Tensor Optimization Problems in Optimal Transport

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Advancement to Ph.D. Candidacy in Applied Mathematics

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January 24, 2025

Transport of a Probability Measure

Random variable $X \sim \mu$ *known*

$$\Big\downarrow \quad \textit{Given} \text{ differentiable } \tau(\,\cdot\,)$$

Random variable $Y = \tau(X) \sim\ ?$

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Notation: $\nu = \tau_{\#}\mu$, read as: ν is the pushforward of μ under *transport map* τ

Computation: $\mu(\mathrm{d}x) = f(x)\,\mathrm{d}x, \quad \nu(\mathrm{d}y) = \tau_{\#}\mu = \dfrac{f\left(\tau^{-1}(y)\right)}{|\,\nabla\tau\left(\tau^{-1}(y)\right)\,|}\,\mathrm{d}y$

Example: 1D Transport of a Probability Measure

Measure Density

$$\mu(\mathrm{d}x) = f(x)\,\mathrm{d}x, x \in \mathcal{X}$$

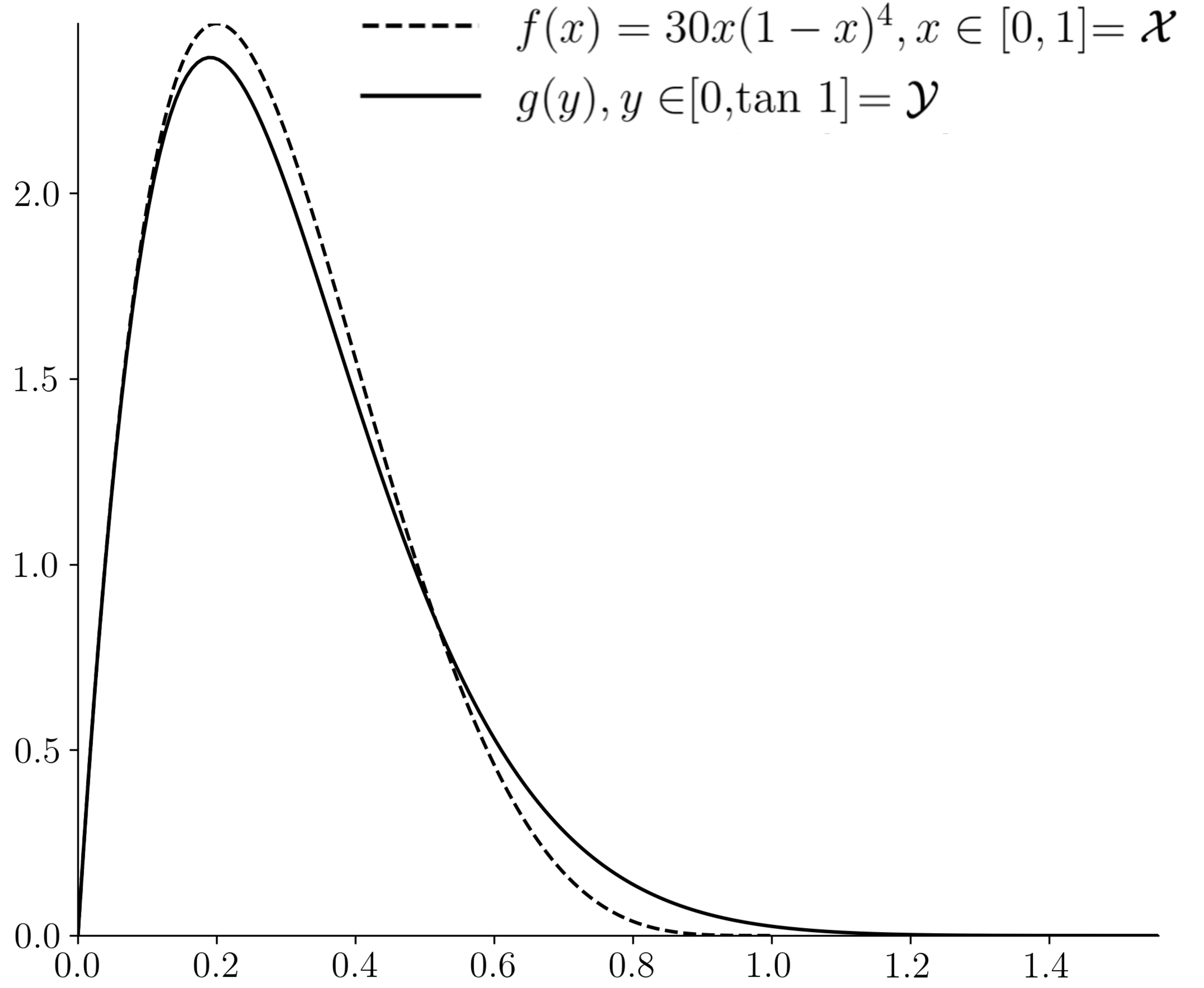
$$\Big\downarrow \; \tau(\cdot) = \tan(\cdot)$$

$$\nu(\mathrm{d}y) = g(y)\,\mathrm{d}y, y \in \mathcal{Y}$$

$$= \frac{f(\arctan y)}{1 + y^2}\,\mathrm{d}y$$

In general, $\mu\left(\tau^{-1}(\mathcal{U})\right) = \nu(\mathcal{U})$

$\forall$ Borel $\mathcal{U} \subseteq \mathcal{Y}$



What is Optimal Transport (OT)?

Given μ, τ, the new measure ν is unique: *nothing to optimize*

Inverse problem: Given μ, ν, the map τ is *underdetermined*

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OT map

$$\tau_{\text{opt}} = \arg\inf_{\tau:\mathcal{X}\to\mathcal{Y}} \int_{\mathcal{X}} c(x, \tau(x))d\mu(x)$$
$$\text{subject to} \quad \tau_{\#}\mu = \nu$$

Ground cost = cost of transporting unit amount of mass from x to $\tau(x)$

Monge formulation, 1781

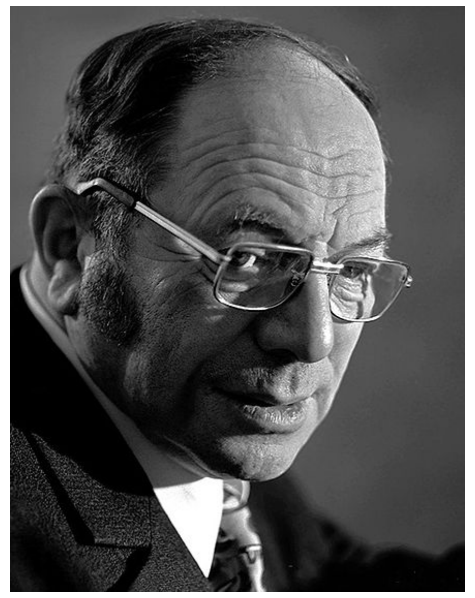
Example: $c(x, y) = \|x - y\|_2^2$, squared minimal geodesic length, etc.

Very Brief History

Gaspard Monge: OT map formulation in 1781 with $c(x, y) = \|x - y\|_1$

Erwin Schrödinger: attempts stochastic interpretation of quantum mechanics in 1931-32

Now called the Schrödinger Bridge (SB): diffusive version of OT



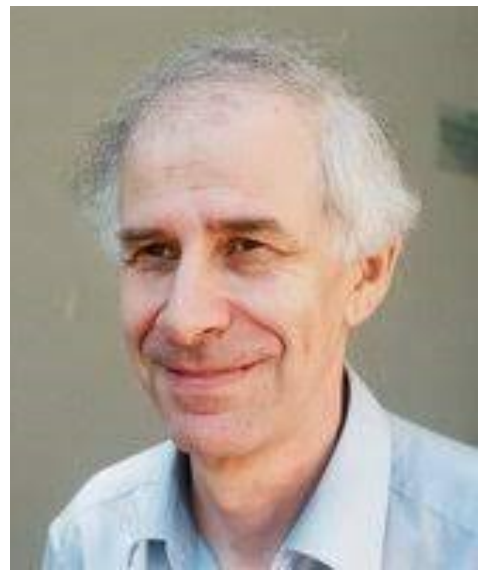
Leonid Kantorovich: OT plan reformulation in 1941

Wins 1975 Nobel prize in Economics for this work

Math for OT takes shape in late 20th - early 21st century

C. Villani

A. Figalli



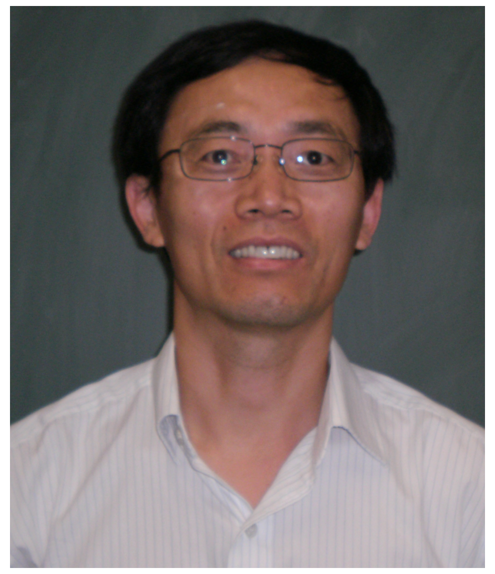
Y. Brenier

J-D. Benamou

R.J. McCann

X-N. Ma

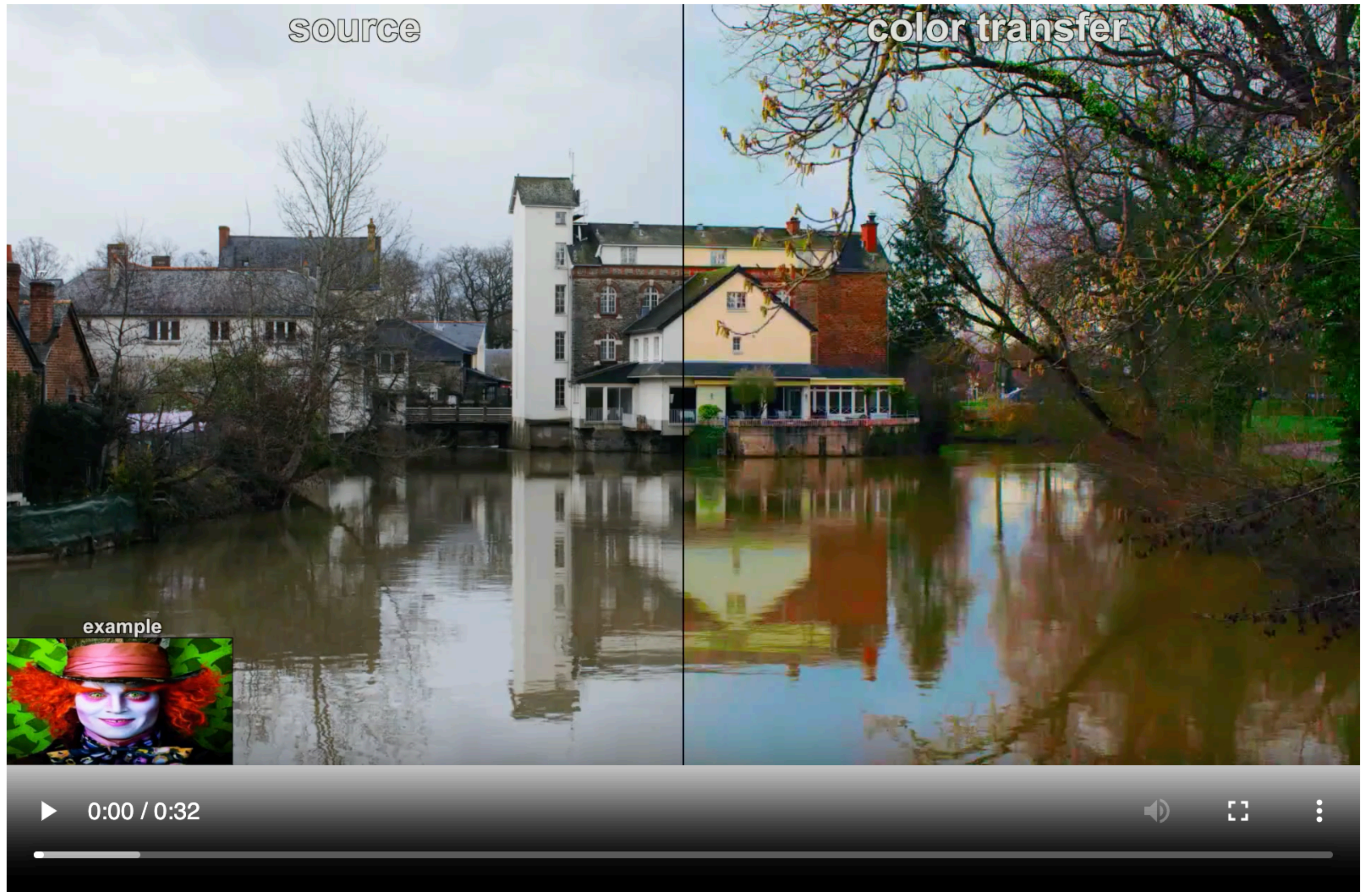
N. Trudinger



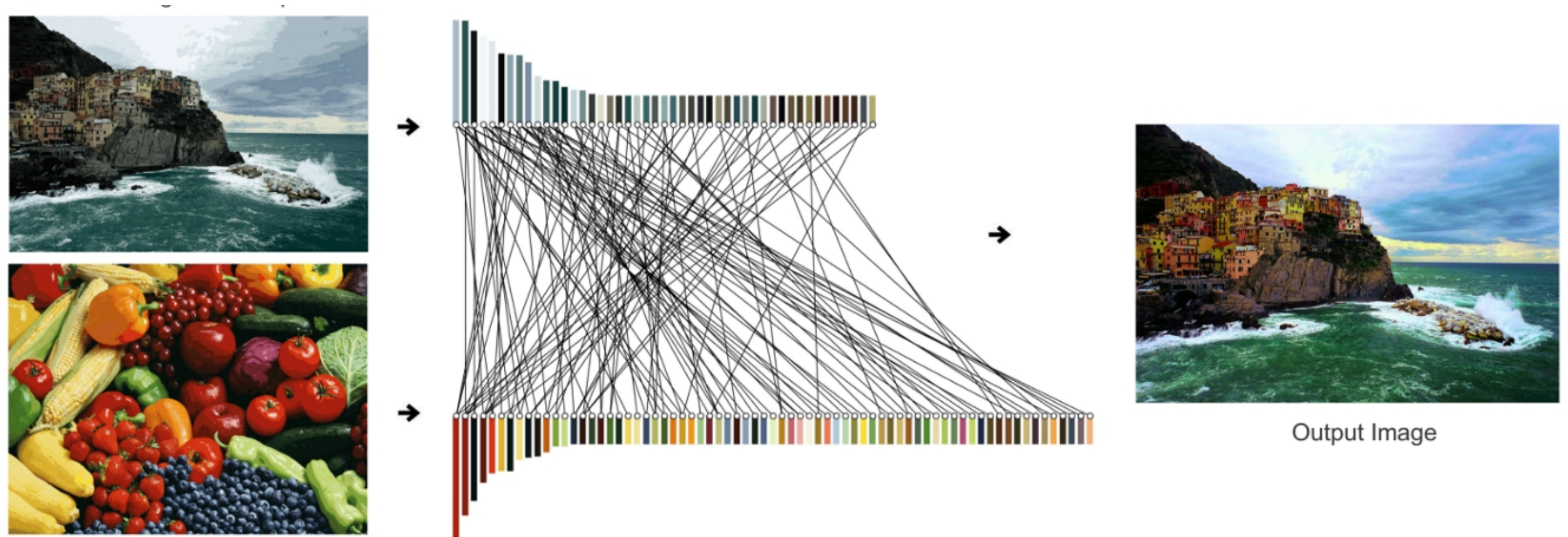
X-J. Wang

AI/ML Applications

OT of color



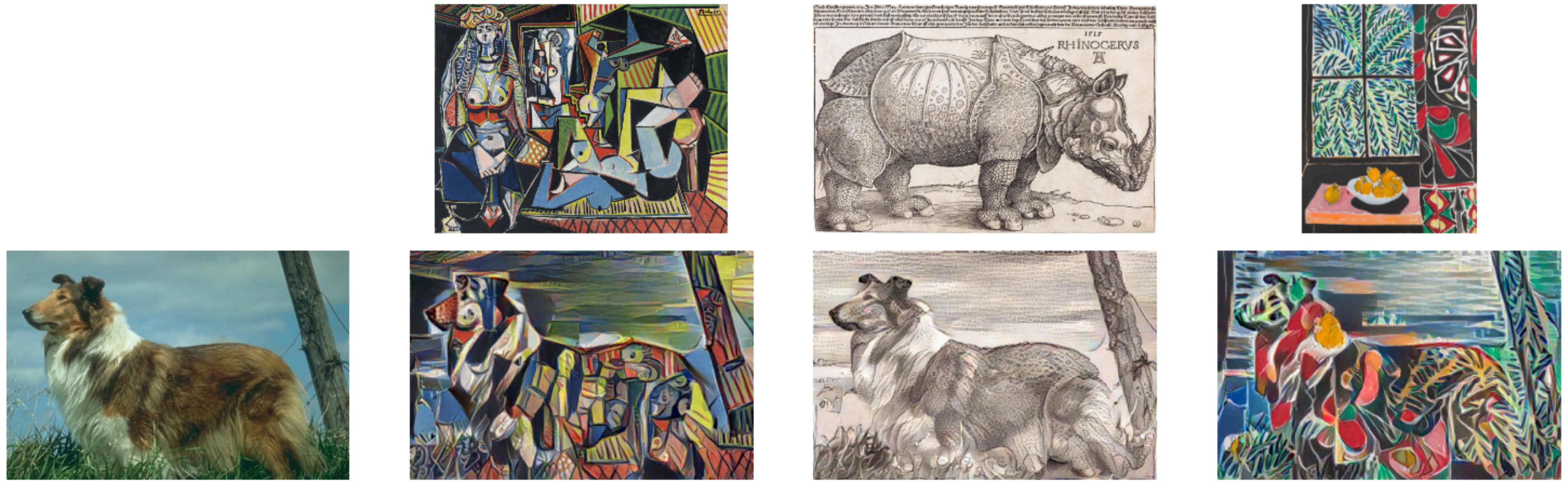
Credit: https://oriel.github.io/color_transfer.html



OT of style

Picasso ν_1 | Dürer ν_2 | Matisse ν_3

μ



Credit: Kolkin, Salavon, Shakhnarovich, CVPR 2019

SB in diffusion model generative AI

Stable diffusion, DALL-E

Credit: https://github.com/Stability-AI/generative-models

Science Applications of SB

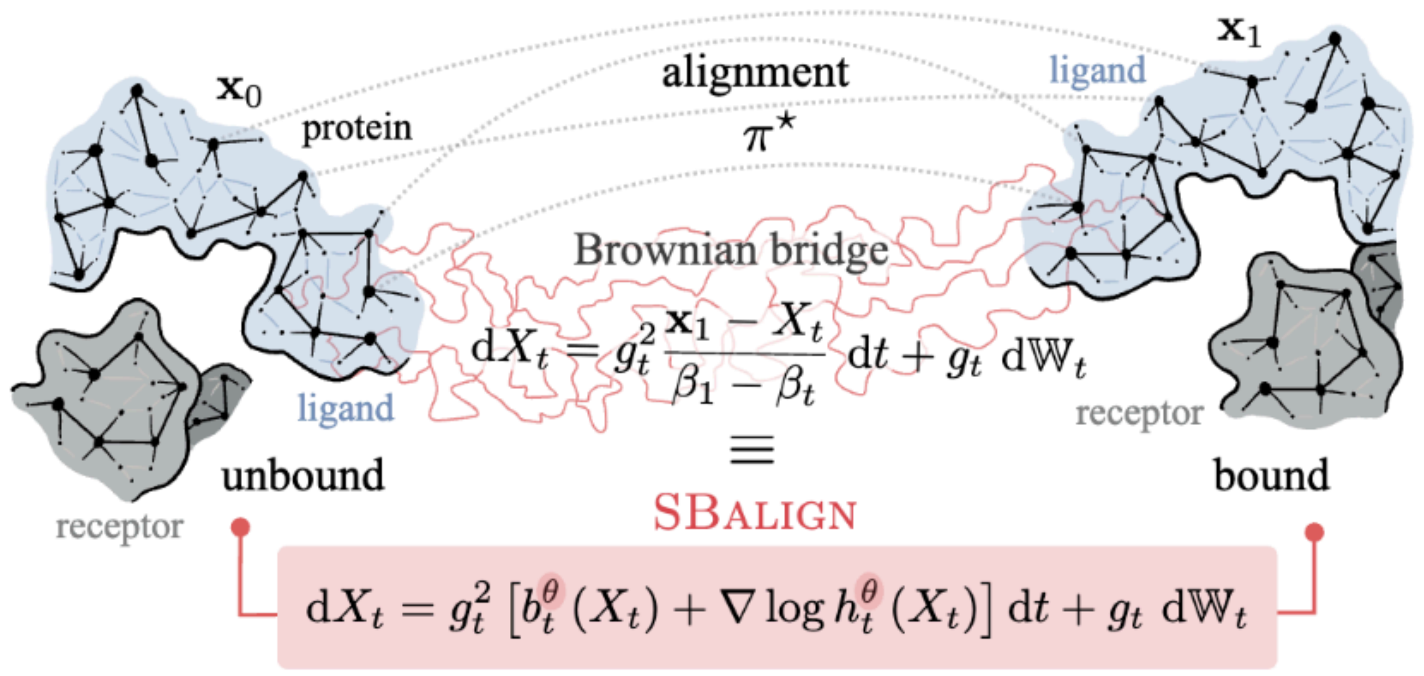
Protein synthesis

UAI 2023

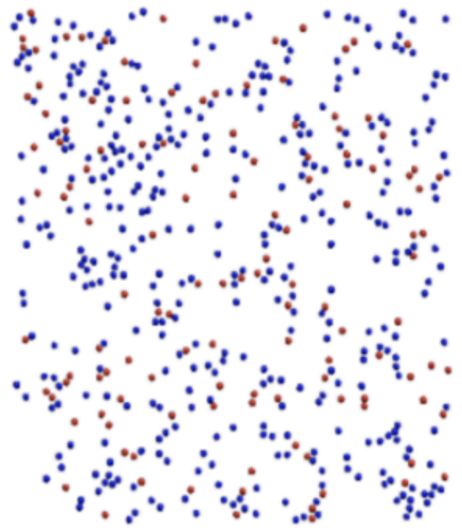
Aligned Diffusion Schrödinger Bridges

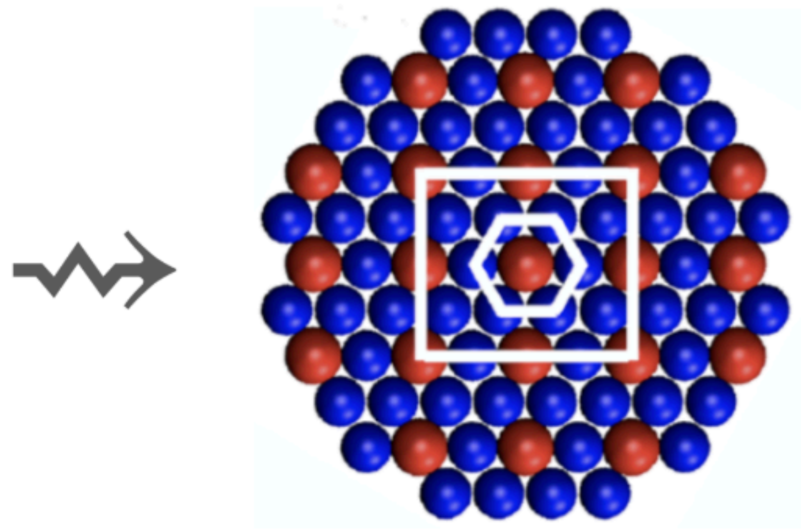
Vignesh Ram Somnath[*1,2] **Matteo Pariset**[*1,3] **Ya-Ping Hsieh**[1]
Maria Rodriguez Martinez[2] **Andreas Krause**[1] **Charlotte Bunne**[1]

