Recht–Ré Noncommutative Arithmetic-Geometric Mean Conjecture is False

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Abstract

Stochastic optimization algorithms have become indispensable in modern machine learning. An unresolved foundational question in this area is the difference between with-replacement sampling and without-replacement sampling — does the latter have superior convergence rate compared to the former? A groundbreaking result of Recht and Ré reduces the problem to a noncommutative analogue of the arithmetic-geometric mean inequality where \(n\) positive numbers are replaced by \(n\) positive definite matrices. If this inequality holds for all \(n\), then without-replacement sampling indeed outperforms with-replacement sampling. The conjectured Recht–Ré inequality has so far only been established for \(n = 2\) and a special case of \(n = 3\). We will show that the Recht–Ré conjecture is false for general \(n\). Our approach relies on the non-commutative Positivstellensatz, which allows us to reduce the conjectured inequality to a semidefinite program and the validity of the conjecture to certain bounds for the optimum values, which we show are false as soon as \(n = 5\).

1. Introduction

The breathtaking reach of deep learning, permeating every area of science and technology, has led to an outsize role for randomized optimization algorithms. It is probably fair to say that in the absence of randomized algorithms, deep learning would not have achieved its spectacular level of success. Fitting an exceedingly high-dimensional model with an exceedingly large training set would have been prohibitively expensive without some form of random sampling, which in addition provides other crucial benefits such as saddle-point avoidance (Fang et al., 2019; Jin et al., 2017). As such, in machine learning computations, stochastic variants of gradient descent (Bottou, 2010; Johnson & Zhang, 2013; Nemirovski et al., 2008), alternating projections (Strohmer & Vershynin, 2009), coordinate descent (Nesterov, 2012), and other algorithms have largely overtaken their classical deterministic counterparts in relevance and utility.

There are numerous random sampling strategies but the most fundamental question, before all other considerations, is deciding between sampling with replacement or sampling without replacement. In the vast majority of randomized algorithms, a random sample is selected or a random action is performed with replacement from a pool, making the randomness in each iteration independent and thus easier (often much easier) to analyze. However, when it comes to practical realizations of these algorithms, one invariably sample without replacement, since they are easier (often much easier) to implement. Take the ubiquitous stochastic gradient descent for example, many if not most implementations would pass through each item exactly once in a random order — this is sampling without replacement. Likewise, in implementations of randomized coordinate descent, coordinates are usually just chosen in a random order — again sampling without replacement.

Apart from its ease of implementation, there are other reasons for favoring without-replacement sampling. Empirical evidence (Bottou, 2009) suggests that in stochastic gradient descent, without-replacement sampling regularly outperforms with-replacement sampling. Theoretical results also point towards without-replacement sampling: Under standard convexity assumptions, the convergence rate of a without-replacement sampling algorithm typically beats a with-replacement sampling one by a factor of \(O(n^{-1/2})\) or \(O(n^{-1})\). This has been established for stochastic gradient descent (Shamir, 2016; Nagaraj et al., 2019) and for coordinate descent (Beck & Tetruashvili, 2013; Wright, 2015).

Recht & Re (2012) proposed a matrix theoretic approach to compare the efficacy of with- and without-replacement sampling methods. Since nearly every common optimization algorithm, deterministic or randomized, works with a linear or quadratic approximation of the objective function locally, it suffices to examine the two sampling strategies on linear or quadratic functions to understand their local
convergence behaviors. In this case, the iteration reduces to matrix multiplication and both sampling procedures are linearly convergent (often called “exponential convergence” in machine learning). The question of which is better then reduces to comparing their linear convergence rates. In this context, Recht & Re (2012) showed that without-replacement sampling outperforms with-replacement sampling provided the following noncommutative version of the arithmetic-geometric mean inequality holds.

**Conjecture 1 (Recht & Re 2012).** Let $n$ be a positive integer, $A_1, \ldots, A_n$ be symmetric positive semidefinite matrices, and $\| \cdot \|$ be the spectral norm. Then for any $m \leq n$,

$$\frac{1}{n^m} \left\| \sum_{1 \leq j_1, \ldots, j_m \leq n} A_{j_1} \cdots A_{j_m} \right\| \geq \frac{(n-m)!}{n!} \left\| \sum_{1 \leq j_1, \ldots, j_m \leq n, j_1, \ldots, j_m \text{ distinct}} A_{j_1} \cdots A_{j_m} \right\|. \tag{1}$$

While one may also ask if (1) holds for other norms, the most natural and basic choice is the spectral norm, i.e., the operator 2-norm. Unless specified otherwise, $\| \cdot \|$ will always denote the spectral norm in this article.

To give an inkling of how (1) arises, consider the Kaczmarz algorithm (Strohmer & Vershynin, 2009) where we attempt to solve an overdetermined linear system $Cx = b$, $C \in \mathbb{R}^{p \times d}$, $p > d$, with ith row vector $e_i^T$ where $e_i \in \mathbb{R}^d$. For $k = 1, 2, \ldots$, the $(k+1)$th iterate is formed with a randomly chosen $i$ and

$$x(k+1) = x(k) + \frac{b_i - \langle e_i, x(k) \rangle}{\| e_i \|^2} e_i.$$

The $k$th error $e(k) = x(k) - x^*$ is then

$$e(k+1) = \left( I - \frac{e_i e_i^T}{\| e_i \|^2} \right) e(k) =: P_{e_i} e(k),$$

where $P_{e_i} \in \mathbb{R}^{d \times d}$, the orthogonal projector onto $\text{span}\{e_i\}$, is clearly symmetric positive semidefinite. A careful analysis would show that the relative efficacy of with- and without-replacement sampling depends on a multitude of inequalities like $\| A^2 + B^2 + AB^2 + BA^2 \| \geq 2 \| AB^2 + BA^2 \|$, which are difficult to analyze on a case-by-case basis. Nevertheless, more general heuristics (Recht & Re, 2012) would lead to (1) — if it holds, then without-replacement sampling is expected to outperform with-replacement sampling. In fact, the gap can be significant — for random Wishart matrices, Recht & Re (2012) showed that the ratio between the two sides of (1) increases exponentially with $m$.

