Preprocessing of Unconstrained Nonlinear Optimization Problems by Symbolic Computation Techniques

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Introduction

Consider the unconstrained nonlinear optimization problem

$$\min_{x \in \mathbb{R}^n} f(x),$$

where $f(x)$:

- $\mathbb{R}^n \rightarrow \mathbb{R}$,
- nonlinear and twice continuously differentiable,
- given by symbolic expression, a formula.

Aim: produce an equivalent problem form by symbolic transformations, what is “simpler”
Symbolic approaches in optimization

There are some examples, mainly in linear and integer programming:

- “presolving” mechanism of the AMPL processor (Gay, 2001)
- LP preprocessing (Mészáros and Suhl., 2003)
- the Reformulation-Optimization Software Engine (Liberti et al., 2010)
- Gröbner bases theory, quantifier elimination and other algebraic techniques for solving optimization problems (Kanno et al., 2008)
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Example: a parameter estimation problem

Consider a parameter estimation problem, minimization of the sum-of-squares form objective function:

$$F(R_{aw}, I_{aw}, B, \tau) = \left[ \frac{1}{m} \sum_{i=1}^{m} |Z_L(\omega_i) - Z'_L(\omega_i)|^2 \right]^{1/2}$$

The original nonlinear model function, based on obvious physical parameters:

$$Z'_L(\omega) = R_{aw} + \frac{B\pi}{4.6\omega} - i \left( I_{aw}\omega + \frac{B \log(\gamma \tau \omega)}{\omega} \right)$$

$\omega_i$ for $i = 1, 2, \ldots, m$: frequencies, $\gamma = 10^{1/4}$, $i$: the imaginary unit
Successful transformation

The original nonlinear model function, based on obvious physical parameters:

\[ Z'_L(\omega) = R_{aw} + \frac{B\pi}{4.6\omega} - i \left( l_{aw}\omega + \frac{B \log(\gamma \tau \omega)}{\omega} \right) \]

parameters: \( R_{aw}, l_{aw}, B, \tau \)

\( \omega; \text{ for } i = 1, 2, \ldots, m: \text{ frequencies}, \gamma = 10^{1/4}, i: \text{ the imaginary unit} \)

A simplified and still equivalent model function exists (linear in the model parameters):

\[ Z'_L(\omega) = R_{aw} + \frac{B\pi}{4.6\omega} - i \left( l_{aw}\omega + \frac{A + 0.25B + B \log(\omega)}{\omega} \right) \]

parameters: \( R_{aw}, l_{aw}, B, A \)

\( A = B \log(\tau) \) changes the problem from nonlinear to linear least squares problem.
Successful transformation

The original nonlinear model function, based on obvious physical parameters:

\[ Z_L'(\omega) = R_{aw} + \frac{B\pi}{4.6\omega} - i \left( I_{aw}\omega + \frac{B\log(\gamma\tau\omega)}{\omega} \right) \]

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\( A = B\log(\tau) \) changes the problem from nonlinear to linear least squares problem.
Aims for our symbolic simplifier method

Let’s find transformations on the formula of a function, that

- eliminate parts of the computation tree,
- help to recognize unimodality,
- give an equivalent form of the optimization problem,
- reduce (at least not extend) the dimension of the problem, and
- can be done automatically.
Unimodality

Definition

The \( n \)-dimensional \( f(x) \) continuous function is \textit{unimodal} on an open set \( X \subseteq \mathbb{R}^n \) if there exists a set of infinite continuous curves such that the curve system is a homeomorphic mapping of the polar coordinate system of the \( n \)-dimensional space, and the function \( f(x) \) grows strictly monotonically along the curves.

Theorem

The continuous function \( f(x) \) is unimodal in the \( n \)-dimensional real space if and only if there exists a homeomorph variable transformation \( y = h(x) \) such that \( f(x) = f(h^{-1}(y)) = y^T y + c \), where \( c \) is a real constant, and the origin is in the range \( S \) of \( h(x) \).
Equivalence

Theorem

If \( h(x) \) is smooth and strictly monotonic in \( x_i \), then the corresponding transformation simplifies the function in the sense that each occurrence of \( h(x) \) in the expression of \( f(x) \) is padded by a variable in the transformed function \( g(y) \), while every local minimizer (or maximizer) point of \( f(x) \) is transformed to a local minimizer (maximizer) point of the function \( g(y) \).

