Testing systems of real quadratic equations for (approximate) solutions

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Solving systems of polynomial equations

Given a system of real polynomial equations

$$p_i(x_1, \ldots, x_n) = 0 \quad \text{for} \quad i = 1, \ldots, m,$$

how hard is it to

a) decide if there is a solution

b) if there is a solution, to find one

c) describe the set of all solutions?

Answer: Generally speaking, pretty hard.
A good reference: S. Basu, R. Pollack, and M.-F. Roy, Algorithms in Real Algebraic Geometry. Second edition, Algorithms and Computation in Mathematics, **10** Springer-Verlag, Berlin, 2006. x+662.

Solving systems of polynomial equations

Two main parameters: the number n of variables and the largest degree d of the equation. Any number of equations can be reduced to one by doubling the degree:

$$p_i\left(x_1, \ldots, x_n\right) = 0 \quad \text{for} \quad i = 1, \ldots, m$$

$$\Updownarrow$$

$$\sum_{i=1}^{m} p_i^2\left(x_1, \ldots, x_n\right) = 0.$$

The complexity of
a) deciding whether there is a solution is roughly $d^{O(n)}$.

b) What does it even mean, to find a solution? One possibility is to use the *Thom encoding* of a real algebraic number: the minimal polynomial and signs of all its derivatives at the desired root. With that, the complexity is roughly $d^{O(n)}$.

c) The complexity of describing the set of solutions can be doubly exponential in n (computing Betti numbers). The problem can also be undecidable (homotopy type).

Systems of quadratic equations

If $d = 1$, we have a system of linear equations which can be solved in $O(n^3)$ time by Gaussian elimination.

What if $d = 2$? Quadratic equations are special.
First, any system of polynomial equations can be reduced to a system quadratic via substitutions of the type

$$y_{ij} := x_i x_j.$$

Second, some systems of quadratic equations naturally arise in applied problems.

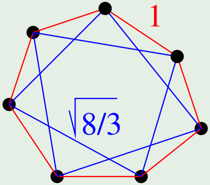
Example (Distance Geometry, Computational Chemistry)

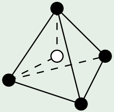
Question: Are there seven points $v_1, v_2, v_3, v_4, v_5, v_7$ in $\mathbb{R}^3$ such that

$$\|v_{(i+1) \mod 7} - v_i\| = 1 \quad \text{and} \quad \|v_{(i+2) \mod 7} - v_i\| = \sqrt{\frac{8}{3}}$$

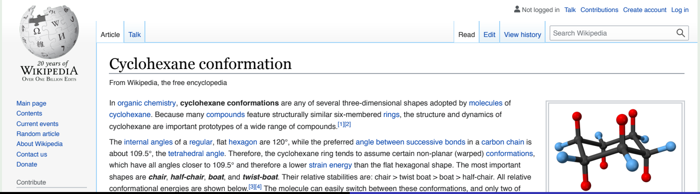
for $i = 1, \ldots, 7$?

Example (Distance Geometry, Computational Chemistry)





The same question for six points.
Check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Cyclohexane conformation

From Wikipedia, the free encyclopedia

In organic chemistry, **cyclohexane conformations** are any of several three-dimensional shapes adopted by molecules of cyclohexane. Because many compounds feature structurally similar six-membered rings, the structure and dynamics of cyclohexane are important prototypes of a wide range of compounds.[1][2]

The internal angles of a regular, flat hexagon are 120°, while the preferred angle between successive bonds in a carbon chain is about 109.5°, the tetrahedral angle. Therefore, the cyclohexane ring tends to assume certain non-planar (warped) conformations, which have all angles closer to 109.5° and therefore a lower strain energy than the flat hexagonal shape. The most important shapes are ***chair***, ***half-chair***, ***boat***, and ***twist-boat***. Their relative stabilities are: chair > twist boat > boat > half-chair. All relative conformational energies are shown below.[3][4] The molecule can easily switch between these conformations, and only two of

Systems of quadratic equations

Another example includes "trust region subproblems", see D. Bienstock, A note on polynomial solvability of the CDT problem, *SIAM J. Optim.* **26** (2016), no. 1, 488–498.