1 We adopt standard convention that any vector $x \in \mathbb{R}^d$ is a column vector; a row vector will always be denoted $x^T$.

**Current status:** Recht & Re (2012) applied results from random matrix theory to show that Conjecture 1 holds with high probability for (i) independent Wishart matrices, and (ii) the incremental gradient method. To date, extensive numerical simulations have produced no counterexample. Conjecture 1 has been rigorously established only in very special cases, notably for $(m, n) = (2, 2)$ (Recht & Re, 2012) and $(m, n) = (3, 3k)$ (Zhang, 2018).

**Our contributions:** We show how to transform Conjecture 1 into a form where the noncommutative Positivestellensatz applies, which implies in particular that for any specific values of $m$ and $n$, the conjecture can be checked via two semidefinite programs. This allows us to show in Section 3 that the conjecture is false as soon as $m = n = 5$. We also establish in Section 2 that the conjecture holds for $m = 2$ and 3 with arbitrary $n$ by extending the approach in Zhang (2018). While the conjectured inequality (1) is clearly sharp (as we may choose all $A_i$’s to be equal) whenever it is true, we show in Section 5 that the $m = 2$ case may nonetheless be improved in a different sense, and we do likewise for $m = 3$ in Section 2. The $m = 4$ case remains open but our noncommutative Positivestellensatz approach permits us to at least check that it holds for $n = 4$ and 5 in Section 3.

Over the next two sections, we will transform Recht and Ré’s Conjecture 1 into a “Loewner form” (Conjecture 1A), a “sum-of-squares form” (Conjecture 1B), and finally a “semidefinite program form” (Conjecture 1C). All four conjectures are equivalent but the correctness of the last one for any $m$ and $n$ is readily checked as a semidefinite program.

2. **Recht–Ré inequality for $m = 2$ and 3**

Our goal here is to establish (1) for a pair and a triple of matrices. In so doing, we take Conjecture 1 a step closer to a form where noncommutative Positivestellensatz applies. There is independent value in establishing these two special cases given that the classical noncommutative arithmetic-geometric-harmonic mean inequality (Bhatia & Holbrook, 2006) is only known for a pair of matrices but nonetheless attracted a lot of interests from linear algebraists. These special cases also have implications on randomized algorithms — take the Kaczmarz algorithm for example, the fact that Conjecture 1 holds for $m = 2$ and 3 implies that if we randomly choose two or three distinct samples, perform the iterations, and sample again, then this “replacing after every two or three samples” strategy will converge faster than a “replacing after every sample” strategy.

We begin by providing some context for the inequality (1). The usual arithmetic-geometric-mean inequality for $n$ non-
negative real numbers \(a_1, \ldots, a_n\), i.e.,

\[(a_1 + \cdots + a_n)/n \geq (a_1 \cdots a_n)^{1/n},\]

is a special case of Maclaurins inequality (Hardy et al., 1988): If we define

\[s_m := \frac{1}{m!} \sum_{1 \leq j_1 < \cdots < j_m \leq n} a_{j_1} \cdots a_{j_m},\]

then \(s_1 \geq \sqrt[n]{a_1} \geq \cdots \geq \sqrt[n]{a_n}\). So \(s_1 \geq \sqrt[n]{s_m}\) gives us

\[\frac{1}{n^m} (a_1 + \cdots + a_n)^m \geq \frac{(n-m)!}{n!} \sum_{1 \leq j_1 < \cdots < j_m \leq n, j_1, \ldots, j_m \text{ distinct}} a_{j_1} \cdots a_{j_m},\]

which is just (1) for 1-by-1 positive semidefinite matrices.

For real symmetric or complex Hermitian matrices \(A, B\), the Loewner order is defined by \(A \succeq B\) iff \(A - B\) is positive semidefinite. The Maclaurins inequality has several noncommutative extensions but we regard the following as the starting point for all noncommutative arithmetic-geometric mean inequalities.

**Proposition 1.** For any unitary invariant norm \(\| \cdot \|\) and Hermitian matrices \(A, B\), \(\|AB + BA\| \leq \|A^2 + B^2\|\) and \(2\|AB + BA\| \leq \|(A + B)^2\|\).

*Proof. Since \(A^2 - B^2 \preceq AB + BA \preceq A^2 + B^2\), by Lemma 2.1 in Bhatia & Kittaneh (2008), the desired inequalities hold for any unitary invariant norm. 

The result was extended to compact operators on a separable Hilbert space and strengthened to \(2\|A^*B\| \leq \|A^*A + B^*B\|\) in Bhatia & Kittaneh (1990), with yet other extensions in Bhatia & Kittaneh (2008; 2000). In Recht & Re (2012), Conjecture 1 was also formulated as an extension of Proposition 1, with the second inequality corresponding to the \(m = n = 2\) case.

Straightforward counterexamples for \(n = 3\) show that we cannot simply drop the norm in (1) and replace the inequality \(\geq\) with the Loewner order \(\succeq\). Nevertheless Conjecture 1 may be written as two Loewner inequalities, as demonstrated by Zhang (2018).

**Conjecture 1A** (Loewner form). Let \(A_1, \ldots, A_n\) be symmetric positive semidefinite and \(A_1 + \cdots + A_n \preceq nI\). Then for any \(m \leq n\),

\[-\frac{n!}{(n-m)!}I \preceq \sum_{1 \leq j_1 < \cdots < j_m \leq n, j_1, \ldots, j_m \text{ distinct}} A_{j_1} \cdots A_{j_m} \preceq \frac{n!}{(n-m)!}I.\]

We prefer this equivalent formulation (2) as the original formulation (1) hides an asymmetry — note that there is an upper bound and a lower bound in (2) and there is no reason to expect that they should have the same magnitude. In fact, as we will see in the later sections, the upper and lower bounds have different magnitudes in every case that we examined.

