Polynomial Optimization and Quantifier Elimination in Quantum Mechanics

Ichio Kikuchi and Akihito Kikuchi*

September 28, 2018

Abstract

In this short notes, we present the formulation of a kind of quantum algorithm, applicable to the polynomial optimization. The present algorithm introduces the quantum effect by means of the coordinate variables, the momentum variables, and the commutators, and the Plank constant, which shall establish the correspondence between the quantum and the classical cases. The formalism is an extension to the polynomial optimization in the “classical” sense; the relations among quantum mechanical values are represented by a semi-algebraic set (by the set of polynomials and sign conditions), and the optimum is searched in this semi-algebraic set. In the context of this formalism, the optimization of the Ising model [QUBO model] will be a special case. However, the computational procedure proposed here is different from the quantum annealing which is now in vogue. We demonstrate the exemplary calculation through quantifier elimination (which is a kind of symbolic computation applicable to optimization and other problems).

1 Introduction

In this article, we give an account of polynomial optimization and quantifier elimination in quantum mechanics. The polynomial optimization is a vast range of algorithms so that one can find the optimum value of the objective function in the set of equations and inequalities: one can also pin up the optimum point in the set of equations and inequalities which are simpler than the initial formula. To this topic deeply related is the quantifier elimination[1, 2, 4]. The latter processes the polynomial formula with quantifiers (s.t. FOR ALL or THERE EXISTS) and breaks down them into a simpler formula without quantifiers. The famous example of the high-school math is this: under what condition does a quadratic equation have real roots?

$$(\exists x) \ ax^2 + bx + c = 0$$

*A.K. is the corresponding author: akihito_kikuchi@gakushikai.jp

The solution is $b^2 - 4ac \geq 0$. (To be exact one should add the extra non-zero condition to a and b)

The physicists are often tempted to search a set of parameters by which the quantum mechanical equation should take the certain value of the solution. In this request, the quantifier elimination is suggestive. But the quantum dynamics is described by the differential equations, while the main objects of quantifier elimination are polynomials.

2 Formulation

We present the formulation of a quantum algorithm, applicable to the polynomial optimization. This formalism is an extension of polynomial optimization, which is a modern numerical technique, in the sense of classical computation. We modify it so that it will admit the presence of quantum fluctuation. Actually, the equations in the quantum mechanics are the differential equations, in contrast to that the object of quantifier elimination is the system of polynomials. Thus our formalism introduces a trick in order to represent the equations in the quantum mechanics by polynomials, from which, we demonstrate how to apply polynomial optimization and quantifier elimination.

The polynomial optimization, the raw material of our scheme, is, in the strict sense, not of the symbolic computation, although the formalism is presented by the symbolic notation. In general, this sort of problem is solved numerically in the framework of the semi-positive definite (SDP) problem[7]. Let us consider the optimization problem in $\mathbb{R}^N$. The basic theory is grounded on the moment problem.

In the standard formulation, we use several matrices defined by the set of the moment. The moment matrix M (with variables $x, y, z, \dots$ and their powers) is defined through this function:

$$M[x^i y^j z^k] = \int x^i y^j z^k d\mu, \quad (1)$$

by means of a certain measure μ such that

$$\int d\mu = 1. \quad (2)$$

In the matrix representation, rows and columns are indexed by $x^i y^j z^k, \dots$, and the above definition should be read as:

$$M[x^{i1} y^{j1} z^{k1}][x^{i2} y^{j2} z^{k2}] = M[x^{i1+i2} y^{j1+j2} z^{k1+k2}].$$

The constraints (including equations and inequalities) are represented by matrices. For example, if it is given by the polynomial

$$f(x, y, z) = \sum a_{pqr} x^p y^q z^r \geq 0$$

the matrix representation is given by the integral like this:

$$R(f)[x^{i1} y^{j1} z^{k1}][x^{i2} y^{j2} z^{k2}] = \sum a_{pqr} \int x^{p+i1+j1} y^{q+i2+j2} z^{r+i3+j3} d\mu.$$

The entries in $R(f)$ are represented by the coefficients a_{pqr} and the entries in M ($M[x^*y^*z^*]$). The inequality or the equation of the polynomial is turned into the semi-definite positiveness of the matrix $R(f)$.

