Approximating Optimal Transport w/ Positive LPs

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Towards Optimal Running Times for Optimal Transport

Jose Blanchet, Arun Jambulapati, Carson Kent, Aaron Sidford

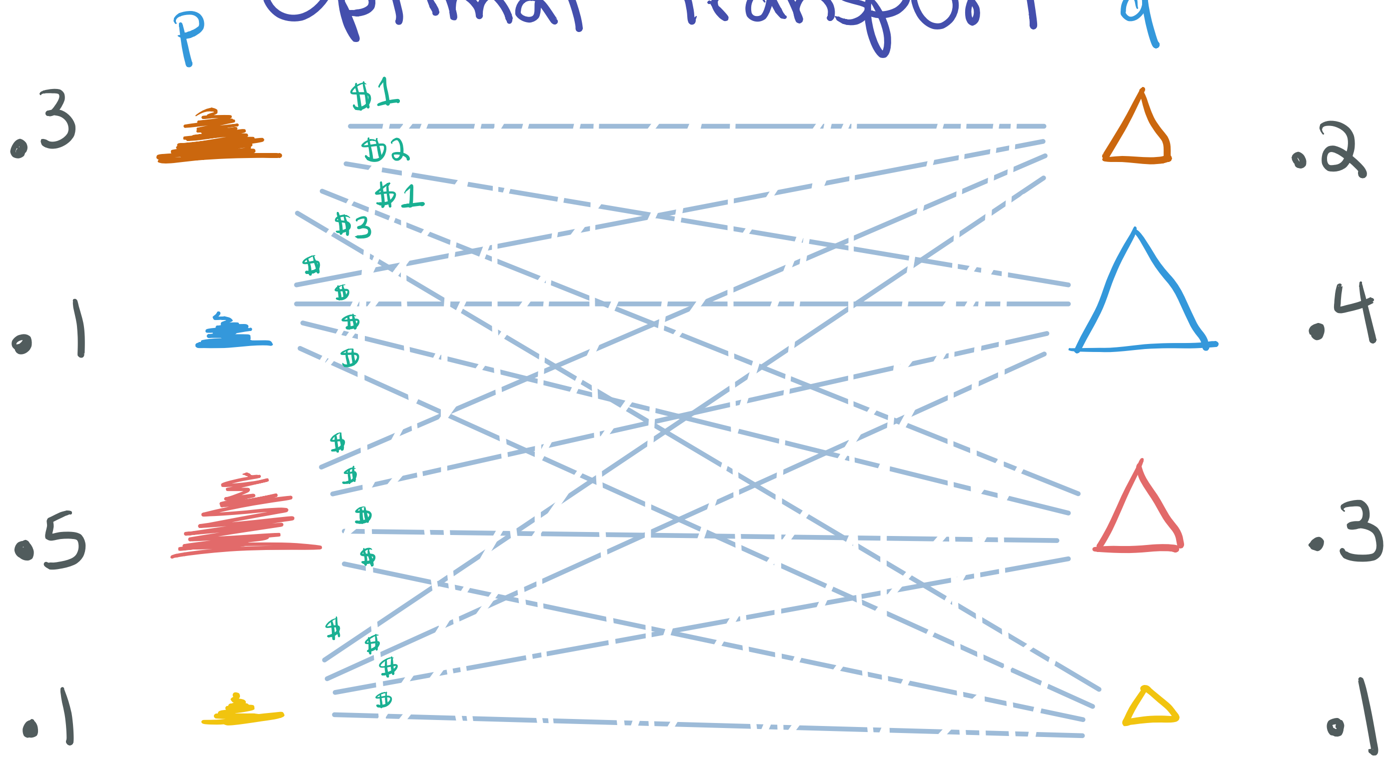
(Submitted on 17 Oct 2018)

In this work, we provide faster algorithms for approximating the optimal transport distance, e.g. earth mover's distance, between two discrete probability distributions $\mu, \nu \in \Delta^n$. Given a cost function $C : [n] \times [n] \to \mathbb{R}_{\geq 0}$ where $C(i,j)$ quantifies the penalty of transporting a unit of mass from i to j, we show how to compute a coupling X between r and c in time $\widetilde{O}\left(n^2/\varepsilon\right)$ whose expected transportation cost is within an additive ε of optimal, where we have assumed that the largest entry of C is bounded by a constant. This improves upon the previously best known running time for this problem of $\widetilde{O}\left(\min\left\{n^{9/4}/\varepsilon, n^2/\varepsilon^2\right\}\right)$.
We achieve our results by providing reductions from optimal transport to canonical optimization problems for which recent algorithmic efforts have provided nearly-linear time algorithms. Leveraging nearly linear time algorithms for solving packing linear programs and for solving the matrix balancing problem, we obtain two separate proofs of our stated running time.
Moreover, we show that further algorithmic improvements to our result would be surprising in the sense that any improvement would yield an $o(n^{2.5})$ algorithm for \textit{maximum cardinality bipartite matching}, for which currently the only known algorithms for achieving such a result are based on fast-matrix multiplication.

