An Extension of the αBB-type Underestimation to Linear Parametric Hessian Matrices

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Problem formulation

Convex underestimators

Let

1. $f : \mathbb{R}^n \mapsto \mathbb{R}$ be a twice-differentiable function,
2. $x_i \in \mathbf{x}_i = [\underline{x}_i, \overline{x}_i]$, $i = 1, \ldots, n$, interval domains for the variables.

Construct a function $g : \mathbb{R}^n \mapsto \mathbb{R}$ satisfying:

1. $f(x) \geq g(x)$ for every $x \in \mathbf{x}$,
2. $g(x)$ is convex on $x \in \mathbf{x}$.

Application

- Deterministic global optimization methods based on branch & bound scheme.
- Rigorous bound on objective and optimal values.
- Rigorous enclosures of constraints.

Forms of underestimators

Forms of underestimators

1. αBB method (Floudas et al., 1995–2013)

$$g(x) := f(x) - \sum_{i=1}^{n} \alpha_i(\overline{x}_i - x_i)(x_i - \underline{x}_i), \qquad (*)$$

2. non-diagonal αBB method (Akrotirianakis et al., 2004, Skjäl et al., 2012)

$$g(x) := f(x) - (\overline{x} - x)^T P(x - \underline{x}) + q(x),$$

   where $q(x)$ is a piecewise linear convex function.

3. γBB method (Akrotirianakis and Floudas, 2004)

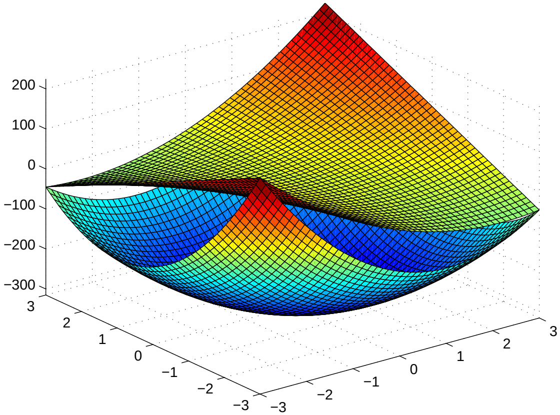
$$g(x) := f(x) - \sum_{i=1}^{n}(1 - e^{\gamma_i(\overline{x}_i - x_i)})(1 - e^{\gamma_i(x_i - \underline{x}_i)}) \qquad (\dagger)$$

Theorem (Floudas and Kreinovich, 2007)

Forms $(*)$ and $(\dagger)$ are the only shift-invariant forms of the gen. scheme

$$g(x) := f(x) - \sum_{i=1}^{n} \alpha_i(g_i(\overline{x}_i) - g_i(x_i))(g_i(x_i) - g_i(\underline{x}_i)).$$

Illustration



Function $f(x)$ and its convex underestimator $g(x)$.

Computation of α

Idea

Choose α large enough to ensure positive semidefinitness of the Hessian of

$$g(x) := f(x) - \sum_{i=1}^{n} \alpha_i(\overline{x}_i - x_i)(x_i - \underline{x}_i),$$

The Hessian of $g(x)$ reads

$$\nabla^2 g(x) = \nabla^2 f(x) + 2\,\mathrm{diag}(\alpha).$$

Interval Hessian matrix

Let $\mathbf{H}$ be an interval matrix enclosing the image of $\nabla^2 f(x)$ over $x \in \mathbf{x}$:

$$\frac{\partial^2}{\partial x_i \partial x_j} f(x) \in \mathbf{h}_{ij} = [\underline{h}_{ij}, \overline{h}_{ij}], \quad \forall x \in \mathbf{x}.$$

Remarks

- Checking positive semidefiniteness of each $H \in \mathbf{H}$ is co-NP-hard (Nemirovskii, 1993).
- Various enclosures for eigenvalues of $H \in \mathbf{H}$.
- Scaled Gerschgorin method enables to express α_i-s.

