Scalable Nearest Neighbor Search for Optimal Transport

Arturs Backurs
TTIC

Yihe Dong
Microsoft Research

Piotr Indyk
MIT

Ilya Razenshteyn
Microsoft Research

Tal Wagner
MIT

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TL;DR

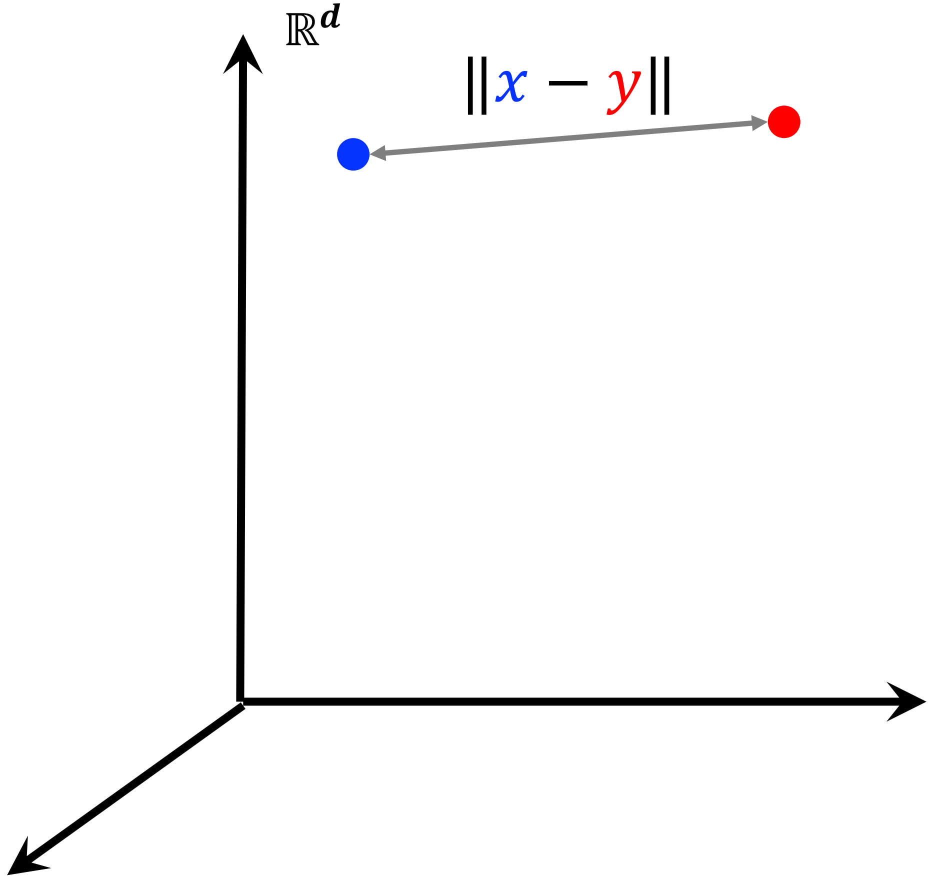
We introduce Flowtree:

- Fast nearest neighbor search algorithm for Optimal Transport
  - a.k.a. Earth Mover Distance, Wasserstein-1 distance
- **Analytically:** Linear running time, worst-case approximation bound
- **Empirically:** Speeds up SOTA by up to 7.4 times
- **Code** publicly available on github: https://github.com/ilyaraz/ot_estimators

Optimal Transport

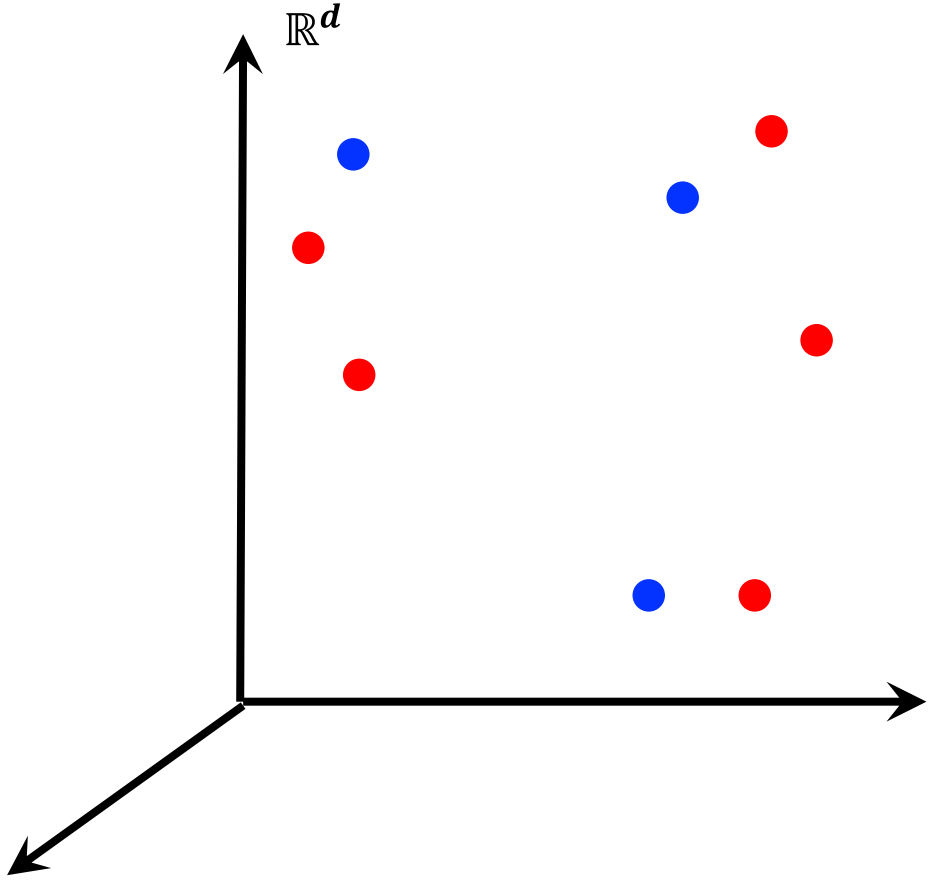
Distance between points x and y:

Euclidean, Manhattan, …



Optimal Transport

Distance between point sets X and Y?