We will next prove Conjecture 1 in its equivalent form Conjecture 1A for \(m = 2\) and \(3\). Our proofs rely on techniques introduced by Zhang (2018) in his proof for the case \(m = 3\), \(n = 3k\), but our two additional contributions are that (i) we will obtain better lower bounds (deferred to Section 5), and (ii) our proof will work for arbitrary \(n\) (not necessarily a multiple of 3).

**Theorem 1** (Recht–Ré for \(m = 2\)). Let \(A_1, \ldots, A_n\) be symmetric positive semidefinite and \(A_1 + \cdots + A_n \preceq nI\). Then

\[-n(n-1)I \preceq \sum_{i \neq j} A_i A_j \preceq n(n-1)I.\]

*Proof. The right inequality in (3) follows from

\[(n-1) \sum_{i,j} A_i A_j - n \sum_{i \neq j} A_i A_j = (n-1) \sum_i A_i^2 - \sum_{i < j} (A_i - A_j)^2 \geq 0,\]

and so

\[\sum_{i \neq j} A_i A_j \preceq n \sum_{i,j} A_i A_j \preceq n(n-1)I.\]

For the left inequality in (3), expand \((\sum_i A_i)^2 \geq 0\) to get

\[\sum_i A_i^2 \geq - \sum_{i \neq j} A_i A_j.\]

Let \(B := nI - \sum_i A_i \succeq 0\) and \(B_i := A_i + \frac{1}{n}B \succeq 0\). So \(\sum_i B_i = nI\). Then

\[-n \sum_{i \neq j} A_i A_j = -(n-1) \sum_{i \neq j} A_i A_j - \sum_j A_j A_j \preceq (n-1) \sum_i A_i^2 - \sum_{i \neq j} A_i A_j = \sum_{i < j} (A_i - A_j)^2 \preceq \sum_{i < j} (B_i - B_j)^2 = (n-1) \sum_i B_i^2 - \sum_{i \neq j} B_i B_j = n \sum_i B_i^2 - (\sum_i B_i)^2 = n \sum_i B_i^2 - n^2 I.\]
Therefore
\[- \sum_{i \neq j} A_i A_j - (n-1)nI \preceq \sum_i B_i^2 - n^2 I = \sum_i (B_i^2 - nB_i).\]

The eigenvalues of $B_i$ fall between 0 and $n$, so the eigenvalues of $B_i^2 - nB_i$ are all nonpositive, i.e., $B_i^2 - nB_i \preceq 0$. Hence $- \sum_{i \neq j} A_i A_j - (n-1)nI \preceq 0$. \hfill \Box

The right inequality of (3) is clearly sharp. In Section 5, we will prove a stronger result, improving the constant in the left inequality of (3) to $(n-1)/4$.

Following Zhang (2018), we write $\mathbb{E}_{i_1, \ldots, i_k}$ for expectation or average over all indices $1 \leq i_1, \ldots, i_k \leq n$, and $\mathbb{E}_{i_1, \ldots, i_k}$ for that over distinct indices $1 \leq i_1, \ldots, i_k \leq n$.

**Theorem 2** (Recht–Ré for $m = 3$). Let $A_1, \ldots, A_n$ be symmetric positive semidefinite and $A_1 + \cdots + A_n \preceq nI$. Then
\[- I \preceq \mathbb{E}_{i,j,k} A_i A_j A_k \preceq I.\]

**Proof.** Let $A, B, C$ be positive semidefinite. Then $ABC \preceq ABA + ABC$. If $B \preceq C$, then $ABA \preceq ACA$.

We start with the right inequality of (4),
\[
\mathbb{E}_{i,j,k} A_i A_j A_k \preceq \mathbb{E}_{i,j,k} \left( (1 - \frac{1}{n}) A_i A_j A_k + \frac{1}{n} A_i A_j A_i \right)
\leq \frac{1}{2} \mathbb{E}_{i,j,k} \left( (A_i + \cdots + A_i) (A_i + \cdots + A_i) \right).
\]

Fix a positive integer $l < n$ whose value we decide later.
\[
\mathbb{E}_{i,j,k} A_i A_j A_k \preceq \mathbb{E}_{i,j,k} \left[ \left( 1 - \frac{1}{l} \right) A_i A_j A_k + \frac{1}{l} A_i A_j A_i \right]
\preceq \frac{1}{2} \mathbb{E}_{i,j,k} \left( (A_i + \cdots + A_i) (A_i + \cdots + A_i) \right).
\]

Since $A_{i_1} + \cdots + A_{i_n} \preceq nI - (A_{i_1} + \cdots + A_{i_1})$, we have
\[
\mathbb{E}_{i,j,k} A_i A_j A_k \preceq \frac{1}{l^2(n-l)} \mathbb{E}_{i_1, \ldots, i_n} \left[ (A_i + \cdots + A_i) (A_i + \cdots + A_i) \right].
\]

Consider the function $f(x) = x^2(n-x)$. Let the line $y = cx + d$ be tangent to $f$ at $x = l$. We require that $c \geq 0$ and $f(x) \leq cx + d$ for $0 \leq x \leq n$. Elementary calculation shows that such a line exists as long as $1/2 \leq l/n \leq 2/3$. Let $A = A_{i_1} + \cdots + A_{i_l}$. As $cA + dI$ and $A(nI - A)A$ are simultaneously diagonalizable, each eigenvalue of $cA + dI - A(nI - A)A$ can be obtained by applying the function $g(x) = cx + d - x^2(n-x)$ to an eigenvalue of $A$. Hence
\[
\mathbb{E}_{i,j,k} A_i A_j A_k \preceq \frac{1}{l^2(n-l)} \mathbb{E}_{i_1, \ldots, i_l} \left[ (A_i + \cdots + A_i) + cI \right],\]
\[
\preceq \frac{1}{l^2(n-l)} \mathbb{E}_{i_1, \ldots, i_l} \left[ (A_i + \cdots + A_i) + cI \right].
\]

where the first inequality follows from the fact that it holds for each eigenvalue. Note that if we choose $A_1 = \cdots = A_n = I$, all inequalities above as well as the right inequality of (4) hold with equality. So as long as $1/2 \leq l/n \leq 2/3$, $c, d$ will give us
\[
\frac{1}{l^2(n-l)} (cl + d) = 1
\]
and thus the right inequality of (4).