Theorem

If \( h(x) \) is smooth, strictly monotonic as a function of \( x_i \), and its range is equal to \( \mathbb{R} \), then for every local minimizer (or maximizer) point \( y^* \) of the transformed function \( g(y) \) there exists an \( x^* \) such that \( y^* \) is the transform of \( x^* \), and \( x^* \) is a local minimizer (maximizer) point of \( f(x) \).
Recognition of redundant variables

Assertion

If a variable $x_i$ appears everywhere in the expression of a smooth function $f(x)$ in a term $h(x)$, then the partial derivative $\frac{\partial f(x)}{\partial x_i}$ can be written in the form $(\frac{\partial h(x)}{\partial x_i})p(x)$, where $p(x)$ is continuously differentiable.

Assertion

If the variables $x_i$ and $x_j$ appear everywhere in the expression of a smooth function $f(x)$ in a term $h(x)$, then the partial derivatives $\frac{\partial f(x)}{\partial x_i}$ and $\frac{\partial f(x)}{\partial x_j}$ can be factorized in the forms $(\frac{\partial h(x)}{\partial x_i})p(x)$ and $(\frac{\partial h(x)}{\partial x_j})q(x)$, respectively, and $p(x) = q(x)$.
Algorithm

1. compute the gradient of the original function,
2. factorize the partial derivatives,
3. determine the substitutable subexpressions and substitute them:
   3.1 if the factorization was successful, then explore the subexpressions that can be obtained by integration of the factors,
   3.2 if the factorization was not possible, then explore the subexpressions that are linear in the related variables,
4. solve the simplified problem if possible, and give the solution of the original problem by transformation, and
5. verify the obtained results.
A successful example

The objective function of the Rosenbrock problem is:

\[ f(x) = 100 \left( x_1^2 - x_2 \right)^2 + (1 - x_1)^2. \]

We run the simplifier algorithm with the procedure call:

\[ \text{symbsimp([x2, x1], 100*(x1^2-x2)^2+(1-x1)^2);} \]

In the first step, the algorithm determines the partial differentials:

\[ dx(1) = -200x_1^2 + 200x_2 \]
\[ dx(2) = 400(x_1^2 - x_2)x_1 - 2 + 2x_1 \]
Then the factorized forms of the partial derivatives are computed:

\[
\text{factor}(dx(1)) = -200x_1^2 + 200x_2,
\]

\[
\text{factor}(dx(2)) = 400x_1^3 - 400x_1x_2 - 2 + 2x_1.
\]

The list of the subexpressions of \( f \), ordered by the complexity in \( x_2 \) is the following:

\[
\{100(x_1^2 - x_2)^2, (x_1^2 - x_2)^2, x_1^2 - x_2, -x_2, x_2, (1 - x_1)^2, x_1^2, 100, 2, -1\}.
\]
A successful example 3

The transformed function at this point of the algorithm is

\[ g = 100y_1^2 + (1 - x_1)^2. \]

Now compute again the partial derivatives and their factorization:

\[ \text{factor(dx(1))} = dx(1) = 200y_1, \]
\[ \text{factor(dx(2))} = dx(2) = -2 + 2x_1. \]

The final simplified function, what our automatic simplifier method produced is

\[ g = 100y_1^2 + y_2^2. \]
Notions on the quality of the results

A: simplifying transformations are possible according to the presented theory,
B: simplifying transformations are possible with the extension of the presented theory,
C: some useful transformations could be possible with the extension of the presented theory, but they not necessarily simplify the problem at all points (e.g. since they increase the dimensionality),
D: we do not expect any useful transformation.

Our program produced ...
1: proper substitutions,
2: no substitutions,
3: incorrect substitutions.

