Space and Time Efficient Kernel Density Estimation in High Dimensions

Arturs Backurs
TTIC

Piotr Indyk
MIT

Tal Wagner
MIT

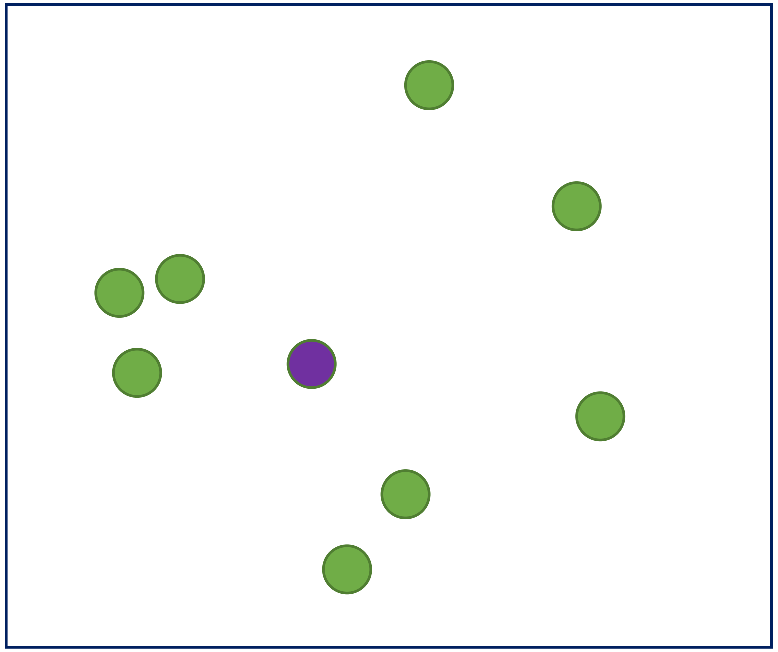
Background:

Density Estimation

Problem: Given a dataset $x_1, \ldots, x_n \in \mathbb{R}^d$,

estimate density at a query point $y \in \mathbb{R}^d$.

How to formalize this?



Background:
Kernel Similarity Measures

Method: Define a similarity measure ("*kernel*"):

$$k: \mathbb{R}^d \times \mathbb{R}^d \rightarrow [0,1]$$

such that the more similar x, y are, the closer $k(x, y)$ to 1.

Examples of popular kernels:

- "Exponential": $k(x, y) = \exp\left(-\frac{\|x-y\|_2}{\sigma}\right)$
- "Laplacian": $k(x, y) = \exp\left(-\frac{\|x-y\|_1}{\sigma}\right)$
- "Gaussian": $k(x, y) = \exp\left(-\frac{\|x-y\|_2^2}{\sigma}\right)$

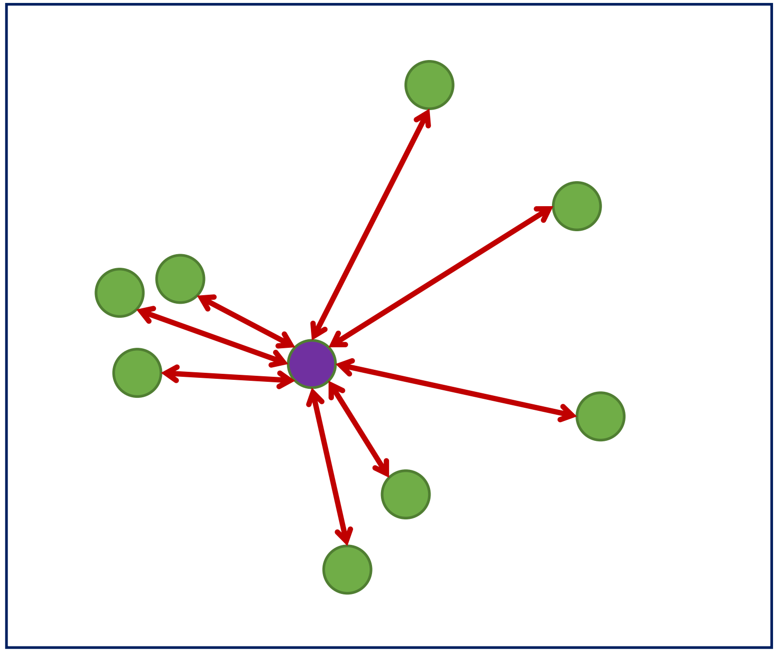
σ is a parameter called *bandwidth*

Background:

