

Cubic regularization and complexity issues for nonconvex optimization

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The problem

We consider the unconstrained nonlinear programming problem:

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

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

Important special case: the **nonlinear least-squares problem**

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

for $x \in \mathbf{R}^n$ and $F : \mathbf{R}^n \rightarrow \mathbf{R}^m$ 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

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

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

The cubic regularization

Change from trust-regions:

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

to cubic regularization:

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

σ is the (adaptive) regularization parameter

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

Cubic regularization highlights

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

- 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

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

- 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 $m_k(s_k) \leq m_k(s_k^c)$

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

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

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:

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

Local convergence theory for cubic regularization (1)

The Cauchy condition:

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

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...

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

first-order global convergence

Under stronger assumptions can show that

If s_k minimizes m_k over subspace with orthogonal basis Q_k ,

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

second-order global convergence

Fast convergence

For fast asymptotic convergence \implies 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**: $\|\nabla_s m_k(s_k)\| \leq \min(1, \|s_k\|) \|g_k\|$

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 $H(x_*)$

\implies **Q-superlinear** convergence of x_k under the g- and s-rules

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

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

\implies **Q-quadratic** convergence of x_k under the s-rule

Function-evaluation complexity (1)

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 $\gamma_3 < 1$

The basic ARC algorithm requires at most

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

for some κ_C independent of ϵ

c.f. steepest descent

Function-evaluation complexity (2)

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

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

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 , the ARC algorithm requires at most

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

for some κ_S independent of ϵ .

c.f. Nesterov & Polyak

Note: an $O(\epsilon^{-3})$ bound holds for convergence to **second-order** critical points.

Function-evaluation complexity (3)

Is the bound in $O(\epsilon^{-3/2})$ sharp? **YES!!!**

Construct a **unidimensional** example with

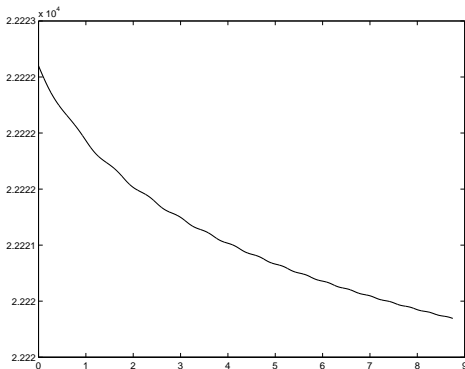
$$x_0 = 0, \quad x_{k+1} = x_k + \left(\frac{1}{k+1}\right)^{\frac{1}{3}+\eta},$$

$$f_0 = \frac{2}{3} \zeta(1+3\eta), \quad f_{k+1} = f_k - \frac{2}{3} \left(\frac{1}{k+1}\right)^{1+3\eta},$$

$$g_k = - \left(\frac{1}{k+1}\right)^{\frac{2}{3}+2\eta}, \quad H_k = 0 \text{ and } \sigma_k = 1,$$

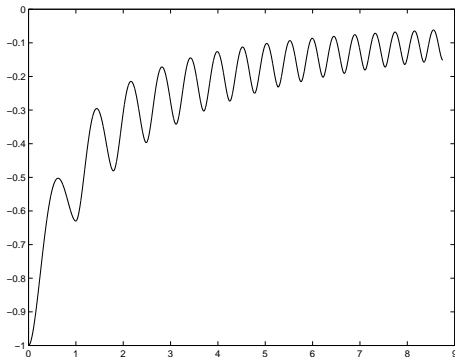
Use Hermite interpolation on $[x_K, x_{K+1}]$.

An example of slow ARC (1)



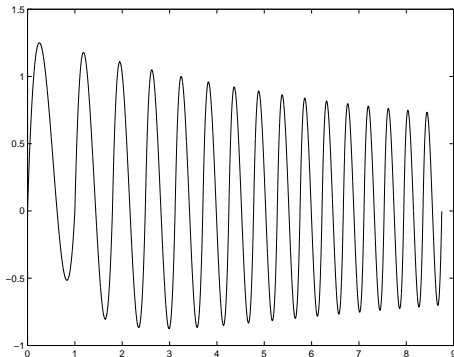
The objective function

An example of slow ARC (2)