[1]Department of Computer Science, ETH Zürich
[2]IBM Research Zürich
[3]Department of Computer Science, EPFL



Material synthesis





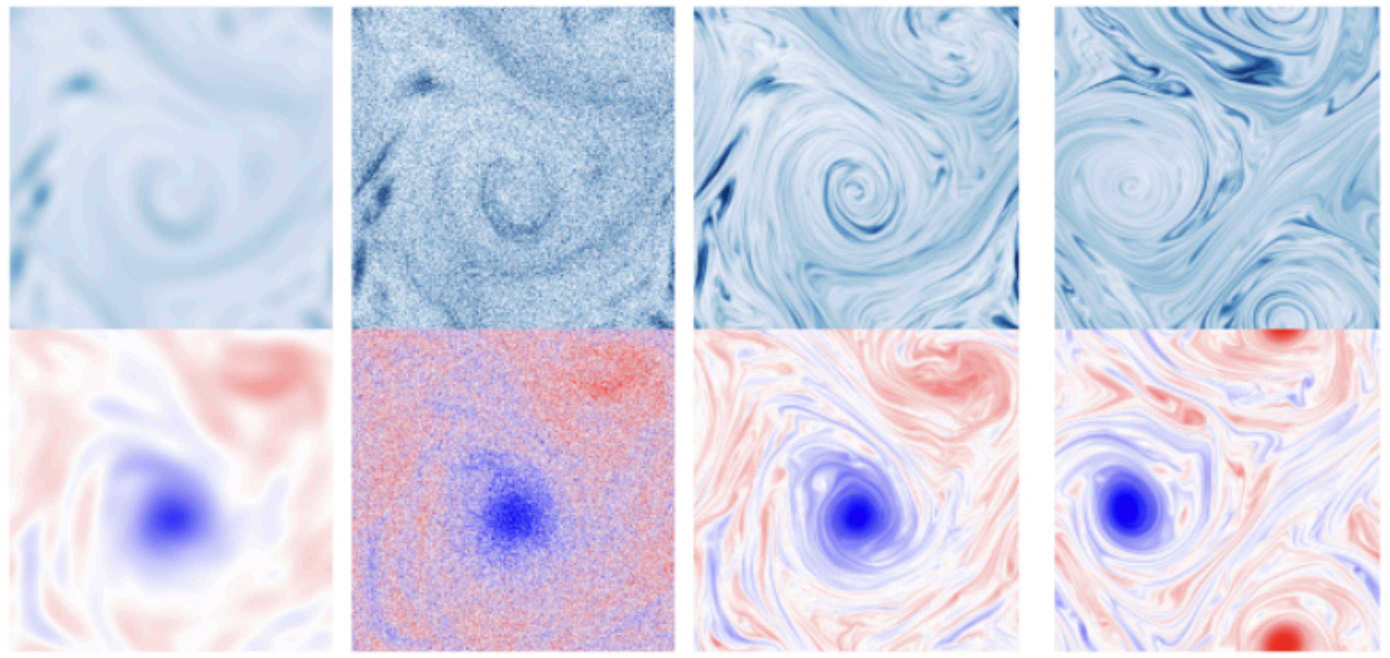
Dispersed particles **Ordered structure**

Superresolution

NeurIPS 2024

Diffusion Schrödinger Bridge Matching

Yuyang Shi* University of Oxford
Valentin De Bortoli* ENS ULM
Andrew Campbell University of Oxford
Arnaud Doucet University of Oxford



Low res **High res**

2024 Hugo Schuck Award by American Automatic Control Council

Outline of This Talk

Mathematical Background

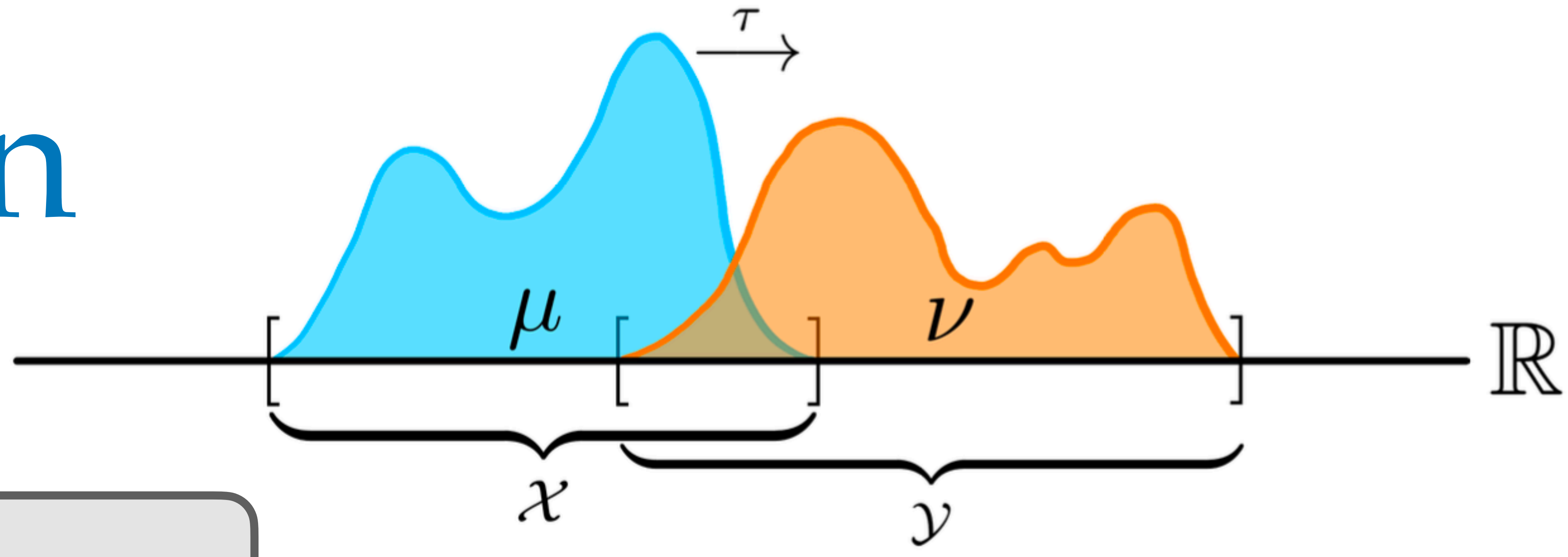
Tensor Optimization for OT Regularity

First computational method for OT regularity

Tensor Optimization for Graph-structured Multimarginal SB

Application in learning computational resource usage

Background: OT Formulation



OT map

$$\tau_{\text{opt}} = \underset{\tau:\mathcal{X}\to\mathcal{Y}}{\arg\inf} \int_{\mathcal{X}} c(x, \tau(x))\,d\mu(x)$$

$$\text{subject to} \quad \tau_{\#}\mu = \nu$$

Ground cost

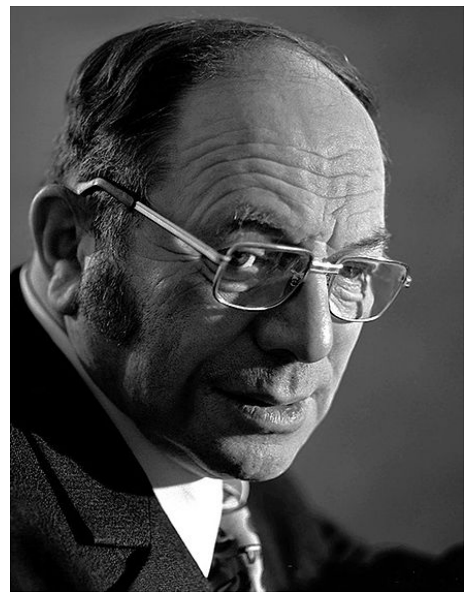
OT plan

$$\pi_{\text{opt}} = \underset{\pi\in\Pi(\mu,\nu)}{\arg\inf} \int_{\mathcal{X}\times\mathcal{Y}} c(x, y)\,d\pi(x, y)$$

The inf value is called the squared Wasserstein distance

Monge formulation, 1781

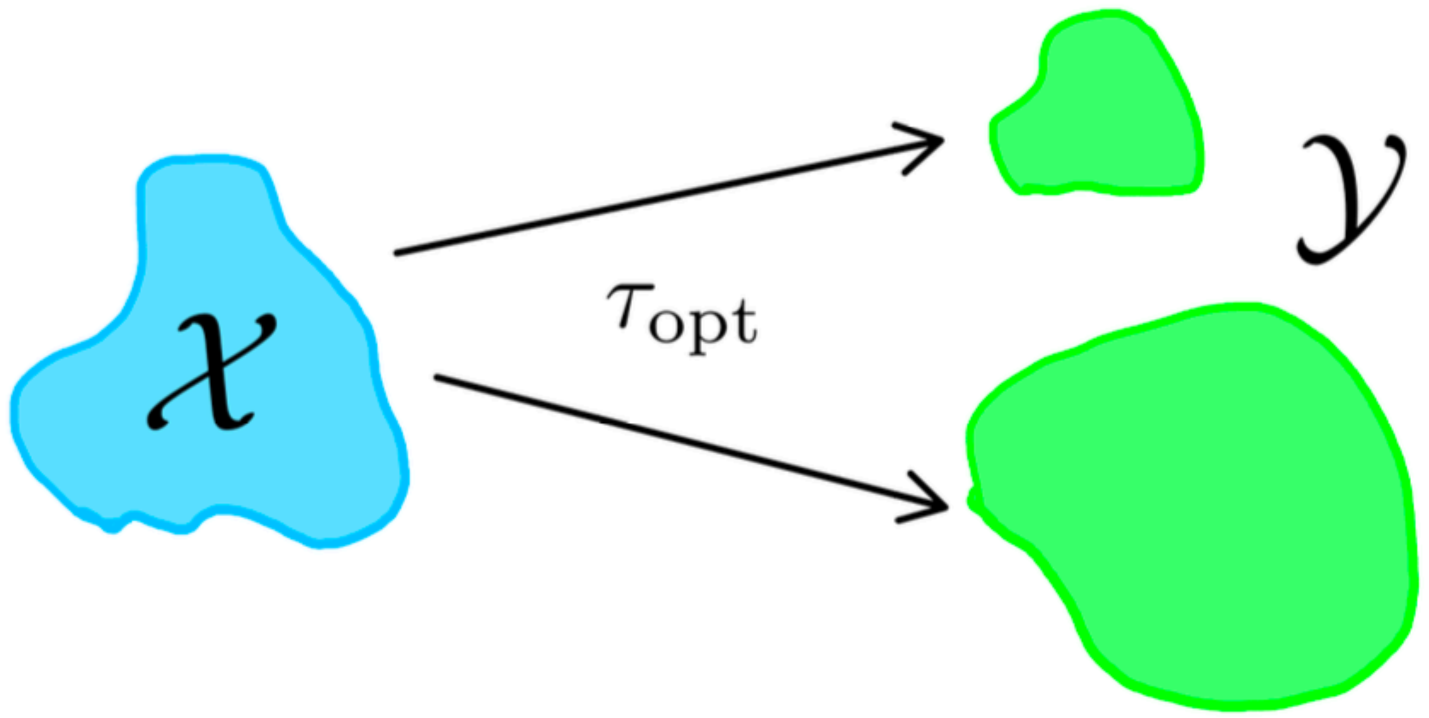
Nonlinear nonconvex program



Kantorovich formulation, 1941

Linear program

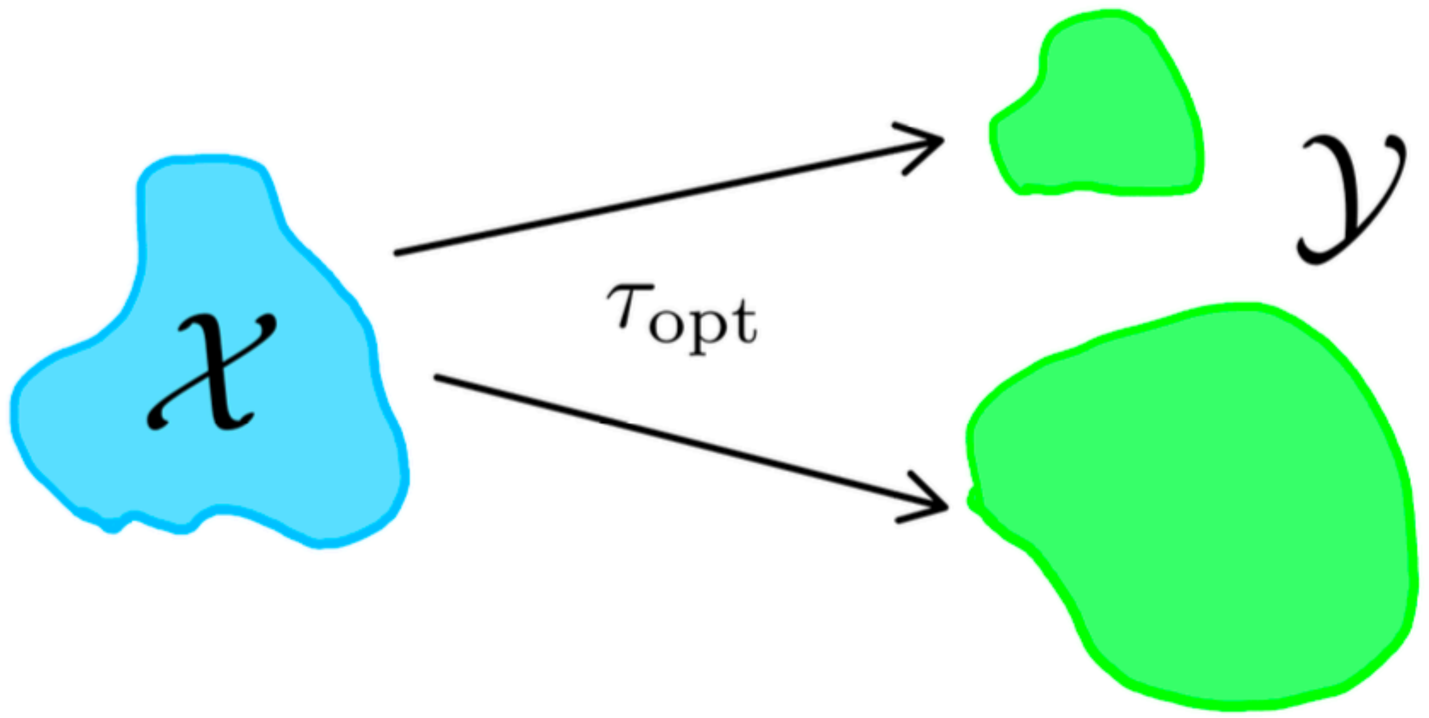
Background: OT Regularity



Question: is τ_{opt} continuous?

Answer: Yes if μ, ν abs. continuous + extra condition on c and manifold

Background: OT Regularity



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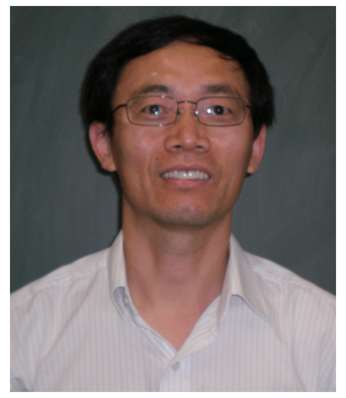
X-N. Ma


N. Trudinger


X-J. Wang

Defn: Ma-Trudinger-Wang (MTW) tensor (2005, 2009)

$$\mathfrak{S}_{(x,y)}(\xi,\eta) := \sum_{i,j,k,l,p,q,r,s} (c_{ij,p}c^{p,q}c_{q,rs} - c_{ij,rs})c^{r,k}c^{s,l}\xi_i\xi_j\eta_k\eta_l$$

$$\forall\, x \in \mathcal{X}, y \in \mathcal{Y}, \xi \in T_x\mathcal{X}, \eta \in T_y^*\mathcal{Y}$$

$$c_{ij,kl} = \partial_{x_i}\partial_{x_j}\partial_{y_k}\partial_{y_l}c(x,y), \quad c^{i,j}(x,y) = \left[((\nabla_x \otimes \nabla_y)c)^{-1}\right]_{i,j}$$

Background: OT Regularity

Defn: MTW(0) and MTW(κ), $\kappa > 0$

If $\mathfrak{S}_{(\cdot,\cdot)}(\xi, \eta) \geq 0 \; \forall (\xi, \eta)$ s.t. $\eta(\xi) = 0$ then c satisfies MTW(0)

If $\exists k > 0$ s.t. $\mathfrak{S}_{(\cdot,\cdot)}(\xi, \eta) \geq \kappa \|\xi\|^2 \|\eta\|^2$ then c satisfies MTW(κ)

Defn: Nonnegative Cost Curvature (NNCC)

If $\mathfrak{S}_{(\cdot,\cdot)}(\xi, \eta) \geq 0 \; \forall (\xi, \eta)$ then c satisfies NNCC

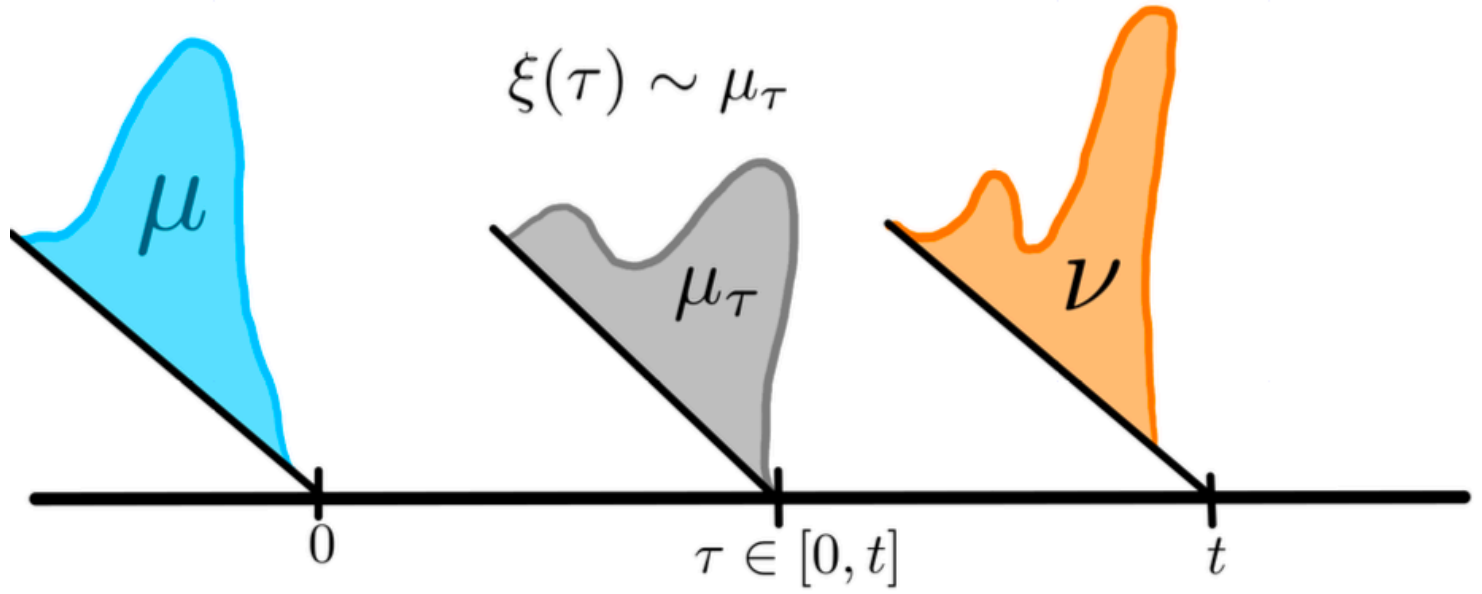
Difficult to verify analytically. **Our approach:** computational certificate

Background: Schrödinger Bridge Problem (SBP)

Static SBP = Kantorovich OT + entropic regularization

$$\pi_{\text{opt}} = \arg\inf_{\pi \in \Pi(\mu,\nu)} \int_{\mathcal{X}\times\mathcal{Y}} (c(x,y) + \varepsilon \log \pi(x,y))d\pi(x,y)$$

Strictly convex program



Continuous SBP = optimization over measure-valued path space

Generates the maximum likelihood trajectory on path space

$$\arg\inf_{M \in \mathcal{P}(\mathcal{X}\times\mathcal{Y})} \int_{\mathcal{X}\times\mathcal{Y}} (c(\boldsymbol{\xi}(0),\boldsymbol{\xi}(t)) + \varepsilon \log M(\boldsymbol{\xi}(0),\boldsymbol{\xi}(t)))M(\boldsymbol{\xi}(0),\boldsymbol{\xi}(t))d\boldsymbol{\xi}(0)d\boldsymbol{\xi}(t)$$

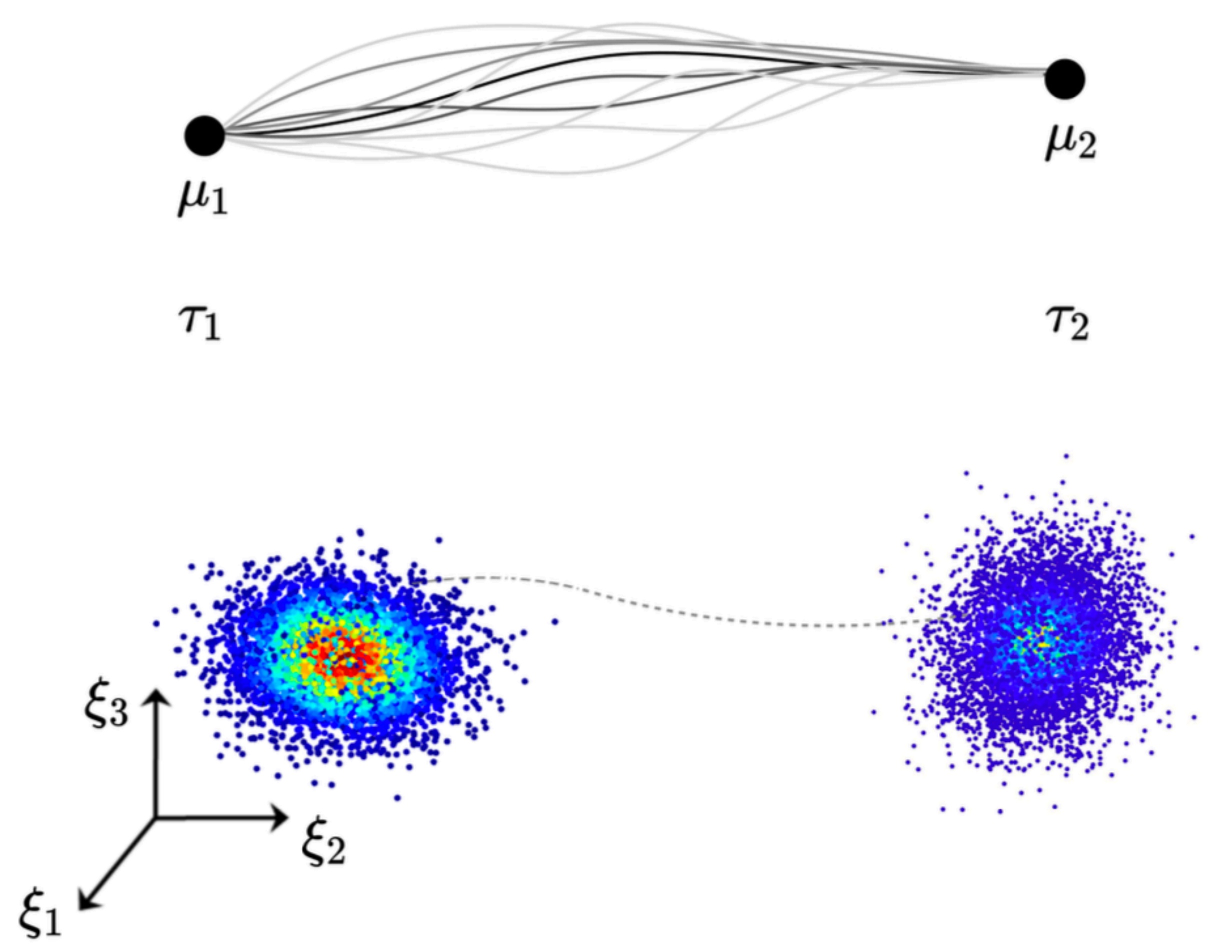
$$\text{subject to} \int_{\mathcal{X}} M(\boldsymbol{\xi}(0),\boldsymbol{\xi}(t))d\boldsymbol{\xi}(0) = \nu, \quad \int_{\mathcal{Y}} M(\boldsymbol{\xi}(0),\boldsymbol{\xi}(t))d\boldsymbol{\xi}(t) = \mu$$