Subjects: Data Structures and Algorithms (cs.DS)

Independent Work

Optimal Transport

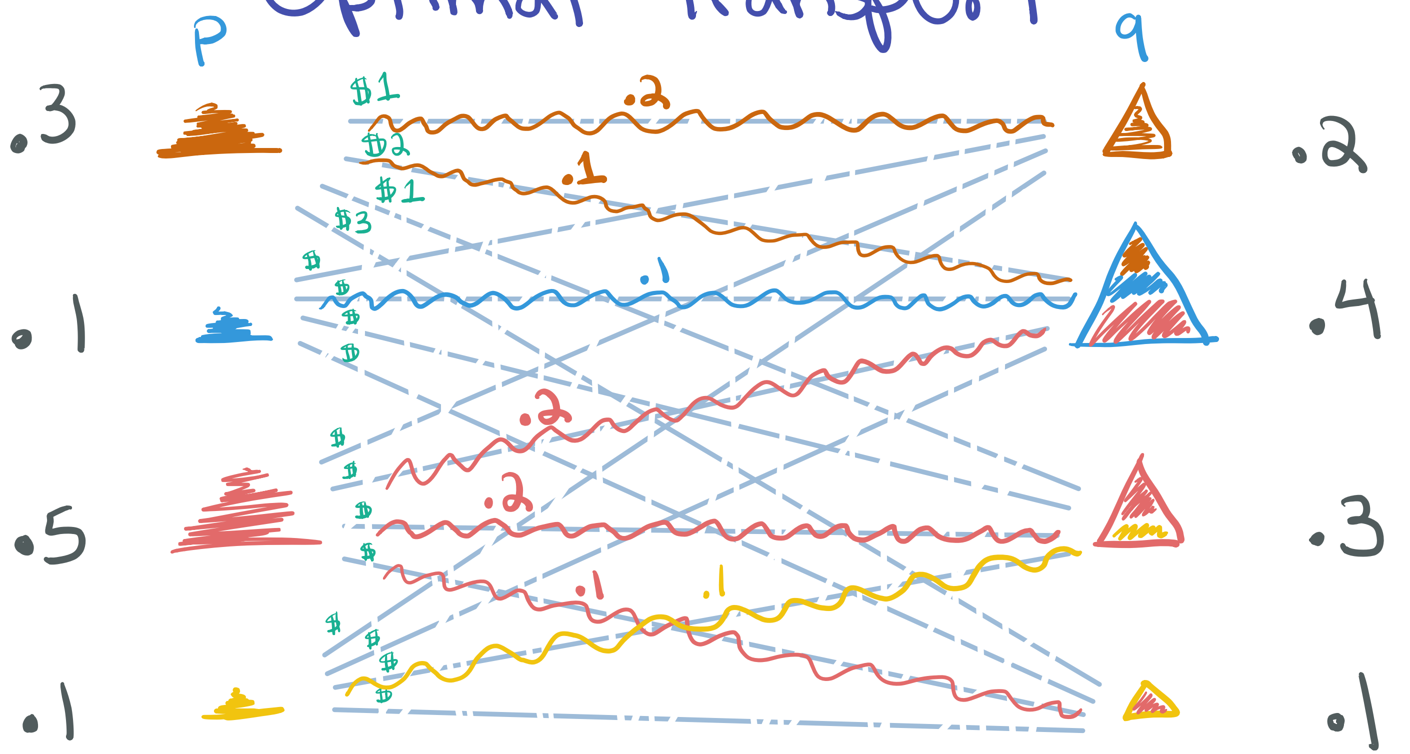


Input: two discrete distributions $p \in \Delta^{\ell}$, $q \in \Delta^{k}$

per-unit costs $\{c_{ij} : i \in [k], j \in [\ell]\}$ for transporting mass

