# Random Walks on the Sphere and Linear Systems of Equations

(or: Stochastic Gradient Descent for Least Squares)

Stefan Steinerberger

Online ICCHA2021

UNIVERSITY of WASHINGTON

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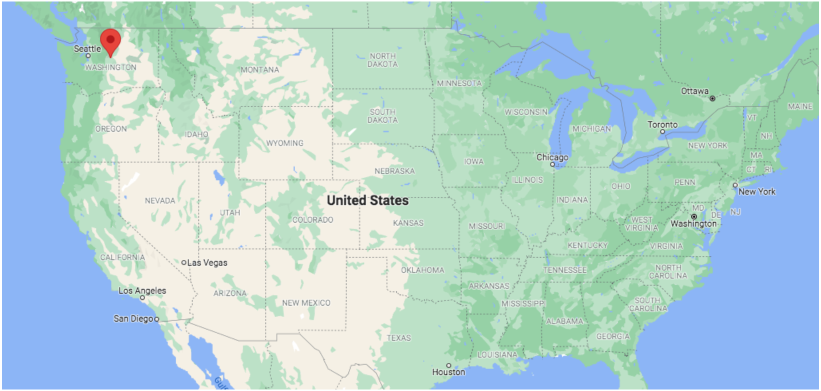


**A Bavarian Town**: Leavenworth, Washington.

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I found it to be **mathematically rich** and naturally leading to **many(!)** open problems! (Some are mentioned in this talk.)

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$$\begin{pmatrix} a_1 \\ a_2 \\ \dots \\ a_n \end{pmatrix} x = b$$

or

$$\forall\ 1 \leq i \leq n : \qquad \langle a_i, x \rangle = b_i.$$

# Linear Systems $\equiv$ Intersection of Hyperplanes

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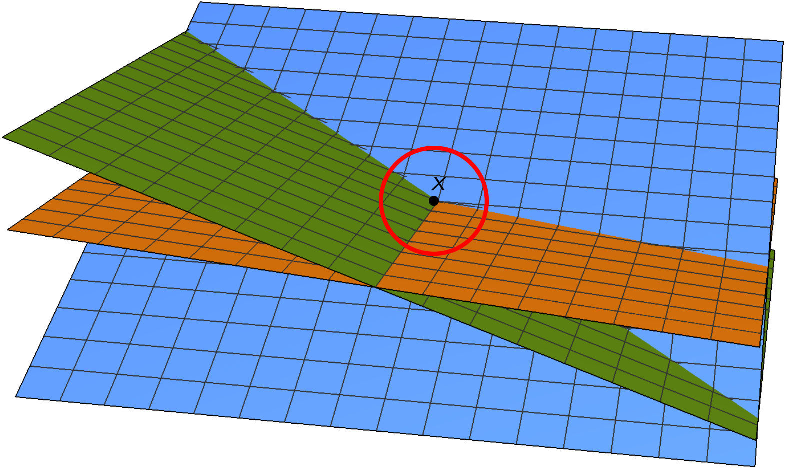

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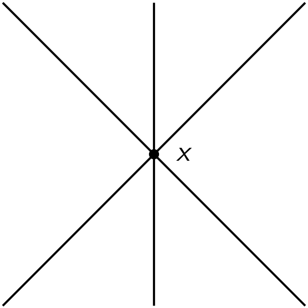
Geometrically, we want to find the intersection of hyperplanes.



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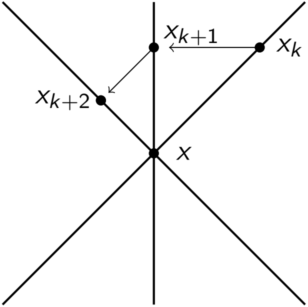

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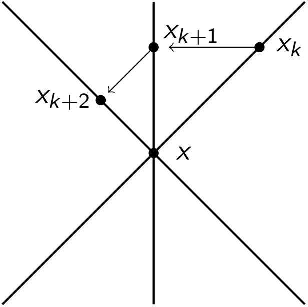


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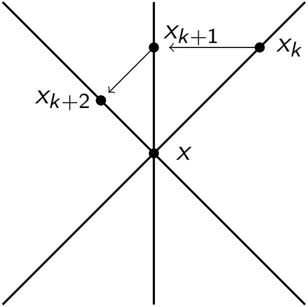


Project iteratively on the hyperplanes given by

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Pythageorean Theorem implies that the distance to the solution always decreases (unless you are already on that hyperplane).