Optimal Transport

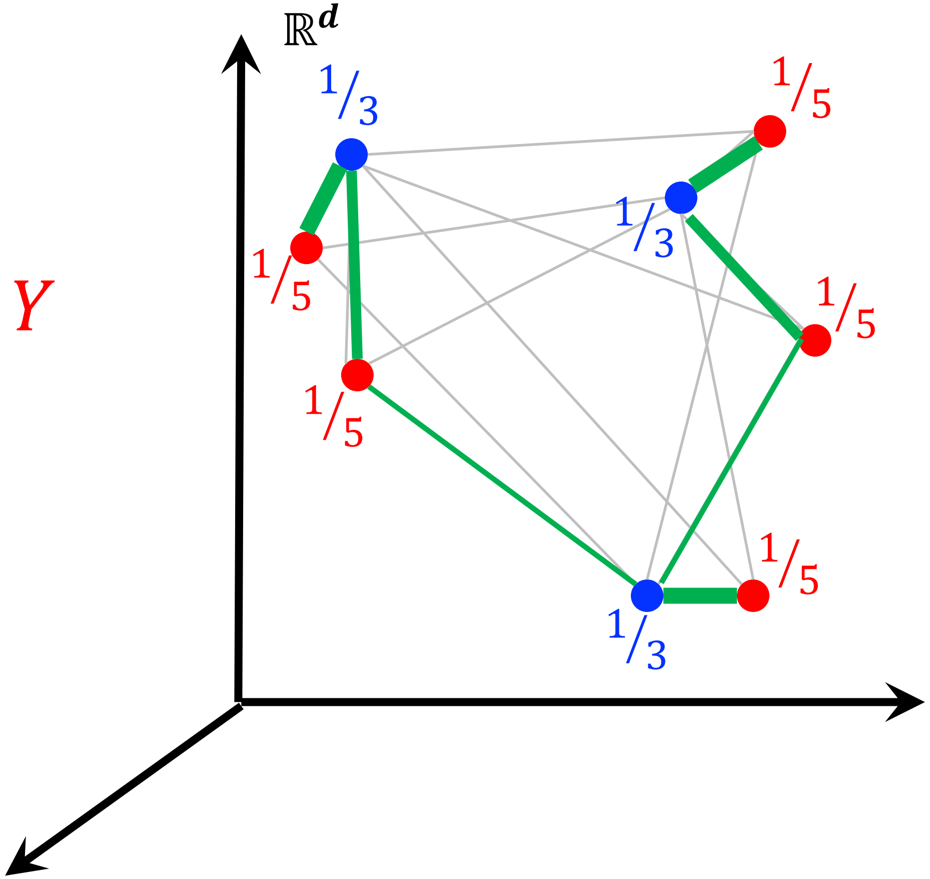
Distance between point sets X and Y?

Choose distributions $\mathcal{D}_X$ on X and $\mathcal{D}_Y$ on Y

- For this talk: uniform distributions

$OT(X, Y)$ = value of minimum-cost flow

from X to Y with demands $\mathcal{D}_X$ and $\mathcal{D}_Y$



$$= \min_{\boldsymbol{F}} \sum_{x \in X,\, y \in Y} \|x - y\| \cdot \boldsymbol{F}(x, y)$$

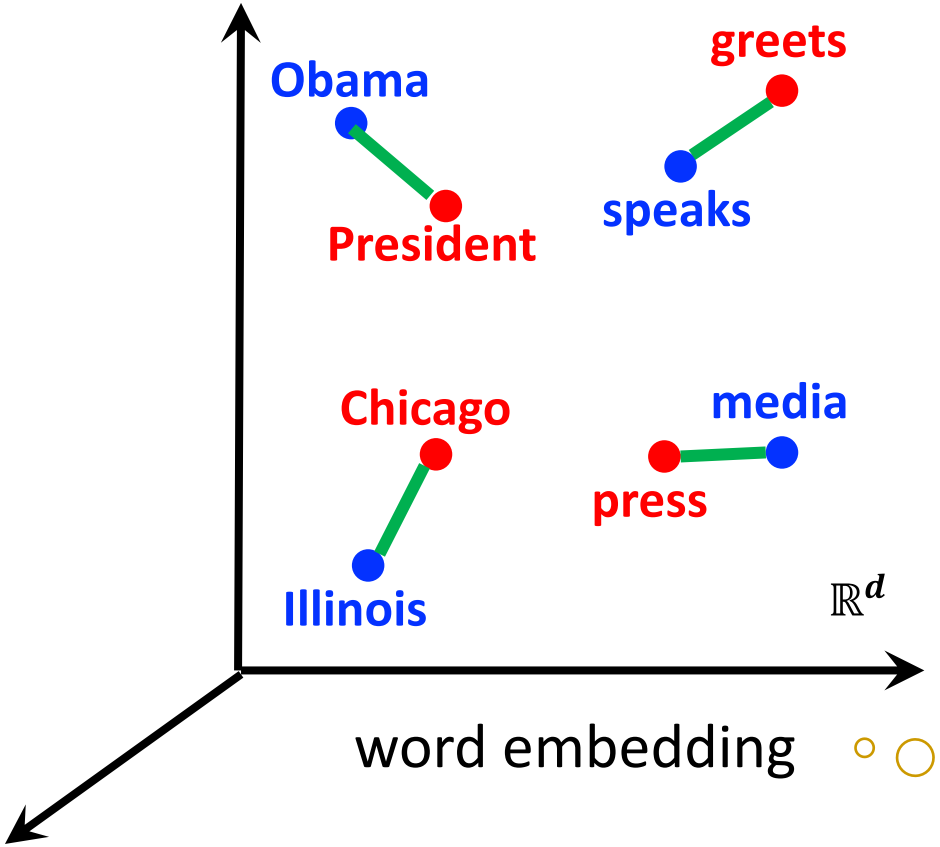
s.t. $\boldsymbol{F}$ is a distribution on $X \times Y$
with marginals $\mathcal{D}_X$ and $\mathcal{D}_Y$

Motivation: “Word Mover Distance”