Background: Discrete SBP

Bi-marginal a.k.a. classical SBP

$$
\begin{aligned}
M_{\text{opt}} = \underset{M \in \mathbb{R}^{n\times n}_{\geq 0}}{\arg\min} \quad & \langle \underset{\mathbb{R}^{n\times n}_{\geq 0}}{\underset{\cap}{C}} + \varepsilon \log M, M \rangle \\
\text{subject to} \quad & \text{proj}_{\sigma}(M) = \underset{\Delta^{n-1}}{\underset{\cap}{\boldsymbol{\mu}_{\sigma}}} \; \forall \sigma \in \{1, 2\}
\end{aligned}
$$

Darker distributional path = more likely



Weighted scattered data:

$$
\{\boldsymbol{\xi}^i(\tau_\sigma)\}_{i=1}^n, \; \mu_\sigma = \frac{1}{n} \sum_{i=1}^{n} \delta\left(\boldsymbol{\xi} - \boldsymbol{\xi}^i(\tau_\sigma)\right)
$$

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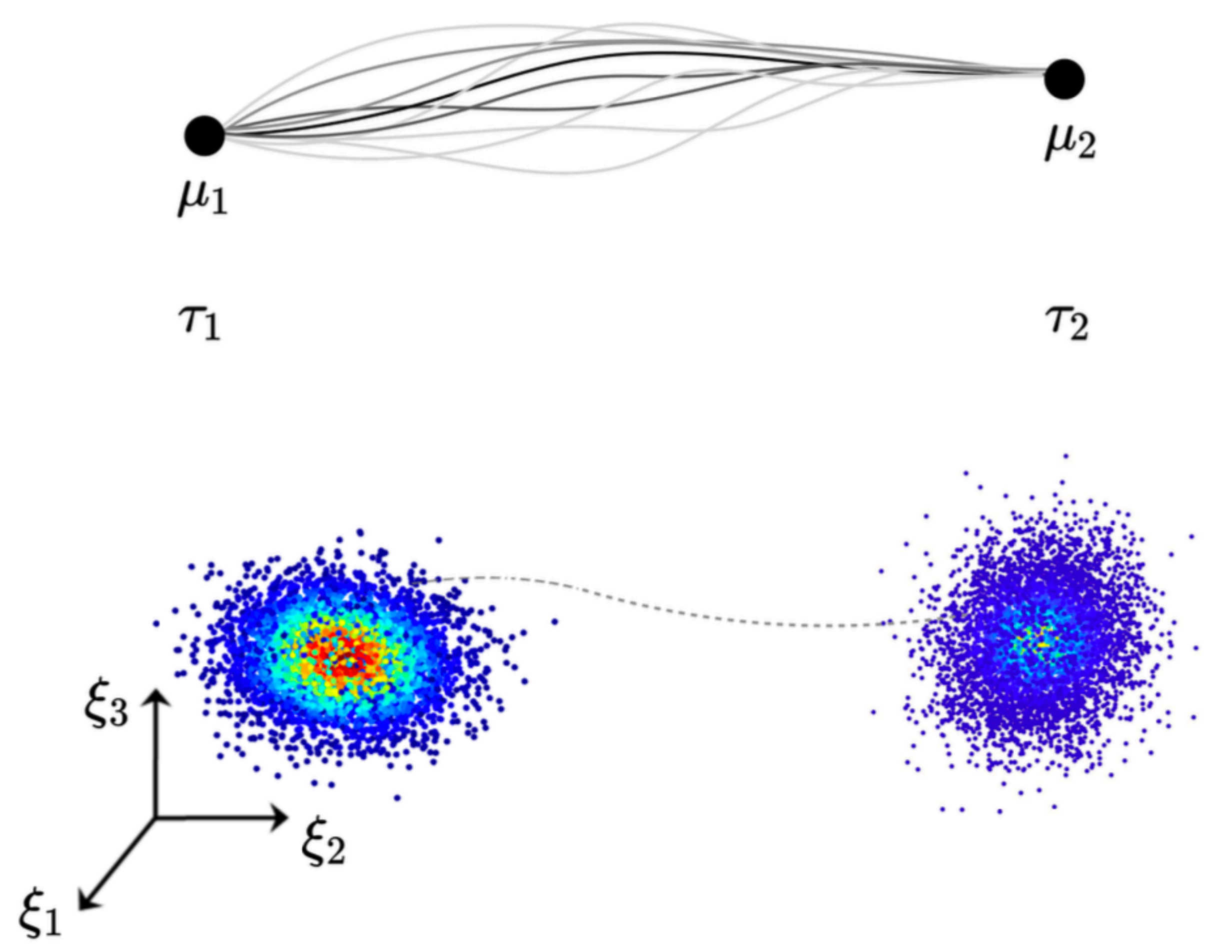

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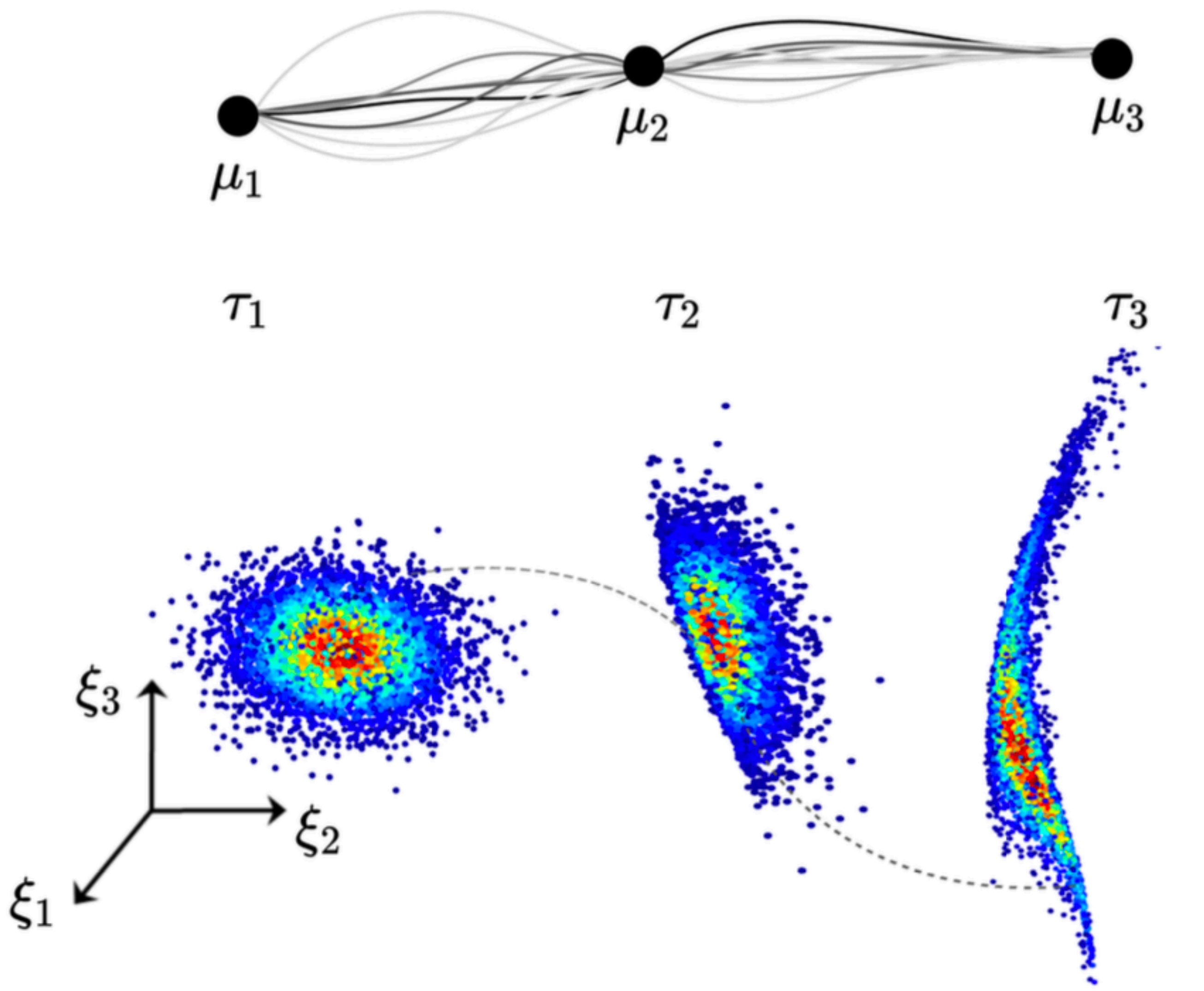
Multimarginal SBP (MSBP)

$$\boldsymbol{M}_{\text{opt}} = \underset{\boldsymbol{M} \in (\mathbb{R}^n)^{\otimes s}_{\geq 0}}{\arg\min} \quad \langle \underset{(\mathbb{R}^n)^{\otimes s}_{\geq 0}}{\underset{\cap}{\boldsymbol{C}}} + \varepsilon \log \boldsymbol{M}, \boldsymbol{M} \rangle$$

$$\text{subject to} \quad \text{proj}_\sigma(\boldsymbol{M}) = \underset{\Delta^{n-1}}{\underset{\cap}{\boldsymbol{\mu}_\sigma}} \quad \forall \sigma \in [\![\underset{\mathbb{N}_{\geq 2}}{\underset{\cap}{s}}]\!]$$



Background: Sinkhorn Iteration to Solve MSBP

Step 1: Let $\boldsymbol{K} := \exp\left(-\boldsymbol{C}/\varepsilon\right) \in \left(\mathbb{R}^n\right)^{\otimes s}_{>0}$, initialize $\boldsymbol{u}_\sigma := \exp\left(\boldsymbol{\lambda}_\sigma/\varepsilon\right) \in \mathbb{R}^n_{>0}$

Step 2: Perform Sinkhorn iterations until (linear) convergence

$$\boldsymbol{u}_\sigma \leftarrow \boldsymbol{u}_\sigma \otimes \boldsymbol{\mu}_\sigma \oslash \operatorname{proj}_\sigma(\boldsymbol{K} \odot \boldsymbol{U}) \quad \forall \boldsymbol{\sigma} \in [\![\boldsymbol{s}]\!]$$

Step 3: $\boldsymbol{M}_{\text{opt}} = \boldsymbol{K} \odot \boldsymbol{U}$ where $\boldsymbol{U} := \otimes_{\sigma=1}^{s} \boldsymbol{u}_\sigma \in \left(\mathbb{R}^n\right)^{\otimes s}_{>0}$

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Trouble: computing $\left[\mathrm{proj}_\sigma\left(\boldsymbol{M}\right)\right]_j = \sum\limits_{i_1,\ldots,i_{\sigma-1},i_{\sigma+1},\ldots,i_s} \boldsymbol{M}_{i_1,\ldots,i_{\sigma-1},j,i_{\sigma+1},\ldots,i_s}$

has $\mathcal{O}(n^s)$ complexity …. more on this later

Tensor Optimization for OT Regularity

Problem Formulation

Assumption A1: MTW tensor is rational in $(x, y) \in \mathcal{X} \times \mathcal{Y}$ semialgebraic

Sufficient but not necessary: c is rational in $(x, y) \in \mathcal{X} \times \mathcal{Y}$ semialgebraic

Problem Formulation

Assumption A1: MTW tensor is rational in $(x, y) \in \mathcal{X} \times \mathcal{Y}$ semialgebraic

Sufficient but not necessary: c is rational in $(x, y) \in \mathcal{X} \times \mathcal{Y}$ semialgebraic

Forward problem:

Given $c, \mathcal{X}, \mathcal{Y}$ as per **A1**, certify / falsify if the ground cost $c : \mathcal{X} \times \mathcal{Y} \mapsto \mathbb{R}_{\geq 0}$ satisfies either MTW(0) or MTW(κ) or NNCC condition

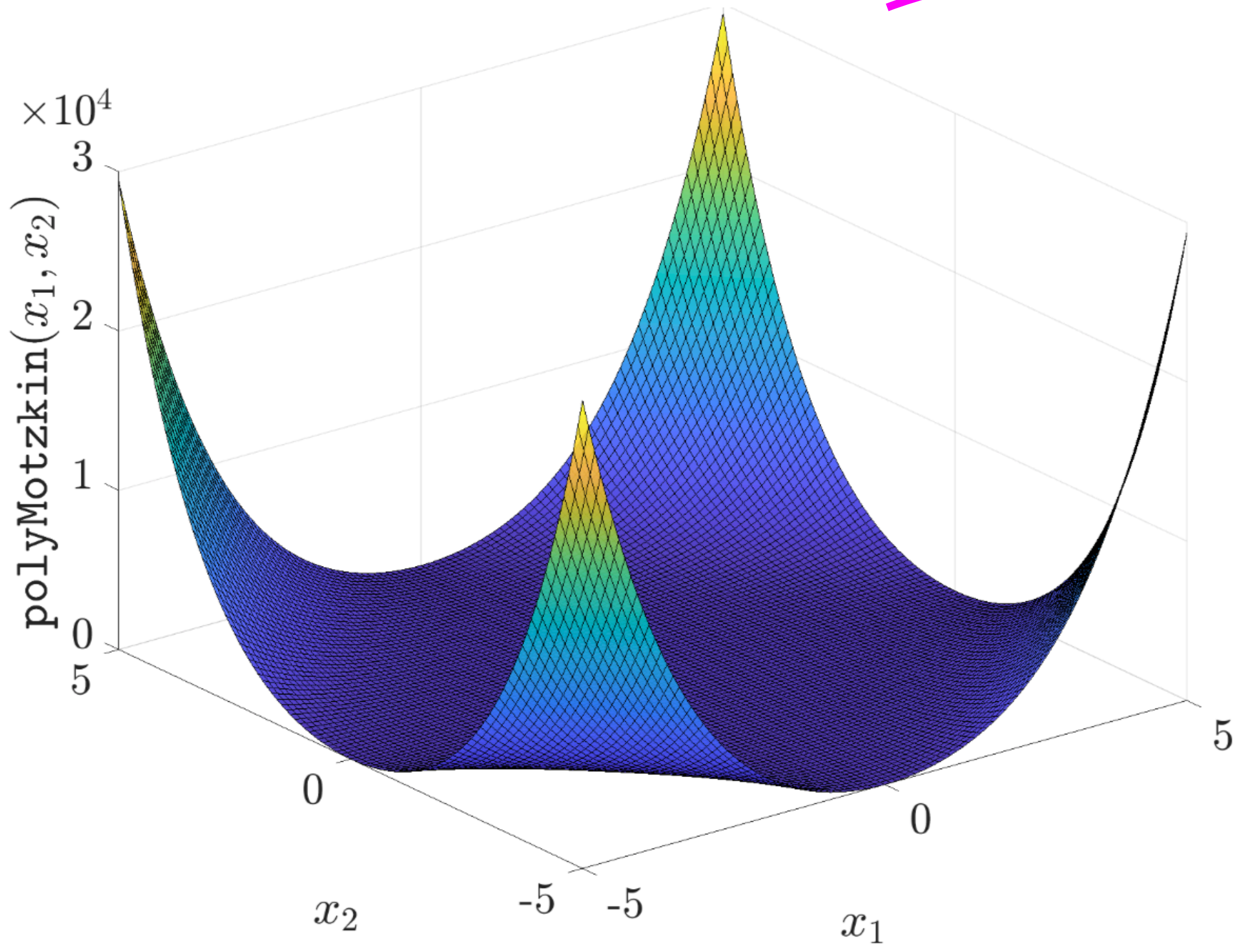
Inverse problem:

Given $c, \mathcal{X}, \mathcal{Y}$ as per **A1**, find semialgebraic $\mathcal{U} \times \mathcal{V} \subseteq \mathcal{X} \times \mathcal{Y}$ such that $c : \mathcal{U} \times \mathcal{V} \mapsto \mathbb{R}_{\geq 0}$ satisfies either MTW(0) or MTW(κ) or NNCC condition

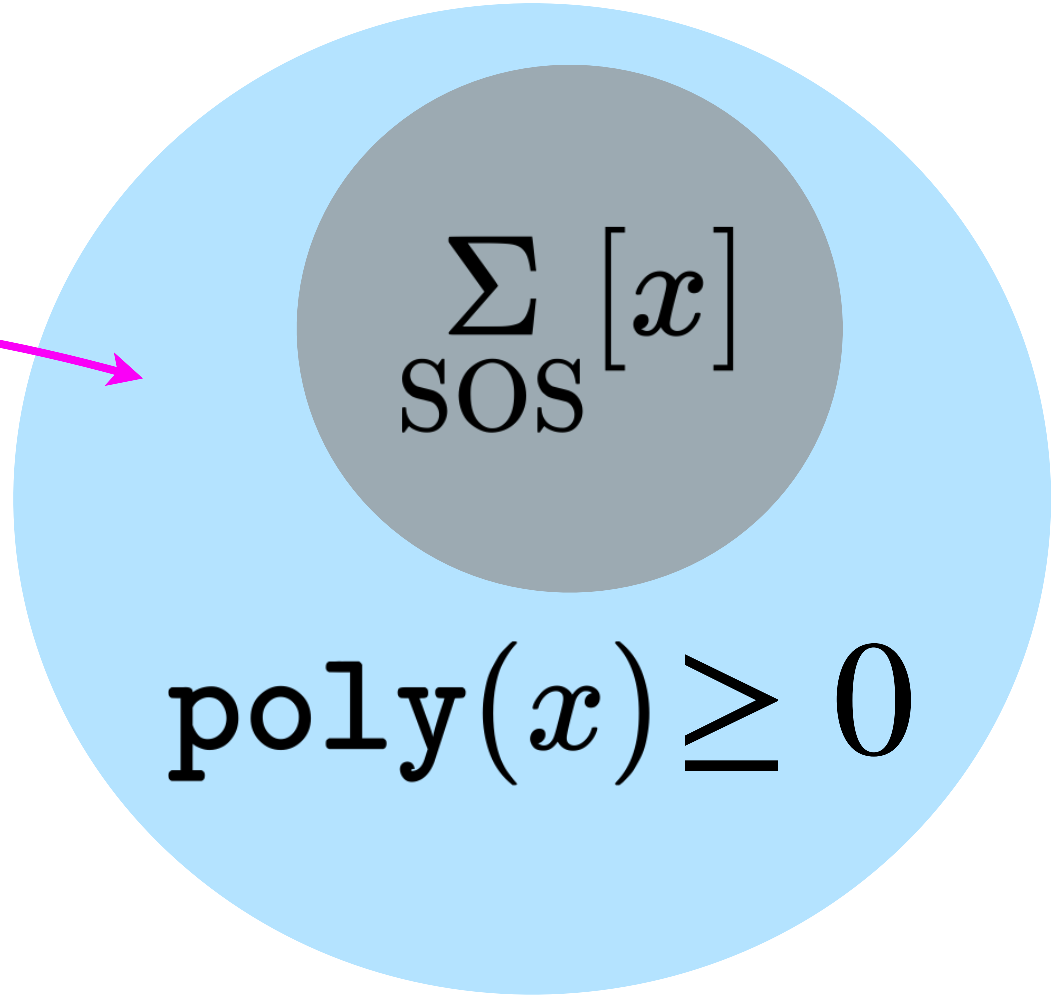
Sum-of-Squares (SOS) Polynomials

$$\texttt{poly}(x) \in \sum_{\mathrm{SOS}}[x] \text{ if } \texttt{poly}(x) = (\texttt{poly}_1(x))^2 + (\texttt{poly}_2(x))^2 + \ldots + (\texttt{poly}_m(x))^2$$

for some $\texttt{poly}_1(x), \texttt{poly}_2(x), \ldots, \texttt{poly}_m(x) \in \mathbb{R}[x], x \in \mathbb{R}^n$



$\texttt{polyMotzkin}(x_1, x_2) := x_1^4 x_2^2 + x_1^2 x_2^4 - 3x_1^2 x_2^2 + 1$



SOS decomposition:

$$\boxed{s \in \sum_{\mathrm{SOS}}[x] \Rightarrow s = Z_d(x)^\top S Z_d(x)}$$

for some $S \succeq 0,\ d \in \mathbb{N}$

where $Z_d(x)$ with monomial entries $(1, x, \ldots, x^d)$ of length $\zeta := \sum_{r=0}^{d} \binom{n+r-1}{r}$

SOS Programming

Defn: Semialgebraic set

Finite union of sets of the form $\{x \in \mathbb{R}^n \mid g(x) \leq 0, g \in \mathbb{R}_{d_g}[x], d_g \in \mathbb{N}\}$

Defn: Polynomial Optimization

Computationally intractable

For $f, g_{i \in [n_g]} \in \mathbb{R}[x]$

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{such that} \quad x \in \mathcal{C} := \{x \in \mathbb{R}^n \mid g_i(x) \leq 0 \forall i \in [\![n_g]\!]\}$$

$$\Updownarrow$$

$$\max_{\gamma \in \mathbb{R}} \gamma \quad \text{subject to} \quad f(x) - \gamma \geq 0 \quad \forall x \in \mathcal{C} \text{ semialgebraic}$$

SOS Programming (contd.)

$$f(x) - \gamma \geq 0 \quad \forall x \in \mathcal{C} \text{ Archimedean}$$

$$\Downarrow \quad \text{Putinar's Positivstellensatz (1993)}$$

$$\exists s_0, s_1, \ldots, s_{n_g} \in \sum_{\text{sos}}[x] \text{ such that } f(x) - \gamma = s_0(x) - \sum_{i \in [n_g]} s_i(x) g_i(x)$$

Defn: SOS tightening of Polynomial Optimization ⇝ Semidefinite program

$$\max_{(\gamma, S_0, S_1, \ldots, S_{n_g}) \in \mathbb{R} \times \underbrace{\mathbb{S}_+^{\zeta} \times \ldots \times \mathbb{S}_+^{\zeta}}_{n_g+1 \text{ times}}} \gamma$$

$$\text{subject to} \quad f(x) - \gamma = Z_d(x)^\top S_0 Z_d(x) - \sum_{i \in [n_g]} Z_d(x)^\top S_i Z_d(x) g_i(x)$$

Semidefinite program (SDP) ⇝ software SOSTOOLS, YALMIP, SOSOPT

Back to Forward Problem

Forward problem:
Given $c, \mathcal{X}, \mathcal{Y}$ as per **A1**, certify/falsify if the ground cost satisfies either MTW(0) or MTW(κ) or NNCC condition

$$\mathcal{X} \times \mathcal{Y} = \{(x,y) \in \mathbb{R}^n \times \mathbb{R}^n \mid m_i(x,y) \leq 0,\ m_i(x,y) \in \mathbb{R}_{d_m}[x,y]\ \forall i \in [\![\ell]\!]\}$$

NNCC forward problem:

$$\begin{aligned} \min \quad & 0 \\ \text{subject to} \quad & \mathfrak{S}_{(x,y)}(\xi,\eta) \geq 0, \quad \forall (x,y) \in \mathcal{X} \times \mathcal{Y},\ \xi \in T_x\mathcal{X},\ \eta \in T_y^*\mathcal{Y} \end{aligned}$$

MTW(κ) forward problem:

$$\begin{aligned} \min \quad & 0 \\ \text{subject to} \quad & \mathfrak{S}_{(x,y)}(\xi,\eta) \geq \kappa \|\xi\|^2 \|\eta\|^2, \\ & \qquad \forall (x,y) \in \mathcal{X} \times \mathcal{Y}, \xi \in T_x\mathcal{X}, \eta \in T_y^*\mathcal{Y} \text{ s.t. } \eta(\xi) = 0. \end{aligned}$$