# 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 thus useful for large matrices.

**Standard Kaczmarz**. We cycle through the indices $i$ and set

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wird wiederum auf $L_1 = 0$ geworfen und gibt den Punkt $x_1^{\dots}, \dots x_n^{\dots}$, usw. Die Konvergenz des Verfahrens ist geometrisch ohne weiteres einleuchtend.

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- stochastic gradient descent for $\|Ax - b\|^2 \to \min$

**Theorem (Strohmer & Vershynin, 2007)**

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- $\|A\|_F$ is the Frobenius norm $\|A\|_F^2 = \sum_{i,j=1}^n a_{ij}^2$.
- $\sigma_n(A)$ is the smallest singular value of $A$.

# Sketch of the Proof

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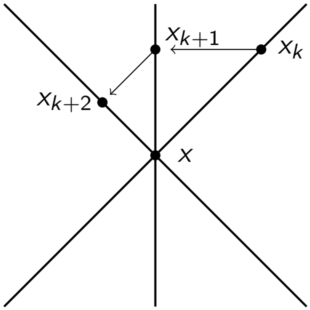

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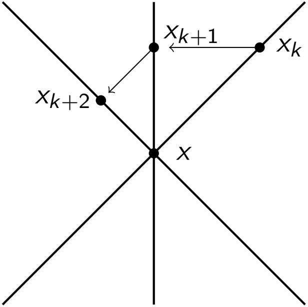
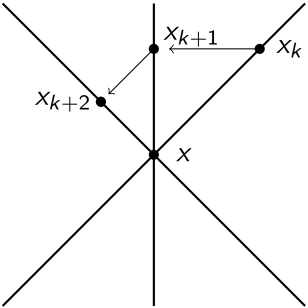



But in numerical experiments, I didn't see that.




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.

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- **Open Problem:** Only Expectation, what can one say about the variance...? Or some other form of deviation from mean?

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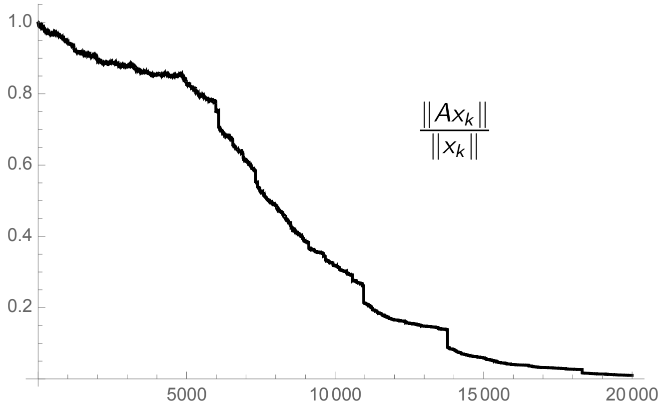
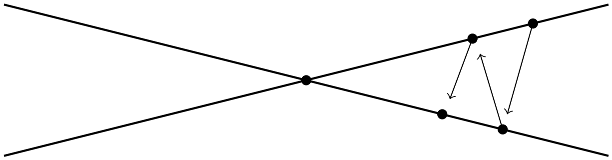



Figure: A sample evolution of $\|Ax_k\|/\|x_k\|$.

# 4. Stuck between a rock and a hard place



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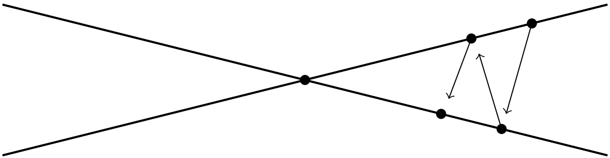

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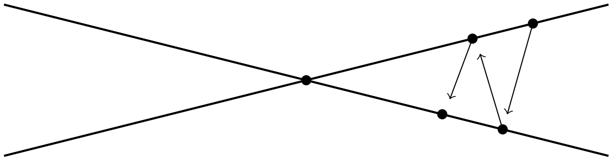
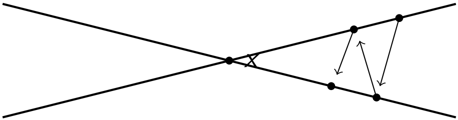


You get trapped in the narrow regions and it's hard to escape. This seems strange because, after all, it is a random process and you might end up on any hyperplane at any point in time.