Kusner et al. (2015): Use OT as distance between text documents

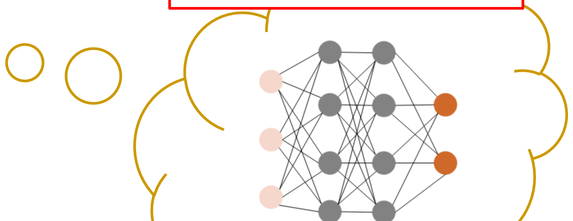
Document 1

Obama
speaks
to
the
media
in
Illinois

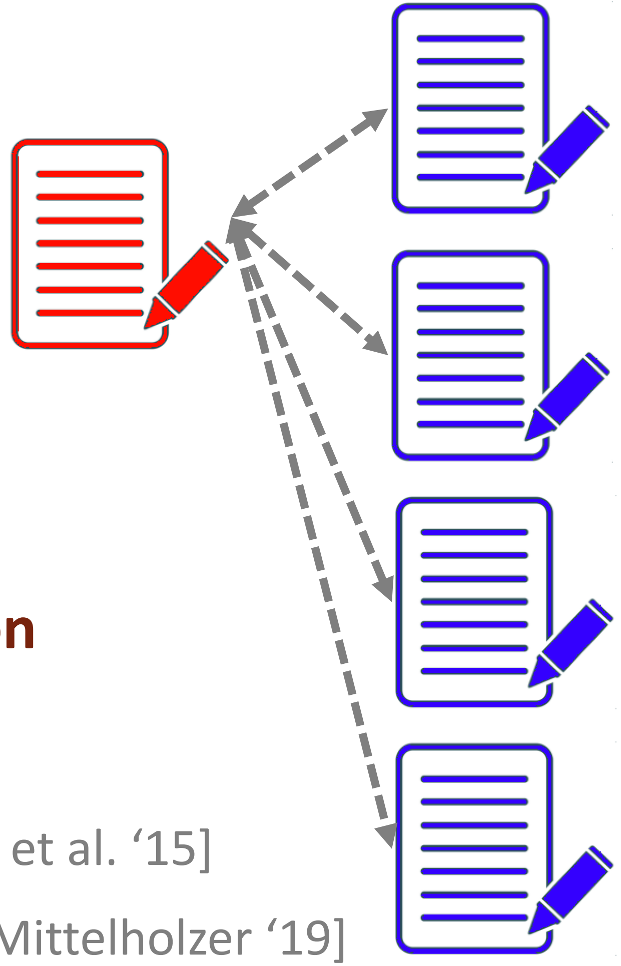


Document 2

The
President
greets
the
press
in
Chicago



OT Nearest Neighbor Search



Exact computation does not scale

Approximate algorithms:

Linear time
Crude approximation

Best of both worlds?

Quadratic time
Fine approximation

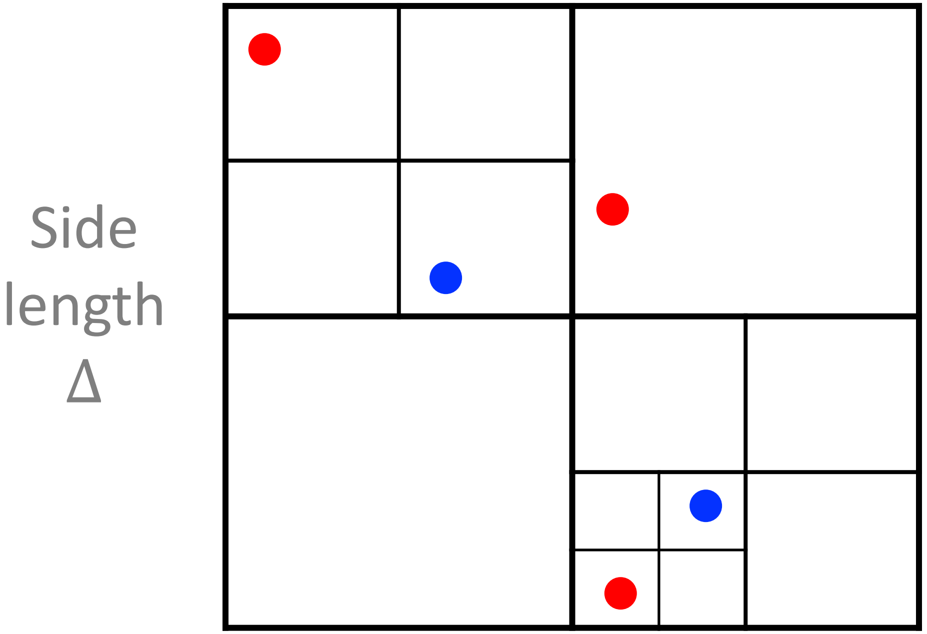
Means	[Kusner et al. ‘15]
TF-IDF	[Luhn ‘57]
Quadtree	[Charikar ’02, Indyk-Thaper ’03]

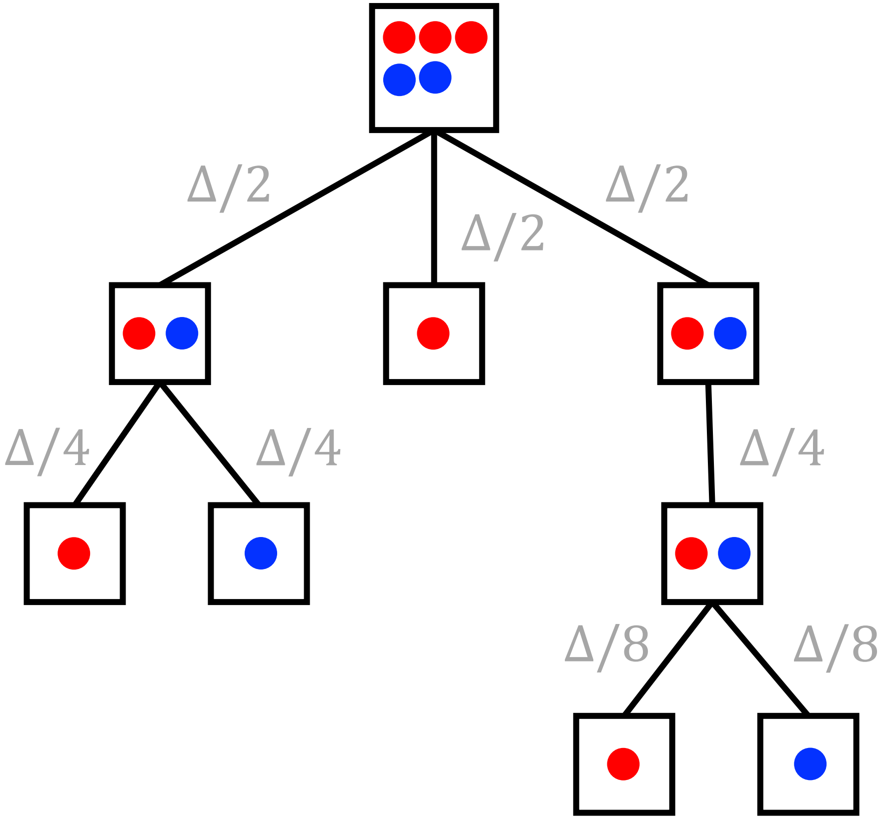
Flowtree:
“Slower” linear time
Fine approximation

