Global minimization of rational functions using semidefinite programming

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Rational function minimization

Let \( p, q, p_1, \ldots, p_k \in \mathbb{R}[x_1, \ldots, x_n] \) (polynomials with real coefficients defined on \( \mathbb{R}^n \)) with \( p \) and \( q \) relatively prime.
Rational function minimization

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p^* := \inf_{x \in S} \frac{p(x)}{q(x)}
\]

where \( S \) is the \textit{semi-algebraic set} given by

\[
S := \{ x \in \mathbb{R}^n : p_i(x) \geq 0, \ i = 1, \ldots, k \}.
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\( p^* \) is not necessarily attained or finite!
Applications

- Least squares approximation of data using rational functions (least squares Padé approximation);
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- stability analysis of certain dynamical systems, including biochemical reactor models.
Possible approaches

- If the infimum is attained one can solve the first order optimality condition equations. Modern review: B. Sturmfels, *Solving Systems of Polynomial Equations*, AMS, 2002. If the inf is not attained ...
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- Global optimization codes — can converge to local minima.
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• Global optimization codes — can converge to local minima.

• Today’s talk: approaches involving semidefinite programming (SDP).
What is SDP?

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\text{subject to} & \sum_{i,j=1}^{n} a_{ij}^{(k)} x_{ij} = b_k \quad \forall \ k = 1, \ldots, m,
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If the data matrices diagonal $\Rightarrow$ LP
Different cases

We investigate SDP-based approaches for the following cases of \( \inf_{x \in S} p(x)/q(x) \):

- \( S = \mathbb{R}^n \) and \( n = 1 \) (Unconstrained minimization: univariate case);
Different cases

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- $S = \mathbb{R}^n$ and $n = 1$ (Unconstrained minimization: univariate case);
- $S = \mathbb{R}^n$ and general $n$ (Unconstrained minimization: general case);
Different cases

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- $S = \mathbb{R}^n$ and $n = 1$ (Unconstrained minimization: univariate case);
- $S = \mathbb{R}^n$ and general $n$ (Unconstrained minimization: general case);
- $S$ is compact, connected and general $n$ (Constrained case);
Unconstrained case

Consider the unconstrained problem.

\[ p^* := \inf_{x \in \mathbb{R}^n} \frac{p(x)}{q(x)} \]

\[ = \sup \left\{ \rho : \frac{p(x)}{q(x)} - \rho \geq 0 \quad \forall x \in \mathbb{R}^n \right\} \]
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We can replace the nonnegativity condition by a simpler one ...
Unconstrained case (ctd)

Theorem (Jibetean) Assume $p^* > -\infty$. Then $q$ does not change sign on $\mathbb{R}^n$. 


This leads us to the theory of nonnegative polynomials.
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Nonnegativity vs SOS

Let $p \in \mathbb{R}[x_1, \ldots, x_n]$. 
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\( p \) is called a \textit{sum of squares} (SOS) if there exist polynomials \( p_i \) such that \( p = \sum_i p_i^2 \).

Nonnegativity and sum of squares are the same if:

- \( n = 1 \) (univariate polynomials) (result by Markov);
- \( d = 2 \) (quadratic polynomials on \( n \) variables);
- \( n = 2 \) and \( d \leq 4 \) (bivariate polynomials of degree at most 4) (result by Hilbert);

In all other cases counterexamples exist.
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The sum of squares cone

We fix a basis of monomials

\[ \tilde{x}_{n,d} := (1, x_1, \ldots, x_n, x_1^2, \ldots, x_n^d) \quad \text{dim:} \binom{n + d}{d}. \]
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**Notation:** We denote the convex cone generated by squares of polynomials on \( \mathbb{R}^n \) of degree at most \( d \) by \( \Sigma_{n,2d}^2 \) (**sum-of-squares (SOS) cone**).
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(We drop the subscripts when they are clear from the context.)
The sum of squares cone (cdt.)

**Theorem:** For a given $f \in \mathbb{R}[x_1, \ldots, x_n]$ of degree $2d$, one has $f \in \Sigma_{n,2d}$ iff

$$f = \tilde{x}_{n,d}^T M \tilde{x}_{n,d}$$

for some $M \succeq 0$ (size $(n+d)^d \times (n+d)^d)$.
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**Implication:** Conic linear optimization over the cone \( \Sigma_{n,d}^2 \) can be done using *semidefinite programming* (SDP);
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**Implication:** Conic linear optimization over the cone \( \Sigma_{n,d}^2 \) can be done using *semidefinite programming* (SDP);

Unconstrained univariate case

If $q$ is nonnegative on $\mathbb{R}$, then

$$\inf_{x \in \mathbb{R}} \frac{p(x)}{q(x)} = \sup_{t,x} \left\{ t : p(x) - tq(x) \geq 0 \ \forall x \in \mathbb{R} \right\}$$

$$= \sup_{t,x} \left\{ t : p(x) - tq(x) \in \Sigma^2 \right\}$$

$$= \sup_{t,x} \left\{ t : p(x) - tq(x) = \tilde{x}^T M \tilde{x} \right\}$$

for some $M \succeq 0$, where

$$\tilde{x}^T = [1 \ x \ x^2 \ldots \ x^{\frac{1}{2} \max\{\deg(p),\deg(q)\}}].$$
Unconstrained univariate case

Let $p(x) - tq(x) = \sum_\alpha a_\alpha(t) x^\alpha$. NB: $a_\alpha(t)$ is affine in $t$. 
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$$a_\alpha(t) = \sum_{i+j=\alpha} M_{ij}, \quad M \succeq 0.$$ 

This is an SDP problem!
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a_{\alpha}(t) = \sum_{i+j=\alpha} M_{ij}, \quad M \succeq 0.
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This is an SDP problem! (Result already obtained by Nesterov for \( q(x) \equiv 1 \).)

