How much patience do you have?
Issues in complexity for nonlinear optimization

Philippe Toint (with Coralia Cartis and Nick Gould)

Namur Center for Complex Systems (naXys), University of Namur, Belgium

(philippe.toint@fundp.ac.be)

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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

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

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

Approximate model minimization

Lipschitz constant L unknown $\Rightarrow$ replace by adaptive parameter σ_k in the model :

$$m(s) \stackrel{\rm def}{=} f(x) + s^T g(x) + \tfrac{1}{2} s^T H(x) s + \tfrac{1}{3}\sigma_k \|s\|_2^3 = T_{f,2}(x,s) + \tfrac{1}{3}\sigma_k \|s\|_2^3$$

Computation of the step:

1. minimize $m(s)$ until an approximate first-order minimizer is obtained:

$$\|\nabla_s m(s)\| \le \kappa_{\rm stop} \|s\|^2$$

(s-rule)

Note: no global optimization involved.

Adaptive Regularization with Cubics (ARC2 or AR2)

Algorithm 1.1: The ARC2 Algorithm

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

Step 1: Termination: If $\|g_k\| \le \epsilon$, terminate.

Step 2: Step computation:

Compute s_k such that $m_k(s_k) \le m_k(0)$ and $\|\nabla_s m(s_k)\| \le \kappa_{\rm stop}\|s_k\|^2$.

Step 3: Step acceptance:

Compute $\rho_k = \dfrac{f(x_k) - f(x_k + s_k)}{f(x_k) - T_{f,2}(x_k, s_k)}$

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

Step 4: Update the regularization parameter:

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

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? YES!
- can we approximately minimize m and retain good worst-case function-evaluation complexity? YES !
- does this work well in practice? yes

Evaluation complexity: an important result

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

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

If H is globally Lipschitz and the s-rule is applied, the ARC2 algorithm requires at most

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

for some $\kappa_{\rm S}$ independent of ϵ.

c.f. Nesterov & Polyak

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

Evaluation complexity: proof (1)

$$f(x_k + s_k) \le T_{f,2}(x_k, s_k) + \frac{L_f}{p}\|s_k\|^3$$

$$\|g(x_k + s_k) - \nabla_s T_{f,2}(x_k, s_k)\| \le L_f \|s_k\|^2$$

Lipschitz continuity of $H(x) = \nabla_x^2 f(x)$

$$\forall k \ge 0 \qquad f(x_k) - T_{f,2}(x_k, s_k) \ge \tfrac{1}{6}\sigma_{\min}\|s_k\|^3$$

$$f(x_k) = m_k(0) \ge m_k(s_k) = T_{f,2}(x_k, s_k) + \tfrac{1}{6}\sigma_k \|s_k\|^3$$

Evaluation complexity: proof (2)

$$\exists \sigma_{\max} \quad \forall k \geq 0 \qquad \sigma_k \leq \sigma_{\max}$$

Assume that $\sigma_k \geq \dfrac{L_f(p+1)}{p\,(1-\eta_2)}$. Then

$$|\rho_k - 1| \leq \frac{|f(x_k+s_k) - T_{f,2}(x_k,s_k)|}{|T_{f,2}(x_k,0) - T_{f,2}(x_k,s_k)|} \leq \frac{L_f(p+1)}{p\,\sigma_k} \leq 1-\eta_2$$

and thus $\rho_k \geq \eta_2$ and $\sigma_{k+1} \leq \sigma_k$.

Evaluation complexity: proof (3)

$$\forall k \ \text{ successful} \qquad \|s_k\| \geq \left(\frac{\|g(x_{k+1})\|}{L_f + \kappa_{\rm stop} + \sigma_{\max}}\right)^{\frac{1}{2}}$$

$$\begin{aligned}
\|g(x_k+s_k)\| &\leq \|g(x_k+s_k) - \nabla_s T_{f,2}(x_k,s_k)\| \\
&\quad + \Big\|\nabla_s T_{f,2}(x_k,s_k) + \sigma_k \|s_k\| s_k\Big\| + \sigma_k \|s_k\|^2 \\
&\leq L_f \|s_k\|^2 + \|\nabla_s m(s_k)\| + \sigma_k \|s_k\|^2 \\
&\leq [L_f + \kappa_{\rm stop} + \sigma_k]\, \|s_k\|^2
\end{aligned}$$

Evaluation complexity: proof (4)

$$\|g(x_{k+1})\| \leq \epsilon \text{ after at most } \frac{f(x_0) - f_{\rm low}}{\kappa}\,\epsilon^{-3/2} \text{ successful iterations}$$