R-WMD	[Kusner et al. ‘15]
ACT	[Atasu-Mittelholzer ‘19]
Sinkhorn	[Cuturi ‘13]

Algorithm

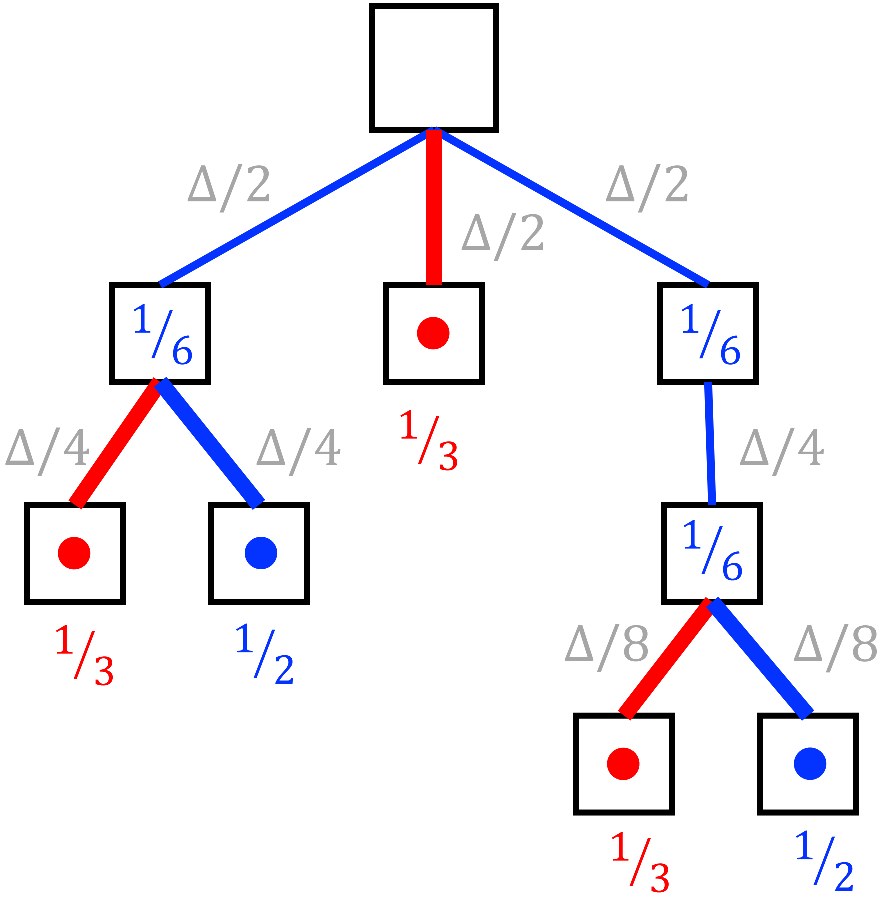
Starting Point: Quadtree





Optimal Transport on a Quadtree

Compute: Optimal flow on tree



Optimal Transport on a Quadtree

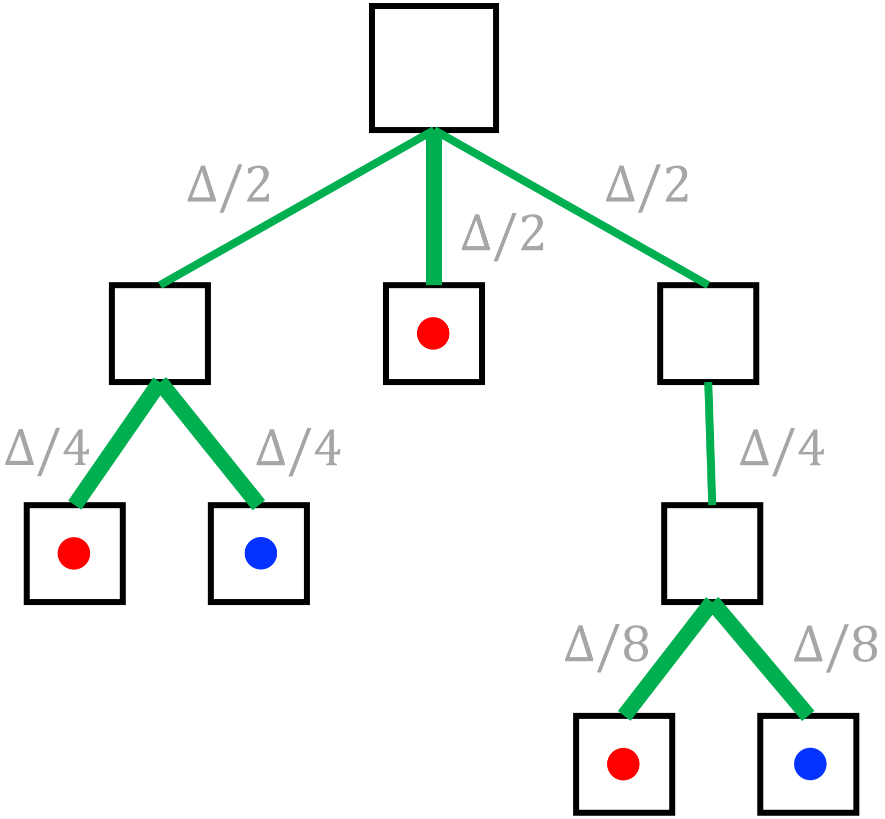
Compute: Optimal flow on tree

Return: Flow cost in tree distance

$$\sum_{\text{Tree edge } e} weight(e) \cdot \boldsymbol{F_T}(e)$$

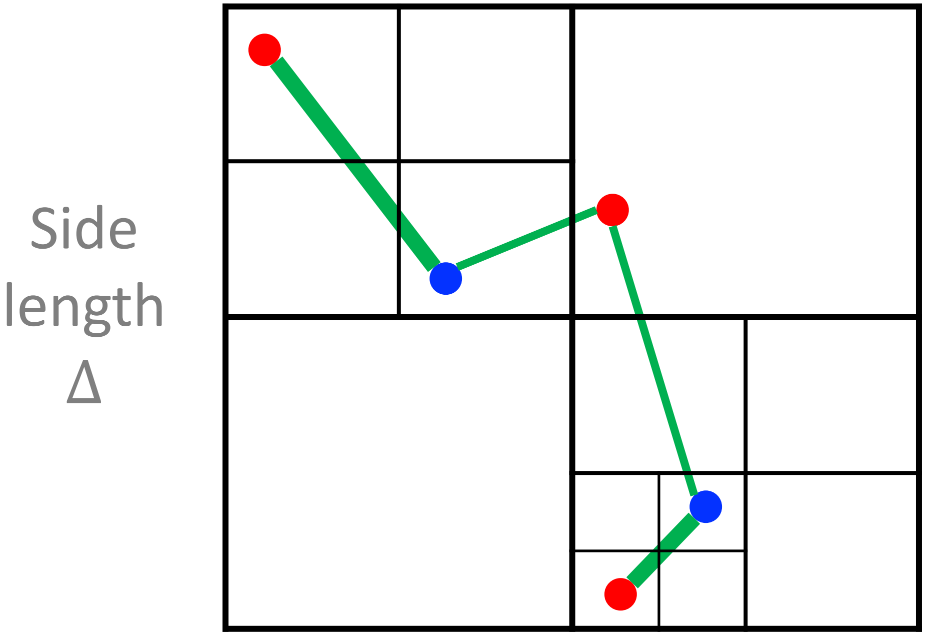
Even faster: ℓ_1-embedding!

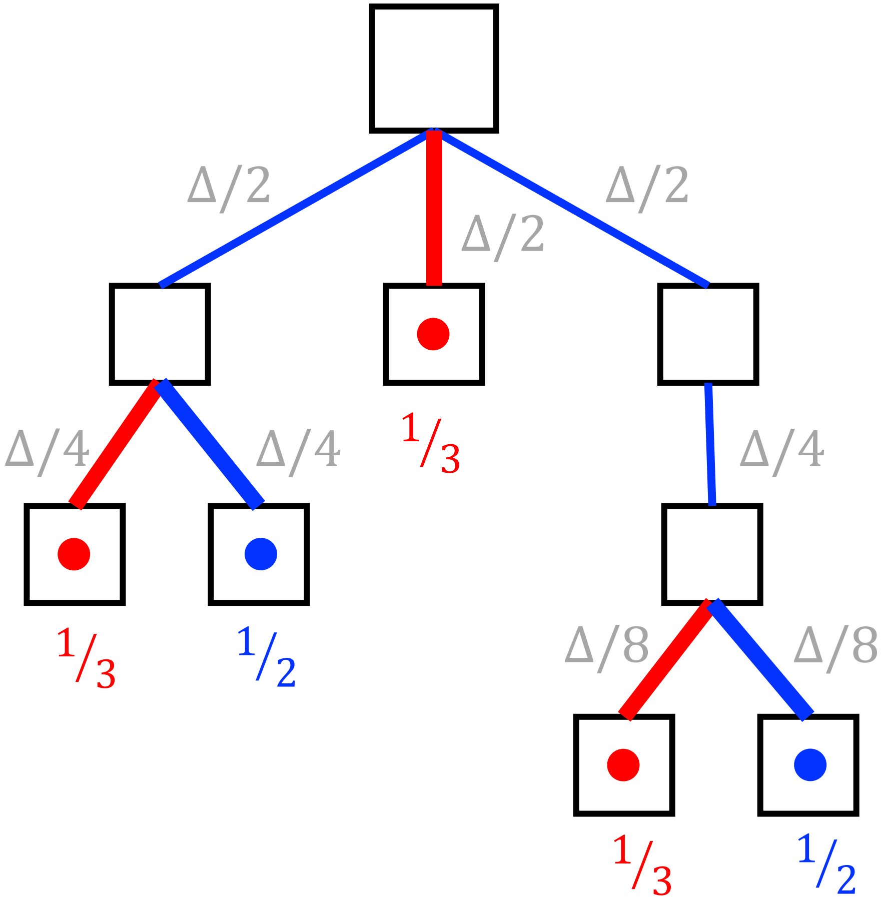
[Kleinberg-Tardos '00, Charikar '02, Indyk-Thaper '03, Le et al. '19, …]