Goal: transport all probability mass from p to q w/ minimum cost

Optimal Transport



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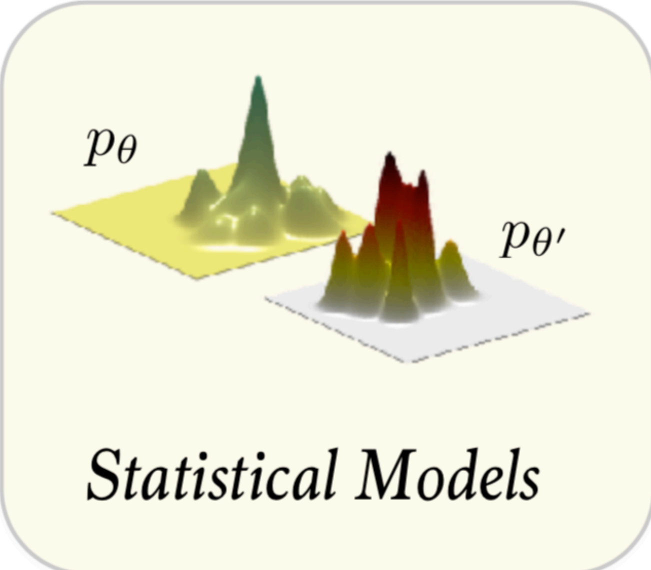
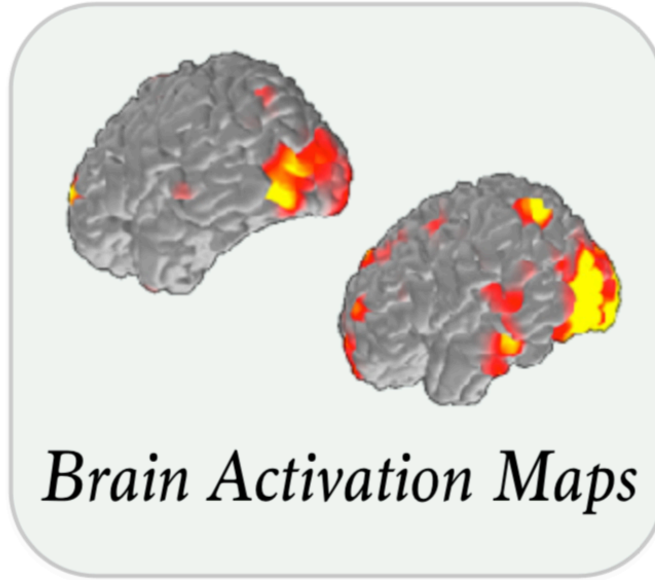
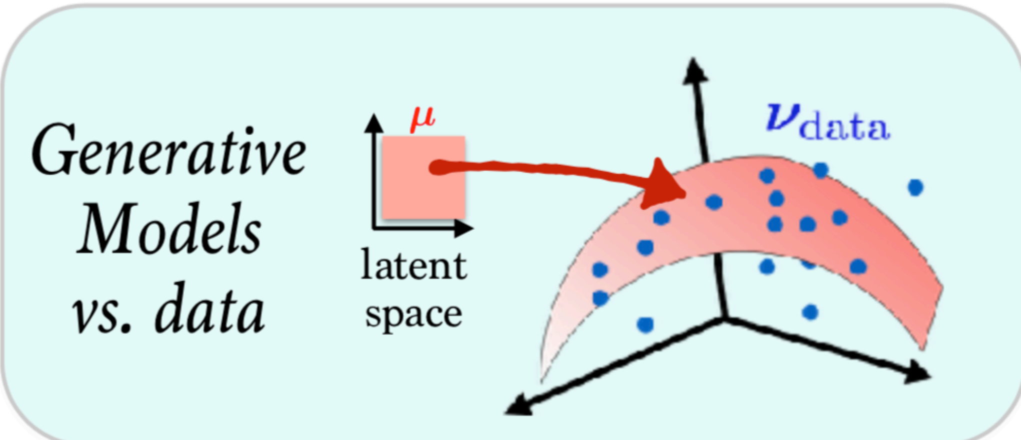
Applications



