An adaptive cubic regularization algorithm for nonconvex optimization with convex constraints and its function-evaluation complexity

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The problem

We consider the unconstrained nonlinear programming problem:

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

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

Important special case: the nonlinear least-squares problem

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

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

A useful observation

Note the following: if

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

Taylor, Cauchy-Schwarz and Lipschitz imply

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

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

The cubic regularization

Change from trust-regions:

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

to cubic regularization:

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

σ is the (adaptive) regularization parameter

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

Cubic regularization highlights

$$f(x+s) \leq m(s) \equiv f(x) + s^T g(x) + \tfrac{1}{2} s^T H(x) s + \tfrac{1}{3} L \|s\|_2^3$$

- Nesterov and Polyak minimize m globally and exactly
  - N.B. m may be non-convex!
  - efficient scheme to do so if H has sparse factors
- global (ultimately rapid) convergence to a 2nd-order critical point of f
- better worst-case function-evaluation complexity than previously known

Obvious questions:

- can we avoid the global Lipschitz requirement?
- can we approximately minimize m and retain good worst-case function-evaluation complexity?
- does this work well in practice?

Cubic overestimation

Assume

- $f \in C^2$
- f, g and H at x_k are f_k, g_k and H_k
- symmetric approximation B_k to H_k
- B_k and H_k bounded at points of interest

Use

- cubic overestimating model at x_k

$$m_k(s) \equiv f_k + s^T g_k + \tfrac{1}{2} s^T B_k s + \tfrac{1}{3} \sigma_k \|s\|_2^3$$

  - σ_k is the iteration-dependent regularisation weight
  - easily generalized for regularisation in M_k-norm $\|s\|_{M_k} = \sqrt{s^T M_k s}$ where M_k is uniformly positive definite

Adaptive Regularization with Cubic (ARC)

Algorithm 1.1: The ARC Algorithm

Step 0: Initialization: x_0 and $\sigma_0 > 0$ given. Set $k = 0$

Step 1: Step computation: Compute s_k for which $m_k(s_k) \leq m_k(s_k^{\mathrm{C}})$

Cauchy point: $s_k^{\mathrm{C}} = -\alpha_k^{\mathrm{C}} g_k$ & $\alpha_k^{\mathrm{C}} = \arg\min_{\alpha \in \mathbf{R}_+} m_k(-\alpha g_k)$

Step 2: Step acceptance: Compute $\rho_k = \dfrac{f(x_k) - f(x_k + s_k)}{f(x_k) - m_k(s_k)}$

and set $x_{k+1} = \begin{cases} x_k + s_k & \text{if } \rho_k > 0.1 \\ x_k & \text{otherwise} \end{cases}$

Step 3: Update the regularization parameter:

$$\sigma_{k+1} \in \begin{cases} (0, \sigma_k] = \frac{1}{2}\sigma_k & \text{if } \rho_k > 0.9 & \textit{very successful} \\ [\sigma_k, \gamma_1 \sigma_k] = \sigma_k & \text{if } 0.1 \leq \rho_k \leq 0.9 & \textit{successful} \\ [\gamma_1 \sigma_k, \gamma_2 \sigma_k] = 2\sigma_k & \text{otherwise} & \textit{unsuccessful} \end{cases}$$

Local convergence theory for cubic regularization (1)

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:

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

(Cartis/Gould/T)

Local convergence theory for cubic regularization (2)

And therefore...

$$\lim_{k\to\infty} \|g_k\| = 0$$

first-order global convergence

Under stronger assumptions can show that

If s_k minimizes m_k over subspace with orthogonal basis Q_k,

$$\lim_{k\to\infty} Q_k^T H_k Q_k \succeq 0$$

second-order global convergence

Fast convergence

For fast asymptotic convergence $\Longrightarrow$ need to improve on Cauchy point: minimize over Krylov subspaces

- g stopping-rule: $\|\nabla_s m_k(s_k)\| \leq \min(1, \|g_k\|^{\frac{1}{2}})\|g_k\|$
- s stopping-rule: $\|\nabla_s m_k(s_k)\| \leq \min(1, \|s_k\| \quad)\|g_k\|$

