Implementing Randomized Matrix Algorithms in Parallel and Distributed Environments

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October 2013

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Outline

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4 Solving ℓ_1 **[regression on MapReduce](#page-23-0)**

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Goal: very large-scale "vector space analytics"

Small-scale and medium-scale:

- Model data by graphs and matrices
- Compute eigenvectors, correlations, etc. in RAM

Very large-scale:

- Model data with flat tables and the relational model
- Compute with join/select and other "counting" in, e.g., Hadoop

Can we "bridge the gap" and do "vector space computations" at very large scale?

- Not obviously yes: exactly computing eigenvectors, correlations, etc. is subtle and uses lots of comminication.
- Not obviously no: lesson from random sampling algorithms is you can get ϵ -approximation of optimal with very few samples.

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Why randomized matrix algorithms?

Traditional matrix algorithms (direct & iterative methods, interior point, simplex, etc.) are designed to work in RAM and their performance is measured in floating-point operations per second (FLOPS).

- **Traditional algorithms** are NOT well-suited for:
	- \blacktriangleright problems that are very large
	- \blacktriangleright distributed or parallel computation
	- \triangleright when communication is a bottleneck
	- \triangleright when the data must be accessed via "passes"

• Randomized matrix algorithms are:

- \blacktriangleright faster: better theory
- \blacktriangleright simpler: easier to implement
- \blacktriangleright implicitly regularize: noise in the algorithm avoids overfitting
- \triangleright inherently parallel: exploiting modern computer architectures
- \triangleright more scalable: modern massive data sets

Traditional algorithms

• for ℓ_2 regression:

- ighthroapoortanal equation ($O(mn^2 + n^2)$ time)
	- \star Pros: high precision & implemented in LAPACK
	- \star Cons: hard to take advantage of sparsity & hard to implement in parallel environments
- \triangleright iterative methods: CGLS, LSQR, etc.
	- \star Pros: low cost per iteration, easy to implement in some parallel environments, & capable of computing approximate solutions
	- \star Cons: hard to predict the number of iterations needed

• for ℓ_1 regression:

- \blacktriangleright linear programming
- \triangleright interior-point methods (or simplex, ellipsoid? methods)
- \blacktriangleright re-weighted least squares
- \blacktriangleright first-order methods

Nearly all traditional algorithms for low-rank matrix problems, continuous optimization problems, etc. boil down to variants of these methods.

(□) (f)

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Over-determined/over-constrained regression

An $\ell_{\bm p}$ *regression problem* is specified by a design matrix $A \in \mathbb{R}^{m \times n}$, a response vector $b \in \mathbb{R}^m$, and a norm $\|\cdot\|_p$:

$$
\text{minimize}_{x \in \mathbb{R}^n} \quad \|Ax - b\|_p.
$$

Assume $m \gg n$, i.e., many more "constraints" than "variables." Given an $\epsilon > 0$, find a $(1 + \epsilon)$ -approximate solution \hat{x} in relative scale, i.e.,

$$
||A\hat{x}-b||_p \leq (1+\epsilon)||Ax^*-b||_p,
$$

where x^* is a/the optimal solution.

- $p = 2$: Least Squares Approximation: Very widely-used, but highly non-robust to outliers.
- $p = 1$: Least Absolute Deviations: Improved robustness, but at the cost of increased complexity.

Large-scale environments and how they scale

- Shared memory
	- ► cores: $[10, 10^3]$ *
	- \blacktriangleright memory: $[100GB, 100TB]$
- Message passing
	- ▶ cores: $[200, 10^5]^\dagger$
	- \blacktriangleright memory: [1TB, 1000TB]
	- ► CUDA cores: $[5 \times 10^4, 3 \times 10^6]^\ddag$
	- GPU memory: [500GB, 20TB]
- **•** MapReduce
	- ▶ cores: $[40, 10^5]$ [§]
	- \triangleright memory: [240GB, 100TB]
	- \triangleright storage: $[100TB, 100PB]^{\P}$
- Distributed computing
	- ► cores: $[-, 3 \times 10^5]$ ^{||}.

