Random Walks on the Sphere and Linear Systems of Equations
(or: Stochastic Gradient Descent for Least Squares)

Stefan Steinerberger

Online ICCHA2021
It would be fun to be in Munich!
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Leavenworth, WA
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The goal of this talk is to tell you about a nice way of (approximately) solving linear systems of equations. It can be interpreted as Stochastic Gradient Descent applied to a classical Least Squares problem – and it can be analyzed rigorously! I found it to be mathematically rich and naturally leading to many (open problems)! (Some are mentioned in this talk.)
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\end{pmatrix} x = b
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or

$$\forall 1 \leq i \leq n : \quad \langle a_i, x \rangle = b_i.$$
Linear Systems \equiv \text{Intersection of Hyperplanes}

\forall 1 \leq i \leq n : \quad \langle a_i, x \rangle = b_i
The Kaczmarz Method

Polish Mathematician

Stefan Kaczmarz
(1895 - 1939/1940)

Circumstances of death in WW2 unclear.
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The method is remarkably simple: we want

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Geometrically, we want to find the intersection of hyperplanes.
The Kaczmarz method

Project iteratively on the hyperplanes given by $\langle a_i, x \rangle = b_i$. The Pythagorean Theorem implies that the distance to the solution always decreases (unless you are already on that hyperplane).
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The Kaczmarz method

If we project $x_k$ onto the hyperplane given by the $i$–th equation $\langle a_i, x \rangle = b_i$ to obtain $x_{k+1}$, then

$$x_{k+1} = x_k + \frac{b_i - \langle a_i, x_k \rangle}{\|a_i\|^2} a_i.$$
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- This is *cheap*: it’s an inner product! We do not even have to load the full matrix into memory.
- This is thus useful for large matrices.
Standard Kaczmarz. We cycle through the indices $i$ and set

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\textbf{Random Kaczmarz.} We pick a \textit{random} equation $i$ and set

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**Random Kaczmarz.** We pick a *random* equation $i$ and set

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- somehow behaves a little better
- used since the 1980s
- stochastic gradient descent for $\|Ax - b\|^2 \to \min$
Theorem (Strohmer & Vershynin, 2007)

Pick the \(i\)-th equation with likelihood proportional to \(\|a_i\|^2\), then

\[
\mathbb{E} \|x_k - x\|^2_2 \leq \left(1 - \sigma_n(A)^2 \|A\|_F^2\right) \|x_0 - x\|^2_2.
\]

\(\|A\|_F\) is the Frobenius norm 
\[
\|A\|_F^2 = \sum_{i,j=1}^n a_{ij}^2.
\]

\(\sigma_n(A)\) is the smallest singular value of \(A\).
Theorem (Strohmer & Vershynin, 2007)

*Pick the $i$−th equation with likelihood proportional to $\|a_i\|^2$, then*

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\mathbb{E} \|x_k - x\|^2_2 \leq \left(1 - \frac{\sigma_n(A)^2}{\|A\|_F^2}\right)^k \|x_0 - x\|^2_2.
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- $\|A\|_F$ is the Frobenius norm $\|A\|^2_F = \sum_{i,j=1}^n a_{ij}^2$.
- $\sigma_n(A)$ is the smallest singular value of $A$. 
Strohmer & Vershynin’s argument is short and elegant (certainly one of the reasons it has inspired a lot of subsequent work).
Sketch of the Proof

Strohmer & Vershynin’s argument is short and elegant (certainly one of the reasons it has inspired a lot of subsequent work).

\[
\mathbb{E} \left| \left\langle \frac{x_k - x}{\|x_k - x\|}, Z \right\rangle \right|^2 = \sum_{i=1}^{m} \frac{\|a_j\|^2}{\|A\|^2_F} \left\langle \frac{x_k - x}{\|x_k - x\|}, \frac{a_j}{\|a_j\|_2} \right\rangle^2 \\
= \frac{1}{\|A\|^2_F} \sum_{i=1}^{m} \left\langle \frac{x_k - x}{\|x_k - x\|}, a_j \right\rangle^2 \\
= \frac{1}{\|A\|^2_F} \left\| A \frac{x_k - x}{\|x_k - x\|} \right\|^2 \\
\geq \frac{1}{\|A\|^2_F} \frac{1}{\|A^{-1}\|^2_2}
\]

