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Two approaches to underestimating quadratic functions

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The Application

A nonconvex mathematical programming problem:

$$\begin{array}{lll} \min & f_0(\boldsymbol{x}) & \\ \text{s.t.} & f_m(\boldsymbol{x}) \leq 0 & i = 1, 2, \ldots, M \\ & \boldsymbol{x}^{\boldsymbol{L}} \leq x \leq \boldsymbol{x}^{\boldsymbol{U}} & \end{array}$$

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Many global optimization algorithms use convex underestimation

- branch-and-bound methods
- lower bounds or proof of infeasibility

A Comparison

I will describe two underestimation methods:

- An αBB variant (Skjäl and Westerlund, 2012)
  - smooth ($\mathcal{C}^2$) functions
  - perturbations

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- An αBB variant (Skjäl and Westerlund, 2012)
  - smooth ($\mathcal{C}^2$) functions
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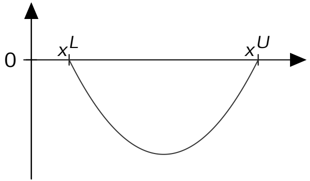
- An underestimation method with roots in algebraic geometry (Jean B. Lasserre and Tung Phan Thanh, 2012)
  - polynomials
  - underestimator of a specified degree

αBB

Perturbations

- All αBB methods use perturbations
- $-\alpha_i(x_i - x_i^L)(x_i^U - x_i)$



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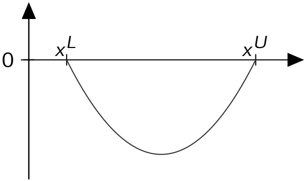

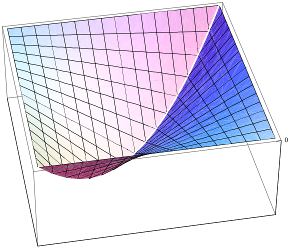

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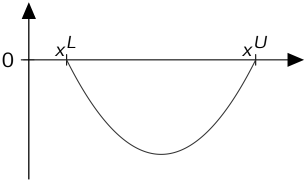
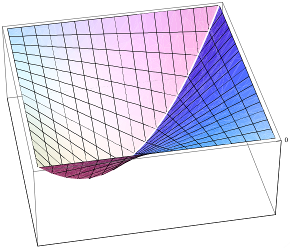
- $-\alpha_i(x_i - x_i^L)(x_i^U - x_i)$
- $\beta_{ij} x_i x_j - \mathrm{conc}(\beta_{ij} x_i x_j)$
- underestimation: ok
- convexity: use a sufficient condition for positive semidefiniteness

$$\nabla^2 f(\boldsymbol{x}) + H^P \succeq 0, \; \forall \boldsymbol{x} \in [\boldsymbol{x}^L, \boldsymbol{x}^U]$$





Parameter Calculation

- Adjiman, Dallwig, Floudas & Neumaier, 1998
  - diagonal
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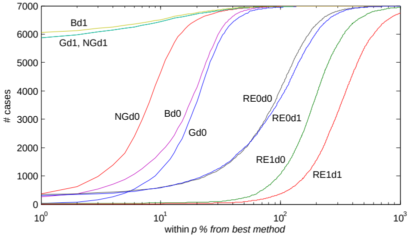
  - additional methods, nondiagonal



(maximum error)

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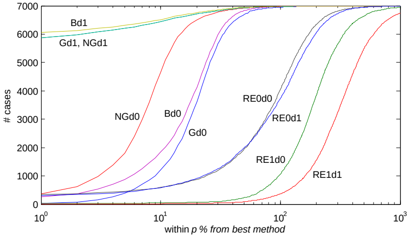
  - diagonal
  - many calculation methods (*e.g.* "Gerschgorin")
- Skjäl & Westerlund, manuscript
  - additional methods, nondiagonal
- The scaled diagonal Gerschgorin method is recommended for general purposes
  - calculation: $O(n^2)$



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Quadratic Functions

- Quadratic functions have constant second derivatives
- No need for interval approximations
- Convexity of the perturbed function is equivalent to

$$H + H^P = H + \begin{bmatrix} 2\alpha_1 & \beta_{1,2} & \cdots & \beta_{1,n} \\ \beta_{1,2} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \beta_{n-1,n} \\ \beta_{1,n} & \cdots & \beta_{n-1,n} & 2\alpha_n \end{bmatrix} \succeq 0$$

