Nonlinear stepsize control, Trust-Region and Regularization Algorithms for Unconstrained Optimization

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Outline

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   - Quadratic
2. Nonlinear stepsize control
3. Conclusions

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The problem

We consider the unconstrained nonlinear programming problem:

$$\text{minimize} \quad f(x)$$

for $x \in \mathbf{R}^n$ and $f : \mathbf{R}^n \to \mathbf{R}$ smooth.

Important special case: the nonlinear least-squares problem

$$\text{minimize} \quad f(x) = \tfrac{1}{2}\|F(x)\|^2$$

for $x \in \mathbf{R}^n$ and $F : \mathbf{R}^n \to \mathbf{R}^m$ smooth.

Work in progress...

Unconstrained optimization — a “mature” area?

$$\underset{x \in \mathbf{R}^n}{\text{minimize}} \;\; f(x) \;\; \text{where} \;\; f \in C^1 \quad (\text{maybe} \quad C^2 \;)$$

Currently two main competing (but similar) methodologies

- **Linesearch methods**
  - compute a descent direction s_k from x_k
  - set $x_{k+1} = x_k + \alpha_k s_k$ to improve f
- **Trust-region methods**
  - compute a step s_k from x_k to improve a model m_k of f within the trust-region $\|s\| \leq \Delta$
  - set $x_{k+1} = x_k + s_k$ if m_k and f “agree” at $x_k + s_k$
  - otherwise set $x_{k+1} = x_k$ and reduce the radius Δ

A useful theoretical observation

Consider trust-region method where

model = true objective function

Then

- model and objective always agree
- trust-region radius goes to infinity

$\Rightarrow$ **a linesearch method**

Nice consequence:

A unique convergence theory!

(Shultz/Schnabel/Byrd, 1985, T., 1988, Conn/Gould/T., 2000)

The keys to convergence theory for trust regions

The Cauchy condition:

$$m_k(x_k) - m_k(x_k + s_k) \geq \kappa_{\rm TR} \|g_k\| \min \left[\frac{\|g_k\|}{1 + \|H_k\|}, \Delta_k \right]$$

The bound on the stepsize:

$$\|s\| \leq \Delta$$

And we derive:

Global convergence to first/second-order critical points

Is there anything more to say?

Regularization Techniques

Is there anything more to say?

Observe the following: if

- f has gradient g and globally Lipschitz continuous Hessian H with constant $2L$

Taylor, Cauchy-Schwarz and Lipschitz imply

$$\begin{aligned} f(x+s) &= f(x) + \langle s, g(x)\rangle + \tfrac{1}{2}\langle s, H(x)s\rangle \\ &\quad + \int_0^1 (1-\alpha)\langle s, [H(x+\alpha s) - H(x)]s\rangle \, d\alpha \\ &\leq \underbrace{f(x) + \langle s, g(x)\rangle + \tfrac{1}{2}\langle s, H(x)s\rangle + \tfrac{1}{3}L\|s\|_2^3}_{m(s)} \end{aligned}$$

$\Longrightarrow$ reducing m from $s = 0$ improves f since $m(0) = f(x)$.

The cubic regularization

Change from

$$\min_s \quad f(x) + \langle s, g(x) \rangle + \tfrac{1}{2}\langle s, H(x)s \rangle \;\; \text{s.t.} \;\; \|s\| \le \Delta$$

to

$$\min_s \quad f(x) + \langle s, g(x) \rangle + \tfrac{1}{2}\langle s, H(x)s \rangle + \tfrac{1}{3}\sigma \|s\|^3$$

σ is the (adaptive) regularization parameter

(ideas from Griewank, Weiser/Deuflhard/Erdmann, Nesterov/Polyak, Cartis/Gould/T)

The keys to convergence theory for cubic regularization

The Cauchy condition:

$$m_k(x_k) - m_k(x_k + s_k) \geq \kappa_{\rm CR} \|g_k\| \min\left[\frac{\|g_k\|}{1 + \|H_k\|}, \sqrt{\frac{\|g_k\|}{\sigma_k}} \right]$$

The bound on the stepsize:

$$\|s\| \leq 3 \min\left[\frac{\|H_k\|}{\sigma_k}, \sqrt{\frac{\|g_k\|}{\sigma_k}} \right]$$

(Cartis/Gould/T)

The main features of adaptive cubic regularization

And the result is. . .