Kernel Density Estimation

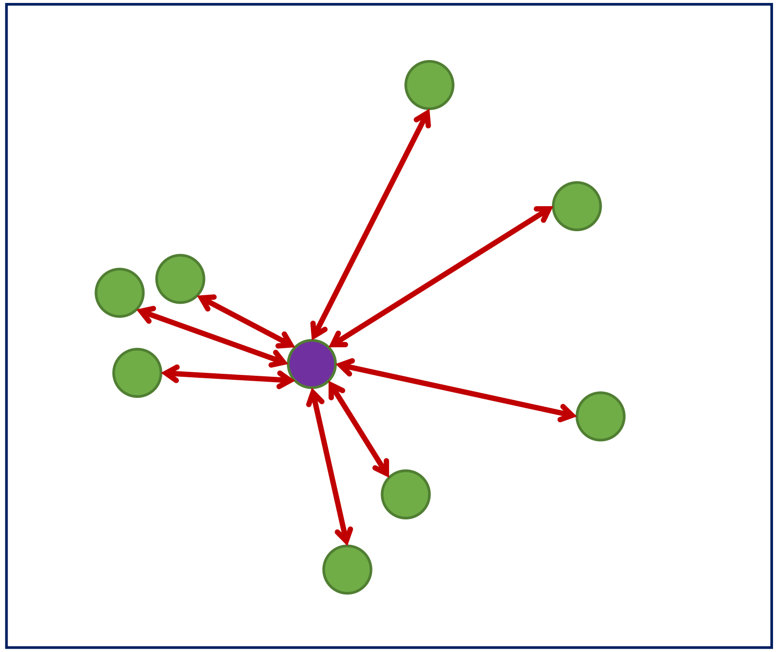
- **Definition**: The Kernel Density Estimation of a query y in a dataset $X = \{x_1, \dots, x\_n\}$ is defined as

$$KDE_X(y) = \frac{1}{n}\sum_{i=1}^{n} k(x_i, y)$$



Fast KDE

- Exact naïve computation: $\Omega(n)$ time, **too slow**
  - Typically there are multiple query points
- **Can we estimate $KDE_X(y)$ efficiently?**



Fast KDE: Uniform Sampling

- Suppose we have the promise: $KDE_X(y) \geq \tau$ for some small $\tau > 0$
  - i.e.: the query y is not too unrelated to the dataset X
- We want a $(1 \pm \varepsilon)$ relative approximation of $KDE_X(y)$
- **Uniform sampling**: If we choose $O\left(\frac{1}{\tau \cdot \varepsilon^2}\right)$ random points $\tilde{X} \subset X$, then

$$KDE_{\tilde{X}}(y) = (1 \pm \varepsilon) KDE_X(y)$$

- Running time: $O\left(\frac{1}{\tau \cdot \varepsilon^2}\right)$. **Can we do better?**

Fast KDE: Hashing-Based Estimators (HBE)

[Charikar & Siminelakis 2017]

- Method based on ***Locality-Sensitive Hashing (LSH)*** [Indyk & Motwani 98]

- **Definition**: The kernel k is ***LSHable*** if there exists a distribution $\mathcal{H}$ over hash functions $h\colon \mathbb{R}^d \to \{0,1\}^*$, such that for every $x, y \in \mathbb{R}^d$,

$$\underbrace{\Pr_{h\sim\mathcal{H}}[h(x) = h(y)]}_{\text{(hash collision probability)}} \approx \sqrt{k(x,y)}$$

Exponential and Laplacian kernels are LSHable

- **Theorem** [Charikar & Siminelakis 2017]: If k is LSHable, we can estimate KDE in time $O\left(\frac{1}{\sqrt{\tau}\cdot\varepsilon^2}\right)$.

