TripleSpin strikes back

New framework for fast structured ML computations

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Plan

Plan

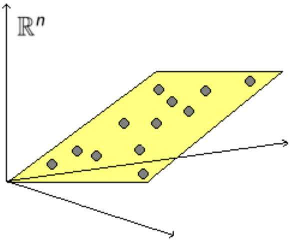
Why random projections? (1/3)

When all you data do not fit into memory:

- Massive data ...
- ... in high dimensionality.

Observation

Lot of high dimensional data with low intrinsic dimension.



Perform dimensionality reduction, e.g.:

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

Why random projections? (2/3)

Founder Lemma: [Johnson and Lindenstrauss, 1984]:

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

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

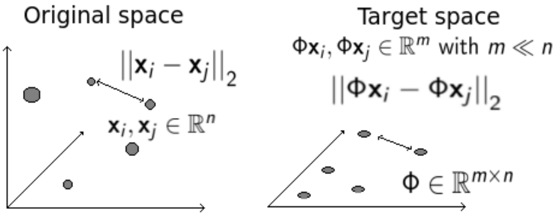
Then there exists a linear map $\Phi : \mathbb{R}^n \to \mathbb{R}^m$ s.t. :

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

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

Why random projections? (3/3)

Dimensionality reduction



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

Properties

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

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 (1/2)

Φ: Dense i.i.d. distribution

- [Johnson and Lindenstrauss, 1984],
- [Frankl and Maehara, 1987]: $\Phi_{i,j} \sim \mathcal{N}(0, \frac{1}{\sqrt{m}})$,
- [Indyk and Motwani, 1998] & [Dasgupta and Gupta, 1999]: simplification of JL lemma's proof,
- [Achlioptas, 2003]: $\Phi_{i,j} \sim \{-1, 1\}$ uniformly,
- [Matoušek, 2008]: $\Phi_{i,j} \sim$ any subgaussian distribution.

Can one sparsify the projection matrix Φ?

Can one sparsify the projection matrix Φ?

Brief random projections evolution (2/2)

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]: $\Phi = \mathbf{PHD}$
  - $\mathbf{P}_{i,j} = \begin{cases} \sim \mathcal{N}(0, \frac{1}{q}) & \text{with probability} \quad q \\ 0 & \text{with probability} \quad 1-q \end{cases}$,
  - $\mathbf{H}$ normalized Hadamard,
  - $\mathbf{D}$ with independent Rademacher (± 1) entries.
- [Matoušek, 2008]: For some $q \in O(\eta^2 m) \leq 1$:

$$\mathbf{P}_{i,j} = \begin{cases} \frac{1}{\sqrt{q}} & \text{with probability} \quad \frac{q}{2} \\ 0 & \text{with probability} \quad 1-q \\ \frac{-1}{\sqrt{q}} & \text{with probability} \quad \frac{q}{2} \end{cases}$$

for $\mathbf{x}$ s.t. $||\mathbf{x}||_\infty / ||\mathbf{x}||_2 \leq \eta$ (i.e. not sparse).

And what is about our *TripleSpin*-family?

Main purpose of *TripleSpin*-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): $O(n \log n)$ 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 $\implies$ only n parameters,
  - 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]: $\mathbf{G}_{circulant}$,
- [Choromanska et al., 2016]: Ψ-regular random matrix.

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

1. Introduction
2. Brief review of TripleSpin family
3. Some applications
4. Conclusion

Definition of *TripleSpin* family

TripleSpin 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

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

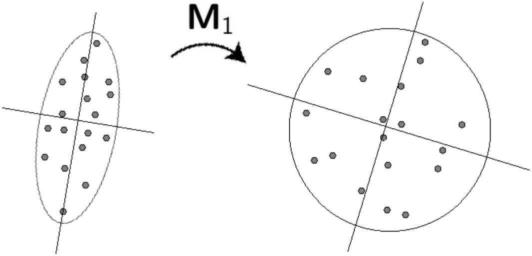
Role of each *TripleSpin* block

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

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

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

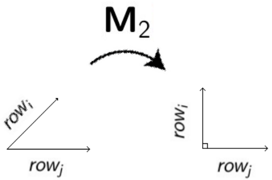
$\hookrightarrow$ Balances data.



