Structured Spinners: Approach for fast and large-scale Machine Learning computations

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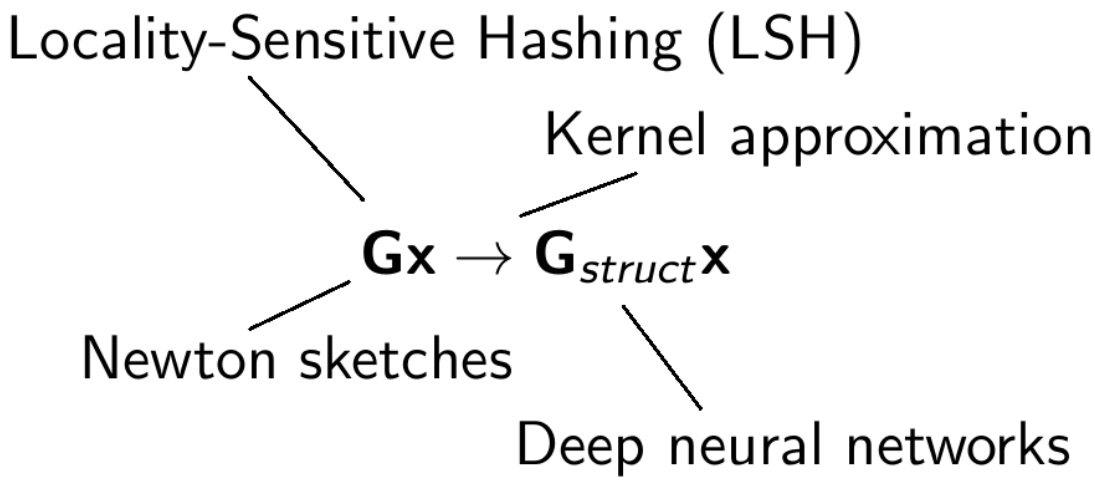
Plan

Plan

Approach for fast and large-scale Machine Learning computations

Structured Spinners' principle

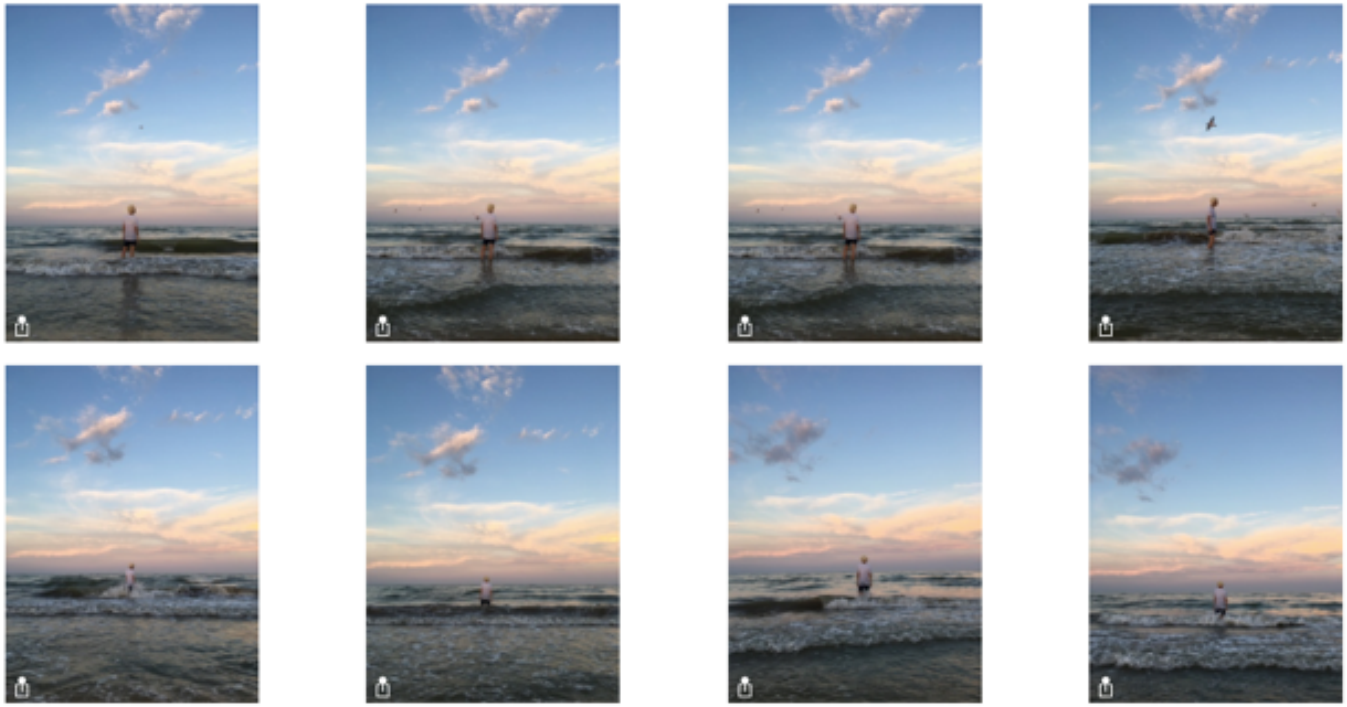
- Replace $\mathbf{Gx}$ by $\mathbf{G}_{struct}\mathbf{x}$ in large-scale ML applications containing random projections, $\mathbf{G}$, $\mathbf{G}_{struct} \in \mathbb{R}^{m \times n}$
- Significant speedups $O(mn) \rightarrow O(n \log m)$
- Memory space savings $O(mn) \rightarrow O(n \log m)$
- Almost no loss of accuracy



Plan

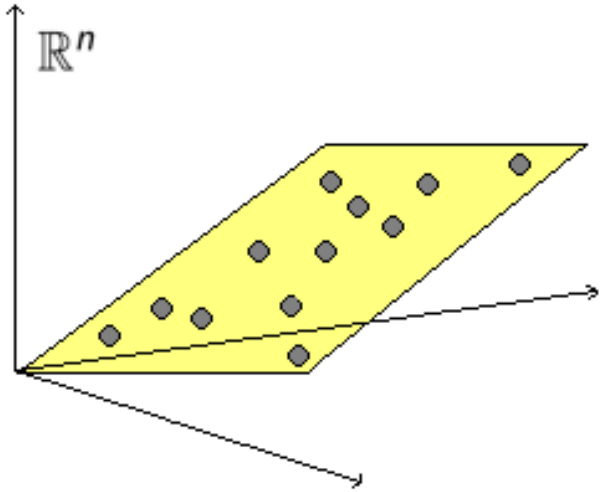
When all your data do not fit into memory...

- Massive data + high dimensionality
- Ex: finding near duplicates in holiday photos



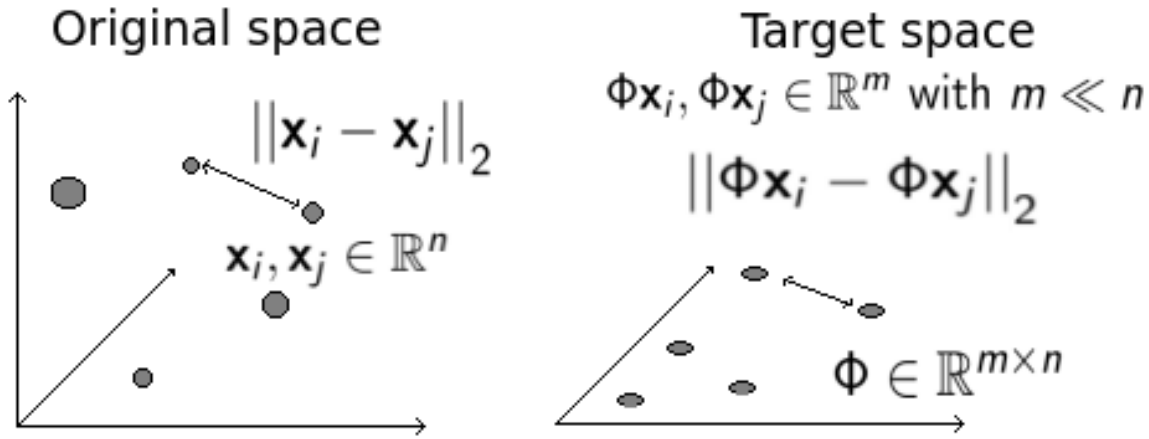
Observation

- Lot of high dimensional data lie on a lower-dimensional manifold
- Concept of intrinsic dimension



- Perform dimensionality reduction / find a suitable projection onto a lower dimensional space

Dimensionality reduction



$$||\Phi\mathbf{x}_i - \Phi\mathbf{x}_j||_2 \approx ||\mathbf{x}_i - \mathbf{x}_j||_2, \; ||\Phi\mathbf{x}_i||_2 \approx ||\mathbf{x}_i||_2$$

Desirable properties of the projection

- Near isometric embedding
- $(1 \pm \epsilon)$ distorsion
- Distance and angle preserved between points

Classical projections

- Principal Component Analysis (PCA)
- Random Projection (RP)

Random projections: theoretical justification

Founder Lemma: [Johnson and Lindenstrauss, 1984]:

Let $\epsilon \in]0,1[$, $\mathcal{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{R}^n$.

Let $m \in \mathbb{N}$, s.t. $m \geq C\epsilon^{-2} \log N$.

Then there exists a linear map $\Phi : \mathbb{R}^n \to \mathbb{R}^m$ s.t. :

$$\forall \mathbf{x}_i, \mathbf{x}_j \in \mathcal{X}, \ (1-\epsilon)||\mathbf{x}_i - \mathbf{x}_j||_2 \leq ||\Phi\mathbf{x}_i - \Phi\mathbf{x}_j||_2 \leq (1+\epsilon)||\mathbf{x}_i - \mathbf{x}_j||_2.$$

- One can take $\Phi =$ **Random** (near orthonormal) which works with high probability.

Random projections applications

- Linear embedding / Dimensionality reduction,
- Approximate nearest neighbor algorithms, e.g.:
  - Random Projection Trees,
  - Locality Sensitive Hashing-based algorithms.
- Compressed sensing,
- Efficient kernel computations via random feature maps,
- Convex optimization algorithms,
- Quantization techniques,
- etc.

$\Longrightarrow$ information retrieval, similarity search, classification, clustering.