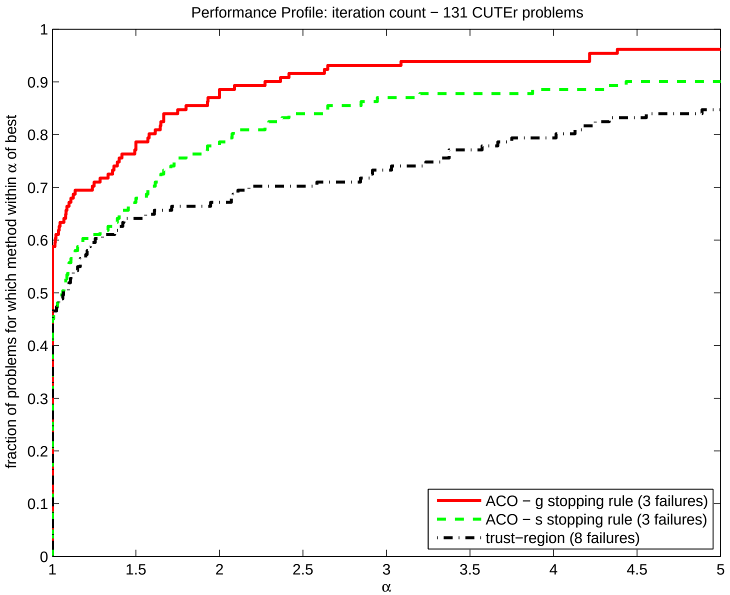
longer steps on ill-conditioned problems

similar (very satisfactory) convergence analysis

best known worst-case complexity for nonconvex problems

excellent performance and reliability

Numerical experience — small problems using Matlab



The quadratic regularization for NLS

Consider the Gauss-Newton method for nonlinear least-squares problems. Change from

$$\min_s \quad \tfrac{1}{2}\|c(x)\|^2 + \langle s, J(x)^T c(x)\rangle + \tfrac{1}{2}\langle s, J(x)^T J(x) s\rangle \;\text{ s.t. }\; \|s\| \leq \Delta$$

to

$$\min_s \quad \|c(x) + J(x)s\| + \tfrac{1}{2}\sigma\|s\|^2$$

σ is the (adaptive) regularization parameter

(idea by Nesterov)

Quadratic regularization: reformulation

Note that

$$\min_{s} \quad \|c(x) + J(x)s\| + \tfrac{1}{2}\sigma\|s\|^2$$

$$\Leftrightarrow$$

$$\min_{\nu,s} \quad \nu + \tfrac{1}{2}\sigma\|s\|^2$$

such that

$$\|c(x) + J(x)s\|^2 = \nu^2$$

exact penalty function for the problem of minimizing $\|s\|$ subject to $c(x) + J(x)s = 0$.

The keys to convergence theory for quadratic regularization

The Cauchy condition:

$$m(x_k) - m(x_k + s_k) \geq \kappa_{\rm QR} \frac{\|J_k^T c_k\|}{\|c_k\|} \min \left[\frac{\|J_k^T c_k\|}{1 + \|J_k^T J_k\|}, \frac{\|J_k^T c_k\|}{\sigma_k \|c_k\|} \right]$$

The bound on the stepsize:

$$\|s\| \leq \frac{1}{2} \frac{\|J_k^T c_k\|}{\sigma_k \|c_k\|}$$

Convergence theory for the quadratic regularization

Convergence results:

Global convergence to first-order critical points

Quadratic convergence to roots

Valid for

- general values of m and n,
- exact/approximate subproblem solution

(Bellavia/Cartis/Gould/Morini/T.)