The objective function should be given by a polynomial like this:

$$g(x, y, z) = \sum c_{pqr} x^p y^q z^r.$$

It is converted into a linear function of the following form

$$O(g) = \sum c_{pqr} M[x^p y^q z^r],$$

where the monomials are replaced by the entries of the momentum matrix.

Formally we assume these matrices are symmetric, real-valued. We find the minimum of the linear objective function $O(g)$ with respect to $M[x^p y^q z^r]$ with the condition that matrices M and $R(f)$ are semi-definite. In the algorithm, we do not determine the measure itself, but we search the values of the moments M which realize the optimum.

For example, optimize the polynomial with two variables:

$$p * p + x * x \tag{3}$$

without constraint.

These variables are used:

$$u = (1, x, p, x * x, xp, p * p).$$

The moment matrix is given as:

$$\begin{pmatrix} 1 & M_x & M_p \\ M_x & M_{xx} & M_{px} \\ M_p & M_{px} & M_{pp} \end{pmatrix}. \tag{4}$$

The problem is: Find the minimum of $M_{xx} + M_{pp}$, with the semi-positive condition of the moment matrix. We find the trivial solution : $M_{xx} = M_{pp} = M_x = M_p = M_{px} = 0$, which satisfy the semi-positive definiteness of the moment matrix, so that the optimum value is zero.

Let us turn to the quantum case. The example polynomial is the model of the 1-dimensional harmonic oscillator, with the momentum p and the coordinate x .

We know that the momentum is given by the differential operator on the wave function. Also, the coordinate x is an operator. The square norm of the wave-function ϕ^2 is integrated to be unity, that is to say, it should be interpreted as a measure mu . In order to construct the moment matrix, we must take into the consideration of the non-commutativity of the p , x :

$$[p, x] = \sqrt{-1}h, \tag{5}$$

where h is the small constant. It will demand the discussion in the complex number. So we would rather make use of $u = h \frac{d}{dx}$, instead of p , in order to go in the real numbers.

We define the extended moment matrix as

$$M[x^i u^j][x^k u^l] = \int (x^i u^k \phi) (x^j u^l \phi) dx. \tag{6}$$

This moment is rearranged by the linear combination of those terms

$$M[x^m u^n] = \int \phi(x^m u^n \phi) dx. \quad (7)$$

The moment matrix is given as:

$$\begin{pmatrix} 1 & M[x] & 0 \\ M[x] & M[xx] & -h/2 \\ 0 & -h/2 & M[-uu] \end{pmatrix} \quad (8)$$

Here we use the relations:

$$M[u][1] = \int \left(h \frac{d}{dx} \phi \right) \phi dx = 0.$$

$$M[u][u] = \int \left(h \frac{d}{dx} \phi \right) \phi \left(h \frac{d}{dx} \phi \right) dx = \int \phi \left(-h^2 \frac{d^2}{dx^2} \right) \phi dx.$$

$$M[u][x] = \int \left(h \frac{d}{dx} \phi \right) (x \phi) dx = \int \phi \left(-h \frac{d}{dx} \cdot x \right) \phi dx = -M[ux] = -M[xu] - h.$$

In order to see the necessity of the existence of $h/2$, let us check the quadratic form:

$$\int [(au + bx) \phi] [(au + bx) \phi] dx (\geq 0) \quad (9)$$

This quadratic form is represented by

$$\begin{aligned} & -a \cdot a M[uu] + b \cdot b \cdot M[xx] + a \cdot b \cdot (-M[ux] + M[xu]) \quad (10) \\ & = -a \cdot a \cdot M[uu] + b \cdot b \cdot M[xx] - a \cdot b \cdot h \\ & = (a, b) \begin{pmatrix} M[-uu] & -h/2 \\ -h/2 & M[xx] \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} (\geq 0) \end{aligned}$$

In this way, the semi-positive definiteness of the quadratic form is replaced by that of the matrix.

In fact, this is an approximation to compute in the finite dimension. The commutators generate an infinite number of terms, but we truncate the infinite dimensional matrix into the finite-dimensional one.