Our Algorithm: Flowtree

Evaluate optimal **tree** flow in **original** metric space



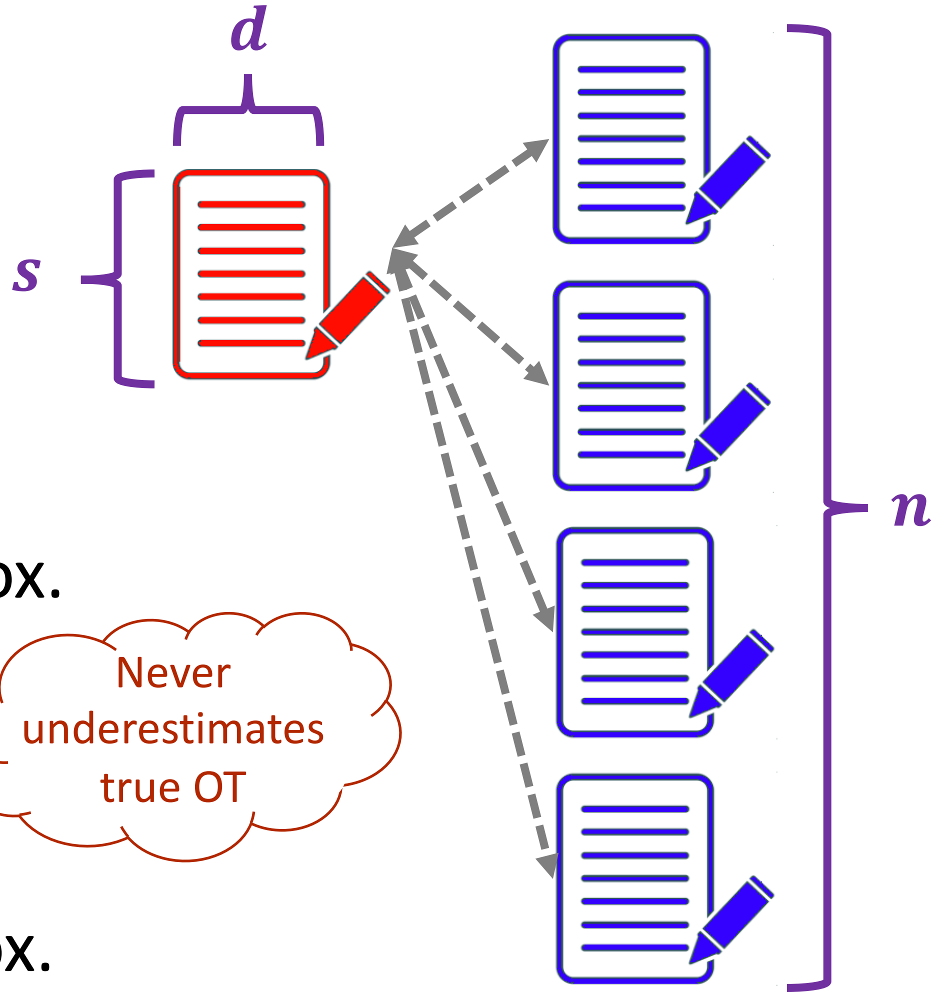


Return: $$\sum_{x\in X,\, y\in Y} \|x-y\|\cdot \boldsymbol{F_T}(x,y)$$

Flowtree: Properties

- **Running time:**
  - **Quadtree**: Linear, ℓ_1 **embedding**
  - **Flowtree**: Linear, does not give embedding
- **Nearest neighbor search approximation:**
  - **Quadtree**: $O(\log(d \cdot \Delta) \cdot \log(s \cdot n))$-approx.
    - Dependence on n is **necessary**
  - **Flowtree**: $O(\log(d \cdot \Delta) \cdot \log s)$-approx.
  - **Flowtree in uniform case**: $O(\log^2 s)$-approx.