Let $\mathcal{S}_k = \{j \leq k \geq 0 \mid \text{iteration } j \text{ is successful}\}$.

$$\begin{aligned}
f(x_0) - f_{\rm low} &\geq f(x_0) - f(x_{k+1}) \geq \sum_{i \in \mathcal{S}_k} \Big[f(x_i) - f(x_i + s_i) \Big] \\
&\geq \frac{1}{10} \sum_{i \in \mathcal{S}_k} \Big[f(x_i) - T_{f,2}(x_i, s_i) \Big] \geq |\mathcal{S}_k| \frac{\sigma_{\min}}{60} \min_i \|s_i\|^3 \\
&\geq |\mathcal{S}_k| \frac{\sigma_{\min}}{60\Big(L_f + \kappa_{\rm stop} + \sigma_{\max}\Big)^{3/2}} \min_i \|g(x_{i+1})\|^{3/2} \\
&\geq |\mathcal{S}_k| \frac{\sigma_{\min}}{60\Big(L_f + \kappa_{\rm stop} + \sigma_{\max}\Big)^{3/2}} \epsilon^{3/2}
\end{aligned}$$

Evaluation complexity: proof (5)

$$k \leq \kappa_u |\mathcal{S}_k|, \quad \text{where} \quad \kappa_u \stackrel{\text{def}}{=} \left(1 + \frac{|\log \gamma_1|}{\log \gamma_2}\right) + \frac{1}{\log \gamma_2} \log\left(\frac{\sigma_{\max}}{\sigma_0}\right),$$

$\sigma_k \in [\sigma_{\min}, \sigma_{\max}]$ + mechanism of the σ_k update.

$$\|g(x_{k+1})\| \leq \epsilon \text{ after at most } \frac{f(x_0) - f_{\rm low}}{\kappa}\,\epsilon^{-3/2} \text{ successful iterations}$$

One evaluation per iteration (successful or unsuccessful).

Evaluation complexity: sharpness

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

Construct a unidimensional example with

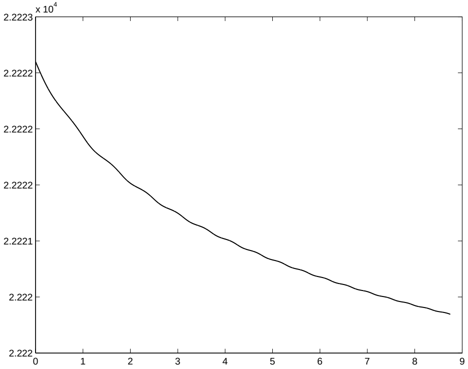
$$x_0 = 0, \quad x_{k+1} = x_k + \left(\frac{1}{k+1}\right)^{\frac{1}{3}+\eta},$$

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

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

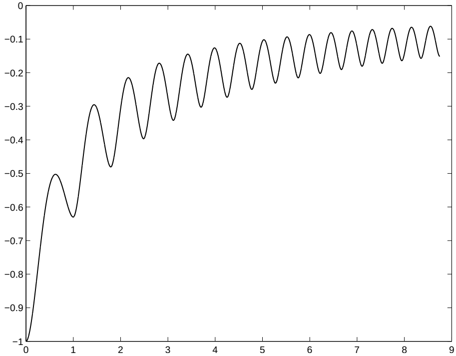
Use Hermite interpolation on $[x_K, x_{k+1}]$.

An example of slow ARC2 (1)



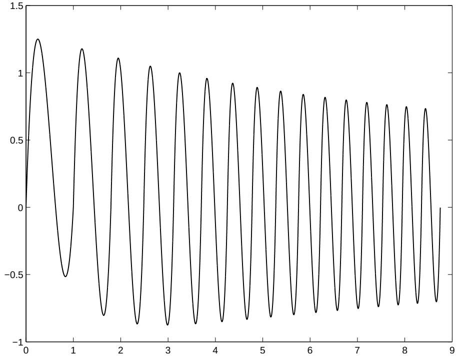
The objective function

An example of slow ARC2 (2)



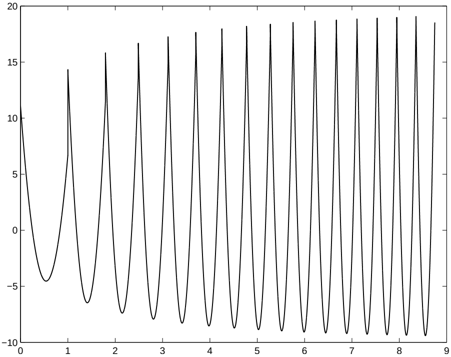
The first derivative

An example of slow ARC2 (3)