Brief random projections evolution

Φ: Dense i.i.d. distribution

- [Frankl and Maehara, 1987]: $\Phi_{i,j} \sim \mathcal{N}(0, \frac{1}{\sqrt{m}})$
- [Achlioptas, 2003]: $\Phi_{i,j} \sim \{-1, 1\}$ uniformly

Φ: Sparse i.i.d. distribution

- [Kane and Nelson, 2010]: #nonzero entries in $\Phi = O(n \log N/\epsilon)$,
- Fast Johnson-Lindenstrauss Transform - FJLT [Ailon and Chazelle, 2006]: $\Phi = \mathbf{PHD}$
  - $\mathbf{P}_{i,j} = \begin{cases} \sim \mathcal{N}(0, \frac{1}{q}) & \text{with probability } q \\ 0 & \text{with probability } 1-q \end{cases}$,
  - $\mathbf{H}$ normalized Hadamard,
  - $\mathbf{D}$ with independent Rademacher (± 1) entries.

$$\mathbf{H}_0 = 1$$

$$\mathbf{H}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$\mathbf{H}_m = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{H}_{m-1} & \mathbf{H}_{m-1} \\ \mathbf{H}_{m-1} & -\mathbf{H}_{m-1} \end{pmatrix}$$

Classical structured matrices

$$\mathbf{H}_0 = 1$$

$$\mathbf{H}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$\mathbf{H}_m = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{H}_{m-1} & \mathbf{H}_{m-1} \\ \mathbf{H}_{m-1} & -\mathbf{H}_{m-1} \end{pmatrix}$$

$$\mathbf{G}_{skew-circ} = \begin{pmatrix} \mathbf{a} & -\mathbf{b} & -\mathbf{c} & -\mathbf{d} & -\mathbf{e} \\ e & a & -b & -c & -d \\ d & e & a & -b & -c \\ c & d & e & a & -b \\ b & c & d & e & a \end{pmatrix}$$

$$\mathbf{G}_{circ} = \begin{pmatrix} \mathbf{a} & \mathbf{b} & \mathbf{c} & \mathbf{d} & \mathbf{e} \\ e & a & b & c & d \\ d & e & a & b & c \\ c & d & e & a & b \\ b & c & d & e & a \end{pmatrix}$$

$$\mathbf{G}_{Toeplitz} = \begin{pmatrix} \mathbf{a} & \mathbf{b} & \mathbf{c} & \mathbf{d} & \mathbf{e} \\ \mathbf{f} & a & b & c & d \\ \mathbf{g} & f & a & b & c \\ \mathbf{h} & g & f & a & b \\ \mathbf{j} & h & g & f & a \end{pmatrix}$$

$$\mathbf{G}_{Hankel} = \begin{pmatrix} \mathbf{a} & \mathbf{b} & \mathbf{c} & \mathbf{d} & \mathbf{e} \\ b & c & d & e & \mathbf{f} \\ c & d & e & f & \mathbf{g} \\ d & e & f & g & \mathbf{h} \\ e & f & g & h & \mathbf{i} \end{pmatrix}$$

$$\mathbf{K} = \mathbf{R}_1 \otimes \mathbf{R}_2 \otimes \ldots \otimes \mathbf{R}_m \in \mathbb{R}^{2^m \times 2^m}$$

$$\mathbf{R}_i \in \mathbb{R}^{2\times 2} \text{ or } \mathbf{R}_i \in \{-1, 1\}^{2\times 2}$$

$$\mathbf{R}_i \mathbf{R}_i{}^T = \mathbf{R}_i{}^T \mathbf{R}_i = \mathbf{I}_2$$

And what is about our *Structured Spinners*-family?

Main purpose of *Structured Spinners*-family

Speed up several machine learning algorithms relying on unstructured random matrices with almost no loss of accuracy!

Arguments

- Speedups:
  - Fast Fourier Transform (FFT) or Fast Hadamard Transform (FHT): $O(n \log m)$ instead of $O(mn)$ for matrix-vector product.
- Less storage:
  - $\mathbf{H}$ is not stored
  - Sparse matrices: diagonal ones
  - Structured matrices: $n \times n$-circulant one $\Longrightarrow$ only n parameters (linear)
  - Structured matrices with ± 1 entries: only bits.

Some of state-of-the-art for structured matrices in applications (1/2)

Approximate Nearest Neighbor search (ANN), e.g.:

- [Andoni et al., 2015]: Locality-Sensitive Hashing (LSH), $\mathbf{HD}_3\mathbf{HD}_2\mathbf{HD}_1$.

Quantization, e.g.:

- [Yu et al., 2014]: $\mathbf{G}_{circulant}$

$$\mathbf{G}_{circulant} = \begin{pmatrix} \mathbf{a} & \mathbf{b} & \mathbf{c} & \mathbf{d} & \mathbf{e} \\ e & a & b & c & d \\ d & e & a & b & c \\ c & d & e & a & b \\ b & c & d & e & a \end{pmatrix}$$

Some of state-of-the-art for structured matrices in applications (2/2)

Kernel approximation via random feature maps
[Rahimi and Recht, 2007, Rahimi and Recht, 2009]

- [Le et al., 2013]: "FastFood", $\frac{1}{\sqrt{n}}\mathbf{SHGPHB}$,
- [Feng et al., 2015]: $\pm 1\mathbf{G}_{circulant}$,
- [Choromanski and Sindhwani, 2016]: "$\mathcal{P}$-model", and Toeplitz-like semi-Gaussian matrices,

  $\sum_{i=1}^{r} \mathrm{Circ}[\mathbf{g}^i]\,\mathrm{SkewCirc}[\mathbf{h}^i]$ for some $\{\mathbf{g}^i, \mathbf{h}^i\}_{i=1}^{r} \in \mathbb{R}^n$.

Plan

Definition of *Structured Spinners* family

Structured Spinners for 3 blocks

$$\mathbf{G} \rightarrow \mathbf{G}_{struct}$$

$$\mathbf{G}_{struct} = \mathbf{M}_3\mathbf{M}_2\mathbf{M}_1 \in \mathbb{R}^{n \times n},$$

where matrices $\mathbf{M}_1, \mathbf{M}_2$ and $\mathbf{M}_3$ satisfy 3 conditions.

Examples

- $[\mathbf{G}_{circ} \mid \mathbf{G}_{skew-circ} \mid \mathbf{G}_{Toeplitz} \mid \mathbf{G}_{Hankel}]\mathbf{D}_2\mathbf{H}\mathbf{D}_1$,
- $\sqrt{n}\,\mathbf{H}\mathbf{D}_{g_1,\ldots,g_n}\mathbf{H}\mathbf{D}_2\mathbf{H}\mathbf{D}_1$,
- $\sqrt{n}\,\mathbf{H}\mathbf{D}_3\mathbf{H}\mathbf{D}_2\mathbf{H}\mathbf{D}_1$.

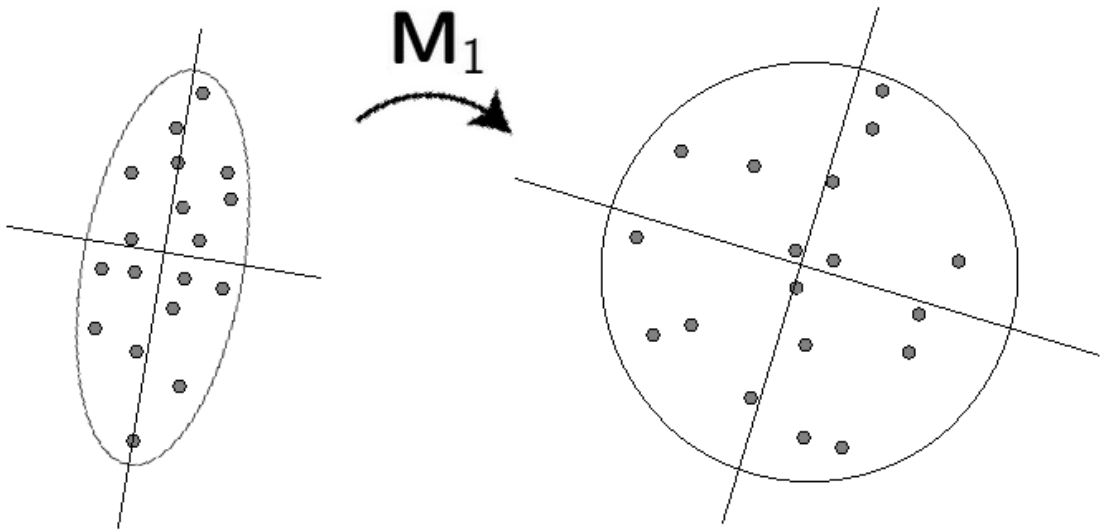
Role of each *Structured Spinner* block

$$\mathbf{G}_{struct} = \mathbf{M}_3\mathbf{M}_2\mathbf{M}_1$$

Role of each *Structured Spinner* block - $\mathbf{M}_1$

$$\mathbf{G}_{struct} = \mathbf{M}_3\mathbf{M}_2\mathbf{M}_1$$

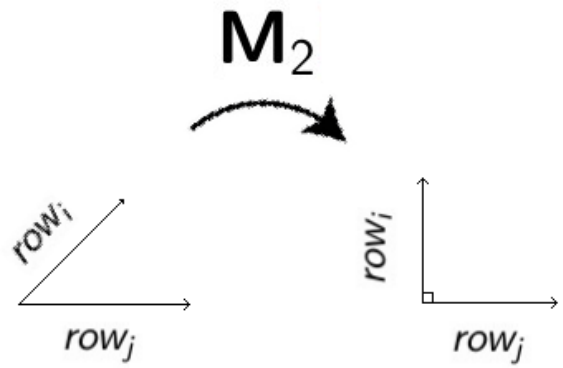
$\hookrightarrow$ Balances data.



Role of each *Structured Spinner* block - $\mathbf{M}_2$

$$\mathbf{G}_{struct} = \mathbf{M}_3\mathbf{M}_2\mathbf{M}_1$$

$\hookrightarrow$ Makes the rows of the final matrix almost independent.



Role of each *Structured Spinner* block - $\mathbf{M}_3$

$$\mathbf{G}_{struct} = \mathbf{M}_3\mathbf{M}_2\mathbf{M}_1$$

$\hookrightarrow$ Budget of randomness.

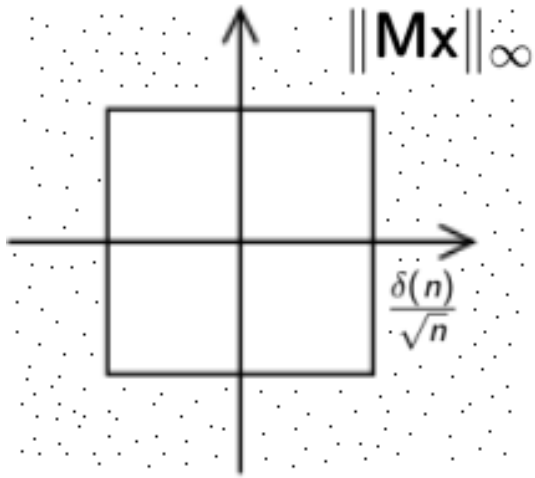
Condition 1 - Balanceness

Condition 1: $\mathbf{M}_1$ and $\mathbf{M}_2\mathbf{M}_1$ are $(\delta(n), p(n))$-balanced isometries.

Definition: $(\delta(n), p(n))$-balanced matrices

A randomized matrix $\mathbf{M} \in \mathbb{R}^{n \times n}$ is $(\delta(n), p(n))$-balanced if it represents an isometry and for every $\mathbf{x} \in \mathbb{R}^n$ with $\|\mathbf{x}\|_2 = 1$ we have:

$$\mathbb{P}[\|\mathbf{M}\mathbf{x}\|_\infty > \frac{\delta(n)}{\sqrt{n}}] \leq p(n).$$



Example

$\mathbf{M}_1 = \mathbf{H}\mathbf{D}_1$, since $\mathbf{H}\mathbf{D}_1$ is $(\log(n), 2ne^{-\frac{\log^2(n)}{8}})$-balanced.