Computation of α

Scaled Gerschgorin method for α

$$\alpha_i := \max\left\{0, -\frac{1}{2}\left(\underline{h}_{ii} - \sum_{j\neq i} |\mathbf{h}_{ij}| d_j / d_i\right)\right\}, \quad i = 1, \dots, n,$$

where $|\mathbf{h}_{ij}| = \max\left\{|\underline{h}_{ij}|, |\overline{h}_{ij}|\right\}$.

- To reflect the range of the variable domains, use $d := \overline{x} - \underline{x}$.

Theorem (H., 2014)

The choice $d := \overline{x} - \underline{x}$ is optimal (i.e., it minimizes the maximum separation distance between $f(x)$ and $g(x)$) if

$$\underline{h}_{ii} d_i - \sum_{j\neq i} |\mathbf{h}_{ij}| d_j \leq 0, \quad \forall i = 1, \dots, n.$$

An idea for improvement

Consider more gentle enclosure of the Hessian matrices than $\mathbf{H}$.

Hessians in linear parametric forms

An idea for improvement

Consider an interval matrix in a linear parametric form

$$H(p) = \sum_{k=1}^{K} H^{(k)} p_k,$$

where $H^{(1)}, \ldots, H^{(K)} \in \mathbb{R}^{n \times n}$ are fixed matrices and $p_1 \in \mathbf{p}_1, \ldots, p_K \in \mathbf{p}_K$.

Assumption

$$\forall x \in \mathbf{x},\ \exists p \in \mathbf{p} :\ \nabla^2 f(x) = H(p).$$

First (stupid) idea

Evaluate

$$\mathbf{H} := H(\mathbf{p}) = \sum_{k=1}^{K} H^{(k)} \mathbf{p}_k$$

and apply the standard method.

Hessians in linear parametric forms

Second idea

Fix $i \in \{1,\dots,n\}$. Then α_i should satisfy

$$-2\alpha_i \le H(p)_{ii} - \sum_{j\ne i} |H(p)_{ij}| d_j/d_i, \quad \forall p \in \mathbf{p}, \forall i = 1,\dots,n. \qquad (*)$$

Define

$$J^+ := \{j \ne i : \underline{H(\mathbf{p})}_{ij} \ge 0\},$$
$$J^- := \{j \notin J^+ \cup \{i\} : \overline{H(\mathbf{p})}_{ij} \le 0\},$$
$$J^0 := \{1,\dots,n\} \setminus (J^+ \cup J^- \cup \{i\}).$$

For $j \in J^0$, find the best upper estimation

$$|H(p)_{ij}| \le \gamma_{ij} H(p)_{ij} + \beta_{ij},$$

Then $(*)$ reads

$$-2\alpha_i \le H(p)_{ii} - \sum_{j\in J^+} H(p)_{ij}\frac{d_j}{d_i} + \sum_{j\in J^-} H(p)_{ij}\frac{d_j}{d_i} - \sum_{j\in J^0}(\gamma_{ij}H(p)_{ij} + \beta_{ij})\frac{d_j}{d_i}$$
$$= \sum_{k=1}^{K}\left(H_{ii}^{(k)} - \sum_{j\in J^+} H_{ij}^{(k)}\frac{d_j}{d_i} + \sum_{j\in J^-} H_{ij}^{(k)}\frac{d_j}{d_i} - \sum_{j\in J^0}\gamma_{ij}H_{ij}^{(k)}\frac{d_j}{d_i}\right)p_k$$
$$- \sum_{j\in J^0}\beta_{ij}\frac{d_j}{d_i}.$$

Hessians in linear parametric forms

Computation of α

Take

$$\alpha_i := \max\left\{0, -\tfrac{1}{2}\underline{h}_i\right\},$$

where

$$\mathbf{h}_i := \sum_{k=1}^{K}\left(H_{ii}^{(k)} - \sum_{j\in J^+} H_{ij}^{(k)}\frac{d_j}{d_i} + \sum_{j\in J^-} H_{ij}^{(k)}\frac{d_j}{d_i} - \sum_{j\in J^0}\gamma_{ij}H_{ij}^{(k)}\frac{d_j}{d_i}\right)\mathbf{p}_k$$
$$- \sum_{j\in J^0}\beta_{ij}\frac{d_j}{d_i}.$$

Proposition

The second idea is never worse than the first idea.

