Optimal Multimarginal Schrödinger Bridge: Minimum Spanning Tree over Measure-valued Vertices

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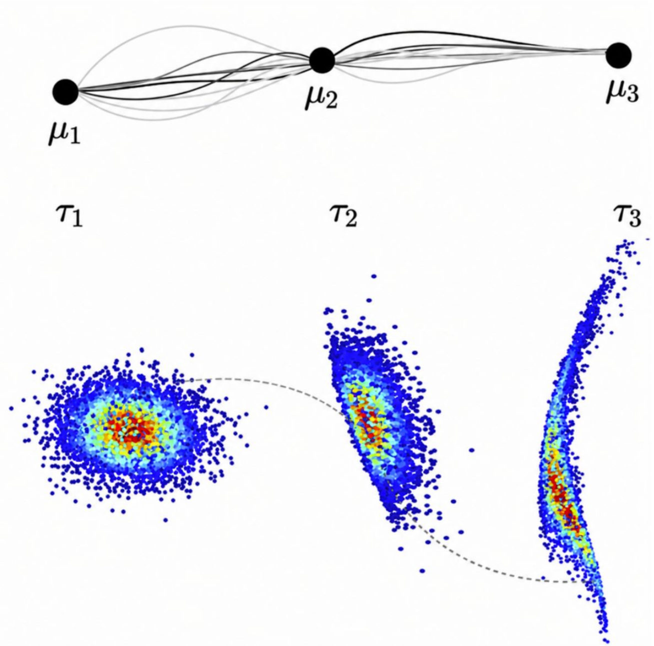
The Multimarginal Schrödinger Bridge Problem

Given $\boldsymbol{s} \in \mathbb{N}_{\geq 2}$ distributions $\boldsymbol{\mu}_{i\in[s]} \in \mathbb{R}^n$, and ground cost $\boldsymbol{C} \in (\mathbb{R}^n)^{\otimes s}_{\geq 0}$,

find the "*optimal measure-valued path* between the distributions"



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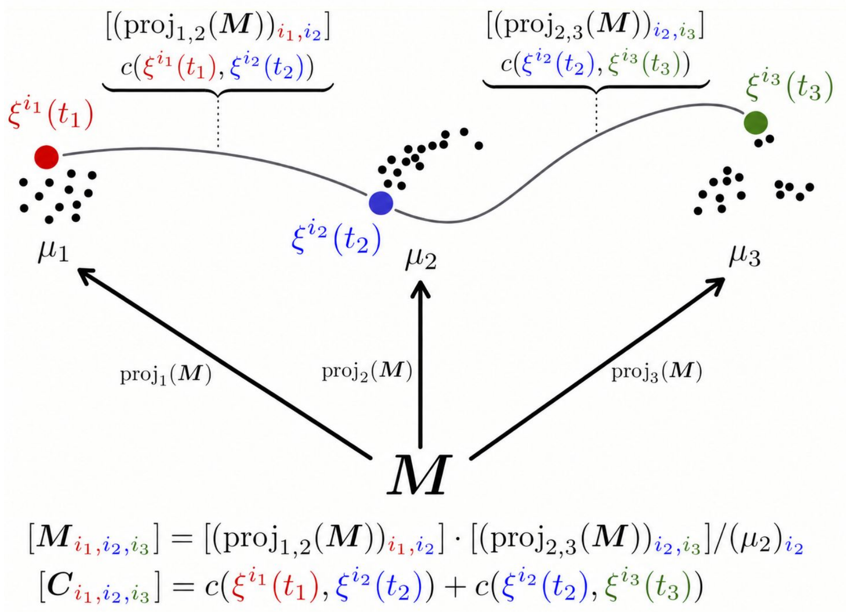
$$\boxed{\begin{aligned} &\min_{\boldsymbol{M}\in(\mathbb{R}^n)^{\otimes s}_{\geq 0}} \langle \boldsymbol{C} + \eta \log \boldsymbol{M}, \boldsymbol{M} \rangle \\ &\text{subject to } \operatorname{proj}_\sigma(\boldsymbol{M}) = \boldsymbol{\mu}_\sigma \quad \forall \sigma \in [\![s]\!] \end{aligned}}$$

Minimizer $\boldsymbol{M}_{\text{opt}}$ is the *MSB*,
with *MSB cost* $\langle \boldsymbol{C} + \eta \log \boldsymbol{M}_{\text{opt}}, \boldsymbol{M}_{\text{opt}} \rangle$

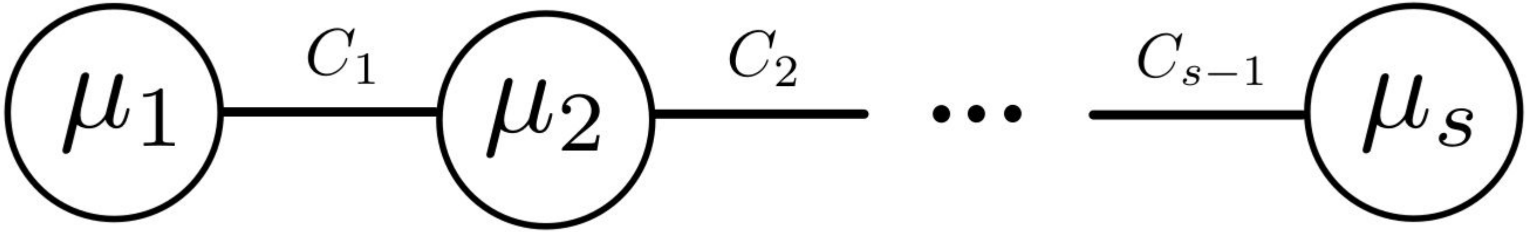
Note that $\langle \boldsymbol{C} + \eta \log \boldsymbol{M}, \boldsymbol{M} \rangle$

