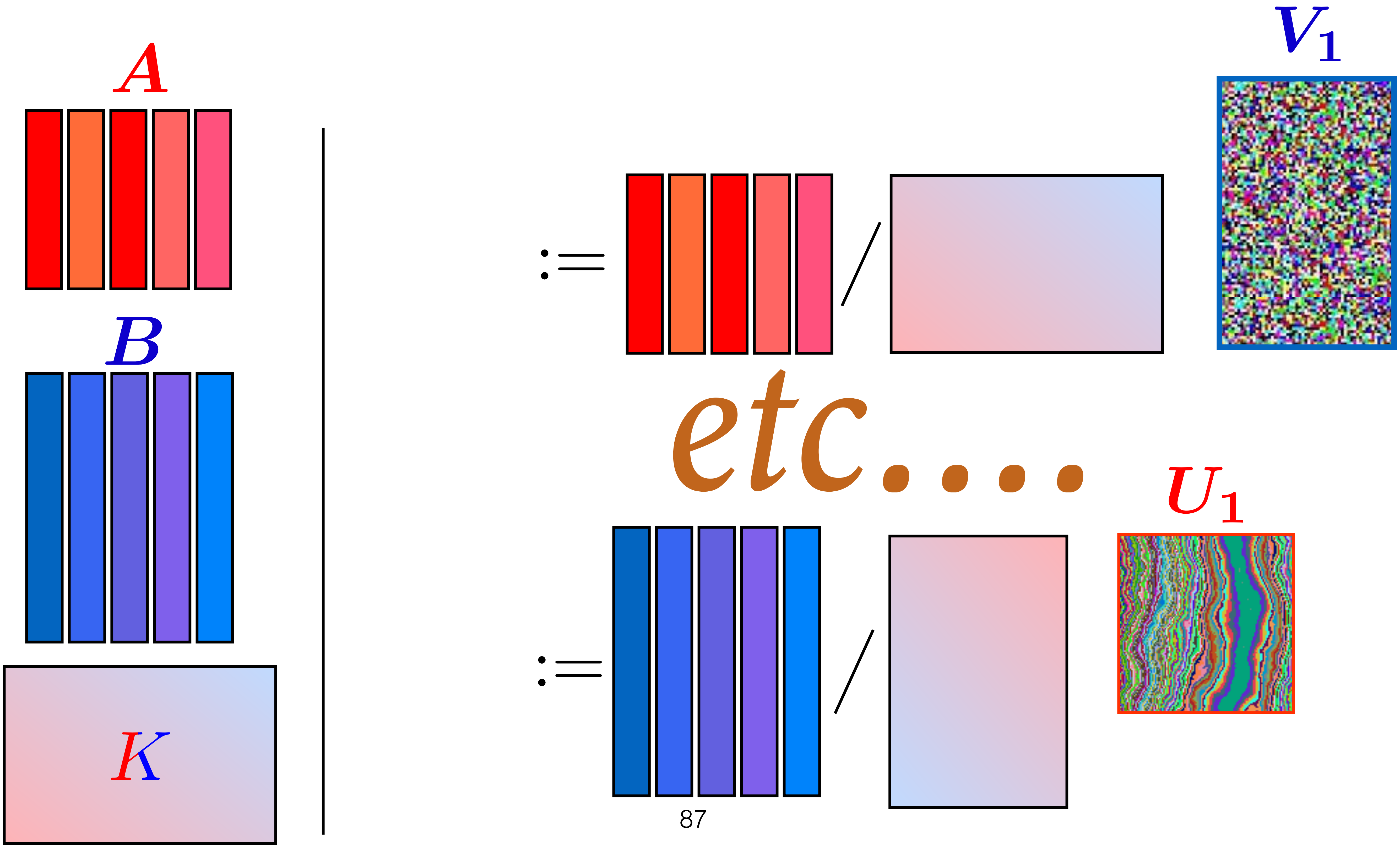
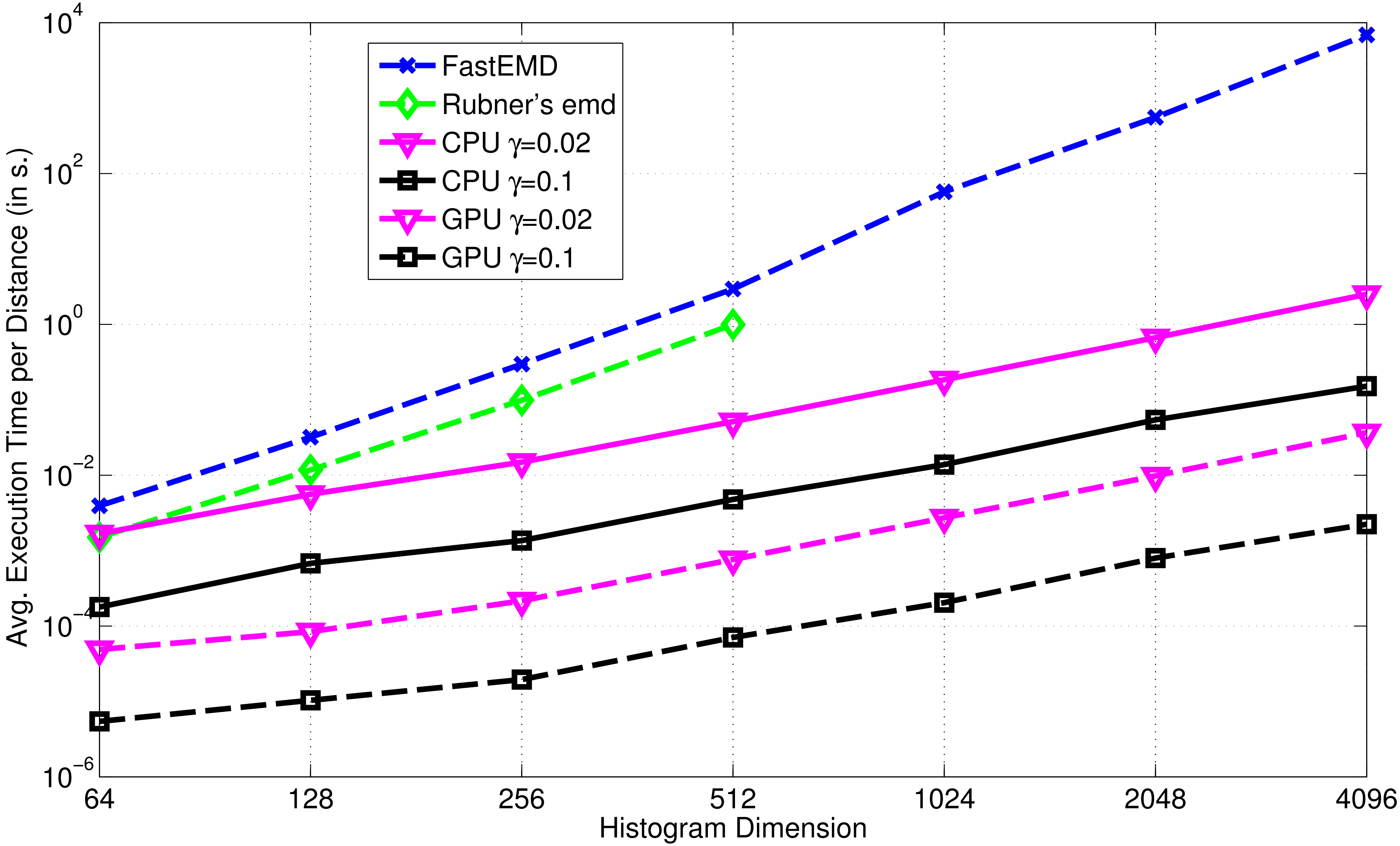
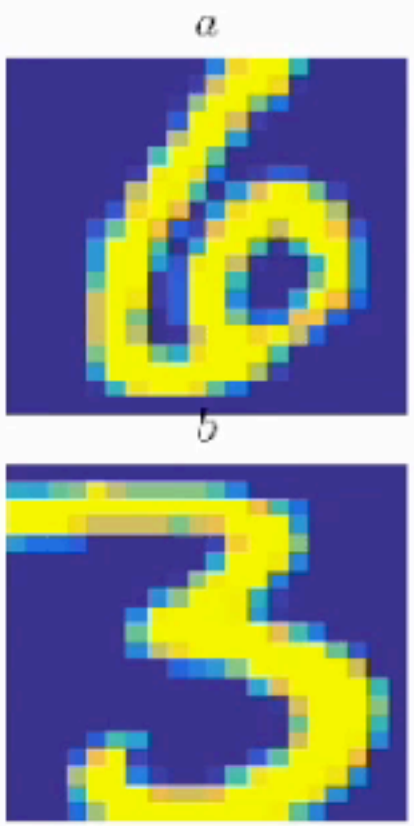


Very Fast EMD Approx. Solver

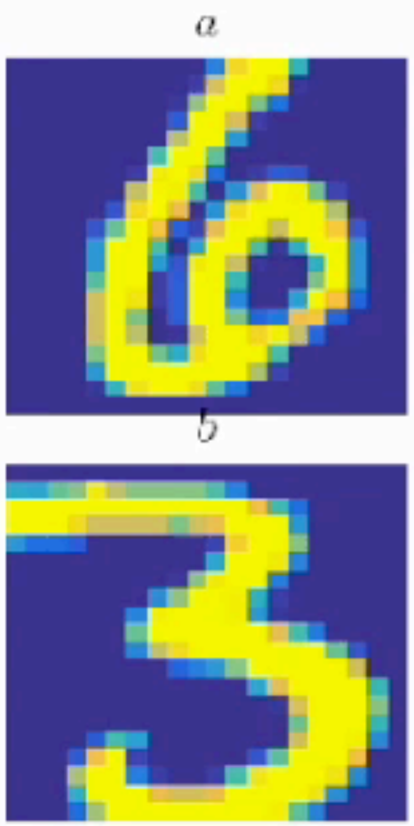


Note. $(\Omega, \boldsymbol{D})$ is a random graph with shortest path metric, histograms sampled uniformly on simplex, Sinkhorn tolerance 10^{-2}.

Very Fast EMD Approx. Solver



Very Fast EMD Approx. Solver



Sinkhorn as a Dual Algorithm

Def. Regularized Wasserstein, $\gamma \geq 0$

$$W_\gamma(\boldsymbol{\mu}, \boldsymbol{\nu}) \stackrel{\text{def}}{=} \min_{\boldsymbol{P} \in U(\boldsymbol{a}, \boldsymbol{b})} \langle \boldsymbol{P}, M_{\boldsymbol{X}\boldsymbol{Y}} \rangle - \gamma E(\boldsymbol{P})$$

REGULARIZED DISCRETE PRIMAL

$$W_\gamma(\boldsymbol{\mu}, \boldsymbol{\nu}) = \max_{\boldsymbol{\alpha}, \boldsymbol{\beta}} \boldsymbol{\alpha}^T \boldsymbol{a} + \boldsymbol{\beta}^T \boldsymbol{b} - \gamma (e^{\boldsymbol{\alpha}/\gamma})^T K (e^{\boldsymbol{\beta}/\gamma})$$

$$\text{where} \quad K = \left[e^{-\frac{\boldsymbol{D}^p(\boldsymbol{x}_i, \boldsymbol{y}_j)}{\gamma}} \right]_{ij}$$

REGULARIZED DISCRETE DUAL

Sinkhorn = *Block Coordinate Ascent* on Dual

Block Coordinate Ascent, *a.k.a Sinkhorn*

$$W_\gamma(\boldsymbol{\mu},\boldsymbol{\nu}) = \max_{\boldsymbol{\alpha},\boldsymbol{\beta}} \boldsymbol{\alpha}^T\boldsymbol{a} + \boldsymbol{\beta}^T\boldsymbol{b} - \gamma(e^{\boldsymbol{\alpha}/\gamma})^T\; K(e^{\boldsymbol{\beta}/\gamma})$$

REGULARIZED DISCRETE DUAL

$$\mathcal{E}(\boldsymbol{\alpha},\boldsymbol{\beta}) = \boldsymbol{\alpha}^T\boldsymbol{a} + \boldsymbol{\beta}^T\boldsymbol{b} - \gamma(e^{\boldsymbol{\alpha}/\gamma})^T\; K e^{\boldsymbol{\beta}/\gamma}$$

Block Coordinate Ascent, *a.k.a Sinkhorn*

$$W_\gamma(\boldsymbol{\mu},\boldsymbol{\nu}) = \max_{\boldsymbol{\alpha},\boldsymbol{\beta}} \boldsymbol{\alpha}^T\boldsymbol{a} + \boldsymbol{\beta}^T\boldsymbol{b} - \gamma(e^{\boldsymbol{\alpha}/\gamma})^T\ K(e^{\boldsymbol{\beta}/\gamma})$$

REGULARIZED DISCRETE DUAL

$$\mathcal{E}(\boldsymbol{\alpha},\boldsymbol{\beta}) = \boldsymbol{\alpha}^T\boldsymbol{a} + \boldsymbol{\beta}^T\boldsymbol{b} - \gamma(e^{\boldsymbol{\alpha}/\gamma})^T\ Ke^{\boldsymbol{\beta}/\gamma}$$

$$\boxed{\nabla_{\boldsymbol{\alpha}}\mathcal{E} = \boldsymbol{a} - e^{\boldsymbol{\alpha}/\gamma}\odot\ Ke^{\boldsymbol{\beta}/\gamma}}$$

$$\boxed{\nabla_{\boldsymbol{\beta}}\mathcal{E} = \boldsymbol{b} - e^{\boldsymbol{\beta}/\gamma}\odot\ K^Te^{\boldsymbol{\alpha}/\gamma}}$$

Block Coordinate Ascent, *a.k.a Sinkhorn*

$$W_\gamma(\boldsymbol{\mu},\boldsymbol{\nu}) = \max_{\boldsymbol{\alpha},\boldsymbol{\beta}} \boldsymbol{\alpha}^T \boldsymbol{a} + \boldsymbol{\beta}^T \boldsymbol{b} - \gamma (e^{\boldsymbol{\alpha}/\gamma})^T \; K (e^{\boldsymbol{\beta}/\gamma})$$

REGULARIZED DISCRETE DUAL

$$\mathcal{E}(\boldsymbol{\alpha},\boldsymbol{\beta}) = \boldsymbol{\alpha}^T \boldsymbol{a} + \boldsymbol{\beta}^T \boldsymbol{b} - \gamma (e^{\boldsymbol{\alpha}/\gamma})^T \; K e^{\boldsymbol{\beta}/\gamma}$$

$$\nabla_{\boldsymbol{\alpha}} \mathcal{E} = \boldsymbol{a} - e^{\boldsymbol{\alpha}/\gamma} \odot \; K e^{\boldsymbol{\beta}/\gamma}$$

$$\boldsymbol{\alpha} \leftarrow \gamma \left(\log \boldsymbol{a} - \log \; K (e^{\boldsymbol{\beta}/\gamma}) \right)$$

$$\nabla_{\boldsymbol{\beta}} \mathcal{E} = \boldsymbol{b} - e^{\boldsymbol{\beta}/\gamma} \odot \; K^T e^{\boldsymbol{\alpha}/\gamma}$$

$$\boldsymbol{\beta} \leftarrow \gamma \left(\log \boldsymbol{b} - \log \; K^T (e^{\boldsymbol{\alpha}/\gamma}) \right)$$

Block Coordinate Ascent, *a.k.a Sinkhorn*

$$W_\gamma(\boldsymbol{\mu},\boldsymbol{\nu}) = \max_{\boldsymbol{\alpha},\boldsymbol{\beta}} \boldsymbol{\alpha}^T\boldsymbol{a} + \boldsymbol{\beta}^T\boldsymbol{b} - \gamma(e^{\boldsymbol{\alpha}/\gamma})^T \; K(e^{\boldsymbol{\beta}/\gamma})$$

REGULARIZED DISCRETE DUAL

Block Coordinate Ascent, *a.k.a Sinkhorn*

$$W_\gamma(\boldsymbol{\mu}, \boldsymbol{\nu}) = \max_{\boldsymbol{\alpha}, \boldsymbol{\beta}} \boldsymbol{\alpha}^T \boldsymbol{a} + \boldsymbol{\beta}^T \boldsymbol{b} - \gamma (e^{\boldsymbol{\alpha}/\gamma})^T \; K (e^{\boldsymbol{\beta}/\gamma})$$

REGULARIZED DISCRETE DUAL

$$(\boldsymbol{u}, \boldsymbol{v}) \stackrel{\text{def}}{=} (e^{\boldsymbol{\alpha}/\gamma}, e^{\boldsymbol{\beta}/\gamma})$$

$$\boldsymbol{u} \leftarrow \frac{\boldsymbol{a}}{K\boldsymbol{v}}$$

$$\boldsymbol{v} \leftarrow \frac{\boldsymbol{b}}{K^T\boldsymbol{u}}$$

Block Coordinate Ascent, *a.k.a Sinkhorn*

$$W_\gamma(\boldsymbol{\mu},\boldsymbol{\nu}) = \max_{\boldsymbol{\alpha},\boldsymbol{\beta}} \boldsymbol{\alpha}^T\boldsymbol{a} + \boldsymbol{\beta}^T\boldsymbol{b} - \gamma(e^{\boldsymbol{\alpha}/\gamma})^T\ K(e^{\boldsymbol{\beta}/\gamma})$$

REGULARIZED DISCRETE DUAL

$$(\boldsymbol{u},\boldsymbol{v}) \stackrel{\text{def}}{=} (e^{\boldsymbol{\alpha}/\gamma}, e^{\boldsymbol{\beta}/\gamma})$$

$$\boldsymbol{\alpha} \leftarrow \gamma\left(\log \boldsymbol{a} - \log\ K(e^{\boldsymbol{\beta}/\gamma})\right)$$

$$\boldsymbol{u} \leftarrow \frac{\boldsymbol{a}}{K\boldsymbol{v}}$$

$$\boldsymbol{\beta} \leftarrow \gamma\left(\log \boldsymbol{b} - \log\ K^T(e^{\boldsymbol{\alpha}/\gamma})\right)$$

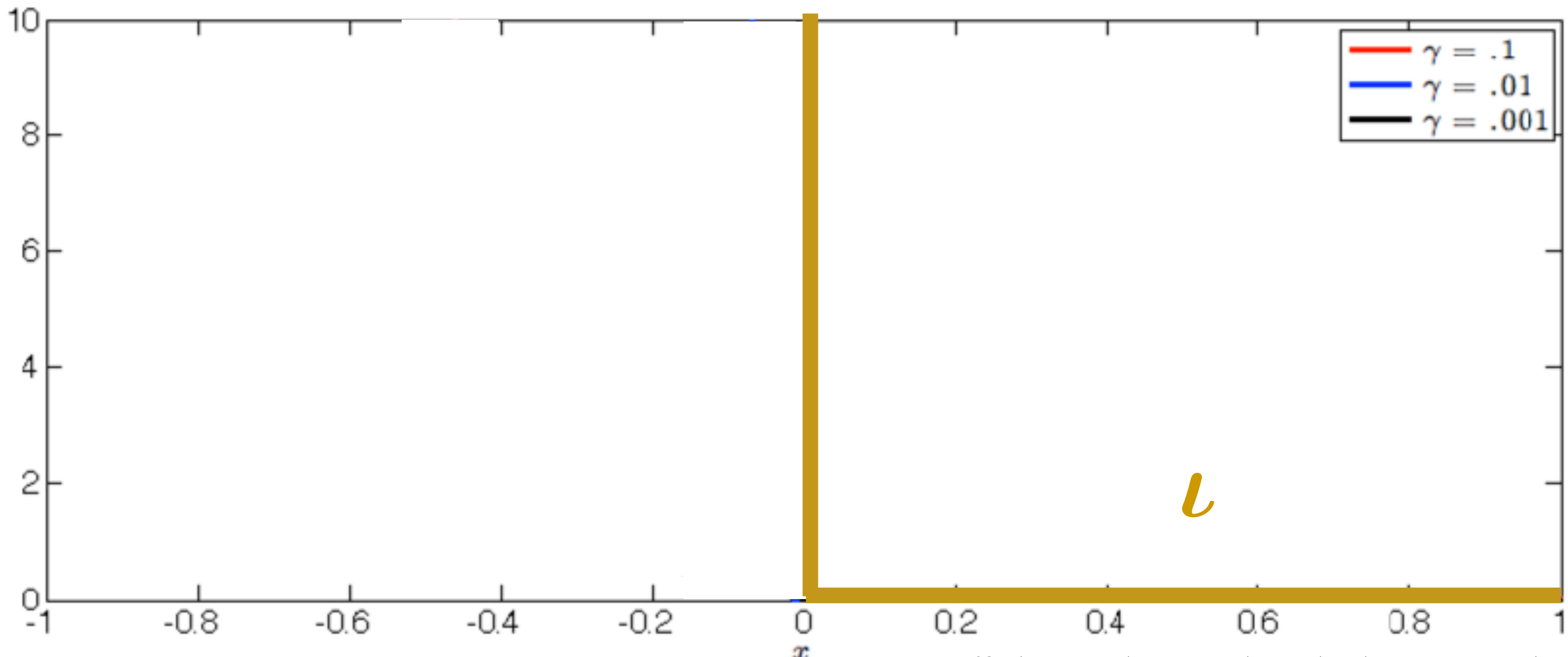
$$\boldsymbol{v} \leftarrow \frac{\boldsymbol{b}}{K^T\boldsymbol{u}}$$

Stochastic Formulation

$$W_p^p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \sup_{\boldsymbol{\varphi}, \boldsymbol{\psi}} \int \boldsymbol{\varphi} d\boldsymbol{\mu} + \int \boldsymbol{\psi} d\boldsymbol{\nu} - \iota_C(\boldsymbol{\varphi}, \boldsymbol{\psi})$$

$$C = \{(\boldsymbol{\varphi}, \boldsymbol{\psi}) | \forall x, y, \boldsymbol{\varphi}(x) + \boldsymbol{\psi}(y) \leq \boldsymbol{D}(x, y)^p\}$$

DUAL



$$\boldsymbol{D}^p(x, y) - (\boldsymbol{\varphi}(x) + \boldsymbol{\psi}(y))$$

Stochastic Formulation

$$W_p^p(\boldsymbol{\mu},\boldsymbol{\nu}) = \sup_{\boldsymbol{\varphi},\boldsymbol{\psi}} \int \boldsymbol{\varphi} d\boldsymbol{\mu} + \int \boldsymbol{\psi} d\boldsymbol{\nu} - \iota_C(\boldsymbol{\varphi},\boldsymbol{\psi})$$

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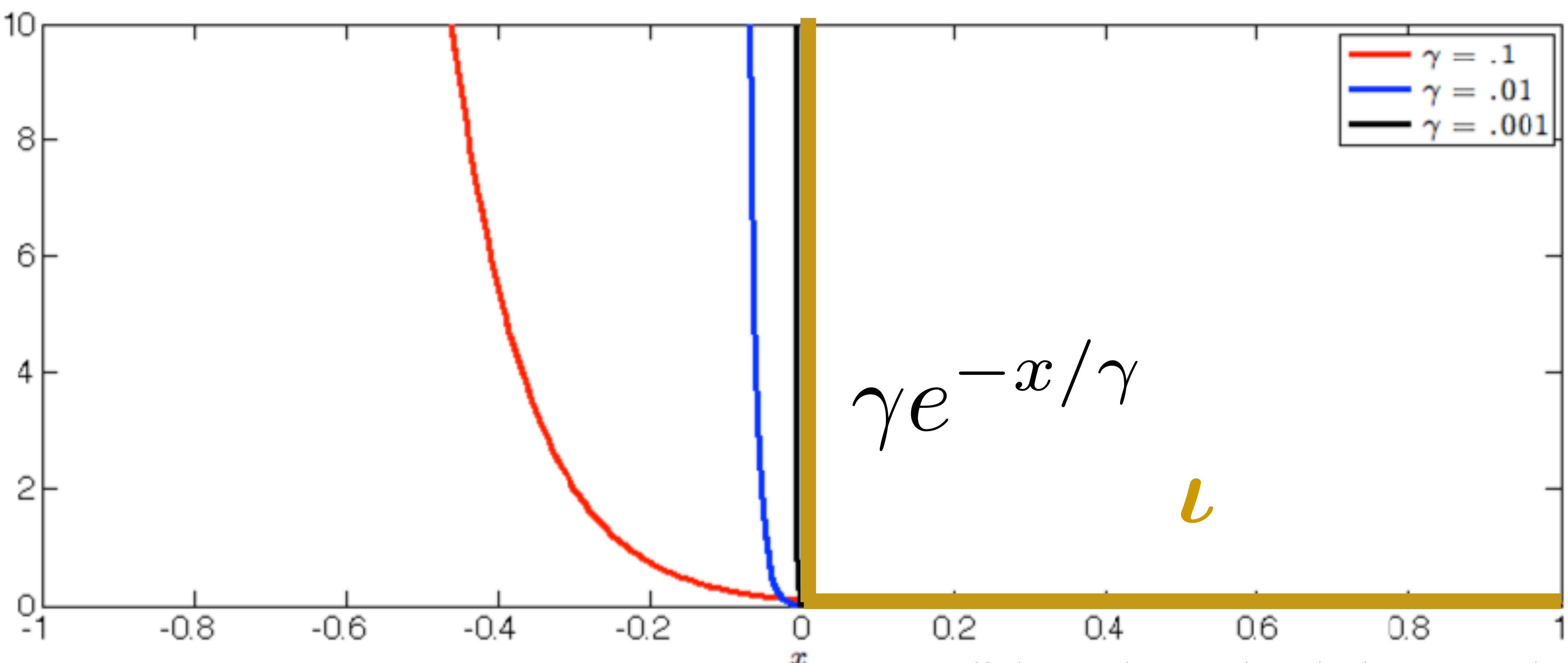
DUAL



$\boldsymbol{D}^p(x,y) - (\boldsymbol{\varphi}(x) + \boldsymbol{\psi}(y))$

Stochastic Formulation

$$W_p^p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \sup_{\boldsymbol{\varphi}, \boldsymbol{\psi}} \int \boldsymbol{\varphi} d\boldsymbol{\mu} + \int \boldsymbol{\psi} d\boldsymbol{\nu} - \iota_C(\boldsymbol{\varphi}, \boldsymbol{\psi})$$

$$C = \{(\boldsymbol{\varphi}, \boldsymbol{\psi}) | \forall x, y, \boldsymbol{\varphi}(x) + \boldsymbol{\psi}(y) \leq \boldsymbol{D}(x, y)^p\}$$

DUAL

regularizing dual *constraints* $\gamma > 0$

$$W_\gamma(\boldsymbol{\mu}, \boldsymbol{\nu}) = \sup_{\boldsymbol{\varphi}, \boldsymbol{\psi}} \int \boldsymbol{\varphi} d\boldsymbol{\mu} + \int \boldsymbol{\psi} d\boldsymbol{\nu} - \iota_C^\gamma(\boldsymbol{\varphi}, \boldsymbol{\psi})$$

$$\iota_C^\gamma(\boldsymbol{\varphi}, \boldsymbol{\psi}) = \gamma \iint e^{(\boldsymbol{\varphi} \oplus \boldsymbol{\psi} - \boldsymbol{D}^p)/\gamma} d\boldsymbol{\mu} d\boldsymbol{\nu}$$

REGULARIZED DUAL

Stochastic Formulation

$$W_p^p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \sup_{\boldsymbol{\varphi}, \boldsymbol{\psi}} \int \boldsymbol{\varphi} d\boldsymbol{\mu} + \int \boldsymbol{\psi} d\boldsymbol{\nu} - \iota_C(\boldsymbol{\varphi}, \boldsymbol{\psi})$$

$$C = \{(\boldsymbol{\varphi}, \boldsymbol{\psi}) | \forall x, y, \boldsymbol{\varphi}(x) + \boldsymbol{\psi}(y) \leq \boldsymbol{D}(x, y)^p\}$$

DUAL

regularizing dual *constraints* $\gamma > 0$

$$W_\gamma(\boldsymbol{\mu}, \boldsymbol{\nu}) = \sup_{\boldsymbol{\varphi}, \boldsymbol{\psi}} \int \boldsymbol{\varphi} d\boldsymbol{\mu} + \int \boldsymbol{\psi} d\boldsymbol{\nu} - \iota_C^\gamma(\boldsymbol{\varphi}, \boldsymbol{\psi})$$

$$\iota_C^\gamma(\boldsymbol{\varphi}, \boldsymbol{\psi}) = \gamma \iint e^{(\boldsymbol{\varphi} \oplus \boldsymbol{\psi} - \boldsymbol{D}^p)/\gamma} d\boldsymbol{\mu} d\boldsymbol{\nu}$$

REGULARIZED DUAL

Smoothed D transforms

$$W_p^p(\boldsymbol{\mu},\boldsymbol{\nu}) = \sup_{\boldsymbol{\varphi}} \int \boldsymbol{\varphi} d\boldsymbol{\mu} + \int \boldsymbol{\varphi}^{\boldsymbol{D}} d\boldsymbol{\nu}.$$

SEMI-DUAL

$$\gamma > 0$$

$$W_\gamma(\boldsymbol{\mu},\boldsymbol{\nu}) = \sup_{\boldsymbol{\varphi}} \int \boldsymbol{\varphi} d\boldsymbol{\mu} + \int \boldsymbol{\varphi}^{\boldsymbol{D},\gamma} d\boldsymbol{\nu}.$$

$$\boldsymbol{\varphi}^{\boldsymbol{D},\gamma} = -\gamma \log \int e^{\frac{\boldsymbol{\varphi}(x) - \boldsymbol{D}(x,\cdot)^p}{\gamma}} d\boldsymbol{\mu}(x)$$

REGULARIZED SEMI-DUAL

Regularized Semidual Wasserstein

$$W_\gamma(\boldsymbol{\mu},\boldsymbol{\nu}) = \sup_{\boldsymbol{\varphi}} \int \boldsymbol{\varphi}\, d\boldsymbol{\mu} + \int \boldsymbol{\varphi}^{\boldsymbol{D},\gamma}\, d\boldsymbol{\nu}.$$

$$\boldsymbol{\varphi}^{\boldsymbol{D},\gamma} = -\gamma \log \int e^{\frac{\boldsymbol{\varphi}(x) - \boldsymbol{D}(x,\cdot)^p}{\gamma}}\, d\boldsymbol{\mu}(x)$$

REGULARIZED SEMI-DUAL

substituting

$$\sup_{\boldsymbol{\varphi}} \int_y \left[\int_x \boldsymbol{\varphi}(x)\, d\boldsymbol{\mu}(x) - \gamma \log \int_x e^{\frac{\boldsymbol{\varphi}(x) - \boldsymbol{D}(x,y)^p}{\gamma}}\, d\boldsymbol{\mu}(x) \right] d\boldsymbol{\nu}(y).$$

REGULARIZED SEMI-DUAL

Stochastic Regularized Semidual

$$\sup_{\varphi} \int_y \left[\int_x \varphi(x) d\mu(x) - \gamma \log \int_x e^{\frac{\varphi(x) - D(x,y)^p}{\gamma}} d\mu(x) \right] d\nu(y).$$

REGULARIZED SEMI-DUAL

Stochastic Regularized Semidual

$$\sup_{\varphi} \int_y \left[\int_x \varphi(x) d\mu(x) - \gamma \log \int_x e^{\frac{\varphi(x) - D(x,y)^p}{\gamma}} d\mu(x) \right] d\nu(y).$$

REGULARIZED SEMI-DUAL

What if μ is a discrete measure?

$\mu = \sum_{i=1}^n a_i \delta_{x_i}$

$\varphi \in L_1(\mu)$ is now just a vector $\alpha \in \mathbb{R}^n$!

