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Exploring Model Energy and Geometry Surfaces Using Sum of Squares Decompositions

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Abstract: The difficulty in exploring potential energy surfaces, which are nonconvex, stems from the presence of many local minima, typically separated by high barriers and often disconnected in configurational space. We obtain the global minimum on model potential energy surfaces without sampling any minima a priori. Instead, a different problem is derived, which is convex and hence easy to solve, but which is guaranteed to either have the same solution or to be a lower bound to the true solution. A systematic way for improving the latter solutions is also given. Because many nonconvex problems are projections of higher dimensional convex problems, Parrilo has recently shown that by obtaining a sum of squares decomposition of the original problem, which can be subsequently transformed to a semidefinite program, a large class of nonconvex problems can be solved efficiently. The semidefinite duality formulation also provides a proof that the global minimum of the energy surface has either been found exactly or has been bounded from below. It additionally provides physical insight into the problem through a geometric interpretation. The sum of squares polynomial representation of the potential energy surface may further reveal information about the nature of the potential energy surface. We demonstrate the applicability of this approach to low-dimensional potential energy landscapes and discuss its merits and shortcomings. We further show how to apply it to geometric problems by obtaining the exact distance of closest approach of anisotropic particles. Efficient molecular dynamics simulations of mixtures of ellipsoids are illustrated.

Introduction

The thermodynamic and kinetic properties of molecular assemblies in chemistry, physics, and biology are often linked to their underlying potential energy surface (PES).[3−5] Even in the simplest cases, exploring potential energy surfaces or even just important regions becomes computationally demanding very rapidly. This is primarily due to the nonconvexity of the underlying potential energy surface. A key step in understanding thermodynamic properties of systems as diverse as nanoscale clusters, proteins, and lipid membranes is the identification of the global minimum. Definite proof typically requires exhaustive sampling of every other minimum in configurational space, a prohibitive task given that the number of local minima on the surface typically grows exponentially with the number of particles in the system.[3,6]

A series of approaches has been proposed to tackle this problem with various degrees of success. Most stochastic methods are variations of the Monte Carlo (MC) method with additional steps introduced to aid barrier crossing between local minima,[7−9] although genetic-based algorithms[10,11] have also been used. Deterministic approaches usually derive from global optimization techniques[12−14] or molecular dynamics.[15] Methods that deform the potential in order to eliminate local minima include hypersurface deformation techniques,[16] such as the distance scaling method[17] and the very successful MC basin-hopping method.[18]

A commonality in most methods is that they require extensive sampling of the local minima of the potential energy surface itself prior to finding the global minimum.

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Not only is this process time-consuming, sensitive to initial conditions, and susceptible to trapping due to high barriers, it crucially provides no proof that a given point on the PES is indeed the global minimum other than that it is the lowest visited to date by the algorithm. It is usually not possible to evaluate how close such a minimum would be to the correct answer to further guide the search. Furthermore, all methods rely to a greater or lesser extent on the topology of the PES being "well behaved" in the sense that the global minimum is connected to other low lying local minima so that it can be reached from them.

A complementary strategy is to abandon the detailed atomic potentials and replace them instead with simpler models. Such coarse-grained models have a rich history and have had successes in recent years in the modeling of both proteins and lipid membranes (for recent reviews, see, for example, refs 19 and 20). These vary from simple to more detailed and have been successful in predicting structural properties as well as thermodynamic phase behavior. The successes of these models seem to share in common an accurate representation of the architecture and shape of the protein and/or lipid. Evidence is accumulating that shows that once this is well represented many of the properties of the units and their assemblies can be captured especially when their mechanical properties play a role.[21,22] At the same time, the shape of the units is often anisotropic. This may be more obvious in lipid molecules, but it turns out to be often the case in proteins as well. In describing such shapes, anisotropic coarse-grained potentials have an advantage over spherical ones in that they capture the interactions properly without introducing artificial long-range potentials or other schemes. Anisotropic potentials have a long history,[23−27] but their use has often been hampered by computing the distance of closest approach correctly and efficiently, a cumbersome task often solved by brute force. It would hence be desirable to capture the shape properties correctly and at the same time have a systematic way to check how close the approximation is from the true answer, that is to have an estimate of the error in comparison with the true problem.

Here we outline a different strategy to address such questions arising from exploring complex (nonconvex) landscapes. A key idea is that instead of sampling the underlying nonconvex function, we approach it from below. A different problem is sought, whose *solution* coincides with the solution of the problem we are interested in. For this approach to be successful, it must be coupled both with a rigorous and systematic way to find such problems that can be easily solved and with a way to evaluate how close the two solutions are. An important mathematical concept that provides such a link is that many nonconvex problems turn out to be projections of higher dimensional convex problems. The great advantage of the latter is that they are efficiently solved since the local minimum is the global minimum. Furthermore, they also allow for physical insight into the system because they possess duality properties. This duality provides geometric interpretations to the original problem and allows us to monitor how close the solution of the derived problem is to the true solution we are seeking. This is coupled with a systematic way to improve on our nonexact solutions. The combination of these features makes this approach appealing because physical insight is revealed about the system while seeking the solution itself.

The approach, originally developed independently by Parrilo[1,2] and Lasserre[28] by drawing together results from two seemingly unconnected fields, algebraic geometry and convex optimization, is based on obtaining a sum of squares (SOS) representation of the original problem. They observed that many nonconvex problems can be represented by finding a suitable globally non-negative polynomial function which is an accurate representation of the nonconvex problem in Euclidean space in which the problem is originally defined. Parrilo and Lasserre realized that although this function must by necessity be nonconvex in the Euclidean space, if well chosen, it may be convex in the vector space of monomials which form a basis for the polynomial. The obvious difficulty is how to choose such a function. Searching the entire space of globally non-negative polynomials is an impossible task; however, the space of SOS functions forms a significant subset of this space. A SOS polynomial is defined as any polynomial that has the following decomposition

$$f^{\mathrm{SOS}} = \sum_{i=1}^{r} (p_i(\mathbf{x}))^2 \geq 0 \qquad (1)$$

where the $p_i(\mathbf{x})$ are polynomials. Suitable subsets of the space of SOS functions can now be found because this search turns out to be convex in the coefficient space of the function and hence efficiently computed using modern convex optimization techniques such as semidefinite programming (SDP). An interesting question is what happens if a suitable SOS cannot be found. The answer, based upon an important theorem in algebraic geometry,[2] is that a lower bound will always be produced in a minimization problem of the type described here, and furthermore this bound can be improved asymptotically to the exact minimum by increasing the complexity of the SOS polynomial in a specific and systematic manner. A central idea is the systematic lifting of a polynomial function in its *coefficient* space (rather than its variables) to a SOS function.

Here we apply this approach in two different but important problems in molecular applications. First, in section II we give the main concepts of the theory and its relation to physical observables by showing how to locate the global minimum in a complex landscape without sampling other minima in configurational space. As a result, it is independent of initial conditions and of any requirement that the minimum be closely related to any other. Either the exact result is found together with a proof, or a lower bound is obtained. In no case is the original function deformed. In the Appendix, we show how to use the method, both in theory and in practice, to obtain a SOS decomposition. By going through each of the steps of an example, we show how the method is implemented and comment on possible choices available. In section III we apply it to a series of low-dimensional examples that exemplifies a range of difficulties encountered in complex landscape problems and which highlight the different capabilities and versatility of this method. In section II.B we show how the SOS approach can be further used to

elegantly and efficiently solve exactly the problem of distance of closest approach of anisotropic particles and interactions. We further show how this can potentially lead to efficient MD simulations by giving an illustration with ellipsoid particles. In section IV we discuss the advantages and shortcomings of the approach and outline future directions.