Example

A class of functions with parametric Hessians:

$$f(x) = \sum_{\ell=1}^{L} c_\ell x_{i_\ell} x_{j_\ell} x_{k_\ell},$$

where $i_\ell, j_\ell, k_\ell \in \{0,\ldots,n\}$ and $x_0 = 1$.

Hessians in linear parametric forms

Example

Let

$$f(x) = x_1^3 + x_1^2 x_2 - 2x_1x_2x_3 + 3x_2x_3^2 - 3x_2^2,$$

where $x \in \mathbf{x} = [0,3] \times [0,3] \times [0,3]$. The Hessian reads

$$\begin{aligned}
\nabla^2 f(x) &= \begin{pmatrix} 6x_1 + 2x_2 & 2x_1 - 2x_3 & -2x_2 \\ 2x_1 - 2x_3 & -6 & -2x_1 + 6x_3 \\ -2x_2 & -2x_1 + 6x_3 & 6x_2 \end{pmatrix} \\
&= \begin{pmatrix} 6 & 2 & 0 \\ 2 & 0 & -2 \\ 0 & -2 & 0 \end{pmatrix} x_1 + \begin{pmatrix} 2 & 0 & -2 \\ 0 & 0 & 0 \\ -2 & 0 & 6 \end{pmatrix} x_2 \\
&+ \begin{pmatrix} 0 & -2 & 0 \\ -2 & 0 & 6 \\ 0 & 6 & 0 \end{pmatrix} x_3 + \begin{pmatrix} 0 & 0 & 0 \\ 0 & -6 & 0 \\ 0 & 0 & 0 \end{pmatrix}.
\end{aligned}$$

- The classical lower bound: -74.1507
- The parametric approach lower bound: -61.5826

Interval computations

Aim

Compute an interval enclosure of the image $f(\mathbf{x}) := \{f(x) : x \in \mathbf{x}\}$.

Interval arithmetic

$$\mathbf{a} + \mathbf{b} = [\underline{a} + \underline{b}, \overline{a} + \overline{b}], \quad \mathbf{a} - \mathbf{b} = [\underline{a} - \overline{b}, \overline{a} - \underline{b}],$$
$$\mathbf{ab} = [\min(\underline{a}\underline{b}, \underline{a}\overline{b}, \overline{a}\underline{b}, \overline{a}\overline{b}), \max(\underline{a}\underline{b}, \underline{a}\overline{b}, \overline{a}\underline{b}, \overline{a}\overline{b})],$$
$$\mathbf{a}/\mathbf{b} = [\min(\underline{a}/\underline{b}, \underline{a}/\overline{b}, \overline{a}/\underline{b}, \overline{a}/\overline{b}), \max(\underline{a}/\underline{b}, \underline{a}/\overline{b}, \overline{a}/\underline{b}, \overline{a}/\overline{b})], \quad 0 \notin \mathbf{b}.$$

Basic functions

$\exp(\mathbf{x}) = [\exp(\underline{x}), \exp(\overline{x})]$, $\mathbf{x}^2 = \ldots$, $\sin(\mathbf{x}) = \ldots$

Natural interval extension

Given an expression for $f(x)$, compute an enclosure by interval arithmetic and basic function evaluation.

Other improvements

Monotonicity checking, interval refinements, ...