- † <http://www.top500.org/list/2011/11/100>
- ‡ <http://i.top500.org/site/50310>

§ <http://www.cloudera.com/blog/2010/04/pushing-the-limits-of-distributed-processing/>

¶ <http://hortonworks.com/blog/an-introduction-to-hdfs-federation/>

k <http://fah-web.stanford.edu/cgi-bin/main.py?qtype=osstats>

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Two important notions: leverage and condition

(Mahoney, "Randomized Algorithms for Matrices and Data," FnTML, 2011.)

- Statistical leverage. (Think: eigenvectors. Important for low-precision.)
	- \triangleright The statistical leverage scores of A (assume $m \gg n$) are the diagonal elements of the projection matrix onto the column span of A.
	- In They equal the ℓ_2 -norm-squared of any orthogonal basis spanning A.
	- \blacktriangleright They measure:
		- \star how well-correlated the singular vectors are with the canonical basis
		- \star which constraints have largest "influence" on the LS fit
		- \star a notion of "coherence" or "outlierness"
	- \triangleright Computing them exactly is as hard as solving the LS problem.
- **Condition number.** (Think: eigenvalues. Important for high-precision.)
	- ► The ℓ_2 -norm condition number of A is $\kappa(A) = \sigma_{\max}(A)/\sigma_{\min}^+(A)$.
	- \triangleright $\kappa(A)$ bounds the number of iterations; for ill-conditioned problems (e.g., $\kappa(A) \approx 10^6 \gg 1$), the convergence speed is very slow.
	- **Computing** $\kappa(A)$ **is generally as hard as solving the LS problem.**

These are [fo](#page-7-0)[r t](#page-9-0)[h](#page-7-0)[e](#page-8-0) ℓ_2 [-](#page-6-0)[n](#page-7-0)[o](#page-13-0)[r](#page-14-0)[m](#page-6-0)[.](#page-7-0) Generalizations exist for the ℓ_1 -norm.

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Meta-algorithm for ℓ_2 -norm regression

(Drineas, Mahoney, etc., 2006, 2008, etc., starting with SODA 2006; Mahoney FnTML, 2011.)

- 1: Using the ℓ_2 statistical leverage scores of A, construct an importance sampling distribution $\{p_i\}_{i=1}^m$.
- 2: Randomly sample a small number of constraints according to $\{ \rho_i \}_{i=1}^m$ to construct a subproblem.
- 3: Solve the ℓ_2 -regression problem on the subproblem.

A naïve version of this meta-algorithm gives a $1 + \epsilon$ relative-error approximation in roughly $O(mn^2/\epsilon)$ time (DMM 2006, 2008). (Ugh.)

Meta-algorithm for ℓ_2 -norm regression, cont.

(Drineas, Mahoney, etc., 2006, 2008, etc., starting with SODA 2006; Mahoney FnTML, $2011.^{\ddagger\ddagger}$)

We can make this meta-algorithm "fast" in RAM:**

- This meta-algorithm runs in $O(mn \log n/\epsilon)$ time in RAM if:
	- \triangleright we perform a Hadamard-based random projection and sample uniformly in a randomly rotated basis, or
	- \triangleright we quickly computing approximations to the statistical leverage scores and using those as an importance sampling distribution.

We can make this meta-algorithm "high precision" in RAM: ††

- This meta-algorithm runs in $O(mn \log n \log(1/\epsilon))$ time in RAM if:
	- \triangleright we use the random projection/sampling basis to construct a preconditioner and couple with a traditional iterative method.

^{∗∗} (Sarl´os 2006; Drineas, Mahoney, Muthu, Sarl´os 2010; Drineas, Magdon-Ismail, Mahoney, Woodruff 2011.)