Computing regularization steps

Iterative techniques. . .

solve the problem in nested Krylov subspaces

- Lanczos → basis of the Krylov subspace
- → factorization of tridiagonal matrices
- different scalar secular equation (solution by Newton's method)

Approach valid for

- trust-region (GLTR),
- cubic and quadratic regularizations

(details in CGT techreport)

A unifying concept: Nonlinear stepsize control

Towards a unified global convergence theory

Objectives:

- recover a unified global convergence theory
- possibly open the door for new algorithms

Idea:

- cast all three methods into a generalized TR framework
- allow this TR to be updated nonlinearly

Towards a unified global convergence theory (2)

Given

- two continuous first-order criticality measures $\psi(x)$ and $\psi(x)\chi(x)$
- an adaptive stepsize parameter δ

define a **generalized radius $\Delta(\delta, \chi(x))$** such that

- $\Delta(\cdot, \chi)$ is C^1, strictly increasing and concave,
- $\Delta(0, \chi) = 0$ for all χ,
- $\Delta(\delta, \cdot)$ is non-increasing
- $$\delta \frac{\partial \Delta}{\partial \delta}(\delta, \chi) \leq \kappa_\Delta \Delta(\delta, \chi)$$
- $\psi(x)$ bounded above
- ...

Towards a unified global convergence theory (3)

- the generalized Cauchy condition:

$$m(x_k) - m(x_k + s_k) \geq \kappa_{\rm N} \chi_k \min \left[\frac{\psi_k}{1 + \|H_k\|}, \Delta(\delta_k, \chi_k) \right]$$

- the generalized bound on the stepsize:

$$\|s\| \leq \Delta(\delta_k, \chi_k)$$

The nonlinear stepsize control algorithm

Algorithm 2.1: Nonlinear Stepsize Control Algorithm

Step 0: Initialization: $x_0 \in \mathbb{R}^n$, δ_0 given. Set $k = 0$.

Step 1: Step computation: Choose a model $m_k(x_k + s)$ and find a step s_k satisfying generalized Cauchy and $\|s_k\| \leq \Delta(\delta_k, \chi_k)$.

Step 2: Step acceptance: Compute $f(x_k + s_k)$ and

$$\rho_k = \frac{f(x_k) - f(x_k + s_k)}{m_k(x_k) - m_k(x_k + s_k)}$$

Set $x_{k+1} = x_k + s_k$ if $\rho_k \geq \eta_1$; $x_{k+1} = x_k$ otherwise.

Step 3: Stepsize parameter update: Choose

$$\delta_{k+1} \in \begin{cases} [\gamma_1 \delta_k, \gamma_2 \delta_k] & \text{if} \quad \rho_k < \eta_1, \\ [\gamma_2 \delta_k, \delta_k] & \text{if} \quad \rho_k \in [\eta_1, \eta_2), \\ [\delta_k, +\infty] & \text{if} \quad \rho_k \geq \eta_2. \end{cases}$$

Set $k \leftarrow k + 1$ and go to Step 1.

Resulting convergence theory

Similar to trust-region convergence theory, but

more work to prove that $\Delta(\delta_k, \chi_k)$ remains bounded away from zero

(assumptions of $\Delta(\delta, \chi)$ crucial here)
and the result is ...

$$\liminf_{k\to+\infty} \psi_k = 0 \quad \text{or} \quad \lim_{k\to+\infty} \chi_k = 0$$

(both true limits if ψ is non-increasing)

Unified first-order convergence theory!

Covers all previous cases

trust regions:

$$\chi_k = \|g_k\|, \qquad \psi_k = 1, \qquad \Delta(\delta, \chi) = \delta$$

cubic regularization:

$$\chi_k = \|g_k\|, \qquad \psi_k = 1, \qquad \delta_k = \frac{1}{\sigma_k}, \qquad \Delta(\delta, \chi) = \sqrt{\delta\chi}$$

quadratic regularization:

$$\chi_k = \frac{\|J_k^T F_k\|}{\|F_k\|}, \quad \psi_k = \|F_k\|, \qquad \delta_k = \frac{1}{\sigma_k}, \qquad \Delta(\delta, \chi) = \delta\chi$$

Conclusions

- Much left to do. . . but very interesting
- Could lead to very untypical methods
  Example:

$$\chi_k = \|g_k\|, \qquad \Delta(\delta, \chi) = \sqrt{\delta\chi}$$

- Meaningful numerical evaluation still needed
- Many issues regarding regularizations still unresolved

Thank you for your attention !

(see `http://perso.fundp.ac.be/~phtoint/publications.html` for references)