II. Theory

A. SOS Decompositions. A different approach to locating the global minimum U^* of a multivariable polynomial, $U(x_i,...x_n) \equiv U$ of degree d is to look for the largest real number λ such that $U - \lambda$ remains non-negative everywhere:

$$U(\mathbf{x}) - \lambda \geq 0, \quad \lambda \in \mathbf{R} \quad \forall \mathbf{x} \in \mathbf{R}^n \tag{2}$$

If we could find the largest λ for which this is true, then we would have found the global minimum of $U(\mathbf{x})$. In this formulation, this problem is at least as difficult to solve as the original problem of locating the global minimum. However, if instead of insisting that the above condition be satisfied, we ask instead that $U(\mathbf{x}) - \lambda$ can be decomposed as a SOS,[1,2,29] that is replace eq 2 with the following condition

$$U(\mathbf{x}) - \lambda \geq f^{\mathrm{SOS}}, \quad \lambda \in \mathbf{R}, \quad \forall \mathbf{x} \in \mathbf{R}^n \tag{3}$$

then the problem becomes considerably easier to solve. Using the definition of eq 1 for a SOS function leads to

$$U - \lambda = \sum_{i=1}^{r} p_i^2 \geq 0 \tag{4}$$

where p_i are polynomial functions of degree $d/2$ in the variables of U.

Being a SOS is a sufficient condition for a function to be non-negative, although not a necessary one. However, the set of SOS polynomials forms a large and significant subset of the set of non-negative polynomials and for reasonably low degree polynomials they are nearly identical. Therefore replacing the non-negativity condition of eq 2 with the SOS condition of eq 4 is a relatively minor relaxation to the problem. When the optimal λ is not the exact global minimum of the function, then it is a lower bound on the global minimum. In fact in a case where only a lower bound is obtained it is possible to improve that bound asymptotically toward the global minimum by increasing the dimensionality and/or degree of the sum of squares relaxation as we will show later. Indeed, both λ and f^{SOS} are guaranteed to bound the original problem from below.[29]

The next step then becomes obtaining the SOS decomposition together with the optimal λ that gives the closest answer to our original problem. The problem becomes tractable by additionally exploiting the theorem[1] that for globally non-negative polynomial functions, there exists a positive semidefinite matrix, $Q \geq 0$, such that

$$U(\mathbf{x}) - \lambda = f^{\mathrm{SOS}} = z(x)^T Q z(x), \quad \text{where } Q \geq 0 \tag{5}$$

so that the problem of eq 4 can now be formulated algebraically. $z(x)$ is the vector of monomials of U with degree less than or equal to half the degree of U and provides a basis for the SOS function decomposition. Monomials are the individual terms (without the coefficients) which when summed together make up a polynomial. Assuming the largest degree monomial in a polynomial is of even degree $2d$, then the monomials which are needed in the basis vector z are all monomials on x_1, ..., x_n of degree $\leq d$. It can be seen that the size of the monomial vector is therefore at most $\binom{n+d}{d}$. Since the variables in z are not algebraically independent, the matrix Q is not unique and may be positive semidefinite in some representations but not in others. The problem now becomes a search for a symmetric positive semidefinite matrix Q that satisfies the constraints imposed by eq 5. Note that the original nonconvex problem in the variables of U has been mapped to a different problem, namely obtaining the polynomial coefficients of the SOS representation, which is equivalent to obtaining the matrix elements of Q, while Q remains positive semidefinite and λ is optimal.

Formally the SOS optimization problem can then be written as

$$\begin{aligned} &\text{Max}: \ \lambda \\ &\text{Subject to}: \ Q \geq 0 \\ &\qquad \mathbf{Tr}(A_i Q) = b_i \ \forall i = 1, ..., m \end{aligned} \tag{6}$$

where b_i are the coefficients of the energy function $U - \lambda$, and the linear constraints on the components of Q are to ensure that the relevant entries in Q sum up to the coefficients of the polynomial. A concrete example of how the A_is appear is given explicitly in the Appendix.

B. SDP and Duality. It turns out that eq 6 is in the form of a primal SDP. SDPs[30,31] are a class of optimization problems over positive definite matrices solvable by polynomial time algorithms such as the very successful primal-dual interior point methods.[32,33] Such methods compute the optimal solution as well as provide certificates (proofs) of optimality. These certificates are based upon a duality theory in which two problems are solved simultaneously. The dual problem solution provides a lower bound on the primal problem. The difference between the primal and dual solutions, referred to as the duality gap, proves whether an exact solution has been found or provides the lower bound to the solution.

We have shown how the original polynomial minimization can be recast as the SDP given by eq 6. In the mathematical community the focus is typically on the primal, with the dual only used to provide the duality gap. However, as we show here there is relevant and interesting physics in the dual problem as well. In our case, the primal problem gives the lower bound to the global minimum as well as the SOS decomposition, while the dual provides the location of this bound in the configurational space.

What has been described so far can be regarded as the primal form of a SOS optimization, in which we have sought to bound the global minimum from below and hopefully exactly. In this primal form the basis has been the monomials that define the polynomial and the variables in looking for the sum of squares decomposition have been the coefficients.

There is also a corresponding dual form of SOS optimization. One way to consider the dual problem is that the basis is now a vector of coefficients and the variables are the values of the monomials. The new variables form the matrix $Y := zz^T$. The effect of this is that if sufficient monomials have been included in z the convex representation of the function is obtained and the coordinates of the global minimum can be found by minimization. Once a solution is obtained, it is possible to confirm if it is correct by verifying whether it is of rank 1.

Both the primal and the dual SOS optimization problems are exactly primal and dual semidefinite programs, respectively, and may be solved using polynomial time primal-dual interior point methods. This latter problem, although in higher dimensions, is now convex and amenable to efficient solutions by SDP. Additionally, the minimization of the potential is carried out concurrently with the search for the SOS coefficients. The theoretical elegance of this methodology coupled with efficient computational techniques allows for SOS decompositions to be found in polynomial time (as long as either the degree of the polynomial or the number of variables are fixed) and additionally provides the proof that the result is indeed a lower bound to the global minimum. If the answer is not exact, then a lower and upper bound on the true solution is known.

C. Convexity and Duality. Duality appears in many places in chemical physics, albeit without this name. It is intimately connected with convexity.[34] Multidimensional convex functions obey a range of useful properties, one of which is that at each point there is at least one hyperplane tangent to the graph, whose slope is the derivative of that function. In fact, this plane belongs to a family of planes that separate the entire configurational space in two parts, below and above the function. Convexity ensures that they never cross the function in more than one point. To demonstrate how duality is related to this, we restrict ourselves to a one-dimensional parabola $f(x) = x^2$, but the argument is completely general. The separating planes now become straight lines (Figure 1). There is a set of lines with slope y which lie below the parabola as long as $yx - d \leq x^2$ where d is the depth. The line will touch tangentially the parabola when $d = 1/4y^2$. Each point on the parabola can be represented as a line which touches the parabola with different slopes y. The envelope of these lines reproduces the parabola itself. In fact, by looking for the maximum slope y, we obtain simultaneously $f(x)$. This is in fact what the Legendre transforms do in thermodynamics where, for example, the Gibbs and Helmholtz free energy are coupled with pressure and volume, respectively. This interpretation was already recognized by Tisza.[35] The dual emphasizes the geometric interpretation of the problem, and in that sense its variables can be interpreted as generalized Lagrange multipliers. It further clarifies how we can obtain information about a function by looking *outside* and bounding it externally from below.

