Lifting Integrality Gaps to Non-Commutative SoS Lower Bounds for Local Hamiltonians

Kareem Diab

University of Miami, Department of Computer Science

Overview

The sum of squares (SoS) hierarchy is a powerful algorithmic framework that subsumes the capabilities of many other known algorithms for optimization problems. Consequently, understanding where sum of squares fails becomes extremely interesting and can be viewed as great evidence for the unconditional hardness of a computational problem. We study the limitations of SoS in the realm of constraint satisfaction problems, and the local Hamiltonian problem from quantum complexity theory. As a hierarchy of semidefinite programs meant to certify polynomial inequalities, each level of the hierarchy comes with a dual program that searches over the space of objects called **pseudo-distributions**. In short, these are a generalization of actual distributions that only care about low degree moments, hence the relaxation. One typically shows an SoS lower bound (or integrality gap) by constructing a pseudo-distribution that assigns an expectation for a polynomial that is strictly greater than the optimum that is trying to be certified.

In this work, we explore several transformations of a constraint satisfaction problem (CSP) to a local Hamiltonian, with the goal of understanding which constructions preserve hardness against the sum-of-squares (SoS) hierarchy, and how the space of pseudo-distributions shifts in the process. The local Hamiltonians we consider represent sums over monomials in noncommuting operator terms, and we accordingly study non-commutative SoS (ncSoS) hierarchies and their dual semidefinite programs over moment matrices, such as the NPA hierarchy.

Construction

A natural construction yields a CSS Hamiltonian from a CSP instance by summing two local Hamiltonians encoding the same instance, one in the Z (computational) basis and one in the X (Hadamard) basis. Consider a 3-XOR instance ψ for example: we convert each constraint over $\{+1, -1\}$ variables, such as $x_i x_j x_k = a_{ijk}$, to a local satisfaction term by replacing each variable x_i with the Pauli operator Z_i, giving a Z-basis Hamiltonian

$$H_Z \;=\; \sum_{(i,j,k)\in\psi} \frac{I + a_{ijk} Z_i Z_j Z_k}{2},$$

where each term contributes 1 on satisfied constraints and 0 on violated ones. The Hamiltonian H_X is defined identically with each Z_i replaced by X_i, encoding the same constraints in the Hadamard basis. The full CSS Hamiltonian is then $H = H_Z + H_X$. Since X_i and Z_i anticommute on each qubit, the two summands do not commute, making this a natural quantization of the original CSP.

Background: Grigoriev's Theorem

We focus specifically on the 3-XOR instances constructed in Grigoriev's SoS lower bounds [1]. A 3-XOR instance ψ over n variables consists of m equations of the form $x_i \oplus x_j \oplus x_k = a_{ijk}$, which can be represented by a bipartite graph where each left vertex (clause) connects to exactly three right vertices (variables). Grigoriev showed that if the number of clauses m is chosen to be sufficiently larger than the number of variables n, and the bipartite graph is sampled randomly, then with high probability the instance satisfies two properties simultaneously:

1. **High unsatisfiability:** $\max_x f_\psi(x) \leq \frac{1}{2} + \delta$ for arbitrarily small $\delta > 0$.
2. **SoS hardness:** degree-$\Omega(n)$ SoS assigns pseudo-expectation 1 to f_ψ, behaving as if the instance were fully satisfiable.

The key property enabling this proof is that random bipartite graphs exhibit small-set expansion with high probability.

Preliminary Results

We study the spectral properties of the CSS Hamiltonians constructed from these instances by analyzing the structure of the underlying *conflict graph* Γ: a graph whose vertices are the local terms of H, with edges between pairs of terms that anticommute. Two terms anticommute precisely when one is an X-type Pauli string and the other is a Z-type Pauli string acting on an odd number of shared qubits. The conflict graph is consequently *bipartite* between H_Z- and H_X-terms, since same-basis terms always commute. We note that Γ is distinct from the bipartite incidence graph of ψ: the former is defined on the Hamiltonian terms and captures their algebraic noncommutativity, while the latter encodes the clause-variable structure of the CSP instance itself.