$$= \eta \, \mathrm{D}_{\mathrm{KL}} (\boldsymbol{M} \parallel \boldsymbol{K})$$

where $\boldsymbol{K} := \exp(-\boldsymbol{C}/\eta)$



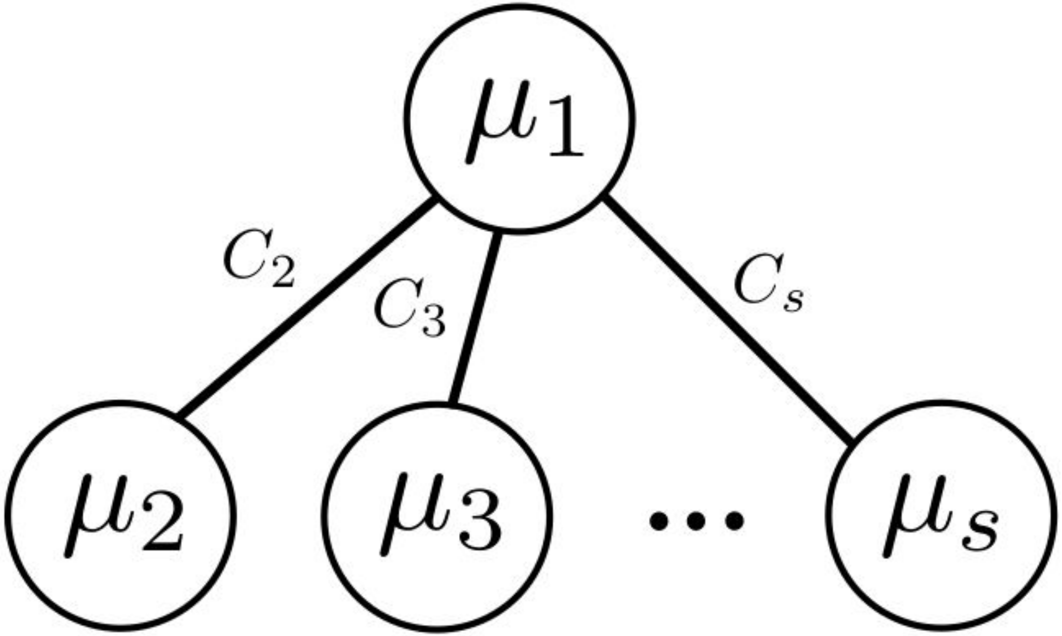
Correspondence Graphs – Path



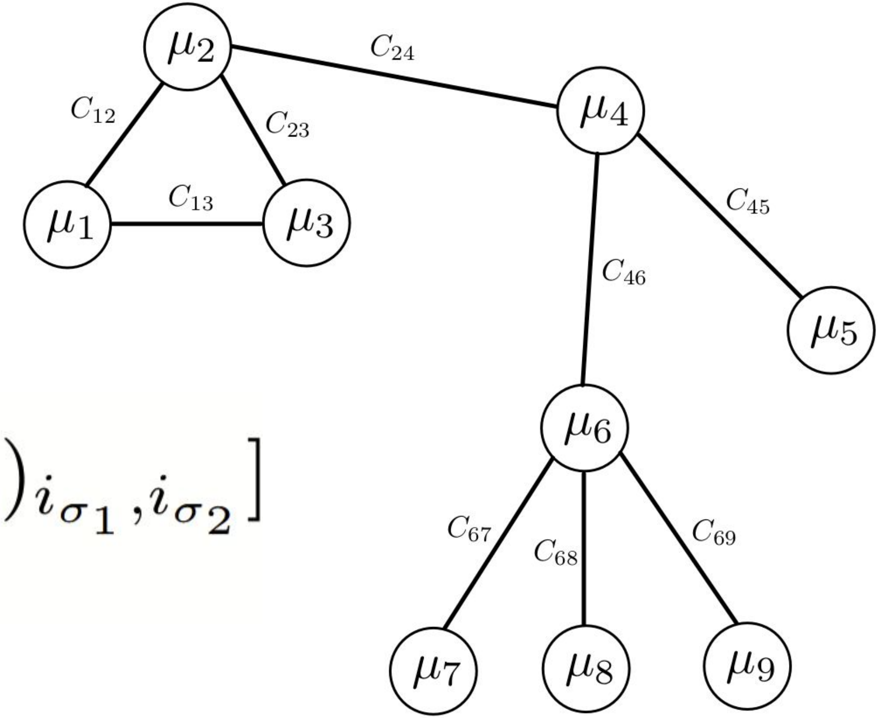
$$[\boldsymbol{C}_{i_{\mathcal{V}}}] = [\boldsymbol{C}_{i_1,\ldots,i_s}] = \sum_{\sigma=1}^{s-1} [(C_\sigma)_{i_\sigma, i_{\sigma+1}}]$$

Correspondence Graphs – Barycenter

$$[\boldsymbol{C}_{i_{\mathcal{V}}}] = \sum_{\sigma=2}^{s} [(C_\sigma)_{i_1, i_\sigma}]$$