D. Different SOS Representations − Beyond Simple Functions. In many cases what makes finding the global minimum energy configuration difficult is as much related to the constraints imposed on the system as to the energy

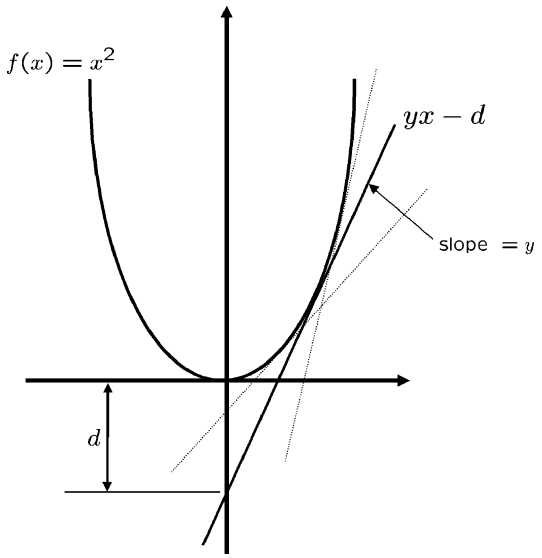

Figure 1. How convexity and duality are related. A set of lines with slope y lie below the parabola $f(x) = x^2$, as long as $yx - d \leq x^2$ where d is the depth. The line will touch tangentially the parabola when $d = 1/4y^2$. Each point on the parabola can be represented as a line which touches the parabola with different slopes y. The envelope of these lines reproduces the parabola itself. In fact, by looking for the maximum slope y, we obtain simultaneously $f(x)$. The relationship between convexity and duality appears in many places in chemical physics. An example of such a relationship are the Legendre transforms in thermodynamics.

surface itself. In these cases it is necessary to include such constraints in the initial statement of the optimization problem. We shall call these constraints necessary constraints. There is also another type of constraint that is often used in optimization, called redundant constraints. These are constraints which repeat what is already stated in another constraint in the problem statement. Although appearing useless at first glance these play a very important role in duality theory in that they bring the lower bound produced by a dual problem closer to the exact solution. By adding these constraints which appear useless in the primal form of the problem, additional variables are added in the dual (lifting) which allows a better bound to be found on the primal objective function.

Once again the analogy carries to SOS optimization. Additional constraints which initially may have appeared to add complexity to the problem allow the formation of progressively better SOS representations which although being higher in dimension, form better representations of the original function when projected back to the original space. Given a problem

$$\begin{aligned} &\min: U(\mathrm{x}) \\ &\text{subject to}: g_i(\mathrm{x}) \geq 0 \; i = 1, ..., m \end{aligned} \tag{7}$$

we can recast this problem as the following SOS problem

$$\begin{aligned} &\max: \lambda \\ &\text{subject to}: U(\mathrm{x}) - \lambda + \sum_{i=1}^{m} p_i(x) g_i(\mathrm{x}) \geq 0 \end{aligned} \tag{8}$$

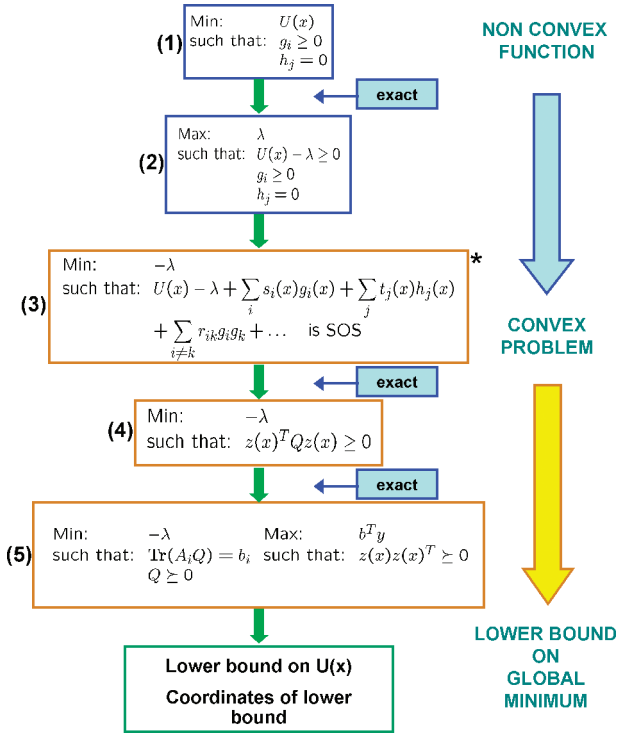

Figure 2. Schematic flowchart of a SOS optimization. The original global energy minimization problem is reformulated in a series of steps: (1) a polynomial optimization including any constraints is transformed to (2) a maximization of a real number λ which will keep the function non-negative. A sufficient but not necessary condition for this to be true is that the function is a SOS, so the problem is rewritten as (3). The constraints can be incorporated as well, and algebraic geometry guarantees the validity of this equation. The additional terms provide a series of hierarchical approximations to the true solution. (4) A function being an SOS is equivalent to finding a positive semidefinite matrix Q where z is a vector of monomials of U. Note that Q relates the coefficients of U and contains λ. Finding Q is equivalent to the semidefinite program given in (5), with the primal (left) and dual (right) problems. Each step is an exact reformulation of the previous apart from (3) which is guaranteed to give an optimal bound to the original problem. When expressed in the appropriate monomial basis the problem of locating the coefficients of Q becomes convex and hence efficiently solvable. However, the SOS function (3) is still a nonconvex function in configuration space and can be a good representation of the original function.

where $p_i(\mathbf{x})$ are undetermined SOS polynomials. These SOS polynomials can be thought of as generalized Lagrange multipliers in the space of non-negative polynomials. By fixing an upper bound on their degree we are again presented with having to solve a semidefinite program. Such representations allow for significantly more elaborate sum of squares relaxations to be found in a systematic manner. Indeed such liftings can be carried out until an exact solution has been obtained or the SDP becomes too large for the computer to solve.

The steps in the methodology are summarized in the flowchart in Figure 2. In the Appendix we show how the method works in practice through a simple example.

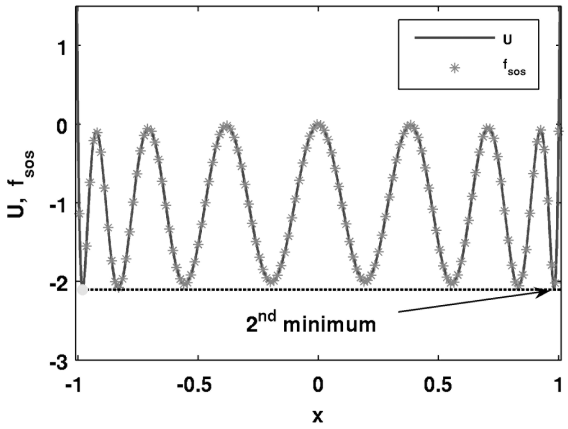

Figure 3. SOS optimization on a multiwell potential $U(-)$ with 8 minima, the leftmost being the global minimum. The second minimum, farthest away in domain space, is very close in value to the global minimum. The global minimum is correctly identified. The SOS function $f^{SOS}(*)$ is in excellent agreement with U. Here, $U = 0.01x - 128.1x^2 + 2688x^4 + -21504x^6 + 84480x^8 - 180224x^{10} + 212992x^{12} - 131072x^{14} + 32768x^{16}$.