Solution to (NNCC) Forward Problem

$$T_x\mathcal{X}, T_y^*\mathcal{Y} \cong \mathbb{R}^n \quad \Longrightarrow \quad \mathfrak{S}_{(x,y)}(\xi,\eta) = (\xi\otimes\eta)^\top \overbrace{F(x,y)}^{\in\mathbb{R}^{n^2\times n^2}}(\xi\otimes\eta)$$

$$[F(x,y)]_{i+n(j-1),k+n(l-1)} = \sum_{p,q,r,s} (c_{ij,p}c^{p,q}c_{q,rs} - c_{ij,rs})c^{r,k}c^{s,l}$$

Thm: SOS Tightening of NNCC Forward Problem $\rightsquigarrow$ SDP

For $F = \frac{F_N}{F_D} \in \mathbb{R}_{N,D}[x,y], N, D \in \mathbb{N}$, if $\exists s_0, s_1, \ldots, s_\ell \in \sum_{\text{sos}}^{n^2}[x,y]$ such that

$$\left(F_N(x,y) + F_N^\top(x,y)\right) - s_0(x,y)F_D(x,y) + \sum_{i\in[\ell]} s_i(x,y)m_i(x,y) \in \sum_{\text{sos}}^{n^2}[x,y]$$

then c satisfies NNCC condition on $\mathcal{X}\times\mathcal{Y}$

Computational Complexity: Forward Problem

Parameters: $\omega \in [2.376, 3]$

$$F = \frac{F_N}{F_D} \in \mathbb{R}_{N,D}[x,y], N, D \in \mathbb{N} \quad \Rightarrow \quad [F]_{i,j} \in \mathbb{R}_{(n^4-1)d_D + d_N, n^4 d_D}[x,y]$$

$$d_N, d_D = \mathcal{O}(ND)$$

$\ell =$ # of polynomial constraints defining $\mathcal{X} \times \mathcal{Y}$ semialgebraic

NNCC complexity: $\mathcal{O}\left(\ell^{5/4} n^{9+5d_N/4} + n^{\omega(4+d_N)} + \ell^{\omega/2} n^{\omega(2+d_N/2)}\right)$

MTW(κ) complexity: $\mathcal{O}\left(\ell^{5/4} n^{9d_N/4} + \ell^{\omega/2+1/4} n^{(\omega/2+1/4)d_N}\right)$

Sub-quadratic in ℓ, polynomial in n

Solution to (NNCC) Inverse Problem

Thm: SOS Tightening of NNCC Inverse Problem $\rightsquigarrow$ SDP

For compact $\Lambda := \{(x,y) \in \mathcal{X} \times \mathcal{Y} \mid \lambda(x,y) \leq 0, \lambda(x,y) \in \mathbb{R}_{d_\lambda}[x,y], d_\lambda \in \mathbb{N}\}$ chosen a priori, let $V_\pm : \Lambda \mapsto \mathbb{R}$ solve

$$
\begin{aligned}
\min_{V \in \mathbb{R}_d[x,y]} \quad & \int_\Lambda V(x,y)dxdy, \\
\text{subject to} \quad & V(x,y) - m_i(x,y) + r_i(x,y)\lambda(x,y) \in \sum_{\text{sos}}[x,y], \quad \forall\, i \in [\![\ell]\!], \\
& V(x,y) \pm F_D(x,y) + s_0(x,y)\lambda(x,y) \in \sum_{\text{sos}}[x,y], \\
& V(x,y) \pm f_j(x,y) + s_j(x,y)\lambda(x,y) \in \sum_{\text{sos}}[x,y], \ \forall j \in [\![\, |\text{pminor}(F_N)|]\!], \\
& s_0(x,y), s_j(x,y), r_i(x,y) \in \sum_{\text{sos}}[x,y] \quad \forall i \in [\![\ell]\!], j \in [\![\, |\text{pminor}(F_N)|]\!],
\end{aligned}
$$

then c satisfies NNCC on $\{(x,y) \in \Lambda \mid V_+(x,y) \leq 0\} \cup \{(x,y) \in \Lambda \mid V_-(x,y) \leq 0\}$

Numerical Results: Forward Problem

Example 1: Perturbed Euclidean Cost

$$c(x,y) = \|x-y\|_2^2 - \varepsilon\|x-y\|_2^4, \quad x,y \in \mathbb{R}^n, \varepsilon > 0$$

Lee & Li (2009): for ε small enough, MTW(0) holds on

$$\mathcal{X} \times \mathcal{Y} := \{(x,y) \in \mathbb{R}^n \times \mathbb{R}^n \mid \|x-y\|_2 \leq 0.5\}$$

But how small is small enough?

We used SOS SDP + bisection to find $\varepsilon_{\max}$ such that MTW(0) holds

Dimensions, n	1	2
$\varepsilon_{\max}$	$0.67(\approx \frac{2}{3})$	$1.05 \cdot 10^{-2}$
Residual	$1.19 \cdot 10^{-7}$	$4.18 \cdot 10^{-7}$

No analytical computation known

in Lee & Li (2009) via nontrivial analysis

Numerical Results: Forward Problem

Example 2: Log Partition Cost (Pal & Wong, 2018; Khan & Zhang, 2020)

used in stochastic portfolio theory

$$c(x,y) = \Psi_{\text{IsoMulNor}}(x-y),\ \Psi_{\text{IsoMulNor}}(x) := \overbrace{\frac{1}{2}\left(-\log x_1 + \sum_{i=2}^{n} x_i^2/x_1\right)}^{\textbf{not rational!}}$$

Our method still applies because $\mathfrak{S}_{(x,y)}(\xi,\eta) \propto \mathfrak{A}_x(\xi,\eta) = \text{poly}(x,\xi,\eta)/x_1^2\xi_n^2$

No analytical method exists to verify MTW(0) for $n > 2$

We can verify MTW(0) for $\mathcal{X} = \mathcal{Y} = \{x \in \mathbb{R}^n \mid x_1 > 0\}\, \forall n \in \mathbb{N}$

Dimensions, n	3	4	5	6
Residual	$1.034 \cdot 10^{-7}$	$4.804 \cdot 10^{-8}$	$4.683 \cdot 10^{-8}$	$3.475 \cdot 10^{-11}$
Total time (s)	0.7220	0.8050	1.2520	1.6690

Numerical Results: Forward Problem

Example 2: Log Partition Cost (Pal & Wong, 2018; Khan & Zhang, 2020)

For $n = 3$, our method discovered SOS decomposition:

$$\mathrm{poly}(x,\xi,\eta) = s(x,\xi,\eta)^\top s(x,\xi,\eta)$$

where $s(x,\xi,\eta) = \begin{bmatrix} 0 & -1.4 & 0 & 0.24 & 0 & 0 \\ 2.4 & 0 & -0.17 & 0 & 0 & 0 \\ 0 & 1.4 & 0 & -0.24 & 0 & 0 \\ -2.4 & 0 & 0.17 & 0 & -0.0002 & 0 \\ 0 & -1.4 & 0 & 0.25 & 0 & -1.2 \\ 2.4 & 0 & -0.17 & 0 & -0.0002 & 0 \\ -1.6 & 0 & -1.9 & 0 & 0 & 0 \\ 0 & 0.52 & 0 & 1.3 & 0 & 0 \\ 0 & 1.4 & 0 & -0.25 & 0 & 0 \\ -0.84 & 0 & 2 & 0 & 0 & 0 \\ 0 & -0.52 & 0 & -1.3 & 0 & 0 \end{bmatrix} \begin{bmatrix} \eta_1\xi_1^2\xi_2 \\ \eta_1\xi_1^2\xi_3 \\ \eta_1\xi_1\xi_2\xi_1 \\ \eta_1\xi_1\xi_3\xi_1 \\ \eta_2\xi_1\xi_2\xi_2 \\ \eta_2\xi_1\xi_2\xi_3 \end{bmatrix}$

Numerical Results: Inverse Problem

Example 3: Perturbed Euclidean Cost Revisited

$$c(x,y) = \|x-y\|_2^2 - \varepsilon\|x-y\|_2^4, \quad x,y \in \mathbb{R}^n, \varepsilon > 0$$

Lee & Li (2009): for $\varepsilon \gg 0$, MTW(0) fails on

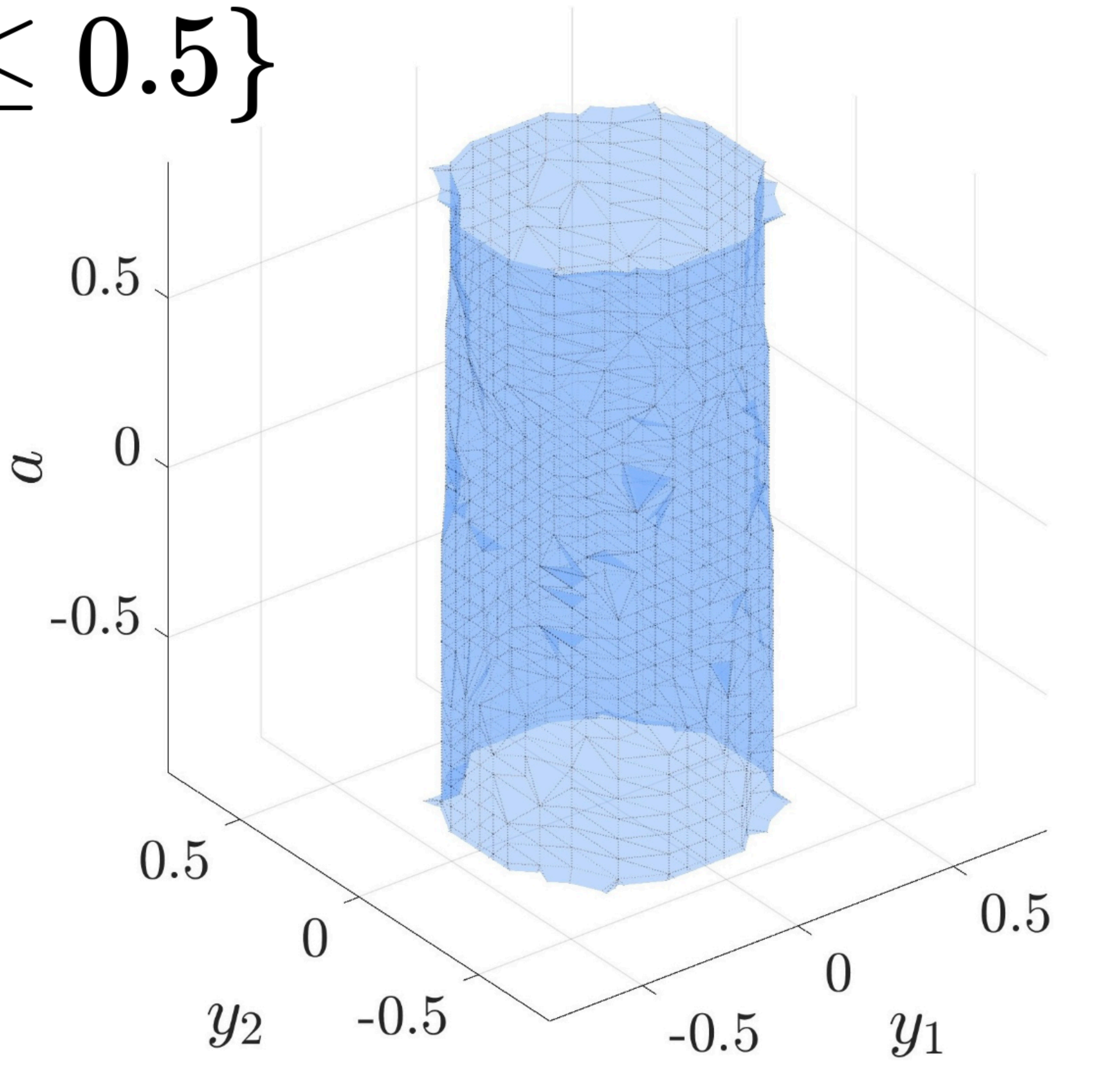
$$\mathcal{X}\times\mathcal{Y} := \{(x,y)\in\mathbb{R}^n\times\mathbb{R}^n \mid \|x-y\|_2 \le 0.5\}$$

Fix $\varepsilon = 1, \Lambda = [-1,1]^2, \mathcal{X} = \{[0,0]\}$

Parameterize $(\xi,\eta) = \left([a,1]^\top, [-1,a]^\top\right)$

Solve MTW(0) inverse problem

Exec time 115 sec, solve time 0.97 sec



Inner approx. of region where MTW tensor ≥ 0

Numerical Results: Inverse Problem

Example 4: Squared Distance Cost for a Surface of Positive Curvature

$$c(x,y) = 3(x_1 - y_1)^2(x_2 + y_2) + 4(x_2^3 + y_2^3) - (4x_2y_2 - (x_1 - y_1)^2)^{\frac{3}{2}}$$

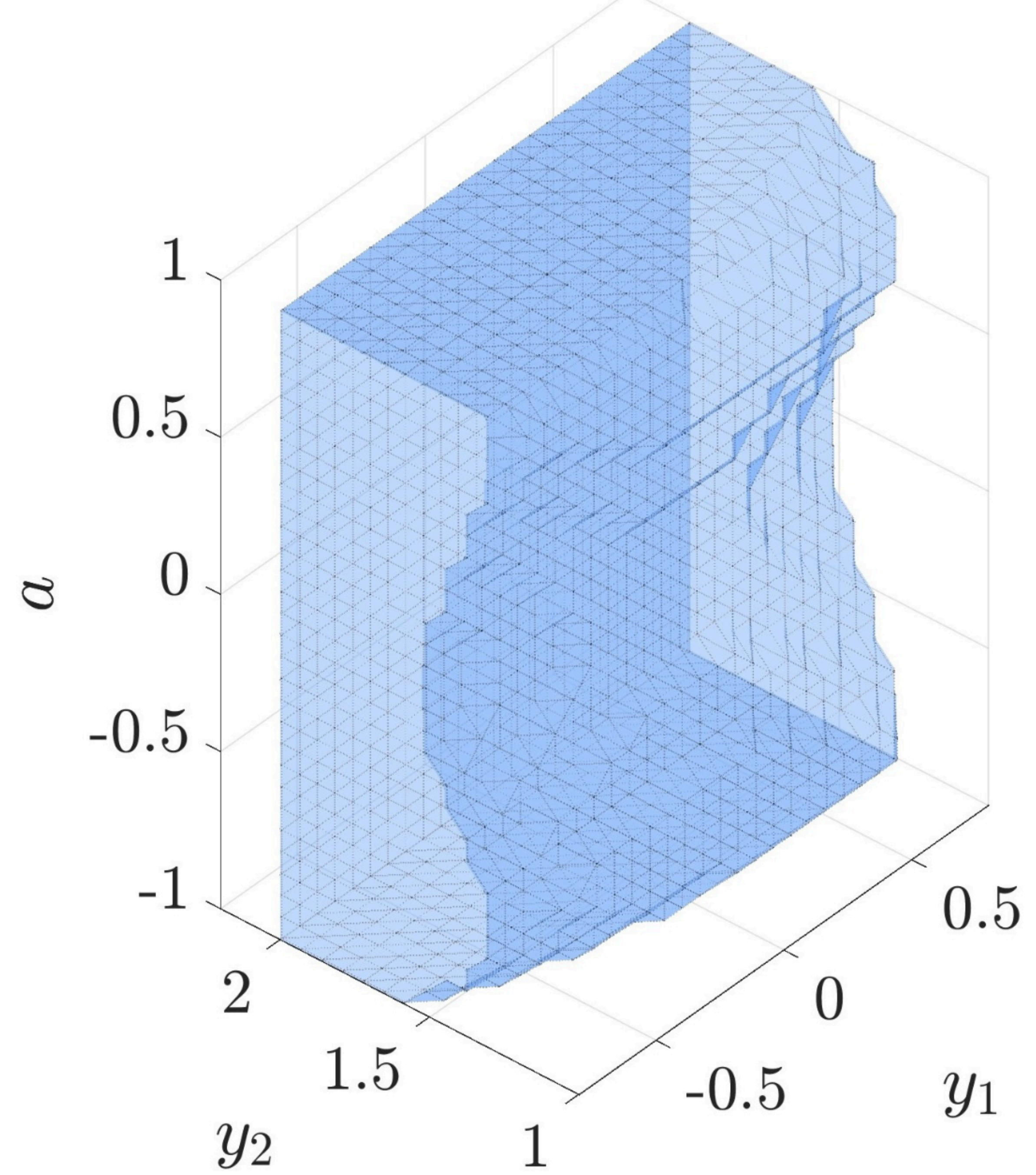
MTW holds around $\{x = y\}$

Fix $\Lambda = [-1,1] \times [0,2]$, $\mathcal{X} \times \mathcal{Y} = \{[0,1]\} \times \{(y_1, y_2) \in [-1,2] \times [0,2] \mid 4y_2 - y_1^2 \geq 0\}$

Parameterize $(\xi, \eta) = \left([a,1]^\top, [-1,a]^\top\right)$

Solve MTW(0) inverse problem

Exec time 119 sec, solve time 19.6 sec



Inner approx. of region where MTW tensor ≥ 0

Recap: SOS Programming for OT Regularity

NNCC, MTW(κ), MTW(0) conditions $\Rightarrow$ regularity of the OT map τ_{opt}

Assumption A1: MTW tensor is rational in $(x, y) \in \mathcal{X} \times \mathcal{Y}$ semialgebraic

$$\Downarrow$$

SOS tightening of forward & inverse problems

$$\Downarrow$$

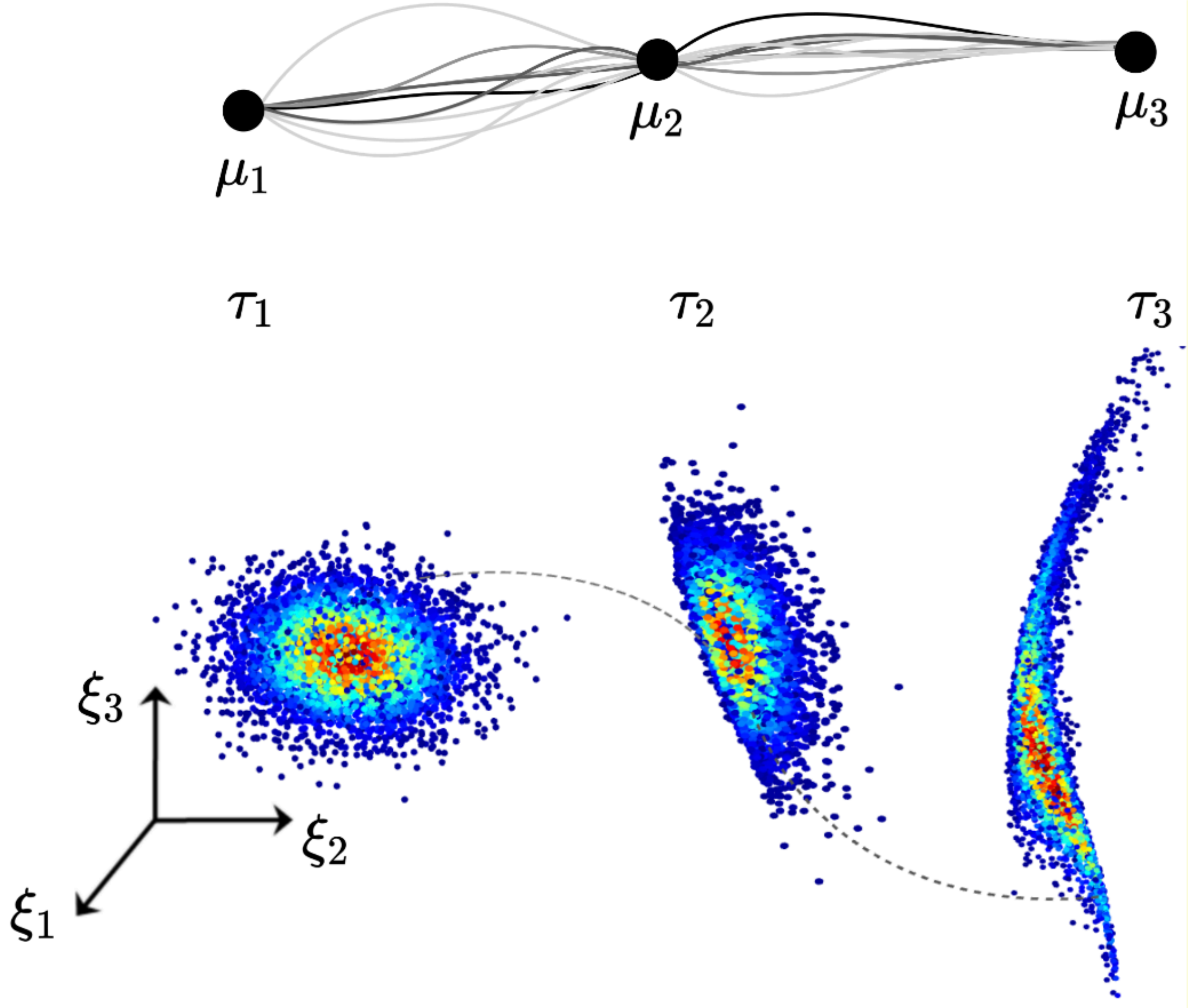
Solve SDP using SOSTOOLS + YALMIP $\rightsquigarrow$ computational certificates

Tensor Optimization for Graph-structured Multi-marginal SB

&

Learning Computational Resource Usage

Motivation: Computational Resource Usage of Multicore Software



Software running on $J \in \mathbb{N}$ CPU cores

Resource usage stochastic process $\boldsymbol{\xi}(\tau) \sim \mu_\tau$

Example: $\boldsymbol{\xi}^j := \begin{pmatrix} \xi_1^j \\ \xi_2^j \\ \xi_3^j \end{pmatrix} = \begin{pmatrix} \text{instructions retired} \\ \text{LLC requests} \\ \text{LLC misses} \end{pmatrix} \quad \forall j \in [\![J]\!]$

"Profiling" in RTOS community: sample $\underbrace{\{\boldsymbol{\xi}^{i,j}(\tau_\sigma)\}_{i=1}^n}_{\text{scattered data}} \forall \sigma \in [\![s]\!]$ where

Time/resource intensive!

$$\tau_1 \equiv 0 < \tau_2 < \ldots < \tau_{s-1} < \tau_s \equiv t, \quad s \geq 2$$

Problem Formulation

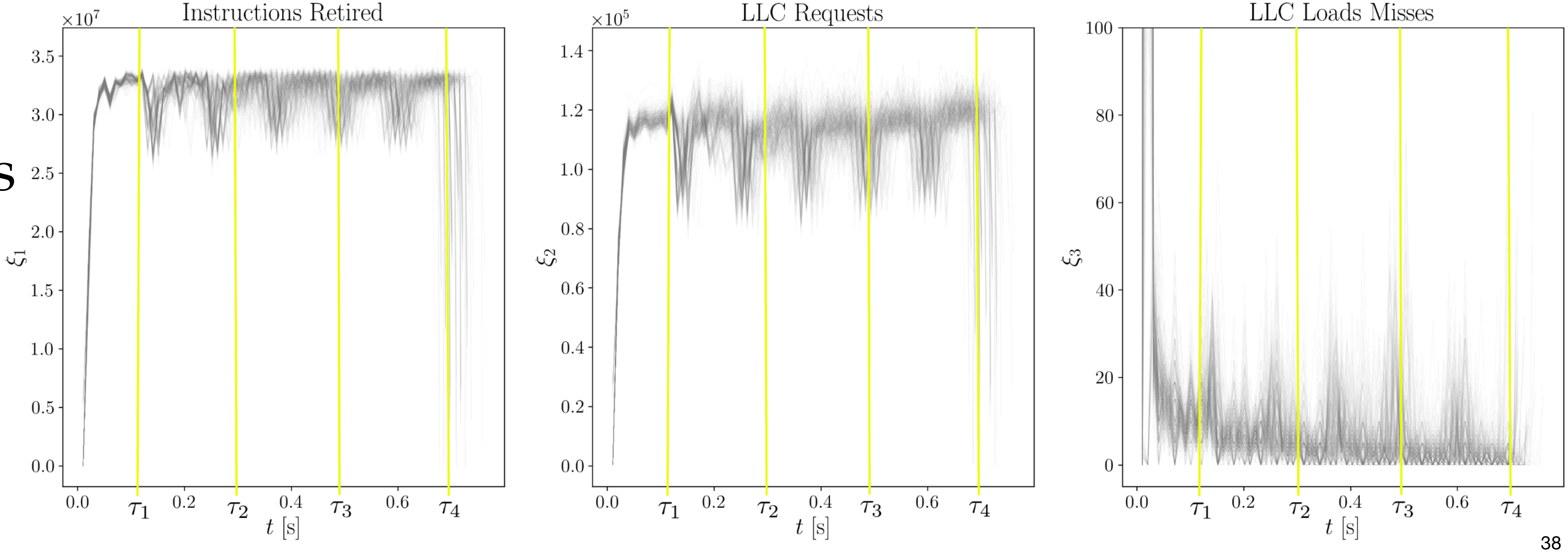
Use (weighted scattered) profile data

$$\{\boldsymbol{\xi}^{i,j}(\tau_\sigma)\}_{i=1}^{n}, \mu_\sigma^j := \frac{1}{n}\sum_{i=1}^{n}\delta\left(\boldsymbol{\xi}^j - \boldsymbol{\xi}^{i,j}(\tau_\sigma)\right) \forall (j,\sigma) \in [\![J]\!] \times [\![s]\!]$$

to learn $\hat{\mu}_\tau \, \forall \tau \in [0, t]$

Typical profiles

$(\tau = 4, J = 1):$



Challenges

Difficult to have first-principle physics based model for combined

S/W+H/W level stochasticity

Learning must be over joint resources (e.g., processor & cache correlated)