Condition 2 - Decorrelation (1/2)

Condition 2: $\mathbf{M}_2 = \mathbf{V}(\mathbf{W}^1, ..., \mathbf{W}^n)\mathbf{D}_{\rho_1,...,\rho_n}$ for some (Λ_F, Λ_2)-smooth set $\mathbf{W}^1, ..., \mathbf{W}^n \in \mathbb{R}^{k \times n}$ and some i.i.d sub-Gaussian random variables $\rho_1, ..., \rho_n$ with sub-Gaussian norm K.

$$\mathbf{V}(\mathbf{W}^1, ..., \mathbf{W}^n) = \begin{pmatrix} \mathbf{W}^1 \\ \mathbf{W}^2 \\ ... \\ \mathbf{W}^n \end{pmatrix} \qquad \mathbf{D}_{\rho_1,...,\rho_n} = \begin{pmatrix} \rho_1 & 0 & \dots & 0 \\ 0 & \rho_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & \rho_n \end{pmatrix}$$

Typically, $K = 1$.

Condition 2 - Decorrelation (2/2)

Definition: (Λ_F, Λ_2)-smooth sets

A deterministic set of matrices $\mathbf{W} = \{\mathbf{W}^1, ..., \mathbf{W}^n\}$, where $\mathbf{W}^i = \{w^i_{k,l}\}_{k,l \in \{1,...,n\}}$ is (Λ_F, Λ_2)-smooth if:

- for $i = 1, ..., n$:

$$\mathbf{W}^i = \begin{pmatrix} \vdots & & \vdots & & \vdots \\ \mathbf{W}^i_1 & \dots & \mathbf{W}^i_l & \dots & \mathbf{W}^i_n \\ \vdots & & \vdots & & \vdots \end{pmatrix}$$

$$\|\mathbf{W}^i_1\|_2 = .. = \|\mathbf{W}^i_l\|_2 = .. = \|\mathbf{W}^i_n\|_2$$

- for $i \neq j$ and $l = 1, ..., n$:

$$\mathbf{W}^i = \begin{pmatrix} \dots & \vdots & \dots \\ \dots & \mathbf{W}^i_l & \dots \\ \dots & \vdots & \dots \end{pmatrix} \quad \mathbf{W}^j = \begin{pmatrix} \dots & \vdots & \dots \\ \dots & \mathbf{W}^j_l & \dots \\ \dots & \vdots & \dots \end{pmatrix}$$

$$(\mathbf{W}^i_l)^T \cdot \mathbf{W}^j_l = 0$$

- $\max_{i,j} \|(\mathbf{W}^j)^T \mathbf{W}^i\|_F \leq \Lambda_F$ and $\max_{i,j} \|(\mathbf{W}^j)^T \mathbf{W}^i\|_2 \leq \Lambda_2$.

Condition 3 - Budget of randomness

Condition 3: $\mathbf{M}_3 = \mathbf{C}(\mathbf{r}, n)$ for $\mathbf{r} \in \mathbb{R}^k$, where $\mathbf{r}$ is random Rademacher (± 1 entries) or Gaussian.

$$M_3 = \begin{pmatrix} \mathbf{r}_1 & \dots & \mathbf{r}_k & 0 & \dots & \dots & \dots & \dots & \dots & 0 \\ 0 & \dots & 0 & \mathbf{r}_1 & \dots & \mathbf{r}_k & 0 & \dots & \dots & 0 \\ & & & & \vdots & \vdots & & & & \\ & & & & \vdots & \vdots & & & & \\ 0 & \dots & \dots & \dots & \dots & \dots & 0 & \mathbf{r}_1 & \dots & \mathbf{r}_k \end{pmatrix}$$

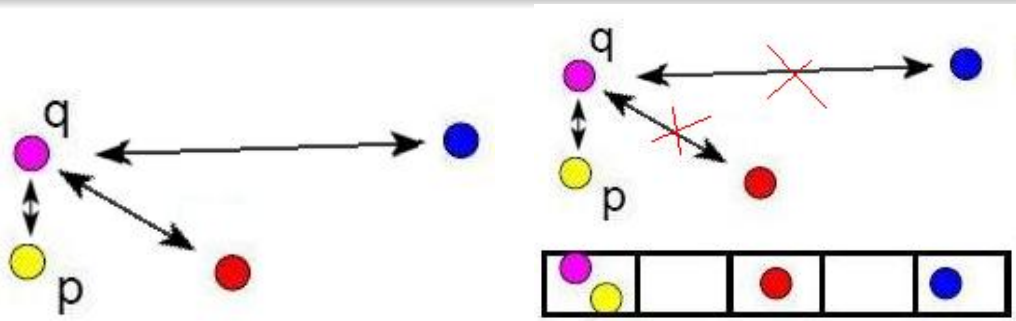
Plan

Plan

Locality-Sensitive Hashing (LSH) for Nearest Neighbor (NN) search

NN search naive approach

- Linear search.
- Prohibitive cost when lots of high dimensional data.
- Solution: Approximate Nearest Neighbor (ANN) search with LSH algorithm in sublinear time.



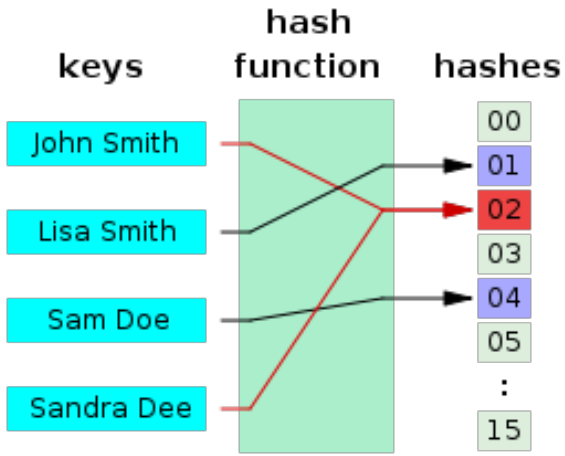
LSH : Two phases

- Build a data structure (hash table) for fast lookup.
- NN search phase: query the database with query point q.

Hashing vs LSH

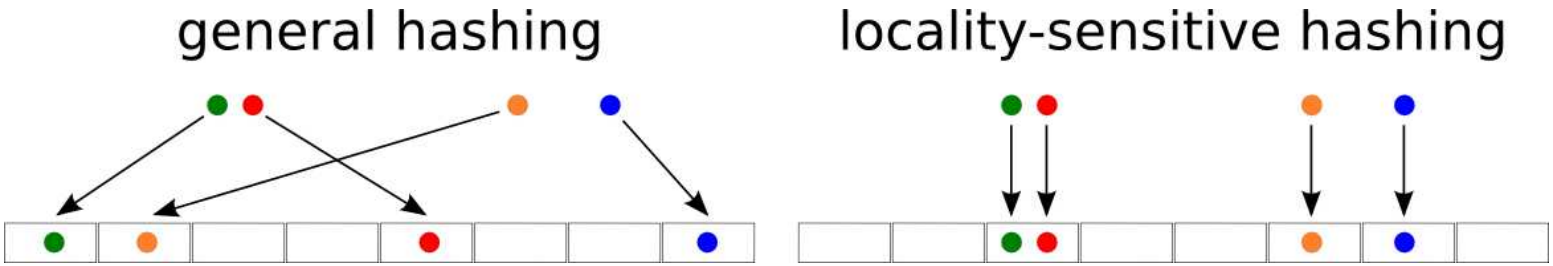
Hashing principle

- Mapping data from a potential high dimensionality to a fixed-size hash value.
- Fast lookup in a database.



LSH principle

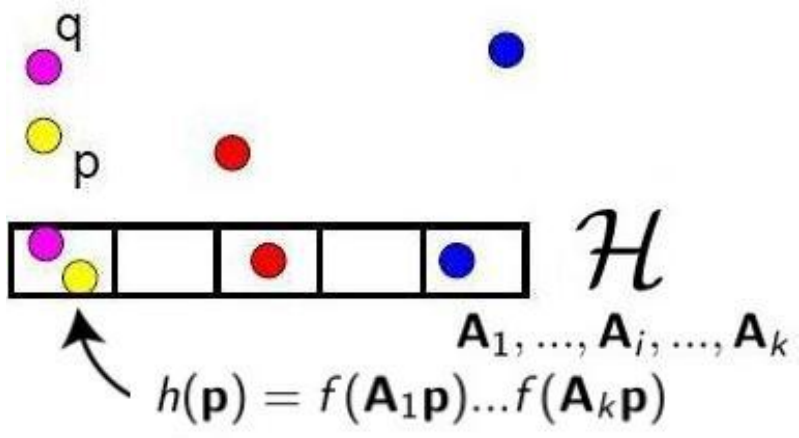
- Exploiting collision probabilities.



LSH in details

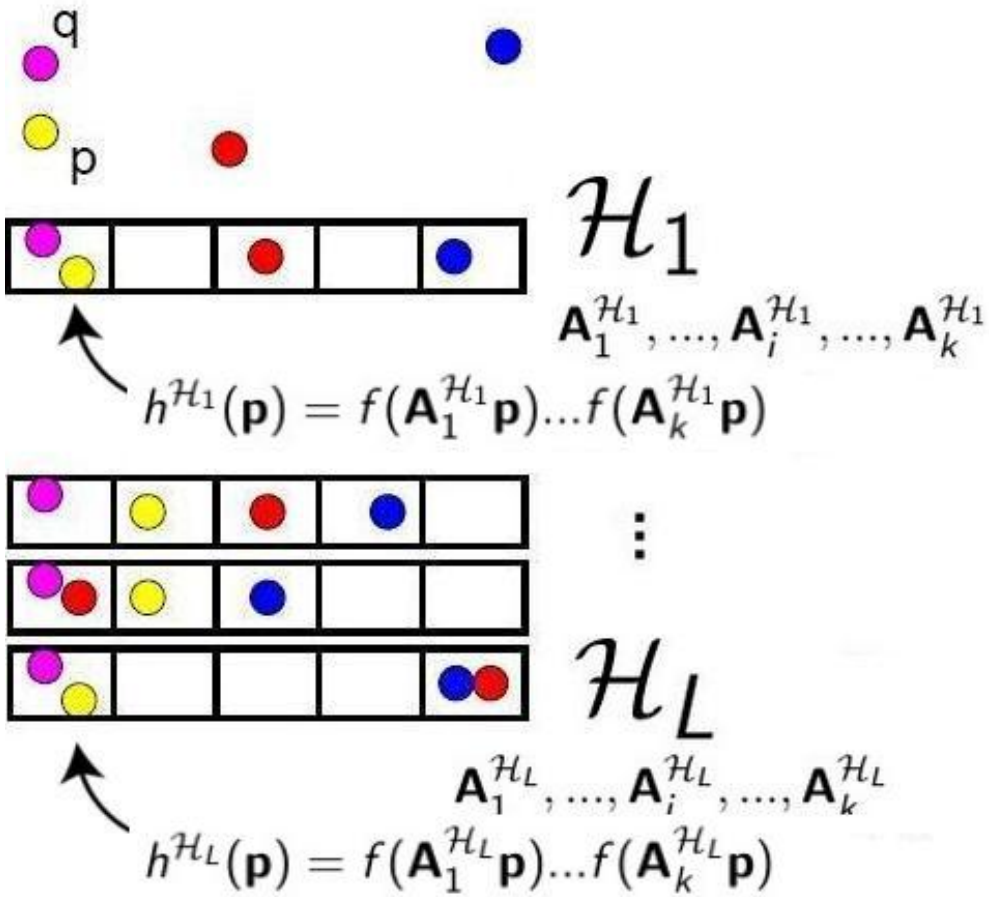
Hash value computation

- Hash value h of a point $\mathbf{x} \in \mathbb{R}^n$ is a combination of k hash function results $h_i, i = 1...k$ s.t. $h_i = f(\mathbf{A}_i\mathbf{x})$ with $\mathbf{A}_i \in \mathbb{R}^{m \times n}$ a projection matrix s.t. $m \ll n$.
- Example: Concatenation: $h = h_1 h_2 ... h_k$.