Results: A system of k quadratic equations in n real variables can be solved (questions a) and b) answered) in $n^{O(k)}$ time. In particular, if k is fixed in advance, in polynomial time.

Testing whether a system of homogeneous quadratic equations has a non-trivial solution: A. Barvinok, Feasibility testing for systems of real quadratic equations, *Discrete Comput. Geom.* **10** (1993), no. 1, 1–13.
In the whole generality: D. Grigoriev and D.V. Pasechnik, Polynomial-time computing over quadratic maps. I. Sampling in real algebraic sets. *Comput. Complexity* **14** (2005), no. 1, 20–52.

Systems of quadratic equations

For the description of the set of solutions (question c)), see S. Basu, D.V. Pasechnik, and M.-F. Roy, Bounding the Betti numbers and computing the Euler-Poincaré characteristic of semi-algebraic sets defined by partly quadratic systems of polynomials, *J. Eur. Math. Soc. (JEMS)* **12** (2010), no. 2, 529–553.

Here is an idea for systems of homogeneous quadratic equations. This is *not* how it has been done, but it shows a useful underlying algebraic structure.

Let

$$q_i(x) = \langle x, Q_i x \rangle \quad \text{for} \quad i = 1, \ldots, k,$$

where Q_i are $n \times n$ symmetric matrices and $\langle \cdot, \cdot \rangle$ is the standard inner product in $\mathbb{R}^n$.

Let

$$\mathbb{S}^{n-1} = \{x \in \mathbb{R}^n : \quad \|x\| = 1\}$$

be the unit sphere endowed with the rotation invariant Borel probability measure μ.

The generating function

Theorem

In a neighborhood of $z_1 = \ldots = z_k = 0$, *we have*

$$\det^{-\frac{1}{2}}\left(I - \sum_{i=1}^{k} z_i Q_i\right) = \sum_{m_1,\ldots,m_k \geq 0} a_{m_1,\ldots,m_k} z_1^{m_1} \cdots z_k^{m_k},$$

where

$$a_{m_1,\ldots,m_k} = \frac{\Gamma\left(m_1 + \ldots + m_k + \frac{n}{2}\right)}{m_1! \cdots m_k! \Gamma\left(\frac{n}{2}\right)} \times \int_{\mathbb{S}^{n-1}} q_1^{m_1}(x) \cdots q_k^{m_k}(x) \; d\mu(x).$$

The generating function

Proof: We note that for

$$q(x) = \langle x, Q_x \rangle,$$

in a neighborhood of $z = 0$, we have

$$\frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{zq(x)/2} e^{-\|x\|^2/2} \ dx = \det^{-\frac{1}{2}} (I - zQ) \, .$$

Consequently,

$$\frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{(z_1 q_1(x) + \ldots + z_k q_k(x))/2} e^{-\|x\|^2/2} \ dx = \det^{-\frac{1}{2}} \left(I - \sum_{i=1}^{k} z_i Q_i \right) .$$

Expanding into the Taylor series in a neighborhood of $z_1 = \ldots = z_k = 0$, we get

$$\det^{-\frac{1}{2}} \left(I - \sum_{i=1}^{k} z_i Q_i \right) = \sum_{m_1, \ldots, m_k \geq 0} b_{m_1, \ldots, m_k} z_1^{m_1} \cdots z_k^{m_k},$$

The generating function

where

$$b_{m_1,\ldots,m_k} = \frac{1}{2^{m_1+\ldots+m_k} m_1! \cdots m_k!} \times \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} q_1^{m_1}(x) \cdots q_k^{m_k}(x) e^{-\|x\|^2/2} \, dx.$$