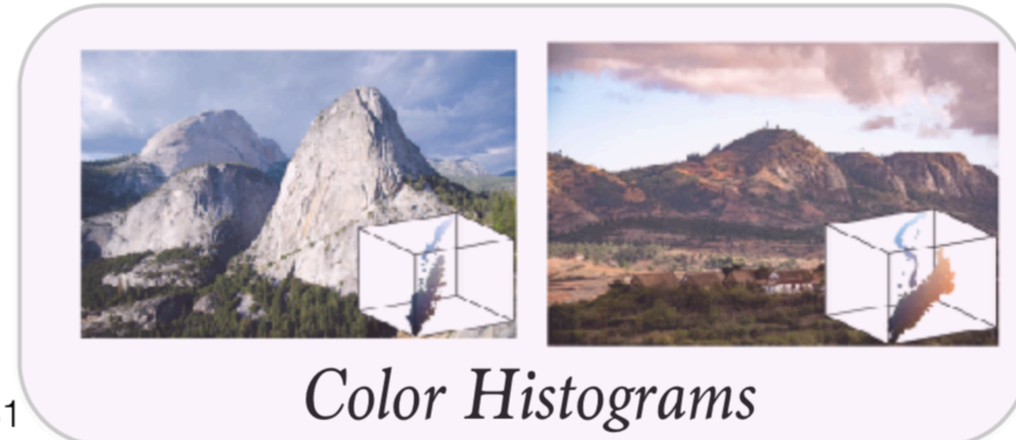
Statistical Models

Bags of features


Brain Activation Maps

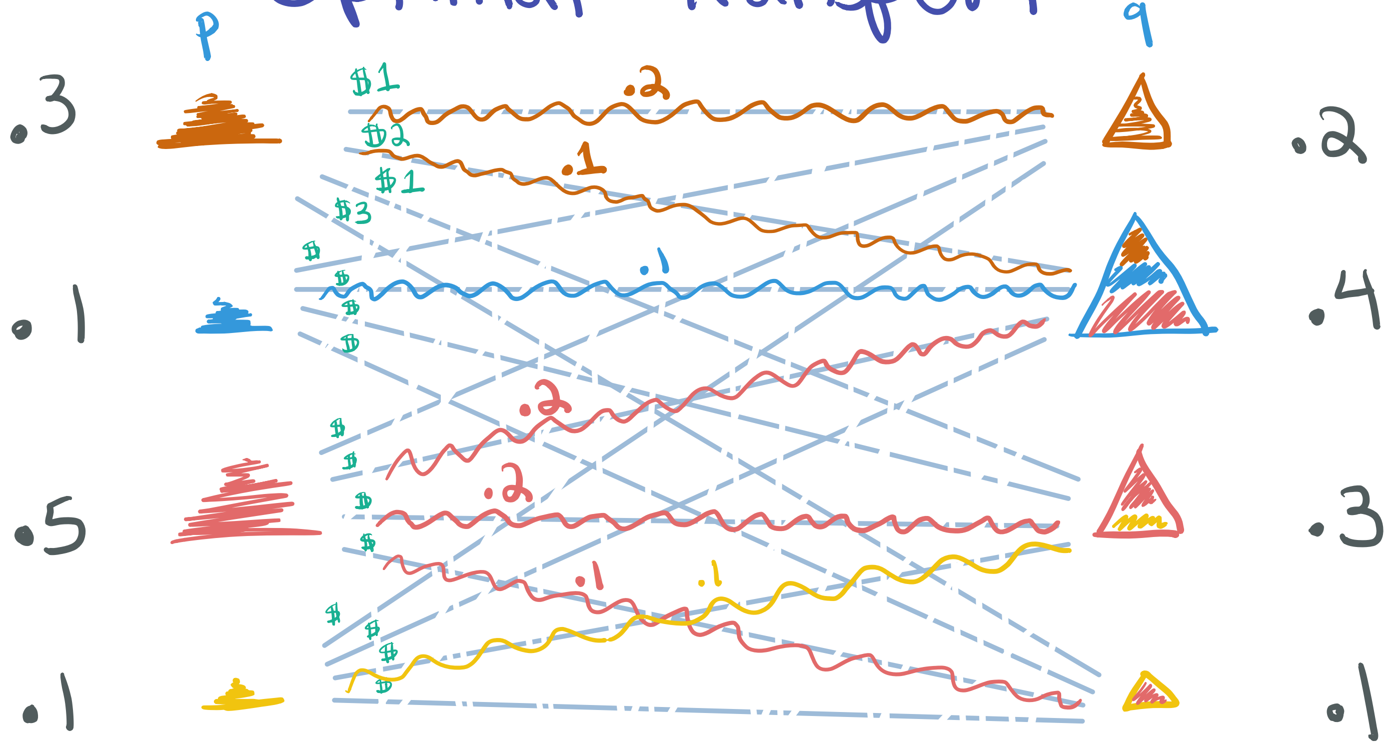


Generative Models vs. data


Color Histograms

Stolen from slides by Marco Cuturi

Optimal Transport



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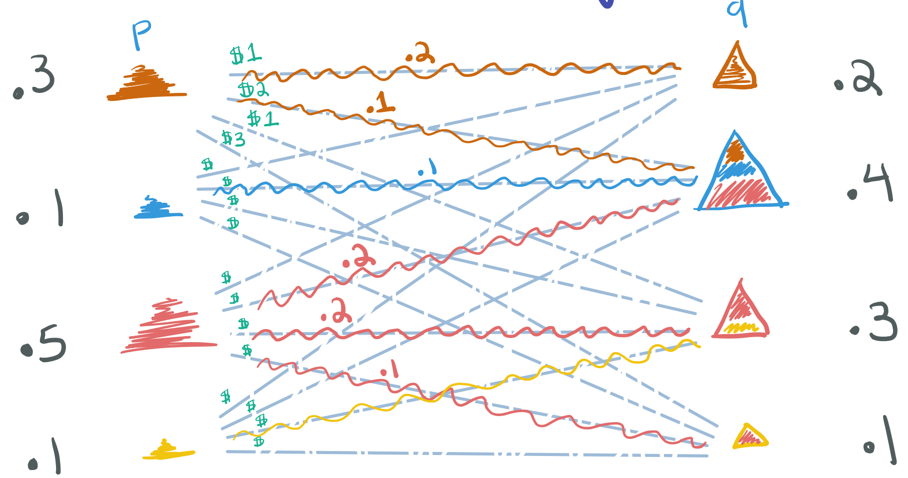
Optimal Transport as an LP