Semi-positive definiteness of the truncated moment matrix demands

$$\begin{aligned} M[xx] & \geq 0 \\ M[-uu] & \geq 0 \\ M[xx]M[-uu] - h^2/4 & \geq 0 \\ M[xx] - M[x]M[x] & \geq 0 \\ \det(M) & \geq 0 \end{aligned}$$

They are not the semi-positive definiteness of the moment matrix itself, but the semi-positiveness of the determinants of the minors taken on the diagonal.

With this condition, the optimum of $M[-uu] + M[xx]$ is obtained at $M[xx] = M[-uu] = 1/2h$. Let us solve this problem by Quantifier

Elimination. We use QEPCAD here[5]. The algorithm is the Cylindrical Algebraic Decomposition (CAD). It processes the polynomials in the given formula and transforms them into additional sets of polynomials, by projecting out the variables one by one. The whole space is divided into cells, the boundaries of which are represented by the generated polynomials, so that the polynomials in the given formula have the invariant signs in each cell. The cells have cylindrical shapes elongated along an axis, although the shapes of bottoms and the tops are arbitrary. One chooses the cells in which the given formula is satisfied, and the union of such cells gives the quantifier-free formula.

In the following computation we denote $M[xx]$, $M[x]$ and $M[uu]$ by MXX, M1X, MUU; We define the total energy by $E = -MUU + MXX$, and we define the Plank constant by H. We ask for the condition of the existence of real points of (MXX, M1X, MUU) in this semi-algebraic set:

```
-MPP >=0
and MXX >= 0
and -M1X^2 + MXX >= 0
and -MUU MXX - 1/4 H^2 >= 0
and M1X^2 MUU -MUU MXX - 1/4 H^2 >=0
and -MUU + MXX = E /\ H > 0
```

We execute the computation in order to process the prenex formula (composed of quantifiers and polynomials) and remove the quantifier with respect to (MXX, M1X, MUU) as follows.

```
=====
Quantifier Elimination
in
Elementary Algebra and Geometry
by
Partial Cylindrical Algebraic Decomposition

Version B 1.69, 16 Mar 2012

by
Hoon Hong
(hhong@math.ncsu.edu)
```

With contributions by: Christopher W. Brown, George E. Collins, Mark J. Encarnacion, Jeremy R. Johnson, Werner Krandick, Richard Liska, Scott McCallum, Nicolas Robidoux, and Stanly Steinberg

```
=====
Enter an informal description between '[' and ']':
[HARMONIC OSCILLATOR]
Enter a variable list:
(E,H,M1X,MUU,MXX)
Enter the number of free variables:
2
```

```

Enter a prenex formula:
(E M1X)(E MUU)(E MXX) [-MUU >=0 /\ MXX >= 0
/\ -M1X^2 + MXX >= 0
/\ -MUU MXX - 1/4 H^2 >= 0
/\ M1X^2 MUU -MUU MXX - 1/4 H^2 >=0
/\ -MUU + MXX = E /\ H > 0 ].

```

=====

```

Before Normalization >
go

```

```

Before Projection (MXX) >
go

```

```

Before Choice >
go

```

```

Before Solution >
go

```

An equivalent quantifier-free formula:

$H > 0 \wedge H - E \leq 0$

===== The End =====

3 Garbage collections, 11339612 Cells and 70 Arrays reclaimed, in 172 milliseconds.
3309571 Cells in AVAIL, 4000000 Cells in SPACE.

System time: 1623 milliseconds.

System time after the initialization: 1570 milliseconds.

The result states that the total energy E is equal to, or greater than H. If one utilizes extra formulae in the quantifier elimination, one can verify $M1X=0$ and $MXX=-MUU=H/2$. (Let us set $H = -MUU+MXX$; by quantifier elimination, we can simplify the following formulae without quantifier:

```

[-MUU >=0 /\ MXX >= 0 /\ -M1X^2 + MXX >= 0
/\ -MUU MXX - 1/4 H^2 >= 0
/\ M1X^2 MUU -MUU MXX - 1/4 H^2 >=0
/\ -MUU + MXX = H ]

```

Then the QEPCAD shall return the simple formulae for M1X, MUU and MXX.)