Stochastic Regularized Semidual

$$\sup_{\boldsymbol{\varphi}} \int_y \left[\int_x \boldsymbol{\varphi}(x) d\boldsymbol{\mu}(x) - \gamma \log \int_x e^{\frac{\boldsymbol{\varphi}(x) - \boldsymbol{D}(x,y)^p}{\gamma}} d\boldsymbol{\mu}(x) \right] d\boldsymbol{\nu}(y).$$

REGULARIZED SEMI-DUAL

What if $\boldsymbol{\mu}$ is a discrete measure?

$$\boldsymbol{\mu} = \sum_{i=1}^n \boldsymbol{a}_i \delta_{\boldsymbol{x}_i}$$

$\boldsymbol{\varphi} \in L_1(\boldsymbol{\mu})$ is now just a vector $\boldsymbol{\alpha} \in \mathbb{R}^n$!

$$\sup_{\boldsymbol{\alpha} \in \mathbb{R}^n} \int_y \left[\sum_{i=1}^n \boldsymbol{\alpha}_i \boldsymbol{a}_i - \gamma \log \sum_{i=1}^n e^{\frac{\boldsymbol{\alpha}_i - \boldsymbol{D}(\boldsymbol{x}_i, \boldsymbol{y})^p}{\gamma}} \boldsymbol{a}_i \right] d\boldsymbol{\nu}(\boldsymbol{y})$$

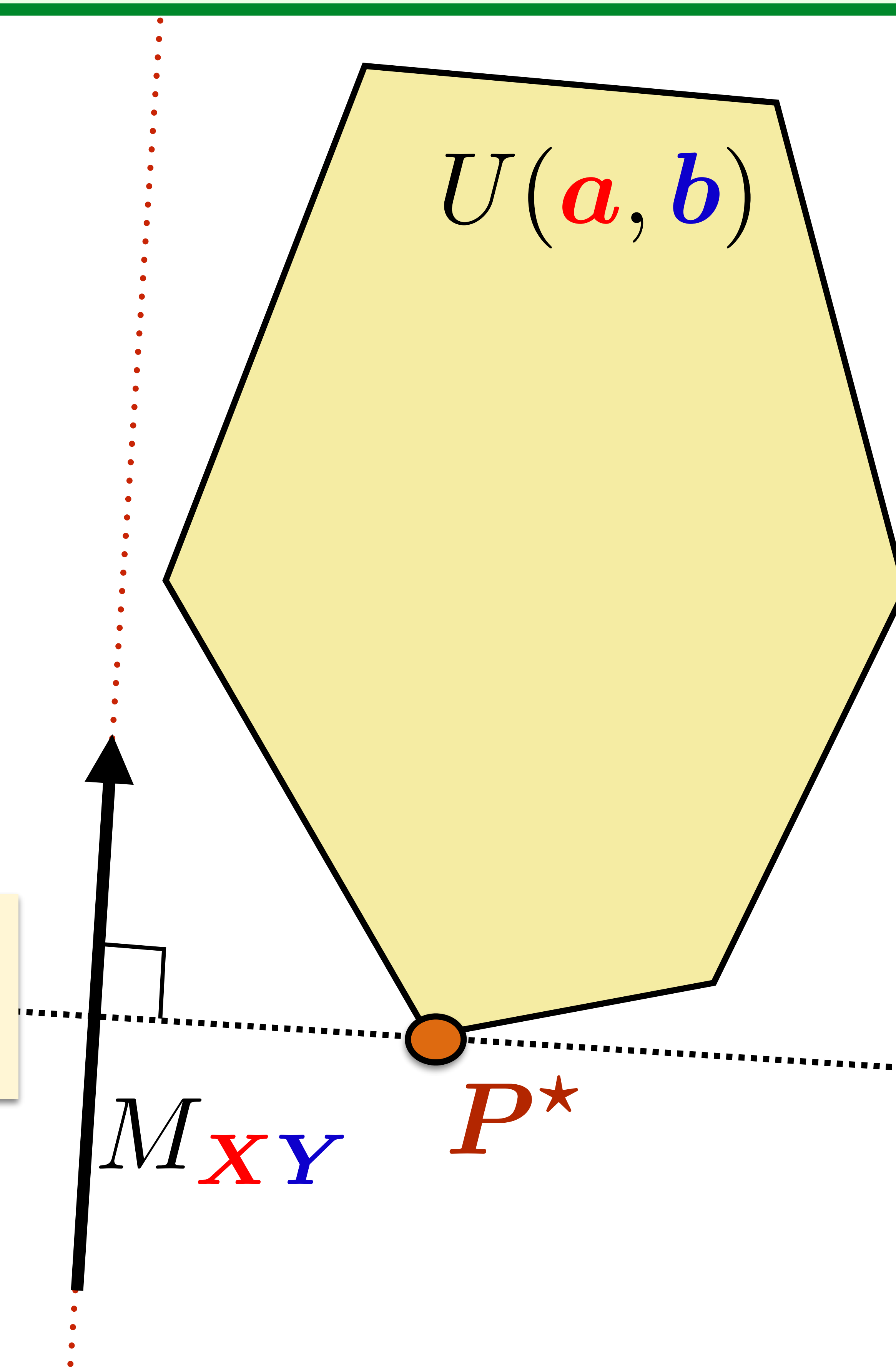
$$= \sup_{\boldsymbol{\alpha} \in \mathbb{R}^n} \mathbb{E}_{\boldsymbol{\nu}} [f(\boldsymbol{\alpha}, \boldsymbol{y})]$$

STOCHASTIC REGULARIZED SEMI-DUAL

Sinkhorn in between W and MMD

$$\boldsymbol{\mu} = \sum_{i=1}^{n} \boldsymbol{a}_i \delta_{\boldsymbol{x}_i} \qquad \boldsymbol{\nu} = \sum_{j=1}^{m} \boldsymbol{b}_j \delta_{\boldsymbol{y}_j}$$

$$W^p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \langle \boldsymbol{P}^\star, M_{\boldsymbol{XY}} \rangle$$

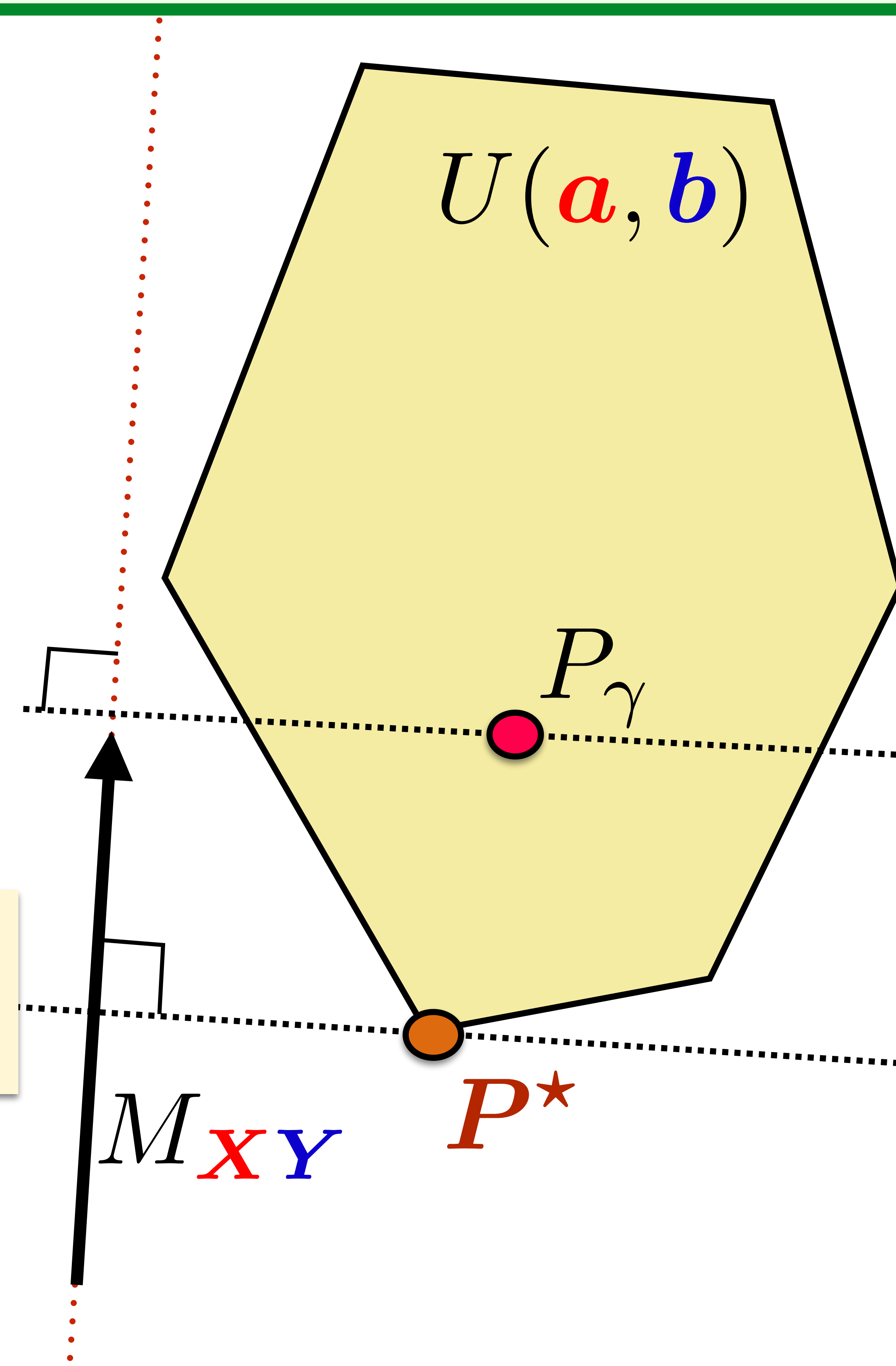


Sinkhorn in between W and MMD

$$\mu = \sum_{i=1}^{n} a_i \delta_{x_i} \qquad \nu = \sum_{j=1}^{m} b_j \delta_{y_j}$$

$$W_\gamma(\mu, \nu) = \langle P_\gamma, M_{\mathbf{XY}} \rangle$$

$$W^p(\mu, \nu) = \langle P^\star, M_{\mathbf{XY}} \rangle$$



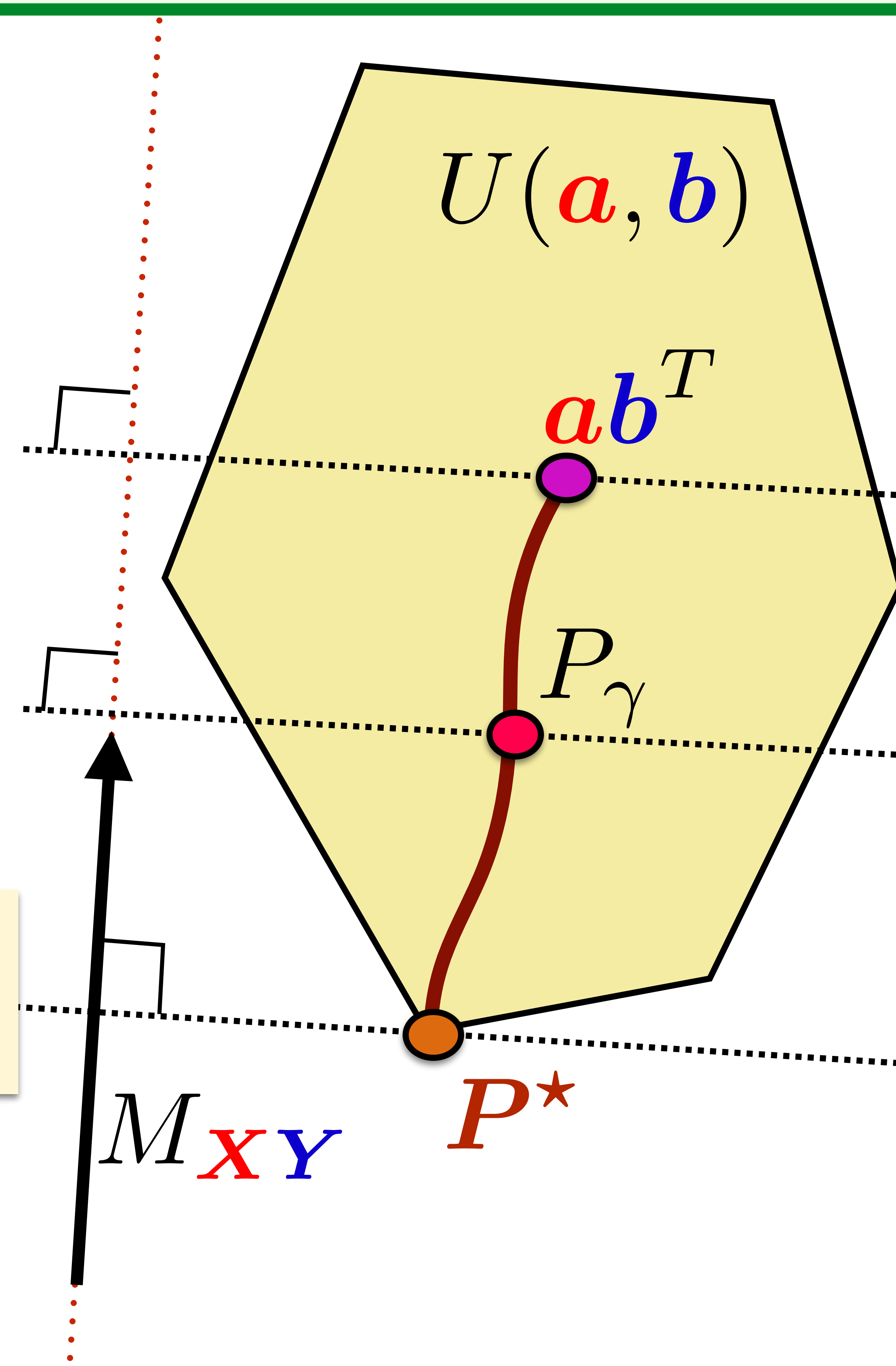
Sinkhorn in between W and MMD

$$\boldsymbol{\mu} = \sum_{i=1}^{n} \boldsymbol{a}_i \delta_{\boldsymbol{x}_i} \qquad \boldsymbol{\nu} = \sum_{j=1}^{m} \boldsymbol{b}_j \delta_{\boldsymbol{y}_j}$$

$$\mathcal{E}(\boldsymbol{\mu}, \boldsymbol{\nu}) = \langle \boldsymbol{a}\boldsymbol{b}^T, M_{\mathbf{XY}} \rangle$$

$$W_\gamma(\boldsymbol{\mu}, \boldsymbol{\nu}) = \langle P_\gamma, M_{\mathbf{XY}} \rangle$$

$$\boxed{W^p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \langle \boldsymbol{P}^\star, M_{\mathbf{XY}} \rangle}$$



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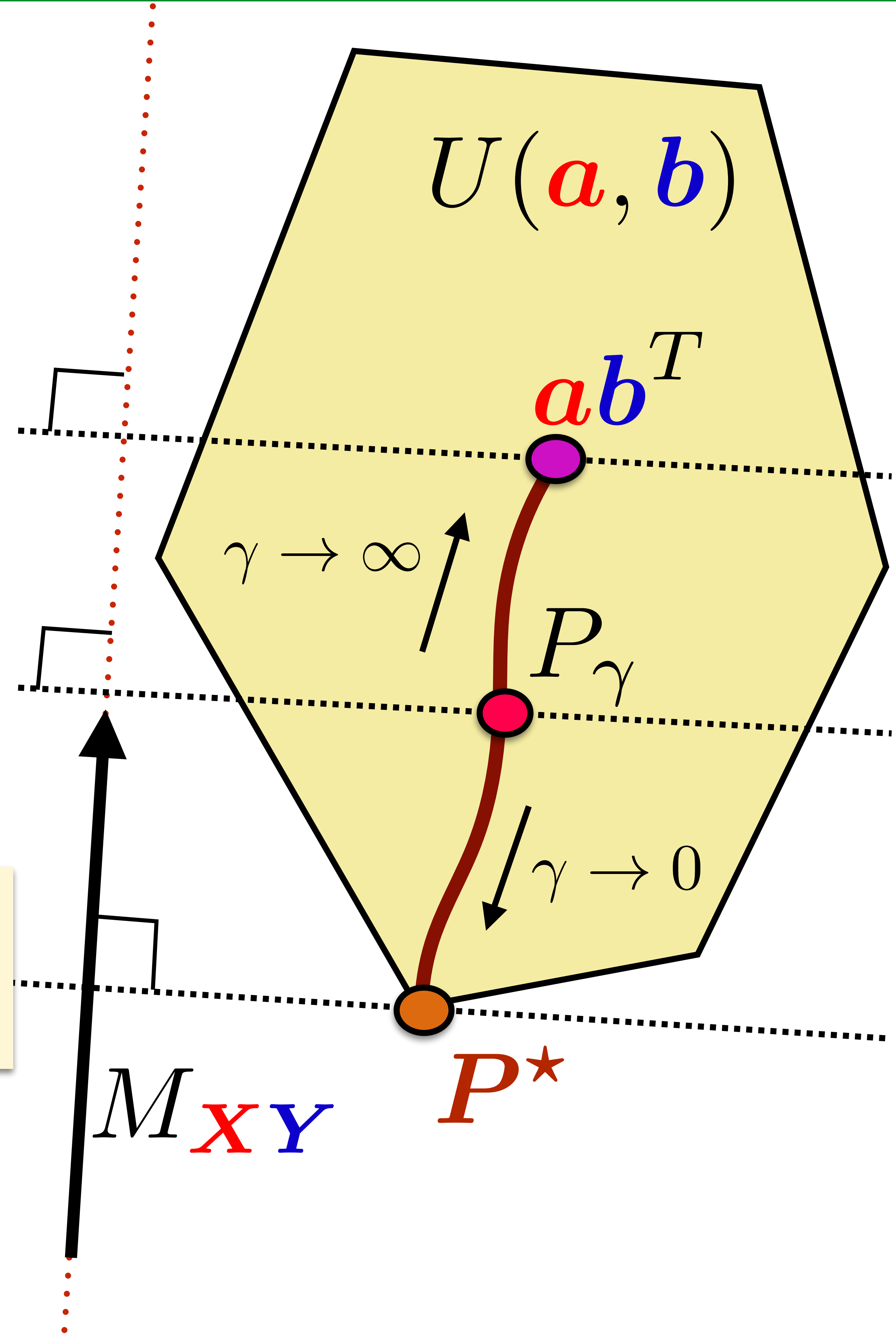
$$\boldsymbol{\mu} = \sum_{i=1}^{n} \boldsymbol{a}_i \delta_{\boldsymbol{x}_i} \qquad \boldsymbol{\nu} = \sum_{j=1}^{m} \boldsymbol{b}_j \delta_{\boldsymbol{y}_j}$$

$$\mathcal{E}(\boldsymbol{\mu}, \boldsymbol{\nu}) = \langle \boldsymbol{a}\boldsymbol{b}^T, M_{\boldsymbol{XY}} \rangle$$

$$W_\gamma(\boldsymbol{\mu}, \boldsymbol{\nu}) = \langle P_\gamma, M_{\boldsymbol{XY}} \rangle$$

$$W^p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \langle \boldsymbol{P}^\star, M_{\boldsymbol{XY}} \rangle$$



Sinkhorn in between W and MMD

$$\mathcal{E}(\boldsymbol{\mu},\boldsymbol{\nu}) = \langle \boldsymbol{a}\boldsymbol{b}^T, M_{\mathbf{X}\mathbf{Y}} \rangle$$

$$\mathcal{MMD}(\boldsymbol{\mu},\boldsymbol{\nu}) = \mathcal{E}(\boldsymbol{\mu},\boldsymbol{\nu}) - \frac{1}{2}(\mathcal{E}(\boldsymbol{\mu},\boldsymbol{\mu}) + \mathcal{E}(\boldsymbol{\nu},\boldsymbol{\nu}))$$

$$W_\gamma(\boldsymbol{\mu},\boldsymbol{\nu}) = \langle P_\gamma, M_{\mathbf{X}\mathbf{Y}} \rangle$$

$$\bar{W}_\gamma(\boldsymbol{\mu},\boldsymbol{\nu}) = W_\gamma(\boldsymbol{\mu},\boldsymbol{\nu}) - \frac{1}{2}(W_\gamma(\boldsymbol{\mu},\boldsymbol{\mu}) + W_\gamma(\boldsymbol{\nu},\boldsymbol{\nu}))$$

$$W^p(\boldsymbol{\mu},\boldsymbol{\nu}) = \langle \boldsymbol{P}^\star, M_{\mathbf{X}\mathbf{Y}} \rangle$$

Sinkhorn in between W and MMD

$$\mathcal{MMD}(\boldsymbol{\mu},\boldsymbol{\nu}) = \mathcal{E}(\boldsymbol{\mu},\boldsymbol{\nu}) - \frac{1}{2}(\mathcal{E}(\boldsymbol{\mu},\boldsymbol{\mu}) + \mathcal{E}(\boldsymbol{\nu},\boldsymbol{\nu}))$$

$$\gamma \to \infty \quad \uparrow$$

$$\bar{W}_\gamma(\boldsymbol{\mu},\boldsymbol{\nu}) = W_\gamma(\boldsymbol{\mu},\boldsymbol{\nu}) - \frac{1}{2}(W_\gamma(\boldsymbol{\mu},\boldsymbol{\mu}) + W_\gamma(\boldsymbol{\nu},\boldsymbol{\nu}))$$

$$\gamma \to 0 \quad \downarrow$$

$$W^p(\boldsymbol{\mu},\boldsymbol{\nu}) = \langle \boldsymbol{P}^\star, M_{\boldsymbol{XY}} \rangle$$

How to compare them?

i.i.d samples $\boldsymbol{x_1, \dots, x_n} \sim \boldsymbol{\mu}$, $\boldsymbol{y_1, \dots, y_m} \sim \boldsymbol{\nu}$,

$$\hat{\boldsymbol{\mu}}_{\boldsymbol{n}} \stackrel{\text{def}}{=} \frac{1}{n} \sum_i \delta_{\boldsymbol{x_i}}, \hat{\boldsymbol{\nu}}_{\boldsymbol{m}} \stackrel{\text{def}}{=} \frac{1}{m} \sum_j \delta_{\boldsymbol{y_j}}$$

Computational properties

Effort to compute/approximate $\boldsymbol{\Delta}(\hat{\boldsymbol{\mu}}_{\boldsymbol{n}}, \hat{\boldsymbol{\nu}}_{\boldsymbol{m}})$?

Statistical properties

$$|\boldsymbol{\Delta}(\boldsymbol{\mu}, \boldsymbol{\nu}) - \boldsymbol{\Delta}(\hat{\boldsymbol{\mu}}_{\boldsymbol{n}}, \hat{\boldsymbol{\nu}}_{\boldsymbol{n}})| \leq f(n)?$$

Sinkhorn in between W and MMD

$$\mathcal{MMD}(\boldsymbol{\mu}, \boldsymbol{\nu}) = \mathcal{E}(\boldsymbol{\mu}, \boldsymbol{\nu}) - \frac{1}{2}(\mathcal{E}(\boldsymbol{\mu}, \boldsymbol{\mu}) + \mathcal{E}(\boldsymbol{\nu}, \boldsymbol{\nu}))$$

$(n+m)^2$

$O(1/\sqrt{n})$ **[see Arthur]**

$$W^p(\boldsymbol{\mu}, \boldsymbol{\nu}) = \langle \boldsymbol{P}^\star, M_{\boldsymbol{XY}} \rangle$$

$O((n+m)nm\log(n+m))$

$O(1/n^{1/d})$

Sinkhorn in between W and MMD

$$\mathcal{MMD}(\boldsymbol{\mu},\boldsymbol{\nu}) = \mathcal{E}(\boldsymbol{\mu},\boldsymbol{\nu}) - \frac{1}{2}(\mathcal{E}(\boldsymbol{\mu},\boldsymbol{\mu}) + \mathcal{E}(\boldsymbol{\nu},\boldsymbol{\nu}))$$

$\boxed{(n+m)^2}$ $\boxed{O(1/\sqrt{n})}$ **[see Arthur]**

$$\bar{W}_\gamma(\boldsymbol{\mu},\boldsymbol{\nu}) = W_\gamma(\boldsymbol{\mu},\boldsymbol{\nu}) - \frac{1}{2}(W_\gamma(\boldsymbol{\mu},\boldsymbol{\mu}) + W_\gamma(\boldsymbol{\nu},\boldsymbol{\nu}))$$

$\boxed{O((n+m)^2)}$ $\boxed{O\left(\frac{1}{\gamma^{d/2}\sqrt{n}}\right)}$ **[GCBCP'18]** **[FSVATP'18]**

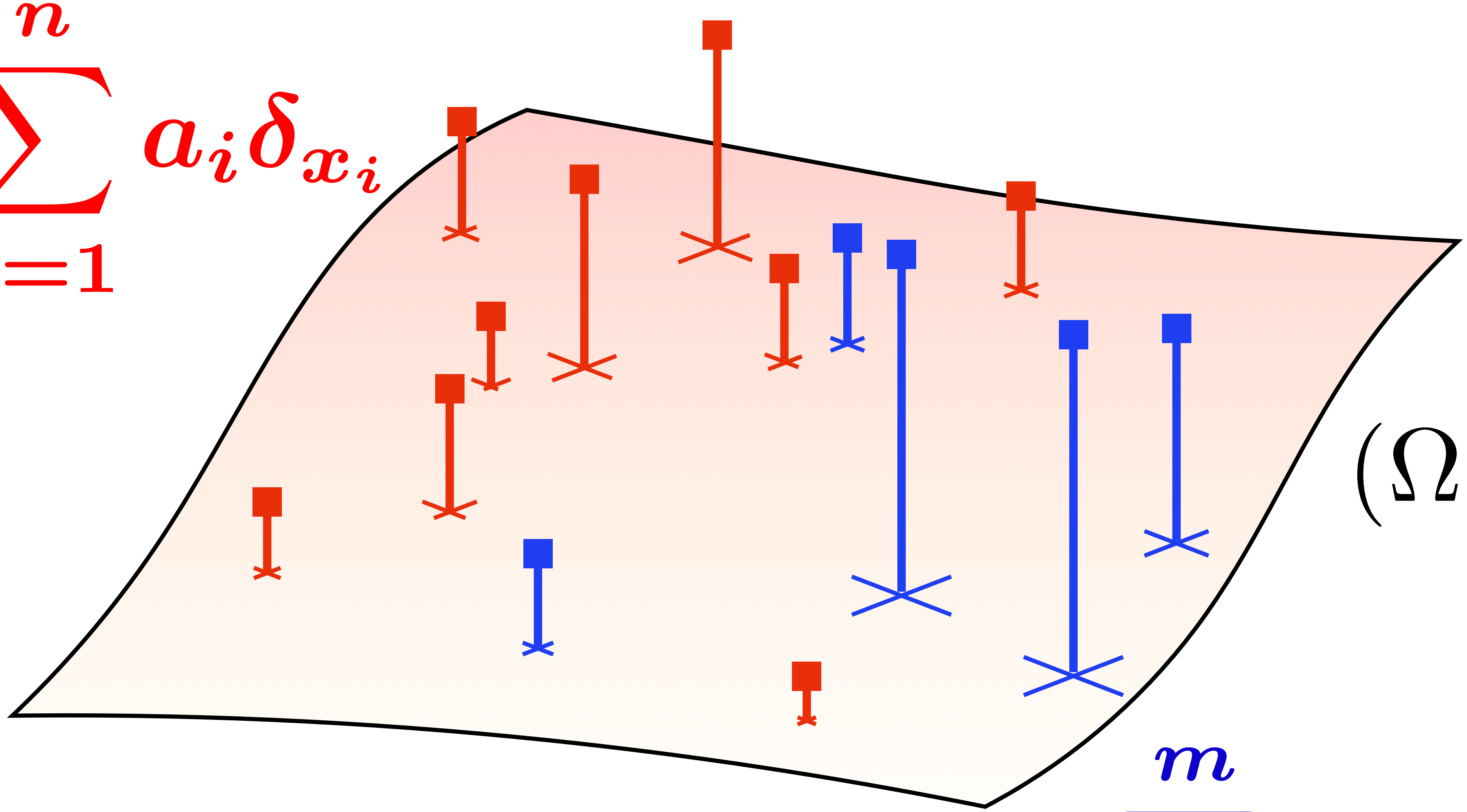
$$W^p(\boldsymbol{\mu},\boldsymbol{\nu}) = \langle \boldsymbol{P}^\star, M_{\boldsymbol{XY}} \rangle$$

$\boxed{O((n+m)nm\log(n+m))}$ $\boxed{O(1/n^{1/d})}$

Differentiability of W

$$W((\boldsymbol{a}, \boldsymbol{X}), (\boldsymbol{b}, \boldsymbol{Y}))$$

$$\boldsymbol{\mu} = \sum_{i=1}^{n} \boldsymbol{a}_i \boldsymbol{\delta}_{\boldsymbol{x}_i}$$



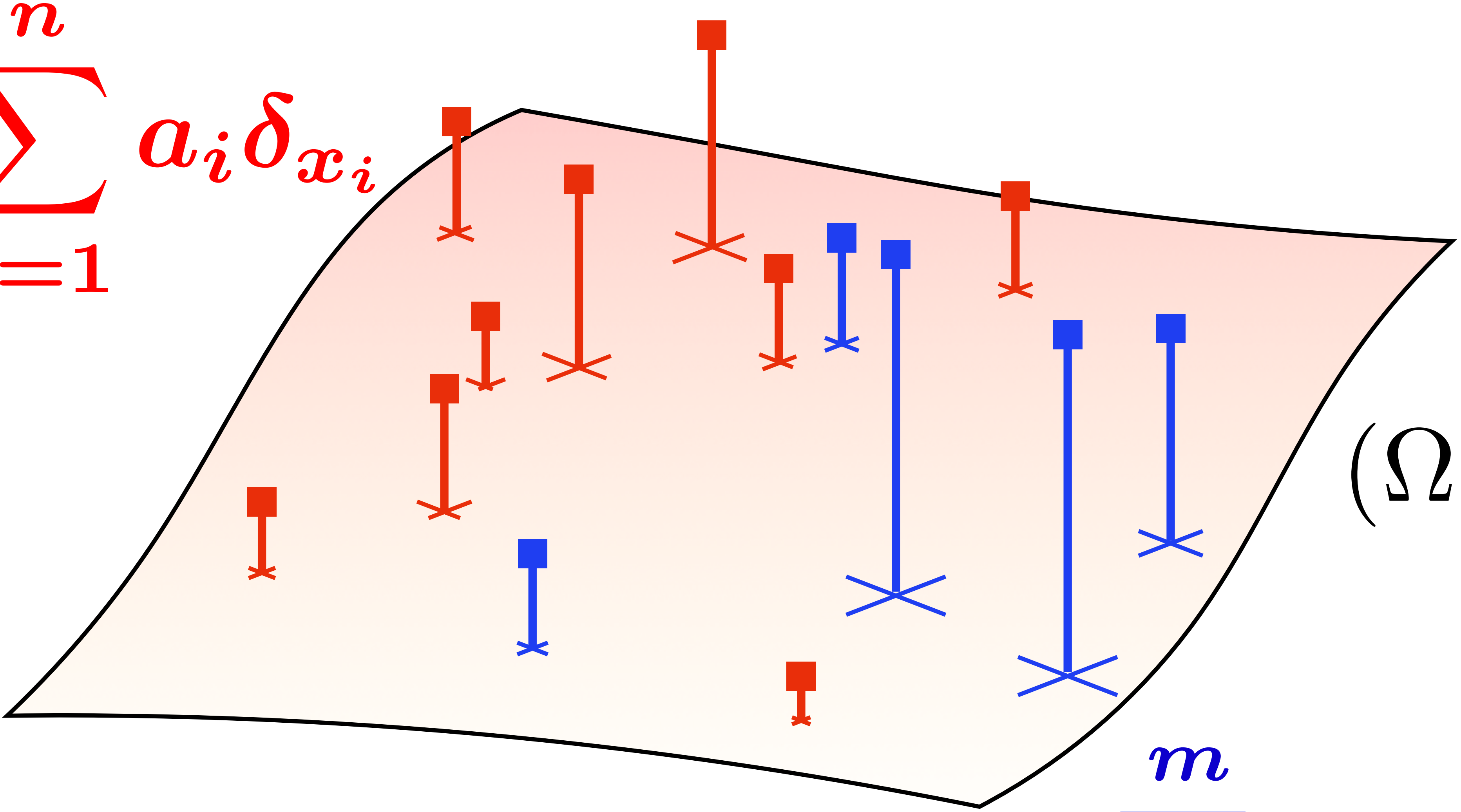
$$(\Omega, \boldsymbol{D})$$

$$\boldsymbol{\nu} = \sum_{j=1}^{m} \boldsymbol{b}_j \boldsymbol{\delta}_{\boldsymbol{y}_j}$$