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

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

$\hookrightarrow$ Budget of randomness.

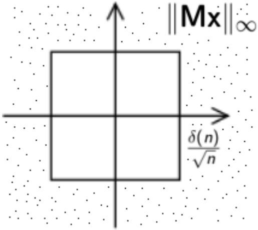
Condition 1

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:

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



Example

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

Condition 2 (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 (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 $i = 1, ..., n$:

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

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

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

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

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

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

Condition 3

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

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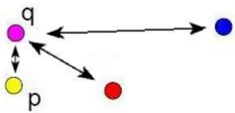
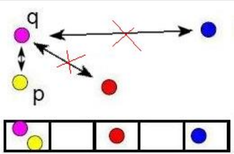
Locality-Sensitive Hashing (LSH) for Nearest Neighbor (NN) search

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.





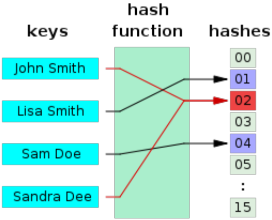
LSH : Two phases

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

Hashing vs LSH

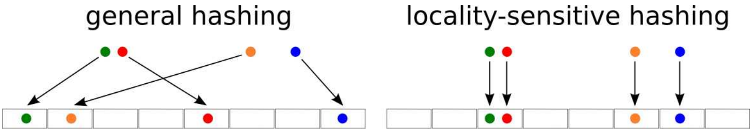
Hashing principle

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



LSH principle

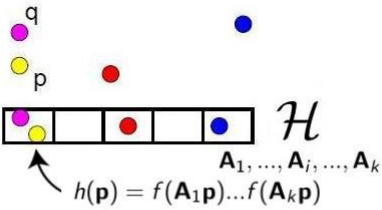
- Exploiting collision probabilities.



LSH in details

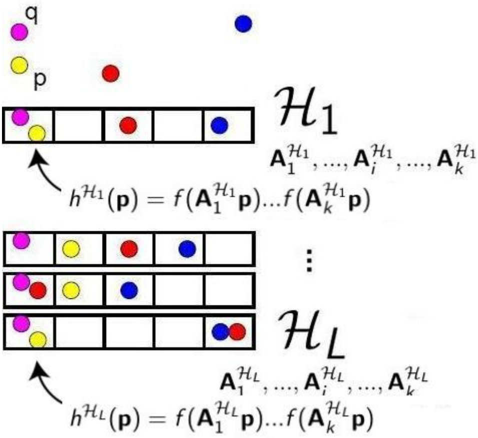
Hash value computation

- 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

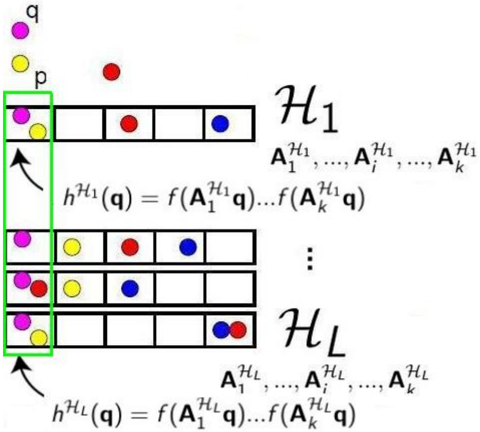
L hash tables



ANN search with LSH

ANN search

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

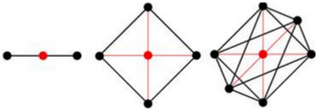


Cross-polytope LSH

Cross-polytope from [Terasawa and Tanaka, 2007]

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

- $h = (2m)^{k-1} h_1 + \ldots + h_k$.
- $\mathbf{G} \in \mathbb{R}^{m \times n}$ 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.