Slopes

Slope form enclosure

$$f(\mathbf{x}) \subseteq f(a) + S(\mathbf{x}, a)(\mathbf{x} - a),$$

where $a \in \mathbf{x}$ and

$$S(x, a) := \begin{cases} \frac{f(x)-f(a)}{x-a} & \text{if } x \neq a, \\ f'(x) & \text{otherwise.} \end{cases}$$

Remarks

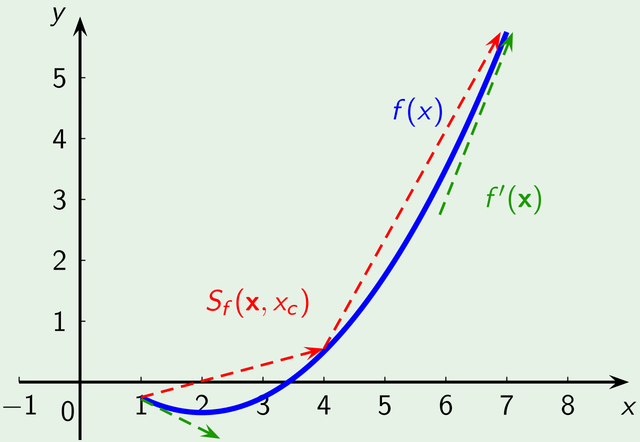
- Slopes can be computed in a similar way as derivatives.
- Slopes can be replaced by derivatives, but slopes gives tighter intervals.

Slopes

Example

$$f(x) = \frac{1}{4}x^2 - x + \frac{1}{2}, \qquad \mathbf{x} = [1, 7].$$

$$f'(\mathbf{x}) = [-\frac{1}{2}, \frac{5}{2}], \qquad S_f(\mathbf{x}, x_c) = [\frac{1}{4}, \frac{7}{4}].$$



Parametric Hessians by slope expansion

Preliminaries

Denote

$$f_{ij}(x) := \frac{\partial^2}{\partial x_i \partial x_j} f(x).$$

Let us have a slope expansion of $f_{ij}(x)$ on $\mathbf{x}$

$$f_{ij}(x) \in f_{ij}(a) + \mathbf{S}_{ij}(\mathbf{x}, a)^T (x - a).$$

Computation of α

$$\alpha_i := \max\left\{0, -\tfrac{1}{2}\underline{h}_i\right\},$$

where

$$\mathbf{h}_i := \left(\mathbf{S}_{ii}(\mathbf{x}, a) - \sum_{j \in J^+} \mathbf{S}_{ij}(\mathbf{x}, a)\frac{d_j}{d_i} + \sum_{j \in J^-} \mathbf{S}_{ij}(\mathbf{x}, a)\frac{d_j}{d_i} - \sum_{j \in J^0} \gamma_{ij}\mathbf{S}_{ij}(\mathbf{x}, a)\frac{d_j}{d_i}\right)^T (\mathbf{x} - a)$$
$$+ f_{ii}(a) - \sum_{j \in J^+} f_{ij}(a)\frac{d_j}{d_i} + \sum_{j \in J^-} f_{ij}(a)\frac{d_j}{d_i} - \sum_{j \in J^0} (\gamma_{ij} f_{ij}(a) + \beta_{ij})\frac{d_j}{d_i}.$$

Parametric Hessians by slope expansion

Choice of the center $a \in \mathbf{x}$

- Quality of the resulting enclosures depends on a.
- Possible choices: x_c, $\underline{x}$, or which one?

Example (Gounaris and Floudas, 2008)

Let

$$f(x) = \left(x_2 - \frac{5.1}{4\pi^2}x_1^2 + \frac{5}{\pi}x_1 - 6\right)^2 + 10\left(1 - \frac{1}{8\pi}\right)\cos(x_1) + 10$$

with $\mathbf{x} = [7, 10] \times [0, 5]$.

- The optimal value: 0.3979
- The classical lower bound: -13.8967
- The parametric approach lower bound with $a = x_c$: -10.9777
- The parametric approach lower bound with $a = \underline{x}$: -27.1285

Conclusion

Conclusion

- Parametric forms of Hessian enclosures enable more delicate construction of convex underestimators
- A parametric form can be obtained by slope expansion.

Open problems

- Choice of the center of slope expansion $a \in \mathbf{x}$