Differentiability of W

$$W((\boldsymbol{a} + \boldsymbol{\Delta a}, \boldsymbol{X}), (\boldsymbol{b}, \boldsymbol{Y})) = W((\boldsymbol{a}, \boldsymbol{X}), (\boldsymbol{b}, \boldsymbol{Y})) + ??$$

$$\boldsymbol{\mu} = \sum_{i=1}^{n} \boldsymbol{a_i \delta_{x_i}}$$



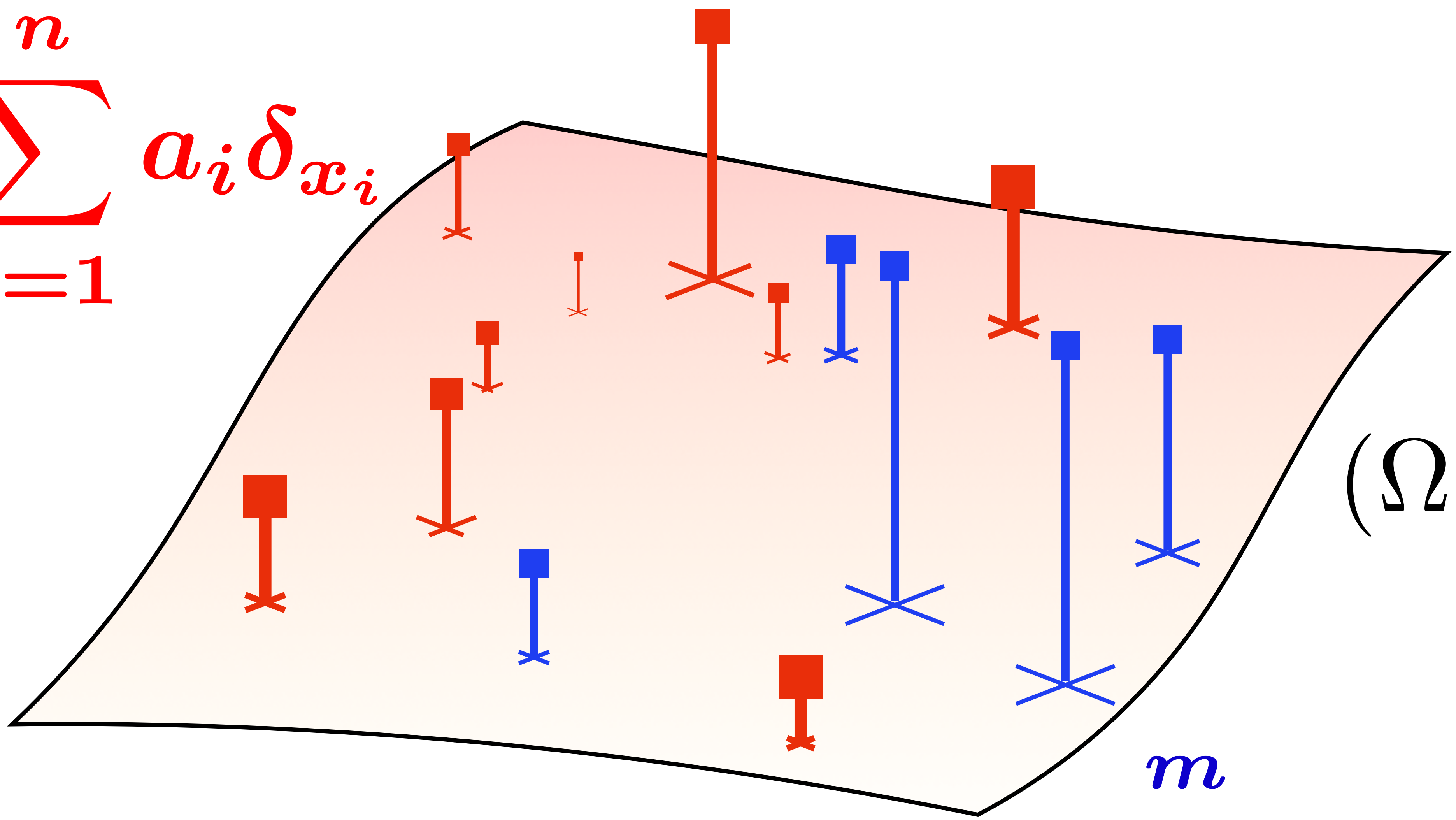
$$(\Omega, \boldsymbol{D})$$

$$\boldsymbol{\nu} = \sum_{j=1}^{m} \boldsymbol{b_j \delta_{y_j}}$$

Differentiability of W

$$W((\boldsymbol{a} + \boldsymbol{\Delta a}, \boldsymbol{X}), (\boldsymbol{b}, \boldsymbol{Y})) = W((\boldsymbol{a}, \boldsymbol{X}), (\boldsymbol{b}, \boldsymbol{Y})) + ??$$

$$\boldsymbol{\mu = \sum_{i=1}^{n} a_i \delta_{x_i}}$$



$$(\Omega, \boldsymbol{D})$$

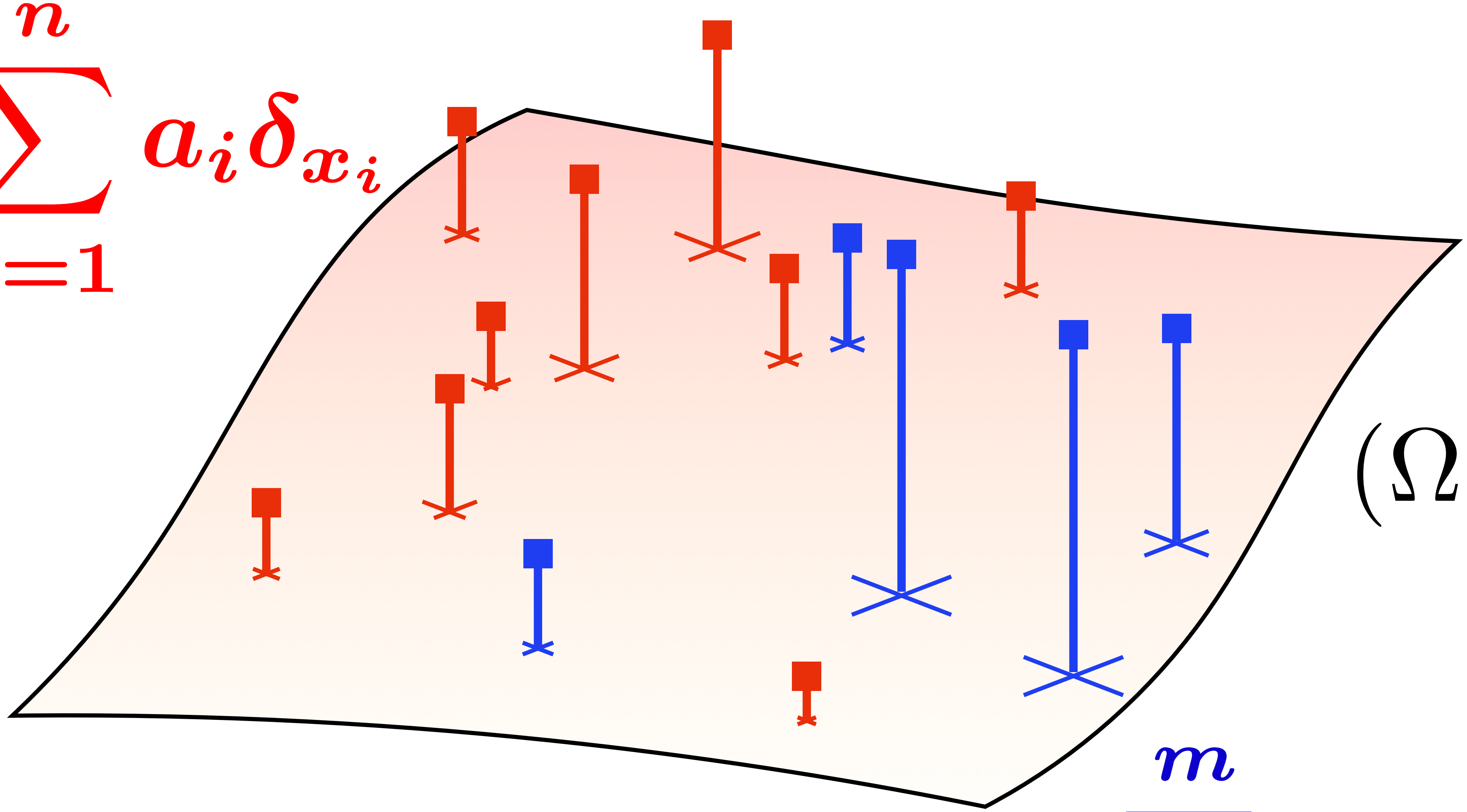
$$\boldsymbol{\nu = \sum_{j=1}^{m} b_j \delta_{y_j}}$$

$$\boldsymbol{a} \leftarrow \boldsymbol{a} + \boldsymbol{\Delta a}$$

Sinkhorn ⇝ *Differentiability*

$$W((\boldsymbol{a}, \boldsymbol{X} + \boldsymbol{\Delta X}), (\boldsymbol{b}, \boldsymbol{Y})) = W((\boldsymbol{a}, \boldsymbol{X}), (\boldsymbol{b}, \boldsymbol{Y})) + ??$$

$$\boldsymbol{\mu = \sum_{i=1}^{n} a_i \delta_{x_i}}$$

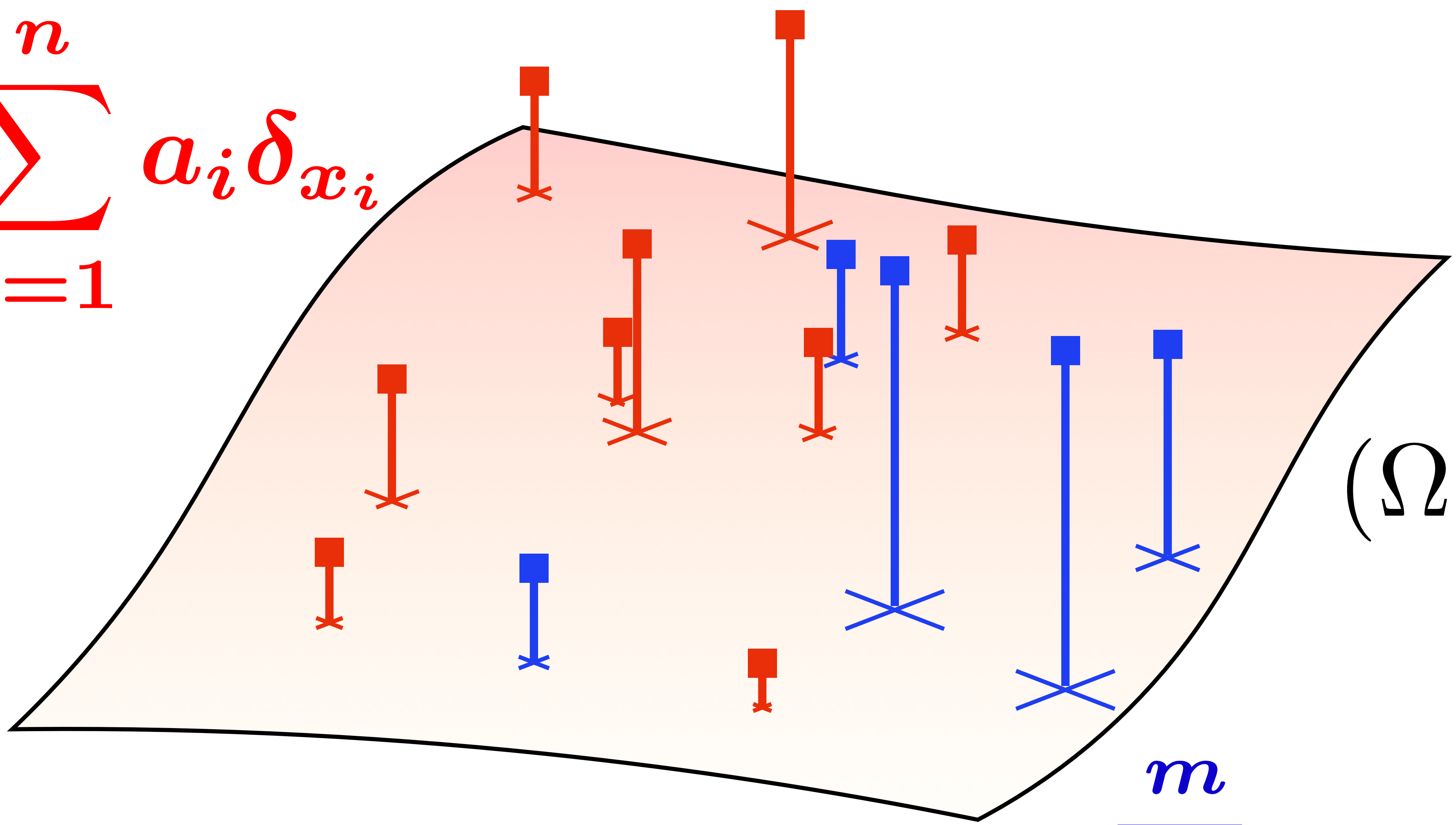


$$\boldsymbol{\nu = \sum_{j=1}^{m} b_j \delta_{y_j}}$$

Sinkhorn ⇝ *Differentiability*

$$W((\boldsymbol{a}, \boldsymbol{X} + \boldsymbol{\Delta X}), (\boldsymbol{b}, \boldsymbol{Y})) = W((\boldsymbol{a}, \boldsymbol{X}), (\boldsymbol{b}, \boldsymbol{Y})) + ??$$

$$\boldsymbol{\mu} = \sum_{i=1}^{n} \boldsymbol{a_i \delta_{x_i}}$$



$$(\Omega, \boldsymbol{D})$$

$$\boldsymbol{X} \leftarrow \boldsymbol{X} + \boldsymbol{\Delta X}$$

$$\boldsymbol{\nu} = \sum_{j=1}^{m} \boldsymbol{b_j \delta_{y_j}}$$

How to decrease W? change weights

$$W_p^p(\boldsymbol{\mu},\boldsymbol{\nu}) = \max_{\substack{\boldsymbol{\alpha}\in\mathbb{R}^n,\boldsymbol{\beta}\in\mathbb{R}^m \\ \boldsymbol{\alpha}\oplus\boldsymbol{\beta}\leq M_{\mathbf{X}\mathbf{Y}}}} \boldsymbol{\alpha}^T\boldsymbol{a} + \boldsymbol{\beta}^T\boldsymbol{b}.$$

DUAL

Prop. $W(\boldsymbol{\mu},\boldsymbol{\nu})$ is convex w.r.t. $\boldsymbol{a}$,

$$\partial_{\boldsymbol{a}} W = \arg_{\boldsymbol{\alpha}} \max_{\boldsymbol{\alpha}\oplus\boldsymbol{\beta}\leq M_{\mathbf{X}\mathbf{Y}}} \boldsymbol{\alpha}^T\boldsymbol{a} + \boldsymbol{\beta}^T\boldsymbol{b}.$$

Prop. $W_\gamma(\boldsymbol{\mu},\boldsymbol{\nu})$ is convex and **differentiable** w.r.t. $\boldsymbol{a}$, $\nabla_{\boldsymbol{a}} W_\gamma = \boldsymbol{\alpha}^\star_\gamma = \gamma\log\boldsymbol{u}$

How to decrease W? change locations

$$W_2^2(\mu,\nu) = \min_{\substack{P\in\mathbb{R}_+^{n\times m}\\ P\mathbf{1}_m=a, P^T\mathbf{1}_n=b}} \langle P, \mathbf{1}_n\mathbf{1}_d^T X^2 + Y^{2T}\mathbf{1}_d\mathbf{1}_m - 2X^TY\rangle$$

PRIMAL

Prop. $p=2, \Omega=\mathbb{R}^d$. $W(\mu,\nu)$ decreases if

$$X \leftarrow Y P^{\star T}\mathbf{D}(a^{-1}).$$

Prop. $p=2, \Omega=\mathbb{R}^d$. $W_\gamma(\mu,\nu)$ is **differentiable** w.r.t. X, with

$$\nabla_X W_\gamma = X - Y P_\gamma^T \mathbf{D}(a^{-1}).$$

Sinkhorn: A Programmer View

Def. For $L \geq 1$, define

$$W_L(\boldsymbol{\mu}, \boldsymbol{\nu}) \stackrel{\text{def}}{=} \langle \boldsymbol{P_L}, M_{\boldsymbol{XY}} \rangle,$$

where $\boldsymbol{P_L} \stackrel{\text{def}}{=} \mathbf{diag}(\boldsymbol{u_L}) K \mathbf{diag}(\boldsymbol{v_L}),$

$\boldsymbol{v_0} = \mathbf{1}_m; l \geq 0, \boldsymbol{u_l} \stackrel{\text{def}}{=} \boldsymbol{a}/K\boldsymbol{v_l}, \boldsymbol{v_{l+1}} \stackrel{\text{def}}{=} \boldsymbol{b}/K^T\boldsymbol{u_l}.$

Prop. $\frac{\partial W_L}{\partial \boldsymbol{X}}, \frac{\partial W_L}{\partial \boldsymbol{a}}$ can be computed recursively, in $O(L)$ kernel $K \times$vector products.

Sinkhorn: A Programmer View

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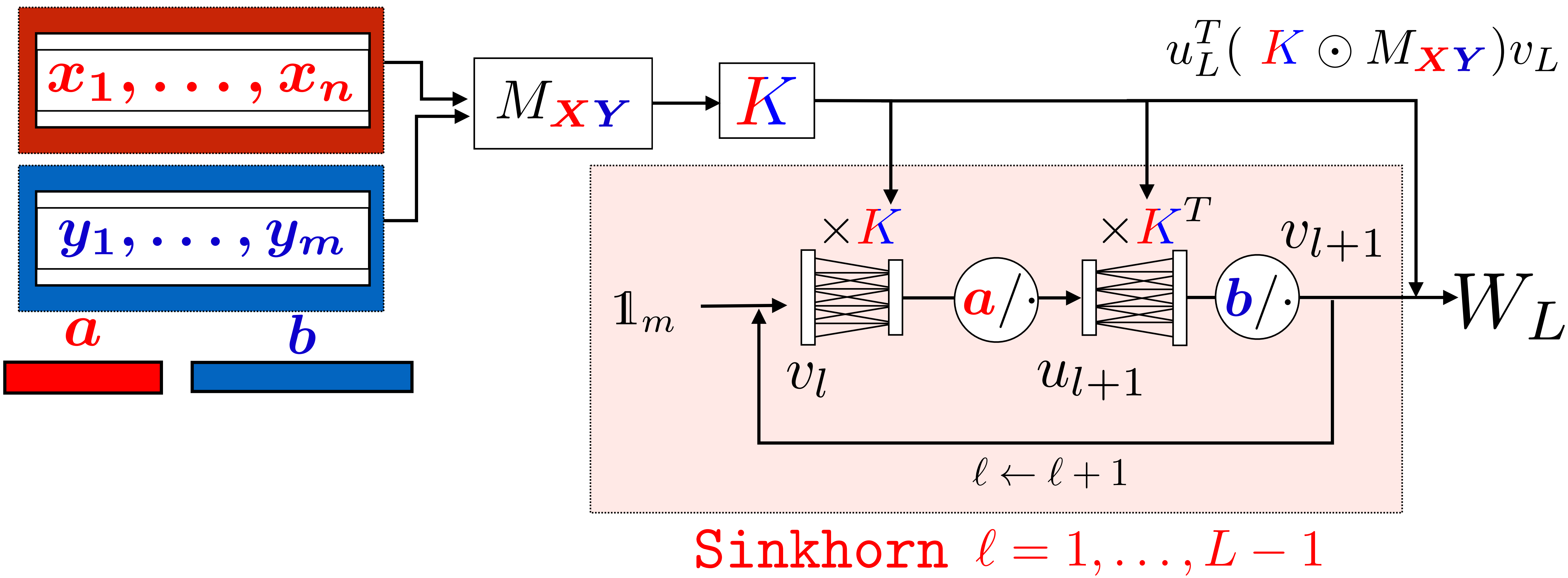
$$W_L(\boldsymbol{\mu}, \boldsymbol{\nu}) \stackrel{\text{def}}{=} \langle \boldsymbol{P_L}, M_{\mathbf{XY}} \rangle,$$



Sinkhorn: A Programmer View

Def. For $L \geq 1$, define

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Prop. $\frac{\partial W_L}{\partial \boldsymbol{X}}, \frac{\partial W_L}{\partial \boldsymbol{a}}$ can be computed recursively, in $O(L)$ kernel $K \times$vector products.

[Hashimoto'16] [Bonneel'16][Shalit'16]

3. Applications

- Wasserstein distances for retrieval
- Wasserstein barycenters
- W for unsupervised learning
- W inverse problems
- W to learn parameters and generative models

The Earth Mover's Distance

The Earth Mover's Distance

The Earth Mover's Distance

[Rubner'98] $\mathrm{dist}(I_1, I_2) = W_1(\boldsymbol{\mu}, \boldsymbol{\nu})$

The Word Mover's Distance

[Kusner'15] $\mathrm{dist}(D_1, D_2) = W_2(\boldsymbol{\mu}, \boldsymbol{\nu})$

Recall

Up to 2010: OT solvers $W_p(\boldsymbol{\mu}, \boldsymbol{\nu}) = ?$

Goal now: use OT as a **loss or fidelity** term

$$\operatorname*{argmin}_{\boldsymbol{\mu} \in \mathcal{P}(\Omega)} F(W_p(\boldsymbol{\mu}, \boldsymbol{\nu_1}), W_p(\boldsymbol{\mu}, \boldsymbol{\nu_2}), \dots, \boldsymbol{\mu}) = ?$$

$$\nabla_{\boldsymbol{\mu}} W_p(\boldsymbol{\mu}, \boldsymbol{\nu_1}) = ?$$

Wassersteinization

[**wos-ur-stahyn-ahy-sey**-sh*uh*-n]
noun.

Introduction of optimal transport into an optimization or learning problem.

cf. least-squarification, L_1ification, deep-netification, kernelization

"Wasserstein + Data" Problems

- Quantization, k-means problem **[Lloyd'82]**

$$\min_{\substack{\boldsymbol{\mu}\in\mathcal{P}(\mathbb{R}^d)\\ |\operatorname{supp}\boldsymbol{\mu}|=k}} W_2^2(\boldsymbol{\mu}, \boldsymbol{\nu}_{\text{data}})$$

- **[McCann'95]** Interpolant

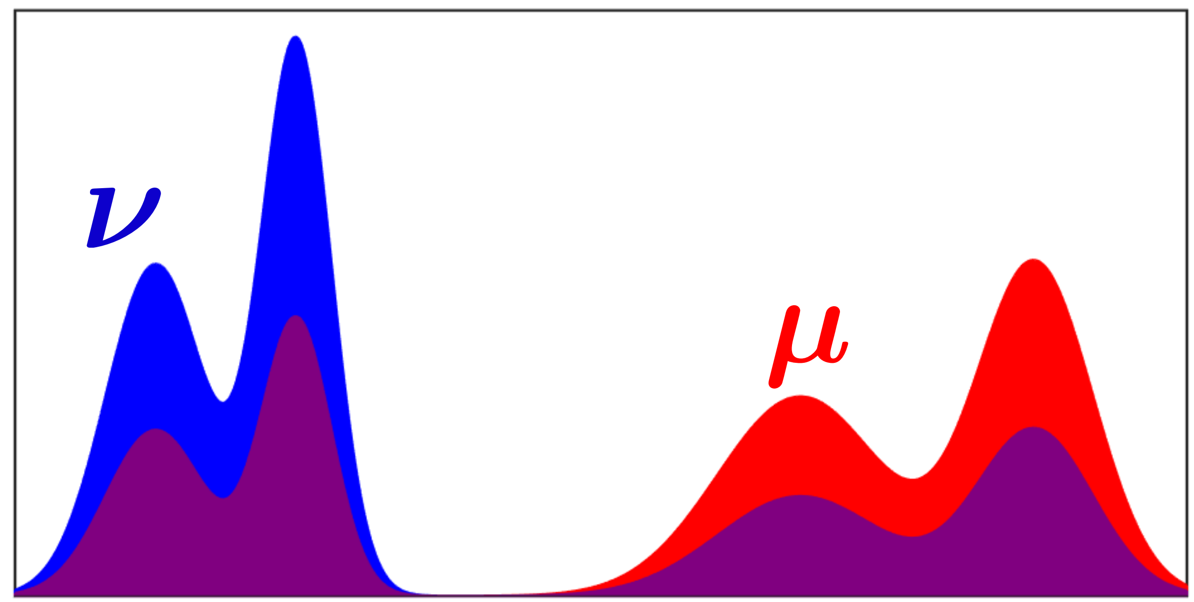
$$\min_{\boldsymbol{\mu}\in\mathcal{P}(\Omega)} (1-t)W_2^2(\boldsymbol{\mu}, \boldsymbol{\nu_1}) + tW_2^2(\boldsymbol{\mu}, \boldsymbol{\nu_2})$$

- **[JKO'98]** PDE's as gradient flows in $(\mathcal{P}(\Omega), W)$.

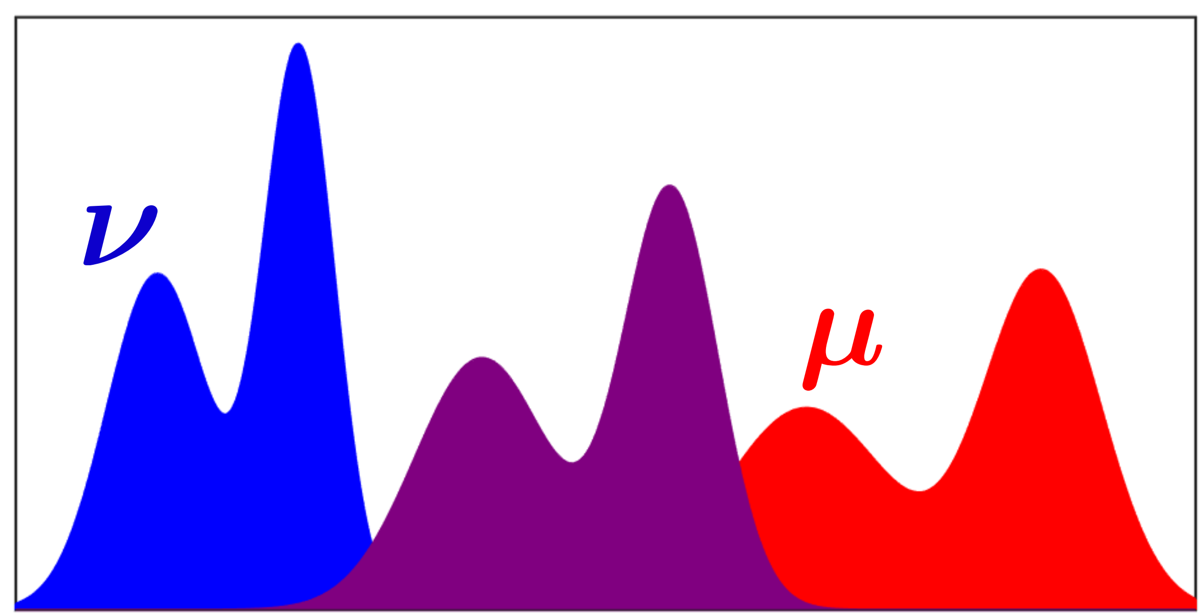
$$\mu_{t+1} = \operatorname*{argmin}_{\boldsymbol{\mu}\in\mathcal{P}(\Omega)} J(\boldsymbol{\mu}) + \lambda_t W_p^p(\boldsymbol{\mu}, \mu_t)$$

Averaging Measures

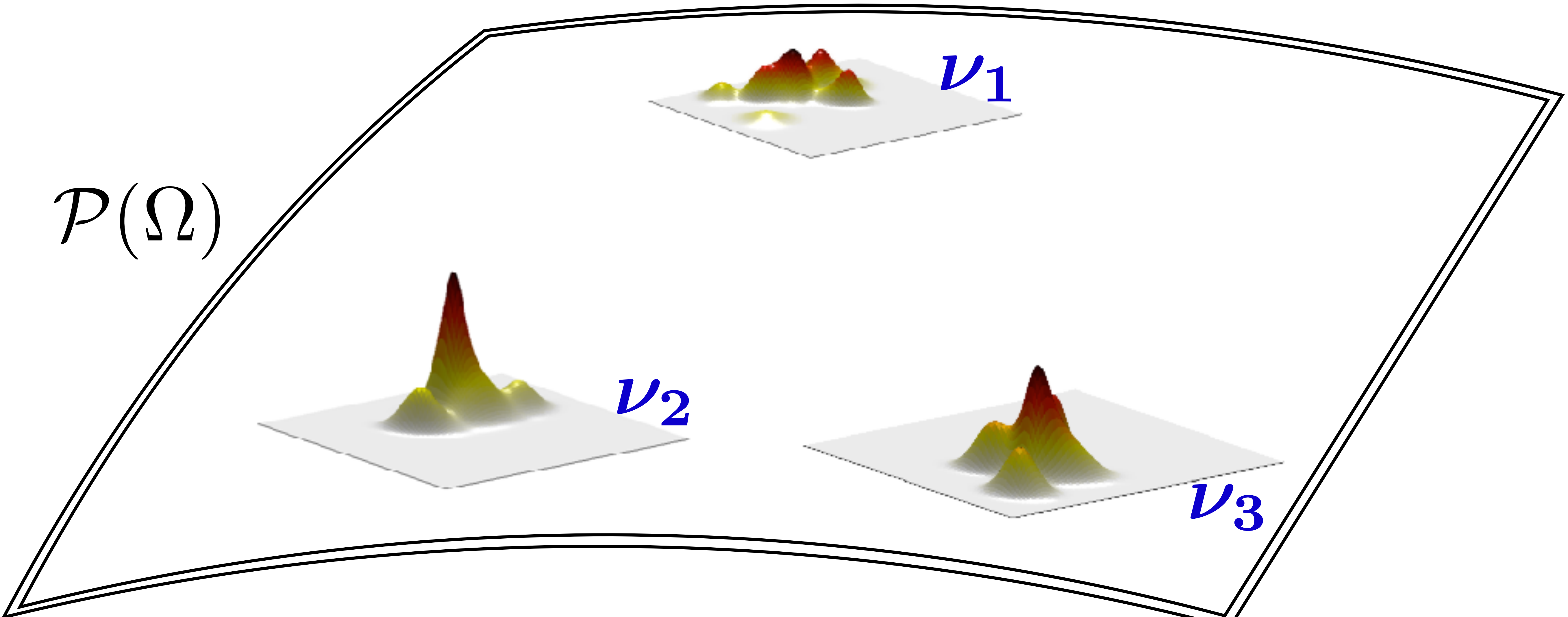
L_2 average



W average

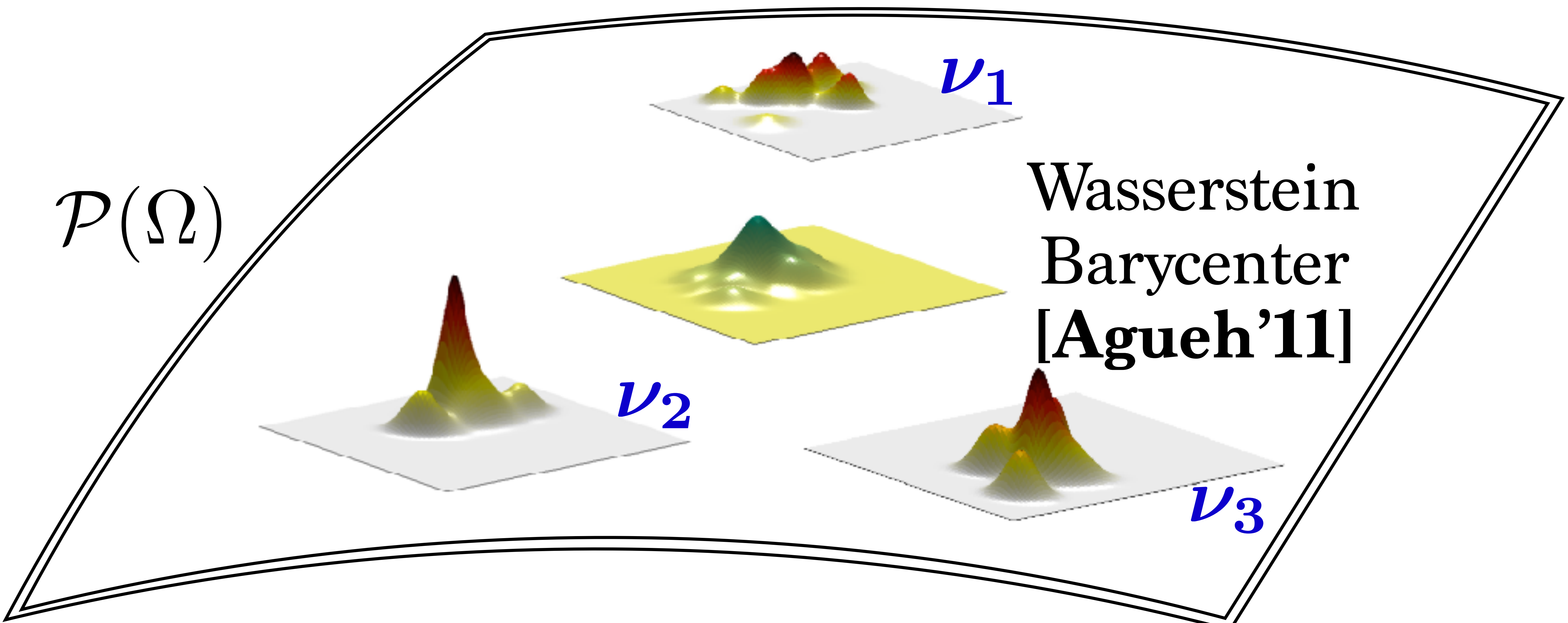


Barycenter for Measures?

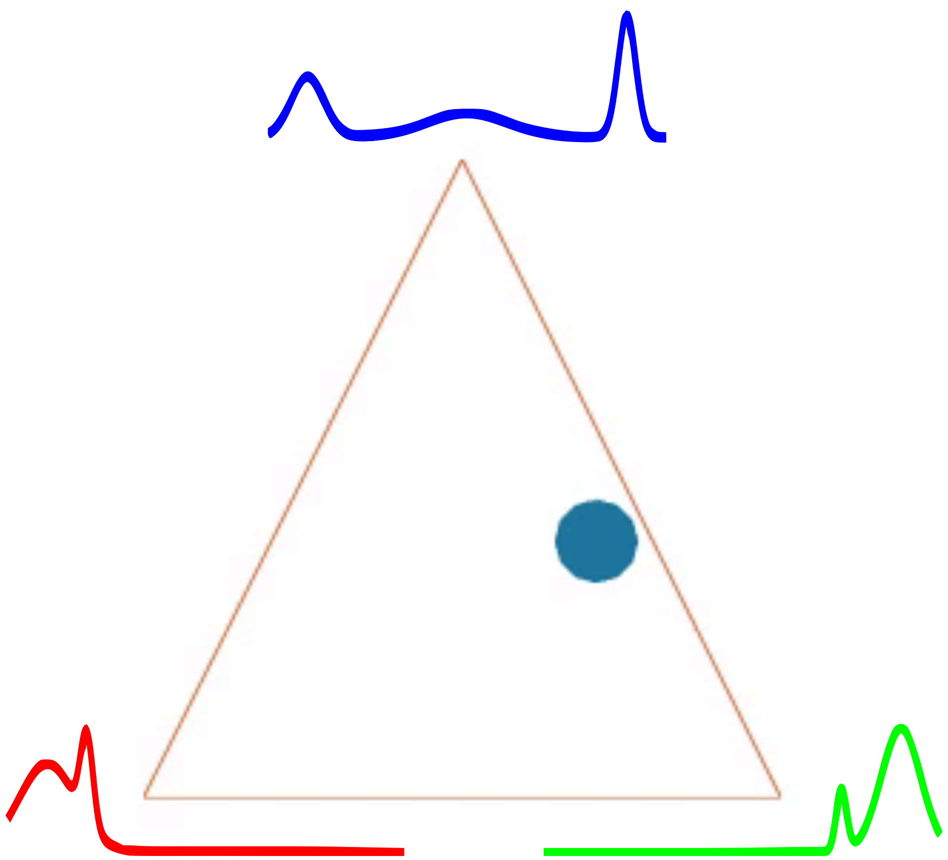


Barycenter for Measures?