Results

A. Global Minimum. To demonstrate the SOS approach in physical applications, we apply it now to model potentials that highlight the versatility of the method in dealing with typical aspects of landscapes that make them difficult to study. Once the problem is formulated theoretically as described above, we use third party Matlab toolboxes to carry out the SOS decomposition: SOSTOOLS, a tool for producing the SOS decompositions of polynomial optimization problems[36] and SeDuMi[37] or SDPT3,[38] SDP solvers which use primal-dual interior point methods. Other minimizations for comparisons were implemented in the Matlab optimization toolbox.

1. Multiwell Potential. To demonstrate the method we apply it first to a potential with many minima whose values are very close to the global minimum but are separated by high barriers (see Figure 3). The typical ratio of barrier height/local minima energy difference is 80. In addition, the minimum closest in energy to the global minimum is furthest apart in domain space. This type of poor connectivity behavior is not uncommon in potential energy surface problems where a number of nodes on the disconnectivity graph[39] have energy levels that are almost identical.

The SOS approach provides the global minimum which in this case is proven to be exact from the duality gap and correctly identifies its location in the coordinate space (Table 1). Additionally, the SOS decomposition we obtained is a faithful representation of the original function (Figure 3). A general feature of the SOS optimization, once formulated theoretically, is that it is carried out once, unlike other methods which may depend on a good initial guess or on the location of the initial conditions, and it provides all the information simultaneously.

We have compared to two other common minimization approaches: the downhill simplex method[40] and the BFGS quasi-Newton scheme,[41] which is used in the basin-hopping algorithm. Unlike SOS, both methods were applied iteratively from a grid of starting points spanning the domain space of

Table 1. Summary of SOS Optimization Results for the Multiwell, Müller, and Golflike Potentials[a]

	1D multiwell	10D multiwell	Müller	golflike
CPU time (s)	0.65	6840.00	10.06	0.80
lower bound	−2.106 [−2.106]	−193.685	−146.674 [−146.674]	−3.539 [−3.537]
configuration	−0.980	see below (*)	(−0.557,1.449)	(4.994,3.995)
duality gap	3.857E-06	7.56E-04	1.366E-4	0.002
primal	2.105998	193.6848	146.6743	3.537
dual	2.106002	193.6855	146.6745	3.539

[a] The CPU time in a standard PC in seconds, the lower bound value with the exact global minimum in brackets, the configurational coordinates of the minimum, the duality gap, and the final values of the primal and dual problem. The 10-dimensional multiwell example was defined as follows: $U = \sum_{i=1}^{10} a_1 x_i + a_2 x_i^2 + a_3 x_i^3 + a_4 x_i^4 + a_5 x_i^5 + a_6 x_i^6$ where $a_1 = 2$, $a_2 = 230$, $a_3 = -28$, $a_4 = -1000$, $a_5 = 1$, $a_6 = 1000$ and the global minimum of −193.685 was located among approximately 59 000 minima at (*)[0.7369, 0.7369, 0.7369, 0.7369, 0.7369, 0.7369, 0.7369, 0.7369, 0.7369, 0.7369].

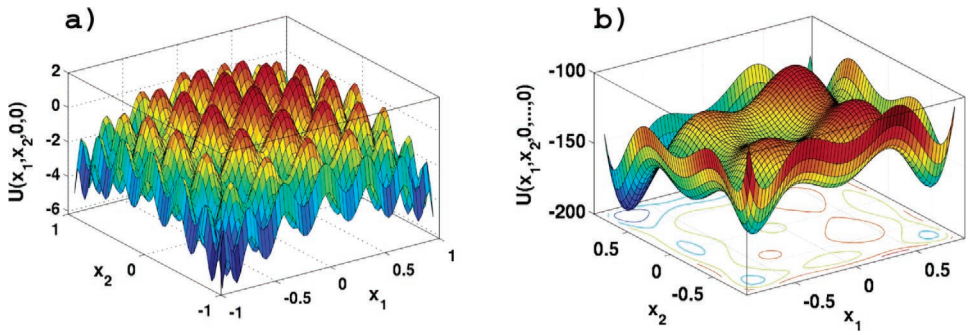

Figure 4. (a) A 2D projection of a four-dimensional 16th degree polynomial multiwell potential with 4096 minima given by $U(x_1, x_2, x_3, x_4) = \sum_{i=1}^{4} a_0 + a_1 x_i + a_2 x_i^2 + a_3 x_i^4 + a_4 x_i^6 + a_5 x_i^8 + a_6 x_i^{10} + a_7 x_i^{12} + a_8 x_i^{14} + a_9 x_i^{16}$ where $a_0 = 1$, $a_1 = 0.5$, $a_2 = -130.1$, $a_3 = 2688$, $a_4 = -21504$, $a_5 = 84480$, $a_6 = -180224$, $a_7 = 212992$, $a_8 = -131072$, $a_9 = 32768$. SOS optimization sucessfully identified the global minimum of $U = -13.977$ to within 0.026 at the point [−0.9792, −0.9792, −0.9792, −0.9792]. (b) A 2D projection of a 10-dimensional 6th degree polynomial multiwell potential given by $U(x_1, x_2, ..., x_{10}) = \sum_{i=1}^{5} a_1 x_i + a_2 x_i^2 + a_3 x_i^3 + a_4 x_i^4 + a_5 x_5 + a_6 x^6 + \sum_{i=6}^{10} b_1 x_i + a_2 x_i^2 + a_3 x_i^3 + a_4 x_i^4 + a_5 x_5 + a_6 x^6 + \sum_{j=i+1,...,10}^{i=1,...,9} r1_{ij} x_i x_j - r2 x_i^2 x_j^4$ where $r1_{ij}$ and $r2_{ij}$ are different numbers chose randomly between 0 and 10. The global minimum (−196.36) is located at [−0.7237, 0.7468, 0.7431, 0.7487, −0.7226, 0.7477, 0.7463, 0.7491, 0.7531, −0.7319]. There are 45 different projections onto different pairs of coordinates. The duality gap is $-2.316E - 3$.

the problem with the grid density being increased until the global minimum was obtained. To succeed in finding the global minimum, at least 10 separate runs from starting points on an evenly spaced grid of points spanning the domain were required. This is in fact more attempts than the number of minima in the domain. The point however remains that these algorithms have no way of establishing that the minimum that they locate is in fact the global minimum.

We note that there is nothing special about the form of the potential presented here. We have tried successfully several multiwell examples with different polynomial representations, more asymmetric wells, and separations with identical success. Interestingly, the method can identify the global minimum even if the wells are nearly degenerate with arbitrarily close energy. In fact, a true degeneracy is reflected in the eigenvalues of the dual solution matrix and can hence be identified and located in the dual solution matrix. This can be very useful in locating often missed degenerate minima by looking at the dual.

The formalism holds for multidimensional problems, and so a generalization of this problem to higher dimensions works in the same fashion. The global minimum ($U = -14.036$, location = [−0.9798, −0.9798, −0.9798, −0.9798]) is identified among on the order of 4100 densely spaced minima (Figure 4 a) of the four-dimensional version of the same potential. At the same time, a 10-dimensional version with now disconnected minima dispersed in a higher 10-dimensional space (of the order of 59 000 minima) worked equally well for uncoupled (Table 1) or coupled variables (Figure 4b).