For a homogeneous polynomial $F(x)$ of degree $2m = 2m_1 + \ldots + 2m_k$, we have

$$\frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} F(x) e^{-\|x\|^2/2} \, dx = \frac{2^m \Gamma\left(m + \frac{n}{2}\right)}{\Gamma\left(\frac{n}{2}\right)} \int_{\mathbb{S}^{n-1}} F(x) e^{-\|x\|^2/2} \, d\mu(x).$$

$\square$

The generating function

Corollary: The integral

$$\int_{\mathbb{S}^{n-1}} q_1^{m_1}(x) \cdots q_k^{m_k}(x) \ d\mu(x)$$

can be computed in $n^{O(1)} \left(m_1 + \ldots + m_k\right)^{O(k)}$ time.

If $q_1, \ldots, q_k : \mathbb{R} \longrightarrow \mathbb{R}$ are positive semidefinite, then for large m,

$$\left(\int_{\mathbb{S}^{n-1}} \left(q_1(x) \ldots q_k(x)\right)^m \ d\mu(x) \right)^{1/m} \approx \max_{x \in \mathbb{S}^{n-1}} q_1(x) \cdots q_k(x).$$

In fact, to approximate the maximum within relative error ϵ, we can choose $m = O\left(\frac{n+km}{\epsilon}\right)$.
Remark: If k is fixed in advance, we can do it in polynomial time *exactly*.

The generating function

Connection to feasibility: Given quadratic forms $q_1, \ldots, q_k : \mathbb{R}^n \longrightarrow \mathbb{R}$, let us define

$$q_i^+ = \|x\|^2 + \epsilon q_i(x) \quad \text{and} \quad q_i^- = \|x\|^2 - \epsilon q_i(x) \quad \text{for} \quad i = 1, \ldots, k$$

and some small $\epsilon > 0$.
Then

$$\begin{aligned} &\max_{x \in \mathbb{S}^{n-1}} q_1^+(x) \cdots q_k^+(x) q_1^-(x) \cdots q_k^-(x) \\ = &\max_{x \in \mathbb{S}^{n-1}} \left(1 - \epsilon^2 q_1^2(x)\right) \cdots \left(1 - \epsilon^2 q_k^2(x)\right) \\ = &\begin{cases} 1 & \text{if} \quad q_i(x) = 0 \quad \text{for some } x \in \mathbb{S}^{n-1} \quad \text{and all } i \\ < 1 & \text{otherwise.} \end{cases} \end{aligned}$$

Computing the integral may allow us to estimate the volume of the set of solutions.

Partition function

What can we do if the number k of equations grows? Here is the idea: Choose a δ-shaped function $F \longrightarrow [0,1]$, such that

$$F(y) = \begin{cases} 1 & \text{if} \quad y = 0 \\ < 1 & \text{if} \quad y \neq 0 \end{cases}$$

and try to compute

$$\frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} F\left(q_1(x)\right) \cdots F\left(q_k(x)\right) e^{-\|x\|^2/2} \, dx.$$

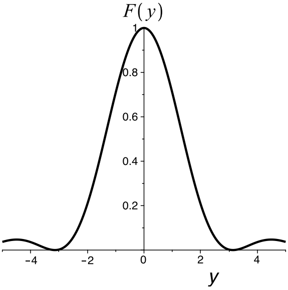
Note that the standard Gaussian probability measure with density $(2\pi)^{-n/2} e^{-\|x\|^2/2}$ is concentrated around $\|x\| = \sqrt{n}$, that is,

$$\mathbf{Prob}\left\{x: \ (1-\epsilon)n \leq \|x\|^2 \leq \frac{n}{1-\epsilon}\right\} \geq 1 - 2e^{-\epsilon^2 n/4} \quad \text{for} \quad 0 < \epsilon < 1.$$