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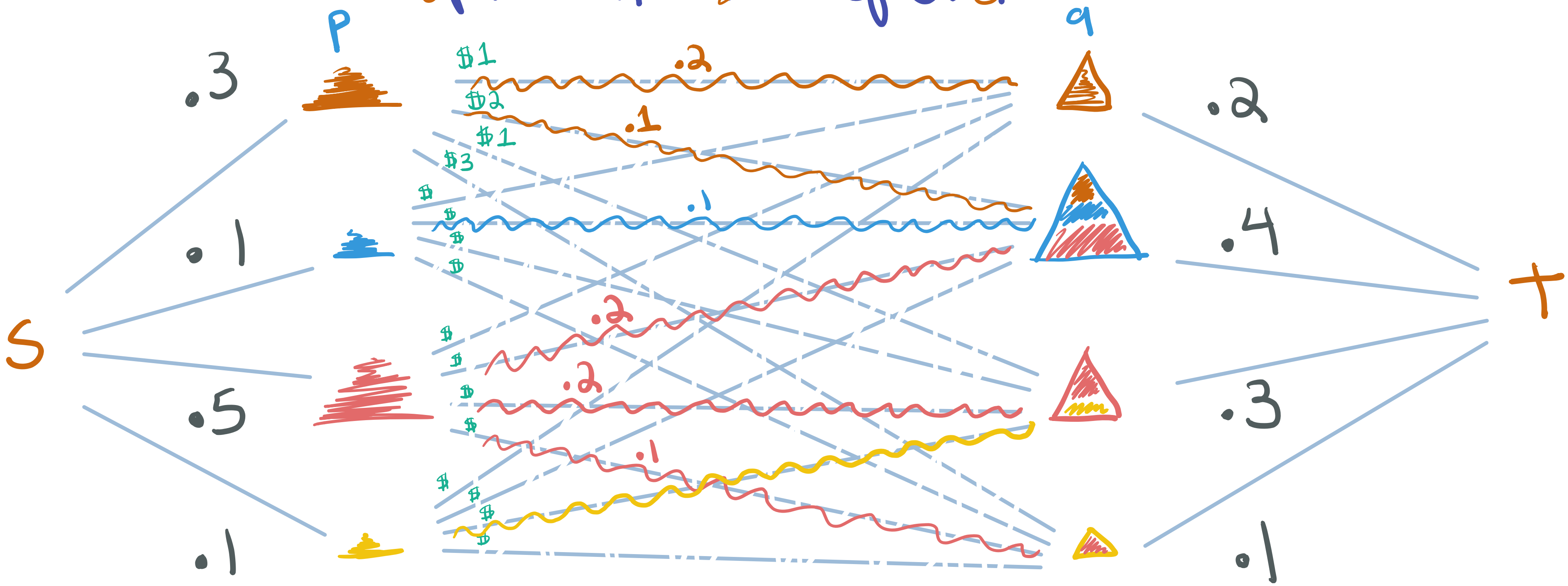
Goal: minimize $\sum_{i=1}^{k} \sum_{j=1}^{\ell} c_{ij}\, p_j\, X_{ij}$ over $X \in \mathbb{R}_{\geq 0}^{k \times \ell}$

s.t. $\sum_{j=1}^{\ell} X_{ij}\, p_j = q_i$ for $i \in [k]$

$\sum_{i=1}^{k} X_{ij} = 1$ for $j \in [\ell]$

(X_{ij} = fraction of p_j's mass transported to q_i)

~~Optimal Transport~~ Min-cost flow



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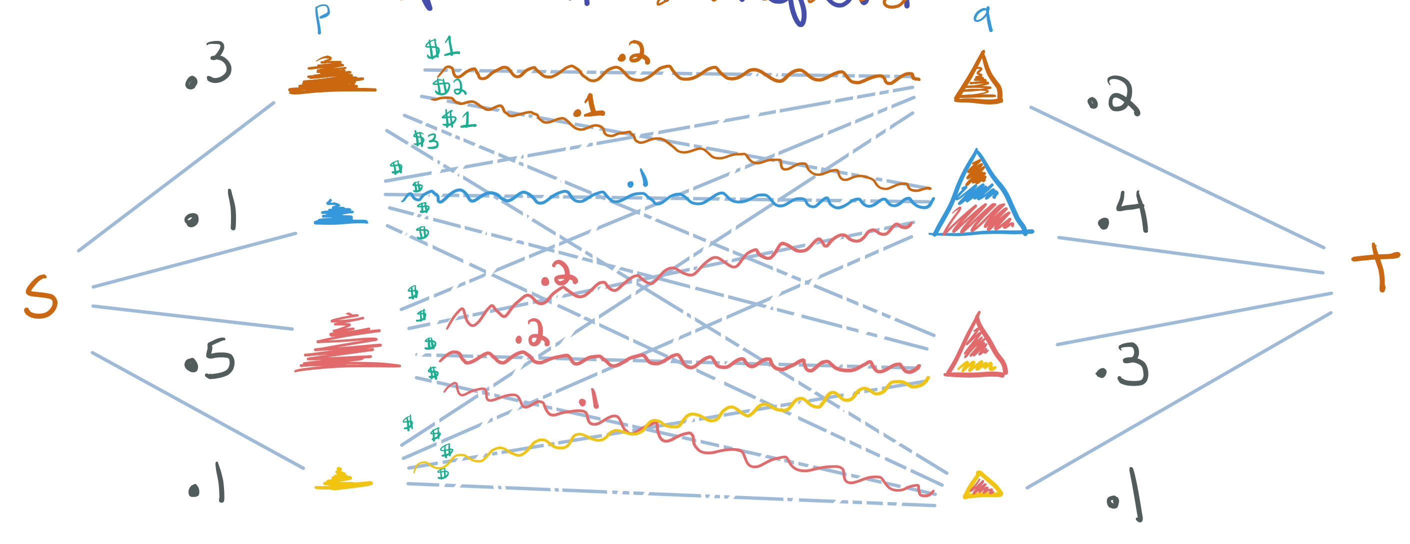
per-unit costs $\{c_{ij} : i \in [k], j \in [\ell]\}$ for ~~transporting mass~~ routing flow

