Tensor Balancing on Statistical Manifold

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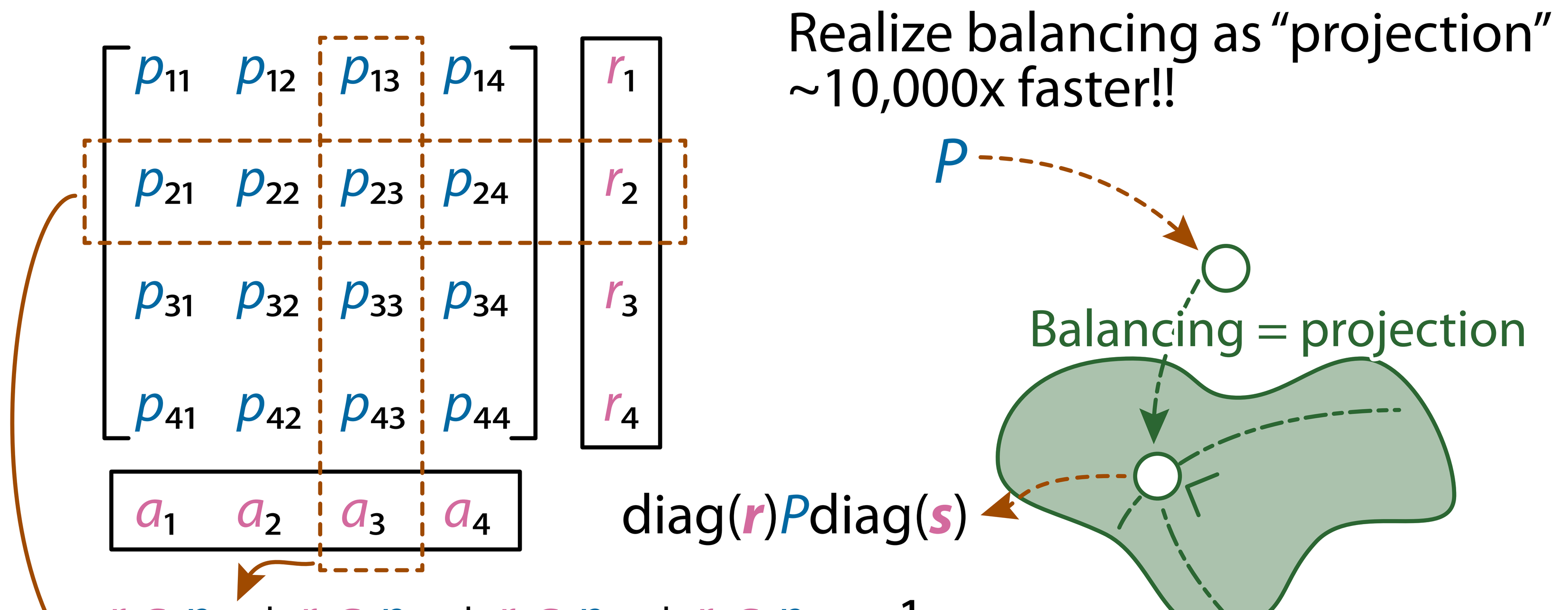
Results

- Balancing of higher order (more than two) tensors is firstly (theoretically) achieved
- A fast balancing algorithm with quadratic convergence using Newton's method (an existing algorithm is linear convergence)
- **[Theory]** We provide dually flat Riemannian manifold of probability distributions with the structured outcome space