If B_k satisfies the Dennis-Moré condition

$$\|(B_k - H_k)s_k\|/\|s_k\| \rightarrow 0 \;\text{ whenever }\; \|g_k\| \rightarrow 0$$

and $x_k \rightarrow x_*$ with positive definite $H(x_*)$

$\Longrightarrow$ Q-superlinear convergence of x_k under the g- and s-rules

If additionally $H(x)$ is locally Lipschitz around x_* and

$$\|(B_k - H_k)s_k\| = O(\|s_k\|^2)$$

$\Longrightarrow$ Q-quadratic convergence of x_k under the s-rule

Function-evaluation complexity

How many function evaluations (iterations) are needed to ensure that

$$\|g_k\| \leq \epsilon?$$

- so long as for very successful iterations $\sigma_{k+1} \leq \gamma_3 \sigma_k$ for $\gamma_3 < 1$
  $\Longrightarrow$ basic ARC algorithm requires at most

  $$\left\lceil \frac{\kappa_{\rm C}}{\epsilon^2} \right\rceil \text{ function evaluations}$$

  for some $\kappa_{\rm C}$ independent of ϵ c.f. steepest descent

- if H is globally Lipschitz, the s-rule is applied and additionally s_k is the global (line) minimizer of $m_k(\alpha s_k)$ as a function of α
  $\Longrightarrow$ ARC algorithm requires at most

  $$\left\lceil \frac{\kappa_{\rm S}}{\epsilon^{3/2}} \right\rceil \text{ function evaluations}$$

  for some $\kappa_{\rm S}$ independent of ϵ c.f. Nesterov & Polyak

Minimizing the model

$$m(s) \equiv f + s^T g + \tfrac{1}{2} s^T B s + \tfrac{1}{3}\sigma \|s\|_2^3$$

- **Small problems:**

  use Moré-Sorensen-like method with modified secular equation (also OK as long as factorization is feasible)

- **Large problems:**

  an iterative Krylov space method

  approximate solution

Numerically sound procedures for computing exact/approximate steps

The main features of adaptive cubic regularization

And the result is. . .

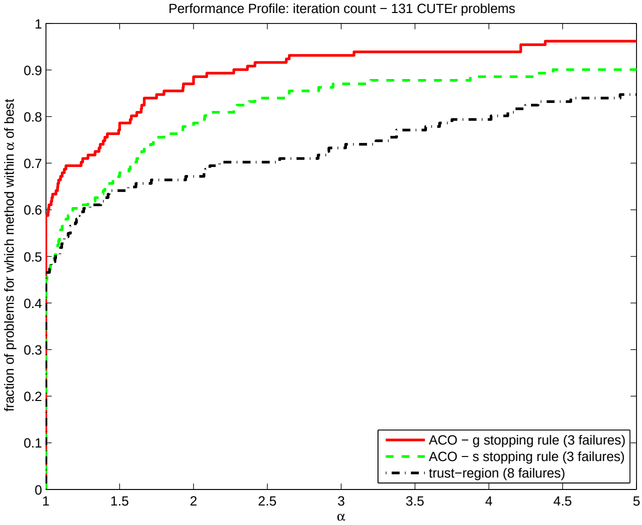
longer steps on ill-conditioned problems

similar (very satisfactory) convergence analysis

best function-evaluation complexity for nonconvex problems

excellent performance and reliability

Numerical experience — small problems using Matlab



The constrained case

Can we apply regularization to the constrained case?

Consider the constrained nonlinear programming problem:

$$\text{minimize} \quad f(x)$$
$$x \in \mathcal{F}$$

for $x \in \mathbb{R}^n$ and $f : \mathbb{R}^n \to \mathbb{R}$ smooth, and where

$$\mathcal{F} \text{ is convex.}$$

Main ideas:

- exploit (cheap) projections on convex sets
- define using the generalized Cauchy point idea
- prove global convergence + function-evaluation complexity

Constrained step computation (1)

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

subject to

$$x + s \in \mathcal{F}$$

σ is the (adaptive) regularization parameter

Criticality measure: (as before)

$$\chi(x) \stackrel{\rm def}{=} \left| \min_{x+d\in\mathcal{F}, \|d\|\leq 1} \langle \nabla_x f(x), d\rangle \right|,$$

The generalized Cauchy point for ARC

Cauchy step: Goldstein-like piecewise linear seach on m_k along the gradient path projected onto $\mathcal{F}$