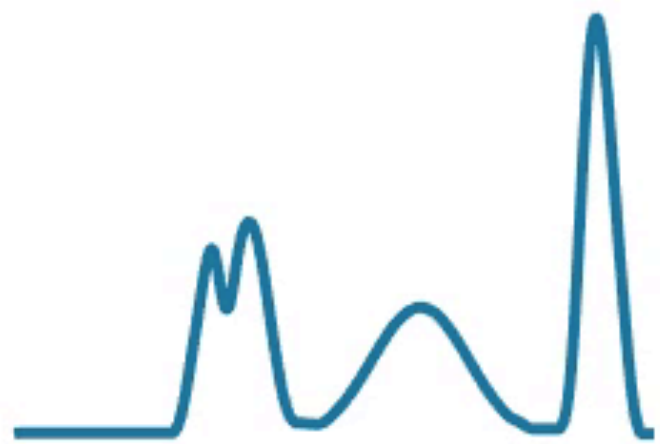
$$\min_{\mu \in \mathcal{P}(\Omega)} \sum_{i=1}^{N} \lambda_i W_p^p(\mu, \nu_i)$$



Barycenter for Measures?



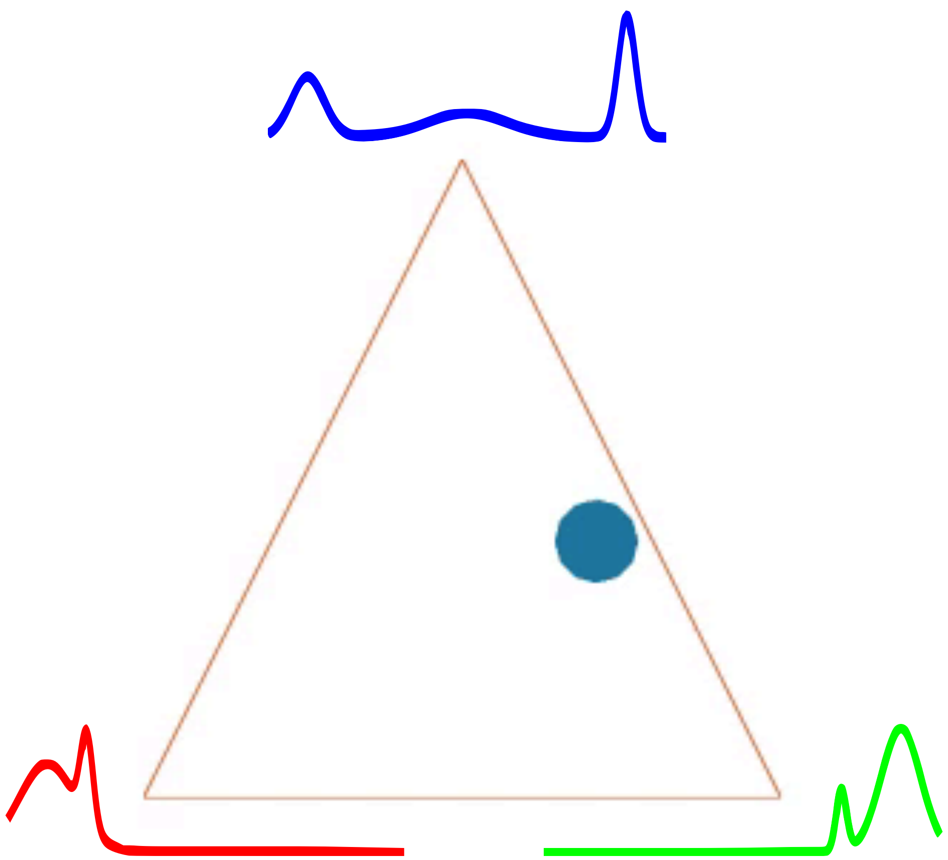
$\lambda \in \Sigma_3$



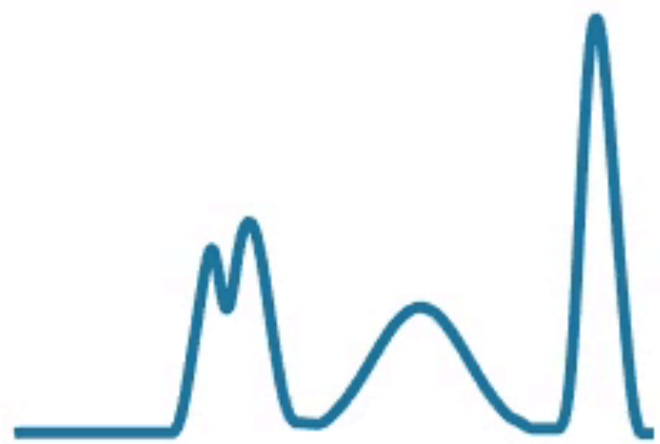
Wasserstein mean

L_2 mean

Barycenter for Measures?



$$\lambda \in \Sigma_3$$

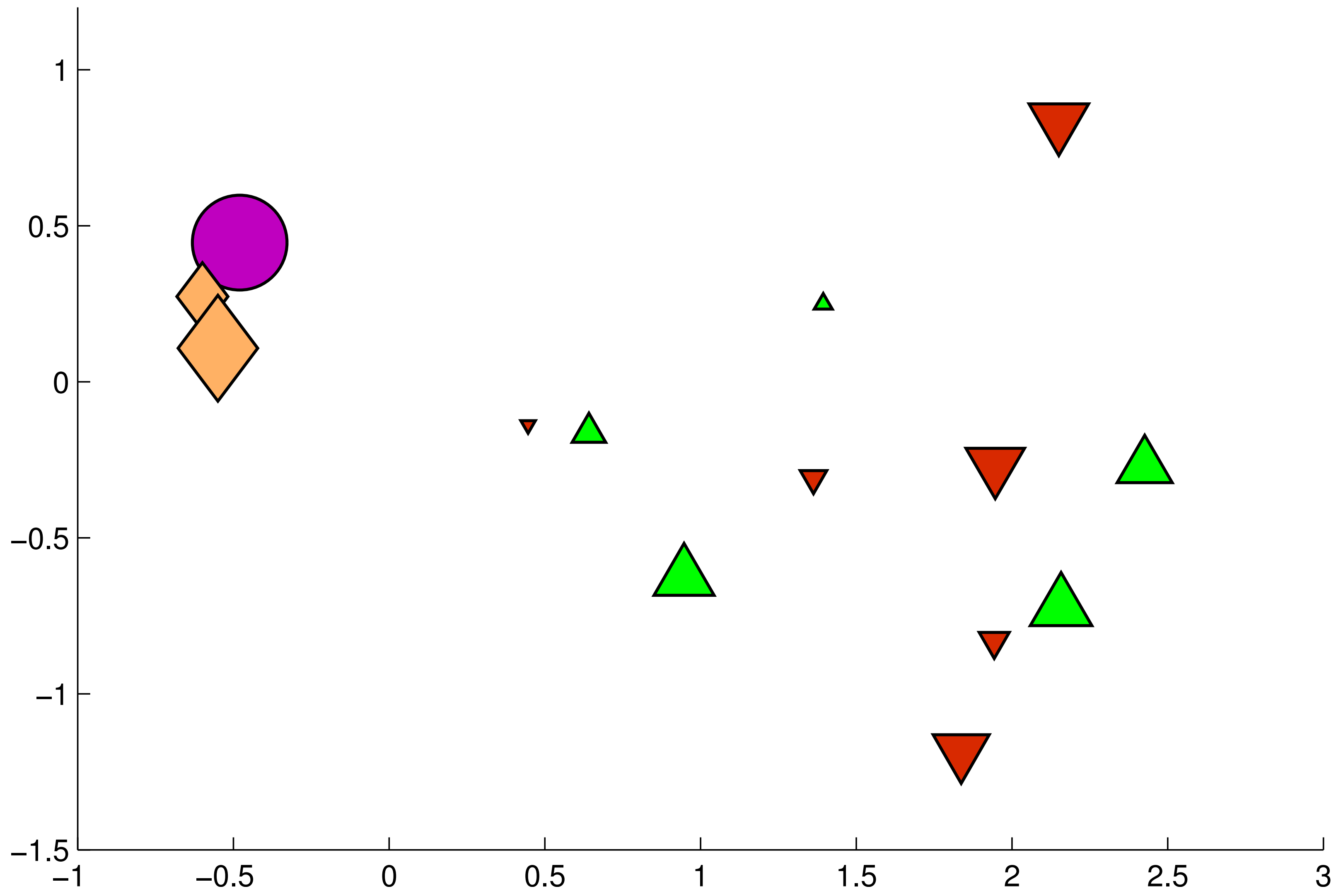


Wasserstein mean

L_2 mean

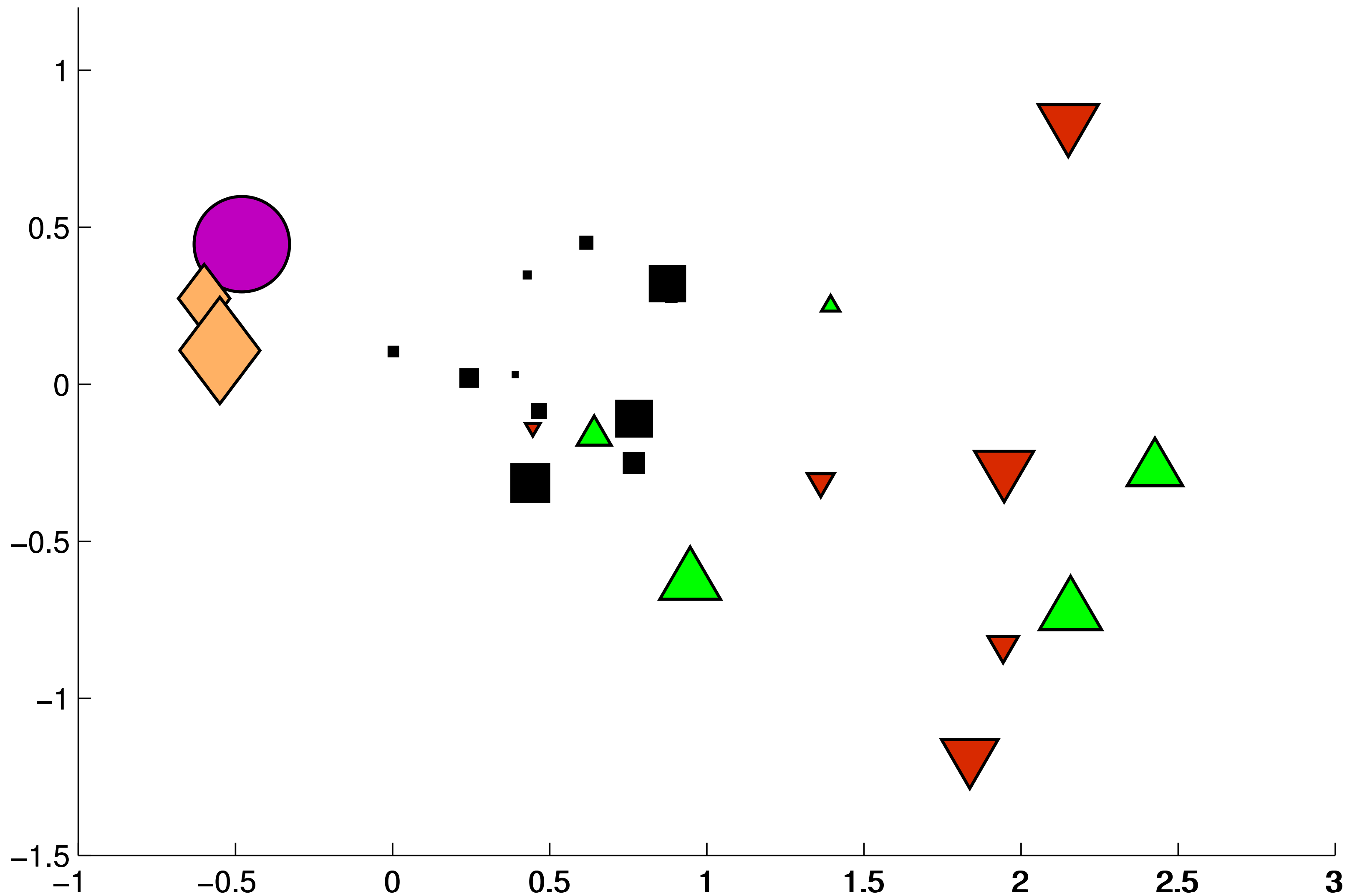
Multimarginal Formulation

- **Exact** solution (W_2) using MM-OT. **[Agueh'11]**



Multimarginal Formulation

- **Exact** solution (W_2) using MM-OT. **[Agueh'11]**



If $|\operatorname{supp} \boldsymbol{\nu_i}| = \boldsymbol{n_i}$, LP of size $(\prod_i \boldsymbol{n_i}, \sum_i \boldsymbol{n_i})$

Averaging Histograms is a LP

When Ω is a finite metric space defined by M.

$$\min_{\boldsymbol{a}\in\Sigma_n} \sum_i \lambda_i W_M(\boldsymbol{a}, \boldsymbol{b_i})$$

Averaging Histograms is a LP

When Ω is a finite metric space defined by M.

$$\min_{\boldsymbol{P_1},\cdots,\boldsymbol{P_N},\boldsymbol{a}} \sum_{i=1}^{N} \lambda_i \langle \boldsymbol{P_i}, M \rangle$$

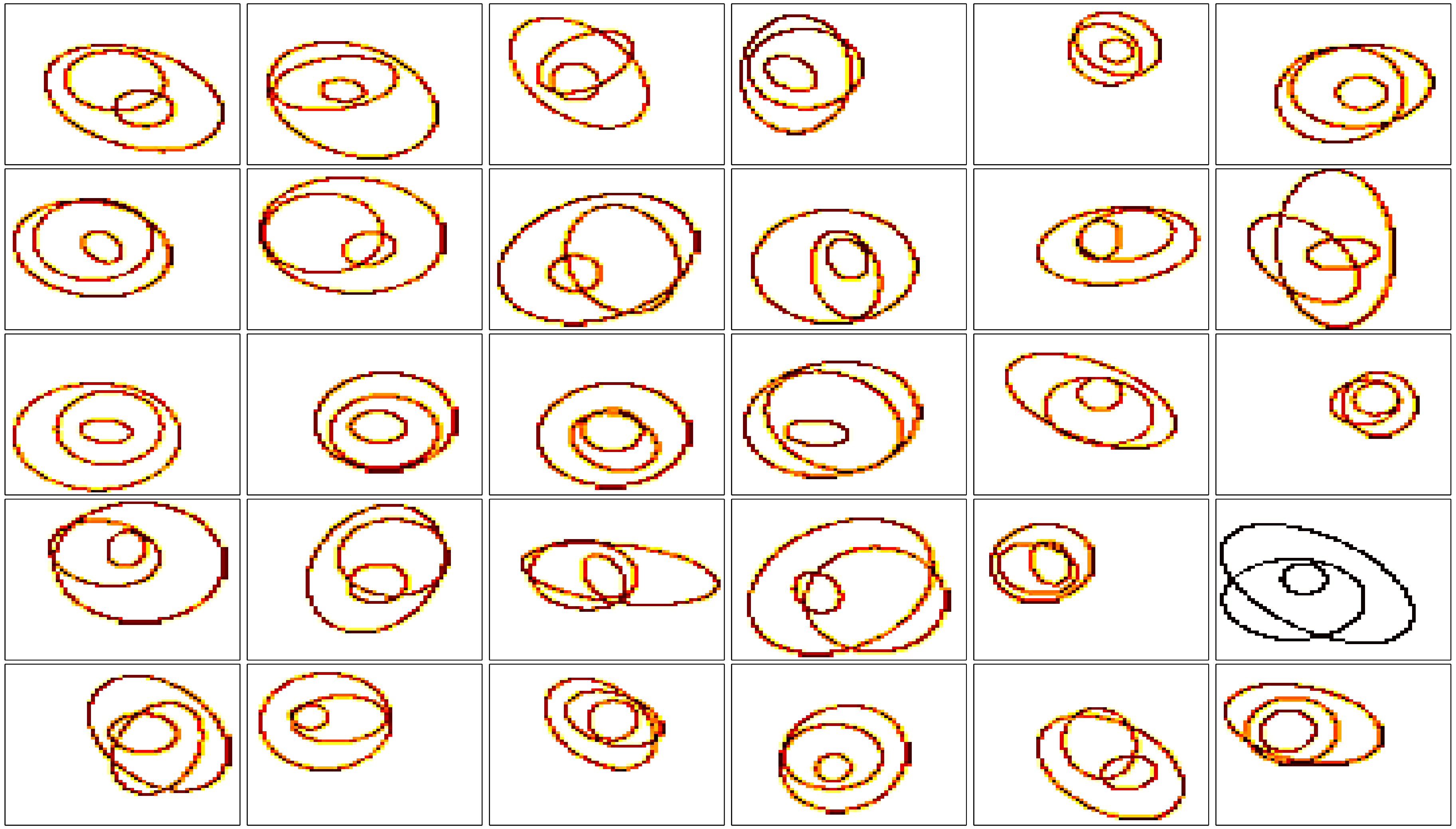
$$\text{s.t. } \boldsymbol{P_i}^T \mathbf{1}_n = \boldsymbol{b_i}, \forall i \leq N,$$

$$\boldsymbol{P_1} \mathbf{1}_n = \cdots = \boldsymbol{P_N} \mathbf{1}_d = \boldsymbol{a}.$$

If $|\Omega| = n$, LP of size $(Nn^2, (2N-1)n)$.

Primal Descent on Regularized W

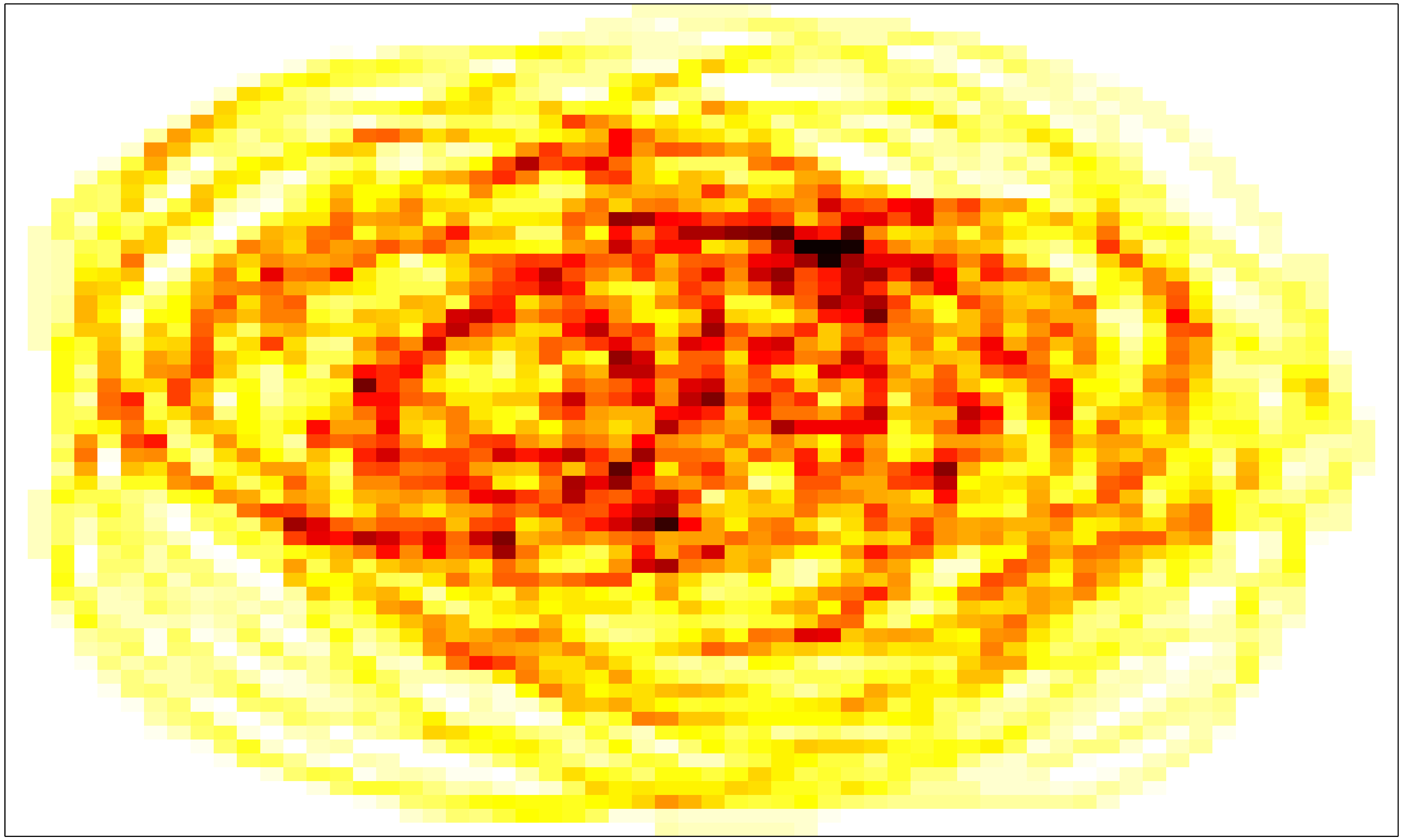
$$\min_{\boldsymbol{a} \in \Sigma_{h \times h}} \sum_{i=1}^{N} \lambda_i W_{\gamma}(\boldsymbol{a}, \boldsymbol{b_i})$$



[Cuturi'14]

Primal Descent on Regularized W

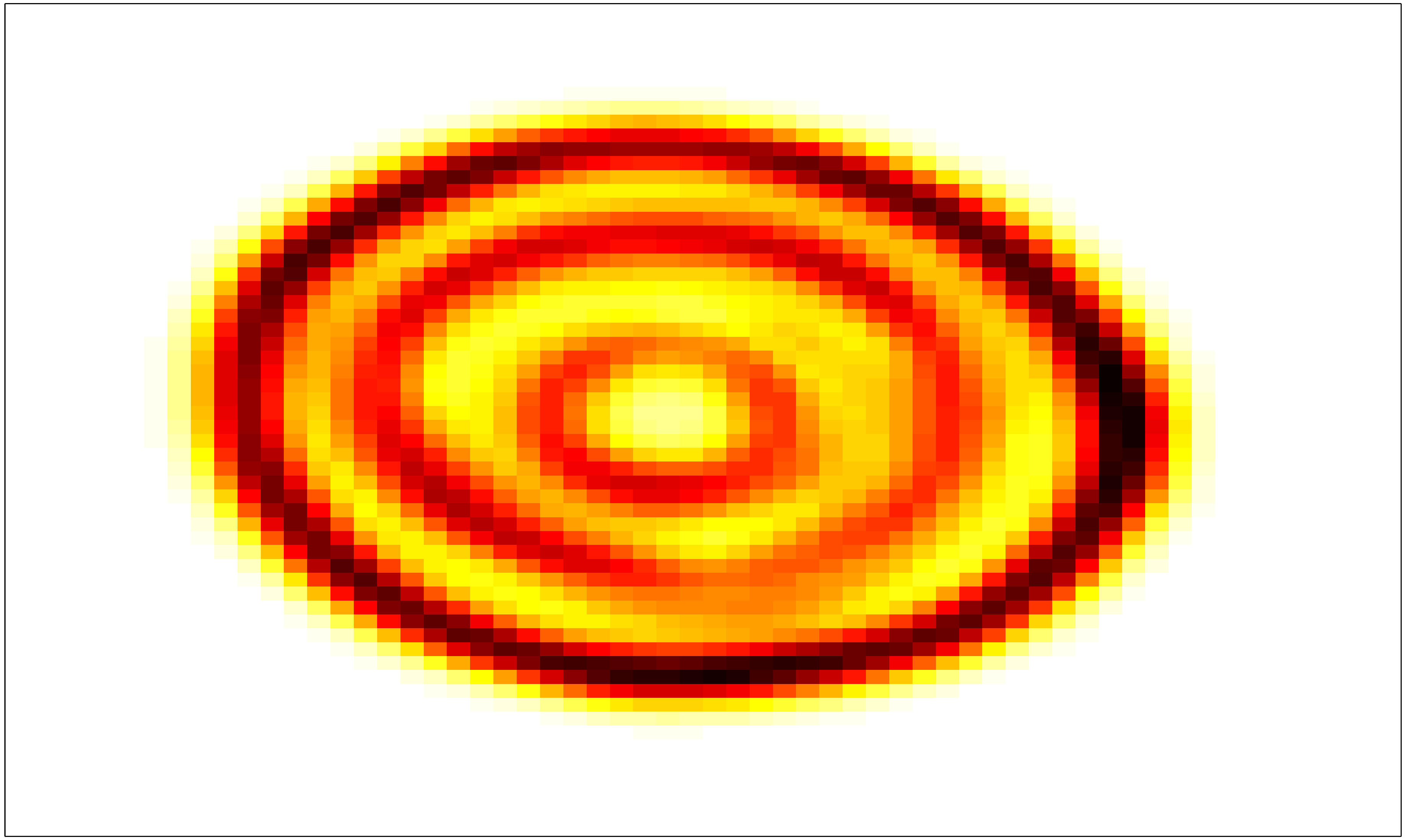
$$\min_{\boldsymbol{a} \in \Sigma_{h \times h}} \sum_{i=1}^{N} \lambda_i W_{\gamma}(\boldsymbol{a}, \boldsymbol{b_i})$$



[Cuturi'14]

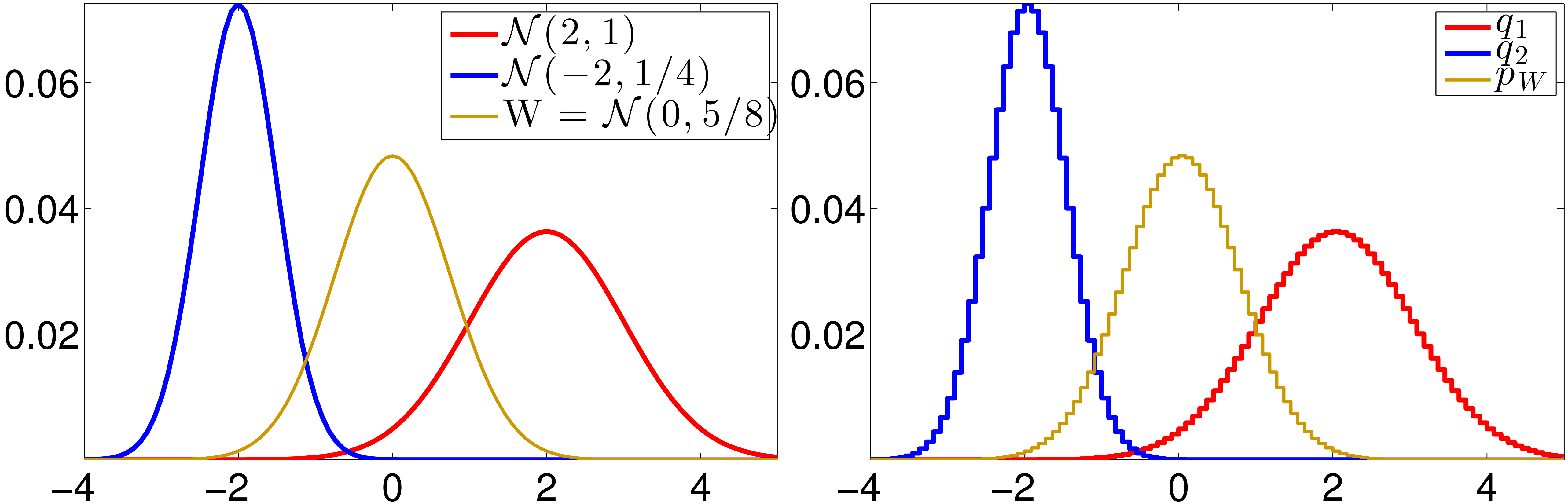
Primal Descent on Regularized W

$$\min_{a \in \Sigma_{h\times h}} \sum_{i=1}^{N} \lambda_i W_{\gamma}(a, b_i)$$

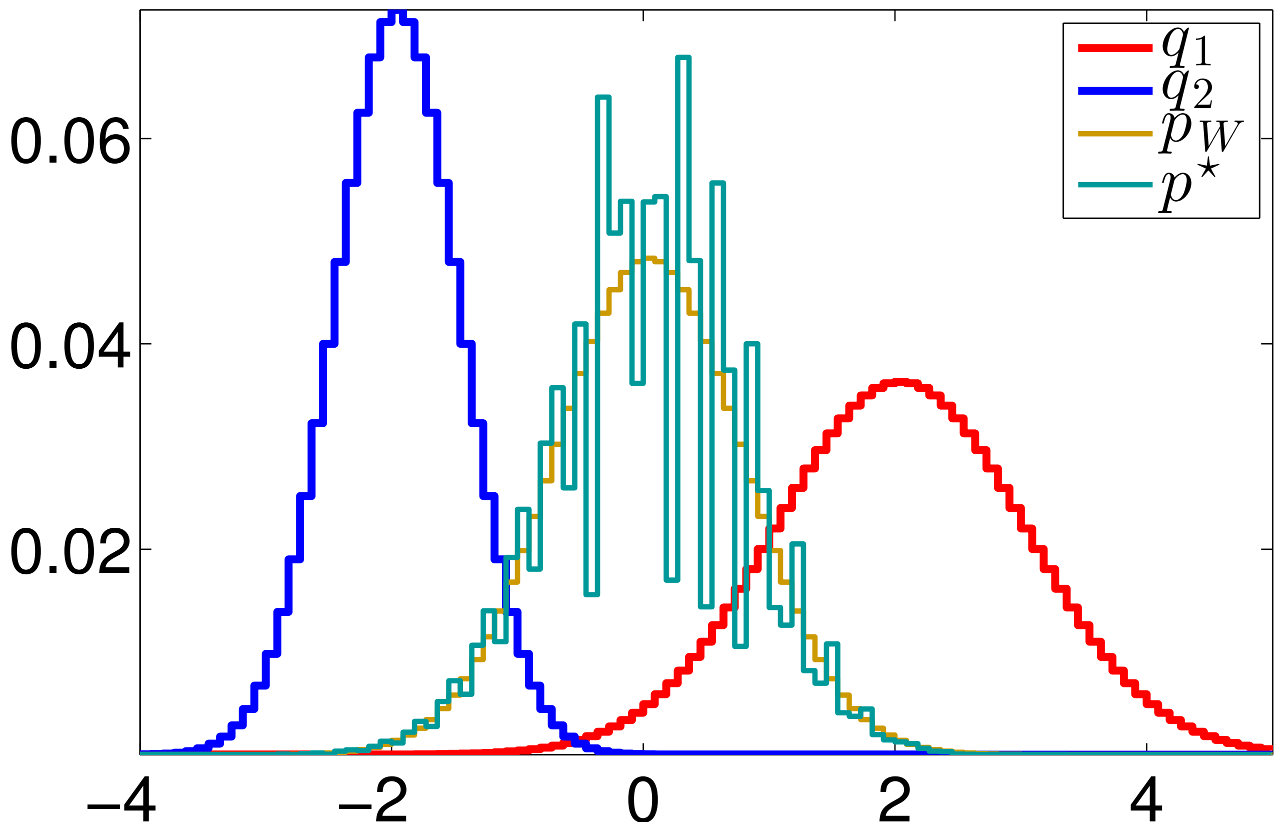


[Cuturi'14]

