Minimizing Polynomials on Semialgebraic Sets

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To Begin

Special thanks to the organizers for...

holding the conference during my spring break
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Notation

We work in $\mathbb{R}[X] := \mathbb{R}[x_1, \ldots, x_n]$. $f \in \mathbb{R}[X]$ is positive semidefinite (psd) if $f$ takes only non-negative values, we write $\sum \mathbb{R}[X]^2$ for the set of sums of squares in $\mathbb{R}[X]$ and say $f \in \mathbb{R}[X]^2$ is sos.
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Given $F = \{g_1, \ldots, g_r\} \subseteq \mathbb{R}[X]$, let $S(F)$ be the basic closed semialgebraic set generated by $F$, i.e., $S(F) = \{\alpha \in \mathbb{R}^n \mid g_i(\alpha) \geq 0, i = 1, \ldots, r\}$. 
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We have two algebraic objects in $\mathbb{R}[X]$ associated to $F$: 

- The **quadratic module** generated by $F$,
  
  $$M(F) := \{s_0 + s_1 g_1 + \cdots + s_r g_r \mid \text{each } s_i \text{ is sos}\}.$$
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  - The **quadratic module** generated by $F$, $M(F) := \{s_0 + s_1g_1 + \cdots + s rg_r \mid \text{each } s_i \text{ is sos} \}$.

  - The **preorder** generated by $F$, $PO(F) := \{\sum_{\epsilon \in \{0,1\}^n} s_\epsilon g_1^{\epsilon_1} \cdots g_r^{\epsilon_r} \mid s_\epsilon \text{ is sos} \}$. 
The Basic Problem

Given $S = S(F)$ and $f \in \mathbb{R}[X]$, find

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An observation: $f^* = \text{maximum} \{ \lambda \in \mathbb{R} \mid f - \lambda \geq 0 \text{ on } S \}$.

Another observation: If $f \in M(F)$ or $f \in PO(F)$, then $f \geq 0$ on $S$. Furthermore, a representation of $f$ in either $M(F)$ or $PO(F)$ is an explicit witness to the non-negativity of $f$ on $S$. 
Some definitions

Throughout, we will fix $F = \{g_1, \ldots, g_r\} \subseteq \mathbb{R}[X]$ and let $S = S(F), M = M(F), \text{ and } P = PO(F)$. 
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Following the above observations, it makes sense to define

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We’ll call this an f **SOS relaxation** of the original problem.
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“$h(X)$ is sos” is equivalent to the existence of a psd matrix $A$ such that

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Using this fact, the computation of \( f_{sos} \) and \( \hat{f}_{sos} \) can be implemented as a semidefinite programming problem (SDP) and hence solved numerically!
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...not precisely the truth, but close enough at this point in the talk!
The Global Case

Suppose we take $S = \mathbb{R}^n$, so that $f^*$ is the global minimum of $f$. Then $f_{sos} = \hat{f}_{sos} = \max\{\lambda \mid f - \lambda \text{ is sos}\}$. 
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The idea of using $f_{sos}$ to approximate $f^*$ in this case goes back to N. Z. Shor in the 1950’s. Computation of $f_{sos}$ gives a lower bound for $f^*$ and when the degree of $f$ is fixed the bound $f_{sos}$ can be computed in polynomial time using an SDP.
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However, the bound may not be useful! For example, if $m$ is the Motzkin polynomial, then $m^* = 0$ but $m - \lambda$ is not sos for any $\lambda$, so that $m_{sos} = -\infty$. 
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Little is known about when this works, how good the bound is, etc.
On the one hand, Parrilo and Sturmfels computed a family of examples of a particular form – with leading form \( \sum x_i^{2d} \) – and found that in all cases tested \( f_{sos} \) was finite and very close to \( f^* \) (within the range of numerical error).
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**Problem**: Explain the experimental results. Find results about when the method works well and/or gives explicit bounds.
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  \Rightarrow Representation Theorems

- Can we define an SDP whose solution is \( f_{sos} \) or \( \hat{f}_{sos} \)?
  \Rightarrow Stability of quadratic modules/preorders.
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\begin{advertisement}
Alex Prestal will be talking about archimedean modules later today. Don’t miss it!
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This means that if \( S \) is compact, then \( \hat{f}_{sos} = f^* \) and if \( M \) is archimedean, then \( f_{sos} = f^* \). That’s the good news.