Find

$$x_k^{\rm GC} = P_{\mathcal{F}}[x_k - t_k^{\rm GC} g_k] \stackrel{\rm def}{=} x_k + s_k^{\rm GC} \quad (t_k^{\rm GC} > 0)$$

such that

$$m_k(x_k^{\rm GC}) \le f(x_k) + \kappa_{\rm ubs}\langle g_k, s_k^{\rm GC}\rangle \qquad \text{(below linear approximation)}$$

and either

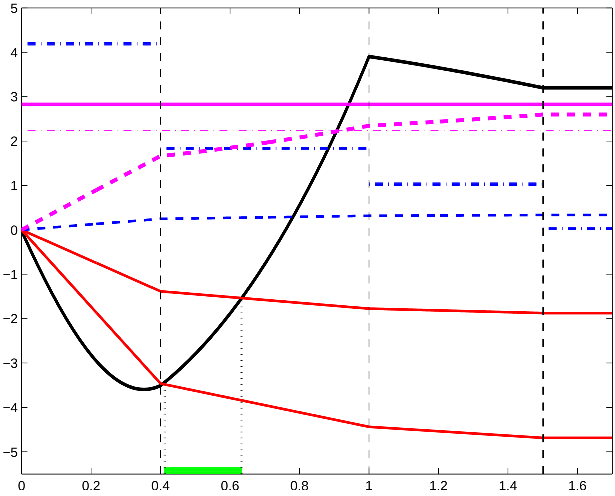
$$m_k(x_k^{\rm GC}) \ge f(x_k) + \kappa_{\rm lbs}\langle g_k, s_k^{\rm GC}\rangle \qquad \text{(above linear approximation)}$$

or

$$\|P_{T(x_k^{\rm GC})}[-g_k]\| \le \kappa_{\rm epp}|\langle g_k, s_k^{\rm GC}\rangle| \qquad \text{(close to path's end)}$$

no trust-region condition!

Searching for the ARC-GCP



$m_k(0+s) = -3.57s_1 - 1.5s_2 - s_3 + s_1 s_2 + 3s_2^2 + s_2 s_3 - 2s_3^2 + \frac{1}{3}\|s\|^3$ such that $s \leq 1.5$

A constrained regularized algorithm

Algorithm 2.1: ARC for Convex Constraints (COCARC)

Step 0: Initialization. $x_0 \in \mathcal{F}$, σ_0 given. Compute $f(x_0)$, set $k = 0$.

Step 1: Generalized Cauchy point. If x_k not critical, find the generalized Cauchy point x_k^{GC} by piecewise linear search on the regularized cubic model.

Step 2: Step calculation. Compute s_k and $x_k^+ \stackrel{\text{def}}{=} x_k + s_k \in \mathcal{F}$ such that $m_k(x_k^+) \leq m_k(x_k^{GC})$.

Step 3: Acceptance of the trial point. Compute $f(x_k^+)$ and ρ_k. If $\rho_k \geq \eta_1$, then $x_{k+1} = x_k + s_k$; otherwise $x_{k+1} = x_k$.

Step 4: Regularisation parameter update. Set

$$\sigma_{k+1} \in \begin{cases} (0, \sigma_k] & \text{if } \rho_k \geq \eta_2, \\ [\sigma_k, \gamma_1 \sigma_k] & \text{if } \rho_k \in [\eta_1, \eta_2), \\ [\gamma_1 \sigma_k, \gamma_2 \sigma_k] & \text{if } \rho_k < \eta_1. \end{cases}$$

Local convergence theory for COCARC

The Cauchy condition:

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

The bound on the stepsize:

$$\|s_k\| \leq 3 \max \left[\frac{\|H_k\|}{\sigma_k}, \left(\frac{\chi_k}{\sigma_k}\right)^{\frac{1}{2}}, \left(\frac{\chi_k}{\sigma_k}\right)^{\frac{1}{3}} \right]$$

And therefore. . .

$$\lim_{k \to \infty} \chi_k = 0$$

(Cartis/Gould/T)

Function-Evaluation Complexity for COCARC (1)

But

What about function-evaluation complexity?

If, for very successful iterations, $\sigma_{k+1} \leq \gamma_3 \sigma_k$ for $\gamma_3 < 1$, the COCARC algorithm requires at most

$$\left\lceil \frac{\kappa_C}{\epsilon^2} \right\rceil \text{ function evaluations}$$

(for some κ_C independent of ϵ) to achieve $\chi_k \leq \epsilon$

c.f. steepest descent

Do the nicer bounds for unconstrained optimization extend to the constrained case?