Never underestimates true OT

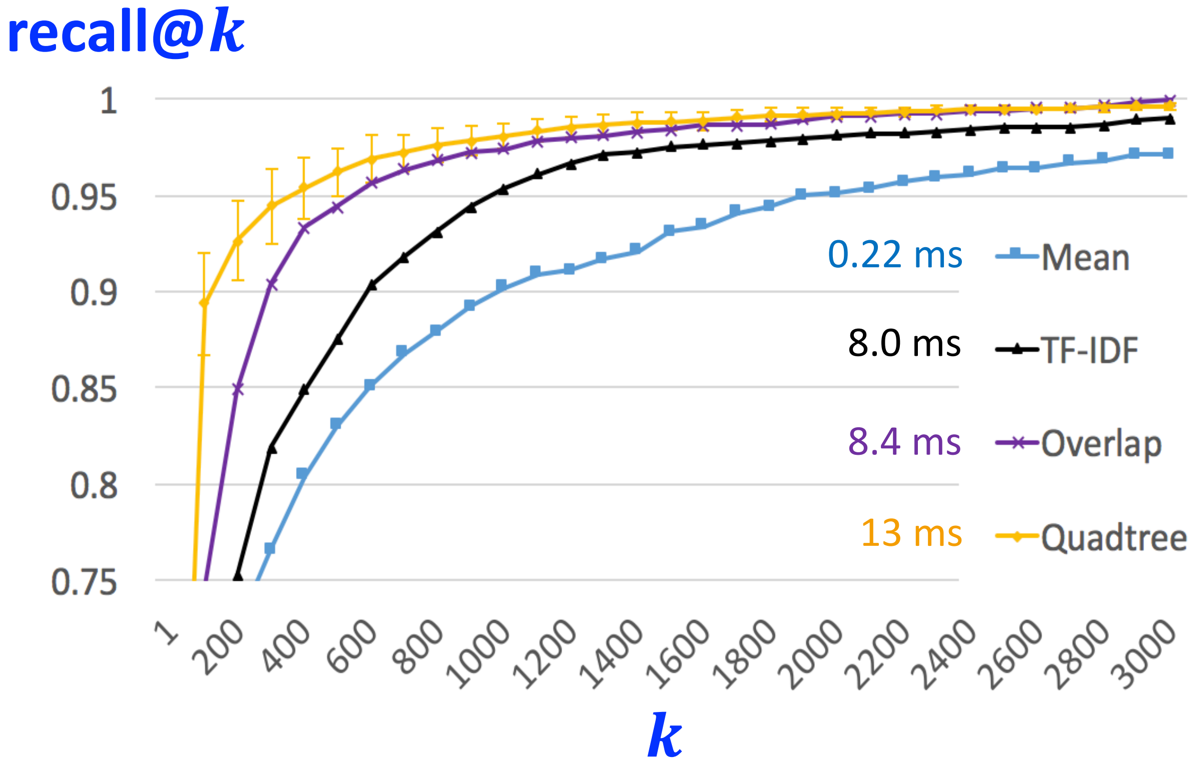


Experiments

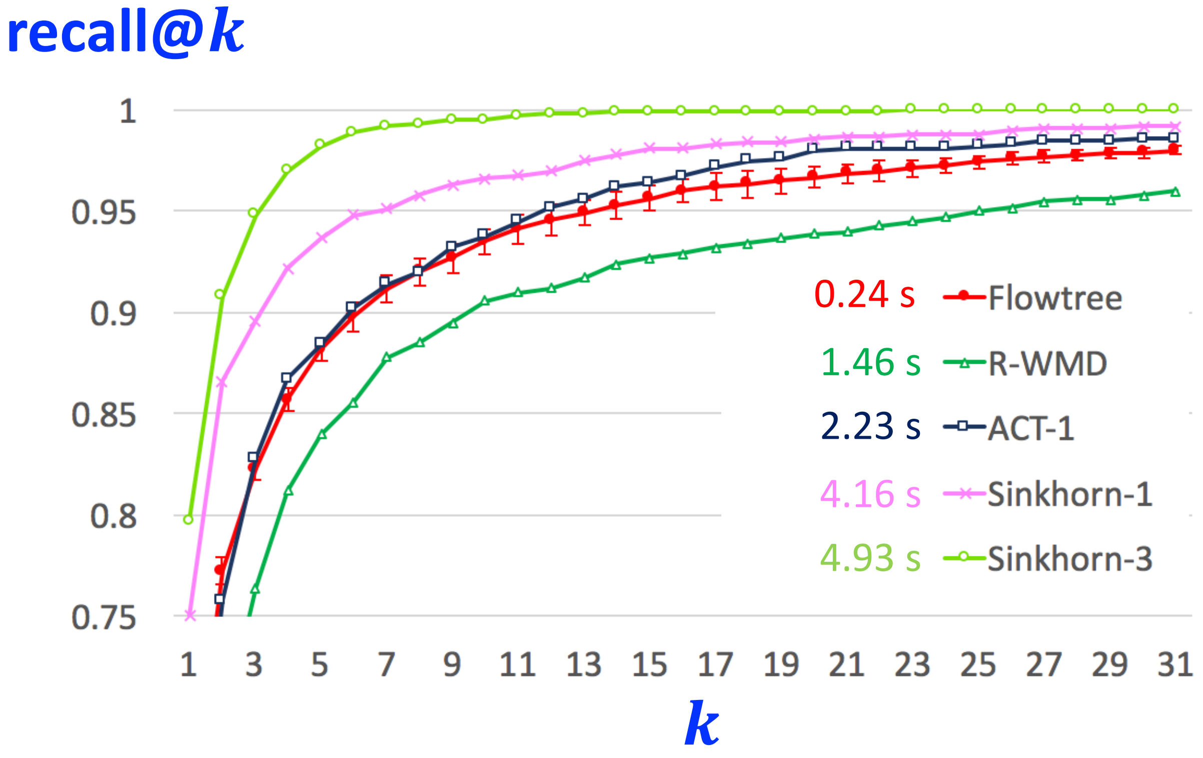
20newsgroups dataset

Individual Algorithm Evaluation

Fast (milliseconds)
Crude approximation

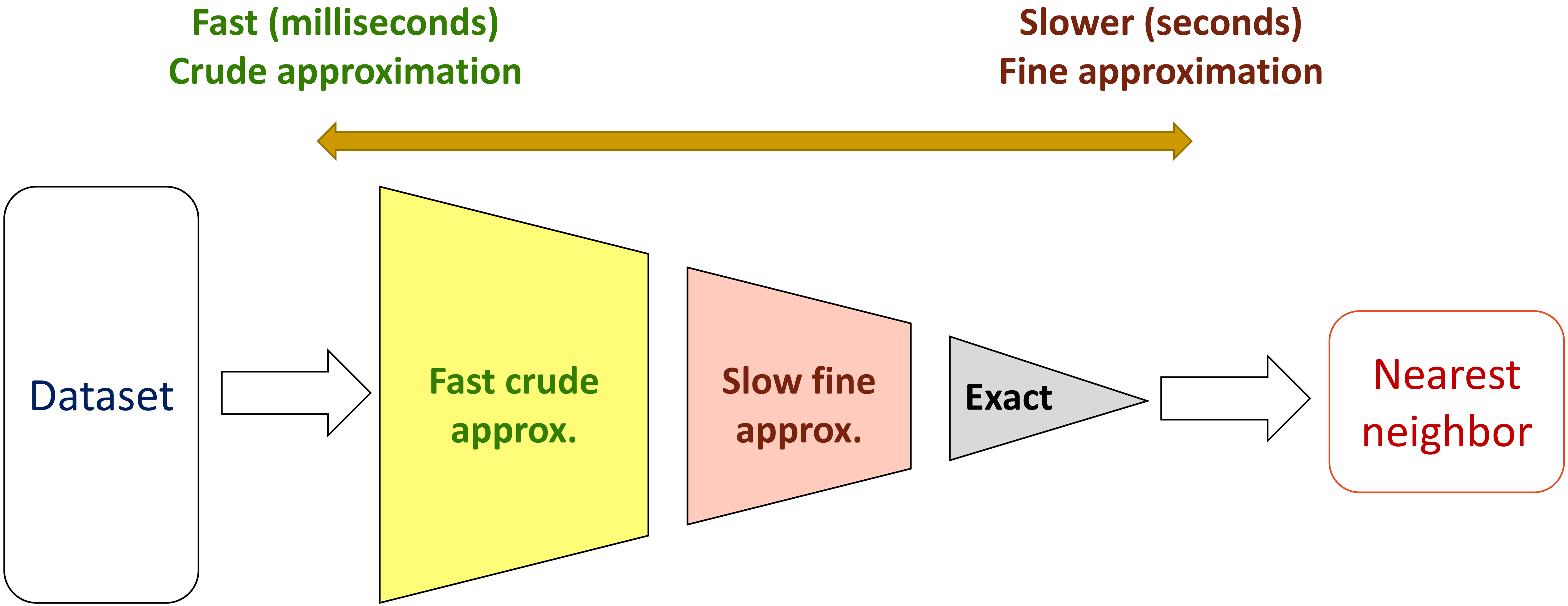


Slower (seconds)