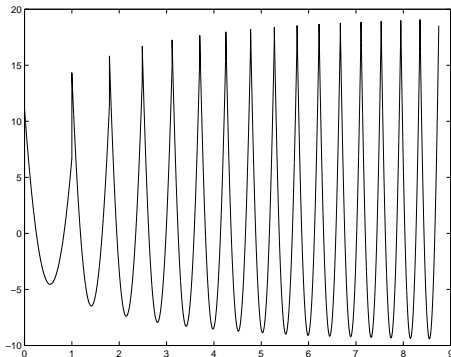
The first derivative

An example of slow ARC (3)



The second derivative

An example of slow ARC (4)



The third derivative

Minimizing the model

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

- 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 . . .

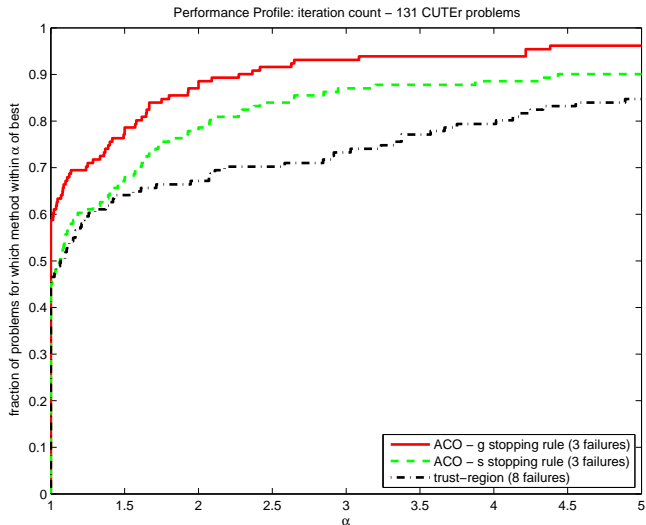
longer steps on ill-conditioned problems

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:

$$\begin{aligned} & \text{minimize} && f(x) \\ & && x \in \mathcal{F} \end{aligned}$$

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

\mathcal{F} 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)

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

subject to

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

σ is the (adaptive) regularization parameter

Criticality measure: (as before)

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

The generalized Cauchy point for ARC

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

Find

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

such that

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

and either

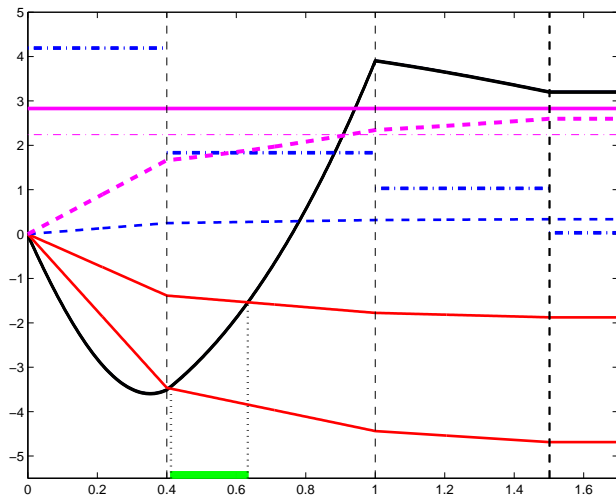
$$m_k(x_k^{\text{GC}}) \geq f(x_k) + \kappa_{\text{lbs}} \langle g_k, s_k^{\text{GC}} \rangle \quad (\text{above linear approximation})$$

or

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

no trust-region condition!

Searching for the ARC-GCP



$$m_k(0+s) = -3.57s_1 - 1.5s_2 - s_3 + s_1s_2 + 3s_2^2 + s_2s_3 - 2s_3^2 + \frac{1}{3}\|s\|^3 \text{ such that } s \leq 1.5$$

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 $m_k(x_k^+) \leq m_k(x_k^{\text{GC}})$.

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:

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

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...