^{††} (Rokhlin & Tygert 2008; Avron, Maymounkov, & Toledo 2010; Meng, Saunders, & Mahoney 2011.)

^{‡‡ (}Mahoney, "Randomized Algorithms for Matrices and Data," FnTML, 2011.[\)](#page-9-0) ← □ ▶ → ← ⑦ ▶ → ← ≧ ▶ → ← ≧

Randomized regression in RAM: Implementations

Avron, Maymounkov, and Toledo, SISC, 32, 1217–1236, 2010.

Conclusions:

- Randomized algorithms "beats Lapack's direct dense least-squares solver by a large margin on essentially any dense tall matrix."
- • These results "suggest that random projection algorithms should be incorporated into future versions of Lapack."

Randomized regression in RAM: Human Genetics

Paschou et al., PLoS Gen '07; Paschou et al., J Med Gen '10; Drineas et al., PLoS ONE '10; Javed et al., Ann Hum Gen '11.

Computing large rectangular regressions/SVDs/CUR decompositions:

- In commodity hardware (e.g., a 4GB RAM, dual-core laptop), using MatLab 7.0 (R14), the computation of the SVD of the dense 2, 240 \times 447, 143 matrix A takes about 20 minutes.
- Computing this SVD is not a one-liner—we can not load the whole matrix in RAM (runs out-of-memory in MatLab).
- Instead, compute the SVD of AAT.
- \bullet In a similar experiment, compute 1,200 SVDs on matrices of dimensions ([appr](#page-11-0)o[x.\)](#page-13-0) [1](#page-11-0), [20](#page-12-0)[0](#page-14-0) \times [45](#page-7-0)0, [00](#page-6-0)0 [\(](#page-7-0)[ro](#page-13-0)[ug](#page-14-0)[hly,](#page-0-0) [a fu](#page-35-0)ll leave-one-out cross-validation experiment). \leftarrow \Box QQ

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A retrospective

Randomized matrix algorithms:

- BIG success story in high precision scientific computing applications and *large-scale* statistical data analysis!
- Can they really be implemented in parallel and distributed environments for *LARGE-scale* statistical data analysis?

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Outline

Algorithm LSRN (for strongly over-determined systems)

(Meng, Saunders, and Mahoney 2011)

- 1: Choose an oversampling factor $\gamma > 1$, e.g., $\gamma = 2$. Set $s = \lceil \gamma n \rceil$.
- 2: Generate $G = \text{randn}(s, m)$, a Gaussian matrix.
- 3: Compute $A = GA$.
- 4: Compute \tilde{A} 's economy-sized SVD: $\tilde{U}\tilde{\Sigma}\tilde{V}^T$.
- 5: Let $N = \tilde{V} \tilde{\Sigma}^{-1}$.
- 6: Iteratively compute the min-length solution \hat{v} to

$$
\text{minimize}_{y \in \mathbb{R}^r} \quad \| A N y - b \|_2.
$$

7: Return $\hat{x} = N\hat{v}$.

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Why we choose Gaussian random projection

(Meng, Saunders, and Mahoney 2011)

Gaussian random projection

- **•** has the best theoretical result on conditioning,
- can be generated super fast,
- \bullet uses level 3 BLAS on dense matrices.
- speeds up automatically on sparse matrices and fast operators,
- \bullet still works (with an extra "allreduce" operation) when A is partitioned along its bigger dimension.

So, although it is "slow" (compared with "fast" Hadamard-based projections i.t.o. FLOPS), it allows for better communication properties.

Theoretical properties of LSRN

(Meng, Saunders, and Mahoney 2011)

- In exact arithmetic, $\hat{x} = x^*$ almost surely.
- The distribution of the spectrum of AN is the same as that of the pseudoinverse of a Gaussian matrix of size $s \times r$.
- $\kappa(AN)$ is independent of all the entries of A and hence $\kappa(A)$.
- For any $\alpha\in(0,1-\sqrt{r/s})$, we have

$$
\mathcal{P}\left(\kappa(AN) \leq \frac{1+\alpha+\sqrt{r/s}}{1-\alpha-\sqrt{r/s}}\right) \geq 1-2e^{-\alpha^2 s/2},
$$

where r is the rank of A.