Fine approximation

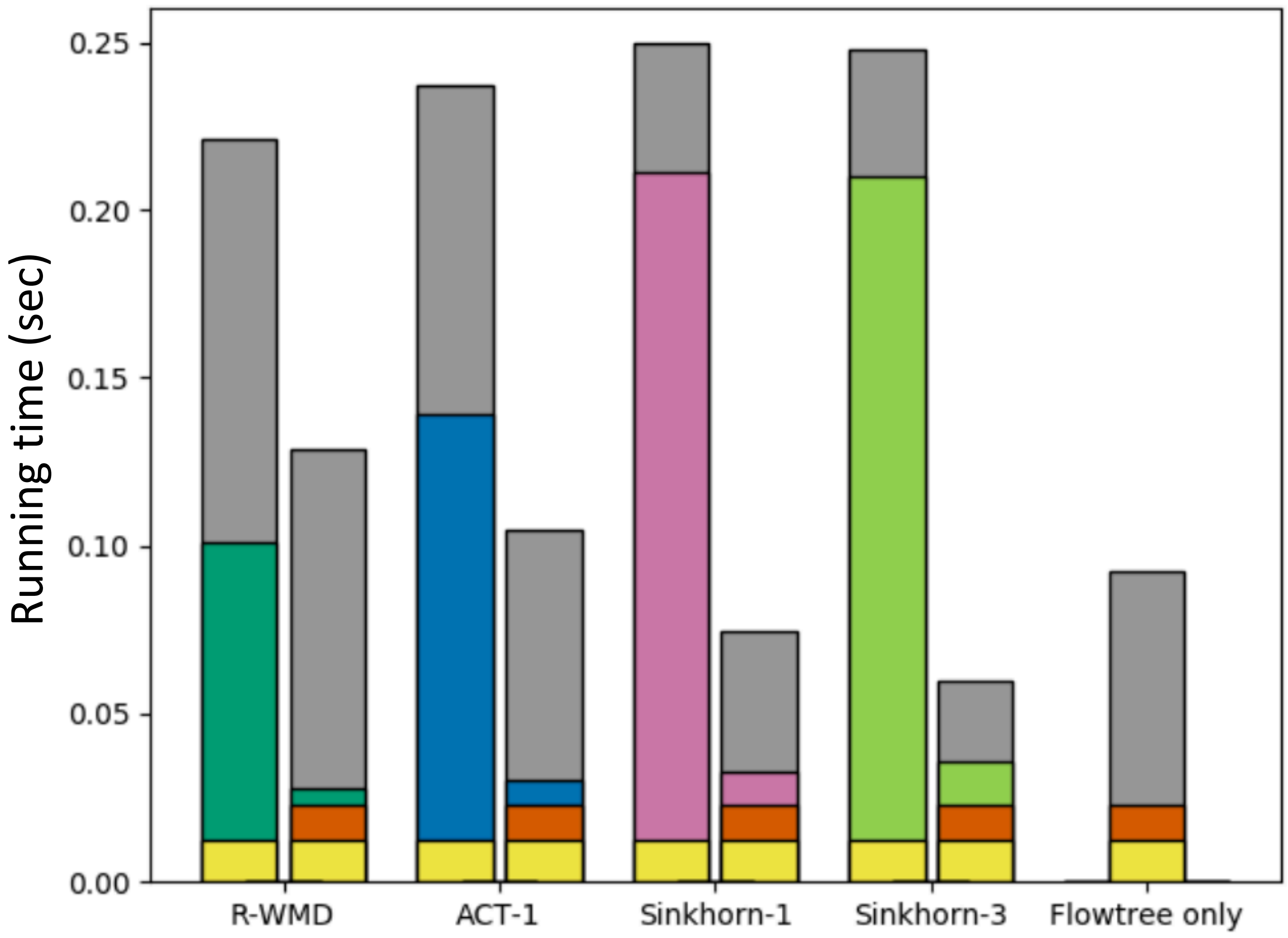


recall@k = % queries whose true nearest neighbor is ranked in top-k returned points

Pipeline Experiments



Pipeline Experiments: Recall@1



1st: 🟨 Quadtree

2nd: 🟩 R-WMD [Kusner et al. '15]

🟦 ACT-1 [Atasu-Mittelholzer'19]