For the left inequality of (4), we start by noting
\[
(A_1 + \cdots + A_{n-1}) A_n (A_1 + \cdots + A_{n-1}) \succeq 0.
\]

Taking expectation, we have $-(n-2)\mathbb{E}_{i,j,k} A_i A_j A_k \succeq \mathbb{E}_{i,j,k} A_i A_j A_k$, and thus
\[
-\mathbb{E}_{i,j,k} A_i A_j A_k
\preceq - \frac{n-2}{n-1} \mathbb{E}_{i,j,k} A_i A_j A_k - \frac{1}{n-1} \mathbb{E}_{i,j,k} A_i A_j A_k
\preceq \frac{1}{2(n-1)} \mathbb{E}_{i,j,k} \left[ (A_i - A_j) A_k (A_i - A_j) \right].
\]

As in the proof of Theorem 1, set $B := nI - \sum_i A_i \succeq 0$ and $B_i := A_i + \frac{1}{n} B \succeq 0$. Then
\[
-\mathbb{E}_{i,j,k} A_i A_j A_k
\preceq \frac{1}{2(n-1)} \mathbb{E}_{i,j,k} \left[ (B_i - B_j) B_k (B_i - B_j) \right]
\preceq \frac{1}{2(n-1)} \mathbb{E}_{i,j,k} B_i B_j B_k.
\]

Let $X_i := B_i (nI - B_i) B_i$ and $Y_i := (nI - B_i) B_i (nI - B_i)$. Routine calculations give
\[
\mathbb{E}_{i,j,k} X_i = (n-1) \mathbb{E}_{i,j,k} B_i B_j B_i,
\]
\[
\mathbb{E}_{i,j,k} Y_i = (n-1) \mathbb{E}_{i,j,k} B_i B_j B_i
\]
\[
+ (n-1)(n-2) \mathbb{E}_{i,j,k} B_i B_j B_k,
\]

which allows us to express $\mathbb{E}_{i,j,k} B_i B_j B_k$ and $\mathbb{E}_{i,j,k} B_i B_j B_k$ in terms of $\mathbb{E}_{i,j,k} X_i$ and $\mathbb{E}_{i,j,k} Y_i$. Then
\[
-\mathbb{E}_{i,j,k} A_i A_j A_k
\preceq \frac{1}{n-1} \mathbb{E}_{i,j,k} B_i B_j B_k - \frac{1}{n-1} \mathbb{E}_{i,j,k} B_i B_j B_k
\preceq \frac{1}{(n-2)(n-1)} \mathbb{E}_{i,j,k} [(n-1) X_i - Y_i].
\]
When we introduce some terminologies. Let $X$ be a monomial of length $d$, i.e., $X = x^i_1 \cdot \ldots \cdot x^i_m$. The monomials span a real finite-dimensional vector space $\mathbb{R}(X_1, \ldots, X_n)$, called the space of noncommutative polynomials. For any $d \in \mathbb{N}$, the finite-dimensional subspace of noncommutative polynomials of degree $\leq d$ will be denoted $\mathbb{R}(X_1, \ldots, X_n)_d$. The transpose of $f \in \mathbb{R}(X_1, \ldots, X_n)$ is denoted $f^\top$ and is defined on monomials by reversing the order of variables $(X_{i_1} \cdot \ldots \cdot X_{i_d})^\top = X_{i_d} \cdot \ldots \cdot X_{i_1}$ and extended linearly to all of $\mathbb{R}(X_1, \ldots, X_n)$. If $f^\top = f$, then $f$ is called symmetric.

The bottom line is that noncommutative polynomials may be evaluated on square matrices of the same dimensions, i.e., they define matrix-valued functions of matrix variables. For our purpose, if $A_1, \ldots, A_n$ are real symmetric matrices, then $f(A_1, \ldots, A_n)$ is also a matrix, but it may not be a symmetric matrix unless $f$ is a symmetric polynomial.

Let $L = \{\ell_1, \ldots, \ell_k\} \subseteq \mathbb{R}(X_1, \ldots, X_n)_1$ be a set of $k$ linear polynomials, i.e., $d = 1$. We will refer to $\ell_1, \ldots, \ell_k$ as linear constraints and $B_L := \{(A_1, \ldots, A_n) \mid \ell_1(A_1, \ldots, A_n) \geq 0, \ldots, \ell_k(A_1, \ldots, A_n) \geq 0\}$. Let $B_L$ be bounded with nonempty interior. Then both $\lambda_1$ and $\lambda_2$ are not bounded from below. Applying Theorem 3 with linear constraints $X_1 \geq 0, \ldots, X_n \geq 0, X_1 + \cdots + X_n \geq 0$. Conjecture 1B becomes the following.

**Conjecture 1B (Sum-of-squares form).** Let $m \leq n \in \mathbb{N}$ and $d = \lfloor m/2 \rfloor$. For the linear constraints $\ell_1 = X_1, \ldots, \ell_n = X_n, \ell_{n+1} = n - X_1 - \cdots - X_n$, let

\[
\lambda_1 = \operatorname{argmin}_{\lambda \in \mathbb{R}} \left\{ \lambda - \sum_{j \neq k} X_{j_1} \cdots X_{j_m} \in \Sigma_d(L) \right\},
\]

\[
\lambda_2 = \operatorname{argmin}_{\lambda \in \mathbb{R}} \left\{ \lambda + \sum_{j \neq k} X_{j_1} \cdots X_{j_m} \in \Sigma_d(L) \right\}.
\]

Then both $\lambda_1$ and $\lambda_2$ are not bounded from below.