LSH in details

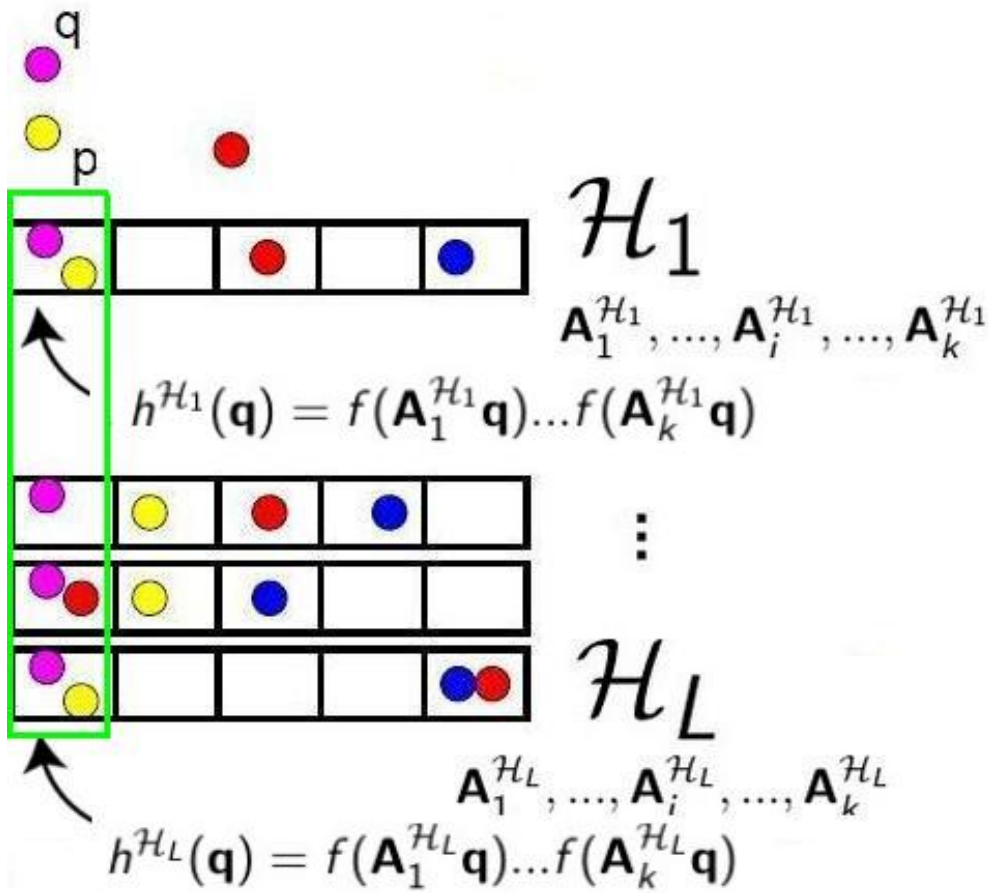
L hash tables



ANN search with LSH

ANN search

- Hash query q.
- Determine pool of candidates (in green).
- Linear scan in the pool of candidates.

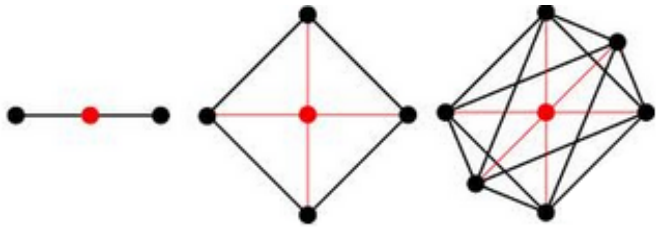


Cross-polytope LSH

Cross-polytope from [Terasawa and Tanaka, 2007]

$$h_i(\mathbf{x}) = f\left(\frac{\mathbf{Gx}}{||\mathbf{Gx}||_2}\right)$$

- $h = (2m)^{k-1}h_1 + ... + h_k$.
- $\mathbf{G} \in \mathbb{R}^{m \times n}$ a random matrix with i.i.d. Gaussian entries.
- $f(\mathbf{y})$ returns the closest vector to $\mathbf{y}$ from the set $\{\pm 1\mathbf{e}_i\}_{1 \leq i \leq m}$, where $\{\mathbf{e}_i\}_{1 \leq i \leq m}$ stands for the canonical basis.



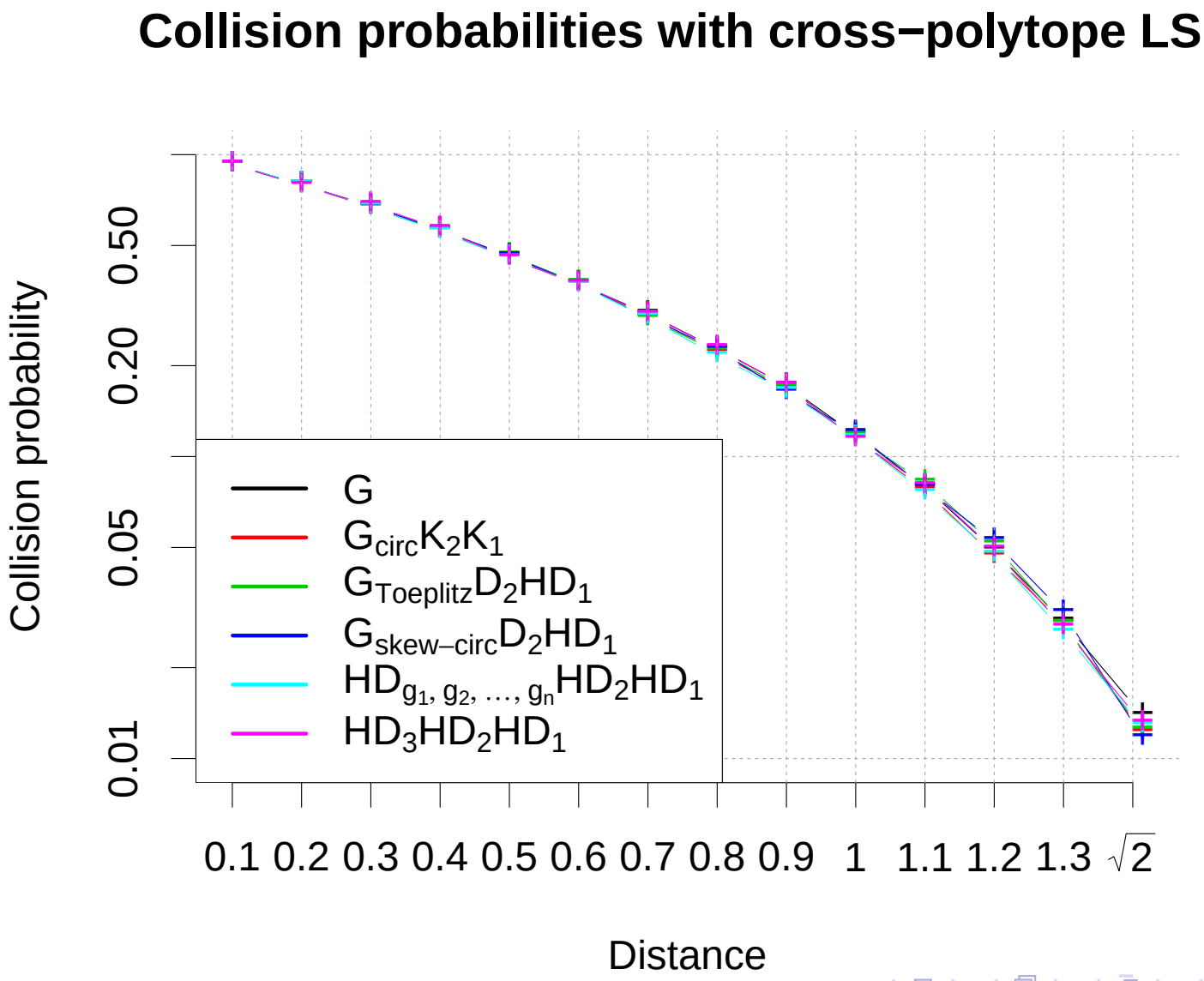
- State-of-the-art cross-polytope LSH [Andoni et al., 2015] $\mathbf{G} \rightarrow \mathbf{HD}_3\mathbf{HD}_2\mathbf{HD}_1$.
- Our variant: $\mathbf{G}_{struct} = \mathbf{M}_3\mathbf{M}_2\mathbf{M}_1$ + theoretical guarantees.