Now for the bad news...
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Suppose $\deg p = 2d$ and $p$ is sos, say

$$p = h_1^2 + \cdots + h_k^2.$$ 

Then comparing leading terms on both sides of the equation, we see that $\deg h_i \leq d$ for all $i$: No “leading term cancellation" is possible. Thus we can implement “maximize $\lambda$ subject to $f - \lambda$ sos" directly as an SDP.
Stability

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However, given $p \in M$, say

$$p = s_0 + s_1g_1 + \cdots + s_rg_r,$$

in general there is no \textit{a priori} bound in terms of $\deg p$ on the $s_i$'s. There can be lots of leading term cancellation in this case!
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The Lasserre Method

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and let

$$f_{sos}^d := \max \{ \lambda \mid f - \lambda \in M_d \}. $$
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**Theorem (Lasserre).** Suppose $M$ is archimedean, then $\{ f_{sos}^d \}$ is an increasing sequence that converges to $f^*$. 

As mentioned above, $M$ is rarely stable. In particular, if $S$ is compact, then $M$ is not stable. Thus even if $f^* = f_{sos}^d$ for some $d$, there is in general no bound on $d$ which does not depend on $f^*$ itself!
As mentioned above, $M$ is rarely stable. In particular, if $S$ is compact, then $M$ is not stable. Thus even if $f^* = f_{sos}^d$ for some $d$, there is in general no bound on $d$ which does not depend on $f^*$ itself!

In general, it seems that little is known about bounds, convergence, etc., However, work of Schweighofer yields a bound in the case where $S = S(\{g\})$ is defined by a single inequality. In this case there is a constant $c \in \mathbb{N}$ depending on $\deg f$ and $g$ and a constant $b \in \mathbb{N}$ depending on $g$ such that

$$f^* - f_{sos}^d \leq \frac{c}{b \sqrt{d}}$$

for large $d$. 
In the case where $S$ is compact, why not use the preorder since it is automatically archimedean? The problem is that the generators of the preorder are all possible products of the elements in $F$ and hence if the set $F$ has $r$ elements, then the preorder has $2^r$ generators.
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Recall that $M$ is archimedean if there is some $N \in \mathbb{N}$ such that $N - \sum x_i^2 \in M$. In practical applications we might know, or can compute, some $N$ so that $S$ is contained in a ball of radius $\sqrt{N}$ about 0. Then we can simply add the polynomial $N - \sum x_i^2$ to $F$ and use the quadratic module.
We assume again that $S = \mathbb{R}^n$ so that $f^*$ is the global minimum of $f$. 
Representations via Gradient Ideals

We assume again that $S = \mathbb{R}^n$ so that $f^*$ is the global minimum of $f$.

The real gradient ideal of $f$, $I_{grad}(f)$, is the ideal in $\mathbb{R}[X]$ generated by the partial derivatives of $f$.

We also consider the gradient variety of $f$,

$$V_{grad}(f) = V(I_{grad}(f)) \subseteq \mathbb{C}^n$$

and

the real gradient variety $V_{grad}^\mathbb{R}(f) = V_\mathbb{R}(I_{grad}(f)) \subseteq \mathbb{R}^n$. 
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We also consider the **gradient variety** of $f$, $V_{\text{grad}}(f) = V(I_{\text{grad}}(f)) \subseteq \mathbb{C}^n$ and

the **real gradient variety** $V_{\text{grad}}^\mathbb{R}(f) = V_{\mathbb{R}}(I_{\text{grad}}(f)) \subseteq \mathbb{R}^n$.

All local and global minima of $f$ occur at points in the real gradient variety of $f$ and so to compute $f^*$ we can minimize $f$ on the real variety $V_{\text{grad}}^\mathbb{R}(f)$. 
There are several recent works on minimizing polynomials via the gradient ideal, among them:

Hanzon and Jibetean apply perturbations of $f$ to produce a sequence $f_\gamma$ with the property that $V_{\text{grad}}(f_\gamma)$ is finite and the minima $f_\gamma^*$ converge to $f^*$. 
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- Jibetean and Laurent give a method for computing $f^*$ via the gradient ideal in the case where the gradient variety is zero-dimensional.
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**Theorem (Demmel, Nie, Sturmfels).** Suppose $I_{\text{grad}}(f)$ is a radical ideal and $f$ is psd, then $f$ is sos modulo $I_{\text{grad}}(f)$. In other words, there is an sos $s \in \mathbb{R}[X]$ and $h \in I_{\text{grad}}(f)$ such that $f = s + h$. 
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There exist counterexamples in the case where $I_{\text{grad}}(f)$ is not radical.

However, if $f > 0$ on $\mathbb{R}^n$, then the assumption that $I_{\text{grad}}(I)$ is radical can be dropped.
Now suppose we want to find the global minimum $f^*$ of $f$, then since $f^*$ occurs at a point in the real gradient variety, fix $N \in \mathbb{N}$ and define the SOS relaxation
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Maximize $\lambda$ subject to

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Optimization via Gradient Ideals

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This problem can be translated into an SDP, and computed numerically. Let $f^*_N$ be the optimal value. If $f(x)$ attains its global minimum $f^*$ then $\lim_{N \to \infty} f^*_N = f^*$. Further, if the gradient ideal is radical, then $f^* = f^*_N$ for some $N$. 