Matrix (Tensor) Balancing

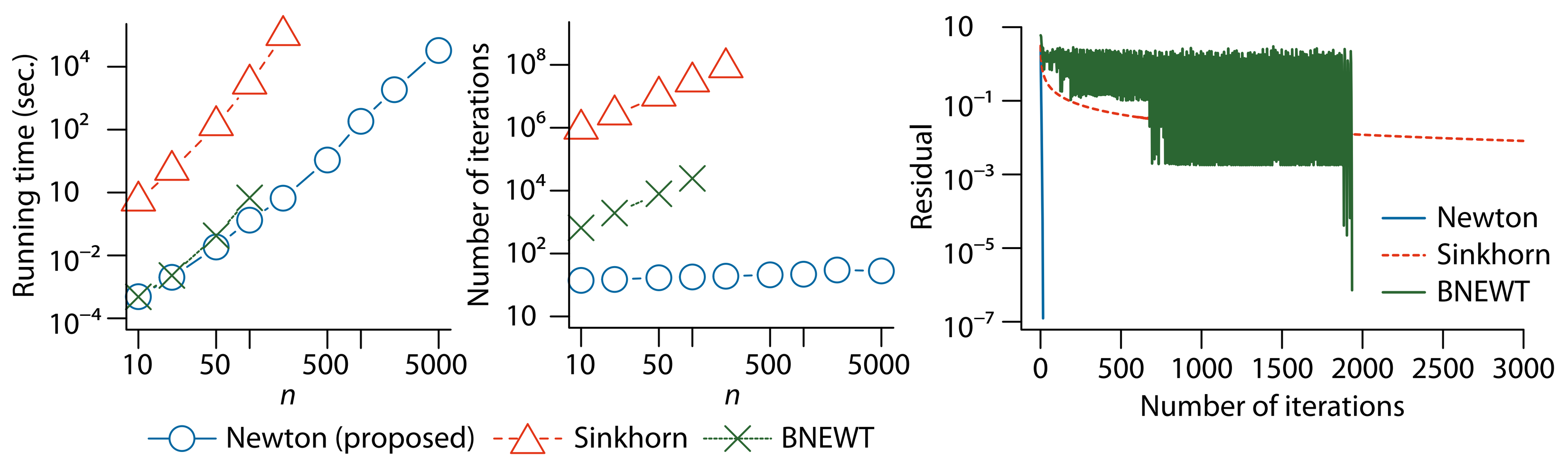


$r_1a_3p_{13} + r_2a_3p_{23} + r_3a_3p_{33} + r_4a_3p_{43} = 1$

$r_2a_1p_{21} + r_2a_2p_{22} + r_2a_3p_{23} + r_2a_4p_{24} = 1$

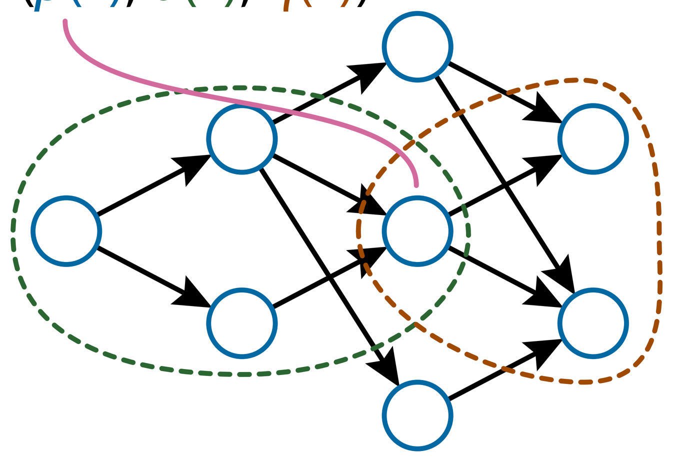
Use geometric structure in Information Geometry

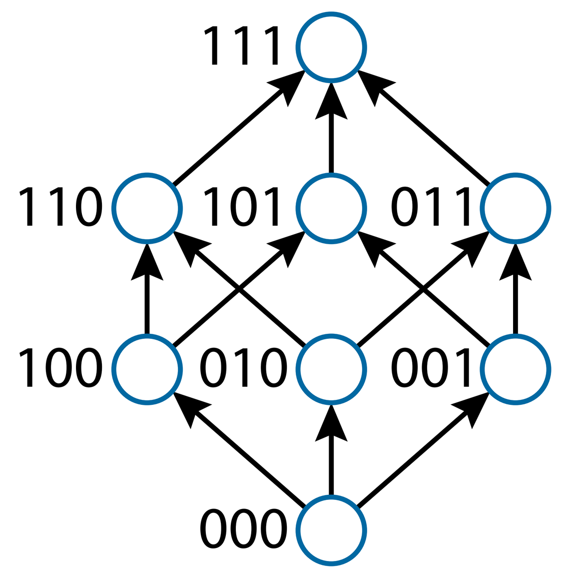
- **Matrix balancing**: Given a nonnegative matrix $P = (p_{ij}) \in \mathbb{R}_+^{n \times n}$, find $\boldsymbol{r}, \boldsymbol{s} \in \mathbb{R}^n$ s.t.
  $(RPS)\mathbf{1} = \mathbf{1}$ and $(RPS)^T\mathbf{1} = \mathbf{1}$
  - R = diag($\boldsymbol{r}$), S = diag($\boldsymbol{s}$), each entry is given as $p'_{ij} = p_{ij}r_is_j$
  - Applications: input-output analysis, Hi-C data analysis, the Sudoku puzzle, and Wasserstein metric approximation
  - Standard balancing algorithm: Sinkhorn–Knopp algorithm



