A Derivative-Free Optimization Algorithm with Low-Dimensional Subspace Techniques for Large-Scale Problems

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- A framework of subspace algorithms
- A practical subspace algorithm: NEWUOAs
- A Numerical results
- Concluding remarks

• The problem

In this talk, to make things simple, we consider unconstrained optimization problem

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- Most of the current methods depend on derivatives.
- In many real-world problems, the derivatives are unavailable.
- Suppose that
 - $\bullet~f$ is smooth, but the derivatives are unavailable;
 - the function evaluation of f is expensive.

• Importance and difficulty

We consider optimization without derivatives one of the most important, open, and challenging areas in computational science and engineering, and one with enormous practical potential.

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Develop optimization algorithms that

- do not use derivatives;
- use function evaluations as less as possible.

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- Two main classes of rigorous methods in DFO:
 - directional methods, like direct search;
 - model-based methods, like trust-region methods.



A. R. Conn, K. Scheinberg, and L. N. Vicente, Introduction to Derivative-Free Optimization, MOS-SIAM Series on Optimization, SIAM, Philadelphia, 2009

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- Trust region technique: Minimize Model Function Subject to Trust Region.
- Model construction: Objective Function $\xrightarrow{\text{Interplolation}}$ Model Function.

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- A linear system with degree of freedom (n+1)(n+2)/2.
- What if $|\mathcal{I}| < (n+1)(n+2)/2$ (for example, $|\mathcal{I}| = O(n)$)?
- Regularization:

$$\min_{Q \in \mathcal{Q}} \mathscr{F}(Q)$$
 s.t. $Q(x) = f(x), \quad x \in \mathcal{I}.$

2. A framework of subspace algorithms

• Why subspace?

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- quadratic-model-based methods:
 - in principle, the degree of freedom of a full quadratic model is (n+1)(n+2)/2;
 - in practice, we hope the algorithms finish the job with number of function evaluations of O(n).
- difficult to exploit the structure.

Basic idea

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- Solve a difficult problem by solving a sequence of easy problems;
- solve a large problem by solving a sequence of small problems.

• Subspace techniques in optimization

- Yuan, Ya-xiang. Subspace techniques for nonlinear optimization. Some topics in industrial and applied mathematics 8 (2007): 206-218.
- Gould, Nick, A. Sartenaer, and Ph L. Toint. On iterated-subspace minimization methods for nonlinear optimization. Rutherford Appleton Laboratory, 1994.

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- Coordinate-search ...

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- Step 3. Solve the Subproblem. Solve the subspace subproblem

$$\min_{d\in\mathcal{S}_k} f(x_k+d)$$

exactly or approximately, obtaining d_k .

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Step 4. Update the Iterate. If $f(x_k + d_k) < f(x_k)$, then

 $x_{k+1} := x_k + d_k$; else $x_{k+1} := x_k$. k := k + 1. Goto Step 2.

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• d_k is exact enough \Leftarrow existing derivative-free algorithms

3. A practical subspace algorithm: NEWUOAs

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July 29, 2013 22 / 36

• NEWUOAs

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- Subproblem solver: NEWUOA.

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- Interpolation set *I_k* ⇒ Quadratic model *Q_k* ⇒ Approximate gradient *ğ_k* = ∇*Q_k(x_k*).
- Subproblem solver: NEWUOA.
 - The parameter RHOEND controls the precision of d_k .



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- $\nabla^2 Q_k$ positive definite, $A_k = [\nabla^2 Q_k]^{-1}$;
- $\nabla^2 Q_k$ not positive definite, $A_k = ?$

• Relatively large problems (n=50, 100, 150, 200)



Fig 1 : Numerical comparison between NEWUOA and NEWUOAs $(au=10^{-2})$

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• Relatively large problems (n=50, 100, 150, 200, cont.)



Fig 2 : Numerical comparison between <code>NEWUOA</code> and <code>NEWUOAs</code> ($au=10^{-4}$)

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• Relatively large problems (n=50, 100, 150, 200, cont.)



Fig 3 : Numerical comparison between NEWUOA and NEWUOAs ($au = 10^{-6}$)

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• Relatively large problems (n=50, 100, 150, 200, cont.)



Fig 4 : Numerical comparison between NEWUOA and NEWUOAs ($au=10^{-8}$)

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Large problems

Tab 1 : The performance of NEWUOAs on some 2000-dimensional problems

| | fstart | $f_{\sf best}$ | #f | CPU (s) |
|----------|--------------|----------------|-------|---------|
| ARWHEAD | 5.997000E+03 | 0.000000E+00 | 16095 | 6.42 |
| BRYBND | 7.200000E+04 | 6.486038E-09 | 50000 | 26.09 |
| DIXMAANE | 1.471453E+04 | 1.000000E+00 | 36264 | 21.12 |
| DIXMAANF | 2.734976E+04 | 1.000000E+00 | 36384 | 31.07 |
| DIXMAANG | 5.069653E+04 | 1.000000E+00 | 36393 | 22.72 |
| DQRTIC | 6.376035E+15 | 1.214880E-38 | 40854 | 14.70 |
| GENHUMPS | 5.122260E+07 | 1.624799E-26 | 36467 | 23.54 |
| LIARWHD | 1.170000E+06 | 2.428807E-24 | 16208 | 6.73 |
| POWER | 2.668667E+09 | 1.423292E-11 | 20130 | 19.19 |
| SPARSQUR | 5.627812E+05 | 6.381755E-30 | 16209 | 9.87 |

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- A framework of subspace algorithms
- A practical subspace algorithm NEWUOAs
- Preconditioning techniques
- New strategy for defining the subspace
- Extend to constrained problems
- General preconditioning techniques

Obrigado! 谢谢! zhang@mat.uc.pt www.zhangzk.net

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Happy birthday!

Happy birthday, Grandpa!