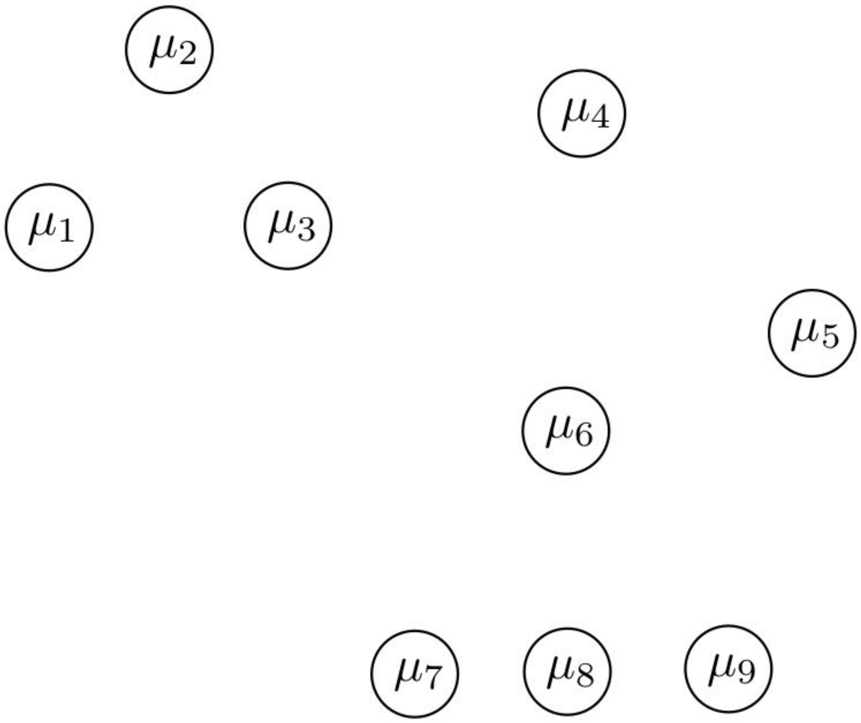


Correspondence Graphs – $\mathcal{G} = (\mathcal{V}, \mathcal{E})$



$$[\boldsymbol{C}_{i_\mathcal{V}}] = \sum_{(\sigma_1,\sigma_2)\in\mathcal{E}} [(C_{\sigma_1\sigma_2})_{i_{\sigma_1}, i_{\sigma_2}}]$$

Correspondence Graphs – ?



$$[\boldsymbol{C}_{i_\mathcal{V}}] = ?$$

Correspondence Graphs – ?

Problem: Find optimal $\mathcal{G}$

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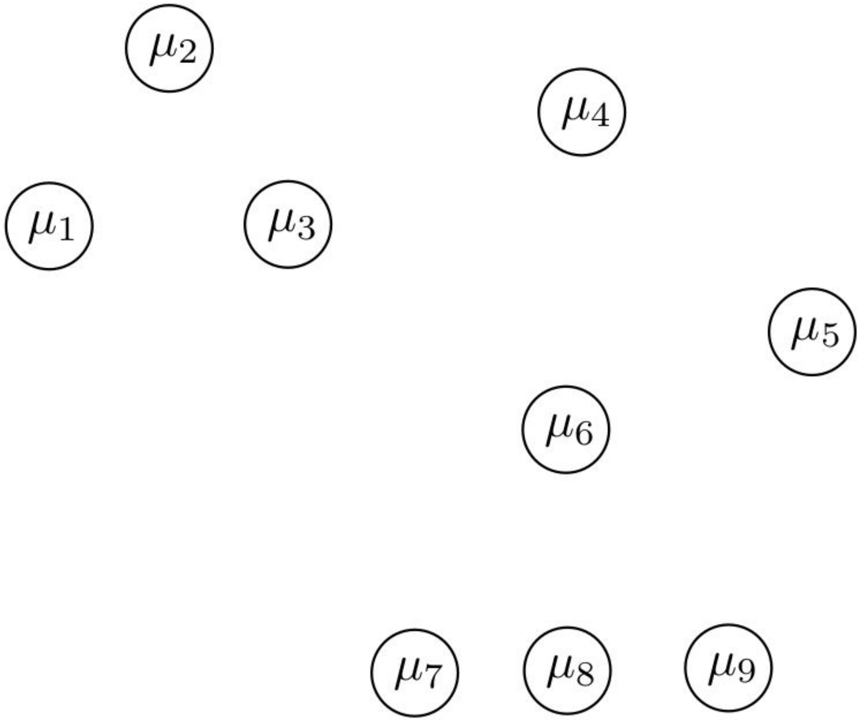


Optimal Multimarginal Schrödinger Bridge Problem

MSB

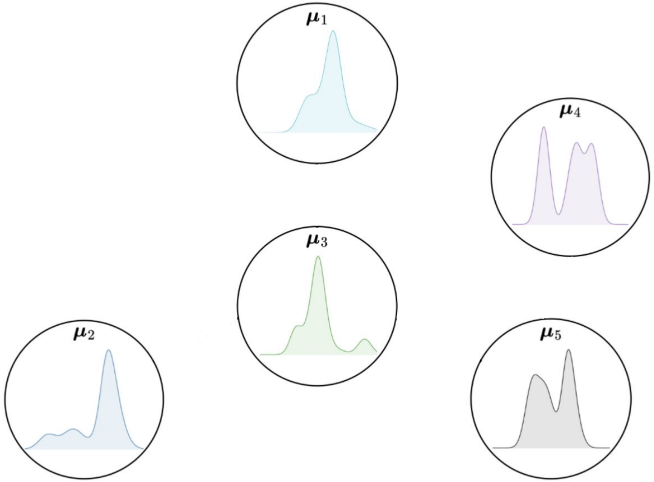
$$\boldsymbol{M}^{\text{opt}} := \underset{\boldsymbol{M}\in\Pi(\mathcal{V})}{\arg\min} \quad \langle \boldsymbol{C} + \eta \log \boldsymbol{M}, \boldsymbol{M} \rangle$$

Definition. *Optimal* MSB

$$\begin{aligned} \mathcal{G}^{\text{opt}} &= \underset{\substack{\mathcal{G}\text{ undirected connected}\\ \text{over vertices } \mathcal{V}}}{\arg\min} \quad \langle \boldsymbol{C}(\mathcal{G}) + \eta \log \boldsymbol{M}^{\text{opt}}(\mathcal{G}), \boldsymbol{M}^{\text{opt}}(\mathcal{G}) \rangle \\ &= \underset{\substack{\mathcal{G}\text{ undirected connected}\\ \text{over vertices } \mathcal{V}}}{\arg\min} \quad \min_{\boldsymbol{M}\in\Pi(\mathcal{V})} \langle \boldsymbol{C}(\mathcal{G}) + \eta \log \boldsymbol{M}, \boldsymbol{M} \rangle \end{aligned}$$

Optimal MSBP: Motivation

Spatial reconstruction



E.g., sensors in a field

Temporal reconstruction

E.g., camera snapshots jumbled in time

Solving for optimal MSB: Reduction to Trees

Proposition 1

$$\mathcal{G}^{\mathrm{opt}} = \underset{\substack{\mathcal{G} \text{ undirected connected} \\ \text{over vertices } \mathcal{V}}}{\arg\min} \; \min_{\boldsymbol{M} \in \Pi(\mathcal{V})} \langle \boldsymbol{C}(\mathcal{G}) + \eta \log \boldsymbol{M}, \boldsymbol{M} \rangle$$ is a tree.