In polynomial optimization (Lasserre, 2015), the commutative Positivstellensatz is used to transform a constrained optimization problem into a sum-of-squares problem that can in turn be transformed into a semidefinite programming (SDP) problem. Helton (2002) has observed that this also applies to noncommutative polynomial optimization problems, i.e., we may further transform Conjecture 1B into an SDP form. The vector space $\mathbb{R}(X_1, \ldots, X_n)_d$ has dimension $q := 1 + n + n^2 + \cdots + n^d$ and a basis comprising all $q$ monomials of degree $\leq d$. We will assemble all basis elements into the feasible set. Note that elements of $B_L$ are $n$ tuples of symmetric matrices. We say that $B_L$ is bounded if there exists $r > 0$ such that all $(A_1, \ldots, A_n) \in B_L$ satisfy $\|A_i\| \leq r, \ldots, \|A_n\| \leq r$. Let $d \in \mathbb{N}$. We write

$$
\Sigma_d(L) := \left\{ \sum_{i=1}^k \sum_{j=1}^p f_{ij} \ell_{ij} \mid f_{ij} \in \mathbb{R}(X_1, \ldots, X_n)_d, \quad k, p_1, \ldots, p_k \in \mathbb{N} \right\}
$$

for the set of noncommutative sum-of-squares generated by $L$. The following theorem is a simplified version of the noncommutative Positivstellensatz, i.e., Theorem 1.1 in Helton et al. (2012), that will be enough for our purpose.

**Theorem 3 (Noncommutative Positivstellensatz).** Let $f$ be a symmetric polynomial with $\deg(f) \leq 2d + 1$ and the feasible set $B_L$ be bounded with nonempty interior. Then

$$
f(A_1, \ldots, A_n) \geq 0 \text{ for all } (A_1, \ldots, A_n) \in B_L
$$

if and only if $f \in \Sigma_d(L)$.

Readers familiar with the commutative Positivstellensatz (Lasserre, 2015) would see that the noncommutative version is, surprisingly, much simpler and neater. To avoid notational clutter, we introduce the shorthand

$$
\sum_{j_i \neq j_k} := \sum_{j_i, j_k} \sum_{j_i \neq j_k} \Lambda_{j_i, j_k}
$$

for sum over distinct indices. Applying Theorem 3 with linear constraints $X_1 \geq 0, \ldots, X_n \geq 0, X_1 + \cdots + X_n \geq 0$. Conjecture 1A becomes the following.

**Conjecture 1A (Sum-of-squares form).** Let $m \leq n \in \mathbb{N}$ and $d = \lfloor m/2 \rfloor$. For the linear constraints $\ell_1 = X_1, \ldots, \ell_n = X_n, \ell_{n+1} = n - X_1 - \cdots - X_n$, let

$$
\lambda_1 = \operatorname{argmin}_{\lambda \in \mathbb{R}} \left\{ - \sum_{j \neq k} X_{j_1} \cdots X_{j_m} \in \Sigma_d(L) \right\},
\]

$$
\lambda_2 = \operatorname{argmin}_{\lambda \in \mathbb{R}} \left\{ \lambda + \sum_{j \neq k} X_{j_1} \cdots X_{j_m} \in \Sigma_d(L) \right\}.
\]
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a $q$-tuple of monomials that we denote by $\beta$. With respect to this basis, any $f \in \mathbb{R}(X_1, \ldots, X_n)_d$ may be represented uniquely as $f = \beta^T u$ for some $u \in \mathbb{R}^q$. Therefore a noncommutative square may be expressed as

$$ \sum_{j=1}^{p} f_j^T f_j = \sum_{j=1}^{p} u_j^T \beta \beta^T u_j = \text{tr} \left( \beta \beta^T \left( \sum_{j=1}^{p} u_j u_j^T \right) \right) $$

by simply writing $f_j = \beta^T u_j, u_j \in \mathbb{R}^q, j = 1, \ldots, p$. Since a symmetric matrix $Y$ is positive semidefinite iff it can be written as $Y = \sum_{j=1}^{p} u_j u_j^T$, we obtain the following one-to-one correspondence between noncommutative squares and positive semidefinite matrices:

$$ \sum_{j=1}^{p} f_j^T f_j \in \mathbb{R}(X_1, \ldots, X_n)_{2d+1}, f_j \in \mathbb{R}(X_1, \ldots, X_n)_d \overset{\text{subject to}}{\implies} \sum_{j=1}^{p} u_j u_j^T \in \mathbb{R}^{n \times q}, u_j \in \mathbb{R}^q. $$

With this correspondence, the two minimization problems in Conjecture 1B become two SDPs.

**Conjecture 1C** (Semidefinite program form). Let $m \leq n \in \mathbb{N}$ and $d = \lfloor m/2 \rfloor$. Let $\beta$ be a monomial basis of $\mathbb{R}(X_1, \ldots, X_n)_d$ and let $X_{n+1} = n - X_1 - \cdots - X_n$. Let $\lambda_1$ be the minimum value of the SDP:

$$ \begin{align*}
\text{minimize} & \quad \lambda - \sum_{j \neq j_0} X_{j_1} \cdots X_{j_m} = \sum_{i=1}^{n+1} \text{tr}(\beta X_i \beta^T Y_i), \\
\text{subject to} & \quad Y_1 \succeq 0, \ldots, Y_{n+1} \succeq 0; \\
& \quad \lambda_1 \leq \lambda_2 \leq n!/(n-m)!. 
\end{align*} \tag{5} $$

and $\lambda_2$ be that of the SDP:

$$ \begin{align*}
\text{minimize} & \quad \lambda + \sum_{j \neq j_0} X_{j_1} \cdots X_{j_m} = \sum_{i=1}^{n+1} \text{tr}(\beta X_i \beta^T Y_i), \\
\text{subject to} & \quad Y_1 \succeq 0, \ldots, Y_{n+1} \succeq 0. \\
& \quad \lambda_1 \leq \lambda_2 \leq n!/(n-m)!. 
\end{align*} \tag{6} $$

Then both $\lambda_1$ and $\lambda_2 \leq n!/(n-m)!$.

Note that the minimization is over the scalar variable $\lambda$ and the matrix variables $Y_1, \ldots, Y_{n+1}$; the equality constraint equating two noncommutative polynomials is simply saying that the coefficients on both sides are equal, i.e., for each monomial, we get a linear constraint involving $\lambda, Y_1, \ldots, Y_{n+1}$ --- the $X_i$’s play no role other than to serve as placeholders for these linear constraints. We may express (5) and (6) as SDPs in standard form with a single matrix variable $Y := \text{diag}(\lambda, Y_1, \ldots, Y_{n+1})$, see (7) for example.

