The Effect of Hessian Evaluations in the Global Optimization αBB Method

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Problem formulation

Convex underestimators

Let

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

Remark

- Deterministic global optimization methods based on branch & bound scheme.
- Rigorous enclosures of global minima and optimal value.
- One has has to bound the optimal value on $\mathbf{x}$ from above and below.

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)

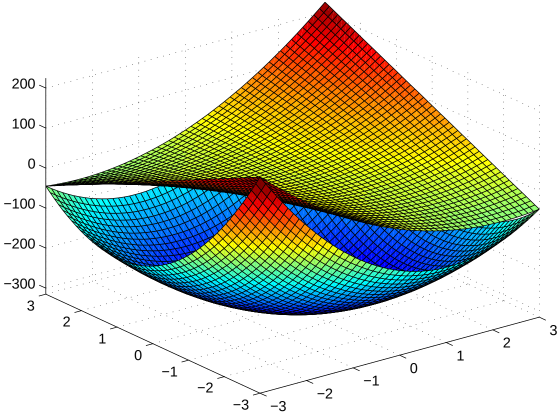
$$g(x) := f(x) - (\overline{x} - x)^T P(x - \underline{x}) + q,$$

3. γBB method (Akrotirianakis and Floudas, 2004)

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

We will consider the form $(*)$.

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

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

Interval Hessian matrix

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

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

Scaled Gerschgorin method for α

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

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

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

Interval computations

Aim

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

Interval arithmetic

$$\mathbf{a}+\mathbf{b} = [\underline{a}+\underline{b}, \overline{a}+\overline{b}], \quad \mathbf{a}-\mathbf{b} = [\underline{a}-\overline{b}, \overline{a}-\underline{b}],$$

$$\mathbf{ab} = [\min(\underline{ab}, \underline{a}\overline{b}, \overline{a}\underline{b}, \overline{a}\overline{b}), \max(\underline{ab}, \underline{a}\overline{b}, \overline{a}\underline{b}, \overline{a}\overline{b})],$$

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

Basic functions

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

General functions

Mean value / slope form: $f(\mathbf{x}) \subseteq f(a) + S(\mathbf{x}, a)(\mathbf{x} - a)$.

Other improvements

Monotonicity checking, interval refinements, …

Symbolic computation of the Hessian

Direct computation of α

Define

$$h_i(x) := \frac{\partial^2}{\partial x_i^2} f(x) - \sum_{j \neq i} \left| \frac{\partial^2}{\partial x_i \partial x_j} f(x) \right| d_j / d_i, \quad i = 1, \ldots, n.$$

The entries of α then follows

$$\alpha_i := \max \left\{ 0, -\frac{1}{2} \underline{h_i(\mathbf{x})} \right\}, \quad i = 1, \ldots, n.$$

Comments

- Do not compute $\mathbf{H}$, and after α, but compute α directly.
- If $0 \notin \frac{\partial^2}{\partial x_i \partial x_j} f(\mathbf{x})$, remove the absolute value.
- Apply symbolic simplifications to the expression for $h_i(x)$.

Example (Gounaris and Floudas, 2008)

Let

$$f(x) = (x_1 + 10x_2)^2 + 5(x_3 - x_4)^2 + (x_2 - 2x_3)^4 + 10(x_1 - x_4)^4,$$

where $x \in \mathbf{x} = [0,1]^4$. It is known that the global minimum is $f^* = 0$.

First, we compute the interval Hessian

$$\nabla^2 f(\mathbf{x}) \subseteq \mathbf{H} = \begin{pmatrix} [-118, 122] & [20, 20] & [0, 0] & [-120, 120] \\ [20, 20] & [176, 248] & [-96, 48] & [0, 0] \\ [0, 0] & [-96, 48] & [-86, 202] & [-10, -10] \\ [-120, 120] & [0, 0] & [-10, -10] & [-110, 130] \end{pmatrix}.$$

and calculate

$$\alpha = (129, 0, 96, 120), \quad f^* \geq -85.1312.$$

Example I.

Example (cont'd)

Let us compute the Hessian matrix symbolically

$$\nabla^2 f(x) = \begin{pmatrix} 2+120(x_1-x_4)^2 & 20 & 0 & -120(x_1-x_4)^2 \\ 20 & 200+12(x_2-2x_3)^2 & -24(x_2-2x_3)^2 & 0 \\ 0 & -24(x_2-2x_3)^2 & 10+48(x_2-2x_3)^2 & -10 \\ -120(x_1-x_4)^2 & 0 & -10 & 10+120(x_1-x_4)^2 \end{pmatrix}.$$

Since all off-diagonal entries are sign stable, we calculate

$$\alpha = (69, 0, 48, 60), \quad f^* \geq -43.2171.$$

Symbolically simplifying $h_1(x)$ to $h_1(x) = -18$, we get

$$\alpha = (18, 0, 0, 0), \quad f^* \geq -1.9768.$$

Example II.

Example (Adjiman et al., 1998)

Let

$$f(x_1, x_2) = \cos(x_1)\sin(x_2) - \frac{x_1}{x_2^2 + 1},$$

where $x_1 \in [-1, 2]$ and $x_2 \in [-1, 1]$. The optimal value is known to be $f^* = -2.02181$.

By the classical αBB method, we compute

$$\nabla^2 f(\mathbf{x}) \subseteq \mathbf{H} = \begin{pmatrix} [-0.8415, 0.8415] & [-5.0000, 4.8415] \\ [-5.0000, 4.8415] & [-18.8415, 20.8415] \end{pmatrix},$$

and get

$$\alpha = (2.0874, 13.1707), \quad f^* \geq -18.4970.$$

Example II.