3 Oscillator Representation in Polynomial Optimization

We can utilize a more convenient representation which gives the exact solution at least to a quadratic polynomial. In the previous section we consider the example of the harmonic oscillator. The quantum harmonic oscillator is modeled by the annihilation and creation operator (b and a). They are given by our notation as follows.

$$a = -u + x \text{ (Creation)}. \quad (11)$$

$$b = u + x \text{ (Annihilation)}. \quad (12)$$

$$E = -u^2 + x^2 = a \cdot b + h. \quad (13)$$

Any powers of x^i are represented by the i -times product of $(a + b)$, so we can formulate the polynomial optimization of $u^2 + f(x)$ (which goes beyond the quadratic one) by the creation and the annihilation operator. The matrix might be represented in the eigenspace represented by the boson-numbers $|0\rangle, |1\rangle, \dots$

As a simple example, let us consider the quantum harmonic oscillator with the shift of origin.

$$E = -u^2 + (x - r)^2 = a \cdot b - r(a + b) + r^2. \quad (14)$$

The optimum is given by shifting the wavefunction of the lowest eigenvalue, from the center at 0 to that at r . The optimum wavefunction (centered at r) is expanded by the series of the eigensolutions (centered at 0), and the coefficients of the expansion are given by analytically. If we do not use the suitable eigenspace, the solution is an approximation by the truncation of the infinite series.

For simplicity, the moment matrix in this exemplary computation is simply set up by the two states $|\phi\rangle$ and $a|\phi\rangle$:

$$\begin{pmatrix} 1 & M_{1,a} \\ M_{a,1} & M_{a,a} \end{pmatrix} \quad (15)$$

In this matrix we see all PERSONA DRAMADICAE. We use the notations such as $M_{a,b} = \int (a\phi)(b\phi)dx$, $M[ab] = \int \phi([a \cdot b]\phi)dx$. In fact it follows that $M_{a,1} = M_{1,b} = M[b]$, $M_{1,a} = M_{1,a} = M[a]$, $M_{a,a} = M[ba]$. Furthermore we can see this:

$$M[a] - M[b] = -2h \int \phi(d\phi/dx)dx = 0. \quad (16)$$

The problem is stated as:

- Minimize $E = M[ba] + h - 2 \cdot r \cdot M[a] + r^2$,
- With the semi-positive definiteness condition of the momentum matrix, that is, $M[ba] - M[a]^2 \geq 0$.

This question is also solvable by the QEPCAD. The prenex formula is represented by

$$(\exists y)(\exists x)[y \geq x^2 \wedge y = -h + 2rx - r^2 + e].$$

This inquiry is to find the tangent line to the parabola, and the solution is given as

$$e - H \geq 0$$

Now we arrive at the exact optimum, without tackling the infinite dimensional series.

We can inquire in another way, with only one quantifier:

$$(\exists y) [y \geq x^2 \wedge y = -H + 2rx - r^2 + e].$$

The solution is

$$x^2 - 2rx + r^2 - e + H \leq 0$$

This implies $e \geq h + (x - r)^2$. So we conclude that $x = M[a] = r$ (the center point of the wavefunction) by the further optimization.

4 Conclusion

We have made a brief account of the “quantum polynomial optimization. It is summarized as

- For a variable x , one introduces the momentum u , and the Plank constant h , and the commutator $[u, x] = h$.
- The set of equations and inequalities are represented by the semi-definite problem of the moment matrices.
- The difference to the normal, classical polynomial optimization is the immutability of the order of the product of variables. $M[ux]$ and $M[xu]$ are not the same items, because of the commutator: $M[ux] = M[xu] + h$; this is the principal condition in order to set up a “quantum” computational scheme. In the limit of $H=0$, we return to the classical computation.
- In order to solve the problems, one can utilize numerical (as is done in the semi-definite problem) or symbolic method (as is in the quantifier elimination)

We know that the Ising model is one of the problems which might find its place in the polynomial optimization. An effective quantum algorithm for this model is the quantum annealing. In the quantum annealing, the quantum fluctuation is introduced rather by a thermodynamic way. One search over the parameter space with the aid of the fluctuation, and finally by quenching it, one arrives at the optimum[8, 9, 10, 11, 12, 13, 15, 16, 17]. Our formalism of quantum optimization goes on a different path. Its main composition comes from the quantum uncertainty, which might act as the fluctuation if one solves the problem by the numerical methods. The analysis of “classical” polynomial optimization from a quantum mechanical viewpoint would be an open problem.