Cross-polytope LSH experiment with *Structured Spinners*

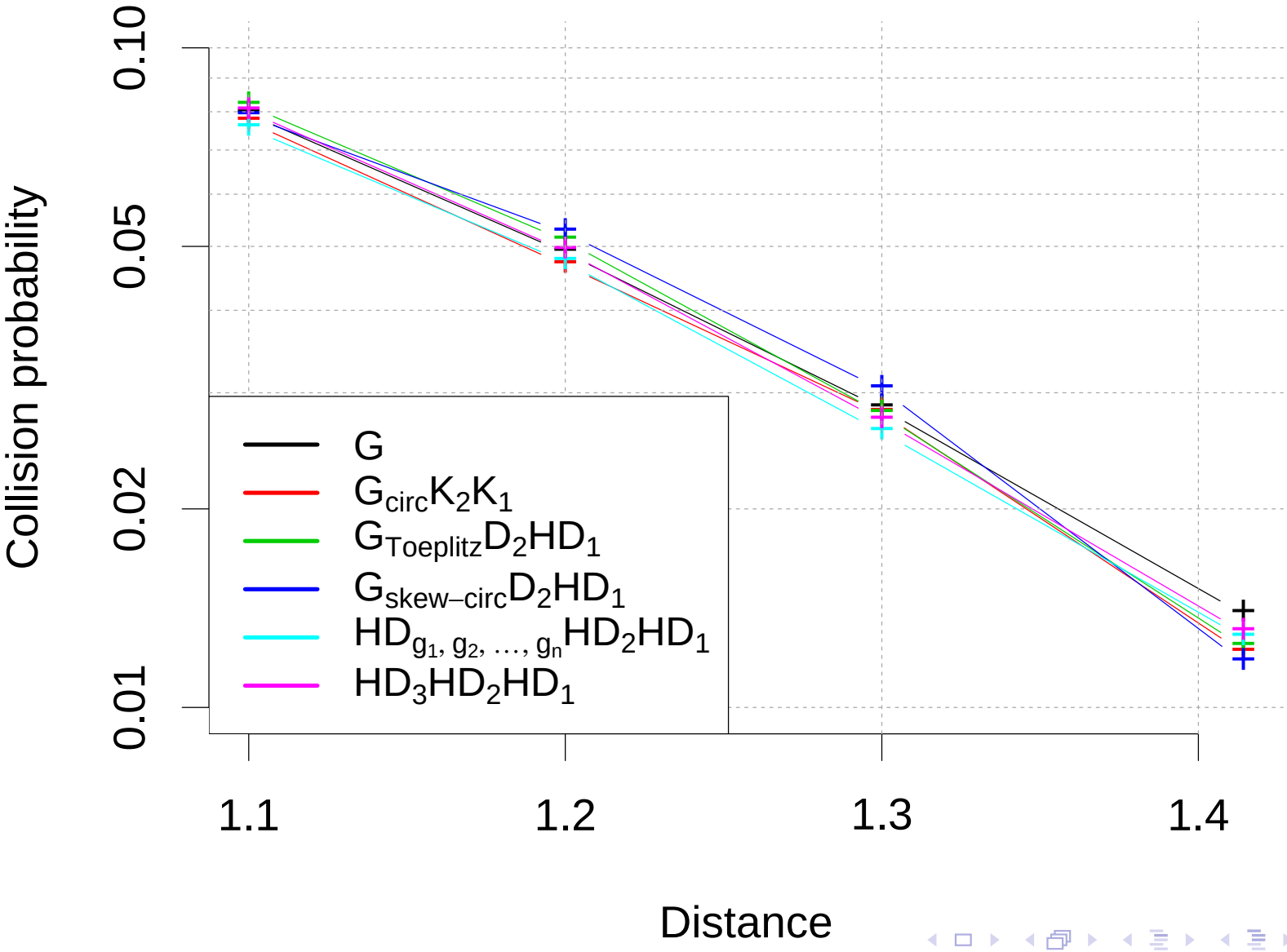
Experimental protocol

- Plot $Pr[h(p) = h(q)]$ as a function of $dist(p, q)$,
- 100 runs,
- $k = 1$,
- Draw points from the hypersphere $\implies \max_{p,q} dist(p, q) = \sqrt{2}$,
- 20000 points per interval of distance:
  $[0, 0.2), [0.2, 0.4), [0.4, 0.6), [0.6, 0.8), [0.8, 1.2), [1.2, \sqrt{2}]$,
- $n = 256$,
- $m = 64$.

Cross-polytope LSH experiment with *Structured Spinners*



Cross-polytope LSH experiment with *Structured Spinners*



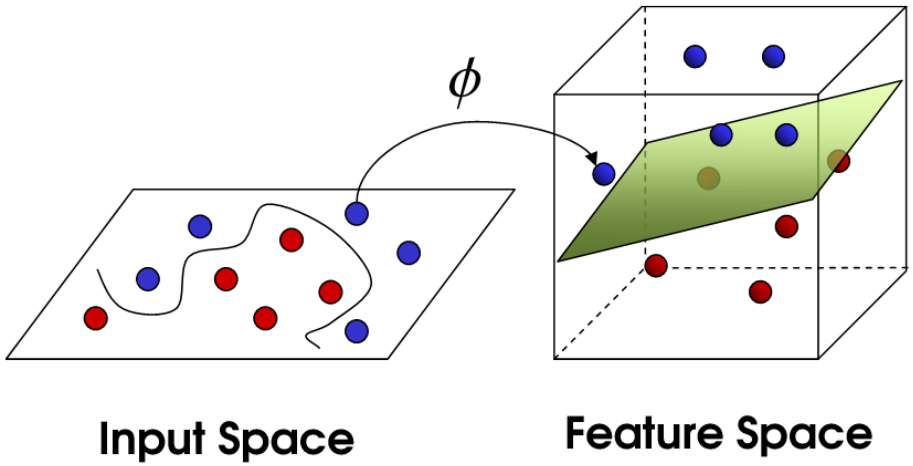
Plan

Kernel methods

Principle

- Goal: To solve nonlinear problems with linear methods.
- How? Map all data into a higher dimensional (possibly infinite) dot product space ν with feature map $\phi : \chi \to \nu$.
- Access to mapped data:

$$\kappa(\mathbf{x}, \mathbf{y}) = \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle$$



Kernel approximation in Support Vector Machines (SVM)

Decision evaluation in SVM: the "kernel trick"

$$f(x) = \langle \mathbf{w},\ \phi(\mathbf{x}) \rangle = \left\langle \sum_{i=1}^{N'} \alpha_i\ \phi(\mathbf{x}_i),\ \phi(\mathbf{x}) \right\rangle = \sum_{i=1}^{N'} \alpha_i\ \kappa(\mathbf{x}_i, \mathbf{x})$$

N' : number of nonzero α_i = number of "support vectors"

Why approximation ?

- Problem: evaluating f cost inscreases as the dataset grows
  N number of training samples.
- Kernel or Gram matrix K:

$$K_{ij} = \kappa(x_i, x_j)$$

$\Longrightarrow$ storage cost: $O(N^2)$

Kernel approximation via random feature maps

Random Kitchen Sinks [Rahimi and Recht, 2007, Rahimi and Recht, 2009]

- $\left\langle \underbrace{z(\mathbf{x})}_{\in\mathbb{R}^k}, z(\mathbf{y}) \right\rangle \approx \left\langle \underbrace{\phi(\mathbf{x})}_{\in\mathbb{R}^D}, \phi(\mathbf{y}) \right\rangle = \kappa(\underbrace{\mathbf{x}}_{\in\mathbb{R}^n}, \mathbf{y})$

  where $k \gg n$; D high, possibly infinite.

- $z(\mathbf{x}) = \frac{1}{\sqrt{k}}\, s(\mathbf{G}\mathbf{x})$,
- random Gaussian matrix $\mathbf{G} \in \mathbb{R}^{k\times n}$ with $k \gg n$, $k = O(n\epsilon^{-2}\log\frac{1}{\epsilon^2})$,
- s is a nonlinearity function.

Still a problem...

- Storage of $\mathbf{G}$: $O(kn)$,
- Computation of $\mathbf{G}\mathbf{x}$: $O(kn)$.

Solution

- Storage of $\mathbf{G}_{struct}$: $O(k\log n)$,
- Computation of $\mathbf{G}_{struct}\mathbf{x}$: $O(k\log n)$.

Experimental protocol for kernel approximation (1/2)

$\mathbf{A} \in \mathbb{R}^{k \times n}$ with $k \gg n$,

Gaussian kernel

- $\kappa_G(\mathbf{x}, \mathbf{y}) = e^{\frac{-||\mathbf{x}-\mathbf{y}||_2^2}{2\sigma^2}}$,
- $\tilde{\kappa}_G(\mathbf{x}, \mathbf{y}) = \frac{1}{k}\, s(\mathbf{Ax})^T s(\mathbf{Ay})$ with $s(x) = e^{\frac{-ix}{\sigma}}$ applied pointwise.

Angular kernel

- $\kappa_0(\mathbf{x}, \mathbf{y}) = 1 - \frac{\theta}{\pi}$ with $\theta = \cos^{-1}\left(\frac{\mathbf{x}^T\mathbf{y}}{||\mathbf{x}||||\mathbf{y}||}\right)$,
- $\tilde{\kappa}_0(\mathbf{x}, \mathbf{y}) = 1 - \frac{dist_{Hamming}(s(\mathbf{Ax}), s(\mathbf{Ay}))}{k}$

with $s(x) = sign(x)$ applied pointwise.

Experiments for kernel approximation (1/4)

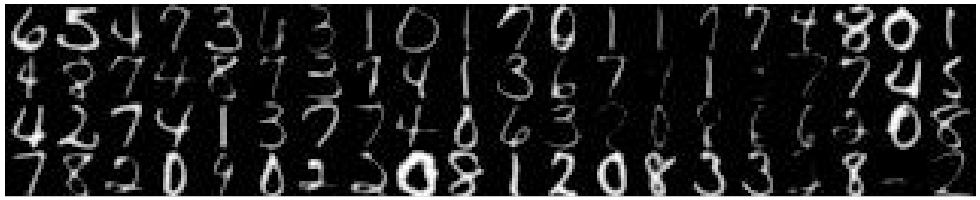
Speedups with Gaussian kernel

$Time(\mathbf{G})/Time(\mathbf{G}_{struct})$

Matrix dimensions	2^9	2^{10}	2^{11}	2^{12}	2^{13}	2^{14}	2^{15}
$\mathbf{G}_{Toeplitz}\mathbf{D}_2\mathbf{H}\mathbf{D}_1$	x1.4	x3.4	x6.4	x12.9	x28.0	x42.3	x89.6
$\mathbf{G}_{skew-circ}\mathbf{D}_2\mathbf{H}\mathbf{D}_1$	x1.5	x3.6	x6.8	x14.9	x31.2	x49.7	x96.5
$\mathbf{H}\mathbf{D}_{g_1,\ldots,g_n}\mathbf{H}\mathbf{D}_2\mathbf{H}\mathbf{D}_1$	x2.3	x6.0	x13.8	x31.5	x75.7	x137.0	x308.8
$\mathbf{H}\mathbf{D}_3\mathbf{H}\mathbf{D}_2\mathbf{H}\mathbf{D}_1$	x2.2	x6.0	x14.1	x33.3	x74.3	x140.4	x316.8

ex: $\mathbf{H}\mathbf{D}_3\mathbf{H}\mathbf{D}_2\mathbf{H}\mathbf{D}_1$, $k = 2^{15}$, $1.382s \rightarrow 4363\mu s$ in comparison with $\mathbf{G}$

Experimental protocol for kernel approximation (2/2)