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

(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

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

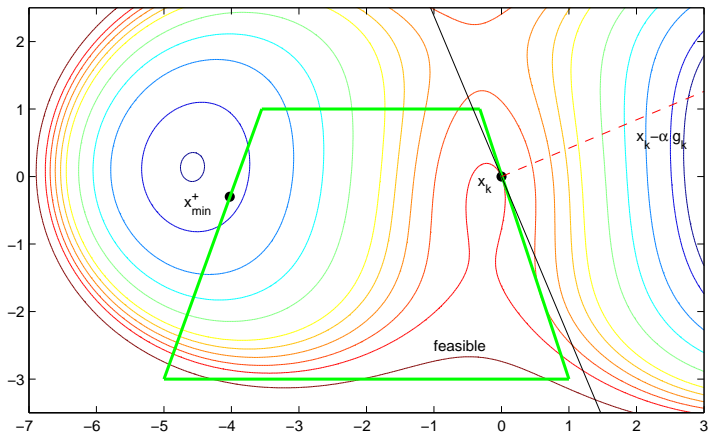
where

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

c.f. the “s-rule” for unconstrained

Note: OK at **local constrained model minimizers**

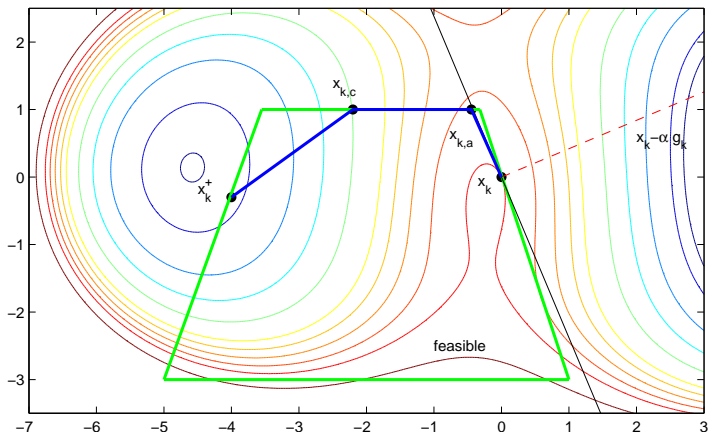
Walking through the pass...



A “beyond the pass” constrained problem with

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

Walking through the pass...with a sherpa



A piecewise descent path from x_k to x_k^+ on

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

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

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

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

Caveat: cost of solving the subproblem

c.f. **unconstrained case!!!**

Without regularization ?

What is known for unregularized (standard) methods?

The **steepest descent method** requires at most

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

for obtaining $\|g_k\| \leq \epsilon$.

Sharp???

Newton's method (when convergent) requires at most

??? function evaluations

for obtaining $\|g_k\| \leq \epsilon$.

Slow steepest descent (1)

For steepest descent, the bound of

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

is sharp on functions with Lipschitz continuous gradients.

As before, construct a **unidimensional** example with

$$x_0 = 0, \quad x_{k+1} = x_k + \alpha_k \left(\frac{1}{k+1} \right)^{\frac{1}{2} + \eta},$$

for some steplength $\alpha_k > 0$ such that

$$0 < \underline{\alpha} \leq \alpha_k \leq \bar{\alpha} < 2,$$

giving the step

$$s_k \stackrel{\text{def}}{=} x_{k+1} - x_k = \alpha_k \left(\frac{1}{k+1} \right)^{\frac{1}{2} + \eta}.$$

Slow steepest descent (1)

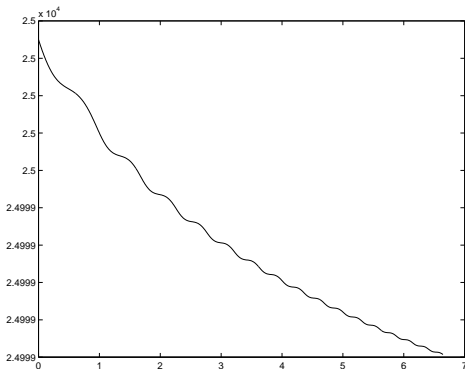
Also set

$$f_0 = \frac{1}{2} \zeta(1 + 2\eta), \quad f_{k+1} = f_k - \alpha_k \left(1 - \frac{1}{2}\alpha_k\right) \left(\frac{1}{k+1}\right)^{1+2\eta},$$

$$g_k = - \left(\frac{1}{k+1}\right)^{\frac{1}{2}+\eta}, \quad \text{and } H_k = 1,$$

