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 $f(x)$:

- $\mathbb{R}^n \to \mathbb{R}$,
- 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)
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Example: a parameter estimation problem

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

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

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

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

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

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parameters: R_{aw}, I_{aw}, B, τ

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

$$Z_L'(\omega) = R_{aw} + \frac{B\pi}{4.6\omega} - \imath\left(I_{aw}\omega + \frac{A + 0.25B + B\log(\omega)}{\omega}\right)$$

parameters: R_{aw}, I_{aw}, B, A

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

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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 *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 $\partial f(x)/\partial x_i$ can be written in the form $(\partial h(x)/\partial x_i)\, p(x)$, 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 $\partial f(x)/\partial x_i$ and $\partial f(x)/\partial x_j$ can be factorized in the forms $(\partial h(x)/\partial x_i)\, p(x)$ and $(\partial h(x)/\partial x_j)\, q(x)$, 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:

```
symbsimp([x2, x1], 100*(x1^2-x2)^2+(1-x1)^2);
```

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

$$\mathtt{dx(1)} = -200x_1^2 + 200x_2$$

$$\mathtt{dx(2)} = 400(x_1^2 - x_2)x_1 - 2 + 2x_1$$

A successful example 2

Then the factorized forms of the partial derivatives are computed:

$$\texttt{factor(dx(1))} = -200x_1^2 + 200x_2,$$

$$\texttt{factor(dx(2))} = 400x_1^3 - 400x_1x_2 - 2 + 2x_1.$$

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:

$$\texttt{factor(dx(1))} = \texttt{dx(1)} = 200y_1,$$

$$\texttt{factor(dx(2))} = \texttt{dx(2)} = -2 + 2x_1.$$

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

ID	Function f	Function g	Substitutions	Result type
Cos	$\cos(e^{x_1} + x_2) + \cos(x_2)$	$\cos(y_1)+\cos(y_2)$	$y_1 = e^{x_1} + x_2, y_2 = x_2$	A1
ParamEst1	$[\frac{1}{3}\sum_{i=1}^{3} \lvert Z_L(\omega_i) - Z_L'(\omega_i)\rvert^2]^{1/2}$	g_1	$y_1 = \omega, y_2 = -R_{aw}, y_3 = I_{aw}, y_4 = B, y_5 = \tau$	A2a
ParamEst2	$[\frac{1}{3}\sum_{i=1}^{3} \lvert Z_L(\omega_i) - Z_L''(\omega_i)\rvert^2]^{1/2}$	$.5773502693 y_5^{1/2}$	$y_1 = \omega, y_2 = -R_{aw}, y_3 = I_{aw}, y_4 = B, y_5$	A3ab
ParamEst3	$[\frac{1}{3}\sum_{i=1}^{3} \lvert Z_L(\omega_i) - Z_L'''(\omega_i)\rvert^2]^{1/2}$	$.5773502693 y_5^{1/2}$	$y_1 = \omega, y_2 = -R_{aw}, y_3 = I_{aw}, y_4 = B, y_5$	A3b
Otis	$(\lvert Z_L(s) - Z_m(s)\rvert^2)^{1/2}$	$(\lvert - Z_L[1] + 1.\frac{y_2}{y_4}\rvert^2)^{1/2}$	$y_1 = s, y_2 = I_C(R_1 + R_2)C_1C_2y_1^3 + (I_C(C_1+C_2)+(R_C(R_1+R_2) + R_1R_2)C_1C_2)y_1^2 + (R_C(C_1+C_2)+R_1C_1+R_2C_2)y_1 + 1, y_4 = (R_1 + R_2)C_1C_2y_1^2 + (C_1+C_2)y_1$	B3

Results for standard Global optimization problems

ID	Function g	Substitutions	Result type
Rosenbrock	$100y_2^2 + (1 - y_1)^2$	$y_1 = x_1, y_2 = y_1^2 - x_2$	A1
Shekel-5	memory error	none	D2
Hartman-3	none	none	D2
Hartman-6	none	none	D2
Goldstein-Prize	none	none	D2
RCOS	$y_2^2 + 10(1 - 1/8/\pi) * \cos(y_1) + 10$	$y_1 = x_1, y_2 = 5/\pi y_1 - 1.275000000 y_1^2/\pi^2 + x_2 - 6$	A1
Six-Hump-Camel-Back	none	none	D2

Other often used global optimization test functions

ID	Function g	Substitutions	Result type
Levy-1	none	none	D2
Levy-2	none	none	D2
Levy-3	none	none	D2
Booth	none	none	C2
Beale	none	none	C2
Powell	$(y_1+10y_2)^2+5(y_3+y_4)^2+(y_2-2y_3)^4+10(y_1+y_4)^4$	$y_1 = x_1, y_2 = x_2, y_3 = x_3, y_4 = -x_4$	D2
Matyas	none	none	D2
Schwefel ($n=2$)	none	none	C2
Schwefel-227	$y_2^2 + .25y_1$	$y_1 = x_1, y_2 = y_1^2 + x_2^2 - 2y_1$	A1
Schwefel-31 ($n=5$)	none	none	D2
Schwefel32 ($n=2$)	none	none	D2
Rastrigin ($n=2$)	none	none	C2
Ratz-4	none	none	C2
Easom	none	none	D2
Griewank-5	none	none	D2

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