Readers acquainted with (commutative) polynomial optimization (Lasserre, 2015) would be familiar with the above discussions. In fact, the only difference between the commutative and noncommutative cases is that $\sum_{i=0}^{d} n^i$, the size of a noncommutative monomial basis, is much larger than $\binom{d+n}{d}$, the size of a commutative monomial basis.

For any fixed values of $m$ and $n$, Conjecture 1C is in a form that can be checked by standard SDP solvers. The dimension of the SDP grows exponentially with $m$, and without access to significant computing resources, only small values of $m, n$ are within reach. Fortuitously, $m = n = 5$ already yields the required violation $144.648 < 120$, showing that Conjecture 1C and thus Conjecture 1 is false in general. We tabulate our results for $m \leq n \leq 5$ in Table 1.

| $m$, $n$ | $\lambda_1$ | $\lambda_2$ | $n!/(n-m)!$ |
|----------|-------------|-------------|--------------|
| $m = 2$, $n = 2$ | 2.0000 | 0.5000 | 2 |
| $m = 2$, $n = 3$ | 6.0000 | 1.5000 | 6 |
| $m = 2$, $n = 4$ | 12.0000 | 3.0000 | 12 |
| $m = 2$, $n = 5$ | 20.0000 | 5.0000 | 20 |
| $m = 3$, $n = 3$ | 6.0000 | 3.4113 | 6 |
| $m = 3$, $n = 4$ | 24.0000 | 8.5367 | 24 |
| $m = 3$, $n = 5$ | 60.0000 | 17.3611 | 60 |
| $m = 4$, $n = 4$ | 24.0000 | 22.4746 | 24 |
| $m = 4$, $n = 5$ | 120.0000 | 80.2349 | 120 |
| $m = 5$, $n = 5$ | 120.0000 | 144.6488 | 120 |

Table 1. Results from the SDPs in Conjecture 1C for $m \leq n \leq 5$. The bold entry for $\lambda_2$ shows that the Recht–Ré conjecture is false for $m = n = 5$ since $144.6488 > 120$.

Indeed, the beauty of the noncommutative Positivstellensatz approach is that it allows us to show that Conjecture 1 is false for $m = n = 5$ without actually having to produce five positive semidefinite matrices $A_1, \ldots, A_5$ that violates the inequality (1). It would be difficult to find $A_1, \ldots, A_5$ explicitly as one does not even know the smallest dimensions required for these matrices to give a counterexample to (1). Our approach essentially circumvents the issue by explicit as one does not even know the smallest dimension of the matrices $A_1, \ldots, A_5$ did not make an appearance anywhere in this article.
4. Verification via Farkas

We take a closer look at the $m = n = 5$ case that provided a refutation to the Recht–Ré conjecture. In this case, the basis $\beta$ has $1 + 5 + 5^2 = 31$ monomials; the SDP in (6) has $1 + 5 + 5^2 + 5^3 + 5^4 + 5^5 = 3906$ linear constraints, $31^2 \times 6 + 1 = 5767$ variables, and takes the form:

\[
\begin{align*}
\text{minimize} & \quad \text{tr}(C_0 Y) \\
\text{subject to} & \quad \text{tr}(C_i Y) = b_i, \quad i = 1, \ldots, 3906, \\
& \quad Y = \text{diag}(\lambda, Y_1, \ldots, Y_6) \succeq 0.
\end{align*}
\]

Here $C_0, C_1, \ldots, C_{3906} \in S_{187}^{+}, b \in \mathbb{R}^{3906}, \lambda$ is a scalar variable, and $Y_1, \ldots, Y_6$ are 31-by-31 symmetric matrix variables. To put (7) into standard form, the block diagonal structure of $Y$ may be further encoded as linear constraints requiring that off-diagonal blocks be zero. The output of our program gives a minimizer of the form $Y^* = \text{diag}(\lambda^*, Y_1^*, \ldots, Y_6^*) \in S_{187}^{+}$ with

\[
\lambda^* = 144.6488, \quad Y_1^*, \ldots, Y_6^* \in S_{31}^{+}.
\]

The actual numerical entries of the matrices appearing in (7) and (8) are omitted due to space constraints; but they can be found in the output of our program (code in supplement).

The values in (8) are of course approximate because of the inherent errors in numerical computations. In our opinion, the gap between the computed 144.6488 and the conjectured 120 is large enough to override any concerns of a mistaken conclusion resulting from numerical errors. Nevertheless, to put to rest any lingering doubts, we will directly show that the conjectured value $\lambda = 120$ is infeasible by producing a Farkas certificate. Consider the feasibility problem:

\[
\begin{align*}
\text{minimize} & \quad 0 \\
\text{subject to} & \quad \text{tr}(C_i Y) = b_i, \quad i = 1, \ldots, 3906, \\
& \quad \text{tr}(C_0 Y) = 120, \\
& \quad Y \succeq 0,
\end{align*}
\]

with $C_0, C_1, \ldots, C_{3906} \in S_{187}^{+}$ and $b \in \mathbb{R}^{3906}$ as in (7). Note that $C_0 = c_1 e_1 e_1^T$ is the matrix with one in the $(1, 1)$th entry and zero everywhere else. So (9) is the feasibility problem of the optimization problem (7) with the additional linear constraint $y_1 = 120$ and where we have disregarded the block diagonal constraints on $Y$. The dual of (9) is

\[
\begin{align*}
\text{maximize} & \quad 120 y_0 + b^T y \\
\text{subject to} & \quad y_0 C_0 + y_1 C_1 + \cdots + y_{3906} C_{3906} \preceq 0.
\end{align*}
\]

Our program produces a Farkas certificate $y \in \mathbb{R}^{3906}$ with $120 y_0 + b^T y \approx 47.3 > 0$, implying that (9) is infeasible.