Proof. We know $\mathcal{G}^{\mathrm{opt}}$ is connected. WTS $\mathcal{G}^{\mathrm{opt}}$ contains no cycles.

Solving for optimal MSB: Reduction to Trees

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$\mathcal{G}^{\mathrm{opt}} = (\mathcal{V}, \mathcal{E})$ contains a cycle $\implies \exists$ removable edge $(\sigma', \sigma'') \in \mathcal{V} \times \mathcal{V}$

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Proof. We know $\mathcal{G}^{\text{opt}}$ is connected. WTS $\mathcal{G}^{\text{opt}}$ contains no cycles.

$\mathcal{G}^{\text{opt}} = (\mathcal{V}, \mathcal{E})$ contains a cycle $\implies \exists$ removable edge $(\sigma', \sigma'') \in \mathcal{V} \times \mathcal{V}$

Let $\mathcal{G}' := (\mathcal{V}, \mathcal{E} \setminus (\sigma', \sigma''))$. Then,

$$[\boldsymbol{C}(\mathcal{G}')_{i_{\mathcal{V}}}] = \sum_{(\sigma_1,\sigma_2) \in \mathcal{E} \setminus (\sigma', \sigma'')} [(C_{\sigma_1 \sigma_2})_{i_{\sigma_1}, i_{\sigma_2}}] < [\boldsymbol{C}(\mathcal{G}^{\text{opt}})_{i_{\mathcal{V}}}] \quad -\!\!\!\times\!\!\!-$$

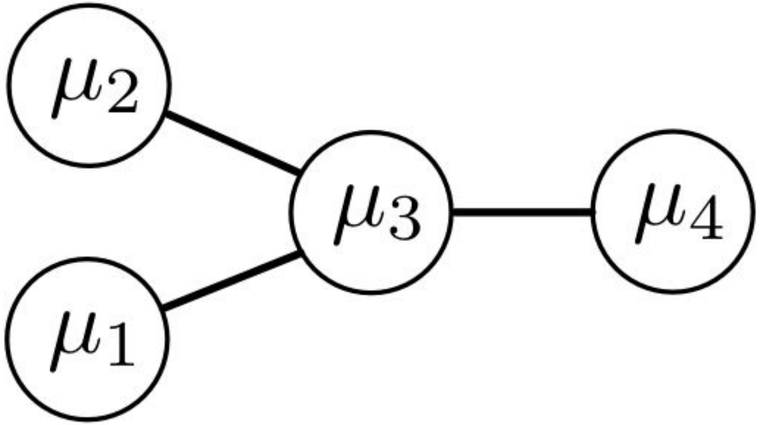
$\blacksquare$

Tree Splitting

$$M_{\mathcal{T}}^{\mathrm{opt}} := \underset{M \in \Pi(\mathcal{V})}{\arg\min}\ \eta\, \mathrm{D_{KL}}(M \parallel K)$$

Exhaustive search over s^{s-2} trees is unfeasible $\Rightarrow$ tree splitting?

$$\mathcal{T} = (\mathcal{V}, \mathcal{E})$$



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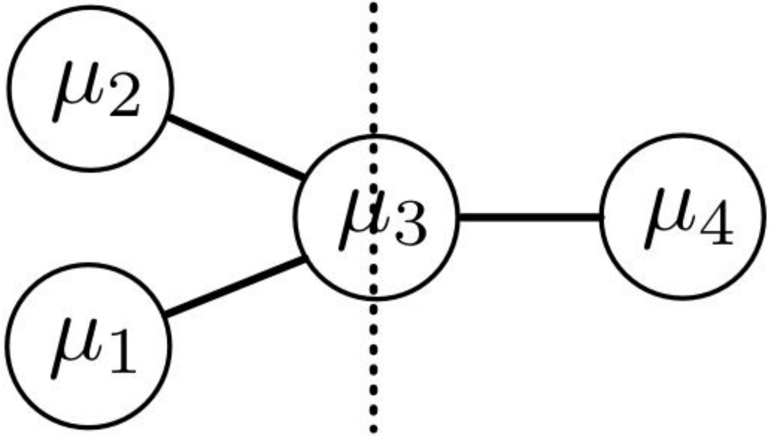


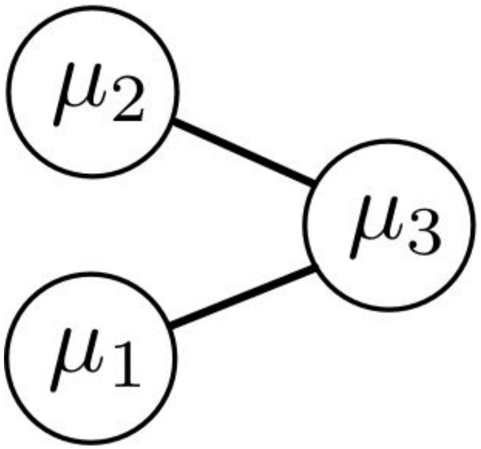
Split $\mathcal{T}$ at μ_σ

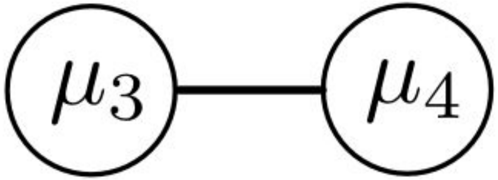
Tree Splitting

$$\boldsymbol{M}_{\mathcal{T}}^{\mathrm{opt}} := \underset{\boldsymbol{M} \in \Pi(\mathcal{V})}{\arg\min}\ \eta\, \mathrm{D}_{\mathrm{KL}}\left(\boldsymbol{M} \,\|\, \boldsymbol{K}\right)$$

Exhaustive search over s^{s-2} trees is unfeasible $\Longrightarrow$ tree splitting?