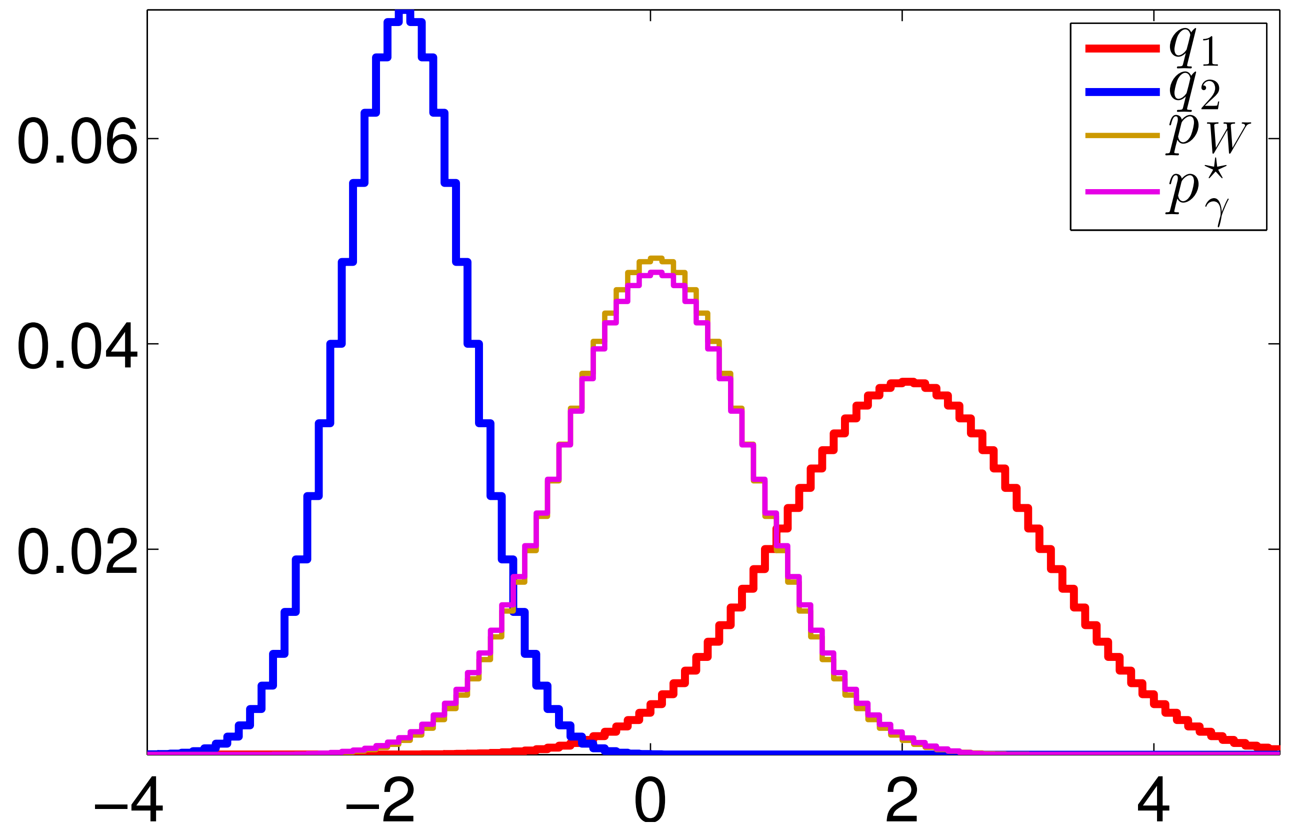
On Regularizing or Not



On Regularizing or Not

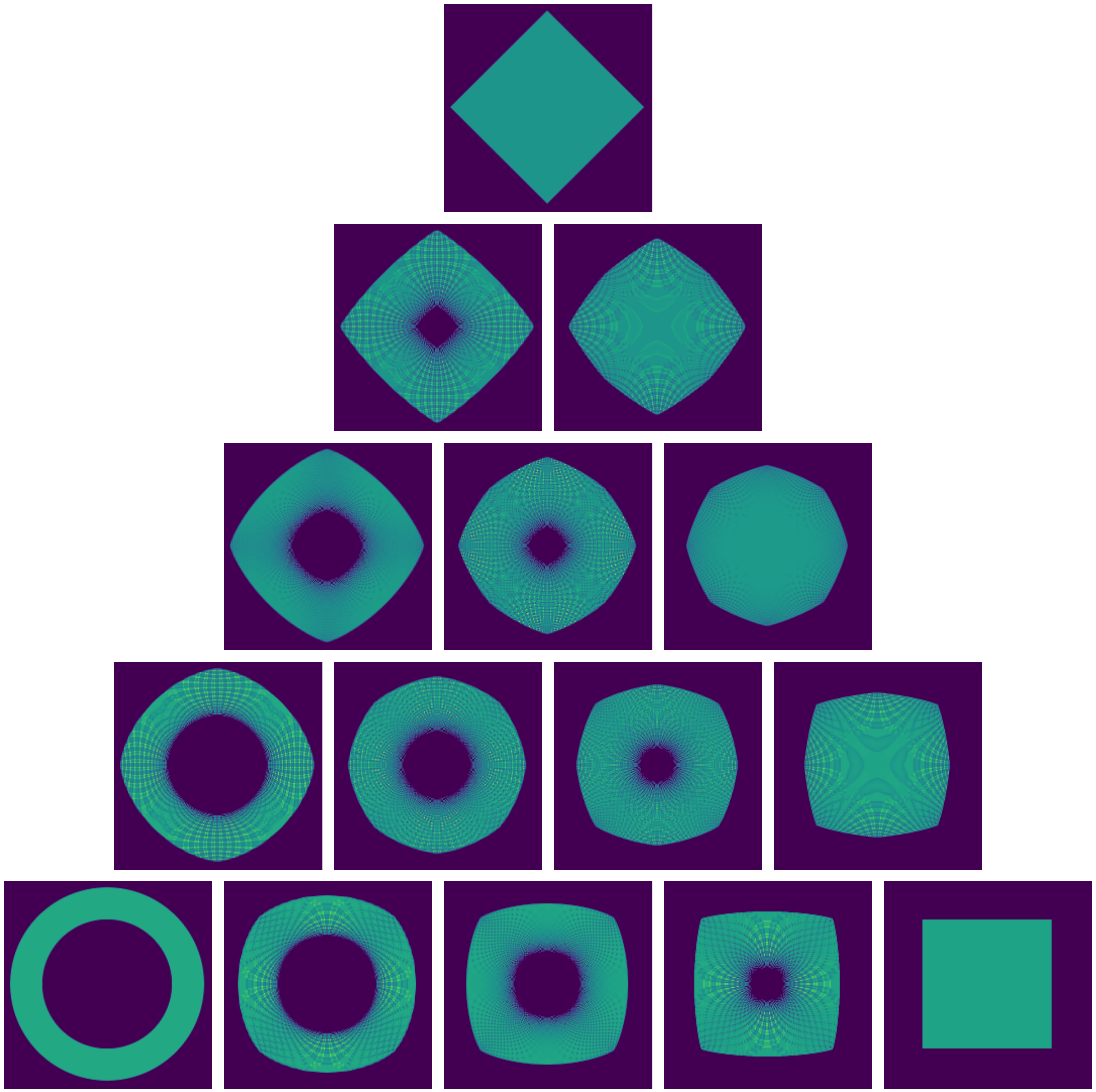


True barycenter



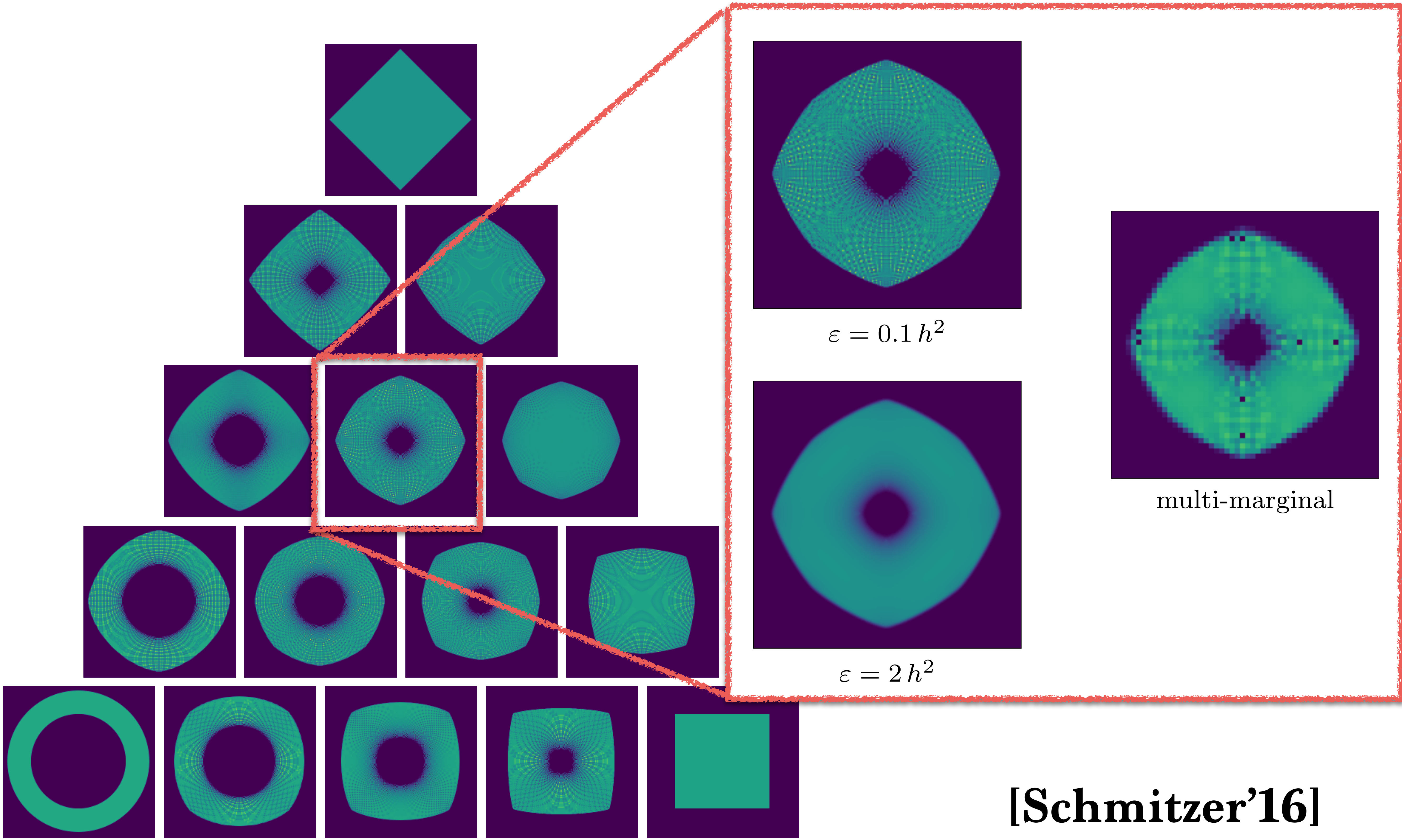
Barycenter using regularized OT

On Regularizing or Not



[Schmitzer'16]

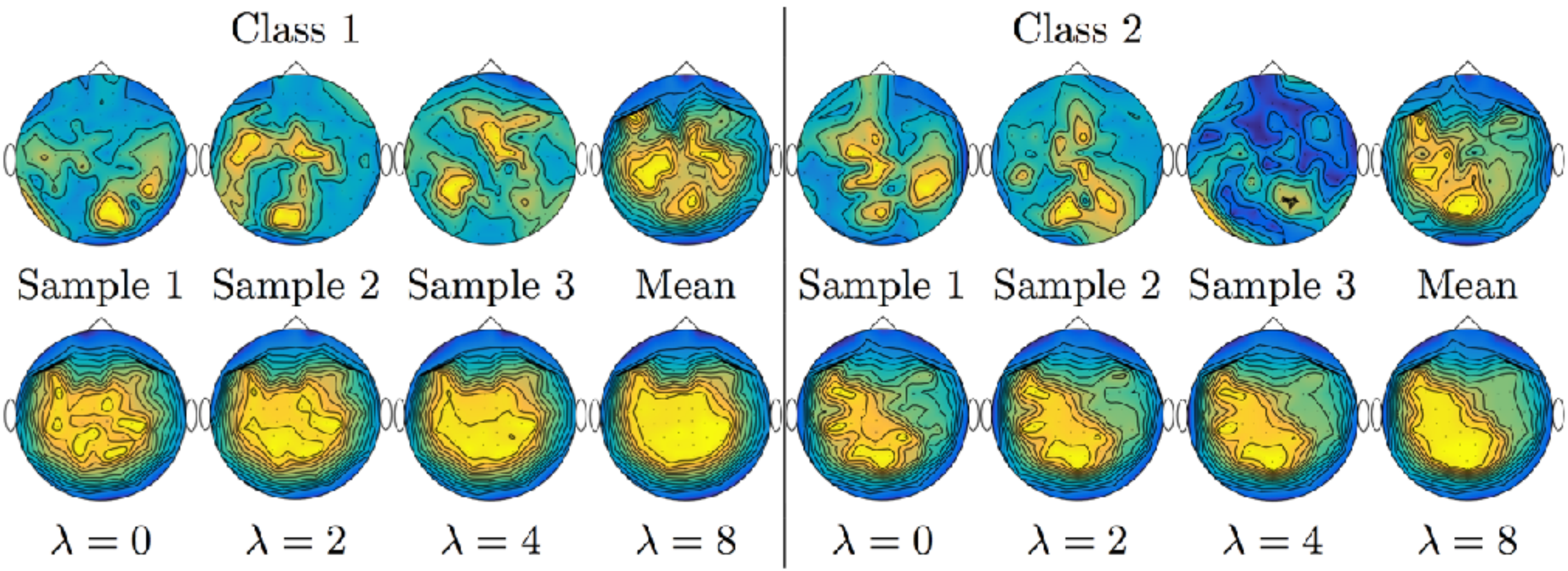
On Regularizing or Not



[Schmitzer'16]

Duality: Regularized Barycenters

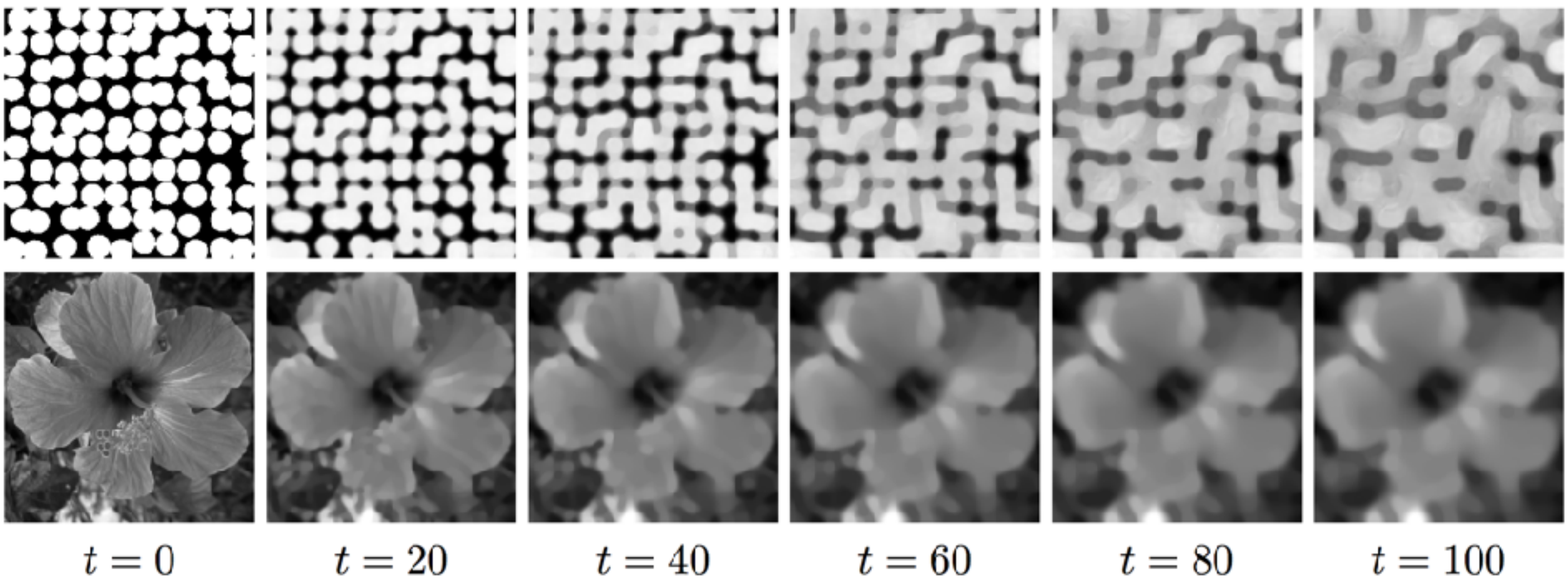
$$\min_{\mu \in \mathcal{P}(\Omega)} \sum_{i=1}^{N} W_{\gamma}(\mu, \nu_i) + \lambda \mathrm{TV}(\mu)$$



A Smoothed Dual Approach for Variational Wasserstein Problems
SIAM Imaging Sciences, 2016 **[CP'16]**

Duality: TV Gradient Flow

$$\mu_{k+1} = \underset{\mu \in \mathcal{P}(\Omega)}{\operatorname{argmin}} W_\gamma(\mu, \mu_k) + \tau \mathrm{TV}(\mu)$$



$t = k\tau$

A Smoothed Dual Approach for Variational Wasserstein Problems **[CP'16]**
SIAM Imaging Sciences, 2016

Regularized OT as KL Projection

$$\mathbf{KL}(P|\,K) = \sum_{ij} P_{ij} \log\left(P_{ij} / \,K_{ij}\right)$$

$$\langle P, M_{\mathbf{XY}}\rangle - \gamma E(P) = \gamma \mathbf{KL}(P|\,K)$$

$$\textbf{Prop.}\;\; P_\gamma = \mathrm{Proj}_{C_{\boldsymbol{a}} \cap C'_{\boldsymbol{b}}}(K)$$

$$C_{\boldsymbol{a}} = \{P | P\mathbf{1}_m = \boldsymbol{a}\},\; C'_{\boldsymbol{b}} = \{P | P^T\mathbf{1}_n = \boldsymbol{b}\}$$

Regularized OT as KL Projection

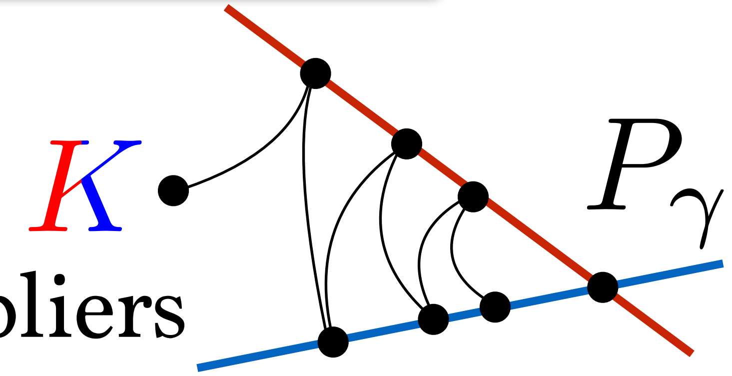
$$\textbf{Prop.}\quad P_\gamma = \mathrm{Proj}_{\mathcal{C}_{\boldsymbol{a}} \cap \mathcal{C}'_{\boldsymbol{b}}}(K)$$

$$\mathcal{C}_{\boldsymbol{a}} = \{P | P\mathbf{1}_m = \boldsymbol{a}\}, \quad \mathcal{C}'_{\boldsymbol{b}} = \{P | P^T\mathbf{1}_n = \boldsymbol{b}\}$$

$$\mathrm{Proj}_{\mathcal{C}_{\boldsymbol{a}}}(P) = \mathbf{D}\left(\frac{\boldsymbol{a}}{P\mathbf{1}_m}\right)P,$$

$$\mathrm{Proj}_{\mathcal{C}'_{\boldsymbol{b}}}(P) = P\,\mathbf{D}\left(\frac{\boldsymbol{b}}{P^T\mathbf{1}_n}\right).$$

1. Sinkhorn = Dykstra's alternate projection
2. Only need to store & update diagonal multipliers



Wasserstein Barycenter = KL Projections

$$\langle P, M_{\mathbf{XY}} \rangle - \gamma E(P) = \gamma \mathbf{KL}(P | K)$$

$$\min_{\boldsymbol{a}} \sum_{i=1}^{N} \lambda_i W_\gamma(\boldsymbol{a}, \boldsymbol{b_i}) = \min_{\substack{\mathbf{P}=[\boldsymbol{P_1},\dots,\boldsymbol{P_N}] \\ \mathbf{P}\in \boldsymbol{C_1}\cap \boldsymbol{C_2}}} \sum_{i=1}^{N} \lambda_i \mathbf{KL}(\boldsymbol{P_i} | K)$$

$$\boldsymbol{C_1} = \{\mathbf{P} | \exists \boldsymbol{a}, \forall i, P_i \mathbf{1}_m = \boldsymbol{a}\}$$

$$\boldsymbol{C_2} = \{\mathbf{P} | \forall i, P_i^T \mathbf{1}_n = \boldsymbol{b_i}\}$$

Wasserstein Barycenter = KL Projections

$$\min_{\boldsymbol{a}} \sum_{i=1}^{N} \lambda_i W_\gamma(\boldsymbol{a}, \boldsymbol{b_i}) = \min_{\substack{\mathbf{P}=[\boldsymbol{P_1},\ldots,\boldsymbol{P_N}]\\ \mathbf{P}\in \boldsymbol{C_1}\cap \boldsymbol{C_2}}} \sum_{i=1}^{N} \lambda_i \mathbf{KL}(\boldsymbol{P_i}|K)$$

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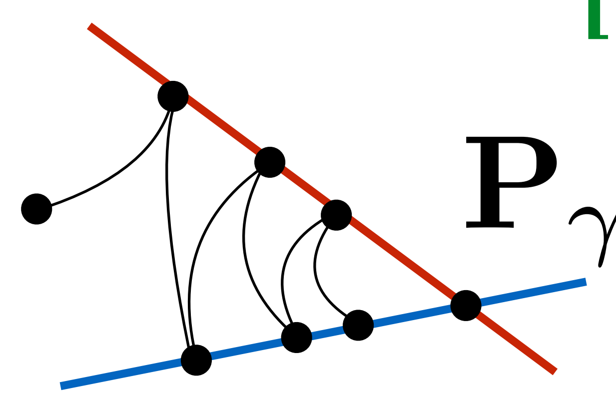
$$\boldsymbol{C_2} = \left\{\mathbf{P} | \forall i, P_i^T \mathbf{1}_n = \boldsymbol{b_i}\right\}$$

[BCCNP'15]

$[\, K \cdots \; K]$



$\mathbf{P}_\gamma$

Wasserstein Barycenter = KL Projections

$$\min_{\boldsymbol{a}} \sum_{i=1}^{N} \lambda_i W_\gamma(\boldsymbol{a}, \boldsymbol{b_i}) = \min_{\substack{\mathbf{P}=[P_1,\dots,P_N] \\ \mathbf{P}\in C_1 \cap C_2}} \sum_{i=1}^{N} \lambda_i \mathbf{KL}(\boldsymbol{P_i}|K)$$

$$C_1 = \{\mathbf{P} | \exists \boldsymbol{a}, \forall i, P_i \mathbf{1}_m = \boldsymbol{a}\}$$

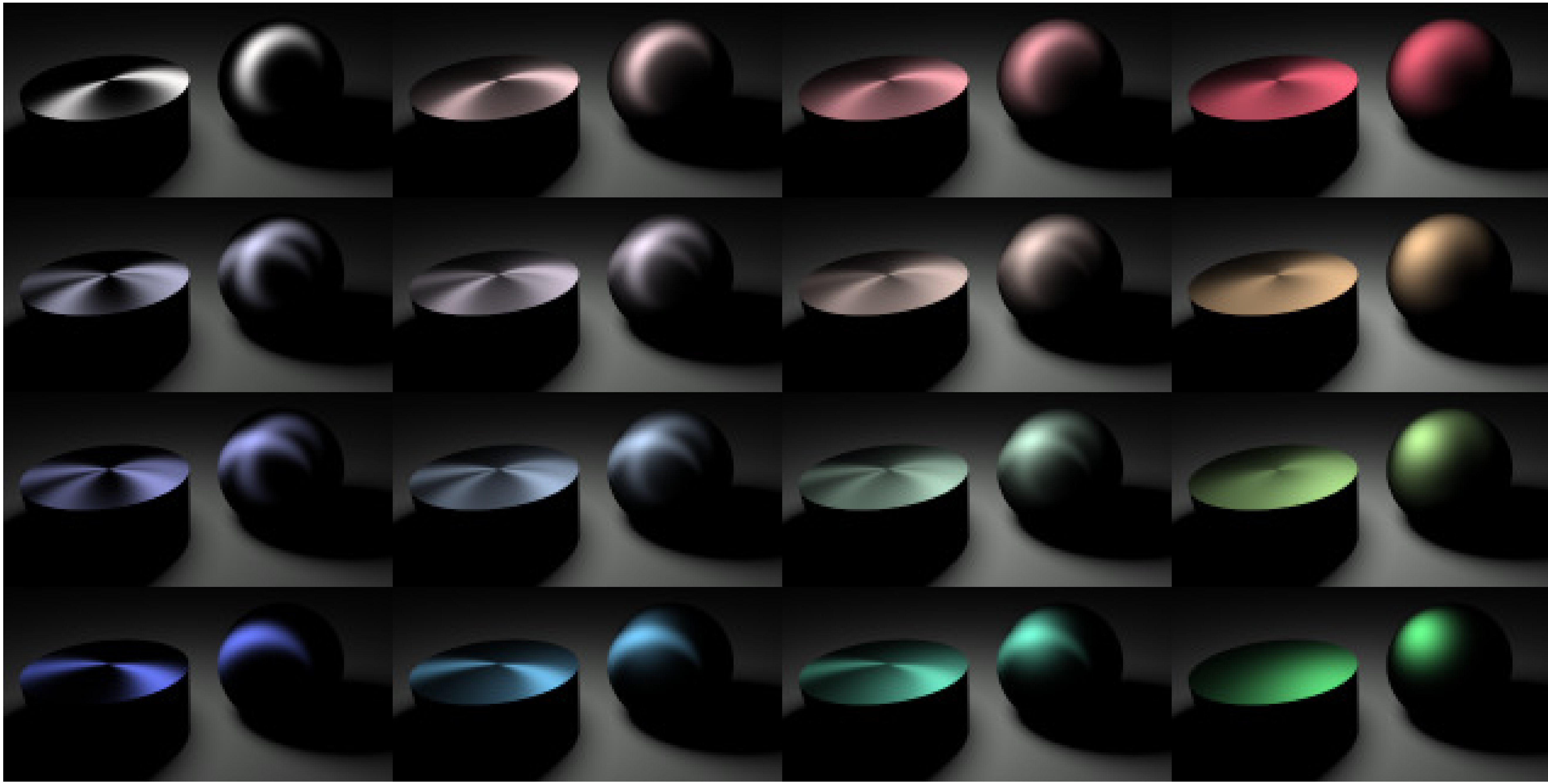
$$C_2 = \left\{\mathbf{P} | \forall i, P_i^T \mathbf{1}_n = \boldsymbol{b_i}\right\}$$

```
u=ones(size(B)); % d x N matrix
while not converged
   v=u.*(K'*(B./(K*u))); % 2(Nd^2) cost
   u=bsxfun(@times,u,exp(log(v)*weights))./v;
end
a=mean(v,2);
```

[BCCNP'15]

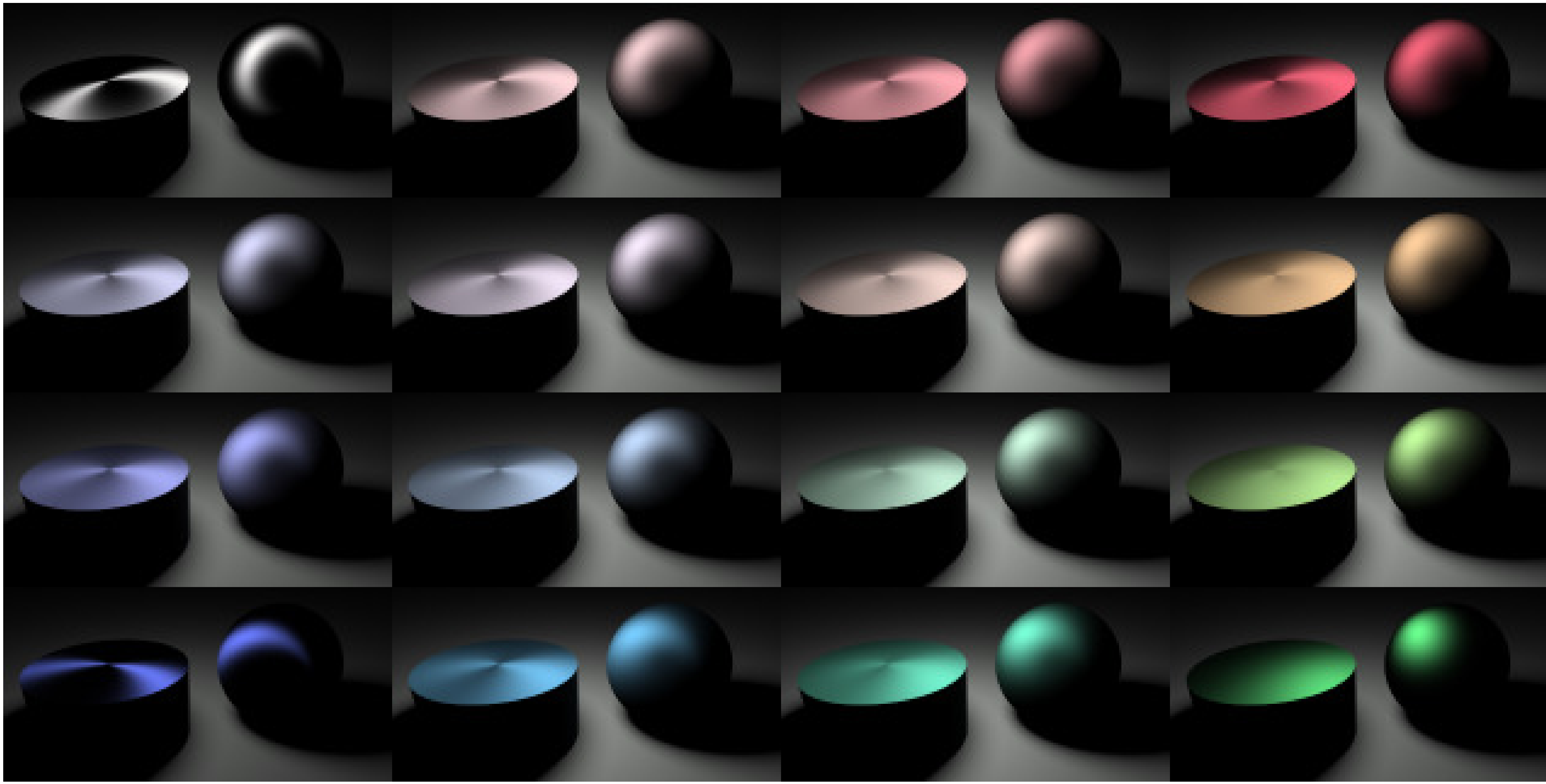
Iterative Bregman Projections for Regularized Transportation Problems
SIAM J. on Sci. Comp. 2015

Applications in Imaging



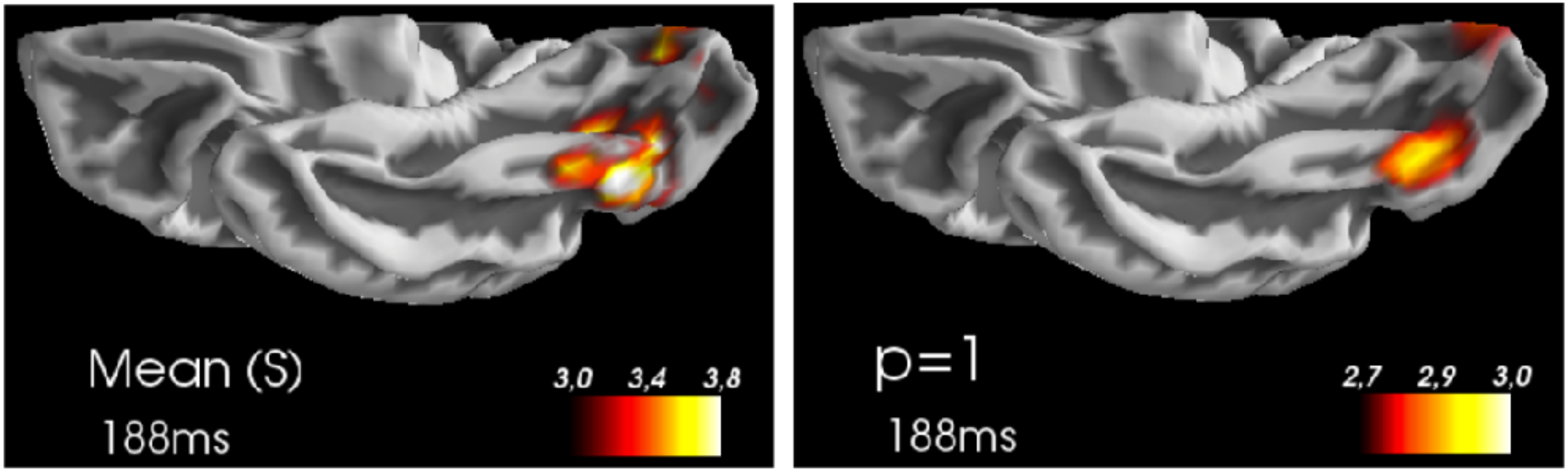
[Solomon'15]

Applications in Imaging



[Solomon'15]

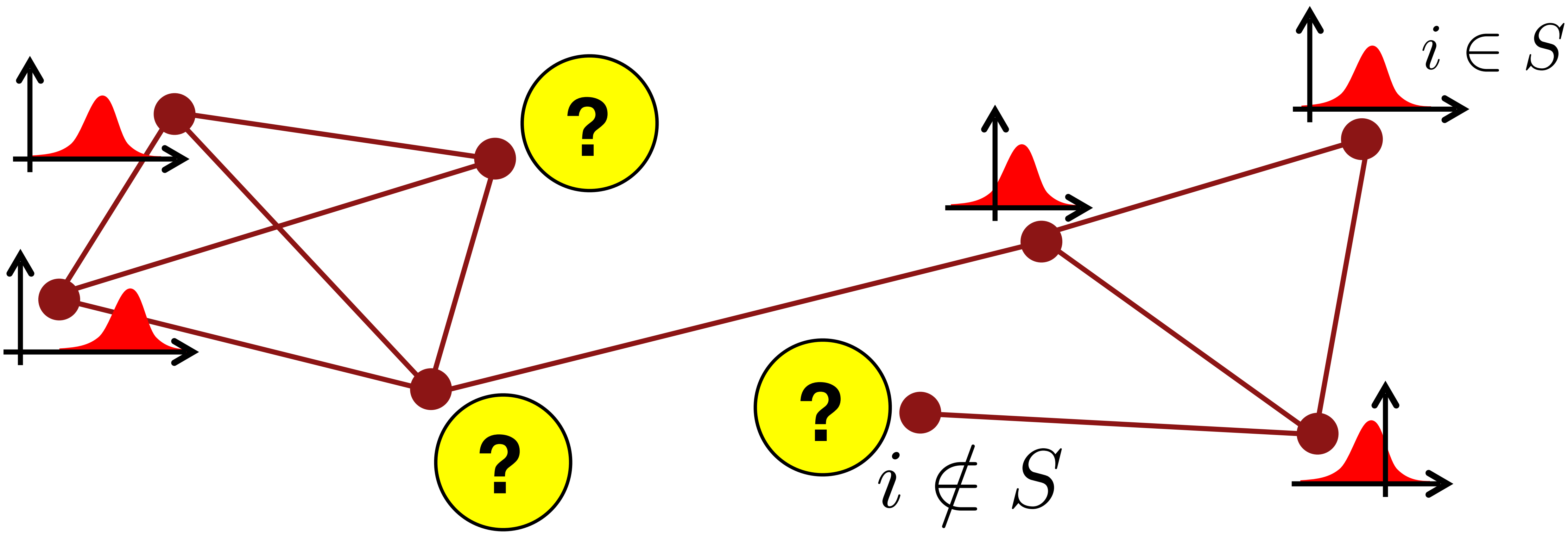
Applications: Brain Imaging



Extension to non-normalized data!
Applied to MEG and fMRI.