Correlation structure among resource states changes with time

Need: nonparametric learning, also desire: learning with optimality

Main Idea

Step 1: Model the spatio-temporal correlation induced by HW+SW architecture by graph structures

Step 2: Solve MSBP over the resulting graph

Step 3: Use the MSBP solution to predict most likely $\hat{\mu}_T$

Steps 1,2: Discrete Graph-structured MSBP

Problem template:
$$\underset{\boldsymbol{M}\in(\mathbb{R}^n)^{\otimes|\Lambda|}_{\geq 0}}{\arg\min}\ \langle \boldsymbol{C}+\varepsilon\log\boldsymbol{M},\boldsymbol{M}\rangle$$

index set capturing graph structure

$$\text{subject to}\ \ \mathrm{proj}_{(j,\sigma)}(\boldsymbol{M})=\boldsymbol{\mu}_\sigma^j\quad\forall(j,\sigma)\in\Lambda$$

Prop: (Strong duality $\rightsquigarrow$ Sinkhorn recursions, complexity: $\mathcal{O}\left(n^{|\Lambda|}\right)$)

Lagrange multipliers

Let $$\underbrace{\boldsymbol{K}:=\exp(-\boldsymbol{C}/\varepsilon)}_{\in(\mathbb{R}^n)^{\otimes|\Lambda|}_{>0}},\ \underbrace{\boldsymbol{u}_\sigma^j:=\exp(\boldsymbol{\lambda}_\sigma^j/\varepsilon)}_{\in\mathbb{R}^n_{>0}\quad\forall(j,\sigma)\in\Lambda},\ \underbrace{\boldsymbol{U}:=\otimes_{(j,\sigma)\in\Lambda}\boldsymbol{u}_\sigma^j}_{\in(\mathbb{R}^n)^{\otimes|\Lambda|}_{>0}}$$

The multi-marginal Sinkhorn recursions

$$\boldsymbol{u}_\sigma^j\leftarrow\boldsymbol{u}_\sigma^j\odot\boldsymbol{\mu}_\sigma^j\oslash\mathrm{proj}_{(j,\sigma)}(\boldsymbol{K}\odot\boldsymbol{U})\ \forall(j,\sigma)\in\Lambda,$$

converges with linear rate to minimizer $\boldsymbol{M}^{\mathrm{opt}}=\boldsymbol{K}\odot\boldsymbol{U}$

$J = 1$: Single CPU Core: Path-structured MSBP

Correlation induced by time

Graph structure: $\mu_1 - \mu_2 - \cdots - \mu_\sigma - \cdots - \mu_s$

Ground cost tensor decomposes: $\boldsymbol{C}(\boldsymbol{\xi}(\tau_1), \ldots, \boldsymbol{\xi}(\tau_s)) = \sum_{\sigma=1}^{s-1} c_\sigma \left(\boldsymbol{\xi}(\tau_\sigma), \boldsymbol{\xi}(\tau_{\sigma+1})\right)$

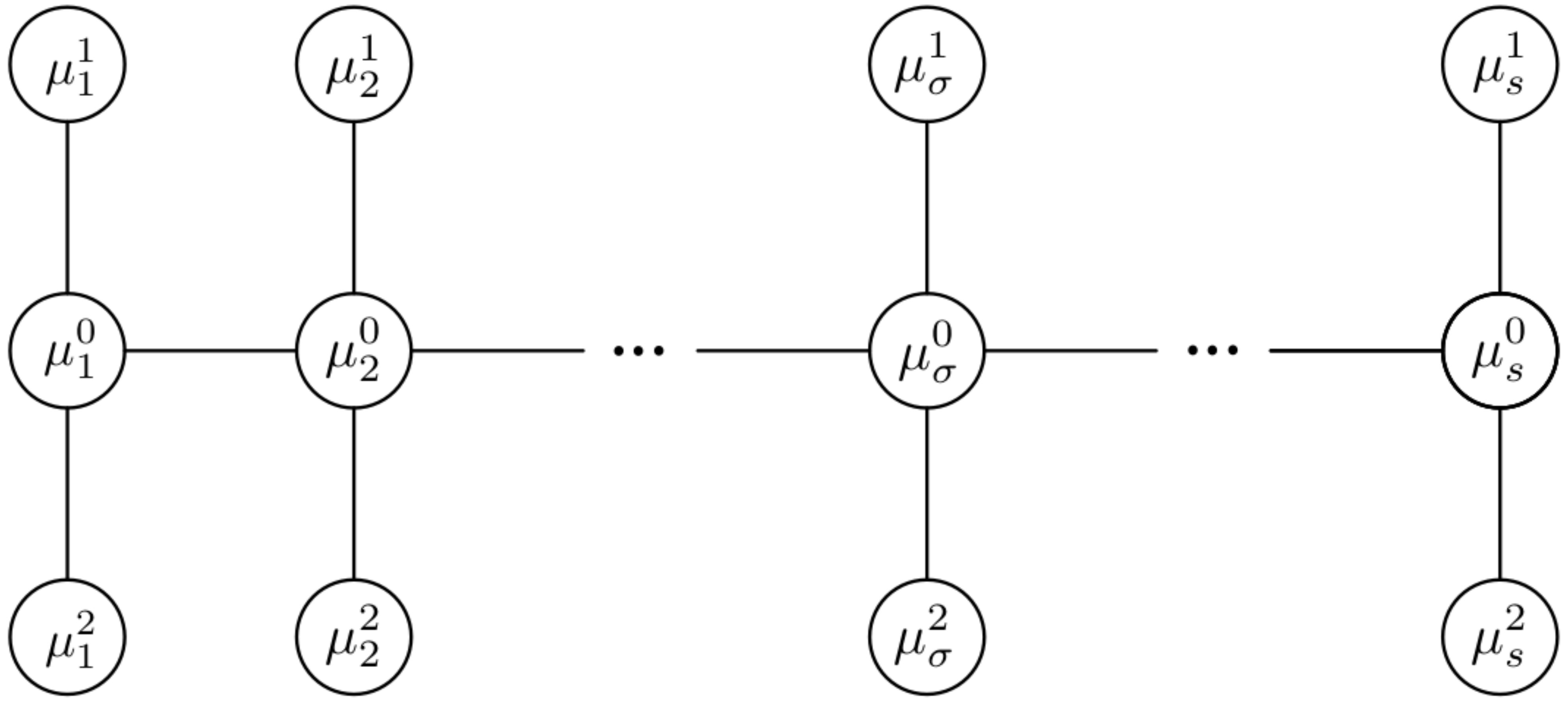
Discrete version: $[\boldsymbol{C}]_{i_1, \ldots, i_s} = \sum_{\sigma=1}^{s-1} [C^\sigma]_{i_\sigma, i_{\sigma+1}}$

$J > 1$: Multiple CPU Cores

Correlation induced by time + CPU cores

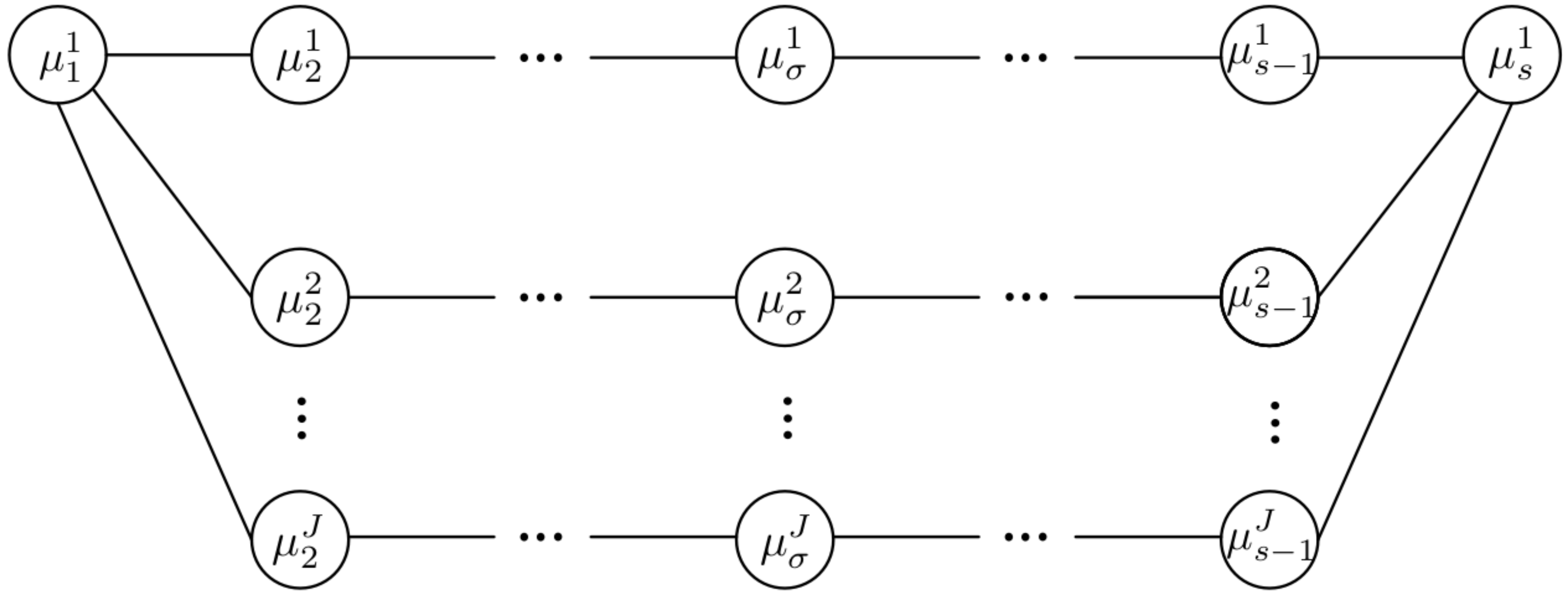
Graph structure:

barycentric (BC)



inter-CPU communication

series-parallel (SP)



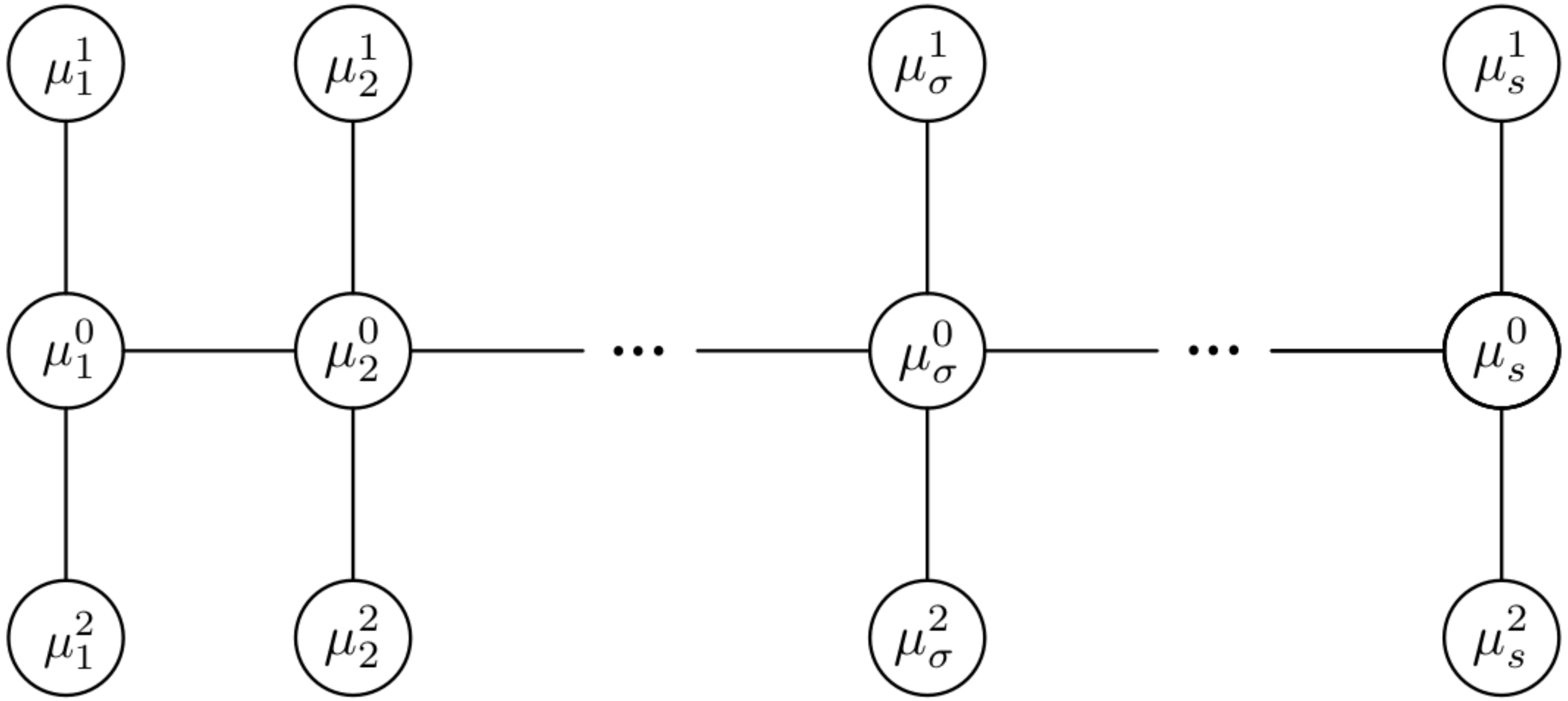
parallel execution

$J > 1$: Multiple CPU Cores: Barycentric MSBP

Idea: phantom CPU resource statistics μ_σ^0 = barycenter of $\{\mu_\sigma^j\}_{j\in[J]} \forall \sigma \in [\![s]\!]$

Index set:

$$\Lambda_{\mathrm{BC}} := (\{0\} \cup [\![J]\!]) \times [\![s]\!]$$

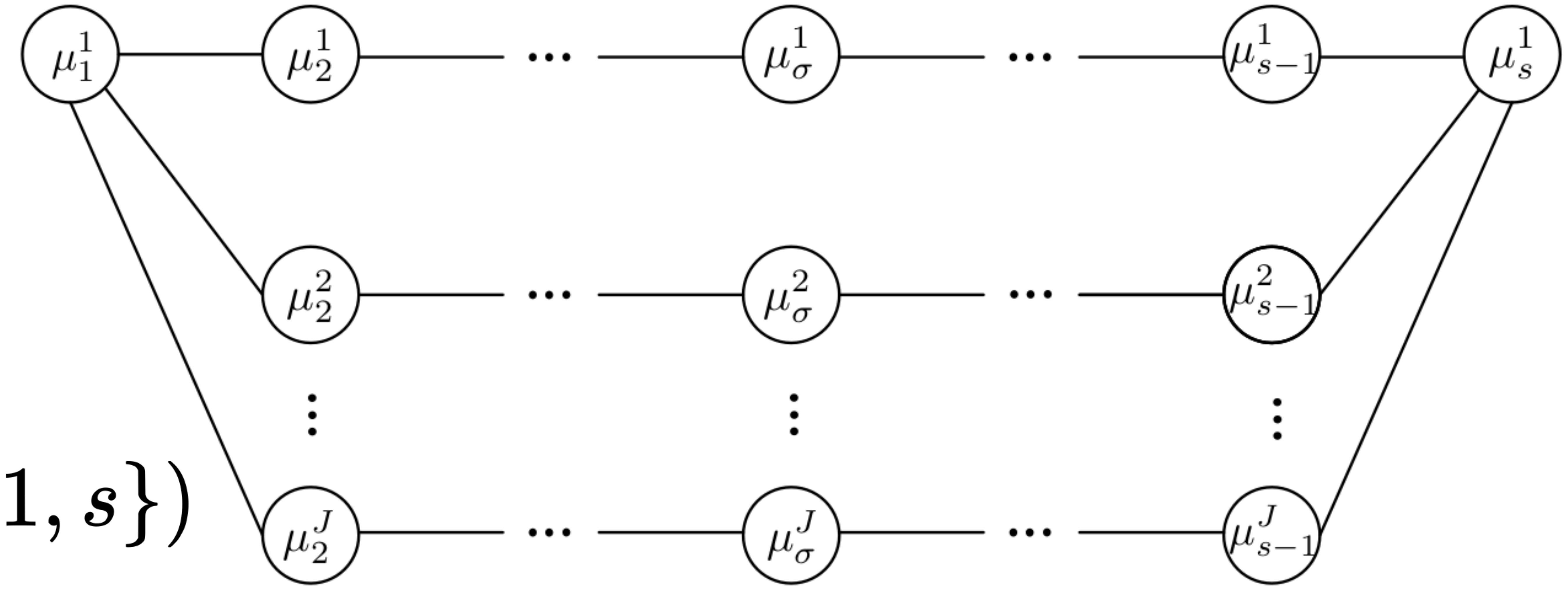


Ground cost tensor decomposition:

$$\boldsymbol{C}(\boldsymbol{\xi}(\tau_1),\dots,\boldsymbol{\xi}(\tau_s)) = \sum_{\sigma=1}^{s-1} c_{0,\sigma}\left(\boldsymbol{\xi}^0(\tau_\sigma),\boldsymbol{\xi}^0(\tau_{\sigma+1})\right) + \sum_{\sigma=1}^{s}\sum_{j=1}^{J} c_{j,\sigma}\left(\boldsymbol{\xi}^j(\tau_\sigma),\boldsymbol{\xi}^0(\tau_\sigma)\right)$$

$J > 1$: Multiple CPU Cores: Series-parallel MSBP

Idea: fork and merge



Index set:

$$\Lambda_{\mathrm{SP}} := (\llbracket J \rrbracket \times \llbracket \boldsymbol{s} \rrbracket) \setminus ((\llbracket J \rrbracket \setminus \{1\}) \times \{1, \boldsymbol{s}\})$$

Ground cost tensor decomposition:

$$\boldsymbol{C}(\boldsymbol{\xi}(\tau_1), \ldots, \boldsymbol{\xi}(\tau_s)) = \sum_{j=1}^{J} \left\{ c_{j,1}\left(\boldsymbol{\xi}^j(\tau_1), \boldsymbol{\xi}^j(\tau_2)\right) + c_{j,s-1}\left(\boldsymbol{\xi}^j(\tau_{s-1}), \boldsymbol{\xi}^j(\tau_s)\right) \right\} + \sum_{\sigma=2}^{s-1} \sum_{j=1}^{J} c_{j,\sigma}\left(\boldsymbol{\xi}^j(\tau_\sigma, \boldsymbol{\xi}^j(\tau_{\sigma+1})\right)$$

$J > 1$: Computational Complexity for MSBP

Structure	General	Path	BC	SP
Index set	Λ	$[\![s]\!]$	Λ_{BC}	Λ_{SP}
# of indices	$\lvert\Lambda\rvert$	s	$(J+1)s$	$J(s-2)+2$
linear in J, s ⟶ $\mathcal{O}(\cdot)$ for $\mathrm{proj}_\sigma(\boldsymbol{M})$	$n^{\lvert\Lambda\rvert}$	$(s-1)n^2$	$(Js)n^2$	$(Js)n^2$

Exact flop count for BC:

$$\underbrace{Js(n_0 n + n_0) + (2n_0) + (2s-2)n_0^2}_{\text{barycenter}}$$

$$\underbrace{Js(n_0 n + n_0) + (3n_0 + n + 2n_0 n) + (2s-2)n_0^2}_{\text{other dist.}}$$

Exact flop count for SP:

$$\underbrace{n + J\left(1 + 2(s-2)\right)n^2}_{\text{end dist.}}$$

$$\underbrace{2n + J\left(1 + 2(s-2)\right)n^2 - n^2}_{\text{other dist.}}$$

Step 3: MSBP Solution to Predicting $\hat{\mu}_\tau$

Given $\tau \in [0, t)$, $j \in [\![J]\!]$, find $\sigma \in \{[\![s]\!] \mid \tau_\sigma \leq \tau < \tau_{\sigma+1}\}$

$$M^{j,\sigma} := \mathrm{proj}_{(j,\sigma),(j,\sigma+1)}(\boldsymbol{M}^{\mathrm{opt}}) : \mu^j_\sigma \to \mu^j_{\sigma+1} \quad \left(\in \mathbb{R}^{n\times n}_{\geq 0}\right)$$

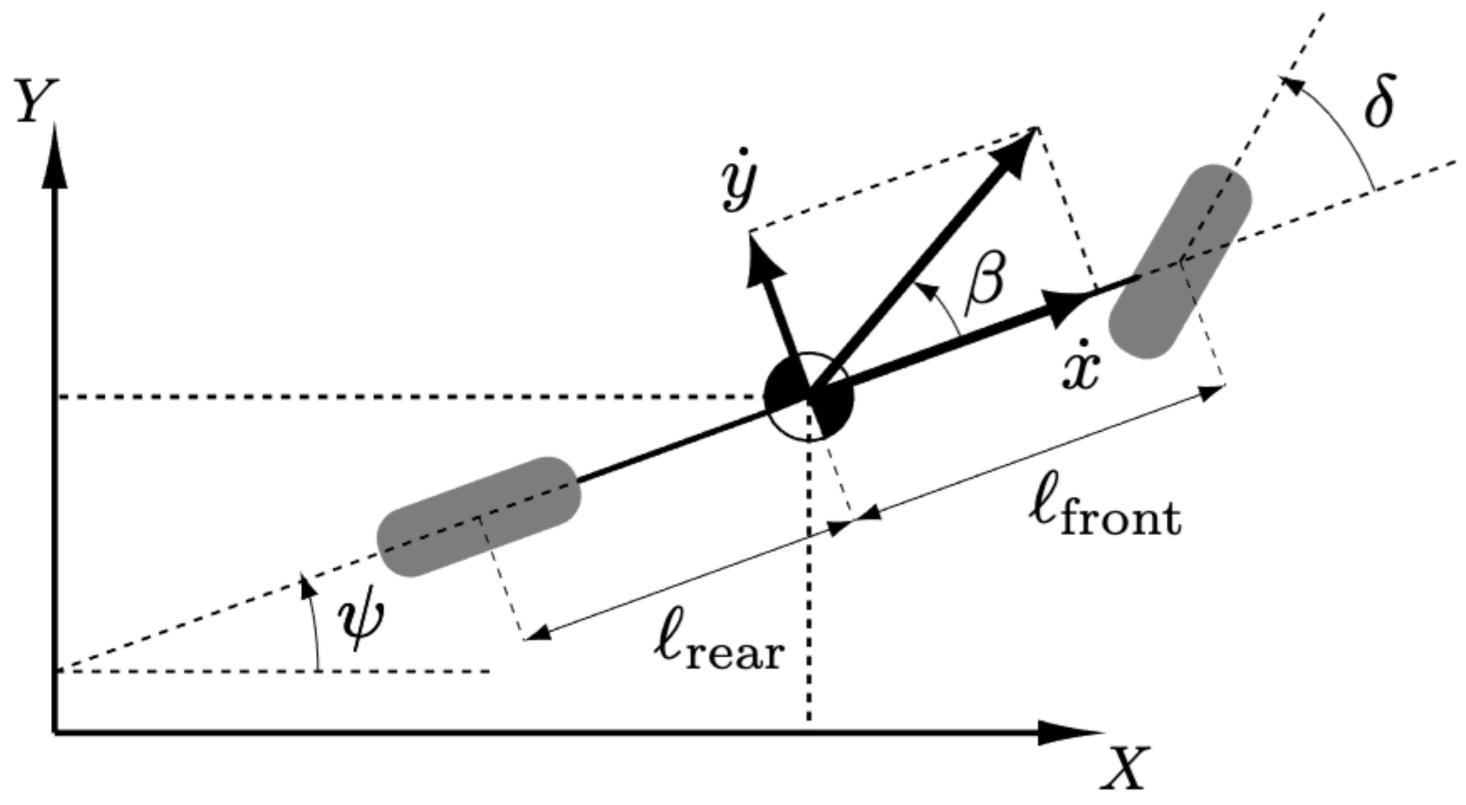
Compute measure interpolating μ^j_σ and $\mu^j_{\sigma+1}$ as:

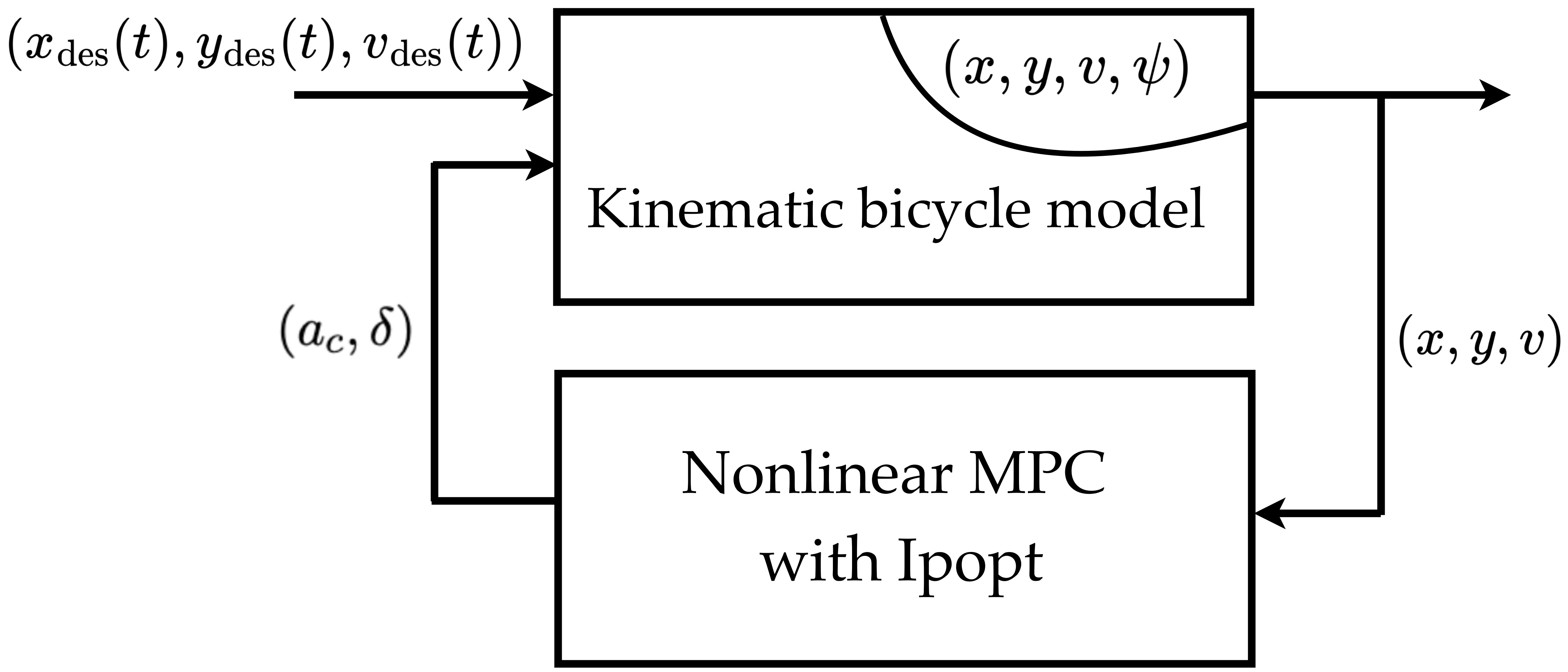
$$\hat{\mu}^j_\tau := \sum_{r=1}^{n}\sum_{\ell=1}^{n}\left[M^{j,\sigma}_{r,\ell}\right]\delta(\boldsymbol{\xi}^j - \widehat{\boldsymbol{\xi}}^j(\tau, \boldsymbol{\xi}^{r,j}(\tau_\sigma), \boldsymbol{\xi}^{\ell,j}(\tau_{\sigma+1})))$$

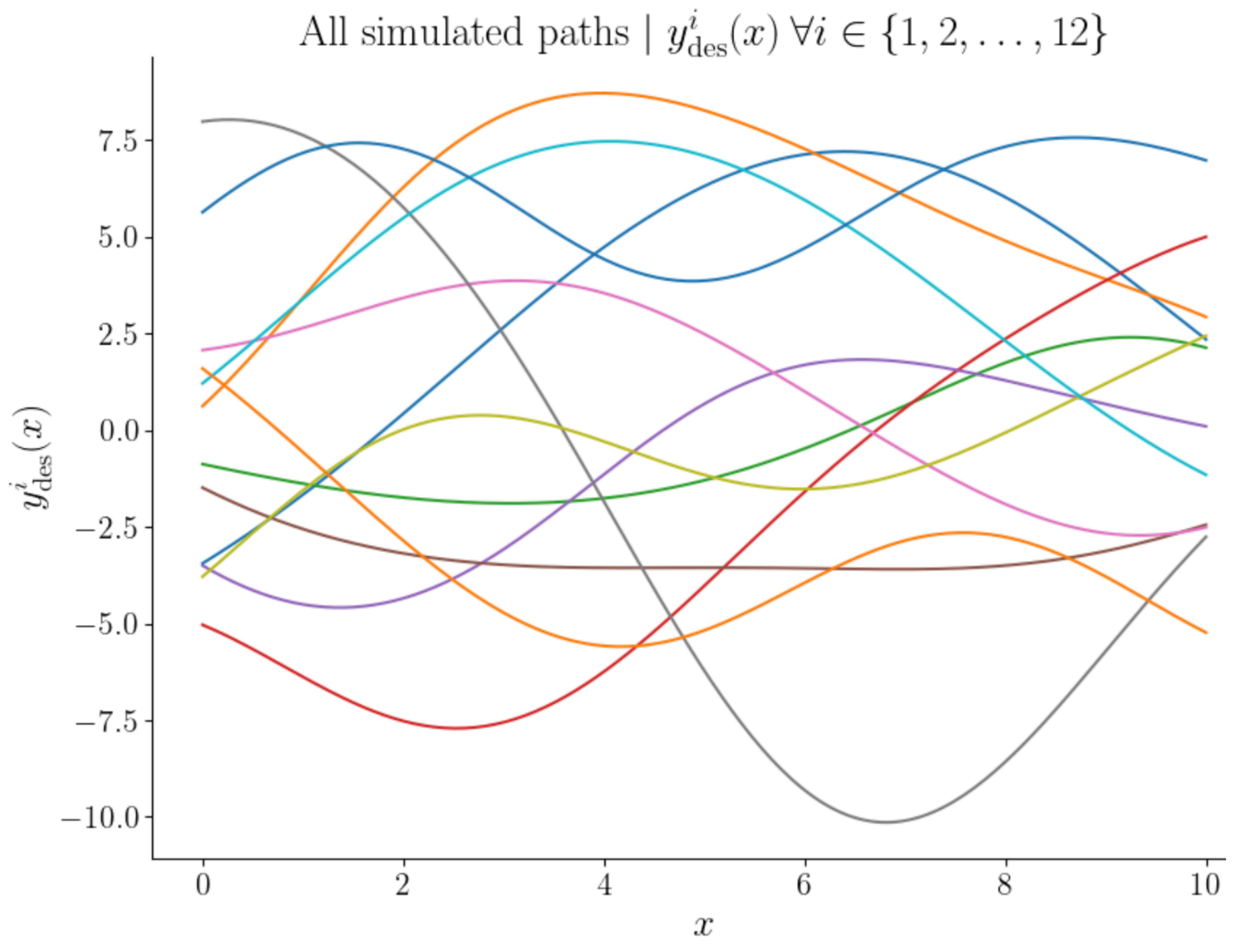
and its support:

$$\widehat{\boldsymbol{\xi}}^j(\tau, \boldsymbol{\xi}^{r,j}(\tau_\sigma), \boldsymbol{\xi}^{\ell,j}(\tau_{\sigma+1})) := (1-\lambda)\boldsymbol{\xi}^{r,j}(\tau_\sigma) + \lambda\boldsymbol{\xi}^{\ell,j}(\tau_{\sigma+1}), \;\; \lambda := \frac{\tau - \tau_\sigma}{\tau_{\sigma+1} - \tau_\sigma} \in [0,1]$$

Case Study: Path Tracking Control Software







$$\boldsymbol{c}_{\text{cyber}} = \begin{pmatrix} \text{alloc. last-level cache} \\ \text{alloc. memory bandwidth} \end{pmatrix}, \quad \boldsymbol{c}_{\text{phys}} = y_{\text{des}}(x) \in \text{GP}\left([x_{\min}, x_{\max}]\right)$$

$$\boldsymbol{\xi} := \begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix} = \begin{pmatrix} \text{instructions retired} \\ \text{LLC requests} \\ \text{LLC misses} \end{pmatrix}$$

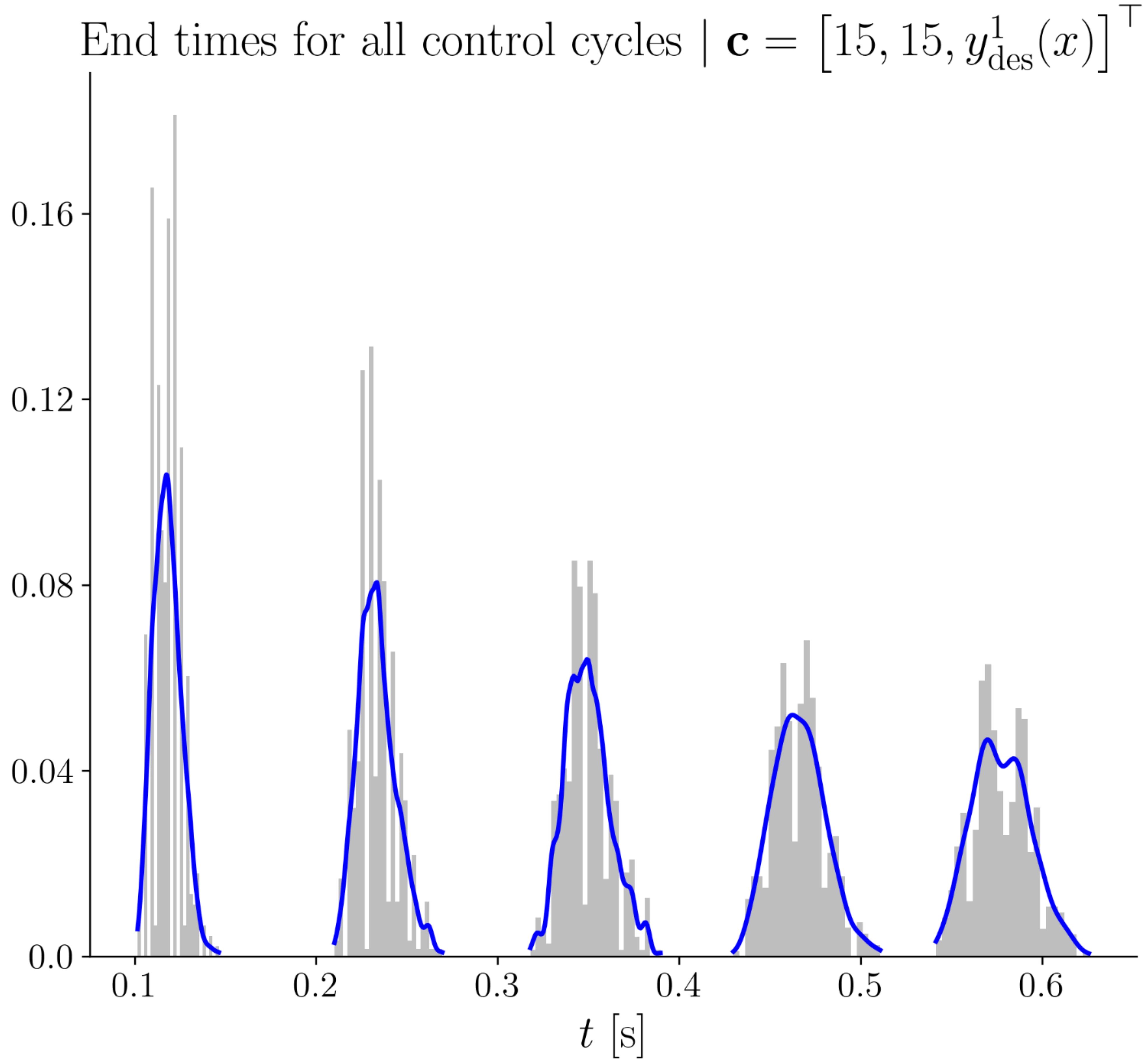
Single core ⇒ Path-structured MSBP

Case Study: Path Tracking Control Software

$n = 500$, $\boldsymbol{c}_{\text{cyber}} = [15 \quad 15]^\top$, $\boldsymbol{c}_{\text{phys}} = y^1_{\text{des}}(x)$, 30 MB LLC, mem. bandwidth

Each profile with $n_c = 5$ control cycles

Cycle No.	Mean	Std. Dev.
#1	0.1181	0.0076
#2	0.2336	0.0106
#3	0.3495	0.0127
#4	0.4660	0.0143
#5	0.5775	0.0159



Sampling period = 5 ms

Case Study: Path Tracking Control Software

Profiles:

H/W-level stochasticity, fixed context $\boldsymbol{c}$

Case Study: Path Tracking Control Software

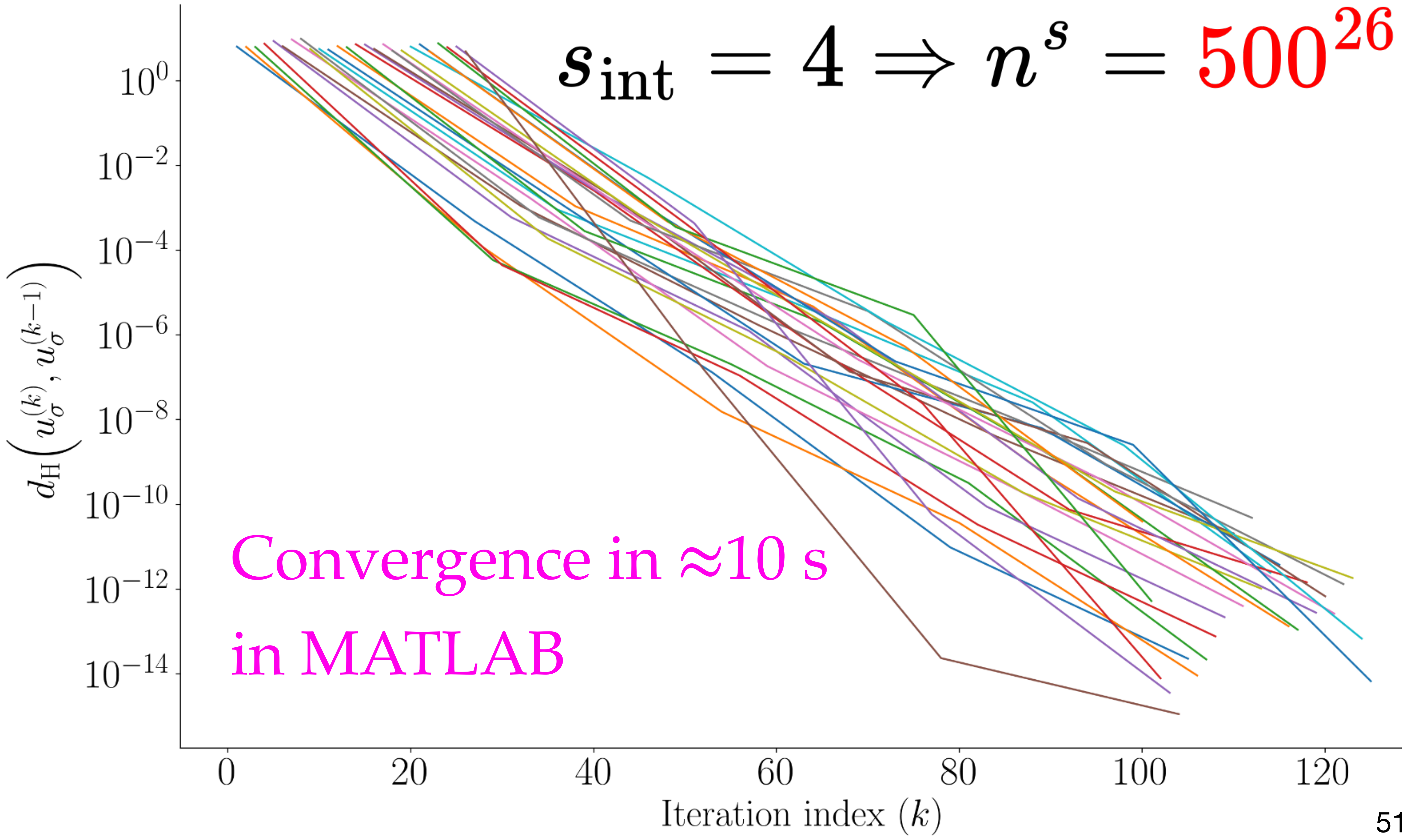
MSBP convergence:

# of marginals $s := 1 + n_c(s_{\text{int}} + 1)$; Euclidean $C^\sigma\ \forall\sigma \in [\![s-1]\!]$

Cost tensor element: $[\boldsymbol{C}]_{i_1,\dots,i_s} = \sum_{\sigma=1}^{s-1} [C]^{\sigma}_{i_\sigma, i_{\sigma+1}}$

$$d_{\text{H}}\left(\boldsymbol{u}, \boldsymbol{v}\right) = \log\left(\frac{\max_{i=1,\dots,n} u_i/v_i}{\min_{i=1,\dots,n} u_i/v_i}\right), \quad \boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^n_{>0}$$

Hilbert projective metric



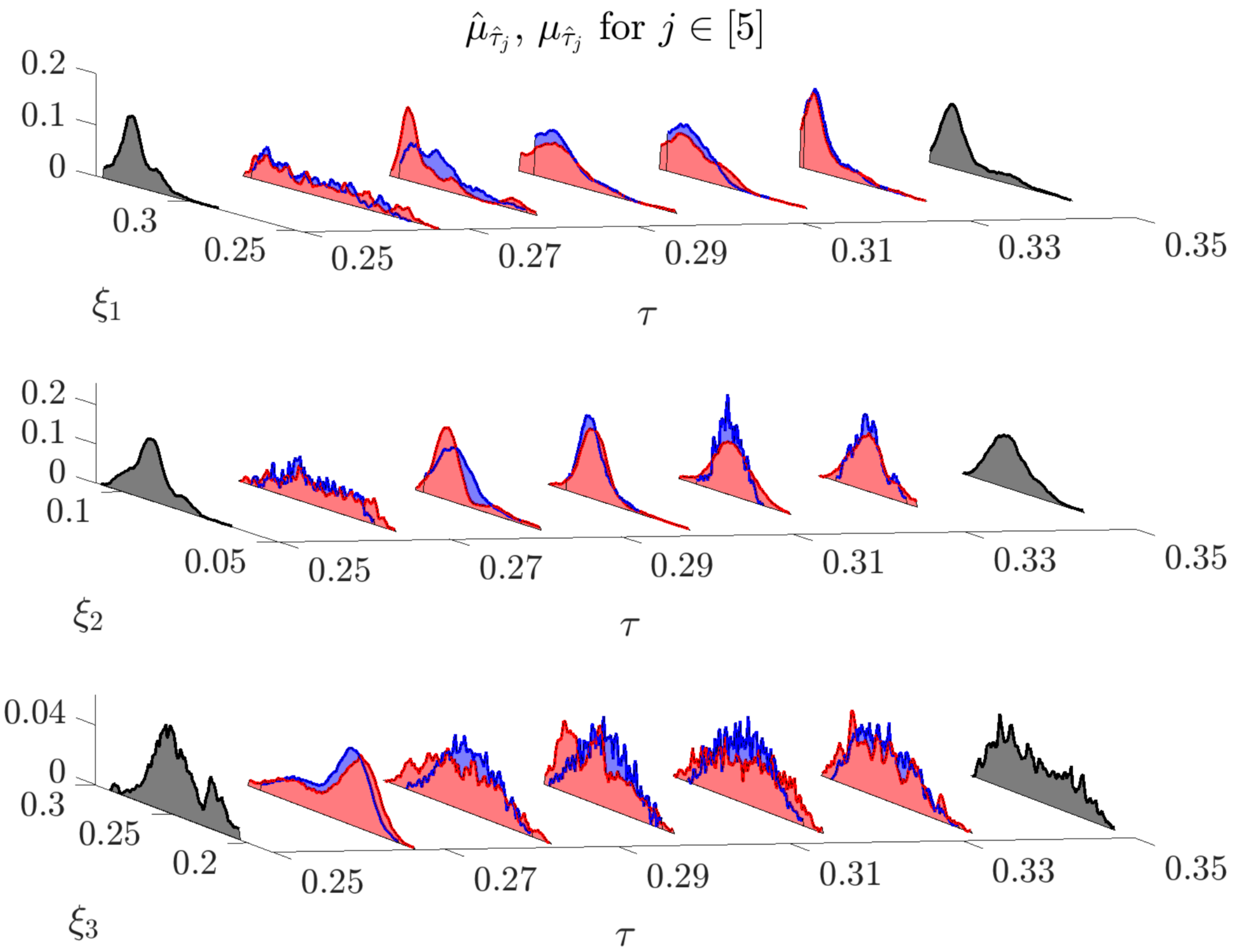
Case Study: Path Tracking Control Software

MSBP prediction vs "hold out" observation, 3rd control cycle, $s_{\text{int}} = 4$:

Predicted $\hat{\mu}$

Measured μ

μ at control-cycle boundaries



Case Study: Path Tracking Control Software

MSBP accuracy:

# of intra-cycle marginals Wasserstein distances $W_j := W(\hat{\mu}_{\hat{\tau}_j}, \mu_{\hat{\tau}_j})\ \forall j \in [\![s_{\text{int}} + 1]\!]$

s_{int}	W_1	W_2	W_3	W_4	W_5
0	2.0489×10^{-4}	-	-	-	-
1	2.2695×10^{-4}	1.1750×10^{-4}	-	-	-
2	5.7717×10^{-4}	0.9163×10^{-4}	0.3794×10^{-4}	-	-
3	2.2413×10^{-4}	1.6432×10^{-4}	1.2345×10^{-4}	0.6010×10^{-4}	-
4	0.6372×10^{-4}	1.2691×10^{-4}	0.9176×10^{-4}	0.6689×10^{-4}	0.2111×10^{-4}

$$\uparrow s_{\text{int}} \quad \Longrightarrow \quad \downarrow \mathbb{E}[W_j]$$