$\mathcal{T}_1 = (\mathcal{V}_1, \mathcal{E}_1)$ $\mathcal{T}_2 = (\mathcal{V}_2, \mathcal{E}_2)$





$$\boldsymbol{M}_{\mathcal{T}_1}^{\mathrm{opt}} := \underset{\mathrm{proj}_{\mathcal{V}_1}(\boldsymbol{M}) \in \Pi(\mathcal{V}_1)}{\arg\min}\ \eta\, \mathrm{D}_{\mathrm{KL}}(\mathrm{proj}_{\mathcal{V}_1}(\boldsymbol{M}) \,\|\, \boldsymbol{K}_1) \quad \boldsymbol{M}_{\mathcal{T}_2}^{\mathrm{opt}} := \underset{\mathrm{proj}_{\mathcal{V}_2}(\boldsymbol{M}) \in \Pi(\mathcal{V}_2)}{\arg\min}\ \eta\, \mathrm{D}_{\mathrm{KL}}(\mathrm{proj}_{\mathcal{V}_2}(\boldsymbol{M}) \,\|\, \boldsymbol{K}_2)$$

Tree Splitting (cont.)

Proposition 2 (Prop. 3.4, Haasler et al.)

For a tree $\mathcal{T} = (\mathcal{V}, \mathcal{E})$ with $\mathcal{T}_1 = (\mathcal{V}_1, \mathcal{E}_1)$, $\mathcal{T}_2 = (\mathcal{V}_2, \mathcal{E}_2)$ as before,

$$[(\boldsymbol{M}_{\mathcal{T}}^{\text{opt}})_{i_{\mathcal{V}}}] = \frac{[(\boldsymbol{M}_{\mathcal{T}_1}^{\text{opt}})_{i_{\mathcal{V}_1}}][(\boldsymbol{M}_{\mathcal{T}_2}^{\text{opt}})_{i_{\mathcal{V}_2}}]}{(\boldsymbol{\mu}_\sigma)_{i_\sigma}}$$

Further, letting $[(\boldsymbol{K}_k)_{i_{\mathcal{V}_k}}] := \prod_{(\sigma_1,\sigma_2)\in\mathcal{E}_k} \exp(-[(C_{\sigma_1,\sigma_2})_{i_{\sigma_1},i_{\sigma_2}}]/\eta)$,

$$\mathrm{D}_{\mathrm{KL}}(\boldsymbol{M}_{\mathcal{T}}^{\text{opt}} \,\|\, \boldsymbol{K}) = \sum_{k=1,2} \mathrm{D}_{\mathrm{KL}}(\boldsymbol{M}_{\mathcal{T}_k}^{\text{opt}} \,\|\, \boldsymbol{K}_k) + H(\boldsymbol{\mu}_\sigma)$$

Tree Splitting (cont.)

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$$\because \quad \boldsymbol{M}_{\mathcal{T}}^{\mathrm{opt}} := \operatorname*{arg\,min}_{\boldsymbol{M}\in\Pi(\mathcal{V})} \eta\, \mathrm{D_{KL}}\left(\boldsymbol{M} \,\|\, \boldsymbol{K}\right) = \operatorname*{arg\,min}_{\substack{\mathrm{proj}_{\mathcal{V}_1}(\boldsymbol{M})\in\Pi(\mathcal{V}_1)\\ \mathrm{proj}_{\mathcal{V}_2}(\boldsymbol{M})\in\Pi(\mathcal{V}_2)}} \eta \begin{pmatrix} \mathrm{D_{KL}}(\mathrm{proj}_{\mathcal{V}_1}(\boldsymbol{M}) \,\|\, \boldsymbol{K}_1) \\ + \mathrm{D_{KL}}(\mathrm{proj}_{\mathcal{V}_2}(\boldsymbol{M}) \,\|\, \boldsymbol{K}_2) + H(\boldsymbol{\mu}_\sigma) \end{pmatrix}$$

Tree Decomposition

Corollary 1

For a tree $\mathcal{T} = (\mathcal{V}, \mathcal{E})$ as before,

$$[(\boldsymbol{M}_{\mathcal{T}}^{\mathrm{opt}})_{i_1,\ldots,i_s}] = \frac{\prod_{(\sigma_1,\sigma_2)\in\mathcal{E}}[(M_{\sigma_1\sigma_2}^{\mathrm{opt}})_{i_{\sigma_1},i_{\sigma_2}}]}{\prod_{\sigma\in[\![s]\!]}(\boldsymbol{\mu}_\sigma)_{i_\sigma}^{\deg(\boldsymbol{\mu}_\sigma)-1}}$$

Further, letting $\mathrm{SB}_\eta\left(\boldsymbol{\mu}_{\sigma_1}, \boldsymbol{\mu}_{\sigma_2}\right) := \mathrm{D_{KL}}\left(M_{\sigma_1\sigma_2}^{\mathrm{opt}} \,\|\, K_{\sigma_1\sigma_2}\right)$,

$$\mathrm{D_{KL}}\left(\boldsymbol{M}_{\mathcal{T}}^{\mathrm{opt}} \,\|\, \boldsymbol{K}\right) = \sum_{(\sigma_1,\sigma_2)\in\mathcal{E}} \mathrm{SB}_\eta\left(\boldsymbol{\mu}_{\sigma_1}, \boldsymbol{\mu}_{\sigma_2}\right) + \sum_{\sigma\in[\![s]\!]} (\deg(\boldsymbol{\mu}_\sigma) - 1) H(\boldsymbol{\mu}_\sigma).$$