So, if we choose $s = 2n \geq 2r$, we have $\kappa(AN) < 6$ w.h.p., and hence we only need around 100 iterations to reach machine precision.

Implementation of LSRN

(Meng, Saunders, and Mahoney 2011)

- Shared memory $(C_{++}$ with MATLAB interface)
	- \triangleright Multi-threaded ziggurat random number generator (Marsaglia and Tsang 2000), generating 10^9 numbers in less than 2 seconds using 12 CPU cores.
	- ▶ A naïve implementation of multi-threaded dense-sparse matrix multiplications.
- Message passing (Python)
	- \triangleright Single-threaded BLAS for matrix-matrix and matrix-vector products.
	- ▶ Multi-threaded BLAS/LAPACK for SVD.
	- \triangleright Using the Chebyshev semi-iterative method (Golub and Varga 1961) instead of LSQR.

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Solving real-world problems

Table: Real-world problems and corresponding running times. DGELSD doesn't take advantage of sparsity. Though MATLAB's backslash may not give the min-length solutions to rank-deficient or under-determined problems, we still report its running times. Blendenpik either doesn't apply to rank-deficient problems or runs out of memory (OOM). LSRN's running time is mainly determined by the problem size and the sparsity.

Iterating with LSQR

(Paige and Saunders 1982)

Code snippet (Python):

u = A. matvec (v) − a l p h a ∗u b e ta = s q r t (comm. a l l r e d u c e (np . d o t (u , u))) . . . v = comm. a l l r e d u c e (A. rma tvec (u)) − b e ta ∗v

Cost per iteration:

- **•** two matrix-vector multiplications
- two cluster-wide synchronizations

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Iterating with Chebyshev semi-iterative (CS) method

(Golub and Varga 1961)

The strong concentration results on $\sigma^\text{max}(A N)$ and $\sigma^\text{min}(A N)$ enable use of the CS method, which requires an accurate bound on the extreme singular values to work efficiently.

```
Code snippet (Python):
```

```
v = comm. all reduce (A, rmatvec (r)) - beta *vx + alpha∗v
r = \alpha alpha *A. matvec (v)
```
Cost per iteration:

- two matrix-vector multiplications
- o one cluster-wide synchronization

LSQR vs. CS on an Amazon EC2 cluster

(Meng, Saunders, and Mahoney 2011)

Table: Test problems on an Amazon EC2 cluster and corresponding running times in seconds. Though the CS method takes more iterations, it actually runs faster than LSQR by making only one cluster-wide synchronization per iteration.

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"Everything generalizes" from ℓ_2 regression to ℓ_1 regression

(But "everything generalizes messily" since ℓ_1 is "worse" that ℓ_2 .)

- A matrix $U \in \mathbb{R}^{m \times n}$ is $(\alpha, \beta, \mathsf{p}=1)$ -conditioned if $|U|_1 \leq \alpha$ and $||x||_{\infty} \leq \beta ||Ux||_1$, $\forall x$; and ℓ_1 -well-conditioned basis if $\alpha, \beta = \text{poly}(n)$.
- Define the ℓ_1 leverage scores of an $m \times n$ matrix A, with $m > n$, as the ℓ_1 -norms-squared of the rows of an ℓ_1 -well-conditioned basis of A.
- Define the ℓ_1 -norm condition number of A, denoted by $\kappa_1(A)$, as:

$$
\kappa_1(A) = \frac{\sigma_1^{\max}(A)}{\sigma_1^{\min}(A)} = \frac{\max_{\|x\|_2=1} \|Ax\|_1}{\min_{\|x\|_2=1} \|Ax\|_1}.
$$

This implies: $\sigma_1^{\min}(A) ||x||_2 \le ||Ax||_1 \le \sigma_1^{\max}(A) ||x||_2, \quad \forall x \in \mathbb{R}$ n .