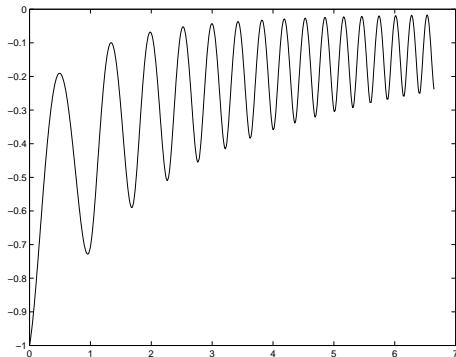
Use Hermite interpolation on $[x_k, x_{k+1}]$.

An example of slow steepest descent (1)



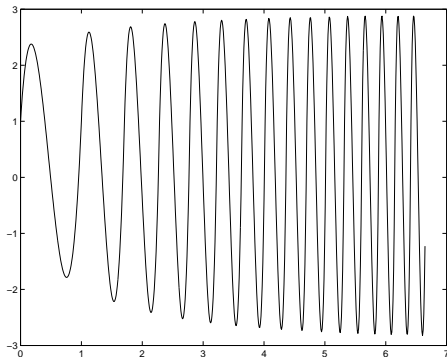
The objective function

An example of slow steepest-descent (2)



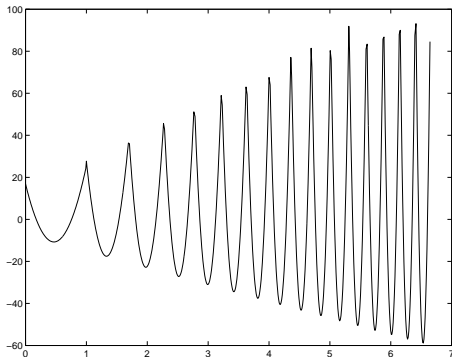
The first derivative

An example of slow steepest-descent (3)



The second derivative

An example of slow steepest descent (4)



The third derivative

Slow Newton (1)

A big **surprise**:

Newton's method may require as much as

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

to obtain $\|g_k\| \leq \epsilon$ on functions with bounded and (segment-wise) Lipschitz continuous Hessians.

Example now **bi-dimensional**

Slow Newton (2)

The conditions are now:

$$x_0 = (0, 0)^T, \quad x_{k+1} = x_k + \begin{pmatrix} \left(\frac{1}{k+1}\right)^{\frac{1}{2}+\eta} \\ 1 \end{pmatrix},$$

$$f_0 = \frac{1}{2} [\zeta(1+2\eta) + \zeta(2)], \quad f_{k+1} = f_k - \frac{1}{2} \left[\left(\frac{1}{k+1}\right)^{1+2\eta} + \left(\frac{1}{k+1}\right)^2 \right],$$

$$g_k = - \begin{pmatrix} \left(\frac{1}{k+1}\right)^{\frac{1}{2}+\eta} \\ \left(\frac{1}{k+1}\right)^2 \end{pmatrix}, \quad \text{and} \quad H_k = \begin{pmatrix} 1 & 0 \\ 0 & \left(\frac{1}{k+1}\right)^2 \end{pmatrix}$$

Use previous example for x_1 and Hermite interpolation on $[x_K, x_{k+1}]$ for x_2 .

More general second-order methods (work in progress)

Assume that, for $\beta \in (0, 1]$, the step is computed by

$$(H_k + \lambda_k I)s_k = -g_k \quad \text{and} \quad 0 \leq \lambda_k \leq \kappa_s \|s_k\|^\beta$$

(ex: Newton, ARC, (TR), ...)

The corresponding method may require as much as

$$\left\lceil \frac{\kappa_C}{\epsilon^{-(\beta+2)/(\beta+1)}} \right\rceil \text{ function evaluations}$$

to obtain $\|g_k\| \leq \epsilon$ on functions with bounded and (segment-wise) β -Hölder continuous Hessians.

Note: ranges from ϵ^{-2} to $\epsilon^{-3/2}$

ARC is optimal within this class

Conclusions

- Many open questions . . . but very interesting
- Algorithm design profits from complexity analysis
- Many issues regarding regularizations still unresolved
- ARC is the optimal second-order method

Many thanks for your attention!