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Pairwise (bimarginal) cost, *additive* Degree dependent, *nonadditive*

Tree Composition – Construction of MSTs

Define $g_{\sigma_1\sigma_2} := \mathrm{SB}_\eta\left(\boldsymbol{\mu}_{\sigma_1}, \boldsymbol{\mu}_{\sigma_2}\right) + H(\boldsymbol{\mu}_{\sigma_1}) + H(\boldsymbol{\mu}_{\sigma_2})$

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$$= \sum_{(\sigma_1,\sigma_2)\in\mathcal{E}} g_{\sigma_1\sigma_2} - \sum_{\sigma\in[\![s]\!]} H(\boldsymbol{\mu}_\sigma)$$

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Structure independent, constant

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Theorem 1

$$\therefore \quad \boxed{\mathcal{G}^{\mathrm{opt}} \underset{\text{(Proposition 1)}}{=} \mathcal{T}^{\mathrm{opt}} \underset{\text{(Corollary 1)}}{=} \operatorname*{arg\,min}_{\mathcal{E}\subset\mathcal{V}\times\mathcal{V}} \sum_{(\sigma_1,\sigma_2)\in\mathcal{E}} g_{\sigma_1\sigma_2}.}$$

Optimal MSB as an MST

Algorithm 1 Optimal MSB as an MST Problem

Require: Distribution set $\mathcal{V} \leftarrow \{\boldsymbol{\mu}_\sigma\}_{\sigma \in [\![s]\!]}$, edge set $\mathcal{E}$ of the complete graph over s vertices, ground cost function c, entropic regularization parameter $\eta > 0$, bimarginal Sinkhorn algorithm `AlgSINK`, MST algorithm `AlgMST`.

for $(\sigma_1, \sigma_2) \in \mathcal{E}$ **do**

$C_{\sigma_1\sigma_2} \leftarrow c(\boldsymbol{x}_{\sigma_1}, \boldsymbol{x}_{\sigma_2})\ \forall(\boldsymbol{x}_{\sigma_1}, \boldsymbol{x}_{\sigma_2}) \in \mathcal{X}_{\sigma_1} \times \mathcal{X}_{\sigma_2}$

$\mathrm{SB}_\eta(\boldsymbol{\mu}_{\sigma_1}, \boldsymbol{\mu}_{\sigma_2}) \leftarrow \mathtt{AlgSINK}(C_{\sigma_1\sigma_2}, \eta, \boldsymbol{\mu}_{\sigma_1}, \boldsymbol{\mu}_{\sigma_2})$

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end for

$\mathcal{T}^{\mathrm{opt}} \leftarrow \mathtt{AlgMST}(\mathcal{V}, \mathcal{E}, \{g_{\sigma_1\sigma_2}\}_{(\sigma_1,\sigma_2)\in\mathcal{V}\times\mathcal{V}})$

- Guaranteed to converge
- Parallelizable

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end for

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- Guaranteed to converge
- Parallelizable

<u>Complexity</u>

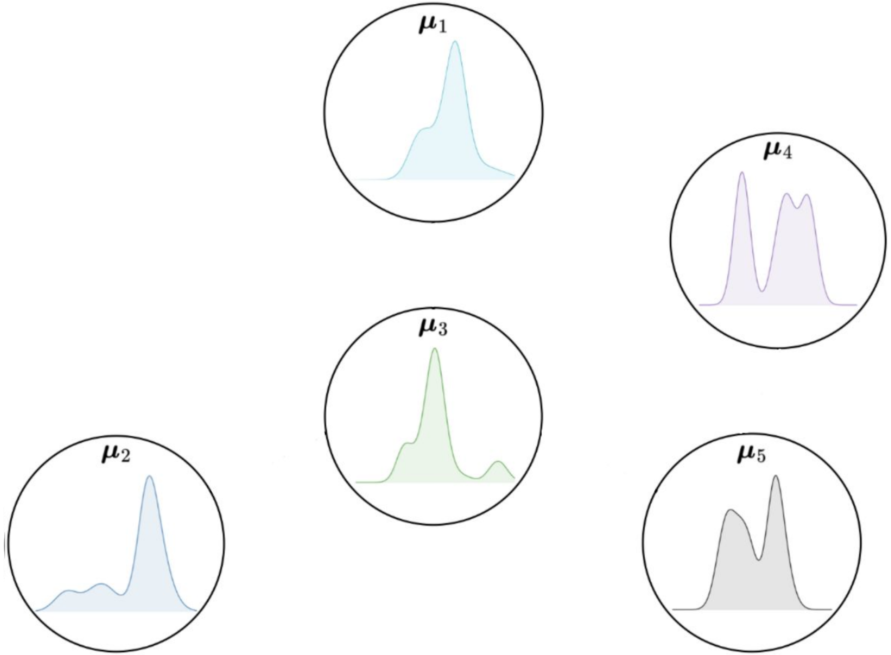
`AlgSINK` $\mathcal{O}\left(n^2\|\boldsymbol{C}\|_\infty^2 \log n/\varepsilon^2\right)$

`AlgMST` $\mathcal{O}\left(s^2\right)$

$$\Downarrow$$

Algorithm 1 $\mathcal{O}\left(s^2 n^2 \|\boldsymbol{C}\|_\infty^2 (\log n)^{-1}/\eta^2\right)$