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- The best perturbation(s) minimize some error measure
  - in literature: the maximum underestimation error
  - a new choice: the average error

Error Measures

- Maximum underestimation error (L^∞-norm)

$$\sum_i \frac{1}{4}(x_i^U - x_i^L)^2 \alpha_i + \sum_i \sum_{j>i} \frac{1}{4} (x_i^U - x_i^L)(x_j^U - x_j^L) |\beta_{ij}|$$

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- Average error (normalized L^1-norm)
  - α_i weight

$$\frac{\int_{[\mathbf{x}^L,\mathbf{x}^U]} (x_i - x_i^L)(x_i^U - x_i)\,\mathrm{d}\mathbf{x}}{\int_{[\mathbf{x}^L,\mathbf{x}^U]} \mathrm{d}\mathbf{x}} = \frac{1}{6}(x_i^U - x_i^L)^2$$

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  - $|\beta_{ij}|$ weight, symbolical integration with Mathematica

$$\frac{1}{12}(x_i^U - x_i^L)(x_j^U - x_j^L)$$

Lasserre & Thanh's Method

Positive Polynomials on $\mathbb{R}^n$

- If a function can be decomposed as a sum of squares it is nonnegative

$$x^2 - 4xy + 5y^2 - 2yz + z^2 = (x - 2y)^2 + (y - z)^2 \geq 0$$

Positive Polynomials on $\mathbb{R}^n$

Hilbert's Seventeenth Problem

Can any nonnegative polynomial be represented as a sum of squares of rational functions?

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- Hilbert showed that a nonnegative polynomial is not in general a sum of squares of polynomials
- Motzkin gave the first example (1966)

$$z^6 + x^4y^2 + x^2y^4 - 3x^2y^2z^2$$

Positive Polynomials on Semialgebraic Sets

- A set is called semialgebraic if it is described by polynomial inequalities

$$\{\boldsymbol{x} \in \mathbb{R}^n : p_1(x) \geq 0, \ldots, p_m(x) \geq 0\}$$

- Let Σ denote all sums of squares of polynomials in $\boldsymbol{x}$; a convex cone

Positive Polynomials on Semialgebraic Sets

Putinar's Positivstellensatz

Let K be a **compact semialgebraic set.** Assume that $p_1 \dots p_m$ have even degrees and that their highest degree homogenous parts have no common zeroes in $\mathbb{R}^n$, except 0. Then **any positive polynomial** p **on** K **belongs to** the cone $\Sigma + p_1\Sigma + \ldots + p_m\Sigma$.

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Underestimation and Convexity

- Lasserre and Thanh use the Positivstellensatz for both properties
  - underestimation:

$$f(x) - h(x) \geq 0, \quad \forall \boldsymbol{x} \in [\boldsymbol{x^L}, \boldsymbol{x^U}]$$

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$$\boldsymbol{y}^T \nabla^2 h(\boldsymbol{x})\, \boldsymbol{y} \geq 0, \quad \forall \boldsymbol{x} \in [\boldsymbol{x}^{\boldsymbol{L}}, \boldsymbol{x}^{\boldsymbol{U}}], \forall \boldsymbol{y} \in \mathbb{R}^n : \|y\| \leq 1$$

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  - the sets are compact semialgebraic

$$\left\{\boldsymbol{x} \in \mathbb{R}^n : (x_i - x_i^L)(x_i^U - x_i) \geq 0, i = 1, \ldots, n\right\}$$

$$\cap \left\{\boldsymbol{y} \in \mathbb{R}^n : 1 - \sum_i y_i^2 \geq 0\right\}$$

Finite-Dimensional Approximation

- The underestimator degree is fixed, $\deg(h) = d$
- The sum-of-squares cones are restricted

$$\Sigma_k := \{p \in \Sigma : \deg(p) \leq 2k\}$$

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- Lasserre & Thanh proved convergence properties as $k \to \infty$
- Elements in Σ_k kan be represented as positive semidefinite matrices

$$(x-2y)^2+(y-1)^2 = \begin{bmatrix} 1 & x & y \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \\ -2 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 & -2 \\ -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ x \\ y \end{bmatrix}$$

$$= \begin{bmatrix} 1 \\ x \\ y \end{bmatrix}^T \underbrace{\begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -2 \\ -1 & -2 & 5 \end{bmatrix}}_{\succeq 0} \begin{bmatrix} 1 \\ x \\ y \end{bmatrix}$$