Improvement of $1/\sqrt{\tau}$ over random sampling; matters in practice [Siminelakis et al. 2019]

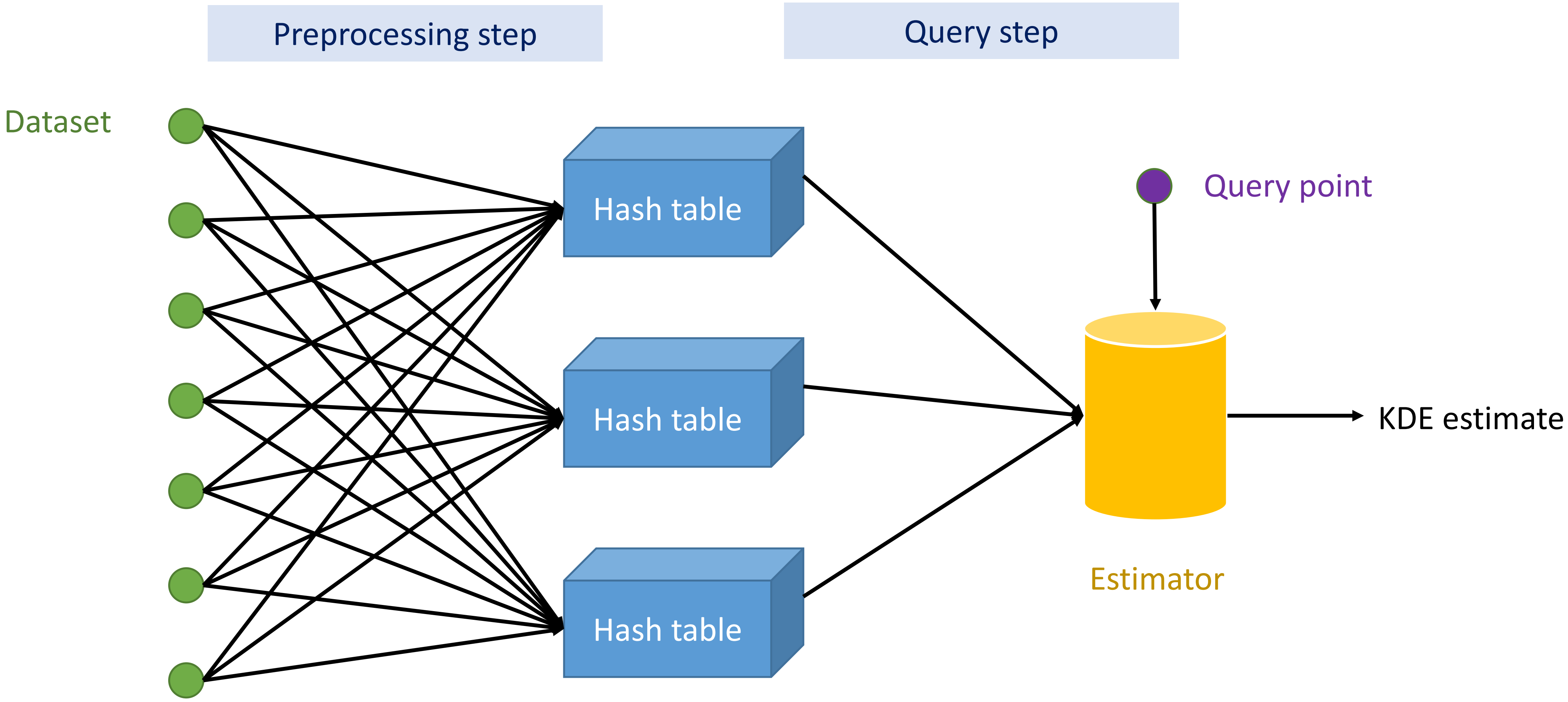
Fast KDE: Our Results

- <u>Drawback of HBE:</u> Requires super-linear preprocessing time and storage space: $O\left(n \cdot \frac{1}{\sqrt{\tau} \cdot \varepsilon^2}\right) = O\left(\frac{1}{\tau\sqrt{\tau} \cdot \varepsilon^4}\right)$
  - Burdens practical implementation [Siminelakis et al. 2019]