Experiment 1 – GMM Vertices



- $n = 25$ samples, $s = 5$
- $s^{s-2} = 125$ possible trees

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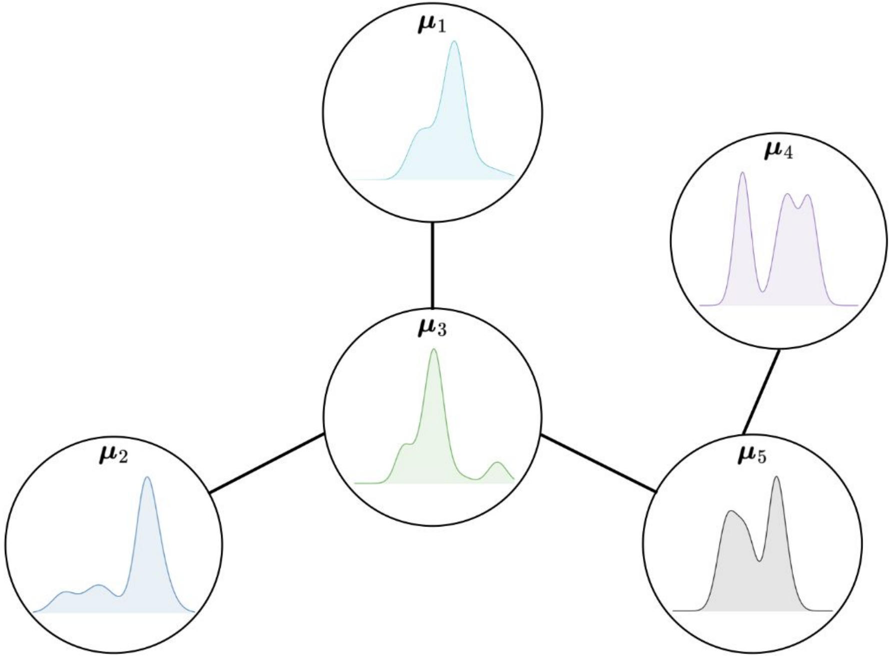

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	Global cost	Pairwise cost
Prüfer code for $\mathcal{T}$	Cost (11)	Cost (21)
3 3 5	0.279922072756287	0.279921946258293
3 3 4	0.295777099784325	0.295776598462776
3 3 3	0.316798945466359	0.316798407793688
5 3 5	0.317890033393032	0.317889978780085
3 5 5	0.319564634628009	0.319562860510066
4 3 5	0.320487973256691	0.320487070929787
3 2 5	0.325540126207581	0.325538361972965
5 3 4	0.333745066643530	0.333744630984569
3 5 4	0.335419414386392	0.335417512714549
4 3 4	0.336342669176185	0.336341723134270

~3s *per tree*

Solved in ~0.226s

Experiment 2 – Porcupines

https://www.youtube.com/watch?v=cCjegaOq2hQ

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$s = 5$

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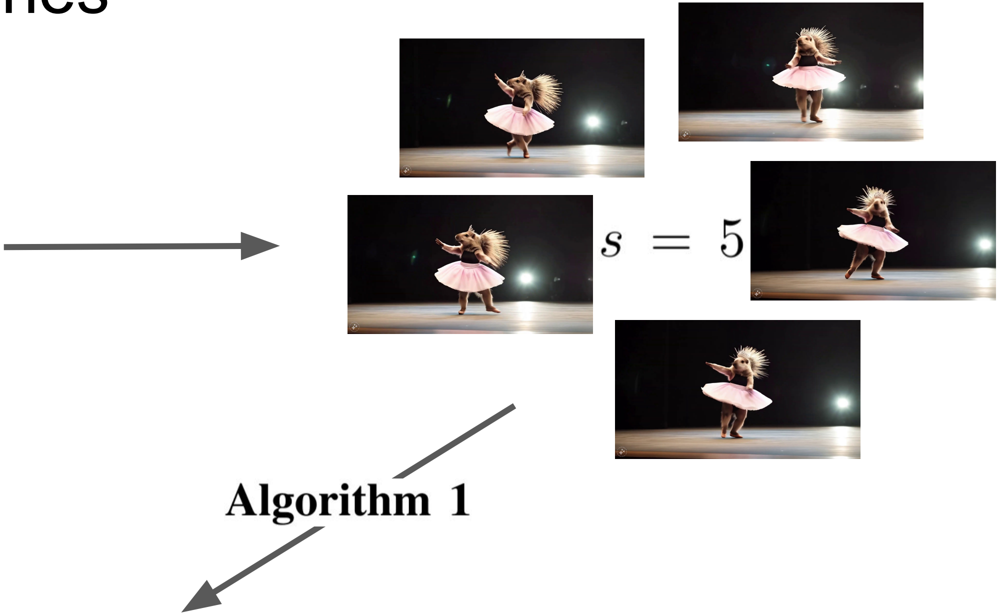
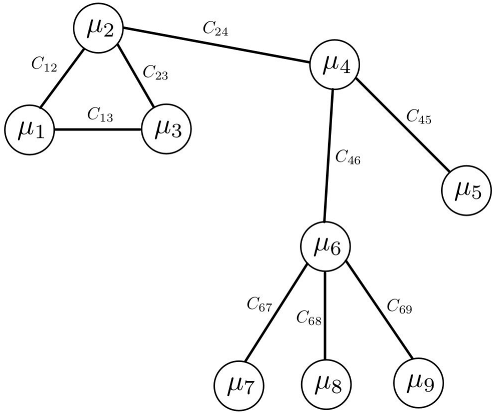