Log-Linear Model on Poset

Each $x \in S$ has a triple: $(p(x), \theta(x), \eta(x))$





- Let $(S, \leq)$ be a poset (= DAG)
- A probability vector $p{:}S \to (0,1)$ s.t. $\sum_{x \in S} p(x) = 1$
  - (Normalized) weight for each node
- We introduce $\theta{:}S \to \mathbb{R}$ and $\eta{:}S \to \mathbb{R}$ as
  $\log p(x) = \sum_{s \leq x} \theta(s)$, $\eta(x) = \sum_{s \geq x} p(s)$
- Our model is generalization of the log-linear model on binary vectors with $\boldsymbol{x} \in \{0,1\}^n = S$:

$$\log p(\boldsymbol{x}) = \sum_i \theta^i x^i + \sum_{i<j} \theta^{ij} x^i x^j + \dots + \theta^{1 \dots n} x^1 x^2 \dots x^n - \psi,$$

$$\eta^i = \mathbf{E}[x^i] = \Pr(x^i = 1),$$

$$\eta^{ij} = \mathbf{E}[x^i x^j] = \Pr(x^i = x^j = 1), \dots$$

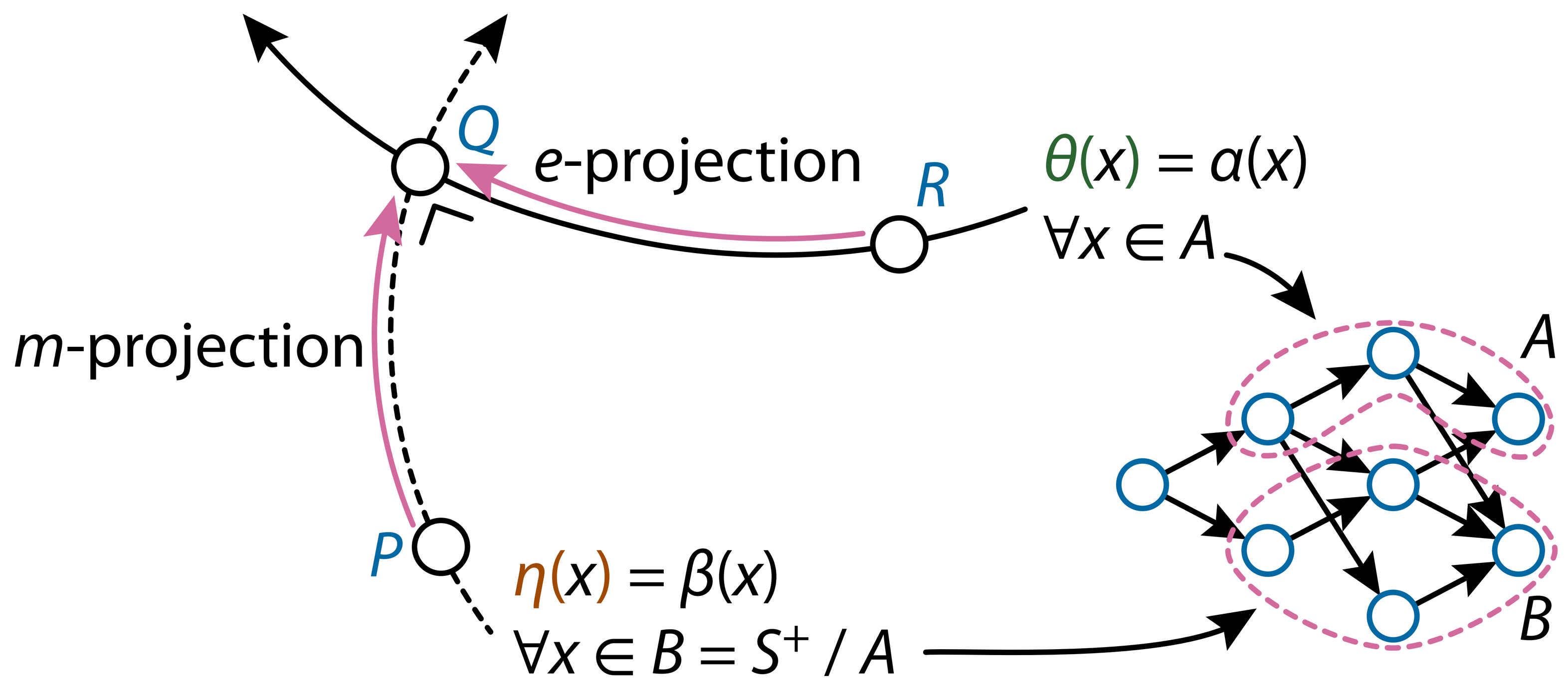
Dually Flat Structure

- θ and η form a dual coordinate system: $\nabla\psi(\theta) = \eta$, $\nabla\varphi(\eta) = \theta$
  - $\psi(\theta) = -\theta(\bot) = -\log p(\bot)$, $\varphi(\eta) = \sum_{x \in S} p(x) \log p(x)$
  - $\psi(\theta)$ and $\varphi(\eta)$ are connected via the Legendre transformation:
    $\varphi(\eta) = \max_{\theta'} \left(\theta'\eta - \psi(\theta')\right)$, $\theta'\eta = \sum_{x \in S \setminus \{\bot\}} \theta'(x)\eta(x)$
- The gradients: $g(\theta) = \nabla\nabla\psi(\theta) = \nabla\eta$, $g(\eta) = \nabla\nabla\varphi(\eta) = \nabla\theta$