Constraints

- The underestimation condition takes the form:

$$f(\boldsymbol{x}) - h(\boldsymbol{x}) = \sigma_0(\boldsymbol{x}) + \sum_{i=1}^{n} \sigma_i(\boldsymbol{x})\,(x_i - x_i^L)(x_i^U - x_i), \qquad \forall \boldsymbol{x}$$

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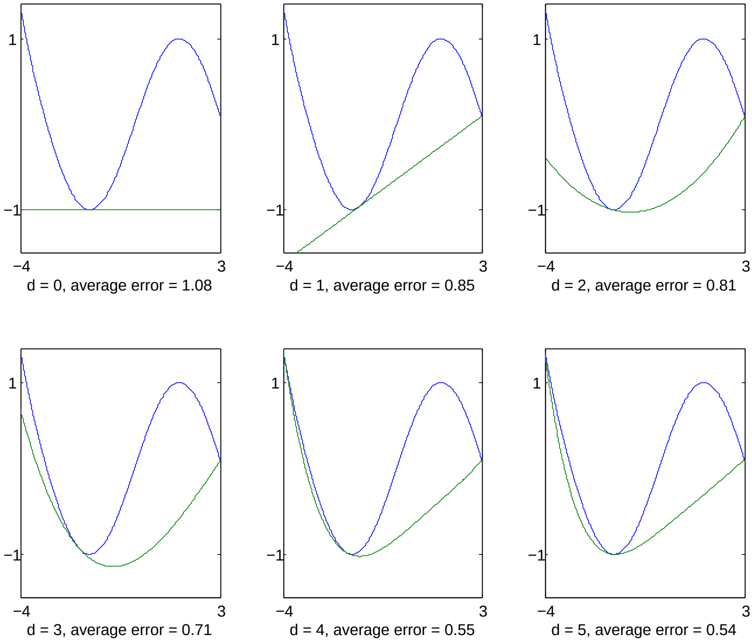
- Rewritten in the monomial basis we get $\binom{n+2k}{n}$ linear constraints

$$f_\alpha - h_\alpha = \sum_{i=0}^{n} \left\langle Z_j, C_\alpha^j \right\rangle$$

involving $n+1$ semidefinite variable matrices

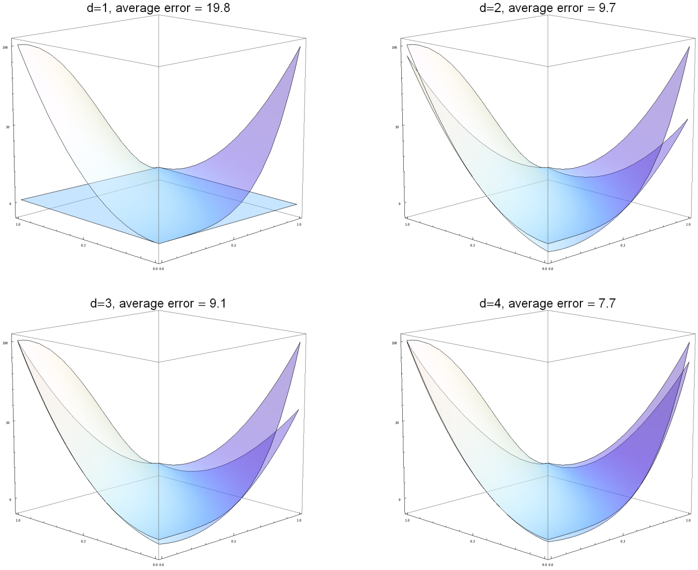
$$Z_j \succeq 0,\ j = 0, 1, \dots, n$$

Example - 1D



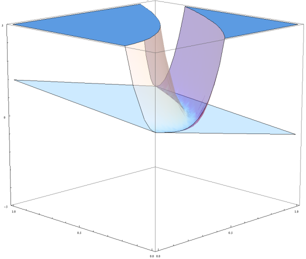
1
−1
−4
3
d = 0, average error = 1.08
d = 1, average error = 0.85
d = 2, average error = 0.81
d = 3, average error = 0.71
d = 4, average error = 0.55
d = 5, average error = 0.54

Example - 2D

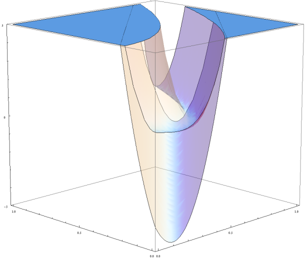

d=1, average error = 19.8
d=2, average error = 9.7
d=3, average error = 9.1
d=4, average error = 7.7