Summary



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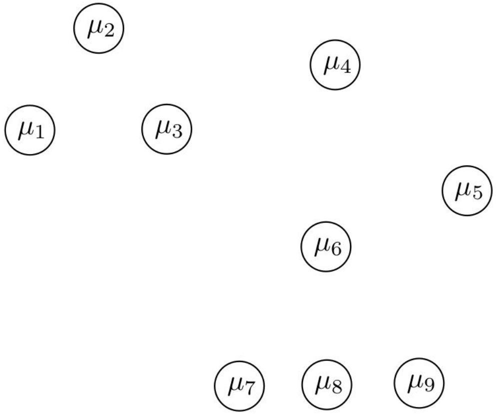
Summary



optimal
MSBP

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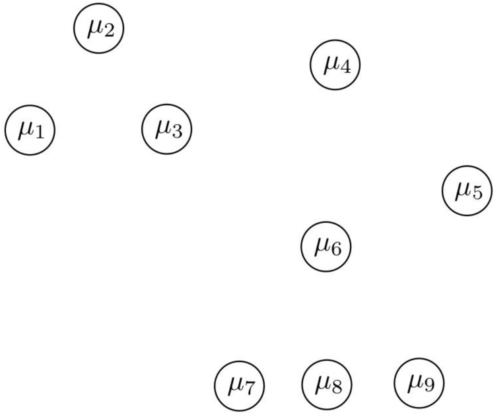
$$\boldsymbol{M}_{\mathcal{T}}^{\mathrm{opt}} := \underset{\boldsymbol{M}\in\Pi(\mathcal{V})}{\arg\min}\ \eta\,\mathrm{D}_{\mathrm{KL}}\left(\boldsymbol{M}\,\|\,\boldsymbol{K}\right)$$

Summary



optimal MSBP

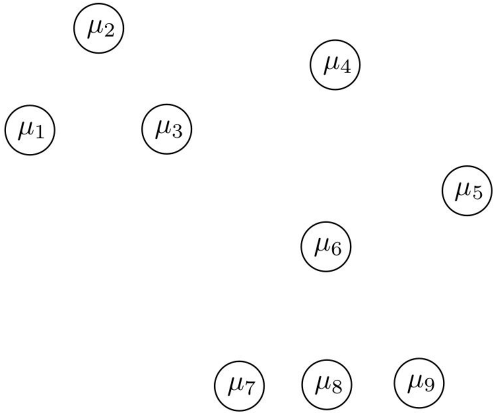
$$\mathcal{G}^{\mathrm{opt}} = \underset{\substack{\mathcal{G} \text{ undirected connected} \\ \text{over vertices } \mathcal{V}}}{\arg\min} \; \min_{\boldsymbol{M} \in \Pi(\mathcal{V})} \eta \, \mathrm{D_{KL}}\left(\boldsymbol{M} \,\|\, \boldsymbol{K}\right)$$

(Proposition 1)

$$\mathcal{G}^{\mathrm{opt}} = \mathcal{T}^{\mathrm{opt}}$$

$$\boldsymbol{M}_{\mathcal{T}}^{\mathrm{opt}} := \underset{\boldsymbol{M} \in \Pi(\mathcal{V})}{\arg\min} \; \eta \, \mathrm{D_{KL}}\left(\boldsymbol{M} \,\|\, \boldsymbol{K}\right)$$

Summary



optimal MSBP

$$\mathcal{G}^{\mathrm{opt}} = \underset{\substack{\mathcal{G} \text{ undirected connected} \\ \text{over vertices } \mathcal{V}}}{\arg\min} \; \min_{\boldsymbol{M} \in \Pi(\mathcal{V})} \; \eta \, \mathrm{D}_{\mathrm{KL}} \left(\boldsymbol{M} \parallel \boldsymbol{K} \right)$$

(Proposition 1)

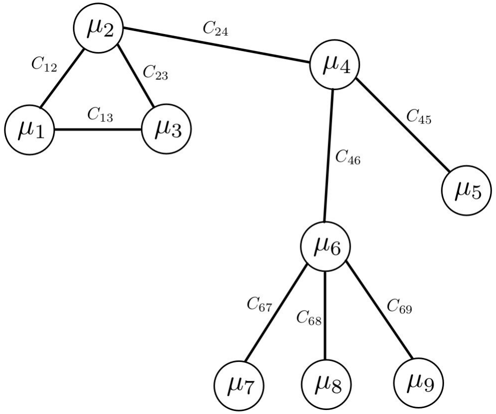
$$\mathcal{G}^{\mathrm{opt}} = \mathcal{T}^{\mathrm{opt}}$$

(Corollary 1)

$$\mathcal{T}^{\mathrm{opt}} = \underset{\mathcal{E} \subset \mathcal{V} \times \mathcal{V}}{\arg\min} \sum_{(\sigma_1, \sigma_2) \in \mathcal{E}} g_{\sigma_1 \sigma_2}$$

$$\boldsymbol{M}_{\mathcal{T}}^{\mathrm{opt}} := \underset{\boldsymbol{M} \in \Pi(\mathcal{V})}{\arg\min} \; \eta \, \mathrm{D}_{\mathrm{KL}} \left(\boldsymbol{M} \parallel \boldsymbol{K} \right)$$

Summary



optimal MSBP

$$\mathcal{G}^{\text{opt}} = \underset{\substack{\mathcal{G}\text{ undirected connected}\\ \text{over vertices }\mathcal{V}}}{\arg\min} \ \min_{\boldsymbol{M}\in\Pi(\mathcal{V})} \eta\, \mathrm{D}_{\mathrm{KL}}\left(\boldsymbol{M} \,\|\, \boldsymbol{K}\right)$$

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Algorithm 1

$$[(\boldsymbol{M}^{\text{opt}}_{\mathcal{T}})_{i_1,\ldots,i_s}] = \frac{\prod_{(\sigma_1,\sigma_2)\in\mathcal{E}}[(M^{\text{opt}}_{\sigma_1\sigma_2})_{i_{\sigma_1},i_{\sigma_2}}]}{\prod_{\sigma\in[\![s]\!]}(\boldsymbol{\mu}_\sigma)_{i_\sigma}^{\deg(\boldsymbol{\mu}_\sigma)-1}}$$

Questions?

Bondar, Georgiy A., and Abhishek Halder. "Optimal Multimarginal Schrödinger Bridge: Minimum Spanning Tree Over Measure-Valued Vertices." *IEEE Control Systems Letters* 9 (2025): 2555-2560.