Partition function

Hence if the integral is large, then there are many x with most $q_i(x) \approx 0$ and if the integral is small, then there are few such x's. The sharper F is peaked at 0, the better we can do. We choose

$$F(y) = \frac{\sin^2 y}{y^2}.$$



Partition function

Main result: There is an absolute constant $\gamma > 0$ (one can choose $\gamma = 0.09$) such that the following holds. Let $q_i : \mathbb{R}^n \longrightarrow \mathbb{R}$, $i = 1, \ldots, k$, be quadratic forms in n real variables $x_1, \ldots, x_n$, such that each q_i depends on at most r variables among $x_1, \ldots, x_n$, has common variables with at most $r - 1$ other forms q_j and satisfies

$$|q_i(x)| \leq \frac{\gamma \|x\|^2}{r} \quad \text{for} \quad i = 1, \ldots, k.$$

Then, for any $0 < \epsilon < 1$, one can compute the value of

$$\frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-\|x\|^2/2} \prod_{i=1}^{k} \frac{\sin^2 q_i(x)}{q_i^2(x)} \, dx$$

within relative error ϵ in quasi-polynomial $(m+n)^{O(\ln(m+n) - \ln \epsilon)}$ time.

Partition function

Suppose that $r = n$ (no restriction on sparseness) and consider the following asymptotic regime:

$$n \longrightarrow \infty, \quad n = km \quad \text{where} \quad m \gg \ln n.$$

Let

$$X = \left\{ x \in \mathbb{R}^n : \quad q_i(x) = 0 \quad \text{for} \quad i = 1, \ldots, k \right\}.$$

We say that "there are many solution" if

$$\textbf{Prob}\left\{ \operatorname{dist}(x, X) \ \leq \ n^{-\gamma} \right\} \ \geq \ n^{-O(k)}$$

for some constant $\gamma > 2$.

We say that the system is "far from having a solution", if for all $x \in \mathbb{R}^n$ such that $\|x\| = \sqrt{n}$, for at least δk of the forms q_i we have $|q_i(x)| > \beta$ for some constants $\delta > 0$ and $\beta > 0$.

Let us copy each form q_i exactly m times in the integral. Then, for systems having "many solutions" the value of the integral is $n^{-O(k)}$, while for systems that are "far from having a solution", the value is $2^{-\Omega(n)}$, so we can tell them apart.

Partition function

Theorem

There is an absolute constant $0 < \gamma_0 < 0.25$ *(one can choose* $\gamma_0 = 0.1$*) such that the following holds. Let* $q_i : \mathbb{R}^n \longrightarrow \mathbb{R}$, $i = 1, \ldots, k$, *be quadratic forms in* n *real variables* $x_1, \ldots, x_n$, *such that each* q_i *depends on at most* r *variables among* $x_1, \ldots, x_n$, *has common variables with at most* $r - 1$ *other forms* q_j *and satisfies*

$$|q_i(x)| \leq \frac{\gamma_0 \|x\|^2}{r} \quad \text{for} \quad i = 1, \ldots, k.$$

Let

$$\phi(z) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-\|x\|^2/2} \prod_{i=1}^{k} \frac{\sin^2 z q_i(x)}{z^2 q_i^2(x)} \, dx.$$

Then for every $z \in \mathbb{C}$ *such that* $|z| \leq 1$, *we have*

$$(1 - 4\gamma_0)^{-n/2} \geq |\phi(z)| \geq 2^{-k/2} (1 + 4\gamma_0)^{-n/2}.$$

Interpolation Lemma

Lemma

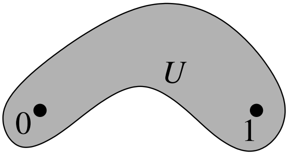
Let $U \subset \mathbb{C}$ be a connected open set containing 0 and 1. Then there is a constant $\gamma = \gamma(U) > 0$ such that the following holds: If

$$g(z) = \sum_{k=0}^{n} c_k z^k, \quad n \geq 2$$

is a polynomial such that $g(z) \neq 0$ for all $z \in U$ then, for any $0 < \epsilon < 1$, the value of $g(1)$, up to relative error ϵ, is determined by the coefficients c_k with $k \leq \gamma (\ln n - \ln \epsilon)$ and can be computed in $n^{O(1)}$ time from those coefficients.