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Meta-algorithm for ℓ_1 -norm regression

- 1: Using an ℓ_1 -well-conditioned basis for A, construct an importance sampling distribution $\{p_i\}_{i=1}^m$ from the ℓ_1 -leverage scores.
- 2: Randomly sample a small number of constraints according to $\{p_i\}_{i=1}^m$ to construct a subproblem.
- 3: Solve the ℓ_1 -regression problem on the subproblem.

A naïve version of this meta-algorithm gives a $1+\epsilon$ relative-error approximation in roughly $O(mn^5/\epsilon^2)$ time (DDHKM 2009). (Ugh.)

But, as with ℓ_2 regression:

- We can make this algorithm run much faster in RAM by
	- **Example 2** approximating the ℓ_1 -leverage scores quickly, or
	- **Performing an** " ℓ_1 projection" to uniformize them approximately.
- We can make this algorithm work at higher precision in RAM at large-scale by coupling with an iterative algorithm.

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Conditioning: finding an ℓ_1 well-conditioned basis

Recall, given an $n \times d$ matrix A and $p \in [1, \infty]$, we want to find a low-distortion embedding $\Pi \in \mathbb{R}^{s \times n}$ s.t. $s = \mathcal{O}(\mathsf{poly}(d))$ and

 $1/\,\mathcal{O}(\mathsf{poly}(d))\cdot\|Ax\|_\rho\leq \|\Pi Ax\|_\rho\leq \mathcal{O}(\mathsf{poly}(d))\cdot\|Ax\|_\rho,\quad\forall x\in\mathbb{R}^d.$

There are two main ways:

Lemma (Conditioning via QR on low-distortion embedding) Given a low-distortion embedding matrix Π of A_p , let R be the "R" matrix from the QR decomposition of ΠA . Then, $A R^{-1}$ is ℓ_p -well-conditioned.

Lemma (Conditioning via ellipsoidal rounding)

Given an $n \times d$ matrix A and $p \in [1,\infty]$, it takes at most $\mathcal{O}(nd^3 \log n)$ time to find a matrix $R \in \mathbb{R}^{d \times d}$ such that $\kappa_p (A R^{-1}) \leq 2d$.

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Making ℓ_1 regression work to low and high precision

Finding a good basis (to get a low-precision solution):

Iteratively solving (to get a medium- to high-precision solution):

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Prior work and evaluations

Evaluate on real and simulated data:

- Simulated data, size ca. $10^9 \times 10^2$, designed to have "bad" nonuniformities.
- Real US Census data, size ca. $10^7 \times 10$, or "stacked" to size ca. $10^{10} \times 10$.

State of the art (due to Portnoy-Koenker, 1997]):

- \bullet Standard solver for ℓ_1 regression is interior-point method ipm, applicable for $10^6 \times 50$ -sized problems.
- \bullet Best previous sampling algorithm for ℓ_1 regression, prqfn, uses an interior-point method on a smaller randomly-co[nst](#page-27-0)[ru](#page-29-0)[ct](#page-27-0)[ed](#page-28-0) [s](#page-29-0)[u](#page-22-0)[b](#page-23-0)[pr](#page-35-0)[ob](#page-22-0)[l](#page-23-0)[em](#page-35-0)[.](#page-0-0)

A MapReduce implementation

Inputs: $A \in \mathbb{R}^{m \times n}$ and κ_1 such that

```
||x||_2 \le ||Ax||_1 \le \kappa_1 ||x||_2, \quad \forall x,
```
 $c \in \mathbb{R}^n$, sample size s, and number of subsampled solutions n_x .