Case Study: Multicore Benchmark

Canneal: quad-core ($J = 4$) benchmark from PARSEC

$$\boldsymbol{c}_{\text{cyber}} = \begin{pmatrix} \text{alloc. last-level cache (MB)} \\ \text{alloc. memory bandwidth (MBps)} \end{pmatrix} := \begin{pmatrix} 24 & 10 & 4 & 2 \\ 125 & 25 & 5 & 1 \end{pmatrix}$$

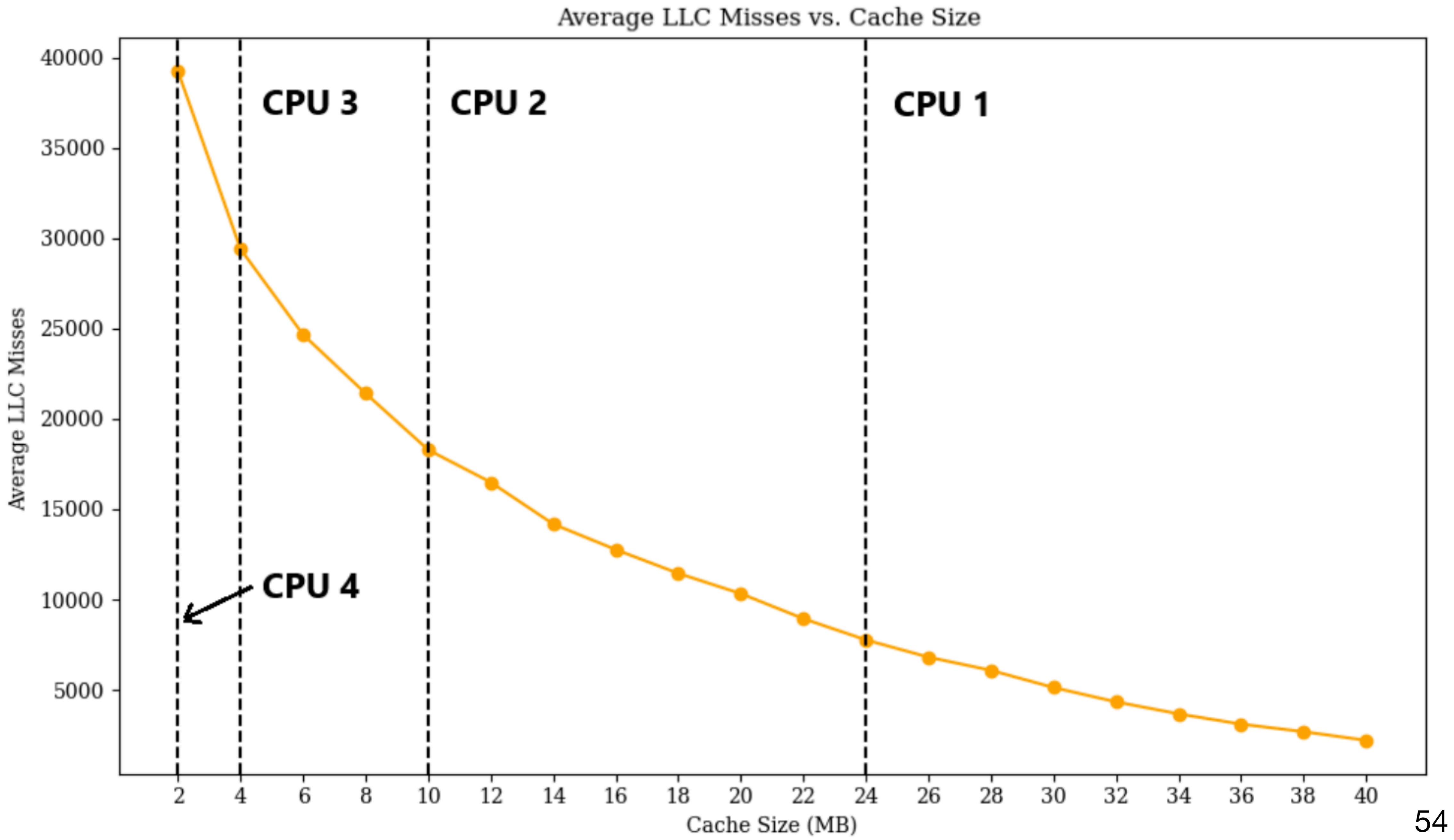
Profiled $n = 400$ times at $\tau_\sigma \in \{0.0, 0.5, 1.5, 2.5, 5.0, 9.5, 10.5\}$, i.e., $s = 7$

Multicore $\Rightarrow$ both BC and SP MSBP

BC: 400^{35} decision variables

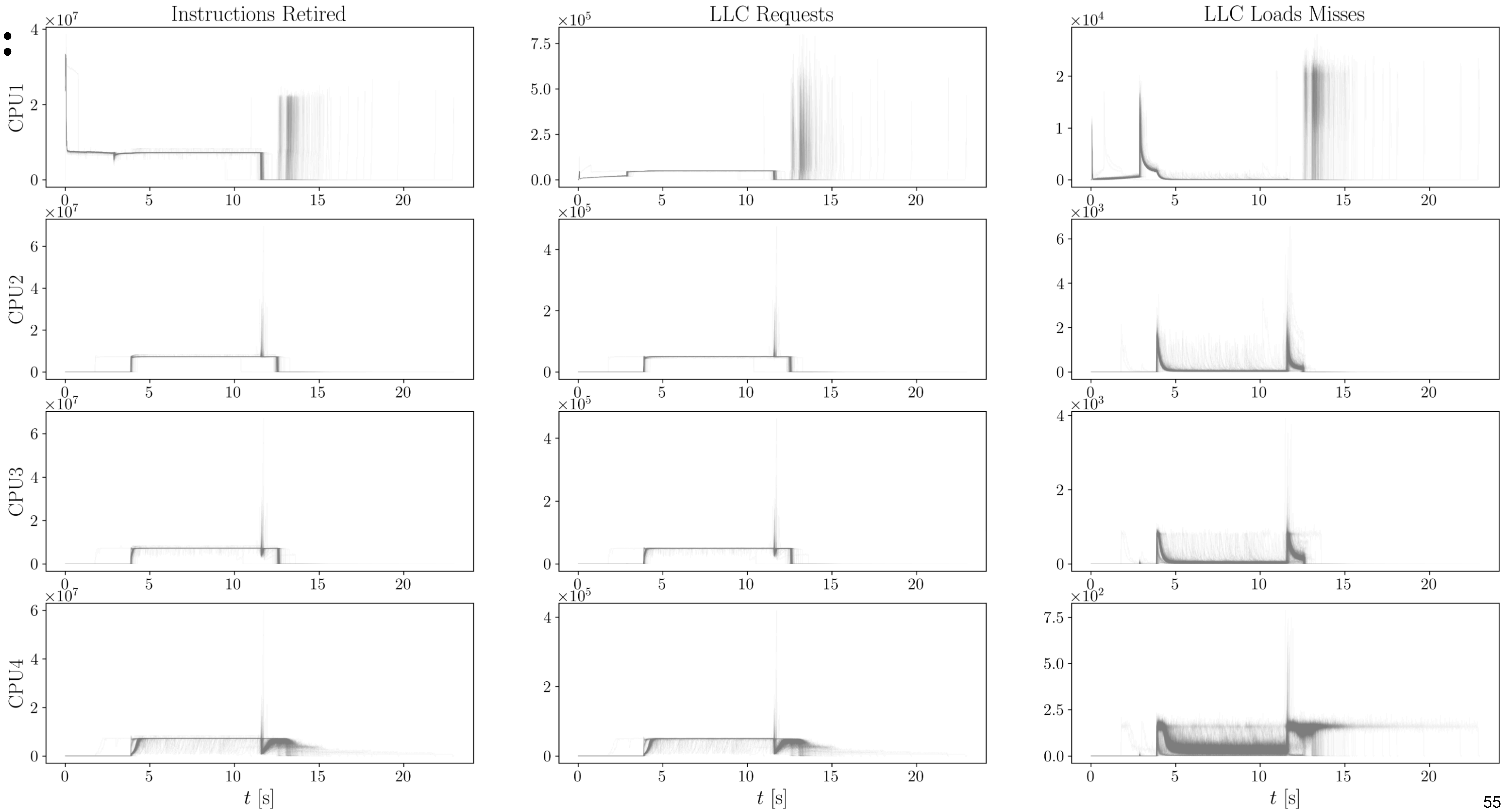
SP: 400^{22} decision variables

Convergence in 0.5 s in MATLAB



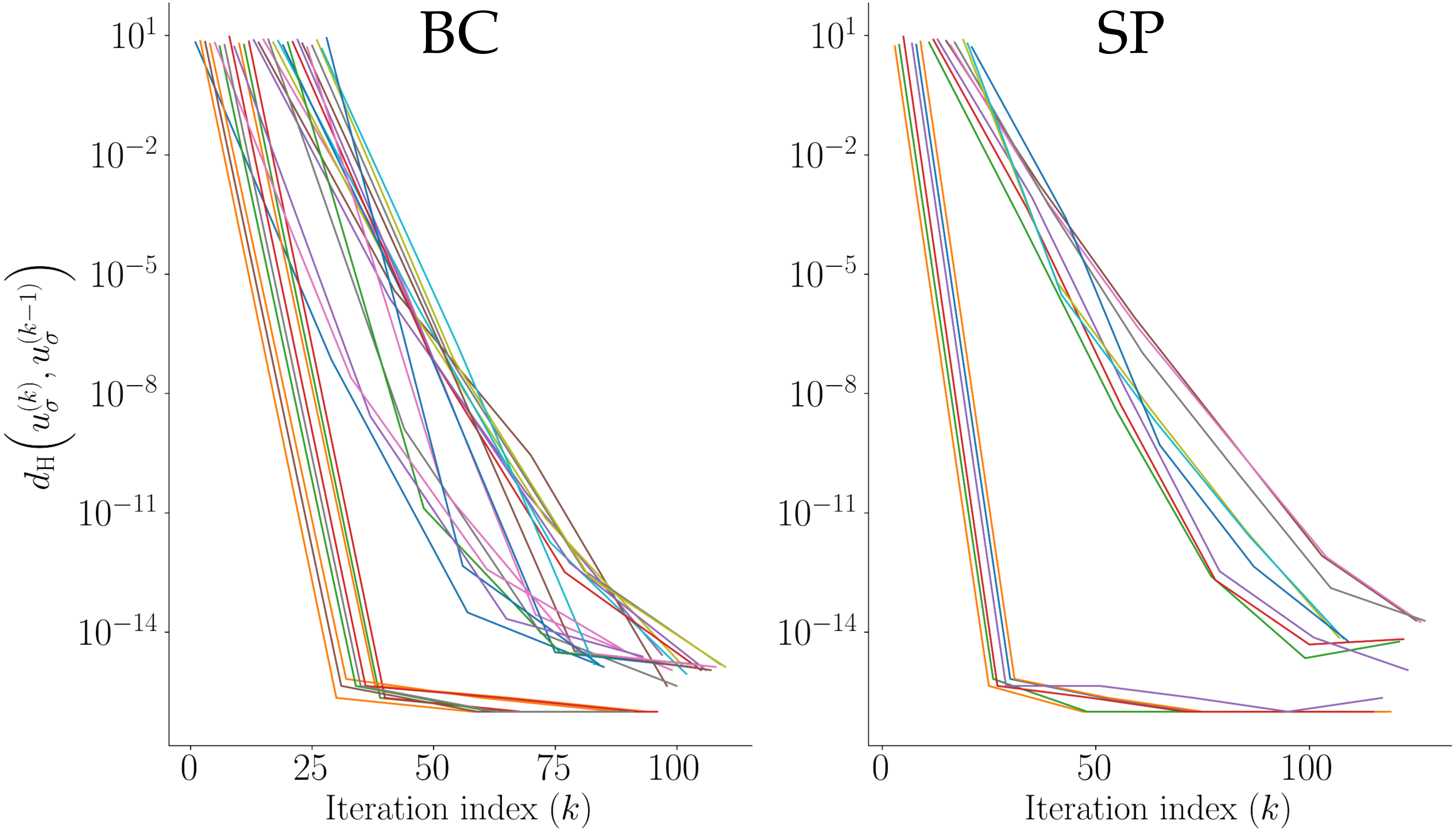
Case Study: Multicore Benchmark

Profiles:



Case Study: Multicore Benchmark

MSBP convergence:



Case Study: Multicore Benchmark

MSBP accuracy:

BC:

CPU core

Wasserstein distances $W_j := W(\hat{\mu}_{\hat{\tau}_j}, \mu_{\hat{\tau}_j})\ \forall j \in [\![s_{\text{int}} + 1]\!]$

j	W_1^j	W_2^j	W_3^j	W_4^j	W_5^j
1	4.077×10^{-5}	1.009×10^{-7}	2.131×10^{-7}	1.976×10^{-7}	1.509×10^{-7}
2	0	1.135×10^{-7}	2.342×10^{-7}	7.684×10^{-8}	8.805×10^{-8}
3	0	1.149×10^{-7}	1.534×10^{-7}	5.752×10^{-8}	6.538×10^{-8}
4	0	3.647×10^{-8}	2.146×10^{-7}	1.906×10^{-7}	9.713×10^{-8}

SP:

j	W_1^j	W_2^j	W_3^j	W_4^j	W_5^j
1	4.079×10^{-5}	1.062×10^{-7}	2.173×10^{-7}	2.110×10^{-7}	1.575×10^{-7}
2	0	1.048×10^{-7}	2.333×10^{-7}	7.303×10^{-8}	9.186×10^{-8}
3	0	1.065×10^{-7}	1.576×10^{-7}	6.394×10^{-8}	6.935×10^{-8}
4	0	5.553×10^{-8}	2.269×10^{-7}	1.857×10^{-7}	9.691×10^{-8}

Case Study: Context-dependent Resource Usage

Idea: account for software's resource allocation / execution context

$$\beta = (\beta_1, \beta_2, \ldots, \beta_b)^\top \in \boldsymbol{\mathcal{B}} \subset \mathbb{R}^b$$

Augment $\eta := [\xi \quad \beta]^\top \in \boldsymbol{\mathcal{X}} \times \boldsymbol{\mathcal{B}} \subset \mathbb{R}^{d+b}$ to form distributions

$$\mu_\sigma := \frac{1}{n_d n_b} \sum_{i=1}^{n_d} \sum_{j=1}^{n_b} \delta(\eta - \eta^{i,j}(\tau_\sigma)), \quad \forall \sigma \in [\![n_s]\!]$$

$$\Downarrow$$

Solve path-structured MSBP for $\mu_\tau, \quad \eta(\tau) \sim \mu_\tau \quad \forall \tau \in [\tau_1, \tau_{n_s}]$

$$\Downarrow$$

Apply Bayes' theorem to obtain $\quad \xi(\tau) \mid \beta \sim \dfrac{\mu_\tau}{\int_{\mathcal{X}} \mu_\tau d\xi}$

Profiling: Context-dependent Resource Usage

Benchmarks: dedup, canneal, fft, radiosity

$$N_{\mathsf{ca}} = N_{\mathsf{bw}} = 20 \implies \mathcal{B} = [\![N_{\mathsf{ca}}]\!] \times [\![N_{\mathsf{bw}}]\!]$$

Profile over $\mathcal{B}' = \{1, 5, 10, 15, 20\}^2 \subsetneq \mathcal{B},\ n_b = |\mathcal{B}'| = 25,\ n_d = 10 \quad \forall \beta \in \mathcal{B}'$

$$\tau = 0.05 \cdot (\sigma - 1)$$

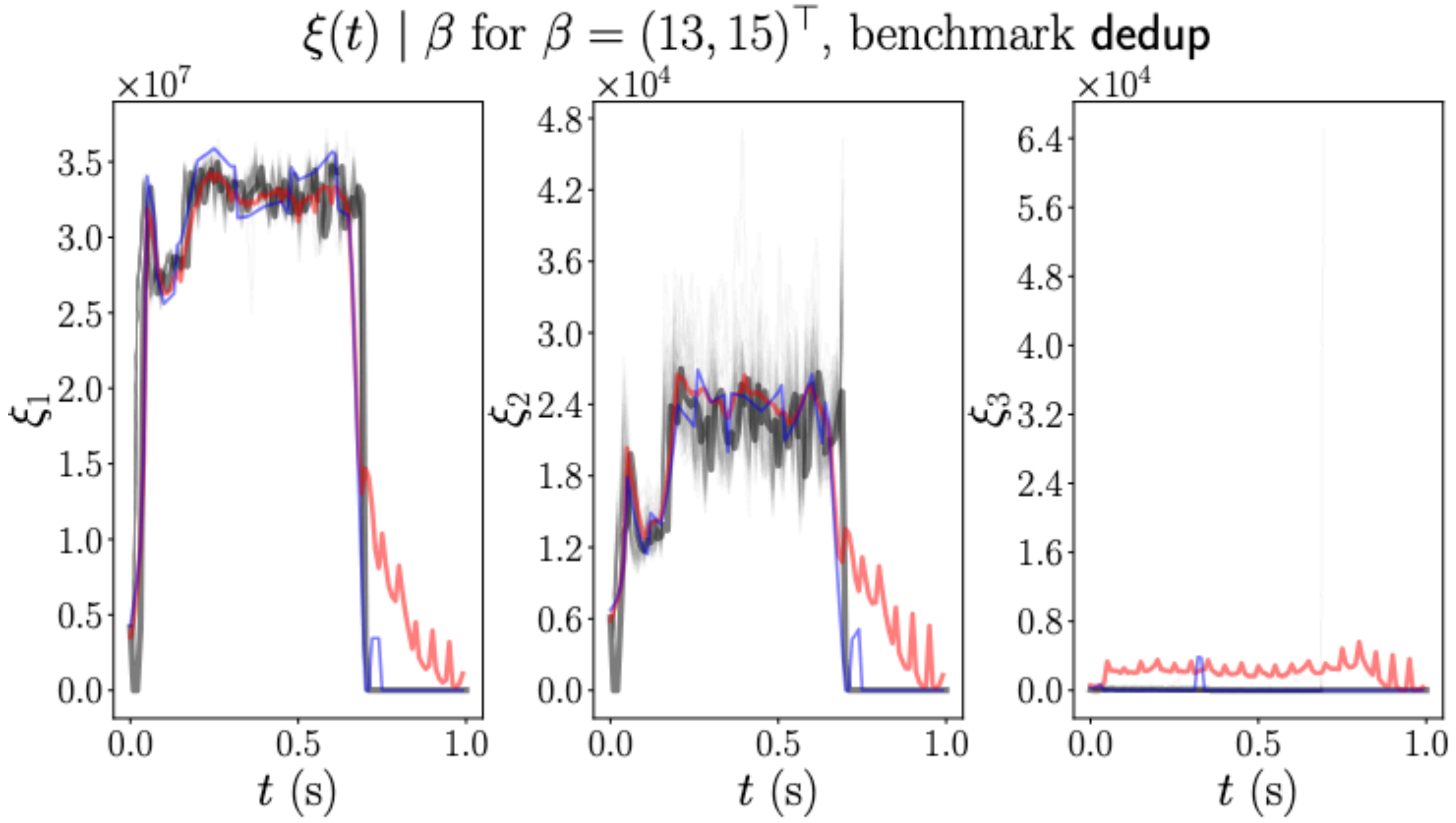
$$\Downarrow$$

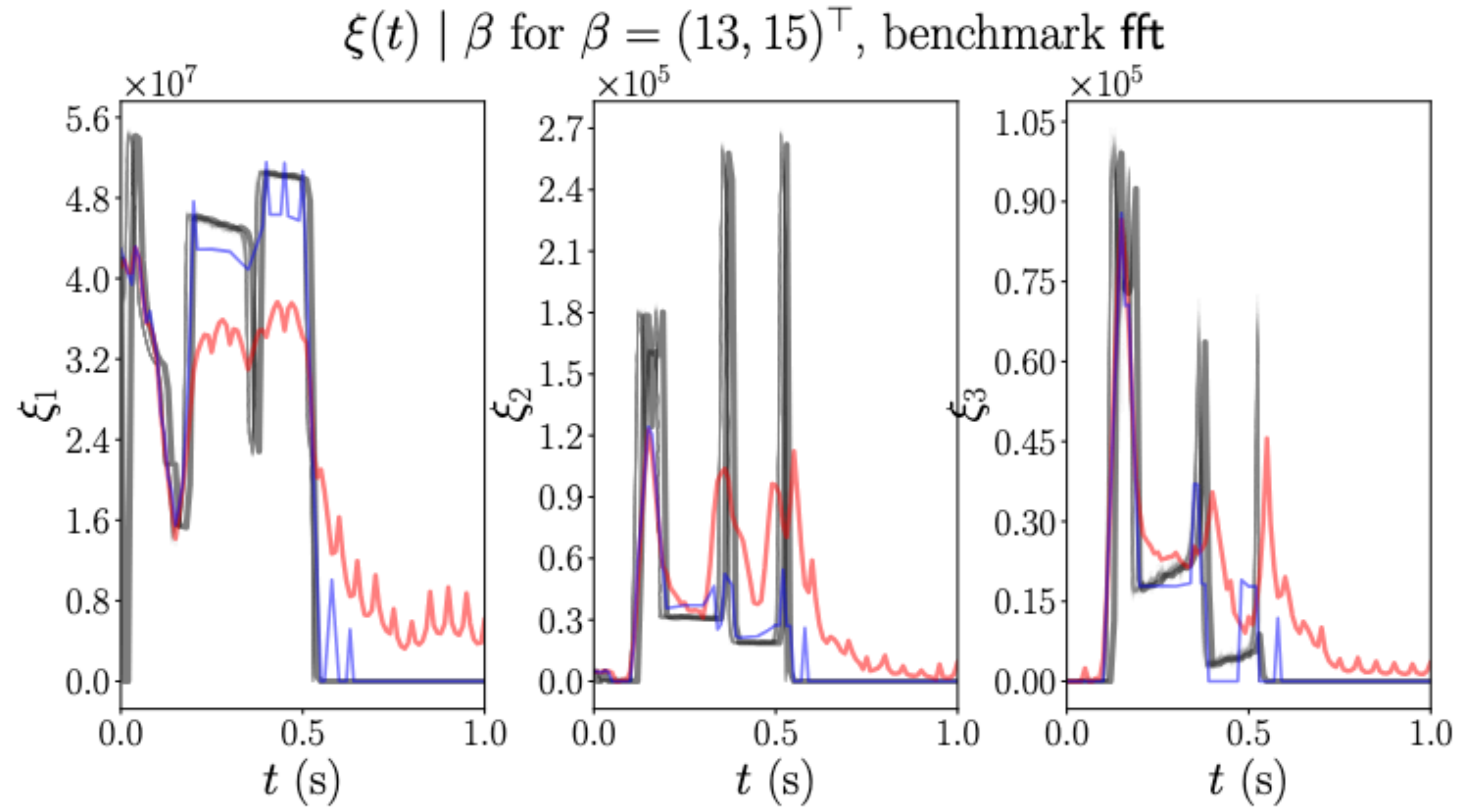
Generate $\xi(\tau)\,|\,\beta$ for all $\tau \in \{0, 0.01, \ldots, \tau_{n_s}\}, \beta \in \mathcal{B}$