$$\begin{cases} g_{xy}(\theta) = \dfrac{\partial \eta(x)}{\partial \theta(y)} = \displaystyle\sum_{s \in S} \zeta(x,s)\zeta(y,s)p(s) - \eta(x)\eta(y) \\ g_{xy}(\eta) = \dfrac{\partial \theta(x)}{\partial \eta(y)} = \displaystyle\sum_{s \in S} \mu(s,x)\mu(s,y)p(s)^{-1} \end{cases}$$

  - Zeta function: $\zeta(s,x) = 1$ if $s \leq x$, $\zeta(s,x) = 0$ otherwise
  - Möbius function: $\mu{:}S \times S \to \mathbb{Z}$ satisfying $\zeta\mu = I$
  - The manifold $(\boldsymbol{\mathcal{S}}, g(\xi))$ is a Riemannian manifold with the set $\boldsymbol{\mathcal{S}}$ of probability vectors and the Riemannian metric $g(\xi)$

e-Projection and *m*-Projection



- *e*-projection and *m*-projection can be computed by Newton's Method
- Each step of Newton's method in *e*-projection:

$$\begin{bmatrix} \vdots \\ \eta^{(t)}_{P_\beta}(x) - \beta(x) \\ \vdots \end{bmatrix} + J \begin{bmatrix} \vdots \\ \theta^{(t+1)}_{P_\beta}(y) - \theta^{(t)}_{P_\beta}(y) \\ \vdots \end{bmatrix} = \mathbf{0},$$

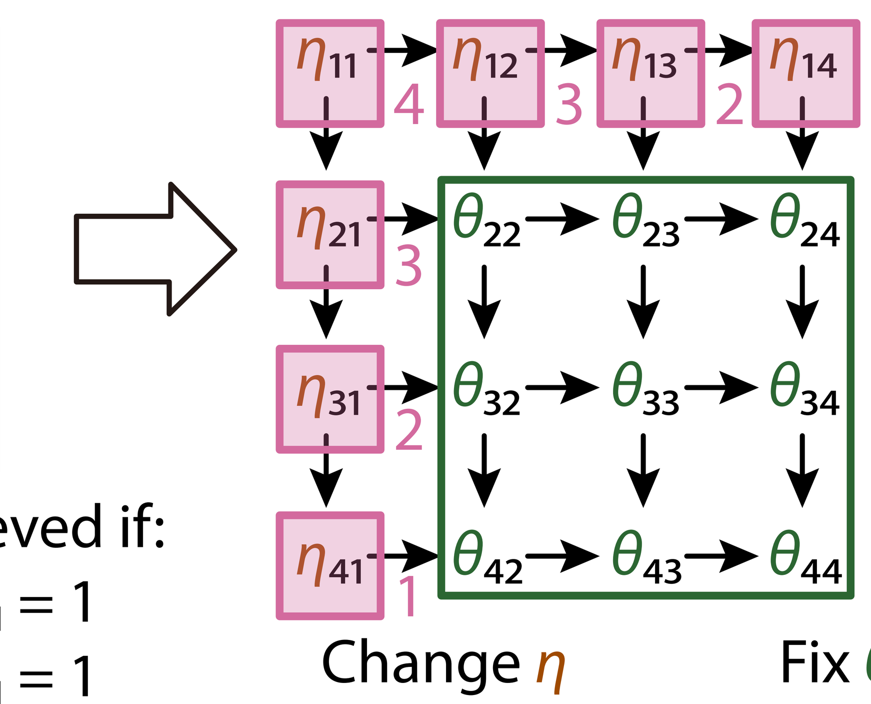
  - J is the $|B| \times |B|$ Jacobian matrix given as

$$J_{xy} = \frac{\partial \eta^{(t)}_{P_\beta}(x)}{\partial \theta^{(t)}_{P_\beta}(y)} = \sum_{s \in S} \zeta(x,s)\zeta(y,s)p_\beta^{(t)}(s) - \eta^{(t)}_{P_\beta}(x)\eta^{(t)}_{P_\beta}(y)$$

for each $x, y \in B$

Balancing = *e*-Projection

$$\begin{bmatrix} p_{11} & p_{12} & p_{13} & p_{14} \\ p_{21} & p_{22} & p_{23} & p_{24} \\ p_{31} & p_{32} & p_{33} & p_{34} \\ p_{41} & p_{42} & p_{43} & p_{44} \end{bmatrix}$$



Matrix balancing is achieved if:

$\eta_{11} = 4, \eta_{21} = 3, \eta_{31} = 2, \eta_{41} = 1$

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