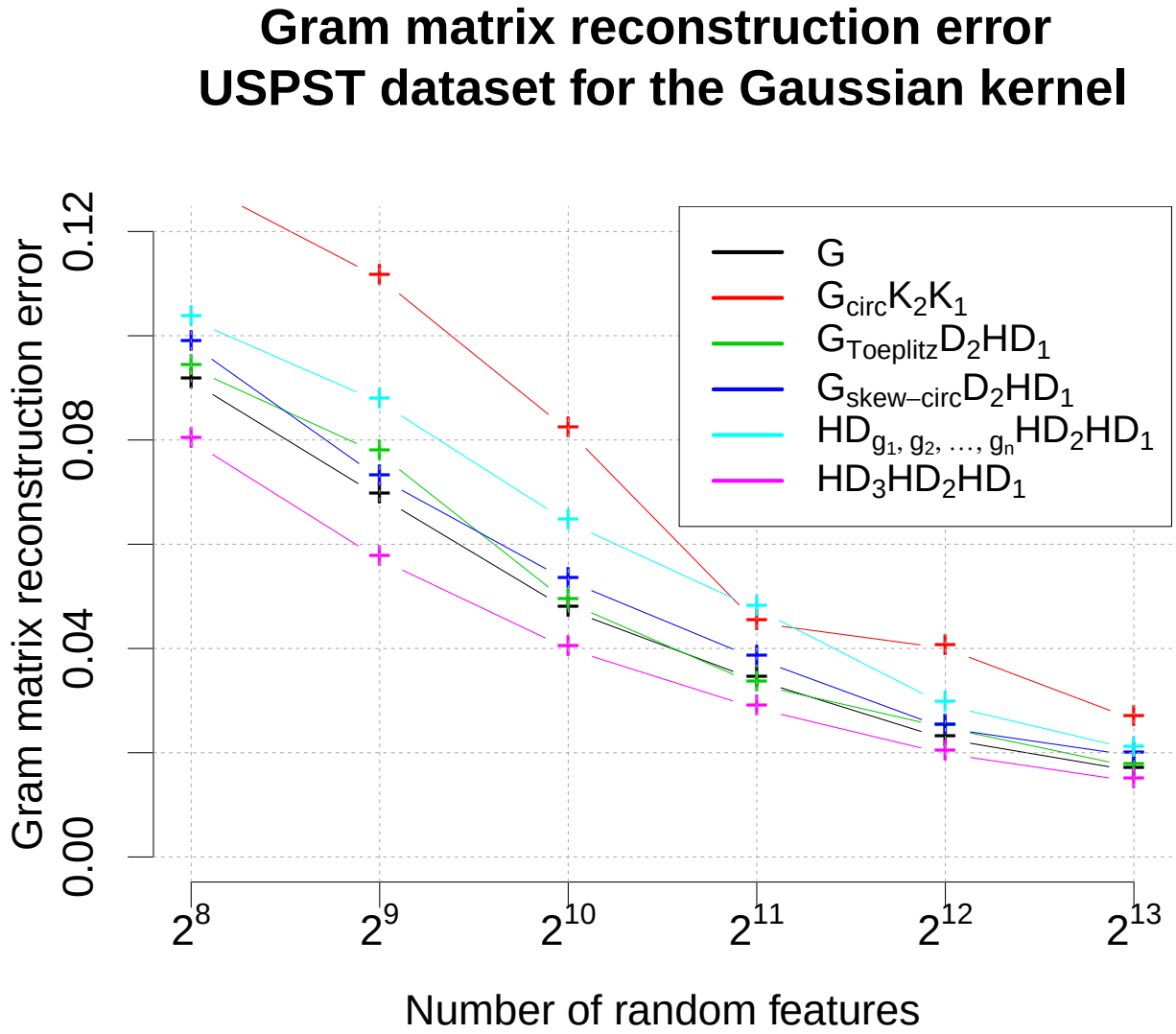
Measure of accuracy

- 10 runs,
- Dataset: USPST,
- 16×16 grayscale images,
- 2007 points of dimensionality 256 ($n = 256$),
- $\sigma = 9.4338$,
- Plots Gram reconstruction error: $\frac{||\mathbf{K} - \tilde{\mathbf{K}}||_F}{||\mathbf{K}||_F}$,
- $\mathbf{K}_{i,j} = \kappa(x_i, x_j)$.

Experiments for kernel approximation (2/3)

$$\frac{||\mathbf{K}-\tilde{\mathbf{K}}||_F}{||\mathbf{K}||_F}$$

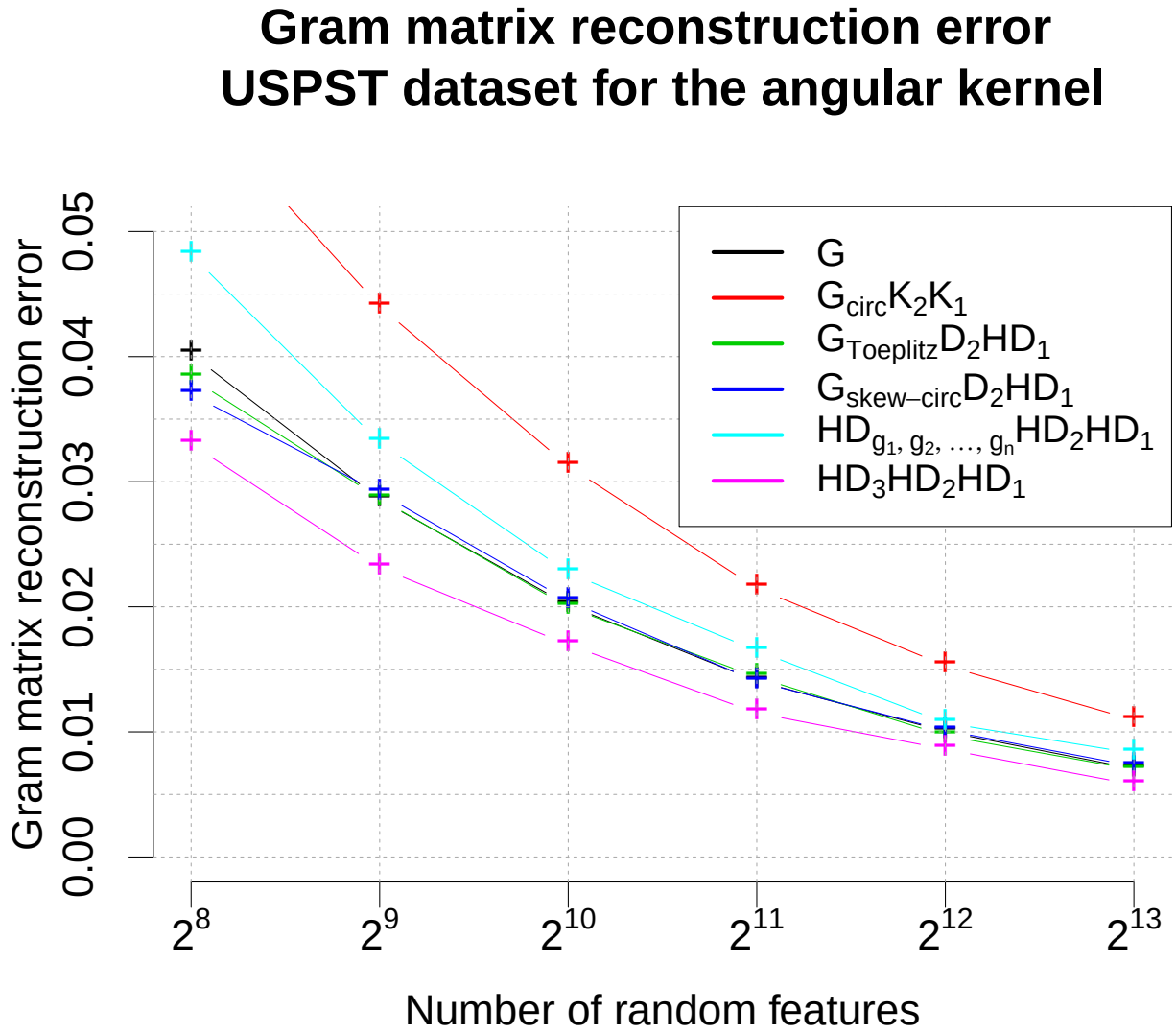
$$\mathbf{K}_{i,j} = \kappa(x_i, x_j)$$



Experiments for kernel approximation (3/3)

$$\frac{||\mathbf{K}-\tilde{\mathbf{K}}||_F}{||\mathbf{K}||_F}$$

$$\mathbf{K}_{i,j} = \kappa(x_i, x_j)$$



Plan

Unconstrained convex optimization with Newton step gradient descent

$$\text{minimize } f(x)$$

where $f : \mathbb{R} \to \mathbb{R}$ is convex and twice continuously differentiable.

- $x^{(t+1)} = x^{(t)} - \mu^{(t)} \nabla^2 f(x)^{-1} \nabla f(x)$
- *Newton decrement:* $\lambda = (\nabla f(x)^T \nabla^2 f(x)^{-1} \nabla f(x))^{1/2}$

  ↳ Used as stopping criterion + in backtracking line search:

  $$\text{while } \lambda^2 = -\nabla f(x)^T \Delta x > \epsilon$$

Principle of Newton sketch's algorithm [Pilanci and Wainwright, 2015]

Newton sketch's algorithm [Pilanci and Wainwright, 2015]

If analytic expression for the square root of the Hessian matrix:

$$x^{(t+1)} = x^{(t)} - \mu \, (\underbrace{(S^{(t)} \, (\nabla^2 f(x^{(t)}))^{1/2})^T}_{(SM)^T} \underbrace{S^{(t)} (\nabla^2 f(x^{(t)}))^{1/2}}_{SM})^{-1} \nabla f(x^{(t)})$$

where $S^{(t)} \in \mathbb{R}^{m \times n}$ is a sequence of isotropic sketchs matrices.

Example for Newton sketch's algorithm (1/2)

Large scale logistic regression problem

$$\min_{x \in \mathbb{R}^n} f(x)$$

$$\text{with } f(x) = \sum_{i=1}^{N} \log(1 + \exp(-y_i a_i^T x))$$

$$N \text{ observations } (a_i, y_i)_{i=1 \dots N}$$

$$\text{s.t. } a_i \in \mathbb{R}^n,$$

$$y_i \in \{-1, 1\}.$$

Example for Newton sketch's algorithm (2/2)

Analytic expressions for the gradient and the Hessian matrix

- $\nabla f(x^{(t)}) = \sum_{i=1}^{n} (\frac{1}{1+\exp(-y_i a_i^T x)} - 1) y_i a_i \ \in \mathbb{R}^n$,
- $\nabla^2 f(x^{(t)}) = A^T diag(\frac{1}{1+\exp(-a_i^T x)}(1 - \frac{1}{1+\exp(-a_i^T x)}))A \ \in \mathbb{R}^{n \times n}$,

  $A = [a_1^T ... a_N^T] \in \mathbb{R}^{N \times n}$, with $N \gg n$,
- We set

  $\nabla^2 f(x^{(t)})^{1/2} = diag(\frac{1}{1+\exp(-a_i^T x)}(1 - \frac{1}{1+\exp(-a_i^T x)}))^{1/2} A \in \mathbb{R}^{N \times n}$.