2. Golflike Potential. A different set of energy landscapes exhibit flat regions with deep and narrow wells which become especially challenging and rapidly intractable for searching algorithms. The reason is that the flat regions provide no energy differences that can guide any search. Exhaustive searching is the only option, which becomes intractable very rapidly as the domain increases. We were able to successfully locate the global minimum of a delta function embedded in a two-dimensional infinite region. Such an example is shown in Figure 5 where the function is almost flat everywhere except in two locations where almost identical delta function wells are present. Note that we have included the entire $\mathbf{R}^2$ domain. The SOS approach correctly identifies the minimum and its location (Table 1). This is also true when the higher energy well becomes wider. The power of this approach comes from the following general simultaneous reasons: (i) the solution is always approached from below so the flatness of the function does not enter, (ii) the minimum is very narrow in configurational space, however, in the lifted space of the coefficients this is no longer necessarily true, and (iii) the set of equations linking the coefficients of the function intersect the cone of positive

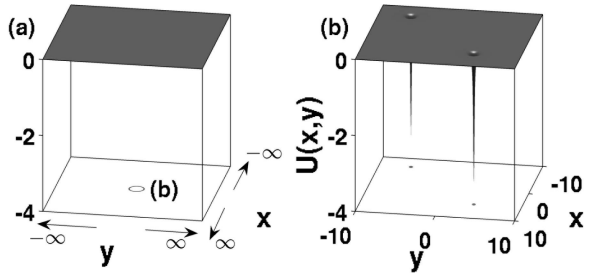

Figure 5. Plot of a golflike potential. U is given by $(-1/\pi)((e_1/((x-5)^2+(y-4)^2+e_1^2))+(e_2/((x+7)^2+(y+6)^2+e_2^2)))$, $e_1 = 0.09$, $e_2 = 0.1$ defined over the entire $\mathbf{R}^2$ domain (left). The area close to the origin (blue circle) is reproduced at greater magnification on the right. The two minima are $U(5, 4) = -3.5369$ (global) and $U(-7, 6) = -3.1832$. In this case the SOS optimization produces a lower bound of $U = -3.539$. The configurational coordinates are obtained correctly to within numerical accuracy.

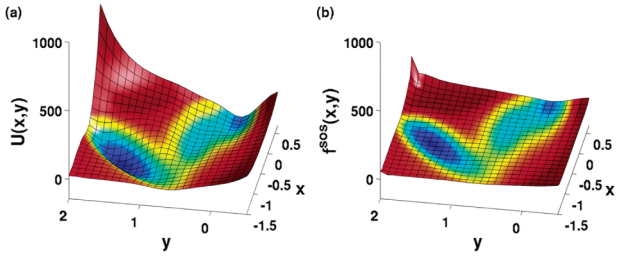

Figure 6. Contour plot of the original fitted Müller potential (a) and its SOS representation (b). The global minimum was identified correctly. f^{SOS} (b) is the projection to the original domain space from the lifted space of the SOS function including the inequality constraints. Much of the original function is preserved within the first order of eq 3, Figure 2.

definite matrices. The possible solutions are now on the boundary of this space and no longer on the interior and hence easy to distinguish near degeneracies even if disconnected in configuration space.

3. Müller Potential. The Müller potential[42] is commonly used[43,44] as a nontrivial test for reaction path methods due to the complexity of its minima structure that leads to a highly contorted reaction coordinate which requires a sharp change of direction at the saddle. The potential surface (Figure 6) contains three minima, with the global minimum of -146.7 at $(-0.558, 1.442)$

$$U(x, y) = \sum_{i=1,\ldots,4} A_i \exp[a_i(x - x_i)^2 + b_i(x - x_i)(y - y_i) + c_i(y - y_i)^2] \tag{9}$$

where $A = (-200, -100, -170, 15)$, $a = (-1, -1, -6.5, 0.7)$, $b = (0, 0, 11, 0.6)$, $c = (-10, -10, -6.5, 0.7)$, $x_i = (1, 0, -0.5, -1)$, $y_i = (0, 0.5, 1.5, 1)$. Its domain is constrained in order to exclude areas where the function is not well behaved. The SOS approach allows for constraints, both equality and inequality, to be incorporated on an equal footing as can be seen in eq 3 of Figure 2. We can take advantage of this powerful tool here by excluding parts of space that are not of interest in the formulation of the problem. The definition of this function includes an exponential so in order to apply the method here we fitted the function in a least squares sense to a polynomial of degree 16, U_f, which contains 153 monomials, 67 of which are odd. (The RMS error normalized by the data range was 0.0015 over the points sampled.) This leads to the minimization of U_f subject to a series of inequality constraints, g_i

$$\begin{aligned} &\max: \lambda \\ &\text{subject to}: U_f - \sum_{i=1}^{4} s_i g_i - \lambda \geq 0 \\ &g1: x \geq -1.5 \; g2: x \leq 0.7 \\ &g3: y \geq -0.5 \; g4: y \leq 2.0 \end{aligned} \tag{10}$$

where s_i are additional SOS functions with unknown coefficients.

The SOS approach succeeded in locating the minimum which is proven to be exact by the duality gap. It is interesting to point out that the final SOS decomposition of the potential is a good representation of the original function (see Figure 6) which may allow for additional properties of the function to be explored in different representations. For example, we were able to correctly locate the elusive saddle through eigenvector following on the SOS function. If more faithful representations were sought, a better bound to the function can be produced by systematically augmenting the dimension of the basis (eq 3, Figure 2) at higher computational cost.

B. Geometry: The Distance of Closest Approach of Anisotropic Coarse-Grained Molecular Units. 1. Formulation. One of the primary challenges in coarse-grained approaches to modeling of complex systems is to produce realistic interparticle potentials and, in particular, to incorporate the geometry or shape of the coarse-grained particles into such a representation of the physical system. In the spherical case this is straightforward as the potential remains isotropic after coarse graining and the interactions are simply functions of the interparticle radial distance. In the general nonspherical case, the interaction can be computed as a force acting at the points of minimum distance between the particles and in the direction of the minimum distance vector. This force can then be resolved into a radial part acting on the center of mass of the particles and a torque acting about the center of mass. The principal difficulty with this approach is how to compute the minimum distance between particles of an arbitrary shape.[25−27]

To formalize this we represent two arbitrary geometrical shapes as $\mathscr{A}$ and $\mathscr{B}$ in the real space $\mathbf{R}^n$, and we define the minimum distance problem as finding $a \in \mathscr{A}$ and $b \in \mathscr{B}$ such that the distance $||a - b||_2$ is a minimum:

$$\begin{aligned} &\min: ||a - b||_2 \\ &\text{such that}: a \in \mathscr{A}, b \in \mathscr{B}. \end{aligned} \tag{11}$$

Finding the minimum distance of closest approach between $\mathscr{A}$ and $\mathscr{B}$ can be formulated as a SOS problem, that is we

search for a function such that (see Figure 2, eq 3)

$$||a - b||_2 - s_1(a, b)g_1(a) - s_2(a, b)g_2(b) \geq 0 \quad (12)$$

where $s_i(a, b)$ are SOS polynomials and $g_1(a) \geq 0$, $g_2(b) \geq 0$ define $\mathscr{A}$ and $\mathscr{B}$, respectively. By "search for a function" we mean "find the coefficients of" such a function. Note that other SOS representations of eq 8 may be required depending on the problem, but we have chosen the most basic representation to make this introduction as clear as possible.

Finally, in analogy to obtaining the global minimum described in the previous section, we can rewrite eq 8 as

$$\begin{aligned} &\max : \lambda \\ &\text{such that} : ||a - b||_2 - s_1(a, b)g_1(a) - s_2(a, b)g_2(b) - \\ &\qquad \lambda \geq 0 \quad (13) \end{aligned}$$

where λ is a real number. The two steps of finding the SOS polynomial and finding its minimum can now be performed simultaneously by solving a semidefinite program. By using the duality, we can also obtain the proof if the minimum distance between the two geometrical shapes has been obtained.