Function-evaluation complexity for COCARC (2)

As for unconstrained, impose a termination rule on the subproblem solution:

- Do not terminate solving $\min_{x_k+s\in\mathcal{F}} m_k(x_k+s)$ before

$$\chi_k^{\mathrm{m}}(x_k^+) \leq \min(\kappa_{\mathrm{stop}}, \|s_k\|)\, \chi_k$$

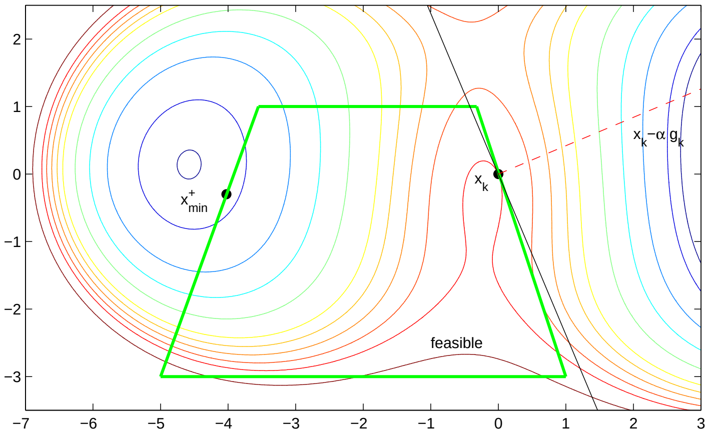
where

$$\chi_k^{\mathrm{m}}(x) \stackrel{\mathrm{def}}{=} \left| \min_{x+d\in\mathcal{F}, \|d\|\leq 1} \langle \nabla_x m_k(x), d \rangle \right|$$

c.f. the "s-rule" for unconstrained

Note: OK at local constrained model minimizers

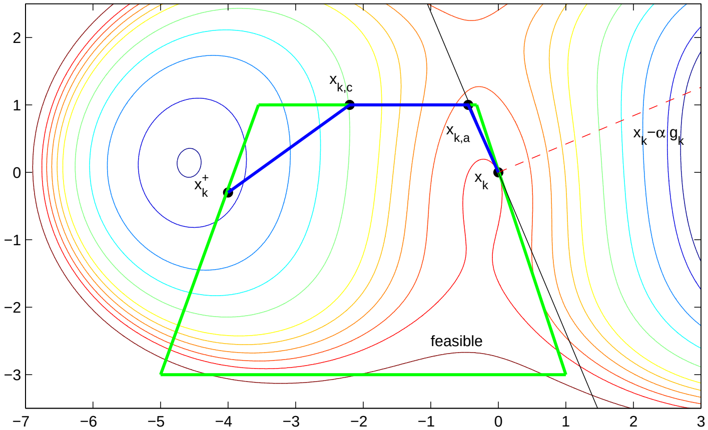
Walking through the pass...



A "beyond the pass" constrained problem with

$$m(x,y) = -x - \tfrac{42}{100}y - \tfrac{3}{10}x^2 - \tfrac{1}{10}y^3 + \tfrac{1}{3}[x^2+y^2]^{\frac{3}{2}}$$

Walking through the pass...with a sherpa



A piecewise descent path from x_k to x_k^+ on

$$m(x,y) = -x - \tfrac{42}{100}y - \tfrac{3}{10}x^2 - \tfrac{1}{10}y^3 + \tfrac{1}{3}[x^2+y^2]^{\frac{3}{2}}$$

Function-Evaluation Complexity for COCARC (2)

Assume also

- $x_k \leftarrow x_k^+$ in a bounded number of feasible descent substeps
- $\|H_k - \nabla_{xx} f(x_k)\| \leq \kappa \|s_k\|^2$
- $\nabla_{xx} f(\cdot)$ is globally Lipschitz continuous
- $\{x_k\}$ bounded

The COCARC algorithm requires at most

$$\left\lceil \frac{\kappa_{\rm C}}{\epsilon^{3/2}} \right\rceil \text{ function evaluations}$$

(for some $\kappa_{\rm C}$ independent of ϵ) to achieve $\chi_k \leq \epsilon$

Caveat: cost of solving the subproblem — c.f. unconstrained case!!!

Conclusions

- Much left to do. . . but very interesting
- Meaningful numerical evaluation still needed for many of these algorithms
- Many issues regarding regularizations still unresolved

Many thanks for your attention!