The second derivative

An example of slow ARC2 (4)



The third derivative

Slow steepest descent (1)

The steepest descent method with requires at most

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

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

Nesterov

Sharp??? YES

Newton's method (when convergent) requires at most

$$O(\epsilon^{-2}) \text{ evaluations}$$

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

Slow Newton (1)

Choose $\tau \in (0,1)$

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

for $k \geq 0$ and

$$f_0 = \zeta(1+2\eta) + \frac{\pi^2}{6}, \quad f_k = f_{k-1} - \frac{1}{2}\left[\left(\frac{1}{k+1}\right)^{1+2\eta} + \left(\frac{1}{k+1}\right)^2\right] \text{ for } k \geq 1,$$

$$\eta = \eta(\tau) \stackrel{\text{def}}{=} \frac{\tau}{4-2\tau} = \frac{1}{2-\tau} - \frac{1}{2}.$$

Slow Newton (2)

$$H_k s_k = -g_k,$$

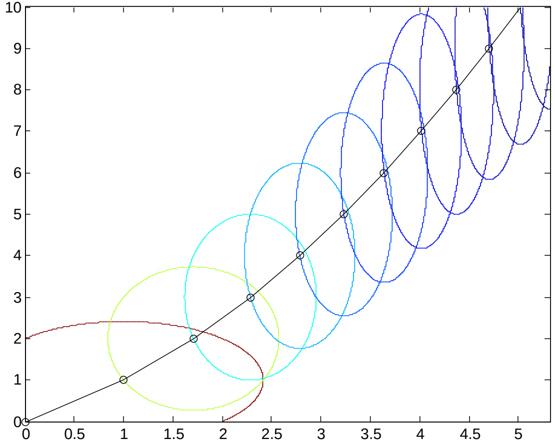
and thus

$$s_k = \begin{pmatrix} \left(\frac{1}{k+1}\right)^{\frac{1}{2}+\eta} \\ 1 \end{pmatrix},$$

$$x_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \qquad x_k = \begin{pmatrix} \sum_{j=0}^{k-1} \left(\frac{1}{j+1}\right)^{\frac{1}{2}+\eta} \\ k \end{pmatrix}.$$

Slow Newton (3)

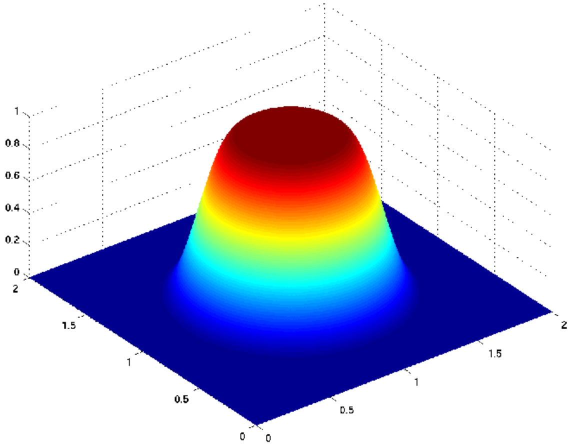
$$q_k(x_{k+1}, y_{k+1}) = f_k + \langle g_k, s_k \rangle + \tfrac{1}{2}\langle s_k, H_k s_k \rangle = f_{k+1}$$



The shape of the successive quadratic models

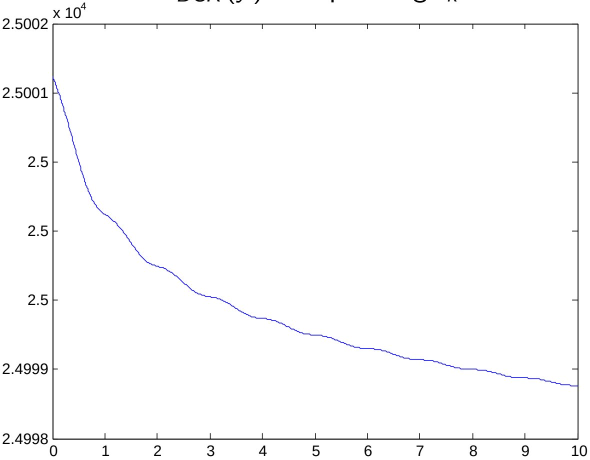
Slow Newton (4)