Goal: ~~transport~~ route all ~~probability mass~~ flow from

p to q w/ minimum cost

~~Optimal Transport~~ Min-cost flow



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Transport = flow $\Rightarrow \tilde{O}(k\ell\sqrt{k\ell})$ exact algorithm

Recent interest in "nearly linear time approximations" in ML community

δ-additive approximations

Transport all probability mass (exactly) with cost within an additive δ of OPT cost

$$\sum_{i=1}^{k} \sum_{j=1}^{\ell} c_{ij} p_j x_{ij} \leq \text{OPT} + \delta$$

$$\left.\begin{aligned} \sum_{j=1}^{\ell} x_{ij} p_j &= q_i \quad \text{for } i \in [k] \\ \sum_{i=1}^{k} x_{ij} &= 1 \quad \text{for } j \in [\ell] \end{aligned}\right\} \text{exact}$$

δ-additive error:

relative to what? normalization?

Existing algorithms parametrized by

$$\|C\|_\infty = \max_{i,j} C_{ij} = \text{max cost}$$

We also consider

$$\langle p, Cq \rangle = \sum_{i,j} p_i C_{ij} q_j = \text{average cost w/r/t } p \times q$$

note that $\langle p, Cq \rangle \leq \|C\|_\infty$

Recent results in approximating transport

[Cuturi 2013]: reduces to convex-min / matrix-scaling by entropy-type regularizer ("Sinkhorn distance")

[Altschuler, Weed, Rigollet 2017] $\tilde{O}\left(k\ell\left(\frac{\|C\|_\infty}{\delta}\right)^3\right)$ Time

[Cohen, Madry, Tsipras, Vladu 2017] $\tilde{O}\left(k\ell\frac{\|C\|_\infty^3}{\delta^2}\right)$ time

[Dvurechensky, Gasnikov, Kroshnin 2018] $\tilde{O}\left(k\ell\left(\frac{\|C\|_\infty}{\delta}\right)^2\right)$ Time

$$\|C\|_\infty = \max_{i,j} C_{ij}$$

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	time	algorithms & techniques
[Altschuler, Weed, Rigollet 2017]	$\tilde{O}\left(k\ell\left(\frac{\lVert C\rVert_\infty}{\delta}\right)^3\right)$	Sinkhorn-Knopp matrix scaling
[Cohen, Madry, Tsipras, Vladu 2017]	$\tilde{O}\left(k\ell\frac{\lVert C\rVert_\infty^3}{\delta^2}\right)$	Boxed-Newton method for matrix scaling w/ fast Laplacian solvers
[Dvurechensky, Gasnikov, Kroshnin 2018]	$\tilde{O}\left(k\ell\left(\frac{\lVert C\rVert_\infty}{\delta}\right)^2\right)$	Sinkhorn-Knopp + accelerated gradient descent analysis

$$\lVert C\rVert_\infty = \max_{i,j} C_{ij}$$

Meanwhile in TCS...

[Sherman, SODA 2017]

$(1+\varepsilon)$-relative approximation in $\tilde{O}(m^{1+o(1)})$ time w/r/t shortest path metric induce by C

here m = #"nonzeroes" in C
(or # edges in graph)

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$$\lVert C\rVert_\infty = \max_{i,j} C_{ij}$$

New sequential runtimes (improving $\tilde{O}\left(k\ell\left(\frac{\|C\|_\infty}{\delta}\right)^2\right)$)

① $\tilde{O}\left(k\ell\left(\frac{\langle q, C_p \rangle}{\delta}\right)^2\right)$ deterministic time

② $\tilde{O}\left(k\ell\,\frac{\|C\|_\infty}{\delta}\right)$ randomized time

New parallel bounds (both deterministic)

③ $\tilde{O}\left(\left(\frac{\langle q, C_p \rangle}{\delta}\right)^3\right)$ depth, $\tilde{O}\left(k\ell\left(\frac{\langle p, C_q \rangle}{\delta}\right)^2\right)$ work

④ $\tilde{O}\left(\left(\frac{\|C\|_\infty}{\delta}\right)^2\right)$ depth, $\tilde{O}\left(k\ell\left(\frac{\|C\|_\infty}{\delta}\right)^2\right)$ work

High level ideas

① Optimal transport is a (positive) LP

② We have really fast relative approximations for positive LPs

③ Make connection between relative approximations and additive approximations by fixing/rounding relative vs additive

(or upper-bounding OPT)

The easiest upper bound

Recall: Goal: minimize $\sum_{i=1}^{k}\sum_{j=1}^{\ell} C_{ij}\, p_j\, X_{ij}$ over $X \in \mathbb{R}_{\geq 0}^{k\times \ell}$

s.t. $\sum_{j=1}^{\ell} X_{ij}\, p_j = q_i$ for $i \in [k]$

$\sum_{i=1}^{k} X_{ij} = 1$ for $j \in [\ell]$

(X_{ij} = fraction of j's mass transported to i)

consider any feasible X.