# 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*

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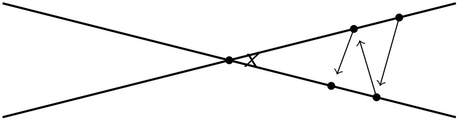


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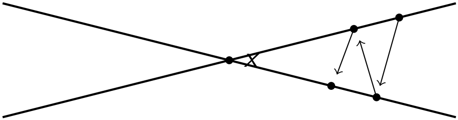


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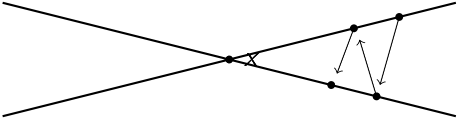


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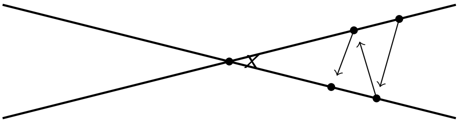


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**Open Problem:** What about variance?
**Open Problem 2:** How do we escape?

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

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

$$\mathbb{E}\left\langle \frac{x_k - x}{\|x_k - x\|}, \frac{x_{k+1} - x}{\|x_{k+1} - x\|} \right\rangle^2 = 1 - \frac{1}{\|A\|_F^2}\left\| A\frac{x_k - x}{\|x_k - x\|}\right\|^2.$$

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

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\end{aligned}$$

**Open Problem:** It would be nice to have more such identities.

# 5. Changing the likelihoods

New idea: maybe we shouldn't pick the likelihoods randomly.

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$$\forall\, 1 \leq i \leq n: \qquad \langle a_i, x \rangle = b_i$$

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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

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- 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 $p \to \infty$.

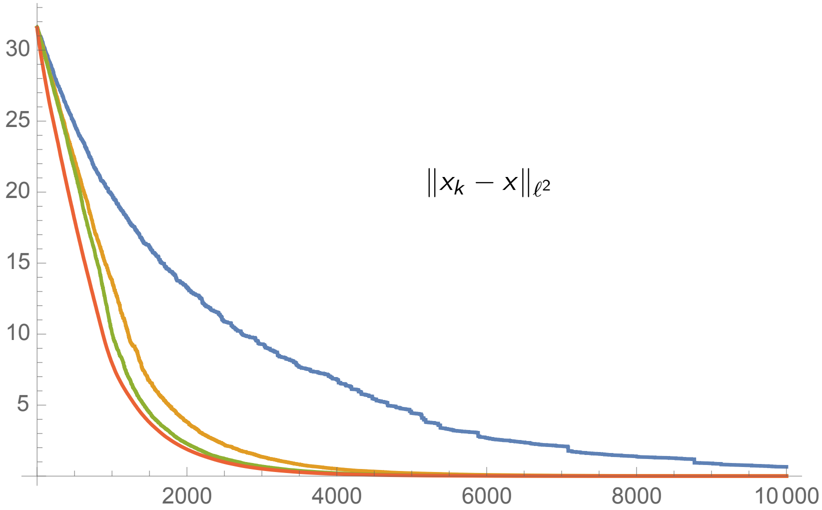


Figure: $\|x_k - x\|_{\ell^2}$ for the Randomized Kaczmarz method (blue), for $p = 1$ (orange), $p = 2$ (green) and $p = 20$ (red).

**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*

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

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

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**Open Problem 2.** The method is *a priori* specified: are there any smarter ways of adapting dynamically along the flow?

# 6. The Magic Bubble

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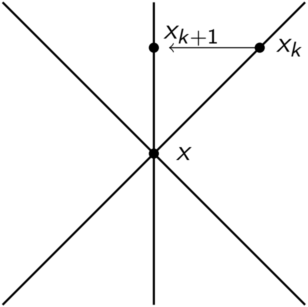
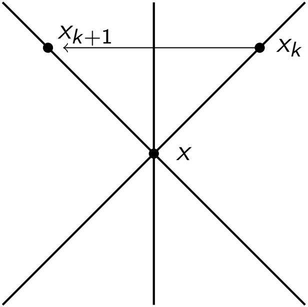



Right now we are projecting...