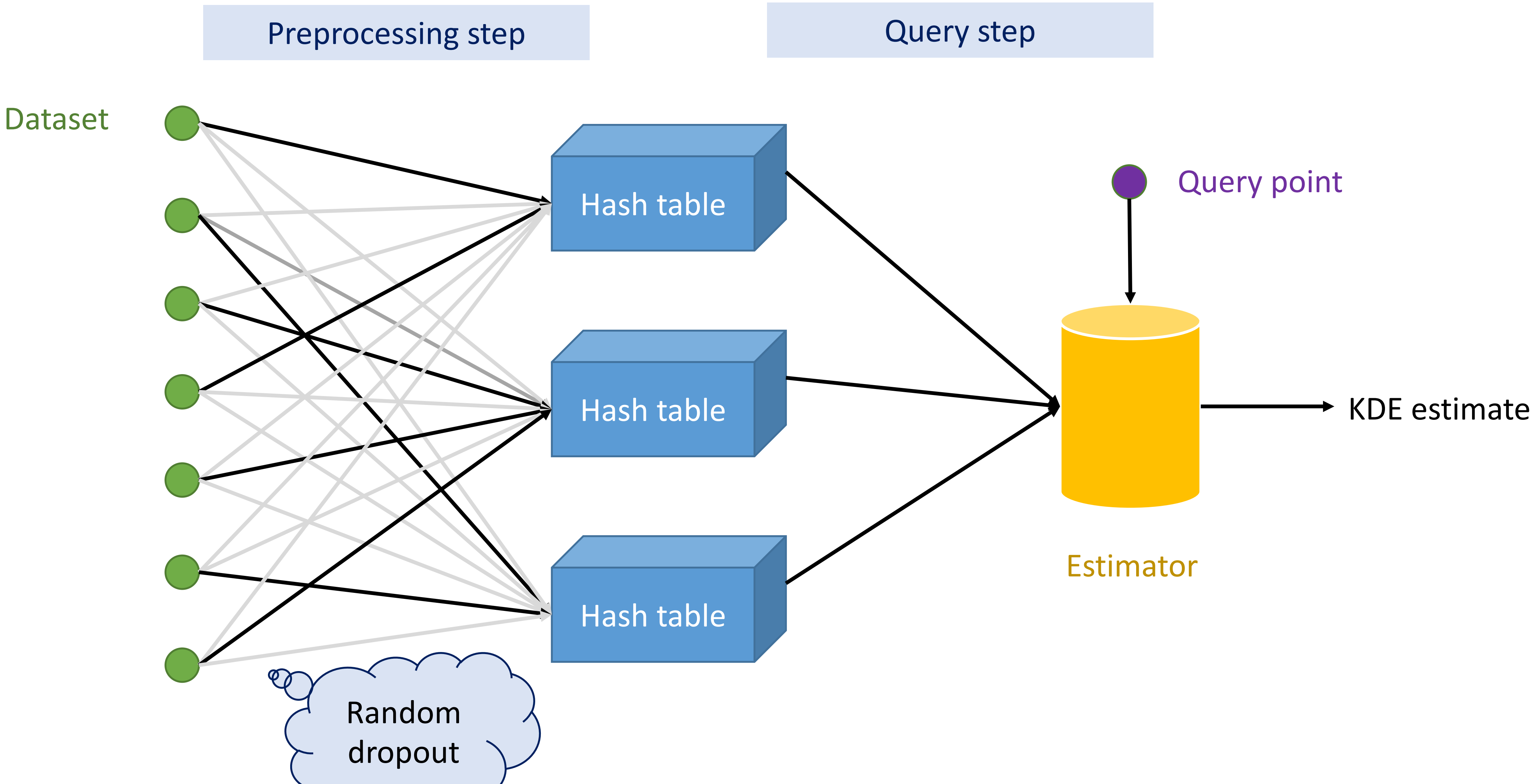
By composing with uniform sampling we can assume $n = 1/(\tau \cdot \varepsilon^2)$

- **<u>This work:</u>** We modify HBE to get the best of both worlds:
  - Preprocessing time and storage space: $O\left(\frac{1}{\tau \cdot \varepsilon^2}\right)$ *(same as uniform sampling)*
  - Query KDE estimation time: $O\left(\frac{1}{\sqrt{\tau} \cdot \varepsilon^2}\right)$ *(same as HBE)*