- Mapper:
	- **1** For each row a_i of A, let $p_i = \min\{s||a_i||_1/(\kappa_1 n^{1/2}), 1\}$.
	- **2** For $k = 1, \ldots, n_{\mathsf{x}}$, emit $(k, a_i/p_i)$ with probability p_i .
- Reducer:
	- \bullet Collect row vectors associated with key k and assemble A_k .
	- **2** Compute $\hat{x}_k = \arg\min_{c \in \mathcal{T}_{x=1}} \|A_k x\|_1$ using interior-point methods.
	- **3** Return \hat{x}_k .

Note that multiple subsampled solutions can be computed in a single pass.

Evaluation on large-scale ℓ_1 regression problem

First (solid) and the third (dashed) quartiles of entry-wise absolute errors (on synthetic data that has "bad" nonuniformities).

First and the third quartiles of relative errors in 1-, 2-, and ∞ -norms on a data set of size 10^{10} × 15. CT (and FCT) clearly performs the best. GT is worse but follows closely. NOCD and UNIF ar[e](#page-29-0) much worse. (S[i](#page-23-0)milar results for size $10^{10} \times 100$ i[f S](#page-35-0)[P](#page-22-0)[C](#page-23-0)[2 i](#page-35-0)[s u](#page-0-0)[sed](#page-35-0).)

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The Method of Inscribed Ellipsoids (MIE)

MIE works similarly to the bisection method, but in a higher dimension.

Why do we choose MIE?

- **o** Least number of iterations
- Initialization using all the subsampled solutions
- Multiple queries per iteration

At each iteration, we need to compute (1) a function value and (2) a gradient/subgradient.

- For each subsampled solution, we have a hemisphere that contains the optimal solution.
- We use all these solution hemispheres to construct initial search region.

Constructing the initial search region

Given any feasible \hat{x} , let $\hat{f} = \|A\hat{x}\|_1$ and $\hat{g} = A^{\mathcal{T}}$ sign $(A\hat{x})$. we have

$$
||x^* - \hat{x}||_2 \le ||A(x^* - \hat{x})||_1 \le ||Ax^*||_1 + ||A\hat{x}||_1 \le 2\hat{f},
$$

and, by convexity,

$$
||Ax^*||_1 \ge ||A\hat{x}||_1 + \hat{g}^\mathcal{T}(x^* - \hat{x}),
$$

which implies $\hat{\mathbf{g}}^{\mathcal{T}} \mathbf{x}^* \leq \hat{\mathbf{g}}^{\mathcal{T}} \hat{\mathbf{x}}$.

Hence, for each subsampled solution, we have a hemisphere that contains the optimal solution.

We use all these hemispheres to construct the initial search region S_0 .

Computing multiple f and g in a single pass

On MapReduce, the IO cost may dominate the computational cost, which requires algorithms that could do more computation in a single pass.

• Single query:

$$
f(x) = ||Ax||_1, \quad g(x) = A^T \mathrm{sign}(Ax).
$$

Multiple queries:

$$
F(X) = \text{sum}(|AX|, 0), \quad G(X) = A^{T} \text{sign}(AX).
$$

An example on a 10-node Hadoop cluster:

- \bullet A : $10^8 \times 50$, 118.7GB.
- A single query: 282 seconds.
- 100 queries in a single pass: 328 seconds.

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MIE with sampling initialization and multiple queries

Comparing different MIE methods on large/LARGE ℓ_1 regression problem.

Conclusion

- Randomized regression in parallel & distributed environments: different design principles for high-precision versus low-precision
	- \blacktriangleright Least Squares Approximation
	- \blacktriangleright Least Absolute Deviations
	- \triangleright Extensions to Quantile Regression, Kernel-based Learning, Etc.
- Algorithms require more computation than traditional matrix algorithms, but they have better communication profiles.
	- \triangleright On MPI: Chebyshev semi-iterative method vs. LSQR.
	- \triangleright On MapReduce: Method of inscribed ellipsoids with multiple queries.
	- \triangleright Look beyond FLOPS in parallel and distributed environments.

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