While this is a consequence of Farkas Lemma for SDP (Lasserre, 1995), all we need is the following trivial version.

**Lemma 1.** Let $m, n \in \mathbb{N}$. Let $C_0, C_1, \ldots, C_m \in S^n$ and $b \in \mathbb{R}^{m+1}$. If there exists a $y \in \mathbb{R}^{m+1}$ with

\[
y_0 C_0 + \cdots + y_m C_m \preceq 0, \quad b^T y > 0,
\]

then there does not exist a $Y \in S^n$ with

\[
\text{tr}(C_0 Y) = b_0, \ldots, \text{tr}(C_m Y) = b_m, \quad Y \succeq 0.
\]

**Proof.** If such a $Y$ exists, then

\[
0 \geq \text{tr}((y_0 C_0 + \cdots + y_m C_m) Y) = y_0 b_0 + \cdots + y_m b_m > 0,
\]

a contradiction. 

Hence a matrix of the form

\[
Y = \text{diag}(120, Y_1, \ldots, Y_6) \in S_{187}^{+}
\]

is infeasible for (7), providing another refutation of Conjecture 1C and thus Conjecture 1. In particular, showing that $\lambda = 120$ is infeasible for (7) does not require any of the values computed in (8). Of course, aside from being the conjectured value of $\lambda_2$, there is nothing special about $\lambda = 120$ — for any $\lambda < 144.6488$, we may similarly compute a Farkas certificate $y$ to show that such a value of $\lambda$ is infeasible for (7).

We conclude with a few words on the computational costs of the SDPs in this and the last section. Our resulting dense linear system for $m = n = 5$ requires $3906 \times 5767 \approx 22$ million floating point storage. Using a personal computer with an Intel Core i7-9700k processor and 16GB of RAM, our SeDuMi (Sturm, 1999) program in Matlab takes 150 seconds. For $m = n = 6$, storage alone would have taken 26 billion floating numbers, beyond our modest computing resources.

5. Improving the Recht–Ré inequality

An unexpected benefit of the noncommutative Positivstellensatz approach is that it leads to better bounds for the $m = 2$ and 3 cases that we know are true. Observe that the values for $\lambda_2$ in Table 1 for $m = 2$ are exactly smaller than the values for $n!/(n-m)!$ by a factor of $1/4$. This suggests that the Recht–Ré inequality (3) for $m = 2$ in Theorem 1 may be improved to

\[
-\frac{1}{4} n(n - 1) I \preceq \sum_{i \neq j} A_i A_j \preceq n(n - 1) I.
\]

Table 1 only shows this for $n = 2, 3, 4, 5$ but in this section, we will give a proof for arbitrary $n \geq 2$. Although our
proof below does not depend on the SDP formulation in (6), the correct coefficients in (11) for arbitrary \( n \) would have been impossible to guess without solving (6) for \( m = 2 \) and some small values of \( n \).

So far we have not explored the symmetry evident in our formulations of the Recht–Ré inequality: In Conjecture 1A, the matrix expression

\[
\lambda I \pm \sum_{j_i \neq j_k} A_{j_1} \cdots A_{j_m}
\]

and the constraints \( A_1 \geq 0, \ldots, A_n \geq 0, A_1 + \cdots + A_n \preceq nI \) are clearly invariant under any permutation \( \sigma \in \mathfrak{S}_n \). In Conjecture 1C, the noncommutative sum-of-squares

\[
\lambda \pm \sum_{j_i \neq j_k} X_{j_1} \cdots X_{j_m} = \sum_{i=1}^{n+1} \text{tr}(\beta X_i \beta^T Y_i), \quad (10)
\]

where \( X_{n+1} = n - X_1 - \cdots - X_n \), is also invariant under \( \mathfrak{S}_n \), and so we may average over all permutations to get a symmetrized sum-of-squares. For commutative polynomials, results from classical invariant theory are often used to take advantage of symmetry (Gatermann & Parrilo, 2004). We will see next that such symmetry may also be exploited for noncommutative polynomials.

Consider the case \( m = 2, n = 3 \). The monomial basis of \( \mathbb{R}(X_1, X_2, X_3)^1 \) is \( \beta = (1, X_1, X_2, X_3) \). The symmetry imposes linear constraints on the matrix variables \( Y_1, Y_2, Y_3, Y_4 \) in (6), requiring them to take the following forms:

\[
Y_1 = \begin{bmatrix} a & b & c \\ b & d & e \\ c & e & f \end{bmatrix}, \quad Y_2 = \begin{bmatrix} a & c & b \\ c & f & e \\ b & e & d \end{bmatrix},
\]

\[
Y_3 = \begin{bmatrix} a & c & b \\ c & f & g \\ c & g & f \end{bmatrix}, \quad Y_4 = \begin{bmatrix} x & y & y \\ y & z & w \\ w & y & z \end{bmatrix}.
\]

These symmetries allow us to drastically reduce the degree of freedom in our SDP. For any \( m = 2, n \geq 2 \), the matrices \( Y_1, \ldots, Y_n \) are always determined by precisely 11 variables that we label \( a, b, c, d, e, f, g, x, y, z, w \). We computed their values explicitly for \( n = 2, 3, 4 \). For \( n = 2 \),

\[
Y_1 = \begin{bmatrix} \frac{5}{2} & -3 & \frac{1}{2} \\ -\frac{3}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix}, \quad Y_3 = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix},
\]

and \( Y_2 \) can be determined from \( Y_1 \). For \( n = 3 \),

\[
Y_1 = \begin{bmatrix} \frac{5}{2} & -1 & 0 \\ -1 & \frac{4}{3} & \frac{1}{3} \\ 0 & \frac{1}{3} & \frac{1}{3} \end{bmatrix}, \quad Y_4 = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix},
\]

and \( Y_2, Y_3 \) can be determined from \( Y_1 \). For \( n = 4 \),

\[
Y_1 = \begin{bmatrix} \frac{15}{4} & -\frac{9}{2} & -\frac{9}{2} & -\frac{1}{2} \\ -\frac{9}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{9}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{bmatrix}, \quad Y_3 = \begin{bmatrix} \frac{3}{2} & -\frac{3}{4} & \frac{3}{4} & \frac{1}{2} \\ -\frac{3}{4} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{3}{4} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{bmatrix}, \quad Y_5 = \begin{bmatrix} \frac{3}{2} & -\frac{3}{4} & \frac{3}{4} & \frac{1}{2} \\ -\frac{3}{4} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{3}{4} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{bmatrix},
\]

and \( Y_2, Y_3, Y_4 \) can be determined from \( Y_1 \). The rational numbers above are all chosen by observing the floating numbers output of the SDP (6).