[Gramfort'16]

Wasserstein Propagation

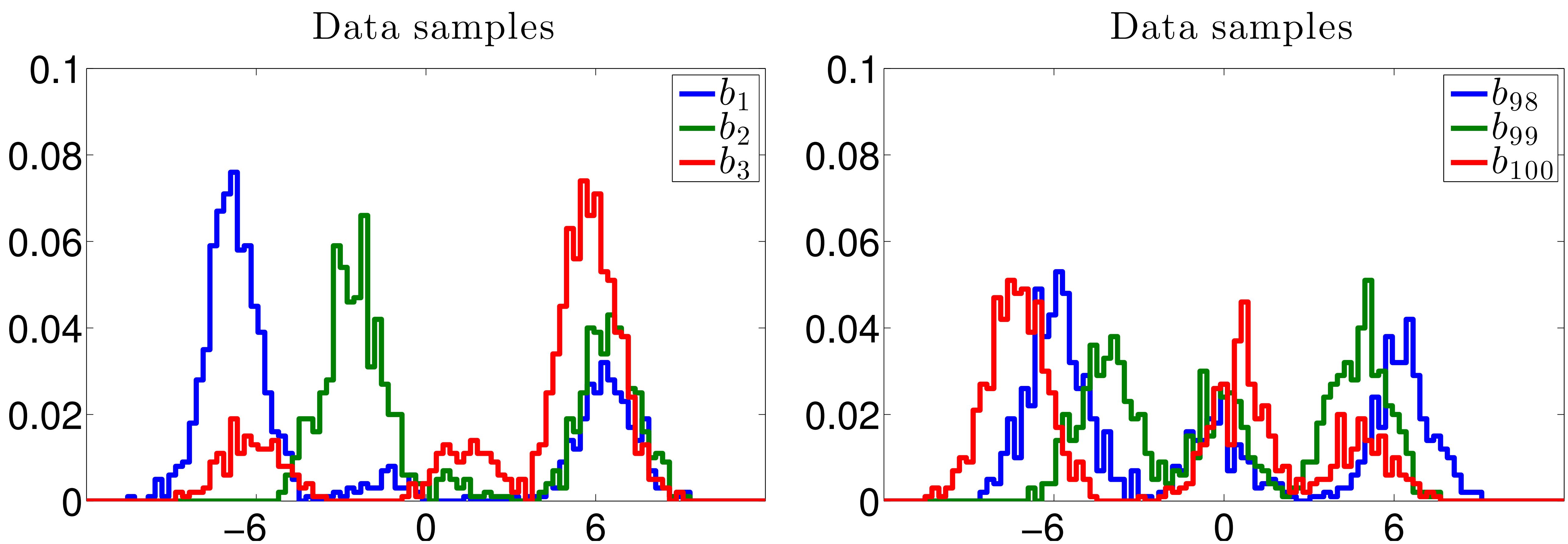


$$\min_{\substack{\mu_i \in \mathcal{P}(\Omega) \\ \mu_i \text{ fixed for } i \in S}} \sum_{(e_1, e_2) \in E} W_2^2(\mu_{e_1}, \mu_{e_2})$$

[Solomon'14]

Dictionary Learning

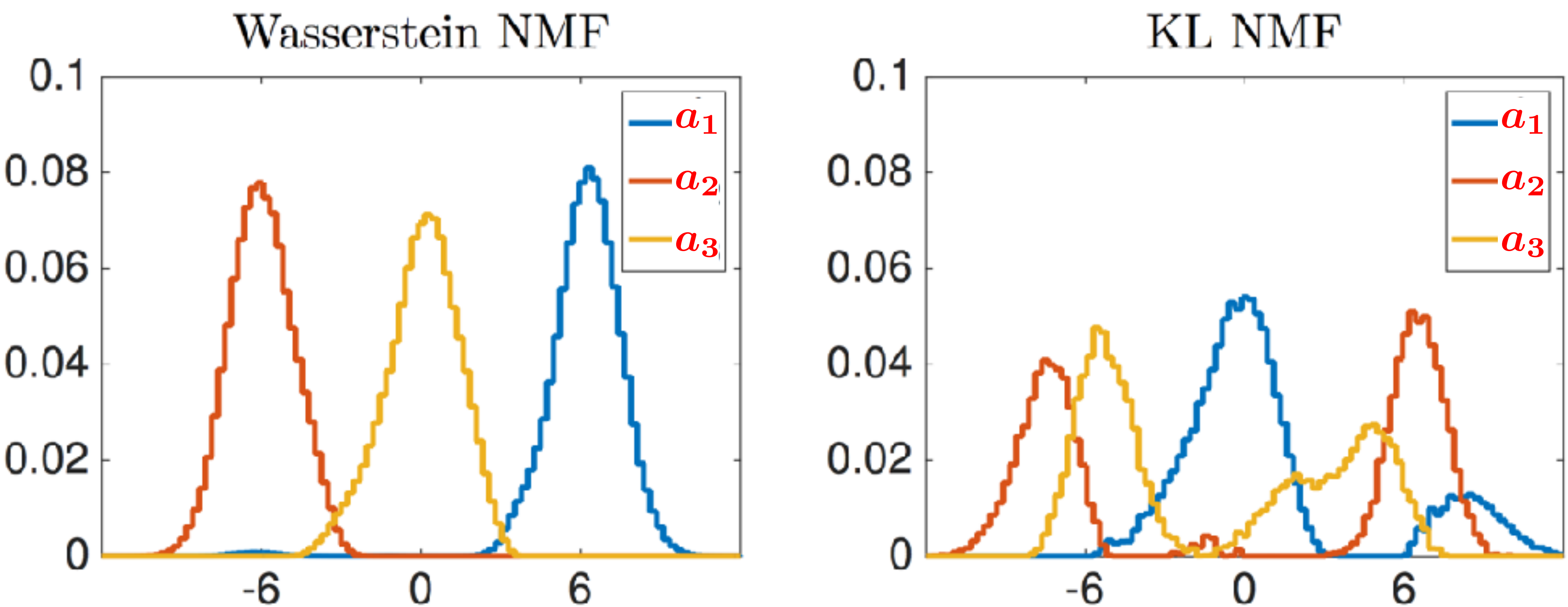
$$\min_{\boldsymbol{A}\in(\Sigma_n)^K,\boldsymbol{\Lambda}\in(\Sigma_K)^N} \sum_{i=1}^N W\left(\boldsymbol{b_i}, \sum_{k=1}^K \boldsymbol{\Lambda_k^i a_k}\right)$$



[Sandler'11] [Zen'14] [Rolet'16]

Dictionary Learning

$$\min_{\boldsymbol{A}\in(\Sigma_n)^K, \boldsymbol{\Lambda}\in(\Sigma_K)^N} \sum_{i=1}^N W\left(\boldsymbol{b_i}, \sum_{k=1}^K \boldsymbol{\Lambda}_{\boldsymbol{k}}^{\boldsymbol{i}} \boldsymbol{a_k}\right)$$



[Sandler'11] [Zen'14] [Rolet'16]

OT Dictionary Learning

- **[Hoffman'98]** proposed to learn dictionaries (topics) for text, seen as histograms-of-words.

$$\Omega = \{\text{words}\}, \quad |\Omega| \approx 13,000$$

- Vector embeddings for words **[Mikolov'13]** **[Pennington'14]** defines geometry:

$$\boldsymbol{D}(\text{public}, \text{car}) = \|x_{\text{public}} - x_{\text{car}}\|^2$$

- Data: 7,034 Reuters, 737 BBC sports news articles

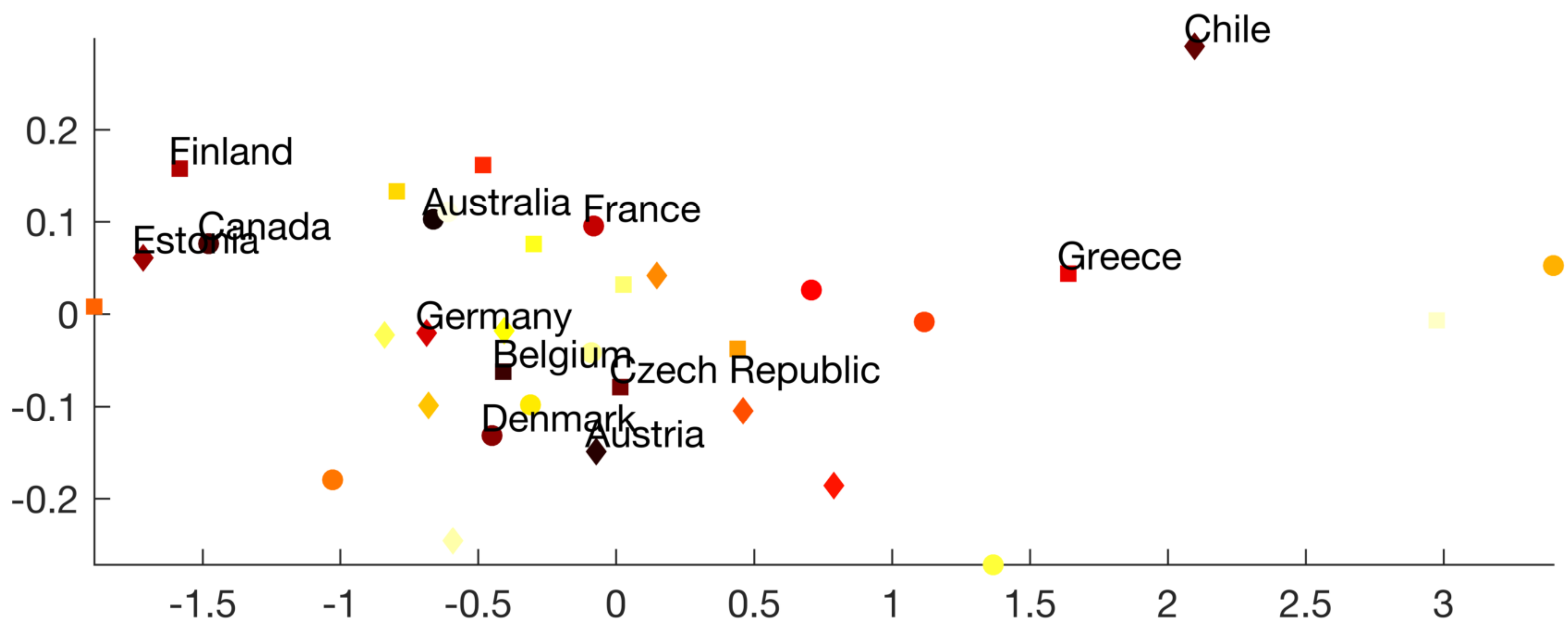
Topic Models

[Rolet'16]

Elliptical Embeddings

Multidimensional Scaling [MDS]

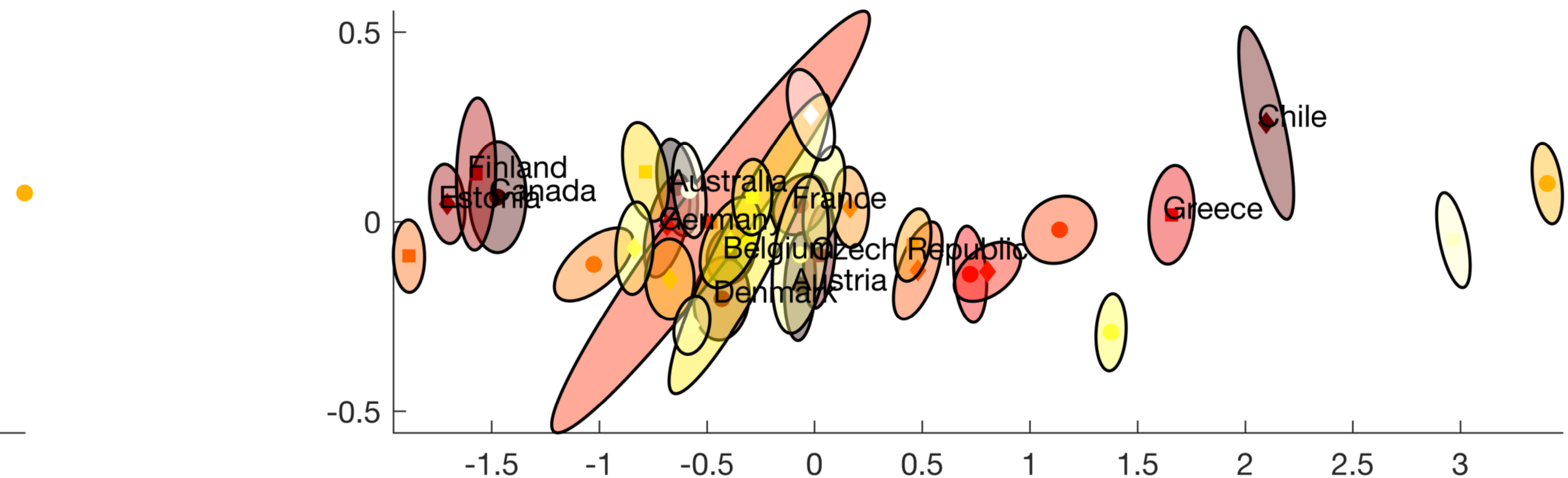
embed a metric space in R^2



Elliptical Embeddings

Multidimensional Scaling [MDS]

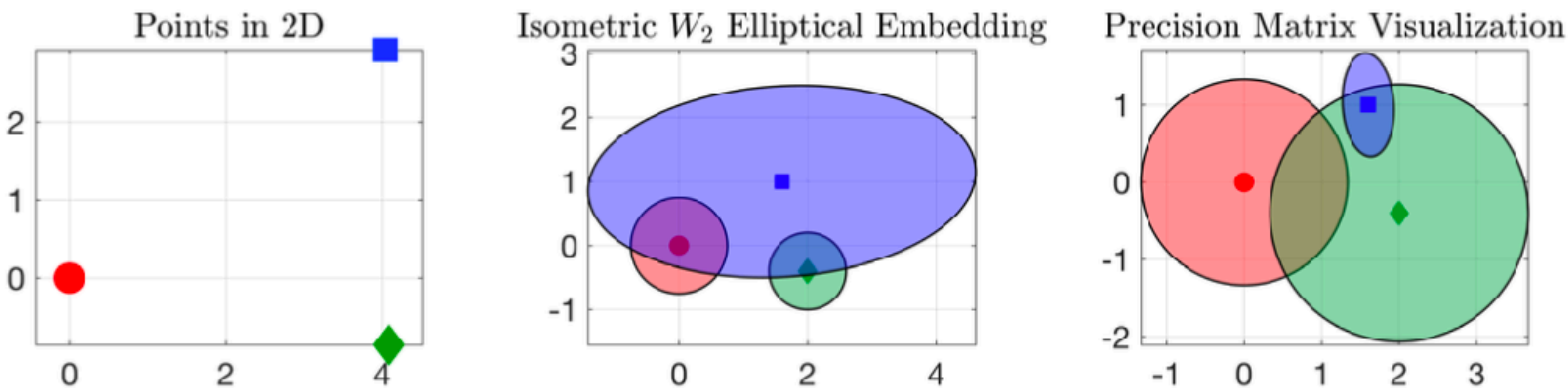
embed a metric space in elliptical distributions in $P(R^2)$, W_2



Elliptical Embeddings

Visualization issue

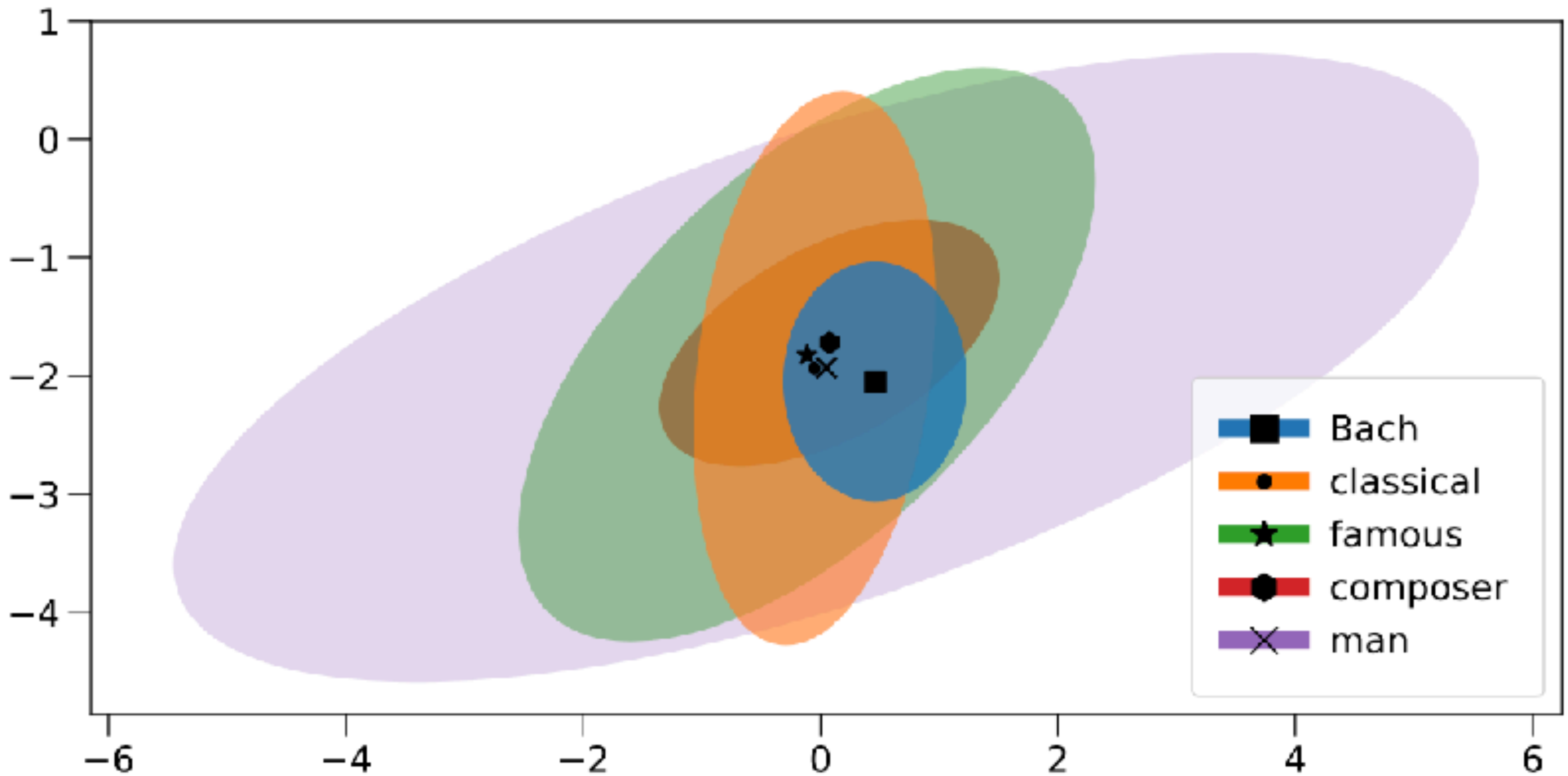
need to shift to precision matrix to recover intuition



Elliptical Embeddings

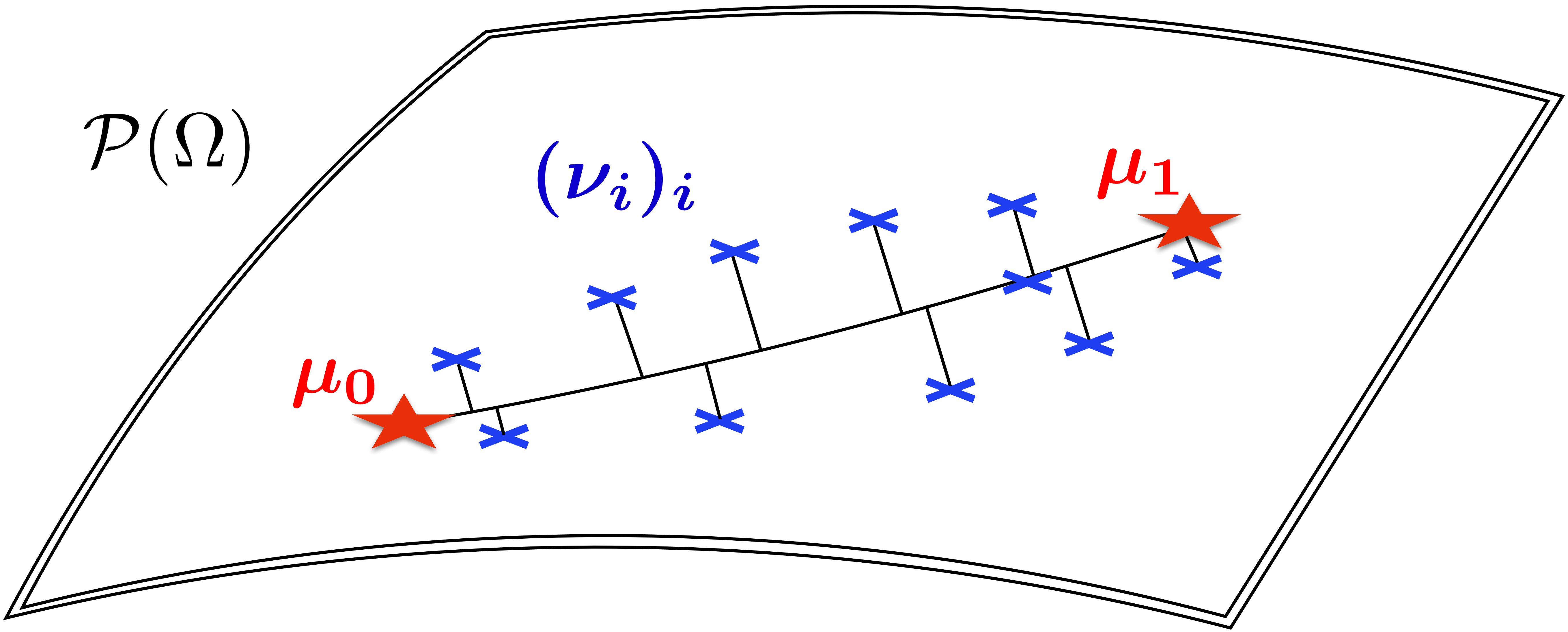
Word Embeddings

Compute elliptical distribution representations for Words

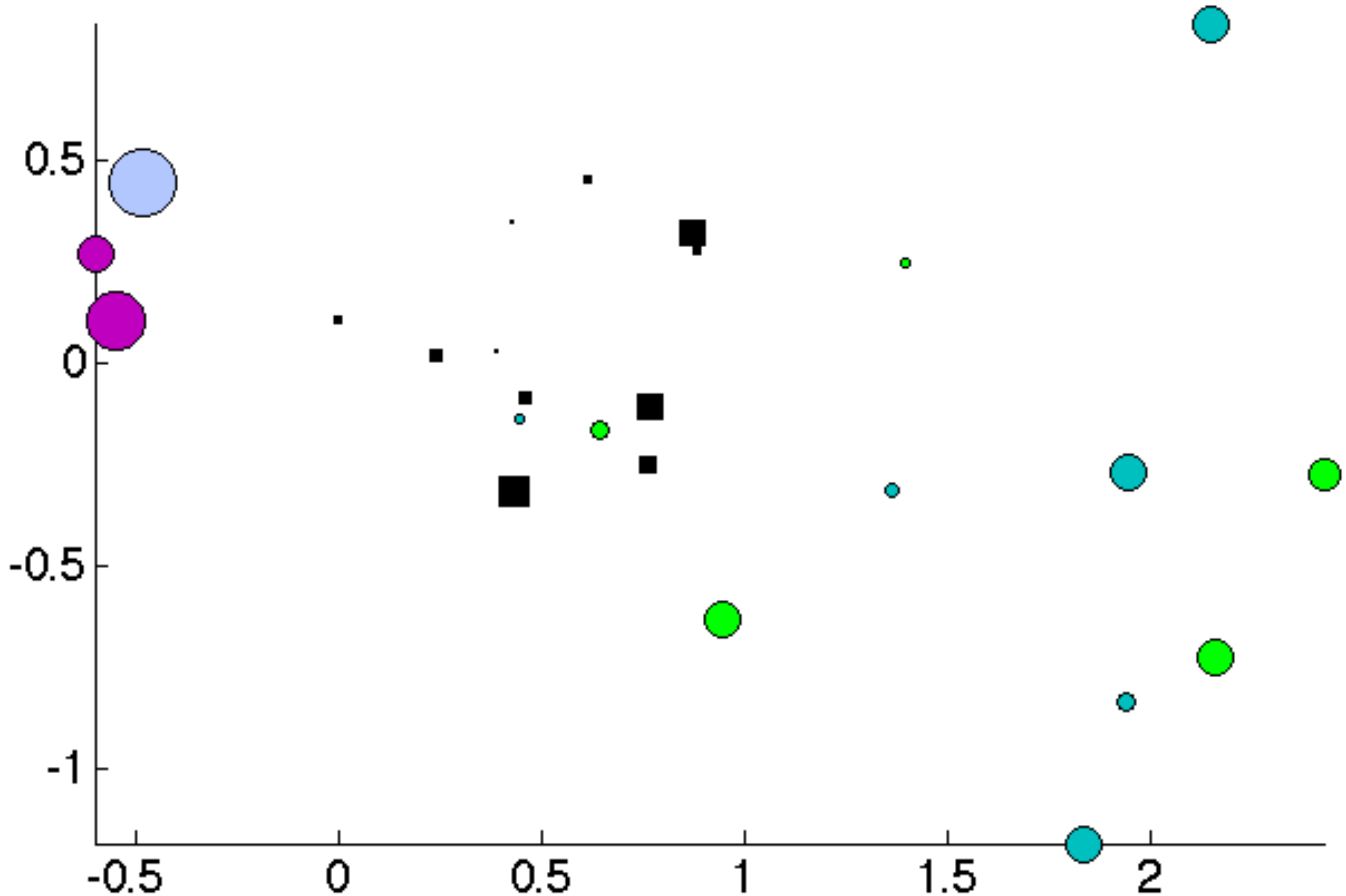


Wasserstein PCA

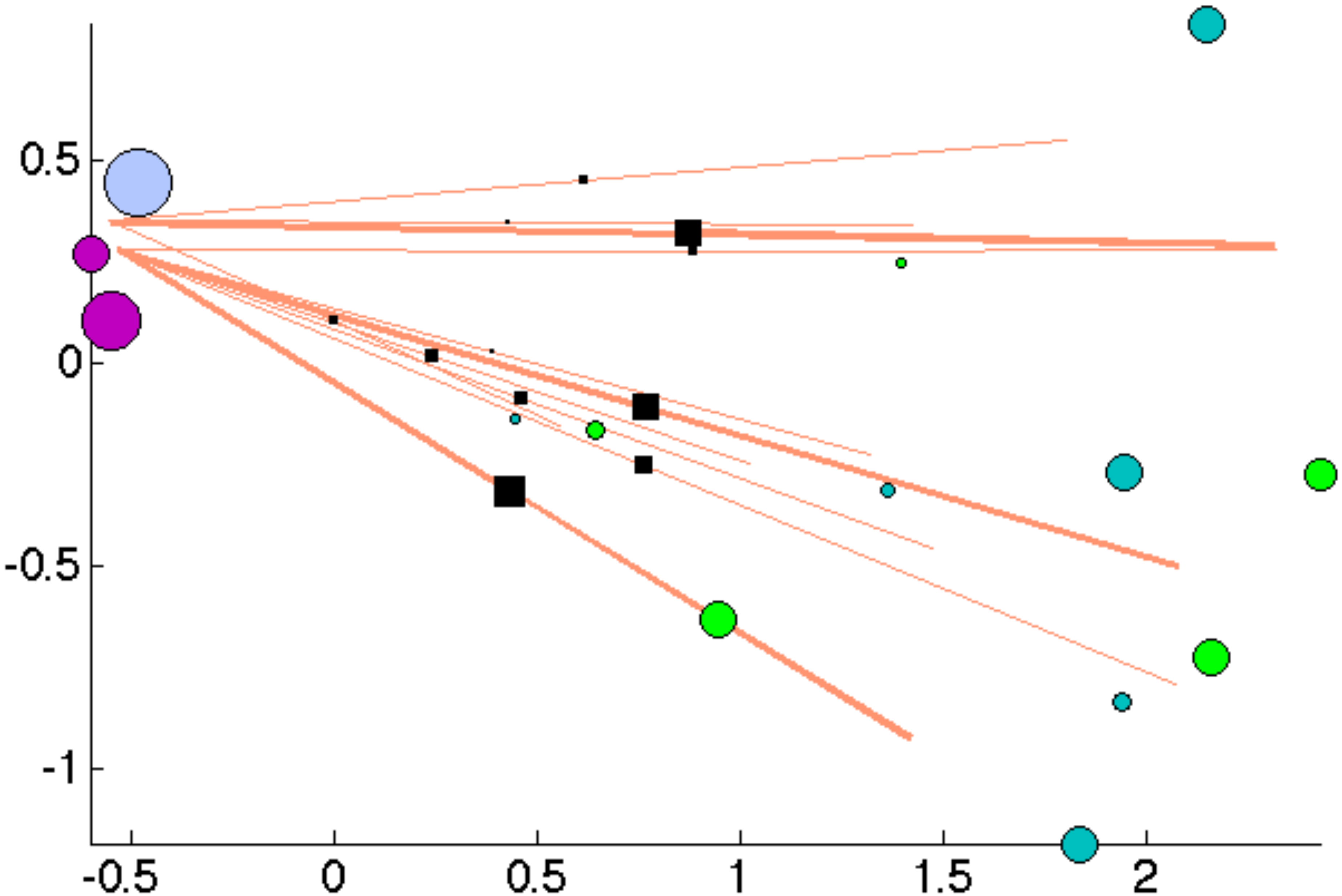
$$\min_{\boldsymbol{\mu_0},\boldsymbol{\mu_1}} \sum_{i=1}^{N} \min_t W_2^2(\rho^t_{\boldsymbol{\mu_0}\to\boldsymbol{\mu_1}}, \boldsymbol{\nu_i})$$