Remark: We say that $w_1 \neq 0$ approximates $w_2 \neq 0$ within relative error ϵ if we can write $w_1 = e^{z_1}$ and $w_2 = e^{z_2}$ with $|z_1 - z_2| \leq \epsilon$.

Interpolation Lemma



If

$$g(z)=\sum_{k=0}^{n} c_k z^k$$

and $g(z) \neq 0$ in an open connected set containing 0 and 1, then, up to relative error $0<\epsilon<1$, the value of $g(1)$ is determined by only $O(\ln n - \ln \epsilon)$ lowest coefficients of g.

Interpolation Lemma: sketch of proof

So we have $g(z) = c_0 + c_1 z + \ldots + c_n z^n$ and $g(z) \neq 0$ for $z \in U$.
Special Case:

$$U = \{z : \ |z| < \beta\} \quad \text{for some} \quad \beta > 1.$$

Consider $f(z) = \ln g(z)$ and its Taylor polynomial at $z = 0$:

$$T_m(z) = f(0) + \sum_{k=1}^{m} \frac{f^{(k)}(0)}{k!} z^k.$$

Claim 1:

$$|f(1) - T_m(1)| \ \leq \ \frac{n}{\beta^m(\beta - 1)(m + 1)}.$$

Claim 2: $f^{(k)}(0)$ is a function of $c_0, \ldots, c_k$.

Interpolation Lemma: sketch of proof

Proof of Claim 1: We have

$$g(z) = g(0) \prod_{i=1}^{n} \left(1 - \frac{z}{\alpha_i}\right) \quad \text{where} \quad |\alpha_i| \geq \beta \quad \text{for} \quad i = 1, \ldots, n.$$

Hence

$$f(z) = f(0) + \sum_{i=1}^{n} \ln\left(1 - \frac{z}{\alpha_i}\right).$$

Now, if $|z| \leq 1$, we have

$$\ln\left(1 - \frac{z}{\alpha_i}\right) = -\sum_{k=1}^{m} \frac{z^k}{k\alpha_i^k} + \eta_i \quad \text{where}$$

$$|\eta_i| = \left| -\sum_{k=m+1}^{\infty} \frac{1}{k\alpha_i^k} \right| \leq \frac{1}{\beta^m(\beta - 1)(m+1)}.$$

Interpolation Lemma: sketch of proof

Proof of Claim 2: We have $f(z) = \ln g(z)$, so

$$f'(z) = \frac{g'(z)}{g(z)} \Longrightarrow g'(z) = f'(z)g(z)$$

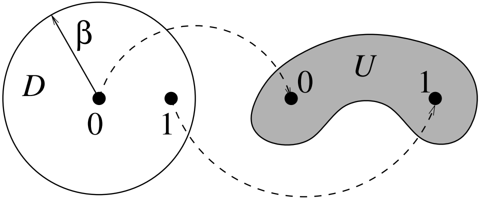
$$\Longrightarrow g^{(k)}(0) = \sum_{j=0}^{k-1} \binom{k-1}{j} f^{(k-j)}(0) g^{(j)}(0),$$

which is a triangular system of linear equations in $f^{(k)}(0)$ with $g(0) \neq 0$ on the diagonal.

General case: Construct an auxiliary disc

$$D = \{z : \ |z| < \beta\} \quad \text{for some} \quad \beta > 1$$

and a polynomial $\phi(z)$ such that $\phi(0) = 0$, $\phi(1) = 1$ and $\phi(D) \subset U$.



Interpolation Lemma: sketch of proof

Consider the composition

$$p(z) = g(\phi(z)).$$

Then $p(z) \neq 0$ for $z \in D$ and, by the special case, to compute $p(1) = g(1)$ within relative error ϵ, we need to access $O(\ln \deg p - \ln \epsilon)$ lowest coefficients of $p(z)$.

Since $\phi(0) = 0$, we need to access $O(\ln \deg g - \ln \epsilon)$ lowest coefficients of $g(z)$.