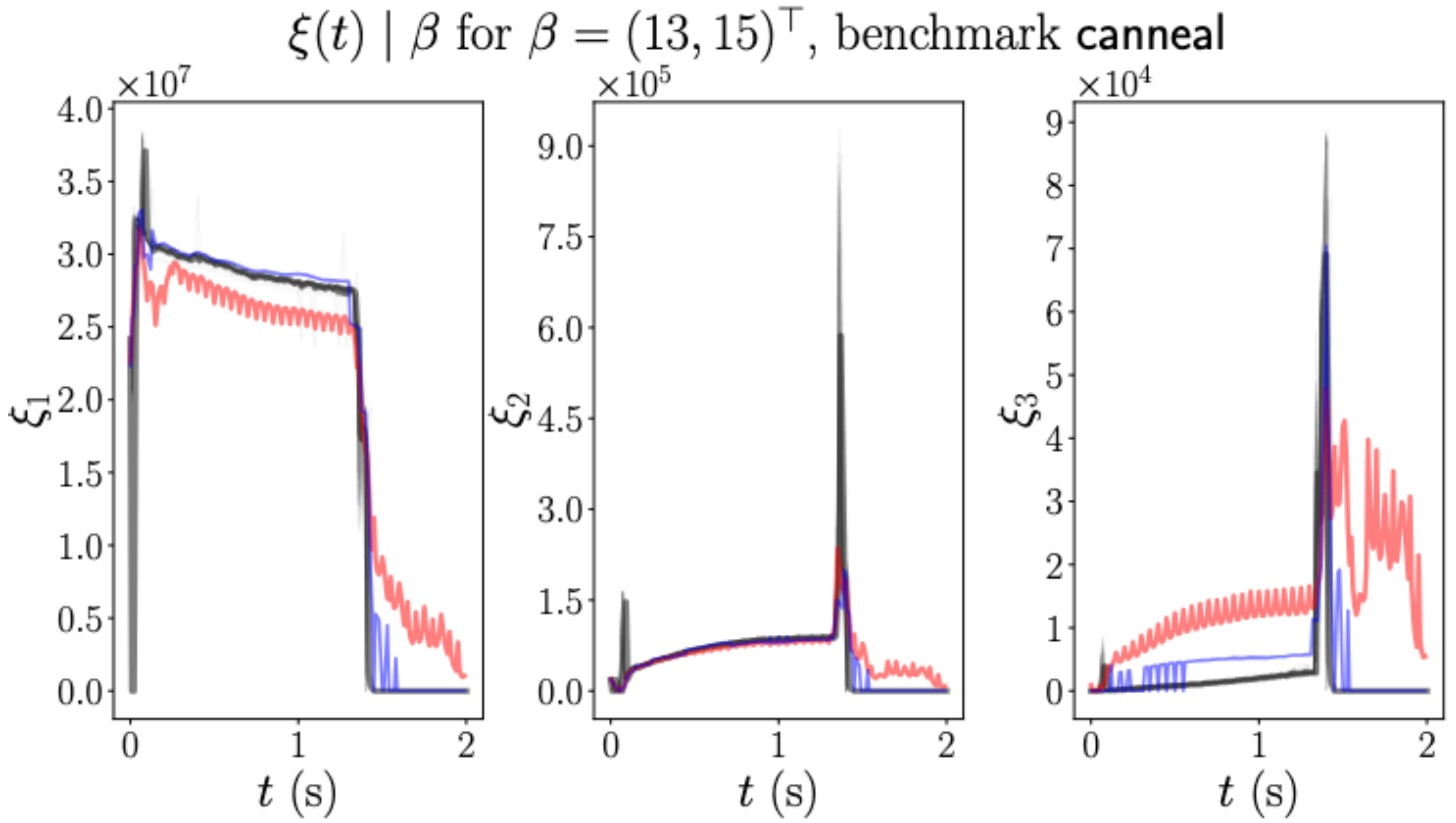
$$\Downarrow$$

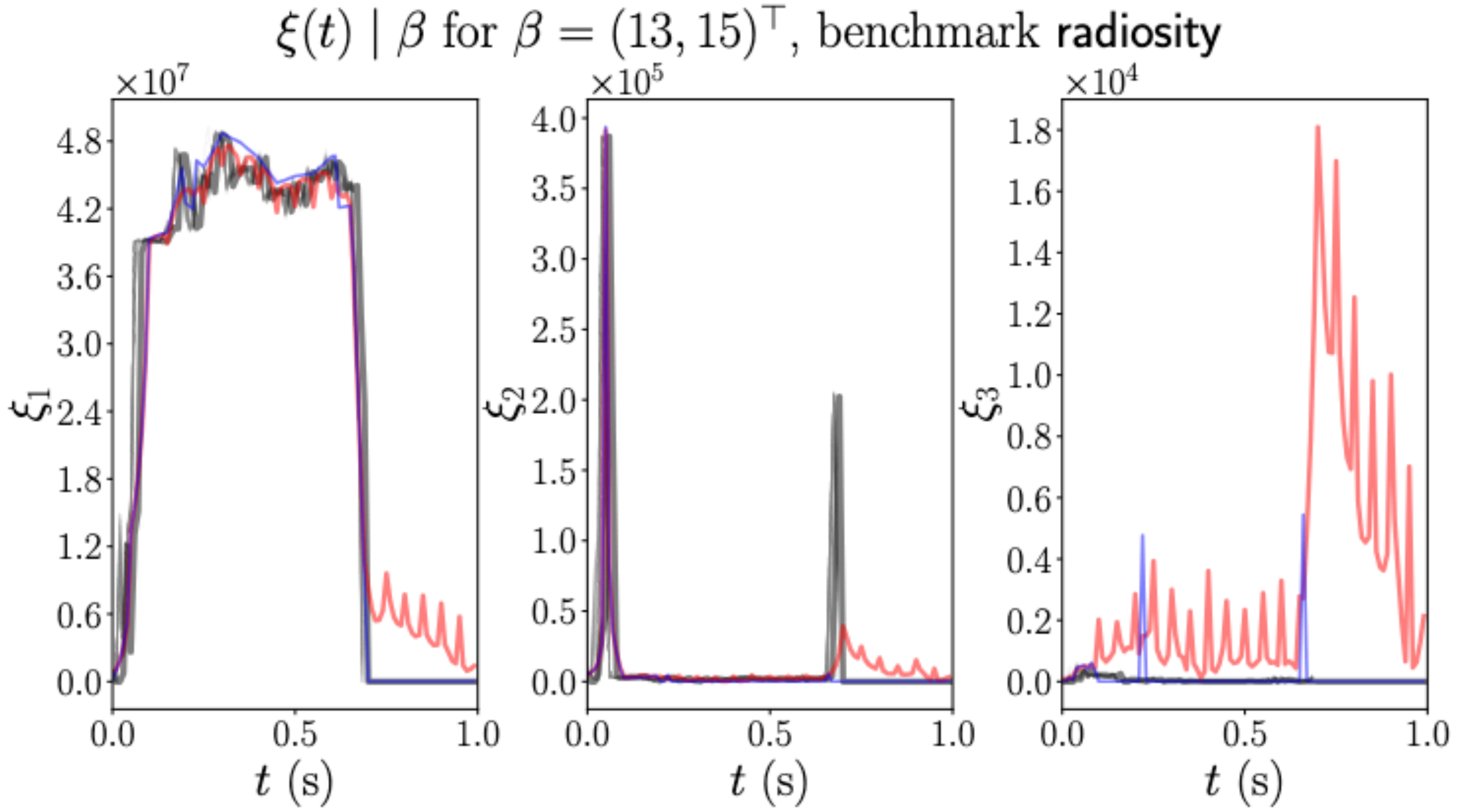
Generate *mean*, *max-likelihood*, and *avg. empirical* profiles for all $\beta \in \mathcal{B}$

Empirical Profiles for Benchmarks









Maximum-likelihood synthetic profile, mean synthetic profile, mean empirical profile, and all empirical profiles

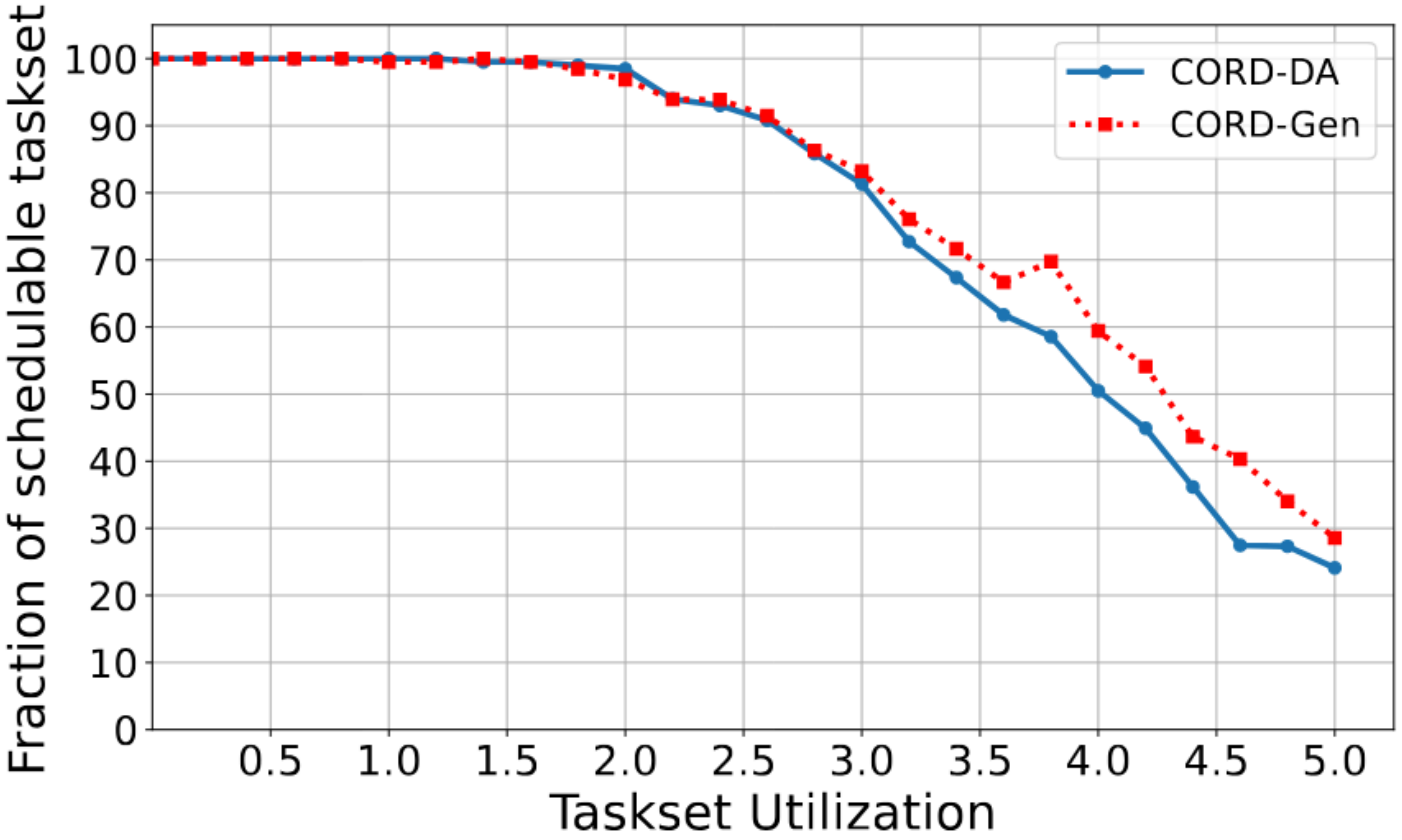
CORD: A Practical Application

Task scheduling *and* resource allocation

Profiles $\forall \beta \in \mathscr{B}$ required

$$\Downarrow$$

Generative profiling (MSBP)



Summary

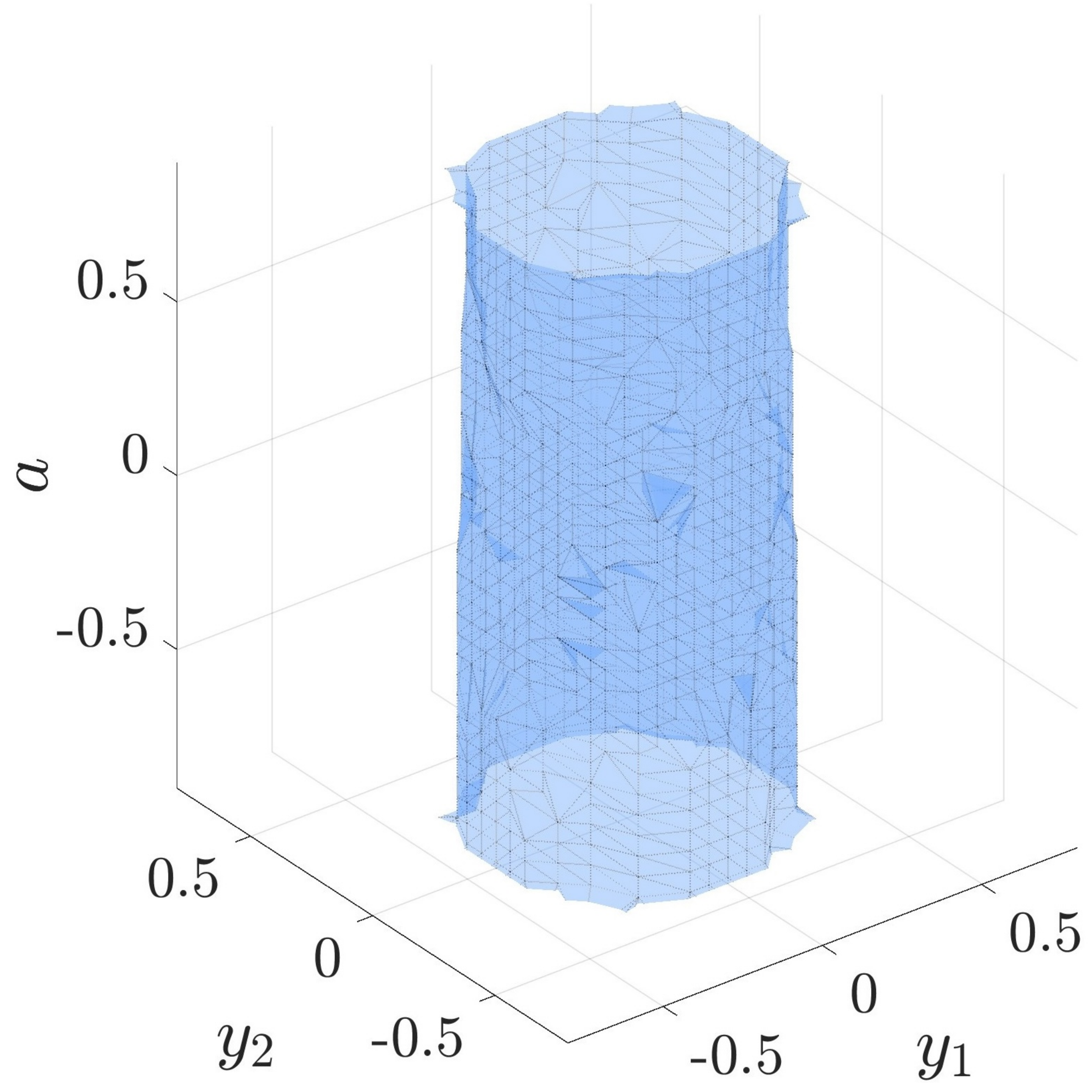
Tensor Optimization for Regularity of OT Maps

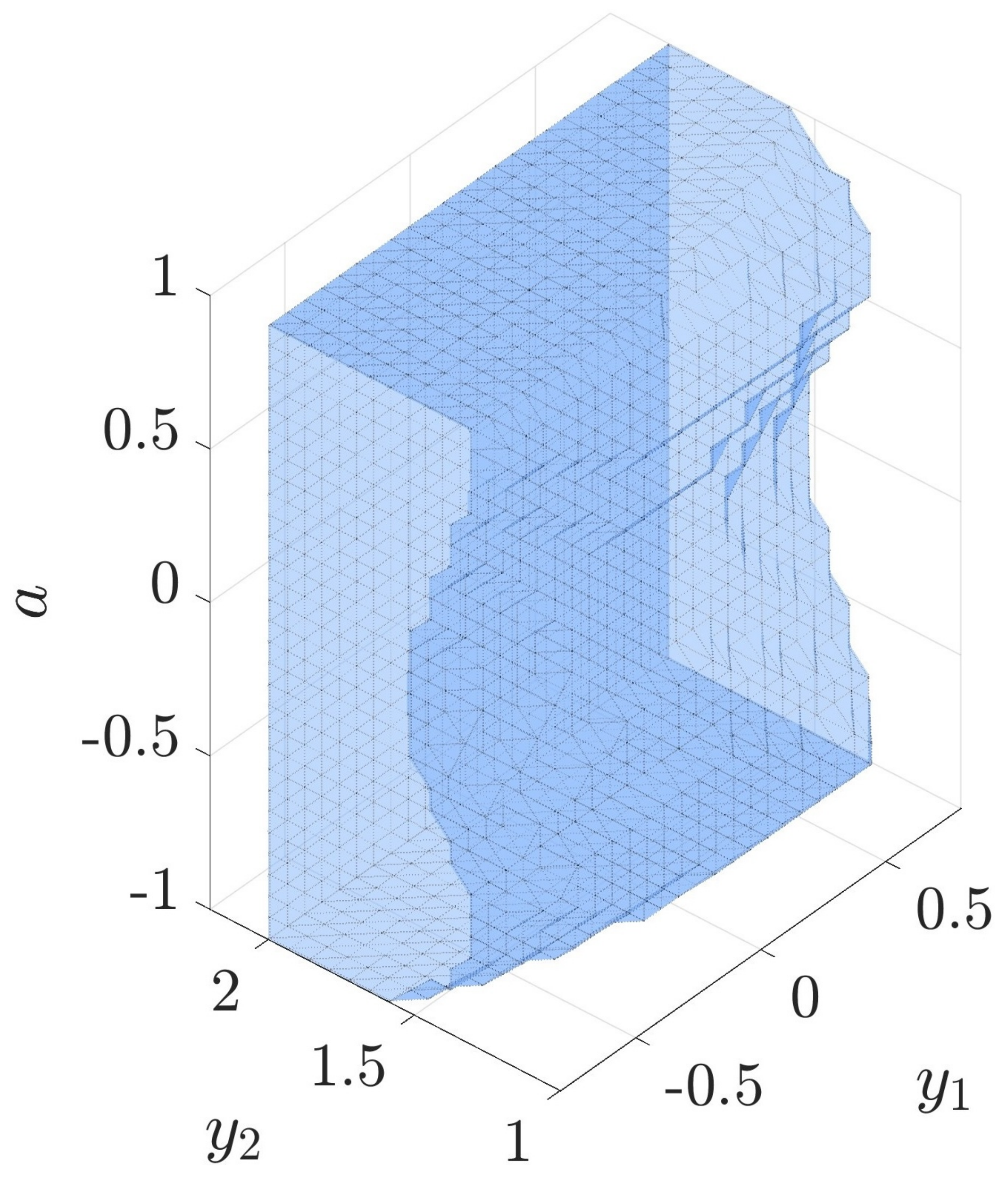
Polynomial complexity for forward problem

c rational over $\mathscr{X} \times \mathscr{Y}$ semi algebraic $\Longrightarrow$ SOS tightening $\Longrightarrow$ SDP

Forward problem: Computational certificate of NNCC and MTW(κ)

Inverse problem: Inner approximation of region of regularity





Tensor Optimization for Graph-structured SB

Graph-structured SBP $\Longrightarrow$ Solve via Sinkhorn

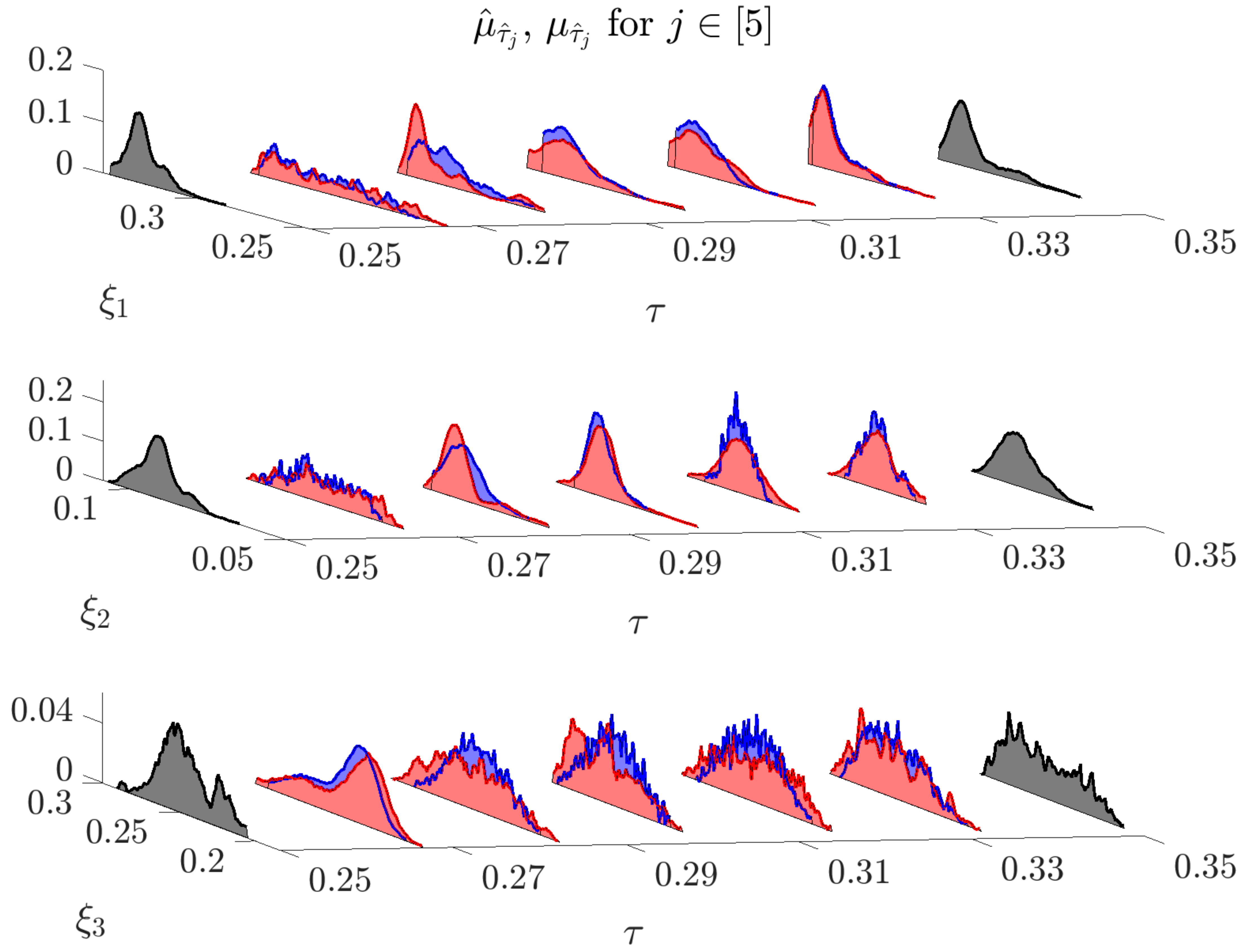
Complexity $\mathcal{O}(n^{|\Lambda|})$

$\Downarrow$

Path, BC, SP graph

$\Downarrow$

Complexity $\mathcal{O}((Js)n^2)$



Linear convergence

Reduce profiling workload

Publications

G.A.B., Gifford, R., Phan, L.T.X., & Halder, A. Path structured multimarginal Schrödinger bridge for probabilistic learning of hardware resource usage by control software. *American Control Conference 2024*

G.A.B., Gifford, R., Phan, L. T. X., & Halder, A. (2024). Stochastic Learning of Computational Resource Usage as Graph Structured Multimarginal Schrödinger Bridge. *Accepted, IEEE Trans. Control Syst. Technology, arXiv:2405.12463.*

Shivakumar, S., **G.A.B.**, Khan, G., & Halder, A. Sum-of-Squares Programming for Ma-Trudinger-Wang Regularity of Optimal Transport Maps. *arXiv:2412.13372.*

Gifford, R., Eisenklam, A., **G.A.B.**, Cai, Y., Sial, T., Phan, L. T. X., & Halder, A. CORD: Co-design of Resource Allocation and Deadline Decomposition with Generative Profiling. *arXiv:2501.08484.*

Future Work Plan

Winter-Summer 2025:

Improving efficiency and tractability in dimension of the SOS-based technique for verification of MTW conditions

Further application of graph-structured SBs for synthetic profiling (e.g., the use of synthetic profiles as system dynamics, accounting for asynchrony)

Generalization of the graph-structured SB problem to include enumeration of optimal graph structure on a set of distributions

Fall-Winter 2025-2026: Publication of theoretical and applied results

Spring-Summer 2026: Composition and defense of dissertation

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