Example (cont'd)

Using the symbolical approach,

$$\nabla^2 f(x) = \begin{pmatrix} -\cos(x_1)\sin(x_2) & -\sin(x_1)\cos(x_2) + \dfrac{2x_2}{(x_2^2+1)^2} \\ -\sin(x_1)\cos(x_2) + \dfrac{2x_2}{(x_2^2+1)^2} & -\cos(x_1)\sin(x_2) + \dfrac{2x_1(x_2^2+1)^2 - 8x_1x_2^2(x_2^2+1)}{(x_2^2+1)^4} \end{pmatrix}.$$

If

$$h_2(x) = -\cos(x_1)\sin(x_2) + \frac{2x_1(x_2^2+1)^2 - 8x_1x_2^2(x_2^2+1)}{(x_2^2+1)^4} - \frac{2}{3}\left| -\sin(x_1)\cos(x_2) + \frac{2x_2}{(x_2^2+1)^2} \right|$$

is simplified to

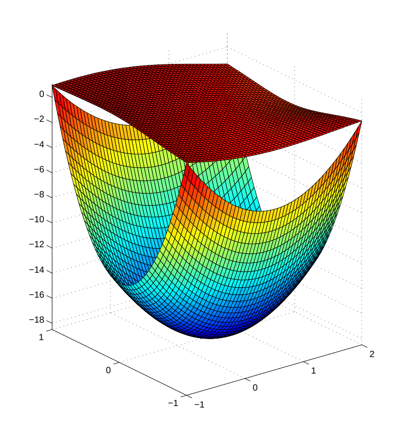
$$h_2(x) = -\cos(x_1)\sin(x_2) + \frac{2x_1(2-6x_2^2)}{(x_2^2+1)^3} - \frac{2}{3}\left| -\sin(x_1)\cos(x_2) + \frac{2x_2}{(x_2^2+1)^2} \right|.$$

we calculate

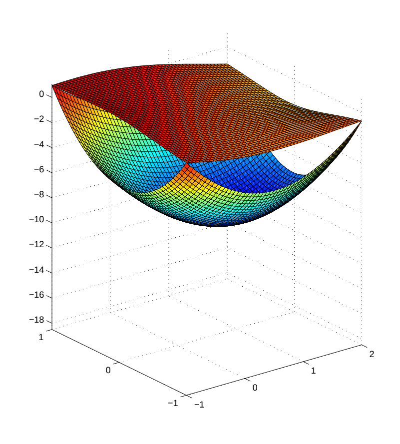
$$\alpha = (1.4208, 5.4208), \qquad f^* \geq -9.3110.$$

Example II.

Example (cont'd)



Traditional approach.



Symbolic approach.

Example III.

Example (Skjäl et al., 2012)

Let

$$f(x_1, x_2) = (1 + x_1 - e^{x_2})^2,$$

where $x_1 \in [0, 1]$ and $x_2 \in [0, 2]$. The optimal value is $f^* = 0$.

By the classical αBB method, we compute

$$f^* \geq -14.46.$$

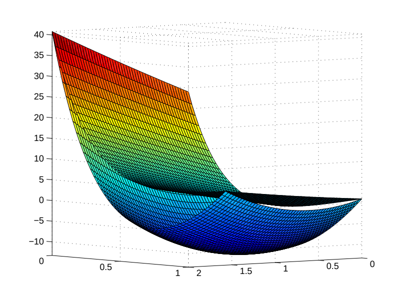
In the symbolic approach, by factoring $h_2(x)$ to

$$h_2(x) = (-3 - 2x_1 + 4e^{x_2})e^{x_2}.$$

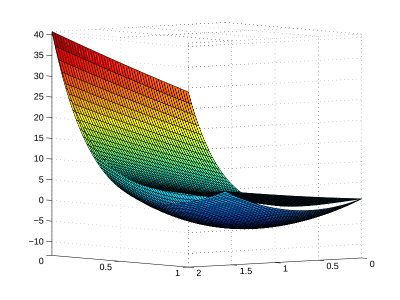
we get

$$f^* \geq -6.5629.$$

Example (cont'd)



Traditional approach.



Symbolic approach.

Further improvements

Recall that

$$\alpha_i := \max\left\{0, -\tfrac{1}{2}\, \underline{h_i(\mathbf{x})}\right\}, \quad i = 1, \dots, n,$$

where

$$h_i(x) := \tfrac{\partial^2}{\partial x_i^2} f(x) - \textstyle\sum_{j \neq i} \left| \tfrac{\partial^2}{\partial x_i \partial x_j} f(x) \right| d_j / d_i, \quad i = 1, \dots, n.$$

Idea: Linearize the absolute values from above.

Proposition

For every $y \in \mathbf{y} \subset \mathbb{R}$ with $\underline{y} < \overline{y}$ one has

$$|y| \leq \alpha y + \beta, \qquad (*)$$

where

$$\alpha = \frac{|\overline{y}| - |\underline{y}|}{\overline{y} - \underline{y}} \quad \text{and} \quad \beta = \frac{\overline{y}|\underline{y}| - \underline{y}|\overline{y}|}{\overline{y} - \underline{y}}.$$

Moreover, if $\underline{y} \geq 0$ or $\overline{y} \leq 0$ then $(*)$ holds as equation.

Conclusion and future work

The main message

- Symbolic evaluation may much more efficient than the automatic one.
- Promising field of research.

Challenge

- Symbolic simplifications of expressions.

Future work

- Handling the absolute value: linearization and numerical testing.

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