- X transports 1 unit of probability mass
- cost per unit of mass $\leq \|C\|_\infty$

$\Rightarrow$ OPT $\leq \|C\|_\infty$,

Better: "Oblivious transport"

Recall: Goal: minimize $\sum_{i=1}^{k}\sum_{j=1}^{\ell} c_{ij} p_j x_{ij}$ over $X \in \mathbb{R}_{\geq 0}^{k\times \ell}$

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consider X where each column $= q$

$$x_{ij} = q_i \quad \forall i,j$$

Then X is feasible with cost

$$\sum_{i=1}^{k}\sum_{j=1}^{\ell} c_{ij} p_j x_{ij} = \sum_{i=1}^{k}\sum_{j=1}^{\ell} c_{ij} p_j q_i = \boxed{\langle q, Cp \rangle}$$

Optimal Transport = 2 diff kinds of LP's

① Positive $\mathcal{L}P$'s

leads to $\langle p, Cq \rangle$-type bounds

② Pure packing $\mathcal{L}P$'s

leads to $\|C\|_\infty$-type bounds

Positive LP's

$$\left\{\begin{array}{c}\text{find } x, \\ \max \langle v,p\rangle, \\ \text{or } \min \langle v,p\rangle\end{array}\right\} \text{ over } x \in \mathbb{R}^n_{\geq 0} \text{ s.t. } \left\{\begin{array}{r} Ax \leq b \\ \text{and } \quad Cx \geq d\end{array}\right\}$$

where $v \in \mathbb{R}^n_{\geq 0}$, $A, C \in \mathbb{R}^m_{\geq 0}$, $b, d \in \mathbb{R}^m_{\geq 0}$ are nonnegative

[Young '14] In $\tilde{O}(N/\varepsilon^2)$ determinstic time,

compute x s.t. $\left\{\begin{array}{l} \langle v,p\rangle \in (1 \pm \varepsilon)\mathrm{OPT} \\ Ax \leq (1+\varepsilon)b \\ Cx \geq (1-\varepsilon)d \end{array}\right.$

Optimal Transport = mixed packing and covering

$$\text{minimize} \sum_{i=1}^{k}\sum_{j=1}^{\ell} c_{ij}\, p_j\, x_{ij} \quad \text{over } X \in \mathbb{R}_{\geq 0}^{k \times \ell}$$

$$\text{s.t.} \quad \sum_{j=1}^{\ell} x_{ij}\, p_j = q_i \qquad \text{for } i \in [k]$$

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"$(1\pm\varepsilon)$ relative approximation" gives $X \in \mathbb{R}_{\geq 0}^{k\times\ell}$

$$\text{s.t.} \begin{cases} \text{cost}(X) \leq \text{OPT} \\ (1-\varepsilon)\, q_i \leq \sum_{j=1}^{\ell} X_{ij}\, p_j \leq q_i \quad \forall i\in[k] \\ 1-\varepsilon \leq \sum_{i=1}^{k} X_{ij} \leq 1 \quad \forall j\in[\ell] \end{cases}$$

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$$X \left\{ \begin{array}{l} \text{underfills } q \\ \text{undertransports } p \end{array} \right\} \text{ by } \varepsilon\text{-mult. factor per coordinate}$$

given X like, we need to convert it to an exact transportation matrix

Rounding $(1\pm\varepsilon)$-APX

Input: $X \in \mathbb{R}_{\geq 0}^{k \times \ell}$ s.t. $\begin{cases} (1-\varepsilon) q_i \leq \sum_{j=1}^{\ell} X_{ij} p_j \leq q_i & \forall i \in [k] \\ 1-\varepsilon \leq \sum_{i=1}^{k} X_{ij} \leq 1 & \forall j \in [\ell] \end{cases}$

High-level sketch

① shrink the flow X

② obliviously transport residual mass

Rounding $(1\pm\varepsilon)$-APX

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① (Shrink the flow) set $Y=(1-\varepsilon)X$

② let $\begin{Bmatrix} \tilde{q} = q - Yp \\ \tilde{p} = p - Y^T p \end{Bmatrix}$ be residual mass

let $\alpha = \sum_i \tilde{p}_i = \sum_j \tilde{q}_j$ = amount of residual mass

③ let Z obliviously transport $\frac{\tilde{p}}{\alpha}$ to $\frac{\tilde{q}}{\alpha}$

(each column of $Z = \frac{1}{\alpha}\tilde{q}$)

then $Z\tilde{p} = \tilde{q}$

Input: $X \in \mathbb{R}^{k \times \ell}_{\geq 0}$ s.t. $\begin{cases} (1-\varepsilon) q_i \leq \sum_{j=1}^{\ell} X_{ij} p_j \leq q_i & \forall i \in [k] \\ 1-\varepsilon \leq \sum_{i=1}^{k} X_{ij} \leq 1 & \forall j \in [\ell] \end{cases}$

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Analysis

① $\tilde{p} \leq 2\varepsilon p$, $\tilde{q} \leq 2\varepsilon q$, $\alpha \geq \varepsilon$ (!!)