# 6. The Magic Bubble

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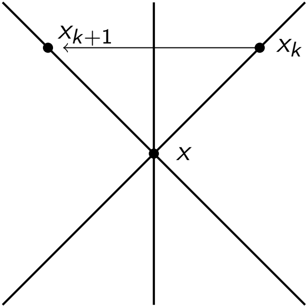
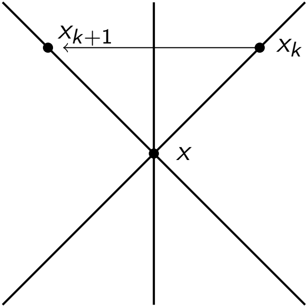


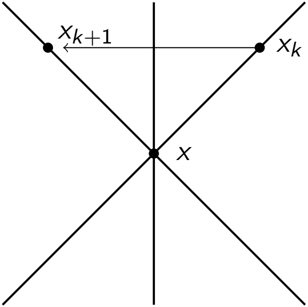

...but we could also be reflecting. Reflection doesn't get us any closer to the solution but it does something else.




We get that, again from Pythagoras,

$$\|x_k - x\| = \|x_{k+1} - x\|.$$

The distance to the true solution stays exactly preserved!




We get that, again from Pythagoras,

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

$$x_{k+1} = x_k + 2\frac{b_i - \langle a_i, x_k\rangle}{\|a_i\|^2} a_i.$$

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- **Open Problem:** Reconstruct a good approximation of the center of a sphere from knowing many points on the sphere.

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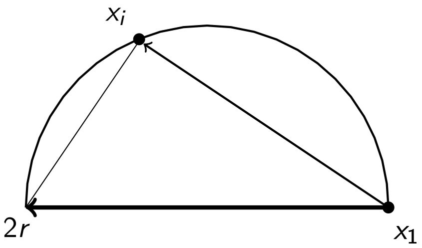


Figure: Thales' Theorem guarantees $\langle x_i - x_1, 2r \rangle = \|x_i - x_1\|^2$.

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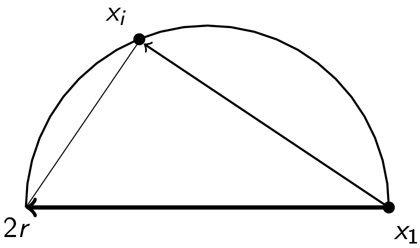


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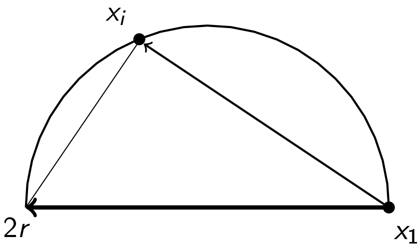


Figure: Thales' Theorem guarantees $\langle x_i - x_1, 2r \rangle = \|x_i - x_1\|^2$.

So we end up with another linear system for $r$.
**Open Problem:** Can this be used for 'upgrading' the quality of the system? It seems that yes, maybe.

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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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So you need roughly $m \sim \|A\|_F^2 \|A^{-1}\|^2$ to decrease by a fixed factor. $\boxed{\textbf{Same as Kaczmarz.}}$

**Question.** How to reconstruct a good approximation of the center of a sphere from knowing many points on the sphere?

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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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$$\mathbb{E}\left\| \frac{1}{m}\sum_{k=1}^{m} x_k \right\|?$$
- Let us use $R$ to denote the random reflection operator. Then
$$\frac{1}{m}\sum_{k=1}^{m} x_k = \frac{1}{m}\sum_{k=1}^{m} R^k x_0.$$

# The Flavor of the Proof

- $$\left\| \sum_{k=1}^{m} R^k x_0 \right\|^2 = \sum_{k,\ell=1}^{m} \left\langle R^k x_0, R^\ell x_0 \right\rangle$$

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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).*

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- 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.*

# References


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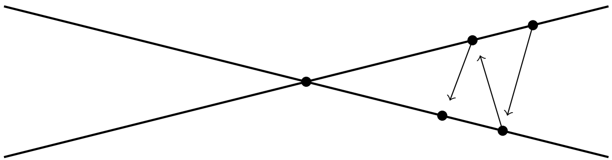

THANK YOU!