Define a support function $s_k(x, y)$ around (x_k, y_k)



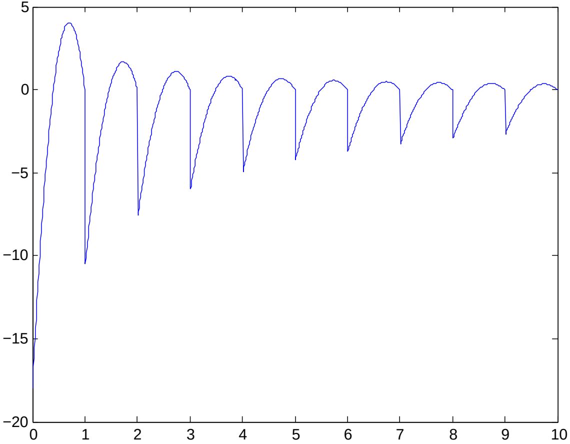
Slow Newton (5)

A background function $f_{BCK}(y)$ interpolating f_k values. . .



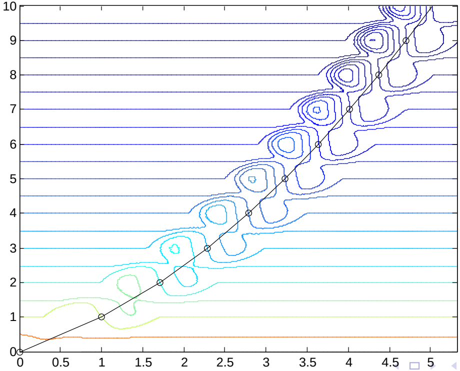
Slow Newton (6)

...with bounded third derivative



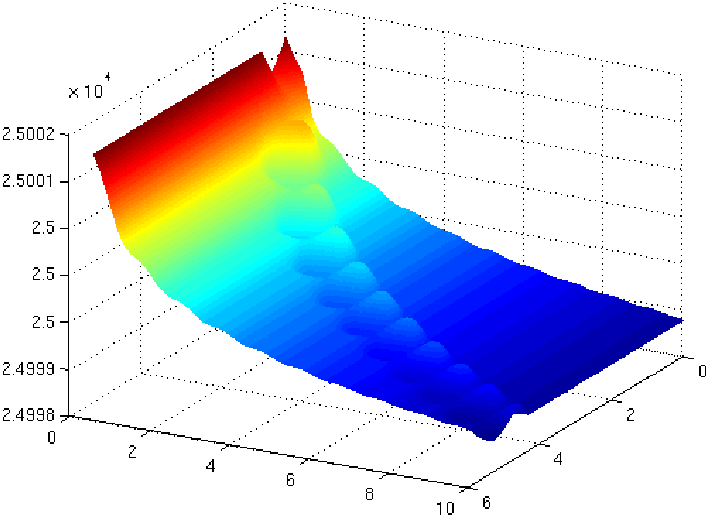
Slow Newton (7)

$$f_{SN1}(x,y) = \sum_{k=0}^{\infty} s_k(x,y) q_k(x,y) + \left[1 - \sum_{k=0}^{\infty} s_k(x,y)\right] f_{BCK}(x,y)$$



Slow Newton (8)

Some steps on a sandy dune. . .



More general second-order methods

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

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

(ex: Newton, ARC2, Levenberg-Morrison-Marquardt, (trust-region), ...)

The corresponding method terminates in at most

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

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

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

ARC2 is optimal within this class

High-order models (1)

What happens if one considers the model

$$m_k(s) = T_{f,p}(x_k, s) + \frac{\sigma_k}{p!}\|s\|_2^{p+1}$$

where

$$T_{f,p}(x,s) = f(x) + \sum_{j=1}^{p} \frac{1}{j!}\nabla_x^j f(x)[s]^j$$

terminating the step computation when

$$\|\nabla_s m(s_k)\| \le \kappa_{\rm stop}\|s_k\|^p$$

???

now the ARp method!

High-order models (2)

ϵ-approx 1rst-order critical point after at most

$$\frac{f(x_0) - f_{\text{low}}}{\kappa}\,\epsilon^{-\frac{p+1}{p}}$$

successful iterations

Moreover

ϵ-approx "q-th order critical point" after at most

$$\frac{f(x_0) - f_{\text{low}}}{\kappa}\,\epsilon^{-\frac{p+1}{p+1-q}}$$

successful iterations

The constrained case

Can we apply regularization to the constrained case?