② cost of the residual routing $= \alpha r$

$$= \frac{1}{\alpha} \langle \tilde{p}, C\tilde{q} \rangle \leq \frac{4\varepsilon^2}{\alpha} \langle q, Cp \rangle \leq 4\varepsilon \langle q, Cp \rangle$$

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Analysis

① $\tilde{p} \leq 2\varepsilon p$, $\tilde{q} \leq 2\varepsilon q$, $\alpha \geq \varepsilon$ (!!)

② cost of the residual routing $= \leq 4\varepsilon \langle p, Cq \rangle$

③ $\Rightarrow 4\varepsilon \langle p, Cq \rangle$ - additive APX in $\tilde{O}(k\ell/\varepsilon^2)$

ie, δ-additive in $\tilde{O}\left(k\ell \left(\frac{\langle p, Cq \rangle}{\delta}\right)^2\right)$ time

Optimal Transport = 2 diff kinds of LP's

① Positive LP's

leads to $\langle p, Cq \rangle$-type bounds

② Pure packing LP's

leads to $\|C\|_\infty$-type bounds

Packing LP's

max $\langle v, x \rangle$ over $x \in \mathbb{R}^n_{\geq 0}$ s.t. $Ax \leq b$

where $v \in \mathbb{R}^n_{\geq 0}$, $A \in \mathbb{R}^m_{\geq 0}$, $b \in \mathbb{R}^m_{\geq 0}$ are nonnegative

[Allen-Zhu, Orecchia '15] In $\tilde{O}(N/\varepsilon)$ randomized time,

compute x s.t. $\begin{cases} \langle v, x \rangle \geq (1-\varepsilon)\,\mathrm{OPT} \\ Ax \leq b \end{cases}$

Optimal Transport = pure packing LP

$$\max \sum_{i,j} x_{ij} p_j \quad \text{over } X \in \mathbb{R}^{k \times \ell}_{\geq 0}$$

$$\text{s.t.} \quad \sum_{j=1}^{\ell} x_{ij} p_j \leq q_i \quad \forall i$$

$$\sum_{i=1}^{k} x_{ij} \leq 1 \quad \forall j$$

$$\text{cost}(X) \leq OPT$$

rewrite "min cost transportation" as

max transport s.t. cost constraint

Optimal Transport = pure packing LP

$$\max \sum_{i,j} X_{ij} p_j \qquad \text{over } X \in \mathbb{R}_{\geq 0}^{k \times \ell}$$

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rewrite "min cost transportation" as max transport s.t. cost constraint

"$(1 \pm \varepsilon)$ relative approximation" gives $X \in \mathbb{R}_{\geq 0}^{k \times \ell}$ s.t. $\text{cost}(X) \leq \text{OPT}$ and transporting all but ε-mass total

Optimal Transport via packing LP

① rewrite "min cost transportation" as "max transport s.t. cost constraint"

② "$(1\pm\varepsilon)$ relative approximation" gives $X \in \mathbb{R}_{\geq 0}^{k \times \ell}$ s.t. $\mathrm{cost}(X) \leq \mathrm{OPT}$ and transporting all but ε-mass total

③ transport remaining ε anyway we want w/ cost $\varepsilon\|C\|_\infty$

$\Rightarrow$ $\varepsilon\|C\|_\infty$ additive APX in $\tilde{O}(k\ell/\varepsilon)$ time

New sequential runtimes (improving $\tilde{O}(k\ell(\frac{\|C\|_\infty}{\delta})^2)$)

① $\tilde{O}(k\ell(\frac{\langle q, C_p \rangle}{\delta})^2)$ deterministic time

② $\tilde{O}(k\ell\frac{\|C\|_\infty}{\delta})$ randomized time

New parallel bounds (both deterministic)

③ $\tilde{O}((\frac{\langle q, C_p \rangle}{\delta})^3)$ depth, $\tilde{O}(k\ell(\frac{\langle p, C_q \rangle}{\delta})^2)$ work

④ $\tilde{O}((\frac{\|C\|_\infty}{\delta})^2)$ depth, $\tilde{O}(k\ell(\frac{\|C\|_\infty}{\delta})^2)$ work

Existing LP solvers do heavy lifting

Conclusion / upshot

① we can solve many LP's very fast; leading to <u>fast</u> approximations

② Maybe more of our TCS tools are better at modern "big data" stuff than we realize!

THANKS