Example - 2D (detail)

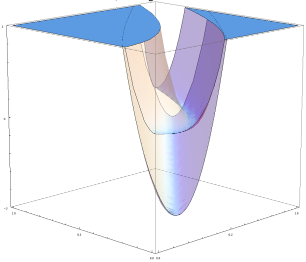
d=1, average error = 19.8



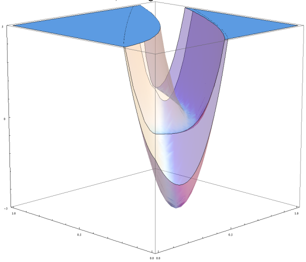
d=2, average error = 9.7



d=3, average error = 9.1



d=4, average error = 7.7



L&T, Quadratic Case

- Lasserre & Thanh's constraints simplify when $\deg(f) = 2, d = 2, k = 1$

$$f(\boldsymbol{x}) - (b + \boldsymbol{a}'\boldsymbol{x} + \boldsymbol{x}'A\boldsymbol{x}) = \sum_{i=1}^{n} \sigma_i (x_i - x_i^L)(x_i^U - x_i) + [\boldsymbol{x}'\ 1]\, C\, [\boldsymbol{x}'\ 1]'$$

$$A \succeq 0,\ C \succeq 0$$

$$\sigma_i \geq 0, \quad \forall i = 1, \ldots, n$$

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- Note the similarity with α perturbations
  $\Rightarrow$ average error better ($\leq$) than diagonal αBB methods
- Nondiagonal αBB was better on a test suite of 300 generated quadratic functions
  - lower average error in all cases, higher minimum in 279 cases

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  - relatively fast
  - introduces additional (linear) constraints and variables
  - slightly tighter and faster in the quadratic case

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  - better for general polynomials
  - a hierarchy of underestimators
  - attractive theoretical convergence
- αBB
  - only requires smoothness
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  - introduces additional (linear) constraints and variables
  - slightly tighter and faster in the quadratic case
- Conclusion: your best choice is problem-dependent!

References

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Thank you for listening!

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Questions?

L&T, Function Form

$$
\begin{cases}
\max\limits_{h \in \mathbb{R}[\mathbf{x}]_d, \sigma_j, \theta_\ell} & \int\limits_{\mathbf{B}} h \, d\lambda \\
 & f(\mathbf{x}) = h(\mathbf{x}) + \sum_{j=0}^{n} \sigma_j(\mathbf{x}) g_j(\mathbf{x}) \quad \forall \mathbf{x} \\
\text{s.t.} & \mathbf{T}h(\mathbf{x}, \mathbf{y}) = \sum_{j=0}^{n} \theta_j(\mathbf{x}, \mathbf{y}) g_j(\mathbf{x}) \\
 & \qquad + \theta_{n+1}(\mathbf{x}, \mathbf{y}) g_{n+1}(\mathbf{x}, \mathbf{y}) \quad \forall \mathbf{x}, \mathbf{y} \\
 & \sigma_0 \in \Sigma[\mathbf{x}]_k, \ \sigma_j \in \Sigma[\mathbf{x}]_{k-1}, \ j \geq 1 \\
 & \theta_0 \in \Sigma[\mathbf{x}, \mathbf{y}]_k, \theta_j \in \Sigma[\mathbf{x}, \mathbf{y}]_{k-1}, \ j \geq 1,
\end{cases}
$$

L&T, SDP Form

$$
\begin{cases}
\max\limits_{h \in \mathbb{R}[\mathbf{x}]_d, \mathbf{Z}_j, \Theta_\ell} & \sum\limits_{\alpha \in \mathbb{N}_d^n} h_\alpha \gamma_\alpha \\
& f_\alpha = h_\alpha + \sum\limits_{j=0}^{n} \langle \mathbf{Z}^j, \mathbf{C}_\alpha^j \rangle, \qquad \forall \alpha \in \mathbb{N}_{2k}^n \\
\text{s.t.} & (\mathbf{T}h)_{\alpha\beta} = \sum\limits_{\ell=0}^{n+1} \langle \Theta_\ell, \Delta_{\alpha\beta}^\ell \rangle, \qquad \forall (\alpha, \beta) \in \mathbb{N}_{2k}^{2n} \\
& \mathbf{Z}^j, \ \Theta^\ell \succeq 0, \quad j = 0, \ldots, n; \ \ell = 0, \ldots, n+1,
\end{cases}
$$