One can obtain a non-trivial upper bound on the maximum eigenvalue of a local Hamiltonian by studying only its anticommutativity properties through the conflict graph. In particular, the Lovász theta function $\vartheta(\Gamma)$ can be computed via a simple semidefinite program and upper bounds the maximum eigenvalue of H. We have identified the conflict graph of these quantized CSPs to be closely related to Johnson-scheme graphs, which allows us to build on the techniques of Hastings and O'Donnell [3], who obtained similar spectral bounds for fermionic Hamiltonians. Understanding $\vartheta(\Gamma)$ for these graphs will provide insight into how the NPA hierarchy performs on such Hamiltonians, since the Lovász theta function is itself equivalent to a degree-2 SoS relaxation. We expect that bounding $\vartheta(\Gamma)$ will help build intuition for the space of pseudo-distributions at low levels of the hierarchy and whether or not there will be an integrality gap.

To complement our progress on the SDP value, we establish a narrow window on the true maximum eigenvalue of these Hamiltonians.

Theorem 1. *Let ψ be a 3-XOR instance with m clauses satisfying $\max_x f_\psi(x) \leq \frac{1}{2} + \delta$, and let $H = H_Z + H_X$ be the CSS Hamiltonian constructed from ψ. Then*

$$(1+\delta)m \;\leq\; \lambda_{\max}(H) \;\leq\; (1+2\delta)m.$$

The lower bound follows by observing that any computational basis state achieving near-optimal energy on H_Z automatically contributes exactly $\frac{m}{2}$ to H_X, since X-type Pauli strings have zero expectation on computational basis states. The upper bound follows from the triangle inequality on operator norms.

There is reason to believe that the NPA hierarchy at low degree is unlikely to detect the unsatisfiability of ψ and may return a value close to $2m$, which would suggest a substantial integrality gap between the true optimum and the NPA value, of order $(1-\delta)m$. However, it is also possible that the anticommutativity of the terms is the primary factor bounding $\lambda_{\max}(H)$, independently of the unsatisfiability of the underlying instance. If this is the case, then the Lovász theta function or low levels of the NPA hierarchy may already certify bounds within the window we established, and the integrality gap may be smaller than anticipated or absent entirely. Distinguishing between these two scenarios is a key open question in our analysis. Regardless of which scenario holds, understanding the space of low-degree pseudo-distributions over these noncommutative polynomials is the central technical challenge going forward.

Connection to NLTS and Further Directions

A secondary motivation for studying these CSS Hamiltonians is to strengthen the analogy between Grigoriev's theorem and the No Low-Energy Trivial States (NLTS) theorem [2]. Both results establish unconditional lower bounds against a restricted model of computation using a form of bipartite expansion: Grigoriev constructs pseudo-distributions that fool the SoS hierarchy, while the NLTS proof uses expansion to certify that low-energy states are well-spread and therefore unreachable by constant-depth circuits. We observe that the CSS Hamiltonians studied here sit naturally at this intersection. If they exhibit ncSoS integrality gaps, they would provide a new class of Hamiltonians with provable hardness guarantees against efficient classical algorithms, and if they additionally satisfy the NLTS property, they would represent a family of Hamiltonians that are simultaneously hard for shallow quantum circuits and for the NPA hierarchy.

We also identify several intermediate problems that may illuminate the main question. First, rather than working with the specific X and Z bases, one could ask whether ncSoS integrality gaps persist for Hamiltonians diagonalized in two arbitrary bases, not necessarily local Pauli bases. This would help clarify what relationship between the two bases is actually necessary to preserve SoS-hardness, and could be approached by taking the second Hamiltonian to be a rotation of H_Z by an arbitrary unitary. Second, we note that the 3-XOR instances used in Grigoriev's theorem are random and thus non-explicit. A promising direction is to first derandomize these instances before performing the quantization. This was recently achieved by Hopkins and Lin [4], who constructed the first explicit SoS-hard 3-XOR instances using small-set high-dimensional expansion inspired by quantum LDPC codes. Their construction relies on algebraic properties of the underlying chain complex of such high-dimensional expanders, and we expect these same properties to be relevant to the analysis of the local Hamiltonians we construct from them.

References

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