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Note that this will always give a finite lower bound for $f^*$. Numerical experiments by Demmel, Nie and Sturmfels suggest that this method outperforms the "pure" SOS method.
Very recently, in joint work with Demmel and Nie, we have generalized the above ideas from the global case to the case of minimizing $f$ on a semialgebraic set.

We assume once again that we have $S = S(F)$, $M = M(F)$, and $P = PO(M)$ and we are trying to find the minimum $f^*$ of $f \in \mathbb{R}[X]$ on $S$. 
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**Theorem.** Suppose $I_{grad}(f)$ is radical and $f \geq 0$ on $S$. Then $f$ is in the preorder $P$ modulo $I_{grad}(f)$, i.e., there is $p \in P$ and $h \in I_{grad}(f)$ so that $f = p + h$. 
Generalization to Semialgebraic Sets

Very recently, in joint work with Demmel and Nie, we have generalized the above ideas from the global case to the case of minimizing \( f \) on a semialgebraic set.

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Again, we can drop the assumption the \( I_{\text{grad}}(f) \) is radical if we assume \( f > 0 \) on \( S \).
Note we do not assume that $S$ is compact.
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On the other hand, we have counterexamples to show that the theorem is not true in general if we replace $P$ by the quadratic module $M$.

If $M$ is archimedean, then the theorem does hold for $M$. 
Application to Optimization

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On the other hand, the traditional local methods in optimization often use the Karush-Kuhn-Tucker (KKT) system for finding $f^*$.

Why not combine these two methods?
Using a KKT System

Our optimization problem is

\[ f^* = \min f \text{ subject to } \]
\[ g_i(x) \geq 0, \quad i = 1, \ldots, r \]
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The KKT system of this is

\[ H \triangleq \nabla f(x) - \sum_{j=1}^{r} \nu_j \nabla g_j(x) = 0, \]

\[ g_j(x) \geq 0, \quad \nu_j g_j(x) = 0, \quad j = 1, \ldots, r, \]

\[ \nu = (\nu_1, \ldots, \nu_r) \text{ are called Lagrange multipliers. Note that we do not require } \nu \geq 0. \]
Under certain regularity conditions, if $f^*$ exists and occurs at an optimizer $x^*$, then the KKT system holds at $x^*$. Then $f^*$ is the minimum of $f$ over the KKT system.
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In $\mathbb{R}[x_1, \ldots, x_n, \nu_1, \ldots, \nu_r]$, define the KKT ideal $I_{KKT}$, KKT preorder $P_{KKT}$, and KKT quadratic module $M_{KKT}$ as follows:

$$I_{KKT} = \langle H_1, \ldots, H_n, \nu_1 g_1, \ldots, \nu_r g_r \rangle,$$

where $H = (H_1, \ldots, H_n)$.

$$P_{KKT} := PO(F) + I_{KKT}$$

$$M_{KKT} := M(F) + I_{KKT}$$
We also define the finite-dimensional analogues of these: $I_{n,KKT}$ are elements of $I_{KKT}$ where each term in the sum has degree $\leq d$, then $M_{d,KKT} = M_d + I_{d,KKT}$ and similarly $P_{d,KKT} = P_d + I_{n,KKT}$. 
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Finally, we define $f_d^*$ to be the maximum $\lambda$ such that $f - \lambda \in M_{d,KKT}$ and $p_d^*$ to be the maximum $\lambda$ such that $f - \lambda \in P_{d,KKT}$. 
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**Theorem.** Assume $f^*$ exists and the optimizer $x^*$ satisfies the KKT system above. The $p^*_d$ converges to $f^*$. Further, if $I_{KKT}$ is a radical ideal, then there is some $N$ such that $p^*_N = f^*$.
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The theorem does not hold in general if we replace $p^*_d$ by $f^*_d$. If the semialgebraic set $S$ is archimedean, then it does hold.
In general, the SOS relaxations are difficult to solve when there are many constraints, which introduces many Lagrange multipliers. In special cases, for example if the semialgebraic set is contained in the non-negative orthant $\mathbb{R}^n_+$, Lagrange multipliers can be removed and the KKT system simplifies considerably, making the computations more efficient.
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Future research could focus on generalizations of this or more general methods for removing Lagrange multipliers.
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Future research could focus on generalizations of this or more general methods for removing Lagrange multipliers.

Also, it’s not always true that the KKT condition holds for the minimizer $x^\ast$. We would like to remove the KKT conditions, or find ones which always hold.
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Conclusions

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I’m Vicki Powers and I approve of this message!