This SOS approach provides a useful general mathematical framework for studying interactions between arbitrarily shaped coarse-grained particles, convex or nonconvex. A popular shape for anisotropic representations is the ellipsoid.[45−48] In this case, it turns out that the equations presented above simplify greatly since ellipsoids have a useful matrix representation, namely as symmetric positive definite matrices whose eigenvalues determine the length of its semiaxes and eigenvectors give their directions.[49]

Equation 7 now becomes

$$\begin{aligned} &\min : ||(c_1 + a) - (c_2 + b)||_2 \\ &\text{such that} : ||A^{-1}a||_2 \leq 1 \ (\mathscr{A}) \quad (14) \\ &\qquad ||B^{-1}b||_2 \leq 1(\mathscr{B}) \end{aligned}$$

where c_1 and c_2 are the centers of the ellipsoids, and A and B are the symmetric positive definite matrices corresponding to particles $\mathscr{A}$ and $\mathscr{B}$, respectively. The search for a globally non-negative representation is now trivial since the norm functions will always be quadratic forms and hence sum of squares.

2. Implementation to MD. We have obtained the minimum distance of closest approach exactly within numerical accuracy as confirmed by the duality gaps and infeasibility information. For an example see Figure 7. We found this to hold for different orientations and particles of varying and disparate size and eccentricity. Typical values reported for the primal and dual objectives were $5.3024e + 04$ with a difference in further than the 6 significant figure. Furthermore, the formulation of eq 10 allowed us to use a more efficient solver[50] since it met the definition of a "second-order cone program" (SOCP) which is a simpler subset of semidefinite programs. Another advantage of this approach is that we can obtain the minimum distances for all pairs of ellipsoids in any current configuration at once in a single step (see Figure 8). Here we show only 32 particles in order to illustrate all the distances at once. Typically, we calculate the minimum distance between approximately 12 000 pairs which takes of the order of 6 s.

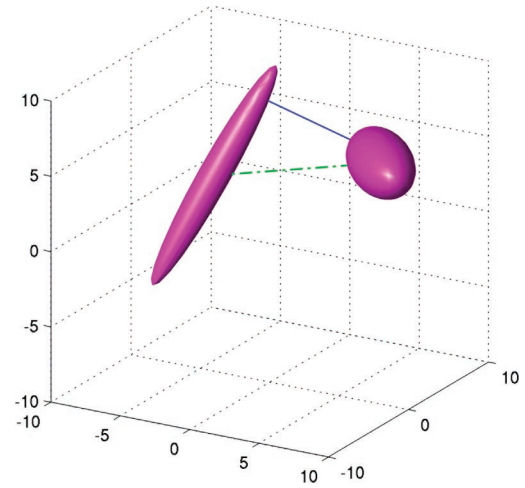

Figure 7. The exact distance of closest approach (6.355763) between two ellipsoid particles given by the SOS approach. Notice that this vector (blue continuous line) differs markedly both in direction and magnitude from the intercenter vector (green dashed line). The semiaxes lengths for the ellipsoids are {8, 1, 1} and {4, 2, 2}, respectively. Their center vectors are [−4, 0, 3] and [8, 0, 6], respectively. The minimum distance vectors are [−1.299203, 2.018481, 7.809342] and [4.874321, 1.910192, 6.302155]. The duality gap ($-1.18E - 7$) verifies the result. The approach works for arbitrary ellipsoids in any orientation.

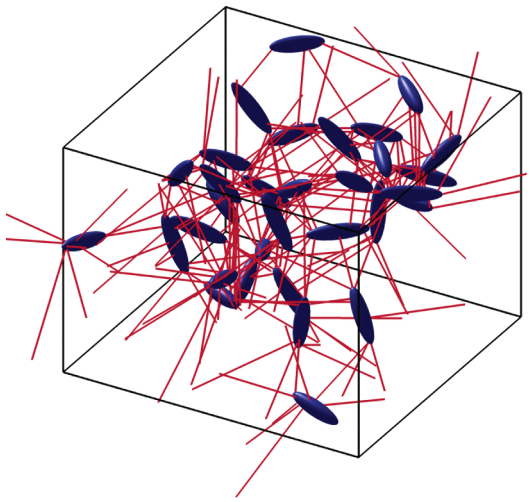

Figure 8. The exact distances of closest approach for all-to-all pair interactions between the particles in a periodic box. Here, only 32 particles are considered for illustrative purposes. The result is obtained at one step.

To show that this can be implemented in an MD simulation, we simulate an NVE ensemble of a binary A−B system of 240 ellipsoids interacting through a Lennard-Jones potential in a box of dimensions 21σ, 20σ, 16σ. The unit of length is σ, unit of energy is ϵ_{11}, while the mass of particle is 1, and the initial temperature is 0.5. Periodic boundary conditions are applied at the sides of the simulation box. The ellipsoids have semiaxis lengths of 3.0σ, 0.5σ, 0.5σ.

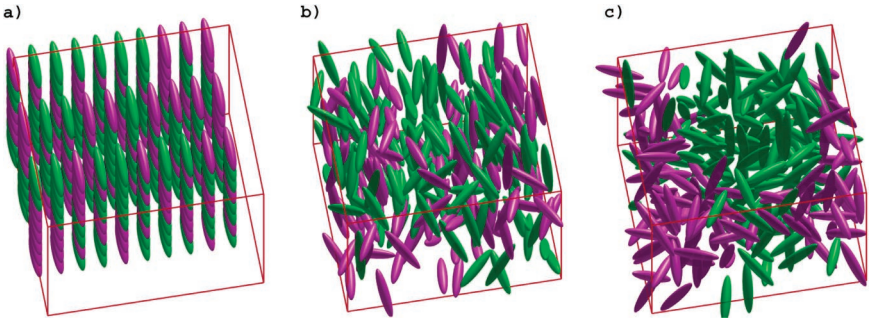

Figure 9. Snapshots from an NVE ensemble MD simulation of a mixture of 240 ellipsoids with semiaxes lengths $\{3.0\sigma, 0.5\sigma, 0.5\sigma\}$ in a box of dimensions {21, 20, 16}. The exact distances of closest approach of all-to-all particles are obtained in one step through the approach described in the text. There are typically 12 000 interactions per configuration. The simulation is initialized in a regular cuboidal array of randomly mixed A and B particles (a) (step 1). By step 500 much of the orientation correlation has disappeared (b), while by step 10 000 (c), a significant region of demixing has formed.

Lennard-Jones interactions are calculated based on distance of closest approach between pairs of ellipsoids using the following parameters: $\sigma_{ij} = 1.0$, $\epsilon_{11} = \epsilon_{22} = 1.0$, while $\epsilon_{12} = 2.0$. Two cutoff parameters are employed. The first ($\mathrm{rcut_{com}} = 9.0$) is a center of mass based spherical cutoff above which distances between ellipsoids are not calculated. A second ($\mathrm{rcut_{md}} = 4.0$) based upon the distance of closest approach between the two ellipsoids is then applied to this remaining set. The simulations were run with time step $\Delta t = 0.005$. Initially the randomized *A*/*B* particles were arranged in a cuboidal array with the principal semiaxis uniformly oriented parallel to the *x* axis. Maxwell−Boltzmann distributed linear velocities were assigned, while the initial angular velocities were zero. The forces and torques were then calculated following the standard way for rigid body dynamics. Time integration of the linear velocities was carried out using a standard leapfrog algorithm, while the angular velocities were integrated using Omelyan's algorithm.[51] The orientation of the ellipsoids was described using quaternions to avoid the singularity issue associated with Euler angles. By step 500 nearly all of the orientation correlation has disappeared (Figure 9b), while by step 15 900 (Figure 9c) significant regions of demixing have formed.