The values of the matrices \( Y_i \)'s for \( n = 2, 3, 4 \) allow us to guess that the variables \( a, b, c, d, e, f, g, x, y, z, w \) are:

\[
a = \frac{5(n-1)}{4}, \quad b = -\frac{3(n-1)}{2n}, \quad c = \frac{3-n}{2n},
\]

\[
d = f = z = \frac{2(n-1)}{n^2}, \quad e = g = w = \frac{n-2}{n^2}, \quad (11)
\]

The proof of our next theorem will ascertain that these choices are indeed correct—they yield the sum-of-squares decomposition in (10) for \( m = 2 \).

**Theorem 4** (Better Recht–Ré for \( m = 2 \)). Let \( A_1, \ldots, A_n \) be positive semidefinite matrices. If \( A_1 + \cdots + A_n \preceq nI \), then

\[
-\frac{1}{4n(n-1)}I \preceq \sum_{i \neq j} A_i A_j \preceq n(n-1)I.
\]

**Proof.** The upper bound has already been established in Theorem 1. It remains to establish the lower bound. We start from the following readily verifiable inequalities

\[
\frac{1}{2n(n-1)}(A_j - A_k)A_i(A_j - A_k) \succeq 0, \quad (12)
\]

\[
\frac{5(n-1)}{4n} \left( I - \frac{6}{5n} A_i + \frac{2(3-n)}{5n(n-1)} \sum_{j \neq i} A_j \right) \succeq 0, \quad (13)
\]

\[
A_i \left( I - \frac{6}{5n} A_i + \frac{2(3-n)}{5n(n-1)} \sum_{j \neq i} A_j \right) \succeq 0,
\]

\[
\frac{n-1}{5n^2} \left( A_i + \frac{2(n-1)}{n-1} \sum_{j \neq i} A_j \right) \succeq 0, \quad (14)
\]
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\[ \frac{1}{2n^2} (A_j - A_k) \left( n - \sum_i A_i \right) (A_j - A_k) \geq 0, \quad (15) \]

\[ \frac{n - 1}{4} \left( I - \frac{2}{n} \sum_i A_i \right) \left( n - \sum_i A_i \right) \geq 0, \quad (16) \]

Sum (12) over all distinct \( i, j, k \); sum (13) over all \( i \); sum (14) over all \( i \); sum (15) over all distinct \( j, k \); add all results to (16). The final inequality is our required lower bound.

For \( n = m = 2 \), the new lower bound is sharp. Take

\[ A_1 = \begin{bmatrix} \frac{3}{2} & 0 \\ 0 & 0 \end{bmatrix}, \quad A_2 = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}, \]

then \( \| A_1 + A_2 \| = 2 \) and the smallest eigenvalue of \( A_1 A_2 + A_2 A_1 \) is \(-1/2\). We conjecture that this bound is sharp for all \( m = 2, n \geq 2 \).

The method in this section also extends to higher \( m \). For example, we may impose symmetry constraints for \( m = n = 3 \) and see if the \( Y_1, Y_2, Y_3, Y_4 \) obtained have rational values, and if so write down a sums-of-squares proof by factoring the \( Y_1 \)'s.

6. Conclusion and open problems

We conclude our article with a discussion of some open problems and why we think the Recht–Ré conjecture, while false as it is currently stated, only needs to be refined.

An immediate open question is whether the conjecture is true for \( m = 4 \): Table 1 shows that it holds for \((m, n) = (4, 4) \) and \((4, 5) \); we suspect that it is true for all \( n \geq 4 \).

As we pointed out after Conjecture 1A, the Recht–Ré inequality as stated in (1) conceals an asymmetry — it actually contains two inequalities, as shown in (2). What we have seen is that the lower bound is never attained in any of the cases we have examined. For \( m = 2 \) and 3, the lower bound is too large, and we improved it in Theorem 4 and the proof of Theorem 2 respectively. For \( m = 5 \), the lower bound is too small, which is why the Recht–Ré inequality is false. A natural follow-up question is then: “What is the correct lower bound?” On the other hand, we conjecture that the remaining half of the Recht–Ré inequality, i.e., the upper bound in (2), holds true for all \( m \leq n \in \mathbb{N} \).

Recht & Re (2012) has another conjecture similar to Conjecture 1 but where the norms appear after the summation.

**Conjecture 2 (Recht & Re 2012).** Let \( A_1, \ldots, A_n \) be positive semidefinite matrices. Then

\[ \frac{1}{n^m} \sum_{1 \leq j_1, \ldots, j_m \leq n} \| A_{j_1} \cdots A_{j_m} \| \geq \frac{(n - m)!}{n!} \sum_{1 \leq j_1, \ldots, j_m \leq n, j_1, \ldots, j_m \text{ distinct}} \| A_{j_1} \cdots A_{j_m} \| . \]

This has been established for \( m = 2 \) and 3 for any unitary invariant norm in Israel et al. (2016). It is not clear to us if the noncommutative Positivstellensatz might perhaps also shed light on this related conjecture.

Lastly, if our intention is to analyze the relative efficacies of with- and without-replacement sampling strategies in randomized algorithms, then it is more pertinent to study these inequalities for random matrices, i.e., we do not just assume that the indices are random variables but also the entries of the matrices. For example, if we want to analyze the Kaczmarz algorithm, then we ought to take expectation not only with respect to all permutations but also with respect to how we generate the entries of the matrices. This would provide a more realistic platform for comparing with- and without-replacement sampling strategies.

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