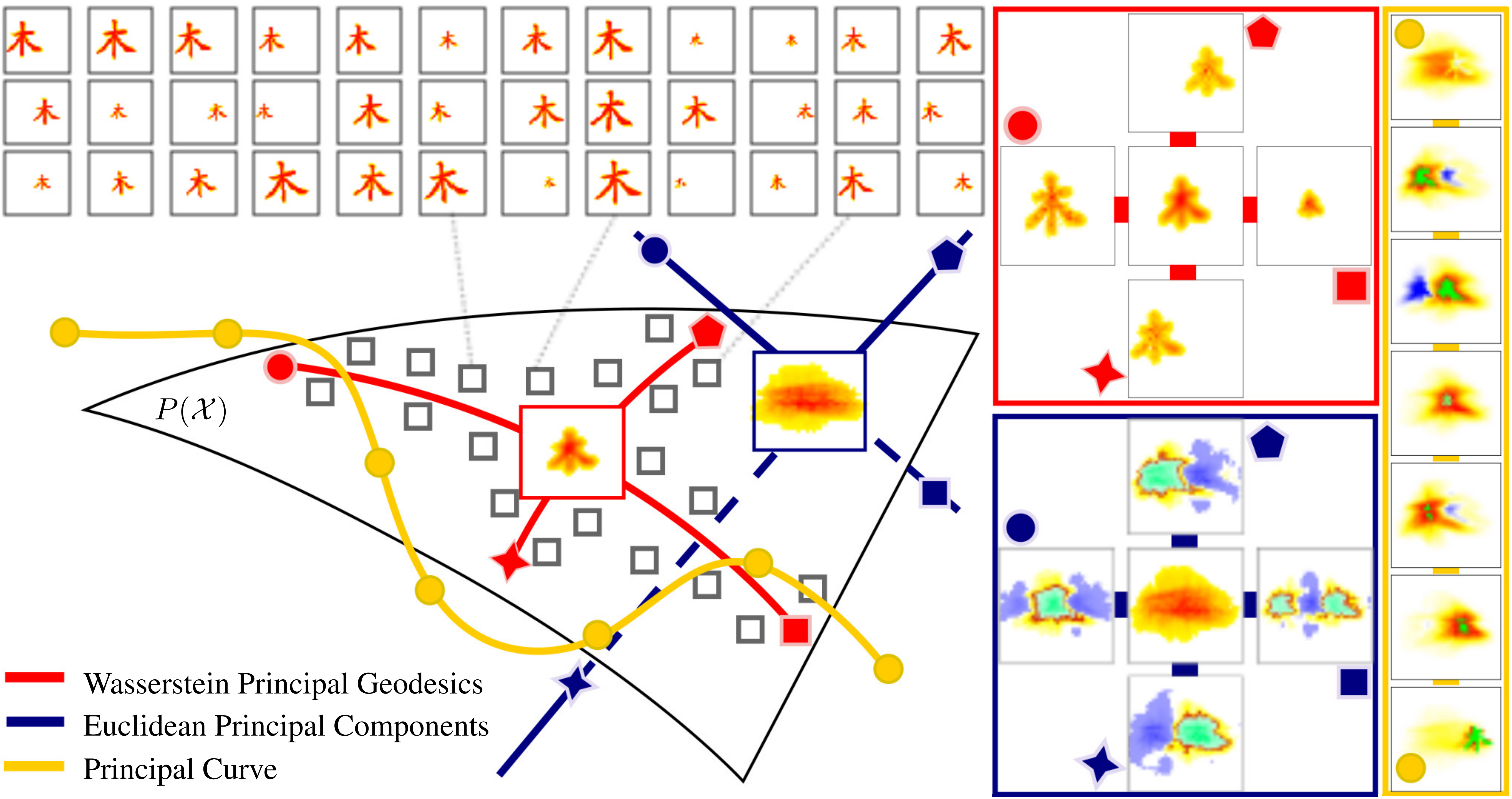
Wasserstein PCA



On Empirical Measures



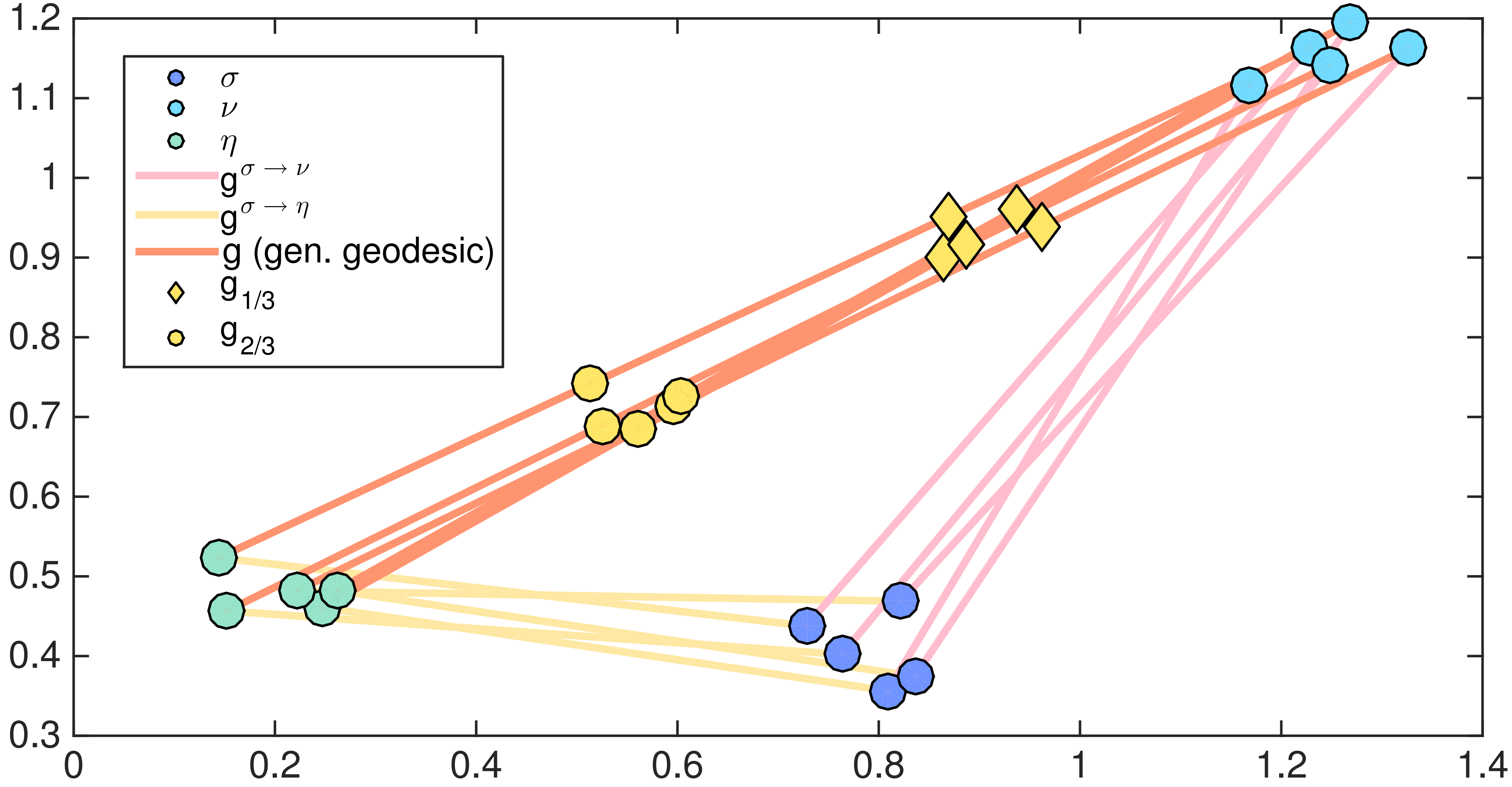
Wasserstein PCA *vs.* Euclidean PCA



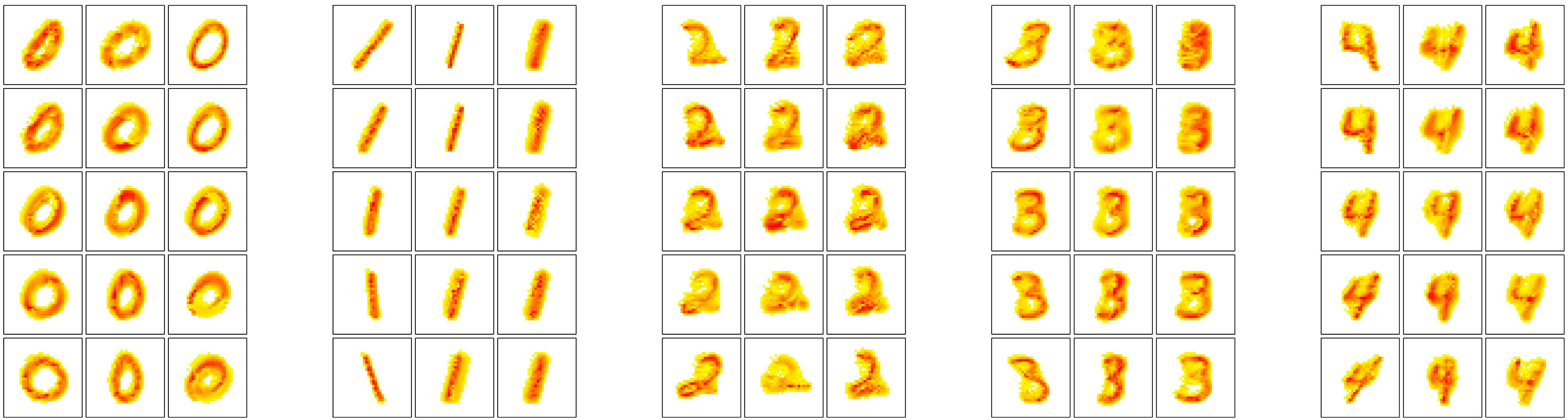
[Ambrosio'06] Generalized Geodesics

$$\min_{\boldsymbol{v_1},\boldsymbol{v_2}\in L^2(\bar{\boldsymbol{\nu}},\Omega)} \quad \sum_{i=1}^{N} \min_{t\in[0,1]} \quad W_2^2\left(g_t(\boldsymbol{v_1},\boldsymbol{v_2}),\boldsymbol{\nu_i}\right)+\lambda R(\boldsymbol{v_1},\boldsymbol{v_2}),$$

$$\text{subject to} \begin{cases} g_t(\boldsymbol{v_1},\boldsymbol{v_2}) = (\mathrm{Id}-\boldsymbol{v_1}+t(\boldsymbol{v_1}+\boldsymbol{v_2}))\,\#\bar{\boldsymbol{\nu}} \\ \mathrm{Id}-\boldsymbol{v_1} \text{ and } \mathrm{Id}+\boldsymbol{v_2} \quad \text{are Monge maps from } \bar{\boldsymbol{\nu}} \end{cases}$$



Generalized Principal Geodesics



For each digit, 1,000 MNIST images

[Seguy'15

Inverse Wasserstein Problems

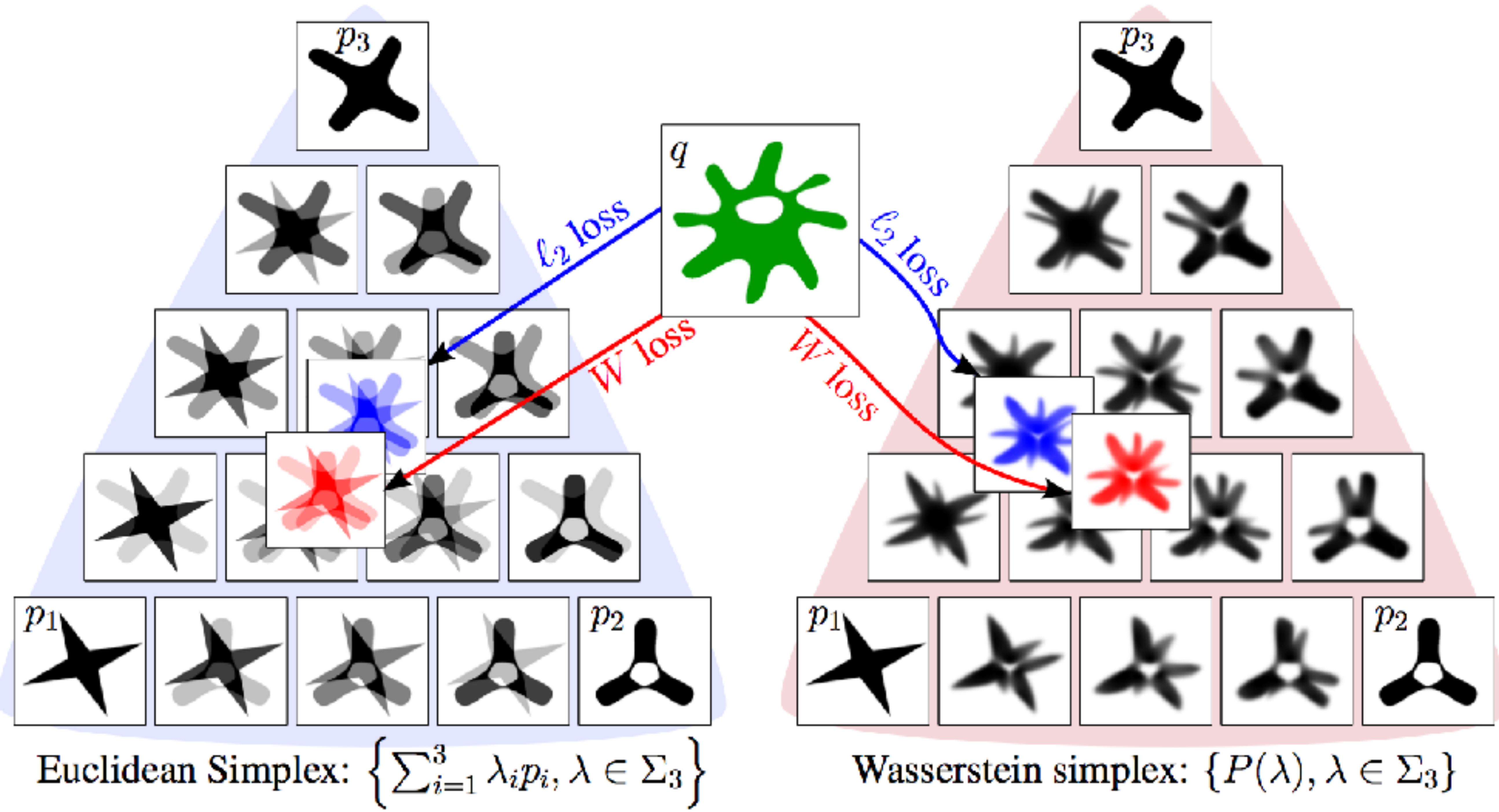
- consider Barycenter operator:

$$\boldsymbol{b}(\lambda) \stackrel{\text{def}}{=} \underset{\boldsymbol{a}}{\operatorname{argmin}} \sum_{i=1}^{N} \lambda_i W_\gamma(\boldsymbol{a}, \boldsymbol{b_i})$$

- address now **Wasserstein inverse problems**:

$$\text{Given } \boldsymbol{a}, \;\; \text{find } \underset{\lambda \in \Sigma_N}{\operatorname{argmin}} \, \mathcal{E}(\lambda) \stackrel{\text{def}}{=} \operatorname{Loss}(\boldsymbol{a}, \boldsymbol{b}(\lambda))$$

Wasserstein Inverse Problems



Barycenters = Fixed Points

Prop. **[BCCNP'15]** Consider $\boldsymbol{B} \in \Sigma_d^N$ and let $\boldsymbol{U_0} = \mathbf{1}_{\boldsymbol{d \times N}}$, and then for $l \geq 0$:

$$\boldsymbol{b}^l \stackrel{\text{def}}{=} \exp\left(\log\left(K^T \boldsymbol{U_l}\right)\lambda\right); \begin{cases} \boldsymbol{V_{l+1}} \stackrel{\text{def}}{=} \dfrac{\boldsymbol{b}^l \mathbf{1}_N^T}{K^T \boldsymbol{U_l}}, \\ \boldsymbol{U_{l+1}} \stackrel{\text{def}}{=} \dfrac{\boldsymbol{B}}{K \boldsymbol{V_{l+1}}}. \end{cases}$$

Using Truncated Barycenters

- instead of using the exact barycenter

$$\underset{\lambda \in \Sigma_N}{\operatorname{argmin}} \mathcal{E}(\lambda) \stackrel{\text{def}}{=} \operatorname{Loss}(\boldsymbol{a}, \boldsymbol{b}(\lambda))$$

- use instead the L-iterate barycenter

$$\underset{\lambda \in \Sigma_N}{\operatorname{argmin}} \mathcal{E}^{(L)}(\lambda) \stackrel{\text{def}}{=} \operatorname{Loss}(\boldsymbol{a}, \boldsymbol{b}^{(L)}(\lambda))$$

- Differente using **the chain rule.**

$$\nabla \mathcal{E}^{(L)}(\lambda) = [\partial \boldsymbol{b}^{(L)}]^T(\boldsymbol{g}), \;\; \boldsymbol{g} \stackrel{\text{def}}{=} \nabla \operatorname{Loss}(\boldsymbol{a}, \cdot)|_{\boldsymbol{b}^{(L)}(\lambda)}.$$

Gradient / Barycenter Computation

function SINKHORN-DIFFERENTIATE$((p_s)_{s=1}^S, q, \lambda)$

$\forall s, b_s^{(0)} \leftarrow \mathbb{1}$

$(w, r) \leftarrow (0^S, 0^{S\times N})$

for $\ell = 1, 2, \ldots, L$ *// Sinkhorn loop*

$\forall s, \varphi_s^{(\ell)} \leftarrow K^\top \frac{p_s}{Kb_s^{(\ell-1)}}$

$p \leftarrow \prod_s \left(\varphi_s^{(\ell)}\right)^{\lambda_s}$

$\forall s, b_s^{(\ell)} \leftarrow \frac{p}{\varphi_s^{(\ell)}}$

$g \leftarrow \nabla \mathcal{L}(p, q) \odot p$

for $\ell = L, L-1, \ldots, 1$ *// Reverse loop*

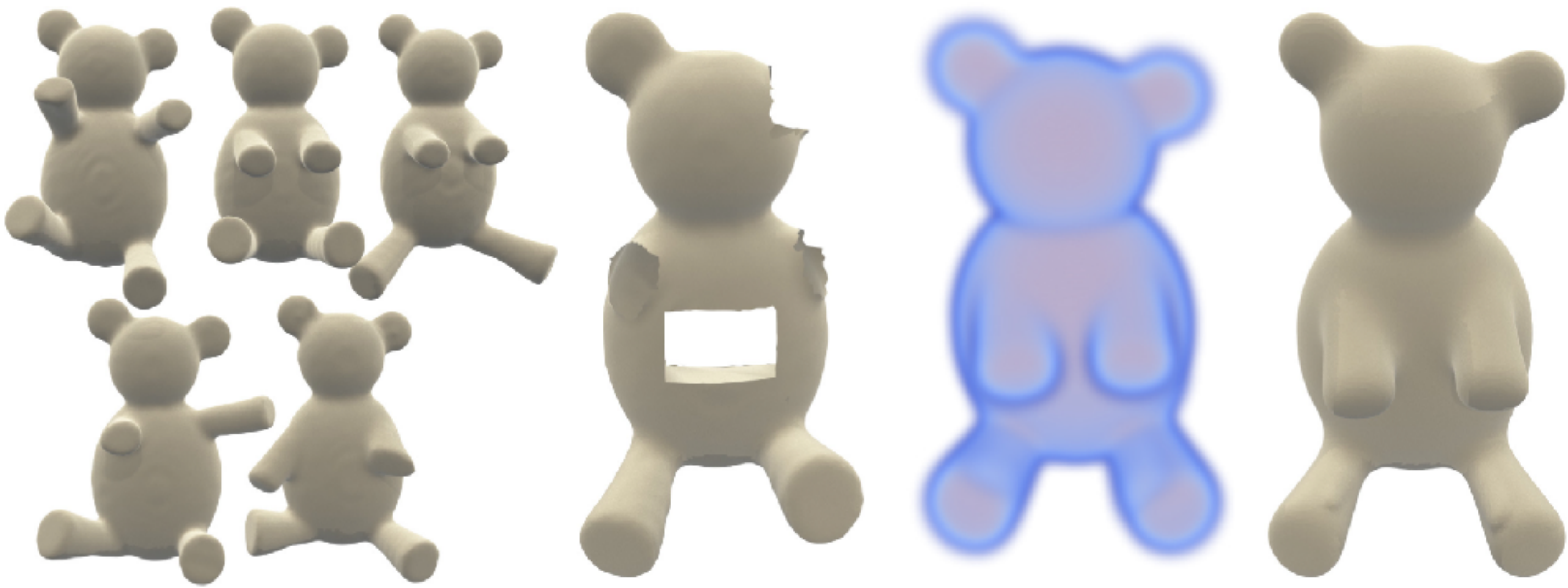
$\forall s, w_s \leftarrow w_s + \langle \log \varphi_s^{(\ell)}, g \rangle$

$\forall s, r_s \leftarrow -K^\top (K(\frac{\lambda_s g - r_s}{\varphi_s^{(\ell)}}) \odot \frac{p_s}{(Kb_s^{(\ell-1)})^2}) \odot b_s^{(\ell-1)}$

$g \leftarrow \sum_s r_s$

return $P^{(L)}(\lambda) \leftarrow p, \nabla \mathcal{E}_L(\lambda) \leftarrow w$

Application: Volume Reconstruction



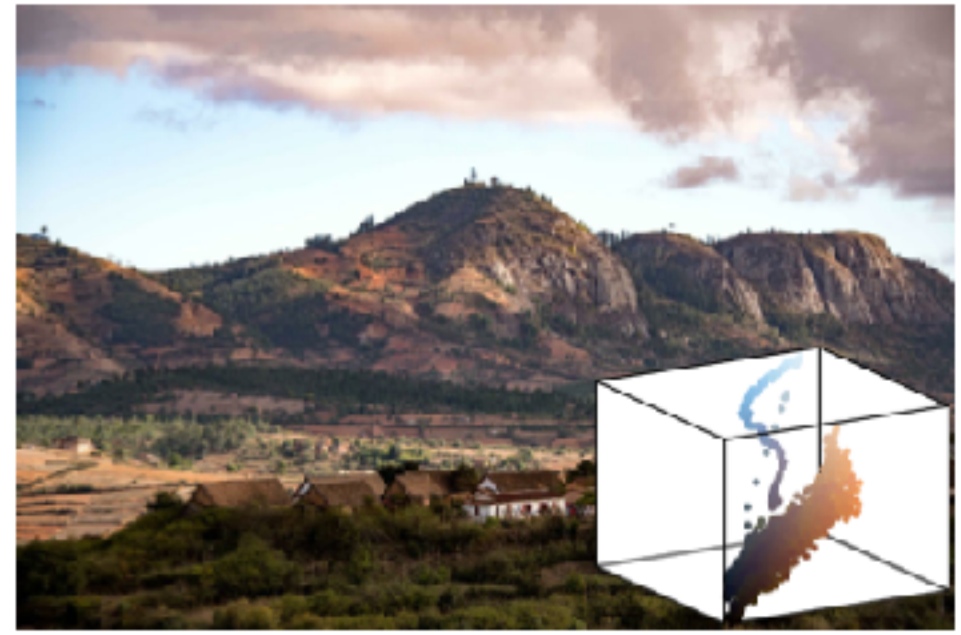
Shape database $(p_1, \ldots, p_5)$ | Input shape q | Projection $P(\lambda)$ | Iso-surface

[Bonneel'16]

Application: Color Grading

Application: Color Grading

$\lambda_0 = 0.03$



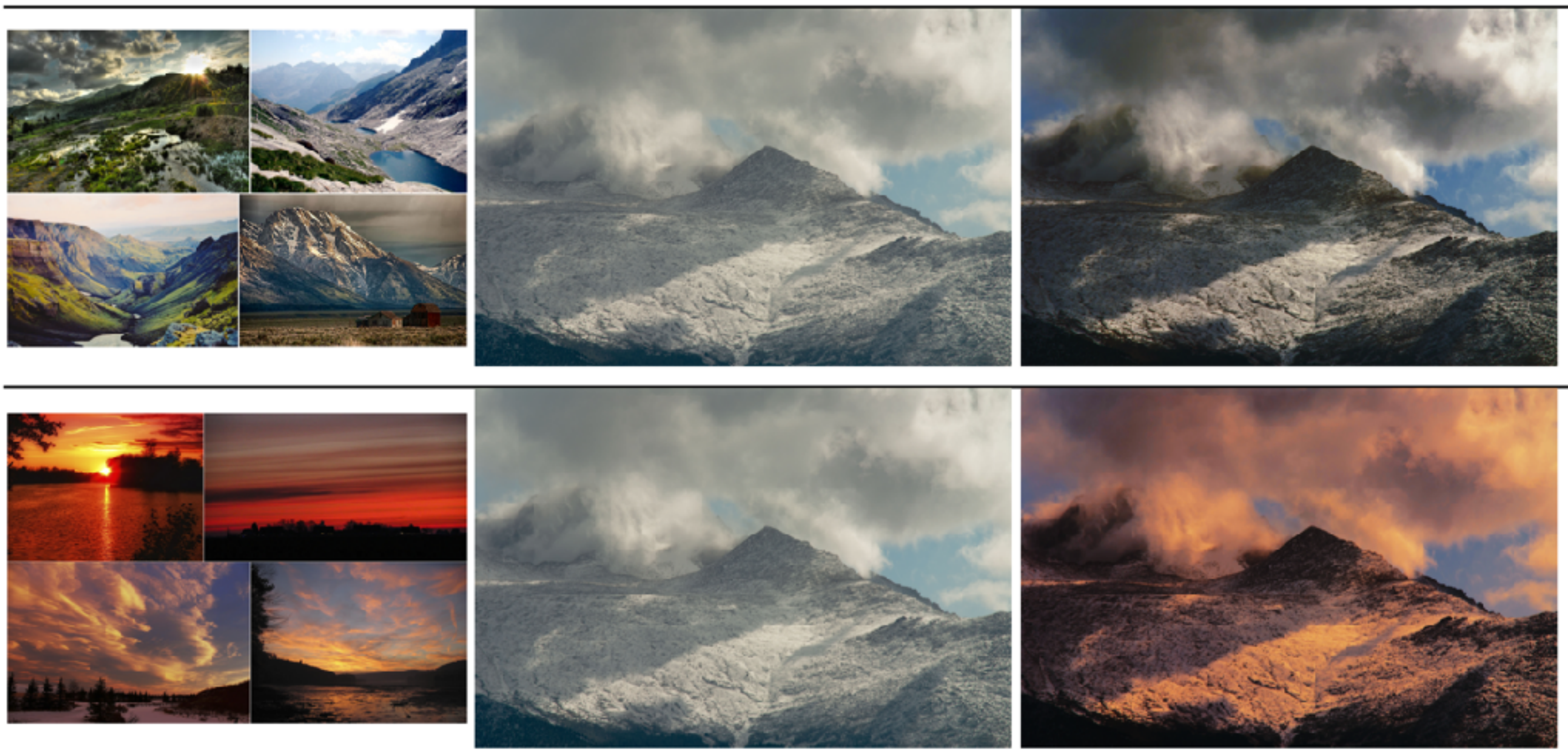
$\lambda_1 = 0.12$

$\lambda_2 = 0.40$

$\lambda_3 = 0.43$

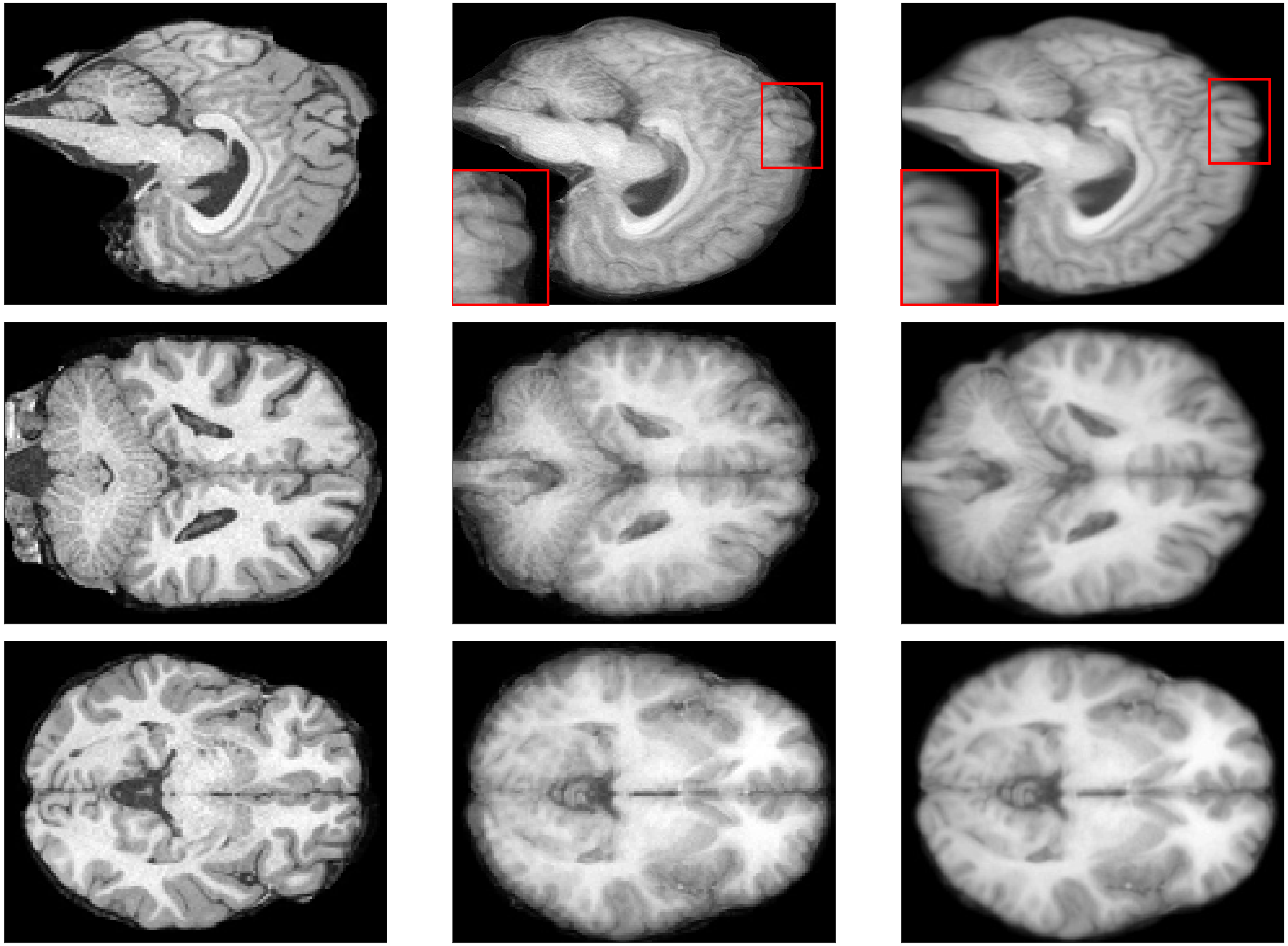
Application: Color Grading

Application: Color Grading



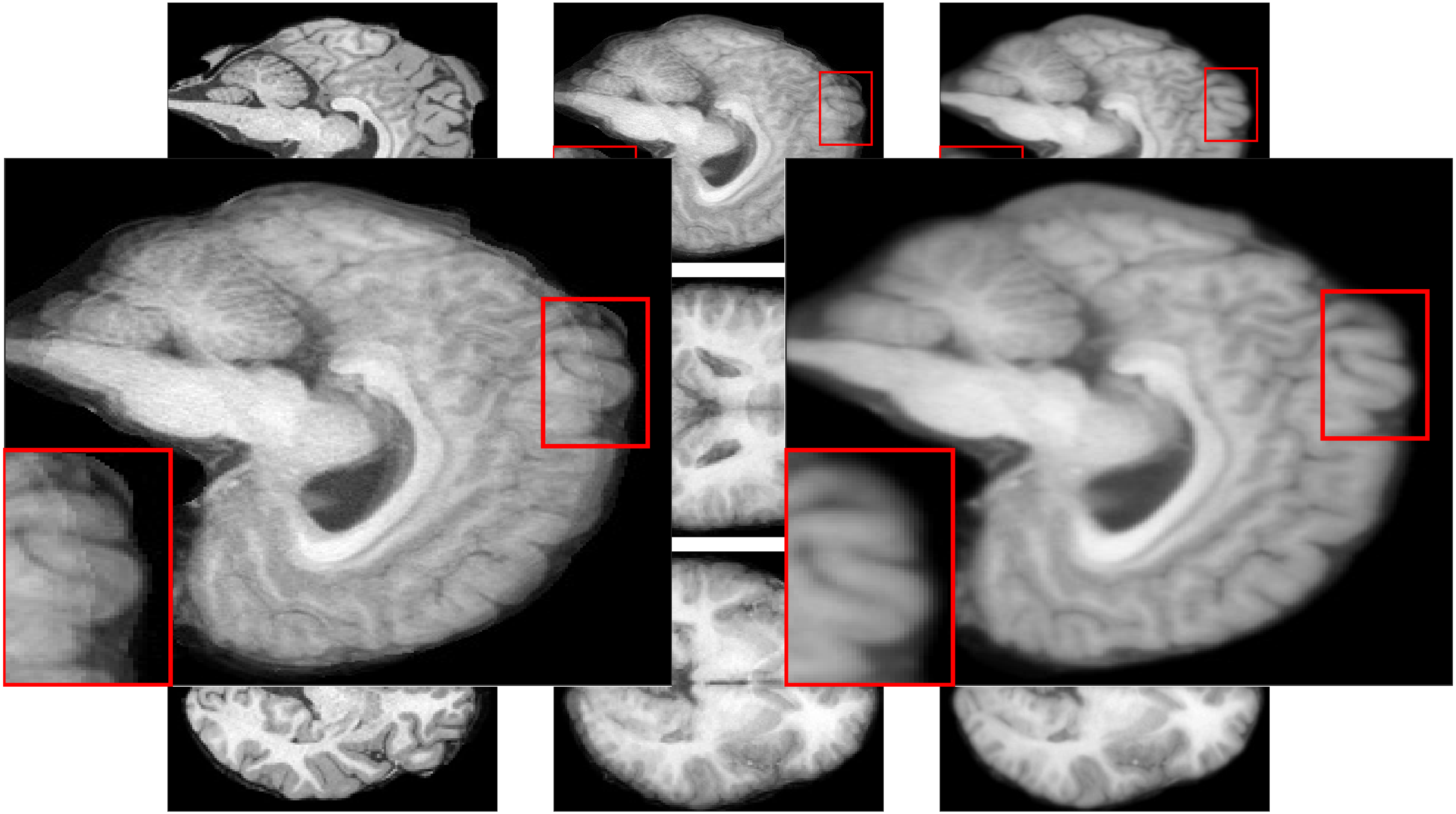
Wasserstein Barycentric Coordinates: Histogram Regression using Optimal Transport, **SIGGRAPH'16** **[BPC'16]**