IV. Discussion

The SOS approach[1] is a rigorous and systematic way to approach complex problems by exploiting both their algebraic and geometric properties. We have applied it here to the identification of the global minimum of model potential energy surfaces which exemplify features that make this problem difficult in physical systems of interest such as narrow and disconnected wells embedded in flat or contorted regions. We have demonstrated the method on low-dimensional problems in which it is possible to gain an understanding of how the method works and how it is different to other approaches. We have also shown that it can be used to solve geometric problems such as obtaining the distance of closest approach of anisotropic coarse-grained particles. It is clear that no method will outperform all other methods for all problems, and it may well be that heuristic approaches may outperform the more formal SOS approach on a given subset of problems. However, the appeal of the SOS approach stems from its generality due to its deep theoretical foundations and efficient computational algorithms.

Another advantage comes from the added physical insight that can be gained by formulating the problem in this way where duality holds. An immediate consequence of duality is the ability to produce a proof when the exact answer has been reached without sampling or comparing to other minima, in contrast to almost all other methods. Second, the geometrical interpretation attached to the dual can lead to insight into the problem, including the identification of degeneracies and symmetries. Furthermore, there is freedom in how to pose a problem, so that constraints (equalities and inequalities) can be incorporated as variables or new variables can be introduced which can lead to efficient answers. This is particularly useful for dealing with more complex potentials that include trigonometric functions and so fitting could be avoided by introducing new variables. This may extend the applicability of the method to certain nonpolynomial functions.

Unlike other methodologies that approximate the functions either by subtracting or adding extra terms, which is known to often alter the behavior of the system especially in multidimensional problems, in this approach the original function is never deformed nor linearized. Rather, an entirely different and higher dimensional problem is sought, which is both convex solvable and whose solution in the space of the original variables coincides with that of the original question. Unlike gradient-based and Monte Carlo methods that use the original function, this approach bounds the function *externally* from below. This is one of the reasons that poorly connected and/or nearly degenerate minima separated by high barriers do not pose the difficulties encountered in the usual sense.

As the complexity of problems attempted increases, it is possible that the exact solution may not be found. In many cases, a "close enough" answer may be adequate. Here, we can quantify the gap between our answer and the exact solution. If the lower bound solution is not adequately close, then further refinement can be sought by seeking a higher dimensional monomial basis by introducing SOS functions, which can be thought here as a generalization of Lagrange multipliers. Accuracy can be systematically increased at the

expense of more computational cost, since there is a proof of the existence of the exact answer in such liftings to higher dimensions. In that respect, this method is closer in spirit to a variational approach but one which is guaranteed to be optimal and may lead eventually, at least in principle, to the right answer of the original problem. Unlike other global approaches, the method allows for insight into the nature of the PES rather than just providing a number. For example, having an explicit SOS polynomial representation of the problem can potentially be useful for studying other properties of the system besides its global minimum. The method also allows for exploiting the geometrical properties of the system which can lead to more efficient ways to simulate dynamics of coarse-grained systems which are often anisotropic.

A number of challenges remain due to the significant scaling of the number of the new variables that occurs as a result of the lifting process which means that, for physical problems, the current limitations on size of SDPs solvable using primal-dual interior point methods need to be overcome. Excluding symmetries and symmetry operations is a promising way in that direction. This is the focus of ongoing research.

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Appendix: How To Obtain the Global Minimum and a SOS Decomposition in Practice

We describe here in detail the process for obtaining a SOS decomposition as well as the global minimum of the function from the SOS decomposition in order to demonstrate how the method works in practice. Note that the decomposition and optimization are carried out simultaneously. We choose a very simple quartic polynomial function to exemplify the method by showing explicitly all the steps involved:

$$U = 2x^4 + 2x^3y - x^2y^2 + 5y^4, \quad x, y \in (-\infty, \infty)$$

For the purposes of this example we omit any constraints. The global minimum (0,0) is straightforward to obtain, but the decomposition is not immediate by standard techniques. The emphasis here is in the implementation of the method in the available software.

1. The first step is to rewrite the problem as a polynomial optimization problem in the form of eq 1 in the flowchart of Figure 2, where U is the function to be minimized subject to all the constraints:

$$\min: \ U(\mathbf{x})$$

$$\text{subject to}: \ g(\mathbf{x}) \geq 0$$

$$h(\mathbf{x}) = 0$$

Although in this example this is straightforward (U is given above and there are no constraints), in certain cases it may be the most difficult step in the calculation.

2. The next step is to introduce an additional real variable, $\lambda \in \mathbf{R}$, such that the minimization problem becomes now a maximization (eq 2, Figure 2):

$$\max: \ \lambda$$

$$\text{subject to}: \ U(\mathbf{x}) - \lambda \geq 0$$

$$g(\mathbf{x}) \geq 0$$

$$h(\mathbf{x}) = 0$$

Although this appears to be a trivial step, it has important theoretical consequences as described in the section Theory and also practical implications. For example, note that the function to be maximized now is a linear function, while all the nonlinear parts are in the constraints. There is no effect on the underlying problem itself, but the benefit is that solutions to the problem (optimal points) that may have been on the interior of the domain space are now on the surface. This makes it possible to find them more efficiently. Our example now becomes

$$\max: \ \lambda$$

$$\text{subject to}: \ 2x^4 + 2x^3y - x^2y^2 + 5y^4 - \lambda \geq 0$$

3. Solving this problem still remains very difficult and often impossible. However, requiring that $2x^4 + 2x^3y - x^2y^2 + 5y^4 - \lambda$ is a SOS instead turns out to be easier to solve. Although not necessarily exact, it often gives a good solution to the original problem we are interested in. In this example, this is equivalent to (eq 3, Figure 2)

$$\min: \ -\lambda$$

$$\text{subject to}: \ 2x^4 + 2x^3y - x^2y^2 + 5y^4 - \lambda \text{ is SOS}$$

4. We now show how to obtain the SOS decomposition. Once we have written our problem in the form above, we can submit it to the software SOSTOOLS which will do precisely that. To proceed, we must define the degree of the SOS basis we want to use. The maximum basis is d where $2d$ is the maximum degree of the function of interest including the constraints. (In this example, $d = 2$.) We now write out the entire vector of monomials whose total degree is less than d

$$z = [x_1, x_2, ..., x_n, x_1^2, ..., x_n^2, x_1x_2, ..., x_{n-1}x_n, ..., x_1^d ..., x_n^d]$$

which in our example is

$$z = [1, x, y, x^2, xy, y^2]$$

The ordering is not particularly important, but we have chosen the ordering that allows for the easiest interpretation of results from SOSTOOLS. If there are symmetry or physical reasons that exclude certain solutions, then we can take advantage of that and not include them in the monomial basis. Additionally, if the problem is of very high dimension, we can start by looking for an approximate solution with a reduced basis and subsequently refine the calculation by increasing the monomials in the basis.