The mistake is due to the incomplete ...
 a: algebraic substitution,
 b: range calculation.
Results for the problems in the original article

<table>
<thead>
<tr>
<th>ID</th>
<th>Function $f$</th>
<th>Function $g$</th>
<th>Substitutions</th>
<th>Result type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cos</td>
<td>$\cos(e^{x_1} + x_2) + \cos(x_2)$</td>
<td>$\cos(y_1) + \cos(y_2)$</td>
<td>$y_1 = e^{x_1} + x_2, y_2 = x_2$</td>
<td>A1</td>
</tr>
<tr>
<td>ParamEst1</td>
<td>$[\frac{1}{3} \sum_{i=1}^{3}</td>
<td>Z_L(\omega_i)</td>
<td>- g_1$</td>
<td>$.5773502693y_5^{1/2}$</td>
</tr>
<tr>
<td>ParamEst2</td>
<td>$[\frac{1}{3} \sum_{i=1}^{3}</td>
<td>Z_L(\omega_i)</td>
<td>- Z_L''(\omega_i)</td>
<td>^2]^{1/2}$</td>
</tr>
<tr>
<td>ParamEst3</td>
<td>$[\frac{1}{3} \sum_{i=1}^{3}</td>
<td>Z_L(\omega_i)</td>
<td>- Z_L''(\omega_i)</td>
<td>^2]^{1/2}$</td>
</tr>
<tr>
<td>Otis</td>
<td>$(</td>
<td>Z_L(s)</td>
<td>- Z_m(s)</td>
<td>^2)^{1/2}$ - $(</td>
</tr>
</tbody>
</table>
Results for standard Global optimization problems

<table>
<thead>
<tr>
<th>ID</th>
<th>Function $g$</th>
<th>Substitutions</th>
<th>Result type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rosenbrock</td>
<td>$100y_2^2 + (1 - y_1)^2$</td>
<td>$y_1 = x_1, y_2 = y_1^2 - x_2$</td>
<td>A1</td>
</tr>
<tr>
<td>Shekel-5</td>
<td>memory error</td>
<td>none</td>
<td>D2</td>
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<tr>
<td>Hartman-3</td>
<td>none</td>
<td>none</td>
<td>D2</td>
</tr>
<tr>
<td>Hartman-6</td>
<td>none</td>
<td>none</td>
<td>D2</td>
</tr>
<tr>
<td>Goldstein-Prize</td>
<td>none</td>
<td>none</td>
<td>D2</td>
</tr>
<tr>
<td>RCOS</td>
<td>$y_2^2 + 10(1 - 1/8/\pi)\cos(y_1) + 10$</td>
<td>$y_1 = x_1, y_2 = 5/\pi y_1 - 1.2750000000y_1^2/\pi^2 + x_2 - 6$</td>
<td>A1</td>
</tr>
<tr>
<td>Six-Hump-Camel-Back</td>
<td>none</td>
<td>none</td>
<td>D2</td>
</tr>
</tbody>
</table>
Other often used global optimization test functions

<table>
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<tr>
<th>ID</th>
<th>Function $g$</th>
<th>Substitutions</th>
<th>Result type</th>
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</thead>
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<td>Levy-1</td>
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<td>D2</td>
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<tr>
<td>Levy-2</td>
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<tr>
<td>Levy-3</td>
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<tr>
<td>Booth</td>
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<td>none</td>
<td>C2</td>
</tr>
<tr>
<td>Beale</td>
<td>none</td>
<td>none</td>
<td>C2</td>
</tr>
<tr>
<td>Powell</td>
<td>$(y_1 + 10y_2)^2 + 5(y_3 + y_4)^2 + (y_2 - 2y_3)^4 + 10(y_1 + y_4)^4$</td>
<td>$y_1 = x_1, y_2 = x_2, y_3 = x_3, y_4 = -x_4$</td>
<td>D2</td>
</tr>
<tr>
<td>Matyas</td>
<td>none</td>
<td>none</td>
<td>D2</td>
</tr>
<tr>
<td>Schwefel $(n = 2)$</td>
<td>none</td>
<td>none</td>
<td>C2</td>
</tr>
<tr>
<td>Schwefel-227</td>
<td>$y_2^2 + .25y_1$</td>
<td>none</td>
<td>A1</td>
</tr>
<tr>
<td>Schwefel-31 $(n = 5)$</td>
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<td>none</td>
<td>D2</td>
</tr>
<tr>
<td>Schwefel-32 $(n = 2)$</td>
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<td>none</td>
<td>D2</td>
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<tr>
<td>Rastrigin $(n = 2)$</td>
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<td>C2</td>
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<td>Ratz-4</td>
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<td>C2</td>
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<td>D2</td>
</tr>
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<td>Griewank-5</td>
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<td>none</td>
<td>D2</td>
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</tbody>
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Bibliography 2

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