3. A Refined Analysis

Here's what I really wanted to know: what does $x^k - x$ do? Looking at the picture, it should be sort of jumping around. $x^k + 1$ $x^k + 2$ But in numerical experiments, I didn't see that.
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But in numerical experiments, I didn’t see that.
Empirically, the (random) sequence of vectors

\[ \frac{x_k - x}{\|x_k - x\|} \]

tends to mainly a linear combination of singular vectors with small singular values.
Theorem (Small Singular Values Dominate, SIMAX 2021)

Let \( v_\ell \) be a (right) singular vector of \( A \) associated to the singular value \( \sigma_\ell \).

\[
\mathbb{E} \langle x_k - x, v_\ell \rangle = \left(1 - \sigma_\ell^2 \|A\|_F^2\right) k \langle x_0 - x, v_\ell \rangle.
\]

▶ Different rate of contraction in different subspaces.
▶ The slowest rate of decay is given by the smallest singular value \( \sigma_n \).
▶ This recovers Strohmer-Vershynin.
▶ Open Problem: Only Expectation, what can one say about the variance...? Or some other form of deviation from mean?
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**Figure:** A sample evolution of $\|Ax_k\|/\|x_k\|$. 
4. Stuck between a rock and a hard place

You get trapped in the narrow regions and it's hard to escape. This seems strange because, after all, it is a random process and you might end up on any hyperplane at any point in time.
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Stuck between a rock and a hard place

Theorem (Slowing down in Bad Regions, SIMAX 2021)

If $x_k \neq x$ and $\mathbb{P}(x_{k+1} = x) = 0$, then

$$\mathbb{E} \left\langle \frac{x_k - x}{\|x_k - x\|}, \frac{x_{k+1} - x}{\|x_{k+1} - x\|} \right\rangle^2 = \quad$$
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Once $x_k - x$ is mainly a linear combination of small singular vectors, this quantity changes very little! We stay trapped!
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Open Problem: What about variance?

Open Problem 2: How do we escape?
\[ E \left\langle \frac{x_k - x}{\|x_k - x\|}, \frac{x_{k+1} - x}{\|x_{k+1} - x\|} \right\rangle^2 = 1 - \frac{1}{\|A\|^2_F} \left\| A \frac{x_k - x}{\|x_k - x\|} \right\|^2. \]

Proof. Well, it’s an identity, how hard can it be?
\[ \mathbb{E} \left( \frac{x_k - x}{\|x_k - x\|}, \frac{x_{k+1} - x}{\|x_{k+1} - x\|} \right)^2 = 1 - \frac{1}{\|A\|_F^2} \left\| A \frac{x_k - x}{\|x_k - x\|} \right\|^2. \]

**Proof.** Well, it’s an identity, how hard can it be?

\[ \mathbb{E} \left( x_k, \frac{x_{k+1}}{\|x_{k+1}\|} \right)^2 = \sum_{i=1}^m \frac{\|a_i\|^2}{\|A\|_F^2} \left( \frac{x_k - \langle a_i, x_k \rangle a_i}{\|a_i\|^2 a_i} \right)^2 = \sum_{i=1}^m \frac{\|a_i\|^2}{\|A\|_F^2} \left( \frac{x_k - \langle a_i, x_k \rangle a_i}{\|a_i\|^2 a_i} \right)^2 \]

\[ = \sum_{i=1}^m \frac{\|a_i\|^2}{\|A\|_F^2} \left\| x_k - \frac{\langle a_i, x_k \rangle}{\|a_i\|^2_a} a_i \right\|^2 = \sum_{i=1}^m \frac{\|a_i\|^2}{\|A\|_F^2} \left\| x_k - \frac{\langle a_i, x_k \rangle}{\|a_i\|^2_a} a_i \right\|^2 \]

\[ = \frac{1}{\|A\|_F^2} \sum_{i=1}^m \left( \|a_i\|^2 - \langle a_i, x_k \rangle^2 \right) = 1 - \frac{1}{\|A\|_F^2} \sum_{i=1}^m \langle a_i, x_k \rangle^2 = 1 - \frac{\|Ax_k\|^2}{\|A\|_F^2}. \]

Open Problem: It would be nice to have more such identities.
\[ \mathbb{E} \left\langle \frac{x_k - x}{\|x_k - x\|}, \frac{x_{k+1} - x}{\|x_{k+1} - x\|} \right\rangle^2 = 1 - \frac{1}{\|A\|^2_F} \left\| A \frac{x_k - x}{\|x_k - x\|} \right\|^2. \]