Application: Brain Mapping



Original | Euclidean projection | Wasserstein projection

Application: Brain Mapping



Original

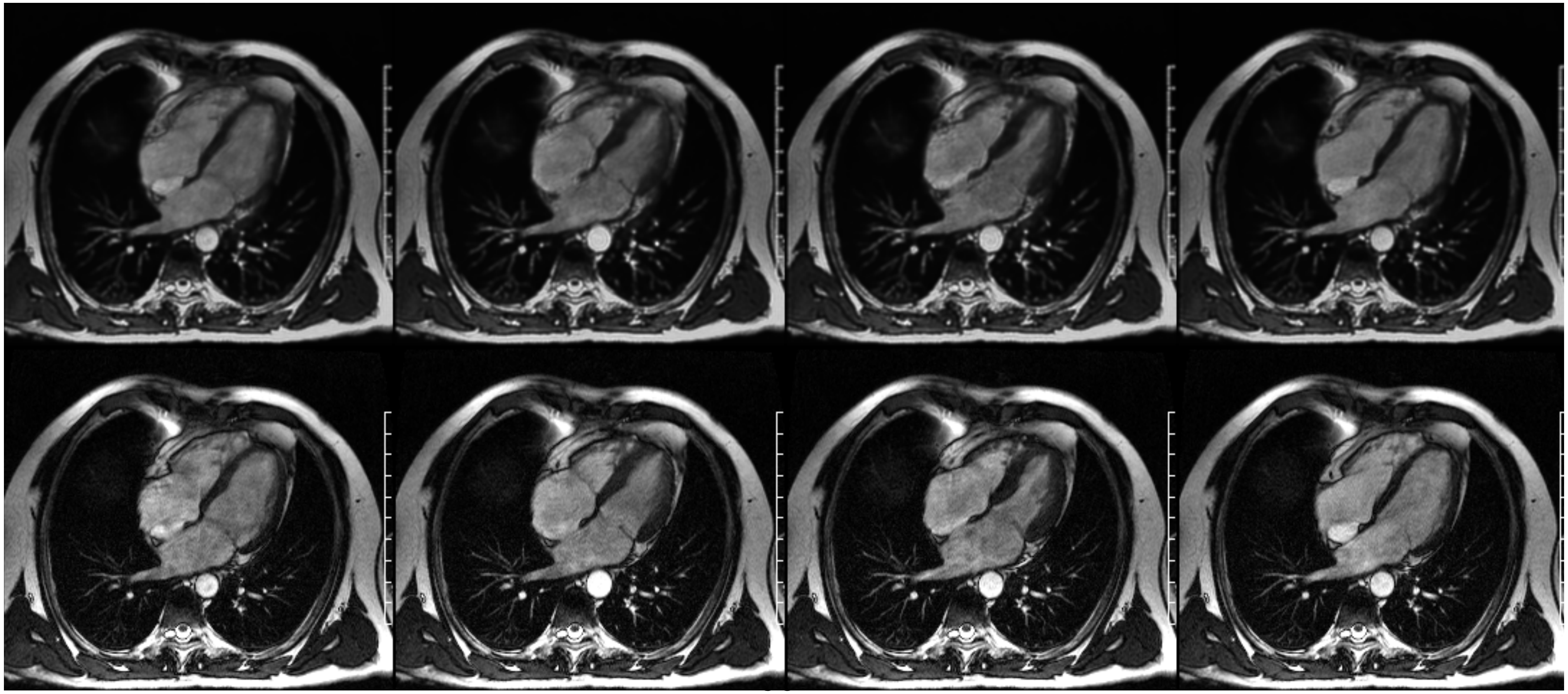
Euclidean projection

Wasserstein projection

end-to-end W Dictionary Learning

$$\min_{\boldsymbol{A}\in(\Sigma_n)^K \boldsymbol{\Lambda}\in(\Sigma_K)^N} \sum_{i=1}^{N} \mathcal{L}\left(\boldsymbol{b_i}, \boldsymbol{a}(\boldsymbol{\lambda_i})\right)$$

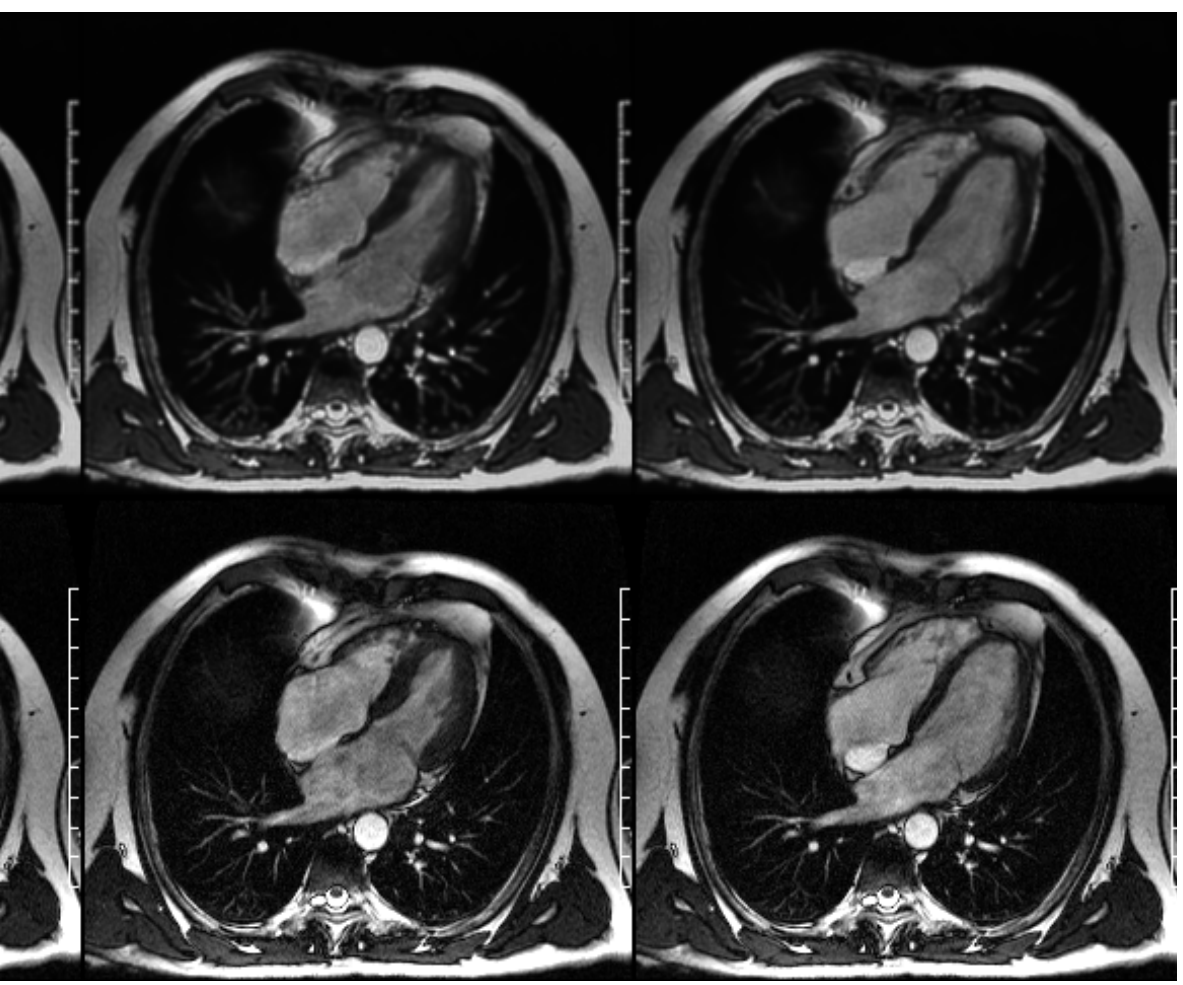
[Schmitz'18]

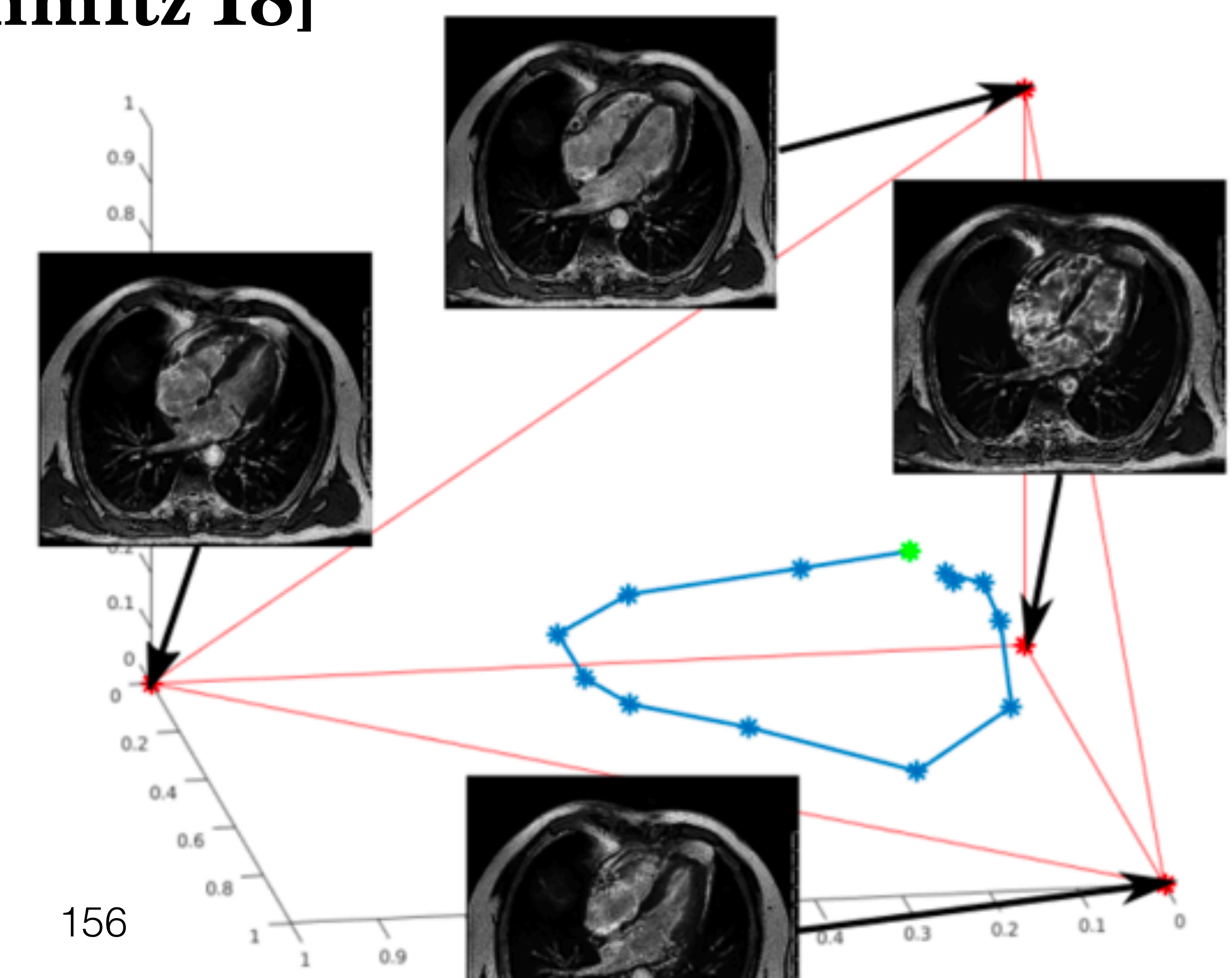


end-to-end W Dictionary Learning

$$\min_{\boldsymbol{A}\in(\Sigma_n)^K \boldsymbol{\Lambda}\in(\Sigma_K)^N} \sum_{i=1}^{N} \mathcal{L}\left(\boldsymbol{b_i}, \boldsymbol{a}(\boldsymbol{\lambda_i})\right)$$

[Schmitz'18]





Distributionally Robust Optimization

$$\nu_{\text{data}} = \frac{1}{n} \sum_{i=1}^{N} \delta_{(x_i, y_i)}$$

Supervised learning

$$\inf_{\theta \in \Theta} \mathbb{E}_{\nu_{\text{data}}}[\mathcal{L}(f_\theta(X), Y)]$$

Learning with Wasserstein Ambiguity

$$\inf_{\theta \in \Theta} \sup_{\mu : W_p(\nu_{\text{data}}, \mu) < \varepsilon} \mathbb{E}_{\mu}[\mathcal{L}(f_\theta(X), Y)]$$

[Esvahani'17]

Distributionally Robust Learning

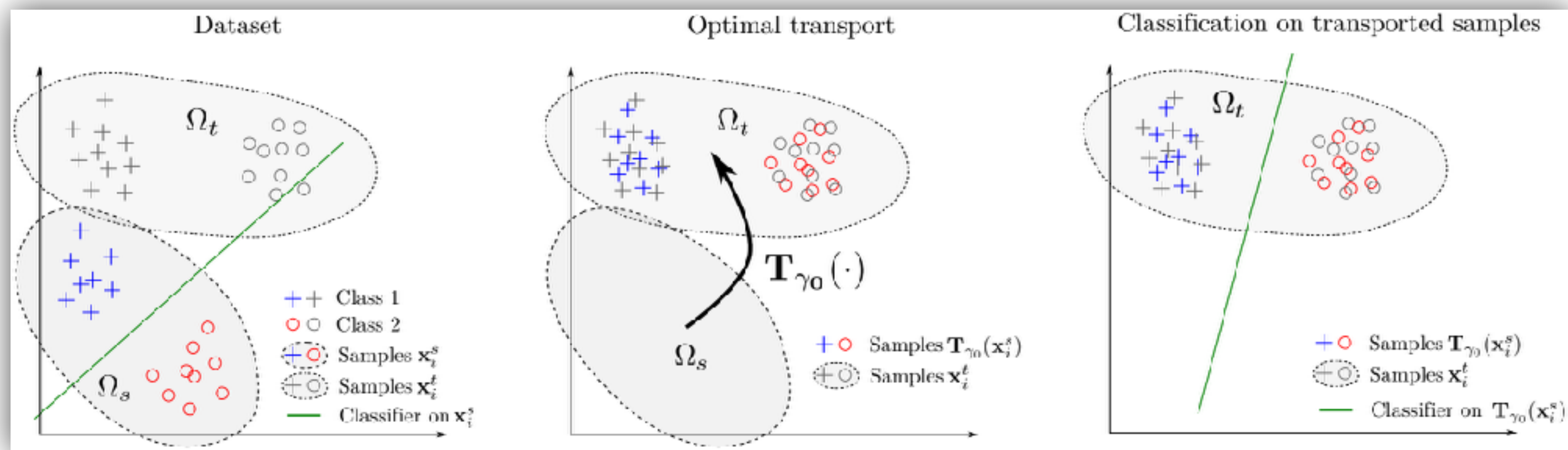
Learning with Wasserstein Ambiguity

$$\inf_{\theta \in \Theta} \sup_{\boldsymbol{\mu} : W_p(\boldsymbol{\nu}_{\mathrm{data}}, \boldsymbol{\mu}) < \varepsilon} \mathbb{E}_{\boldsymbol{\mu}}[\mathcal{L}(f_\theta(X), Y)]$$

Advantages:

- Bound on out-of-sample performance
- Converges as size of dataset increases
- Often reduces to a finite convex program (e.g. when f is element-wise max over elementary concave functions)

Domain Adaptation



1. Estimate transport map
2. Transport labeled samples to new domain
3. Train classifier on transported labeled samples

[Courty'16]

Learning with a Wasserstein Loss

$$\text{Dataset } \{(x_i, y_i)\}, x_i \in \mathbb{R}^p, y_i \in \mathbb{R}^n_+$$

x_i

husky
snow
sled
slope
men

y_i

Goal is to find $f_{\boldsymbol{\theta}}$: Images $\mapsto$ Labels

Learning with a Wasserstein Loss

$$\min_{\boldsymbol{\theta} \in \Theta} \sum_{i=1}^{N} \mathcal{L}(f_{\boldsymbol{\theta}}(x_i), y_i)$$

x_i

husky
snow
sled
slope
men

y_i

Which loss $\mathcal{L}$ could we use?

Learning with a Wasserstein Loss

$$\min_{\boldsymbol{\theta} \in \Theta} \sum_{i=1}^{N} \mathcal{L}(f_{\boldsymbol{\theta}}(x_i), y_i)$$

dog driver winter ice $f_{\boldsymbol{\theta}}(x_i)$	husky snow sled slope men y_i

Which loss $\mathcal{L}$ could we use?

Learning with a Wasserstein Loss

$$\min_{\boldsymbol{\theta}\in\Theta} \sum_{i=1}^{N} \mathcal{L}(f_{\boldsymbol{\theta}}(x_i), y_i)$$

$$\mathcal{L}(\boldsymbol{a}, \boldsymbol{b}) = \min_{\boldsymbol{P}\in\mathbb{R}^{nm}} \langle \boldsymbol{P}, M \rangle + \varepsilon \mathrm{KL}(\boldsymbol{P}\mathbf{1}, \boldsymbol{a}) + \varepsilon \mathrm{KL}(\boldsymbol{P}^T\mathbf{1}, \boldsymbol{b}) - \gamma E(\boldsymbol{P})$$

1. Generalizes Word Mover's to label clouds
2. Sinkhorn algorithm can be generalized

[Frogner'15] [Chizat'15][Chizat'16]

Minimum Kantorovich Estimation

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Statistics & Probability Letters 76 (2006) 1298–1302

STATISTICS & PROBABILITY LETTERS

www.elsevier.com/locate/stapro

On minimum Kantorovich distance estimators

Federico Bassetti[a], Antonella Bodini[b], Eugenio Regazzini[a,*]

Use *Wasserstein distances* to define a loss between data and model.

$$\min_{\boldsymbol{\theta} \in \Theta} W(\boldsymbol{\nu}_{\mathrm{data}}, p_{\boldsymbol{\theta}})$$

Minimum Kantorovich Estimators

$$\min_{\boldsymbol{\theta}\in\Theta} W(\boldsymbol{\nu}_{\text{data}}, f_{\boldsymbol{\theta}\sharp}\boldsymbol{\mu})$$

[Bassetti'06] 1st reference discussing this approach.

$$\text{Challenge: } \nabla_{\boldsymbol{\theta}} W(\boldsymbol{\nu}_{\text{data}}, f_{\boldsymbol{\theta}\sharp}\boldsymbol{\mu})?$$

[Montavon'16] use regularized OT in a finite setting.

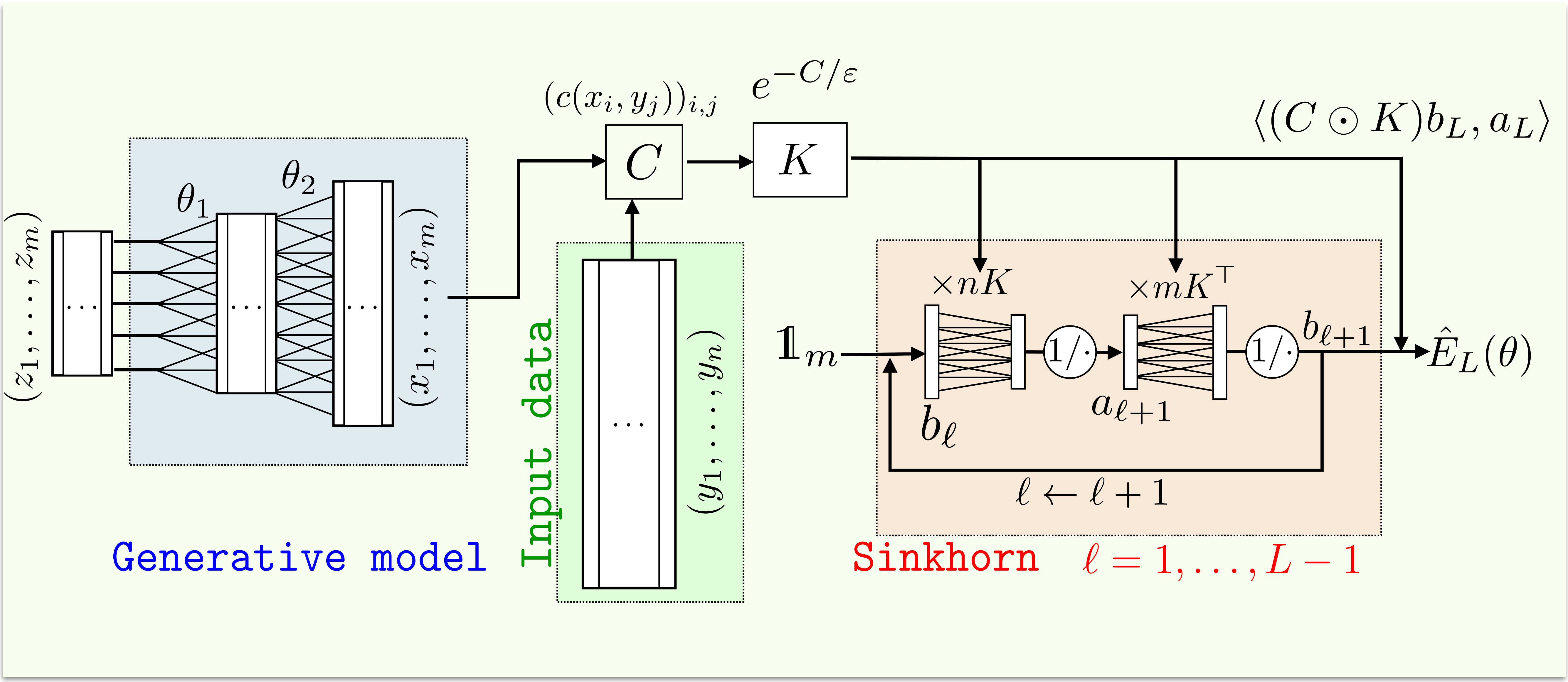
[Arjovsky'17] *(WGAN)* uses a NN to approximate dual solutions and recover gradient w.r.t. parameter

[Bernton'17] *(Wasserstein ABC)*

[Genevay'17, Salimans'17] *(Sinkhorn approach)*

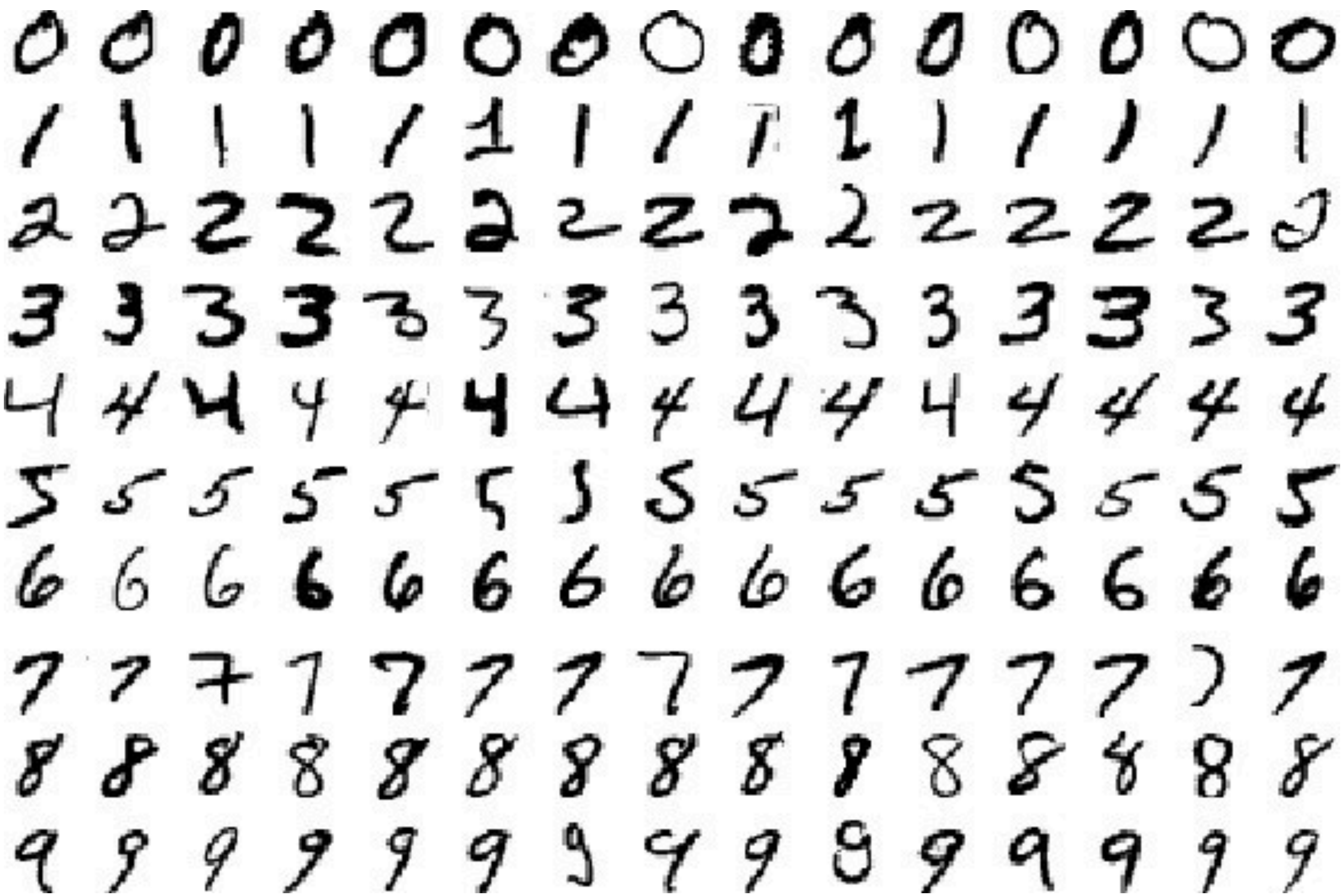
Proposal: Autodiff OT using Sinkhorn

Approximate W loss by the transport cost $\bar{W}_L$ after L Sinkhorn iterations.



[GPC'17]

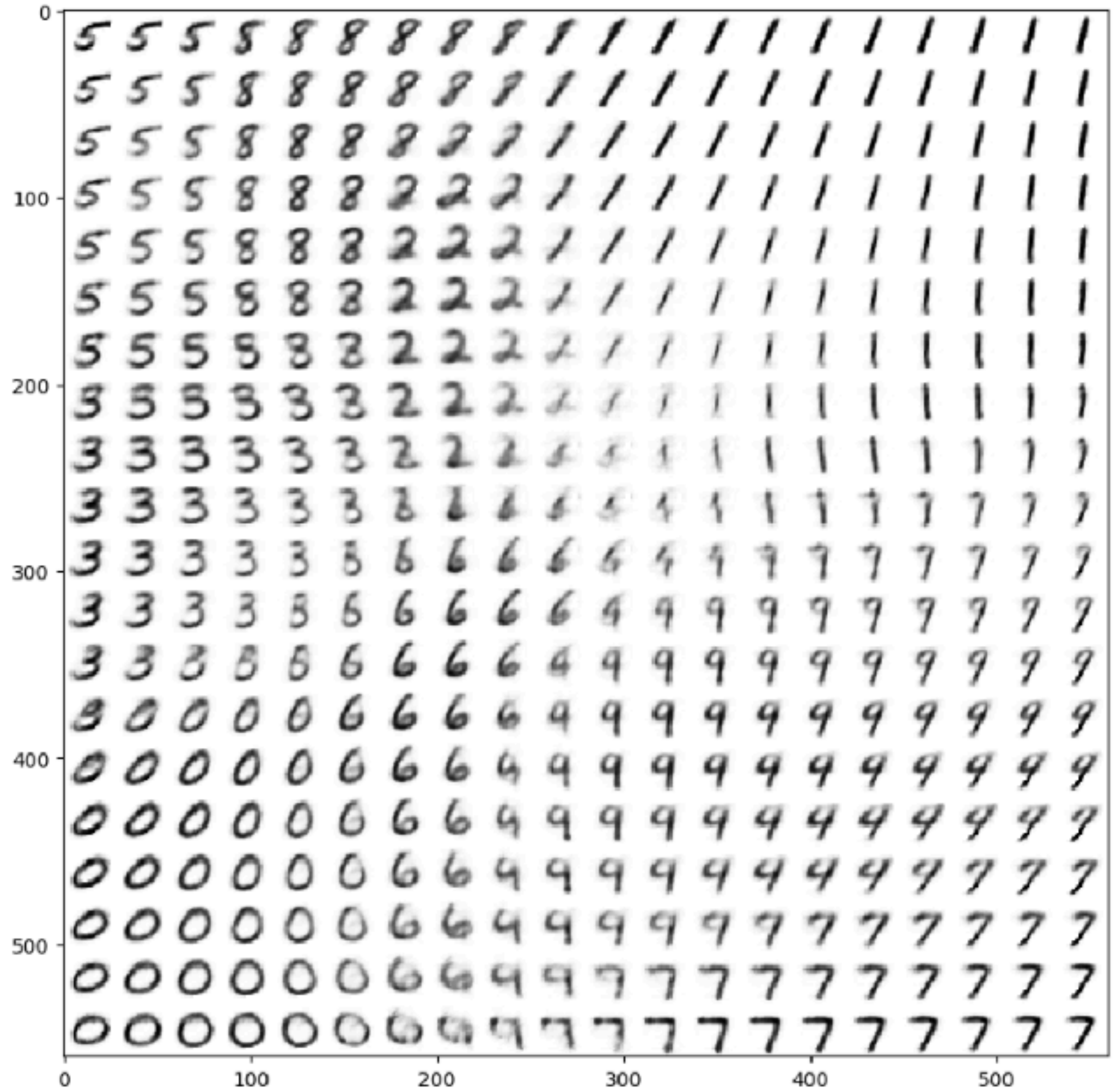
Example: MNIST, Learning $f_{\boldsymbol{\theta}}$



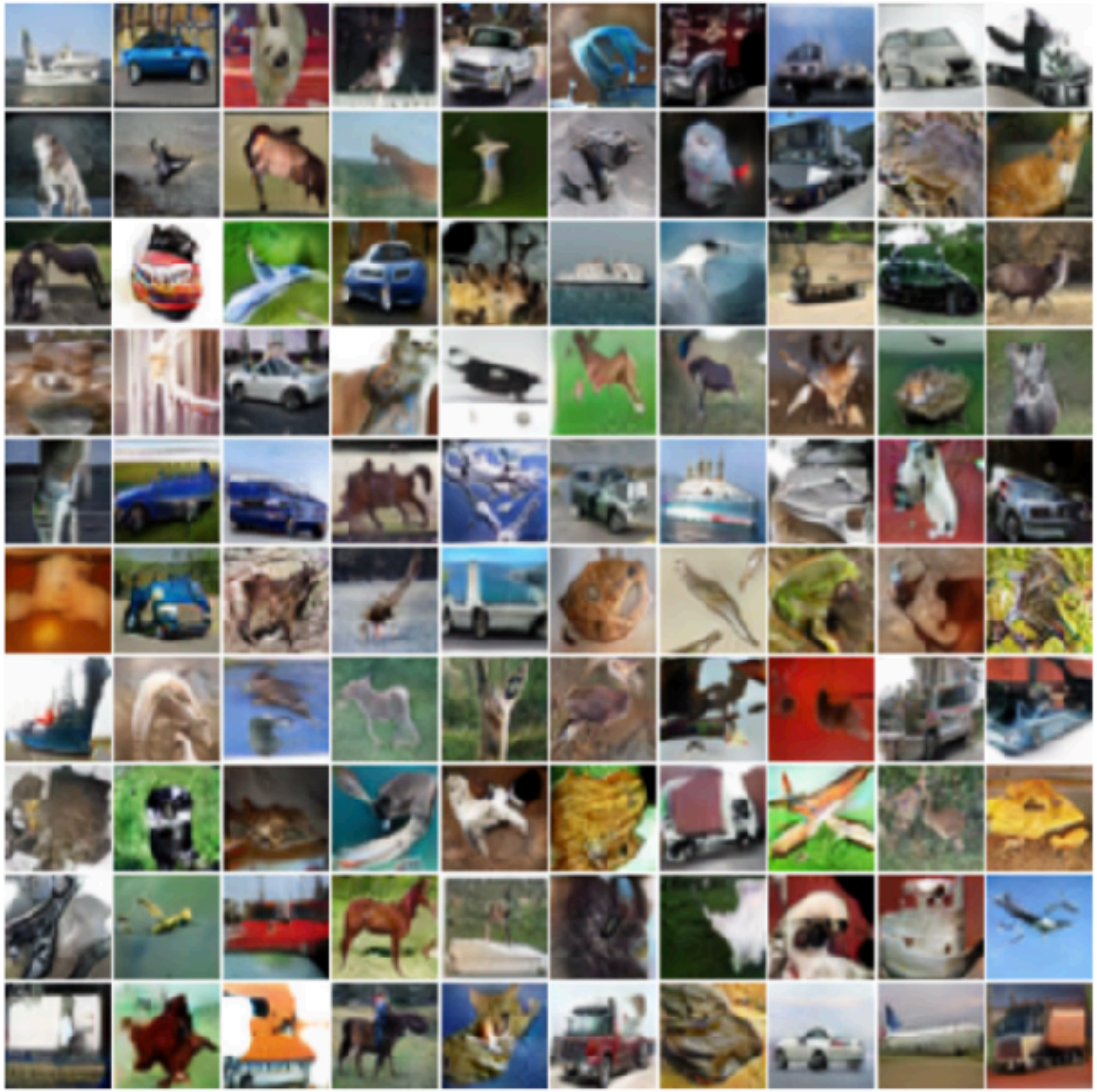
Example: MNIST, Learning $f_{\boldsymbol{\theta}}$

Latent space

$[0,1]^2$



Example: Generation of Images



arxiv.org/pdf/1710.05488

[Salimans'18]

Example: Generation of Images

arxiv.org/pdf/1710.05488

[Salimans'18]

Concluding Remarks

- *Regularized* OT is much faster than OT.
- *Regularized* OT can interpolate between W and the *MMD / Energy distance (MMD)* metrics.
- The solution of *regularized OT* is *“auto-differentiable”*.
- **Many open problems remain!**

What I could not talk about...

- Very large supply of maths...
- **Statistical** challenges to compute W.
- If **linear assignment** = Wasserstein, then **quadratic assignment** = Gromov-Wasserstein.
- Wasserstein gradient flows (a.k.a. **JKO** flow).
- **Dynamical** aspects of optimal transport
- Transporting vectors and matrices
- Applications to sampling.

https://optimaltransport.github.io/