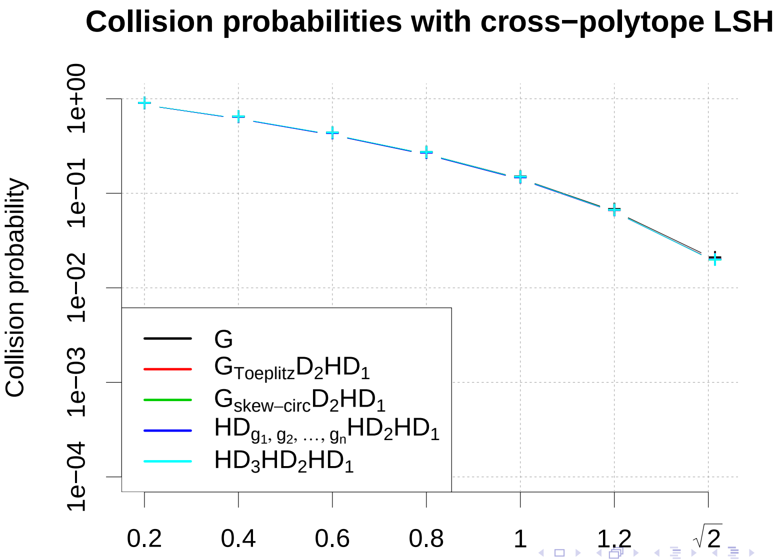
- State-of-the-art cross-polytope LSH [Andoni et al., 2015] $\mathbf{G} \rightarrow \mathbf{HD}_3\mathbf{HD}_2\mathbf{HD}_1$.
- Our variant: $\mathbf{G}_{struct} = \mathbf{M}_3\mathbf{M}_2\mathbf{M}_1$ + theoretical guarantees.

Cross-polytope LSH experiment with *TripleSpin*-matrices

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 *TripleSpin*-matrices



Plan

Kernel methods

Principle

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

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

- <u>Example:</u> the Gaussian radial basis function or Gaussian kernel,

$$\kappa(\mathbf{x}, \mathbf{y}) = e^{\frac{-||\mathbf{x}-\mathbf{y}||_2^2}{2\sigma^2}}.$$

Why kernel approximation?

Decision evaluation in kernel machines: 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.
- $z(\mathbf{x}) = \frac{1}{\sqrt{k}} s(\mathbf{Gx})$,
- 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 $\mathbf{Gx}$: $O(kn)$.

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

  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
$\mathbf{H}\mathbf{D}_{g_1,\dots,g_n}\mathbf{H}\mathbf{D}_2\mathbf{H}\mathbf{D}_1$	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

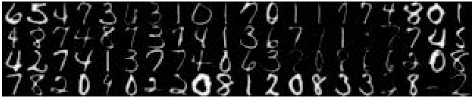
Experiments for kernel approximation (2/4)

Speedups with Gaussian kernel

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

$(n = 2^{11})$ k	2^{11}	2^{12}	2^{13}	2^{14}	2^{15}
$\mathbf{G}_{Toeplitz}\mathbf{D}_2\mathbf{H}\mathbf{D}_1$	x5.97	x6.68	x6.51	x6.52	x6.95
$\mathbf{G}_{skew-circ}\mathbf{D}_2\mathbf{H}\mathbf{D}_1$	x6.61	x6.73	x6.54	x6.65	x7.36
$\mathbf{H}\mathbf{D}_{g_1,\ldots,g_n}\mathbf{H}\mathbf{D}_2\mathbf{H}\mathbf{D}_1$	x13.74	x11.35	x10.86	x10.82	x11.90
$\mathbf{H}\mathbf{D}_3\mathbf{H}\mathbf{D}_2\mathbf{H}\mathbf{D}_1$	x10.67	x11.39	x10.22	x10.36	x11.8

Experimental protocol for kernel approximation (2/2)



Source [1]