**Proof.** Well, it's an identity, how hard can it be?

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\mathbb{E} \left\langle x_k, \frac{x_{k+1}}{\|x_{k+1}\|} \right\rangle^2 = \sum_{i=1}^m \frac{\|a_i\|^2}{\|A\|^2_F} \left\langle x_k, \frac{x_k - \frac{\langle a_i, x_k \rangle}{\|a_i\|^2} a_i}{\|x_k - \frac{\langle a_i, x_k \rangle}{\|a_i\|^2} a_i\|} \right\rangle^2
= \sum_{i=1}^m \frac{\|a_i\|^2}{\|A\|^2_F} \left\langle x_k, \frac{x_k - \frac{\langle a_i, x_k \rangle}{\|a_i\|^2} a_i}{\|x_k - \frac{\langle a_i, x_k \rangle}{\|a_i\|^2} a_i\|} \right\rangle^2
= \sum_{i=1}^m \frac{\|a_i\|^2}{\|A\|^2_F} \left\| x_k - \frac{\langle a_i, x_k \rangle}{\|a_i\|^2} a_i \right\|^4
= \sum_{i=1}^m \frac{\|a_i\|^2}{\|A\|^2_F} \left( 1 - \frac{\langle a_i, x_k \rangle^2}{\|a_i\|^2} \right)
= \frac{1}{\|A\|^2_F} \sum_{i=1}^m \left( \|a_i\|^2 - \langle a_i, x_k \rangle^2 \right) = 1 - \frac{1}{\|A\|^2_F} \sum_{i=1}^m \langle a_i, x_k \rangle^2 = 1 - \frac{\|Ax_k\|^2}{\|A\|^2_F}. \]

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5. Changing the likelihoods

New idea: maybe we shouldn’t pick the likelihoods randomly.
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\[ \forall 1 \leq i \leq n : \quad \langle a_i, x \rangle = b_i \]

so maybe we should pick equations where \(|\langle a_i, x \rangle - b_i|\) is large?
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so maybe we should pick equations where $|\langle a_i, x \rangle - b_i|$ is large?

This is known as the maximum residual method. It is known since (at least) the 1990s that this is faster (Feichtinger, Cenker, Mayer, Steier and Strohmer, 1992), (Griebel and Oswald, 2012), ...
Proposed fix: choose the $i$–th equation with likelihood proportional to

$$
\mathbb{P}(\text{we choose equation } i) = \frac{|\langle a_i, x_k \rangle - b|^p}{\|Ax_k - b\|_{\ell_p}^p}.
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- in practice, no difference between $p = 20$ and $p = 10^{100}$
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$$\mathbb{P}(\text{we choose equation } i) = \frac{|\langle a_i, x_k \rangle - b|^p}{\|Ax_k - b\|^{lp}_{lp}}.$$ 

- for $p = 0$, every equation is picked with equal likelihood
- for $p$ large, the large deviations are more likely to be picked
- in practice, no difference between $p = 20$ and $p = 10^{100}$
- the method ‘converges’ to maximum residual as $p \to \infty$. 
Figure: $\|x_k - x\|_{\ell^2}$ for the Randomized Kaczmarz method (blue), for $p = 1$ (orange), $p = 2$ (green) and $p = 20$ (red).
Theorem (Weighting is better, Math. Comp, 2021)

Let \(0 < p < \infty\), let \(A\) be normalized to having the norm of each row be \(\|a_i\| = 1\). Then

\[
\mathbb{E} \|x_k - x\|_2^2 \leq \left(1 - \inf_{x \neq 0} \frac{\|Ax\|_{\ell^p+2}^{p+2}}{\|Ax\|_{\ell^p} \|x\|_{\ell^2}^2}\right)^k \|x_0 - x\|_2^2.
\]
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Let $0 < p < \infty$, let $A$ be normalized to having the norm of each row be $\|a_i\| = 1$. Then

$$\mathbb{E} \|x_k - x\|_2^2 \leq \left(1 - \inf_{x \neq 0} \frac{\|Ax\|_{\ell_p}^{p+2} \|x\|_2^2}{\|Ax\|_{\ell_p} \|x\|_2^2} \right)^k \|x_0 - x\|_2^2.$$ 

This is at least the rate of Randomized Kaczmarz ($p = 0$):

$$\inf_{x \neq 0} \frac{\|Ax\|_{\ell_p}^{p+2} \|x\|_2^2}{\|Ax\|_{\ell_p} \|x\|_2^2} \geq \frac{\sigma_n^2}{\|A\|_F^2}. $$

Open Problem.