HBE Scheme

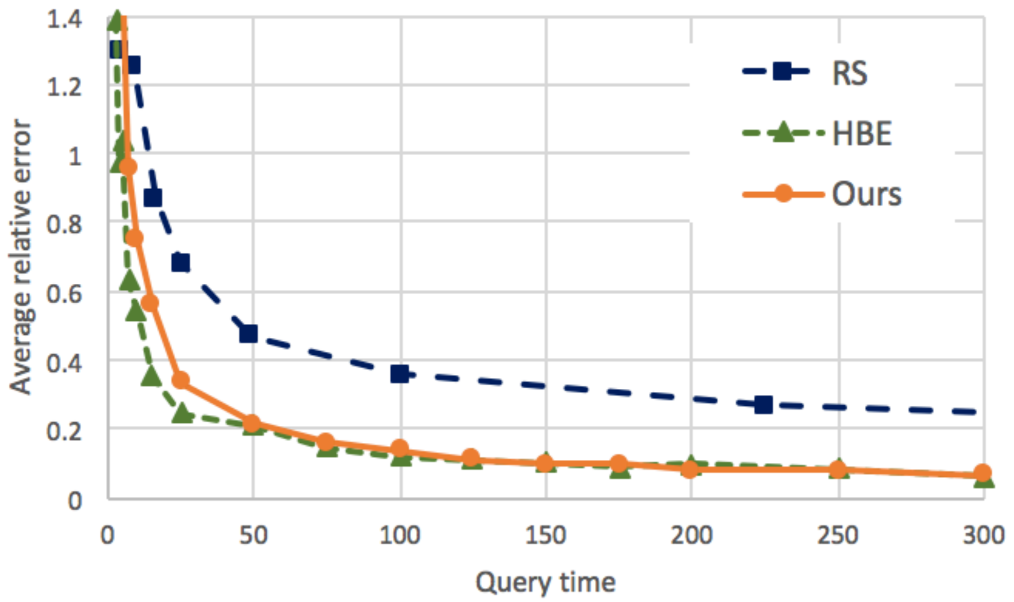

Preprocessing step
Query step
Dataset
Hash table
Hash table
Hash table
Query point
Estimator
KDE estimate

Space-Efficient HBE Scheme

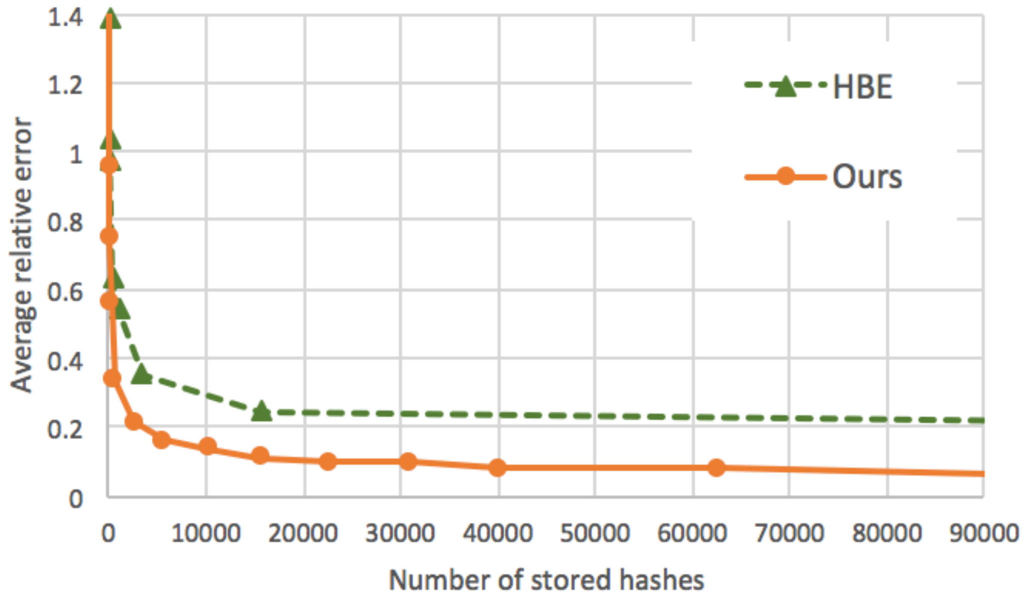


Representative Experiments (more in paper)

- Forest cover type dataset*, Laplacian kernel



Our query time is similar to HBE and better than uniform sampling (RS)



Our storage space and preprocessing time improve over HBE

* Jock A Blackard and Denis J Dean, Comparative accuracies of artificial neural networks and discriminant analysis in predicting forest cover types from cartographic variables, Computers and electronics in agriculture 24 (1999), no. 3, 131–151

References

- Moses Charikar, Paris Siminelakis. **Hashing-based-estimators for kernel density in high dimensions.** FOCS 2017
- Piotr Indyk, Rajeev Motwani. **Approximate nearest neighbors: towards removing the curse of dimensionality.** STOC 1998
- Paris Siminelakis, Kexin Rong, Peter Bailis, Moses Charikar, Philip Levis. **Rehashing kernel evaluation in high dimensions.** ICML 2019