Finally, we point out this: a polynomial set algebraically describes a geometrical object – which is the object of algebraic geometry, and the quantifier elimination is the fruit of this big tree. In our algorithm, we always corporate with geometrical objects through the algebraic idea. Here we dare to say: we arrive at the wave geometry, as a counterpart of Wave

Dynamics. Our wave geometry does not have the direct touch to the “wavefunction, but it tries to determine the moments (or the expectation values) in the framework of polynomial relations. And the moment problem is built on the measure theory, which, in our case, can be interpreted to be the square norm of the wavefunction. Here remains a problem: can we directly determine the measure μ which gives the optimum? In fact, the computation of wave function is the everyday work of theoretical physicists: in the materials science, the manifold of wavefunction can be computed with high accuracy (with the parameter system of the atomic arrangement), as one does in the first principles molecular dynamics or the molecular orbital method. These well-developed techniques in quantitative simulation seem to be the future resources of another algorithm in the quantum polynomial optimization.

References

- [1] D. S. Arnon, G. E. Collins, S. McCallum, “Cylindrical Algebraic Decomposition I: The Basic Algorithm” Purdue University, Computer Science Technical Reports, 82-427, (1982).
- [2] S. McCallum, “Solving Polynomial Strict Inequalities Using Cylindrical Algebraic Decomposition”, The computer journal, Vol. 36, No.5, 432-438
- [3] H. Hong, M. S. El-Din, “Variant Real Quantifier Elimination, Algorithm and Application”, preprint.
- [4] C. Chen, M. M. Maza, “Quantifier Elimination By Cylindrical Algebraic Decomposition Based on Regular Chains”, ISSAC-2014 ACM 978-1-4503-2501-1/14/07
- [5] <http://www.usna.edu/CS/qepcad/B/QEPCAD.html>
- [6] C.T.Abdallah, P.Dorato, R.Liska, S.Steinberg, W.Yang, “Applications of Quantifier Elimination Theory to Control Theory”, University of New Mexico, UNM Digital Repository, Electrical and Computer Engineering Technical Reports, 9-14-1995.
- [7] J.B.Lassere ”Global optimization with polynomials and the problem of moments”, SIAM Journal on Optimization, 11(2001), 796-817
- [8] D-Wave, An Introduction to Quantum Computing, D-Wave Style, QuAASI2016 Workshop, July 2016.
- [9] M M. Nevisi et al. Simulating a quantum annealer with GPU-based Monte Carlo algorithms, D-Wave, 2016.
- [10] E.Crossn, A.W.Harrow, Simulated Quantum Annealing Can Be Exponentially Faster then Classical Simulated Annealing, arXiv:1691.03030v2.
- [11] F.Keukart et al., Traffic flow optimization using a quantum annealer, arXiv:1708.01625v2.
- [12] Steve Adachi, Near-Term Application of Quantum Annealing, Lockheed Martin Corporation, 2016.

- [13] Andrew Lucas, Ising formulations of many IP problems, arXiv:1302.5843v3.
- [14] Dan Padilha, Solving NP-Hard Problems on an Adiabatic Quantum Computer, Thesis, in UNSW AUSTRALIA, 2014.
- [15] Elliot Snow-Kropka, COMPILING PROGRAMS FOR ADIABATIC COMPUTER, Dalhousie University, 2014.
- [16] T. Kadowaki and H. Nishimori, "Quantum annealing in the transverse Ising model" Phys. Rev. E 58, 5355 (1998)
- [17] A. B. Finilla, M. A. Gomez, C. Sebenik and D. J. Doll, "Quantum annealing: A new method for minimizing multidimensional functions" Chem. Phys. Lett. 219, 343 (1994)