Newton sketch's algorithm, complexity analysis (1/2)

Comparison

- Exact Newton:

$$\nabla^2 f(x)^{-1}$$

$$\nabla^2 f(x^{(t)}) = A^T diag(\frac{1}{1+\exp(-a_i^T x)}(1 - \frac{1}{1+\exp(-a_i^T x)}))A$$

$$Cost = O(Nn^2 + n^3) \ (n \ll N)$$

Newton sketch's algorithm, complexity analysis (2/2)

Comparison

- Exact Newton:

$$Cost = O(Nn^2 + n^3) \ (n \ll N)$$

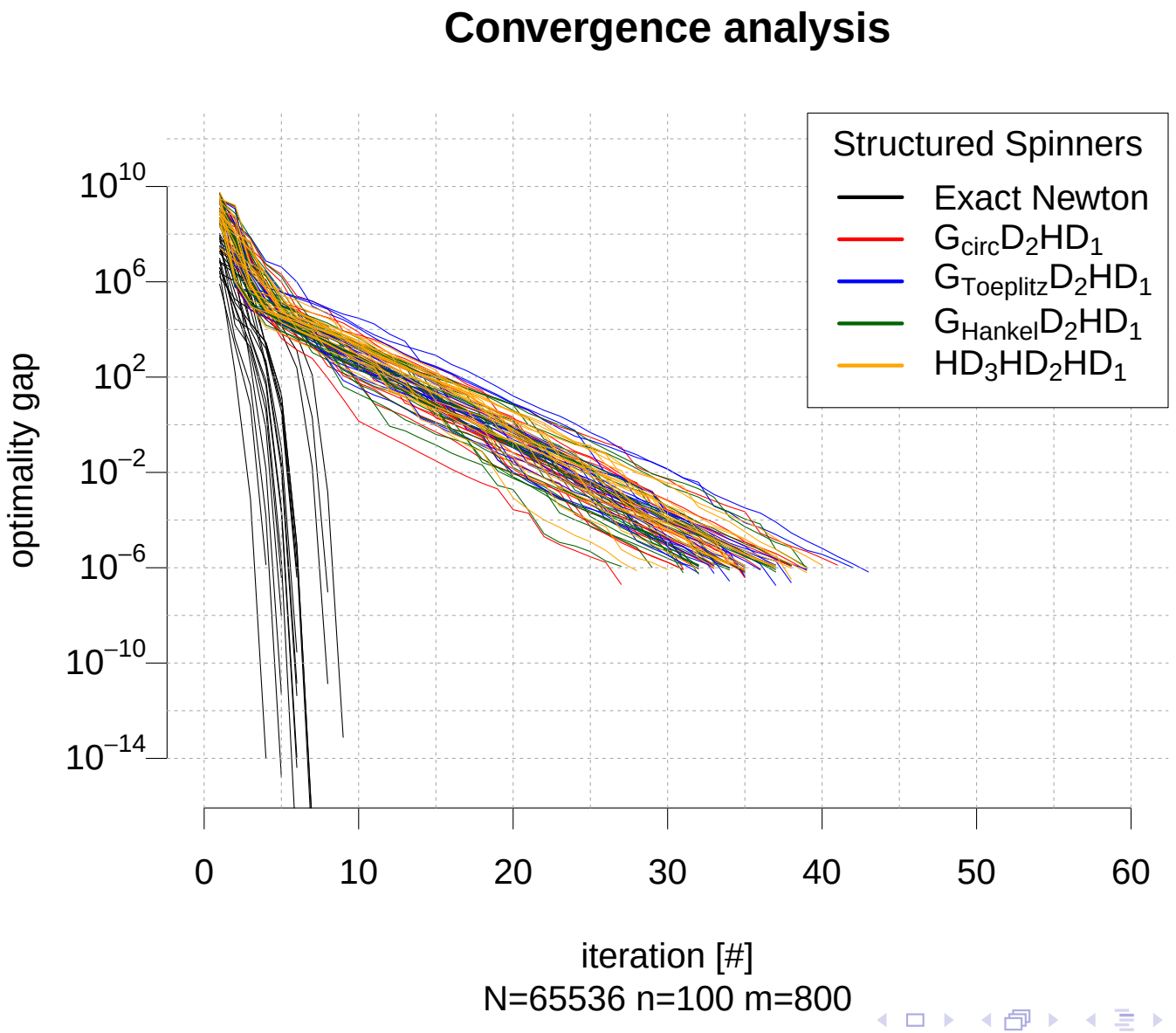
- Sketching: $((\underbrace{S^{(t)} \ (\nabla^2 f(x^{(t)}))^{1/2})^T}_{(SM)^T} \ \underbrace{S^{(t)}(\nabla^2 f(x^{(t)}))^{1/2}}_{SM} \ )^{-1}$

$$\nabla^2 f(x^{(t)})^{1/2} = diag(\frac{1}{1+\exp(-a_i^T x)}(1 - \frac{1}{1+\exp(-a_i^T x)}))^{1/2} A \in \mathbb{R}^{N \times n}$$

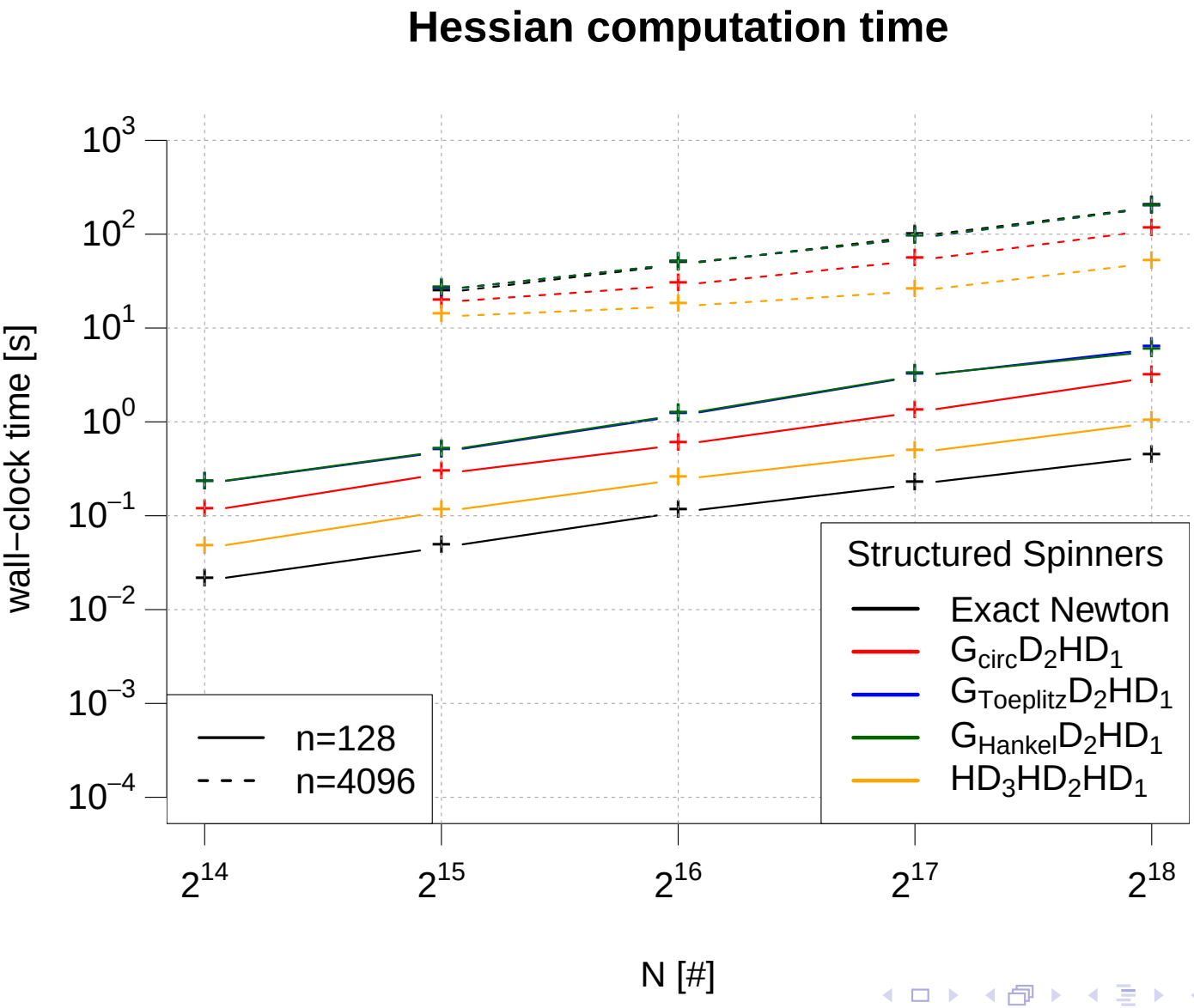
$$Cost = O(3nN \log N + mn^2 + n^3) \text{ with } m \ll N$$

Critical issue: when is $O(3nN \log N + mn^2)$ better than $O(Nn^2)$?

Experimental results (1/2)



Experimental results (2/2)

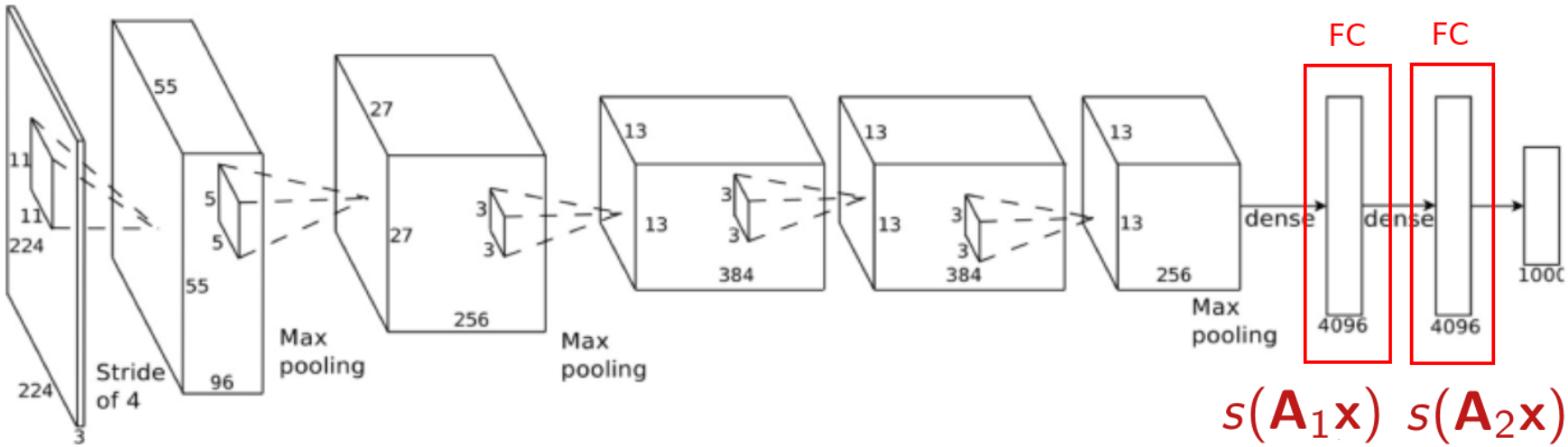


Plan

Plan

Deep neural networks and parameters

- Explosion of deep neural networks (e.g. convolutional networks) applications: with billions of parameters!
- Standard architecture: convolutional and fully-connected layers
- Convolutional layers: most of the computational effort
- Fully-connected layers: 90% of the parameters!
- Necessity to reduce the number of parameters for deployment on embedded mobile devices (speed up train + test time)