🟪 Sinkhorn-1 [Cuturi'13]

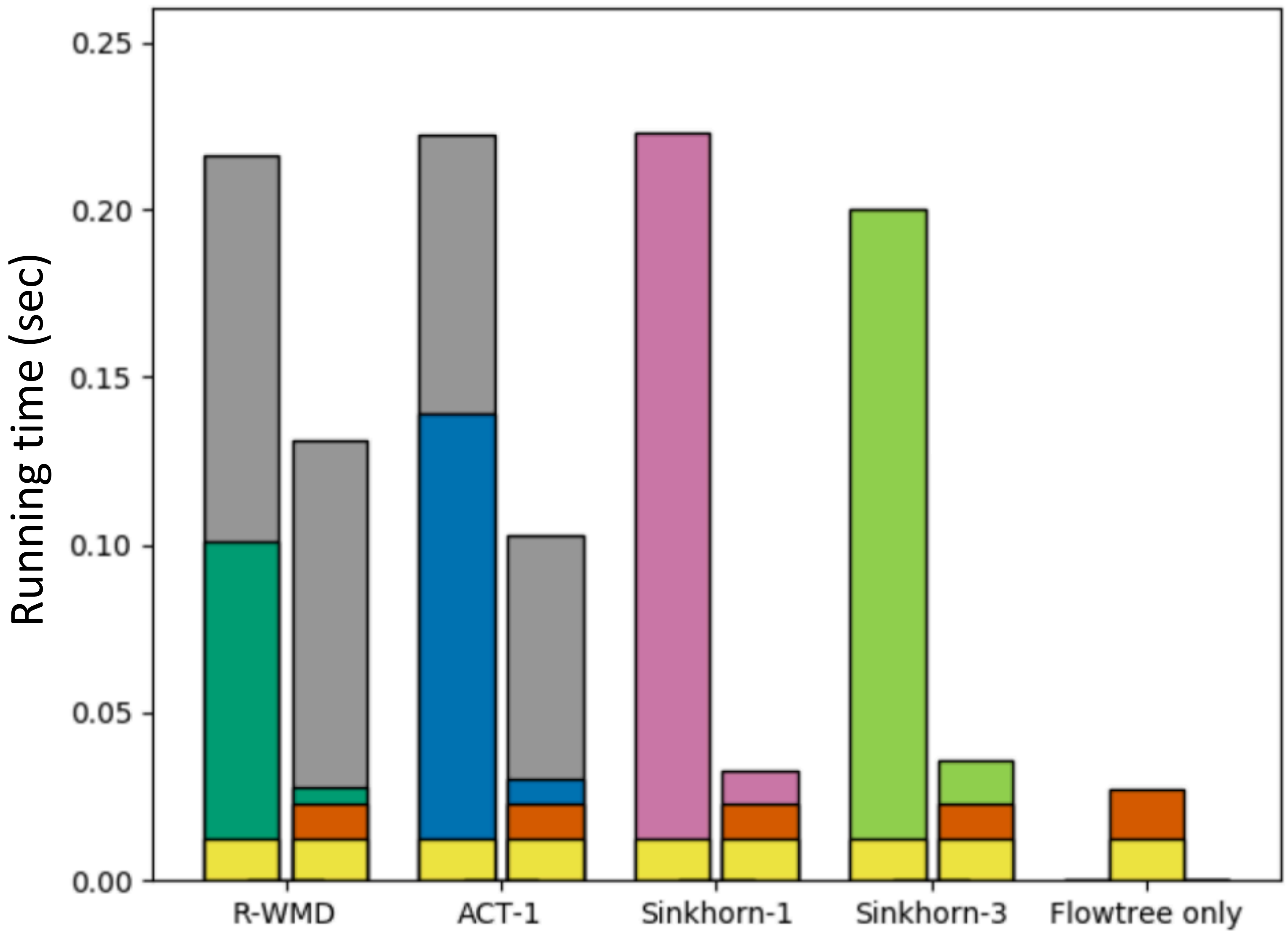
🟩 Sinkhorn-3

3rd: ⬜ Exact

New: 🟧 Flowtree

x3.7 speed up

Pipeline Experiments: Recall@5



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Conclusion

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Thank you