Is there any structure in $x_k - x$?

Open Problem 2.

The method is a priori specified: are there any smarter ways of adapting dynamically along the flow?
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...but we could also be reflecting. Reflection doesn’t get us any closer to the solution but it does something else.
We get that, again from Pythagoras,

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The distance to the true solution stays exactly preserved! The formula stays simple

\[ x_{k+1} = x_k + 2 \frac{b_i - \langle a_i, x_k \rangle}{\|a_i\|^2} a_i. \]
This gives us a new approach to the problem.

Start with some arbitrary $x_0 \in \mathbb{R}^n$. Generate a sequence of vectors in $\mathbb{R}^n$ via $x_{k+1} = x_k + 2b_i - \langle a_i, x_k \rangle \frac{a_i}{\|a_i\|^2}$. You can pick the $i$ any way you like. Do this for a while until you are happy. You end up with a set \{ $x_0, \ldots, x_n$ \} such that $\|x_k - x\|$ is constant. They are all on a sphere around the true solution.

Open Problem: Reconstruct a good approximation of the center of a sphere from knowing many points on the sphere.
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**Figure:** Thales’ Theorem guarantees $\langle x_i - x_1, 2r \rangle = \|x_i - x_1\|^2$.

Open Problem: Can this be used for ‘upgrading’ the quality of the system? It seems that yes, maybe.
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![Diagram of Thales' Theorem](image)

**Figure:** Thales’ Theorem guarantees $\langle x_i - x_1, 2r \rangle = \|x_i - x_1\|^2$.

So we end up with another linear system for $r$. 
One could certainly do exact reconstruction. Suppose we have $x_1, x_2, \ldots, x_{n+1}$ all on a sphere in $\mathbb{R}^n$.

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So we end up with another linear system for $r$.

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**Theorem (Applied Mathematics Quarterly, 2021)**

If the \(i\)–th hyperplane is picked with likelihood proportional to \(\|a_i\|^2\), the arising random sequence of points \((x_k)_{k=1}^{\infty}\) satisfies

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\mathbb{E} \left\| x - \frac{1}{m} \sum_{k=1}^{m} x_k \right\| \leq \frac{1 + \|A\|_F \|A^{-1}\|}{\sqrt{m}} \cdot \|x - x_1\|.
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So you need roughly \( m \sim \|A\|_F^2 \|A^{-1}\|^2 \) to decrease by a fixed factor. **Same as Kaczmarz.**
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Simple Averaging already leads to something as good as Random Kaczmarz!
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Flavor of the Proof.

▶ We can assume w.l.o.g. that $x = 0$ and that the sphere has radius 1. What can we say about

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▶ Let us use $R$ to denote the random reflection operator. Then

$$\frac{1}{m} \sum_{k=1}^m x_k = \frac{1}{m} \sum_{k=1}^m R^k x_0.$$
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\[ \left\| \sum_{k=1}^{m} R^k x_0 \right\|^2 = \sum_{k, \ell=1}^{m} \langle R^k x_0, R^\ell x_0 \rangle \]
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A Decorrelation Lemma
We have, for any \( x \in \mathbb{R}^n \), and any \( k \in \mathbb{N} \),

\[ \left| \mathbb{E} \left\langle x, R^k x \right\rangle \right| \leq \left( 1 - \frac{2 \sigma_n^2}{\|A\|_F^2} \right)^k \|x\|^2. \]

(Proof by Induction).
Summary

- The Kaczmarz method is a geometrically beautiful iterative method for solving linear system.

- By replacing projection with reflection, we introduce a random reflection process on the sphere that is pretty interesting.

- Given points on a sphere, how do you estimate the location of the center of the sphere?

- Taking the average leads to a method that is as good as Random Kaczmarz. Anything better leads to a better method.
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- Taking the average leads to a method that is as good as Random Kaczmarz. *Anything better leads to a better method.*
References

1. Randomized Kaczmarz converges along small singular vectors, SIMAX 2021

Thank you!