5. The basis of monomials allows us to construct a matrix Q. Finding the SOS decomposition is equivalent to finding a suitable positive semidefinite matrix, $Q \geq 0$, such that

$$U - \lambda = z^T Q z$$

This Q matrix is an $r \times r$ symmetric matrix in unknown variables q_{ij}. The problem now becomes (eq 4, Figure 2)

$$\min : \ -\lambda$$

$$\text{subject to} : \ z^T Q z \geq 0$$

So in this example we want to find the entries of Q such that

$$U - \lambda = \begin{bmatrix} 1 \\ x \\ y \\ x^2 \\ xy \\ y^2 \end{bmatrix}^T \begin{bmatrix} q_{11} - \lambda & q_{12} & q_{13} & q_{14} & q_{15} & q_{16} \\ q_{12} & q_{22} & q_{23} & q_{24} & q_{25} & q_{26} \\ q_{13} & q_{23} & q_{33} & q_{34} & q_{35} & q_{36} \\ q_{14} & q_{24} & q_{34} & q_{44} & q_{45} & q_{46} \\ q_{15} & q_{25} & q_{35} & q_{45} & q_{55} & q_{56} \\ q_{16} & q_{26} & q_{36} & q_{46} & q_{56} & q_{66} \end{bmatrix} \begin{bmatrix} 1 \\ x \\ y \\ x^2 \\ xy \\ y^2 \end{bmatrix}$$

and Q remains positive semidefinite.

6. Note that the entries of Q and the coefficients of the monomials of the function of interest define a set of linear constraints. In our example, this leads to the following set of linear equations:

$$\begin{array}{lllll} q_{11} - \lambda = 0, & q_{13} = 0, & 2q_{16} + q_{33} = 0, & q_{36} = 0, & q_{66} = 5, \\ q_{12} = 0, & q_{15} = q_{23} = 0, & q_{35} + q_{26} = 0, & q_{56} = 0, & 2q_{14} + q_{22} = 0, \\ q_{43} + q_{45} = 0, & 2q_{46} + q_{55} = -1, & q_{24} = 0, & 2q_{45} = 2 & q_{44} = 2 \end{array}$$

In fact, our original problem can be rewritten as

$$\min : \ -\lambda$$

$$\text{subject to} : \ \mathbf{Tr}(A_i, Q) = b_i, \ \forall i = 1, ..., 15$$

$$Q \geq 0$$

where the A_i are matrices representing the coefficients in the linear constraints. For example, A_{10} is

$$\begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{11}$$

and $b_{10} = 0$. It turns out that the linear objective function to be minimized, the linear constraints, and the constraint $Q \geq 0$ form a statement of a general class of problems, semidefinite programs, that are solved efficiently and possess interesting duality properties. If we define C to be a 6×6 matrix with zeros everywhere except a -1 in the (1, 1) entry and b with

$$b = [0, 0, 0, 0, 5, 0, 0, 0, 0, 0, 0, -1, 0, 2, 2]$$

then we have the primal form of a semidefinite program[1]

$$\min : \ \mathbf{Tr}(C, Q)$$

$$\text{subject to} : \ \mathbf{Tr}(A_i, Q) = b_i, \ \forall i = 1, ..., m,$$

$$Q \geq 0$$

where m is the number of constraints. The dual form is easily formulated as

$$\max : \ b^T y$$

$$\text{subject to} : \ C - \sum_i A_i y_i \geq 0$$

SOSTools now invokes an SDP solver to obtain the solution we are interested in. Semidefinite programs are commonly solved using path following interior point methods in which the primal and dual formulations are solved simultaneously. Commonly used solvers include SeDuMi and SDPT3. Both solvers are indeed variations of the primal-dual interior point algorithm and will solve this problem very easily. For small to medium sized problems SeDuMi is extremely robust indeed, but in larger sparse problems we found SDPT3 to be more effective at finding solutions. For this example, we report solutions from SeDuMi. Once the SDP solver has completed its solution a number of checks must be made to ensure proper convergence. The checks are more or less standard for most SDP solvers such as SeDuMi or SDPT3.

(a) Check that the primal solution is feasible.

(b) Check that the dual solution is feasible.

(c) Check the duality gap.

The duality gap is defined as the difference between the primal and dual solutions. It must be checked manually, and in our example the primal solution is $-8.1518E - 10$, the dual solution is $-6.0227E - 10$, and the gap is $-2.1291E - 10$. This gives us the proof that we have found the exact minimum.

7. Upon solving the semidefinite program, a primal and dual solution matrix are produced. These will allow us to locate the global minimum and find the SOS decomposition. In our example, the solution matrices are

Primal:

$$\begin{bmatrix} 0.0000 & 0.0000 & 0.0000 & -0.0000 & -0.0000 & -0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & -0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & -0.0000 & -0.0000 \\ -0.0000 & 0.0000 & 0.0000 & 2.0000 & 1.0000 & -1.3214 \\ -0.0000 & -0.0000 & -0.0000 & 1.0000 & 1.6427 & -0.0000 \\ -0.0000 & 0.0000 & -0.0000 & -1.3214 & -0.0000 & 5.0000 \end{bmatrix}$$

Dual:

$$\begin{bmatrix} 1.0000 & 0.0000 & -0.0000 & 0.0000 & -0.0000 & 0.0000 \\ 0.0000 & 0.0000 & -0.0000 & -0.0000 & -0.0000 & 0.0000 \\ -0.0000 & -0.0000 & 0.0000 & -0.0000 & 0.0000 & -0.0000 \\ 0.0000 & -0.0000 & -0.0000 & 0.0000 & -0.0000 & 0.0000 \\ -0.0000 & -0.0000 & 0.0000 & -0.0000 & 0.0000 & -0.0000 \\ 0.0000 & 0.0000 & -0.0000 & 0.0000 & -0.0000 & 0.0000 \end{bmatrix}$$

From the primal solution matrix we can extract the global minimum of the function to be $\lambda = q_{11} = 0.000$. Interpretation of the dual solution matrix is obtained by noting that

the dual solution matrix in a sum of squares SDP solution should correspond to the matrix zz^T. Therefore we can conclude that the first row and the first column are equal to z provided the first entry in z is 1. Therefore we can read off the location of the global minimum to be the vector $(x, y) = (0, 0)$. It is important to check the rank of the dual solution matrix which should be 1 if the relaxation is exact.

8. Finding the SOS decomposition: Before we do this it is worth noting that the primal solution matrix can be divided into 4 (3×3) submatrices and that only one of these is nonzero. From this we can see that the SOS decomposition in fact only requires a smaller basis of monomials namely $z = [x^2, xy, y^2]$. There are in fact ways of identifying such reductions in basis size, and these will be discussed in a later publication. To see the SOS decomposition, we must factorize the matrix, and here we take the Cholesky factorization of the (3×3) matrix:

$$L = \begin{bmatrix} 1.4142 & 0.0000 & 0.0000 \\ 0.7071 & 1.0690 & 0.0000 \\ -0.9344 & 0.6180 & 1.9352 \end{bmatrix}$$

Each row contains a single square within the SOS with each entry in each row being the coefficient of the corresponding entry in z. So we can reconstruct the SOS as

$$f^{\mathrm{SOS}} = (1.4142x^2)^2 + (0.7071x^2 + 1.0690xy)^2 + (-0.9344x^2 + 0.6180xy + 1.9352y^2)^2$$

The SOS decomposition is not necessarily unique, and other decompositions may be also be found; however, the global minimum and location will be unique provided that this is the case for the energy function being minimized. If the global minimum is not unique, then this will be evident from the rank of the dual matrix which will be greater than 1. Often the nonuniqueness is as a result of a symmetry in the function which may not be apparent upon initial examination. Examining the eigenvalues of the dual solution matrix gives information as to in which degrees of freedom the degeneracies lie.

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