Plan

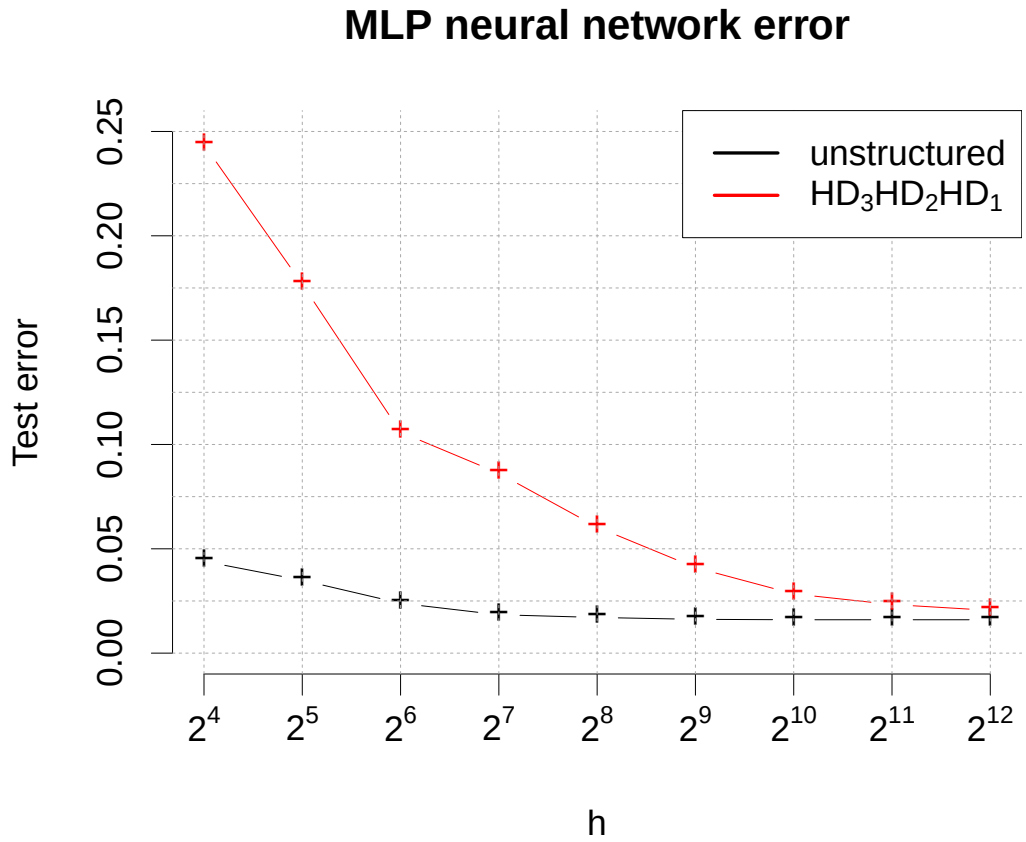
Related work

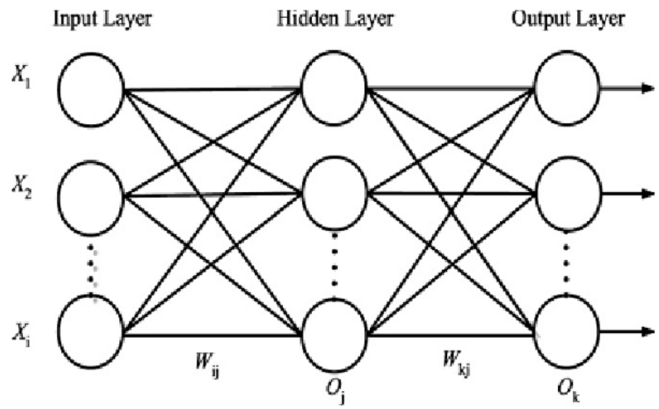
Some structured neural networks

- Deep Fried Convnets [Yang et al., 2015]: **SHGPHB** (Fastfood)
- [Moczulski et al., 2016]: $\mathbf{ACDC}^{-1}$, $\mathbf{A}$, $\mathbf{D}$ diagonal, $\mathbf{C}$ is the discrete cosine transform
- [Denil et al., 2013]: **UV**, fix $\mathbf{U} \in \mathbb{R}^{m \times r}$ and learn $\mathbf{V} \in \mathbb{R}^{r \times n}$, $r \ll m, n$
- [Sainath et al., 2013]: low-rank matrix factorization **UV**
- [Xue et al., 2013]: $\mathbf{U}(\mathbf{\Sigma}\mathbf{V}^T)$, $\mathbf{U} \in \mathbb{R}^{m \times r}$, $\mathbf{\Sigma} \in \mathbb{R}^{r \times r}$, $\mathbf{V} \in \mathbb{R}^{n \times r}$ (after training)

Plan

Structured MLP with 2 fully-connected layers on MNIST



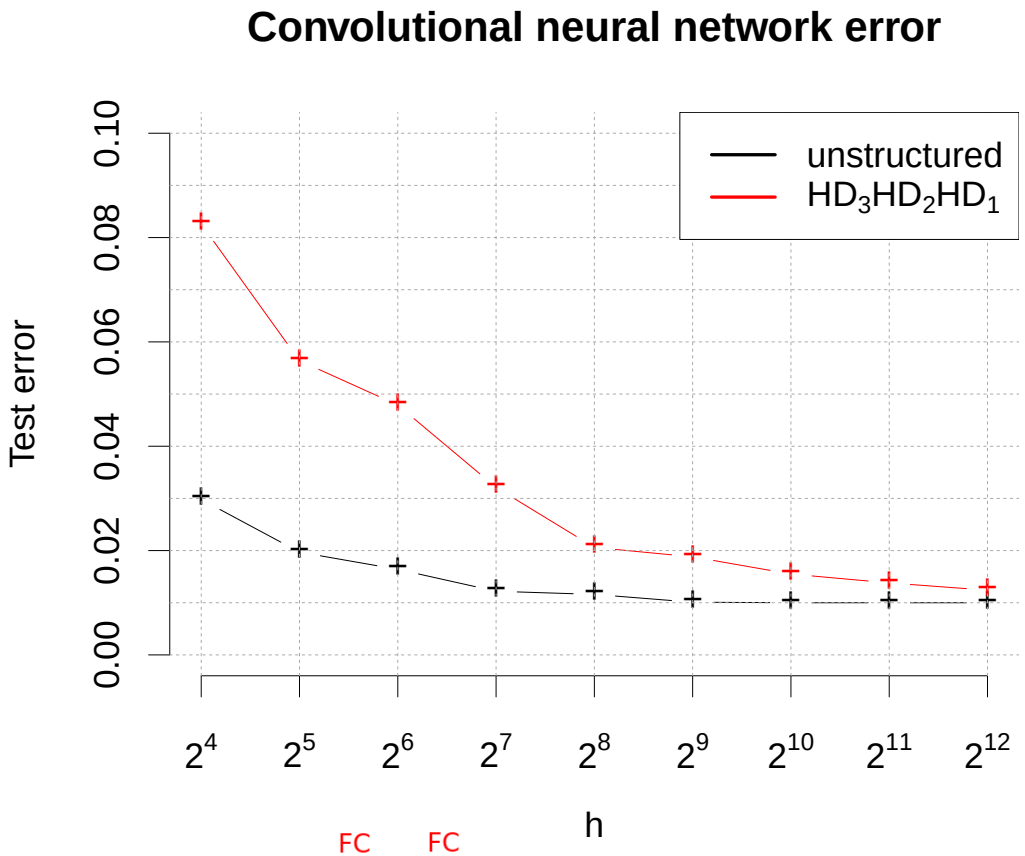


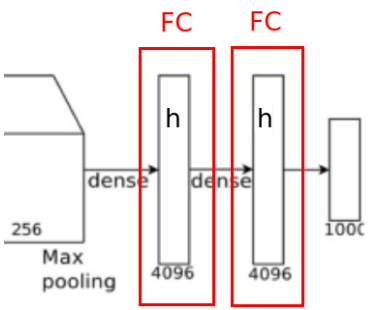
$s(\mathbf{A}_1\mathbf{x})$ $s(\mathbf{A}_2\mathbf{x})$

Running time (in μs), h: size of the hidden layers

h	2^4	2^5	2^6	2^7	2^8	2^9	2^{10}	2^{11}	2^{12}
unstructured	42.9	51.9	72.7	99.9	163.9	350.5	716.7	1271.5	2317.4
$HD_3HD_2HD_1$	109.2	121.3	109.7	114.2	117.4	123.9	130.6	214.3	389.8

Structured convolutional network on MNIST





$s(\mathbf{A}_1\mathbf{x})$ $s(\mathbf{A}_2\mathbf{x})$

- Conv. layer with filter size 5×5, 4 feature maps + ReLU + Max Pooling (region 2×2 and step 2×2)
- Conv. layer with filter size 5×5, 6 feature maps + ReLU + Max Pooling (region 2×2 and step 2×2)
- FC layer (h outputs) + ReLU
- FC layer (10 outputs)
- LogSoftMax.

Plan

Conclusion

Structured Spinners paper brings:

- a general structured paradigm for large scale machine learning computations with random matrices, providing computational speedups and storage compression with various applications:
  - kernel approximations via random feature maps
  - dimensionality reduction algorithms
  - deep learning
  - convex optimization via Newton sketches
  - quantization wit random projection trees
- theoretical guarantees on the effectiveness of the structured approach.

Open question

Can one obtain computation speedups for these matrices from the *Structured Spinners* model for which the Fast Fourier Transform trick does not work ?

Thank you for your attention!

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Kronecker matrices

Gaussian or discrete Kronecker matrix

$$\mathbf{K} = \mathbf{R}_1 \otimes \mathbf{R}_2 \otimes \ldots \otimes \mathbf{R}_m \in \mathbb{R}^{2^m \times 2^m}$$

$$\mathbf{R}_i \in \mathbb{R}^{2\times 2} \text{ or } \mathbf{R}_i \in \{-1, 1\}^{2\times 2}$$

$$\mathbf{R}_i \mathbf{R}_i^T = \mathbf{R}_i^T \mathbf{R}_i = \mathbf{I}_2$$

Kronecker product [Zhang et al., 2015]

$$\text{For } \mathbf{A} \in \mathbb{R}^{k_1, \times d_1}, \ \mathbf{B} \in \mathbb{R}^{k_1, \times d_1},$$

$$\mathbf{A} \otimes \mathbf{B} = \begin{pmatrix} \mathbf{A}_{11}\mathbf{B} & \ldots & \mathbf{A}_{1d_1}\mathbf{B} \\ \mathbf{A}_{21}\mathbf{B} & \ldots & \mathbf{A}_{2d_1}\mathbf{B} \\ \vdots & \ddots & \vdots \\ \mathbf{A}_{k_1 1}\mathbf{B} & \ldots & \mathbf{A}_{k_1 d_1}\mathbf{B} \end{pmatrix} \in \mathbb{R}^{k_1 k_2 \times d_1 d_2}$$

Thank you for your attention!