Measure of accuracy

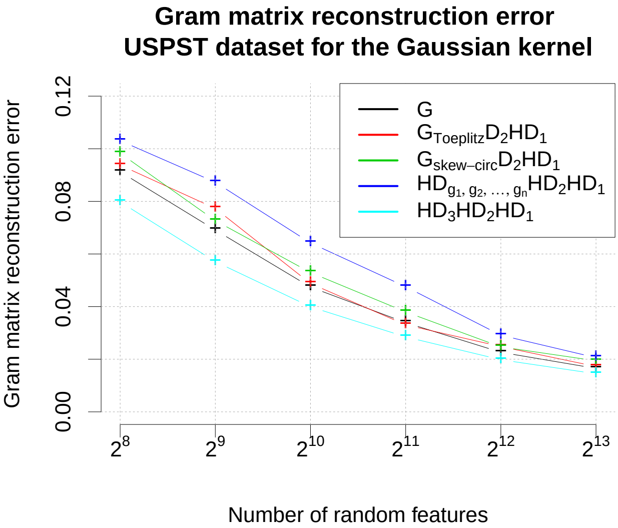
- 10 runs,
- Dataset: USPST,
- 16×16 grayscale images,
- 2007 points of dimensionality 256 ($n = 256$),
- $\sigma = 9.4338$,
- Plots Gram reconstruction error: $\frac{||\mathbf{K}-\tilde{\mathbf{K}}||_F}{||\mathbf{K}||_F}$,
- $\mathbf{K}_{i,j} = \kappa(x_i, x_j)$.

[1] http://statweb.stanford.edu/~tibs/ElemStatLearn/data.html

Experiments for kernel approximation (3/4)

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

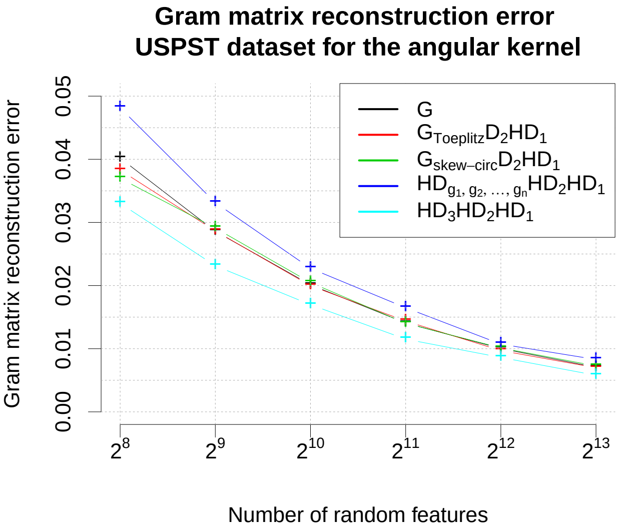
$$\mathbf{K}_{i,j} = \kappa(x_i, x_j)$$



Experiments for kernel approximation (4/4)

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

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



Plan

Brief review of unconstrained convex optimization (1/5)

The unconstrained optimization problem

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

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

Descent methods

- $x^{(t+1)} = x^{(t)} + \mu^{(t)} \Delta x^{(t)}$,
- $f(x^{(t+1)}) < f(x^{(t)})$,
- $\mu^{(t)} > 0$ except when $x^{(t)}$ is optimal,
- $\Delta x^{(t)}$ is the *step* or *search direction*,
- $\mu^{(t)}$ is called the *step size* or *step length*.

Brief review of unconstrained convex optimization (2/5)

General descent method

given a starting point x

repeat

  Determine a descent direction Δx

  Backtracking line search. Choose a step size $\mu > 0$

  Update. $x := x + \mu\Delta x$

until stopping criterion is satisfied;

Brief review of unconstrained convex optimization (3/5)

Gradient descent method with Newton step

Newton step: $\Delta x = -\nabla^2 f(x)^{-1} \nabla f(x)$ (vs. $\Delta x = -\nabla f(x)$)

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:

$$\lambda^2 = -\nabla f(x)^T \Delta x$$

Brief review of unconstrained convex optimization (4/5)

Newton's method

given a starting point x, tolerance $\epsilon > 0$

repeat

Compute the Newton step Δx and λ^2.

Stopping criterion. **quit** if $\lambda^2 \leq \epsilon$

Backtracking line search. Choose a step size $\mu > 0$

Update. $x := x + \mu \Delta x$

until stopping criterion is satisfied;

Brief review of unconstrained convex optimization (5/5)

Backtracking line search

given a descent direction Δx, $\alpha \in (0, 0.5)$, $\beta \in (0, 1)$

$\mu := 1$

while $\underline{f(x + \mu \Delta x) > f(x) + \alpha \mu \nabla f(x)^T \Delta x}$ **do**