Example

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\frac{p(x)}{q(x)} := \frac{x^2 - 2x}{(x + 1)^2}.
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\]

Equivalent problem: \(\sup t\) such that

\[
(1-t)x^2 - 2(1+t)x - t = \begin{bmatrix} 1 \\ x \end{bmatrix}^T \begin{bmatrix} M_{00} & M_{01} \\ M_{10} & M_{11} \end{bmatrix} \begin{bmatrix} 1 \\ x \end{bmatrix},
\]

(2)

for some \(M \succeq 0\).
Example (ctd)

From (2):

\[ M_{00} = -t, \quad M_{01} = M_{10} = -(1 + t), \quad M_{11} = 1 - t. \]
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We therefore get

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\min_{x \in \mathbb{R}} \frac{p(x)}{q(x)} = \max_{t, M} \frac{p(x)}{q(x)} = \max_t \quad \text{such that}
\]

\[
M = \begin{bmatrix} -t & -(1 + t) \\ -(1 + t) & 1 - t \end{bmatrix} \succeq 0.
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such that

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\]

Note that the optimal value is \( p^* = -1/3. \)
Constrained case

Consider a semi-algebraic set

\[ S = \{ x \in \mathbb{R}^n : p_i(x) \geq 0 \ (i = 1, \ldots, k) \} . \]
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General constrained problem: find

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General constrained problem: find

\[ p^* = \inf_{x \in S} \frac{p(x)}{q(x)} . \]

One can treat the *unconstrained multivariate problem* by adding an *artificial constraint* \[ \|x\|^2 \leq R \] for some ‘large’ \( R \).
Constrained case

**Theorem (Jibetean)** Assume that $S$ is open and connected (or the (partial) closure of such a set). If $p^* > -\infty$ then $q$ does not change sign on $S$.

Assuming $q(x) \geq 0$ on $S$, then

$$\frac{p(x)}{q(x)} \geq \alpha \ \forall x \in S \iff p(x) - \alpha q(x) \geq 0 \ \forall x \in S.$$
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$$\frac{p(x)}{q(x)} \geq \alpha \ \forall x \in S \iff p(x) - \alpha q(x) \geq 0 \ \forall x \in S.$$  


**Consequence**

$$\inf_{x \in S} \frac{p(x)}{q(x)} = \sup \{ \rho : p(x) - \rho q(x) \geq 0 \ \forall x \in S \}.$$
Constrained multivariate case

Technical assumption: $S$ is compact and there exists a

$$\bar{p} \in \Sigma^2 + p_1 \Sigma^2 + \ldots + p_k \Sigma^2$$

such that $\{x : \bar{p}(x) \geq 0\}$ is compact.
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Theorem (Putinar): For a given polynomial $p_0$ one has $p_0(x) > 0$ for all $x \in S$ iff

$$p_0 \in \Sigma^2 + p_1 \Sigma^2 + \ldots + p_k \Sigma^2.$$
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If \( p \) and \( q \) have no common roots in \( S \), then by Putinar’s and Jibetean’s theorems:

\[ p^* = \sup \left\{ \rho : p(x) - \rho q(x) > 0 \; \forall x \in S \right\} \]
\[ = \sup \left\{ \rho : (p - \rho q) \in \Sigma^2 + p_1 \Sigma^2 + \ldots + p_k \Sigma^2 \right\} \]
\[ \geq \sup \left\{ \rho : (p - \rho q) \in \Sigma_{1,t}^2 + p_1 \Sigma_{1,t}^2 + \ldots + p_k \Sigma_{1,t}^2 \right\} \]
\[ := \rho_t \quad \text{(for any integer } t \geq 1). \]
Constrained multivariate case

We have that $\rho_i \leq \rho_{i+1} \leq p^*$ and – if $p$ and $q$ have no common roots in $S$ –

$$\lim_{{t \to \infty}} \rho_t = p^*.$$
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Computation of $\rho_t$: SDP problem with matrices of size $\binom{n+t}{t} \times \binom{n+t}{t}$ and at most $\max\{\deg(p),\deg(q)\}$ constraints — "polynomial" complexity for $t = O(1)$. 
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These results by already obtained by Lasserre for $q(x) \equiv 1$ (polynomial objective function).

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Return to the unconstrained case

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Artificial constraint $\|x\|^2 \leq R$ for some ‘sufficiently large’ $R$.  

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Now we have \( \min_{x \in S} \frac{p(x)}{q(x)} \) where \( S \) is the compact semi-algebraic set

\[ S := \left\{ x \in \mathbb{R}^n : R - \|x\|^2 \geq 0 \right\} . \]
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No a priori choice for \( R \) available in general.
Software

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*GloptiPoly* and *SOStools* extremely useful to prove *global optimality* in small problems.
Discussion

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- SDP approach competitive with state-of-the-art global optimization software.
Discussion

- We have extended results by Nesterov, Lasserre and Parrilo to include rational objective functions.
- Techniques from real algebraic geometry available to compute all KKT points, but SDP approach computationally attractive. See: P. Parrilo and B. Sturmfels. Minimizing polynomial functions, 2001. (Available at arXiv.org e-Print archive)
- SDP approach competitive with state-of-the-art global optimization software.
- Need for large-scale (parallel?) SDP solvers to solve the large SDP relaxations.