$\quad \mu := \beta \mu$

end

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

Newton's method of unconstrained convex optimization

$$x^{(t+1)} = x^{(t)} - \mu^{(t)} \nabla^2 f(x)^{-1} \nabla f(x)$$

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

Is of interest where we have an analytic expression for the square root of the Hessian matrix. The problem is cast as the following:

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

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

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

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

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

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

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

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

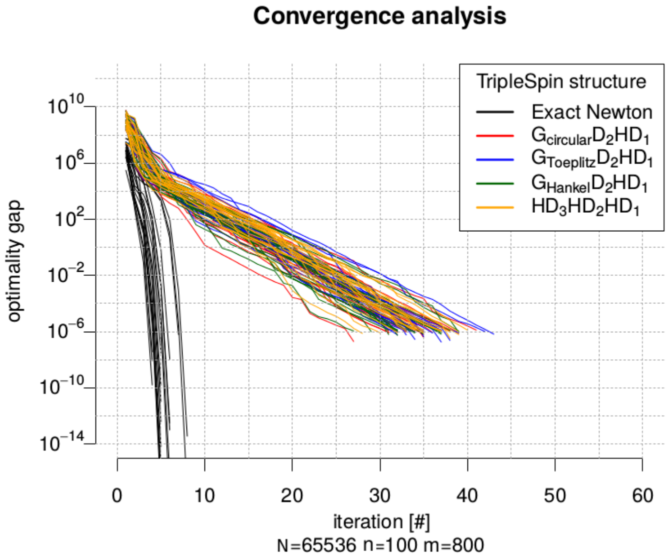
Analytic expressions for the gradient and the Hessian matrix

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

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

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

Experimental results (1/2)



Newton sketch's algorithm, complexity analysis (1/3)

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 (2/3)

Comparison

- Exact Newton:

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

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

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

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

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

Newton sketch's algorithm, complexity analysis (3/3)

Comparison

- Exact Newton:

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

- Sketching: $Cost = O(3nN \log N + mn^2 + n^3)$ with $m \ll N$

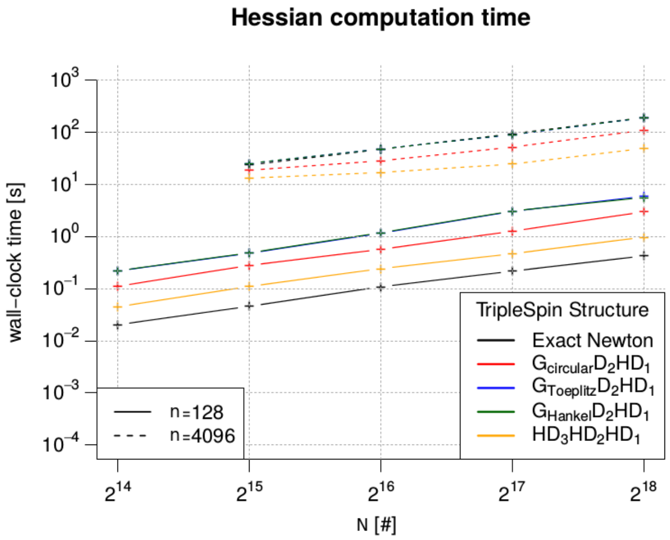
- Sub-sampling (m rows):

$$(\underbrace{SampleRows(\ (\nabla^2 f(x^{(t)}))^{1/2})^T}_{(M)^T}\ \underbrace{SampleRows((\nabla^2 f(x^{(t)}))^{1/2}}_{M}\ ))^{-1}$$

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

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

Experimental results (2/2)



Plan

Conclusion

TripleSpin paper brings:

- first theoretical guarantees for the fastest known cross-polytope LSH [Andoni et al., 2015] based on the $\mathbf{HD}_3\mathbf{HD}_2\mathbf{HD}_1$ structured matrix,
- a general structured paradigm for large scale machine learning computations with random matrices, providing computational speedups and storage compression.

Questions

- Can one obtain computations speedups for these matrices from the *TripleSpin* model for which the Fast Fourier Transform trick does not work ?
- Theoretical guarantees for learning with structured matrices ? (work in progress)

Thank you for your attention!

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Hadamard transform - recursive definition

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

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

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

Thank you for your attention!