Consider the constrained nonlinear programming problem:

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

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

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

Ideas:

- exploit (cheap) projections on convex sets
- use appropriate termination criterion

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

Constrained step computation

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

subject to

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

- minimization of the cubic model until an approximate first-order critical point is met, as defined by

$$\chi_m(s) \leq \kappa_{\text{stop}}\|s\|^2$$

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

Note: OK at local constrained model minimizers

A constrained regularized algorithm

Algorithm 4.1: ARC for Convex Constraints (ARC2CC)

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

Step 1: Termination. If $\chi_f(s_k) \leq \epsilon$, terminate.

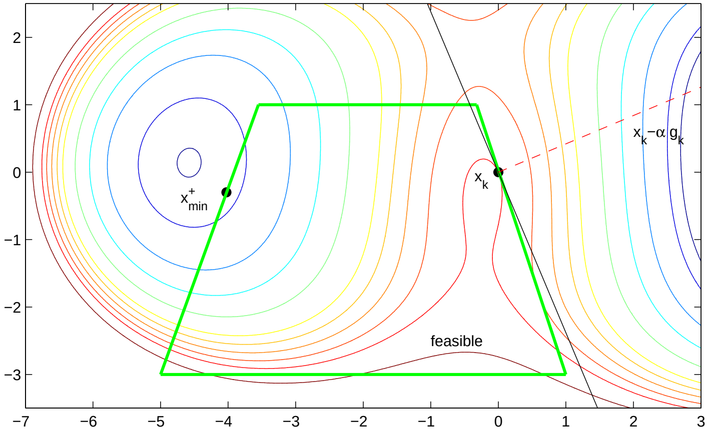
Step 2: Step calculation. Compute s_k and $x_k^+ \stackrel{\text{def}}{=} x_k + s_k \in \mathcal{F}$ such that $\chi_m(s_k) \leq \kappa_{\text{stop}} \|s_k\|^2$.

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

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

Walking through the pass...



A "beyond the pass" constrained problem with

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

Evaluation Complexity for ARC2CC

The ARC2CC algorithm requires at most

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

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

Caveat: cost of solving the subproblem!

Higher-order models/critical points: $\left\lceil \frac{\kappa_{\rm C}}{\epsilon^{(p+1)/(p+1-q)}} \right\rceil$ evaluations

Identical to the unconstrained case!!!

The general constrained case

Consider now the general NLO (slack variables formulation):

$$\begin{array}{ll} \text{minimize}_x & f(x) \\ \text{such that} & c(x) = 0 \quad \text{and} \quad x \in \mathcal{F} \end{array}$$

Ideas for a second-order algorithm:

1. get $\|c(x)\| \leq \epsilon$ (if possible) by minimizing $\|c(x)\|^2$ such that $x \in \mathcal{F}$ (getting $\|J(x)^T c(x)\|$ small unsuitable!)
2. track the "trajectory"

$$\mathcal{T}(t) \stackrel{\text{def}}{=} \{x \in \mathbb{R}^n \mid c(x) = 0 \quad \text{and} \quad f(x) = t\}$$

for values of t decreasing from f(first feasible iterate) while preserving $x \in \mathcal{F}$

First-order complexity for general NLO (1)

Sketch of a two-phases algorithm:

feasibility: apply ARC2CC to

$$\min_x \nu(x) \stackrel{\text{def}}{=} \|c(x)\|^2 \quad \text{such that} \quad x \in \mathcal{F}$$

at most $O(\epsilon_P^{-1/2}\epsilon_D^{-3/2})$ evaluations

tracking: successively

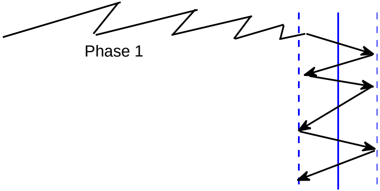
- apply ARC2CC (with specific termination test) to

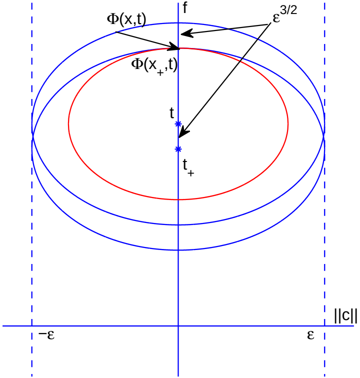
$$\min_x \mu(x) \stackrel{\text{def}}{=} \|c(x)\|^2 + (f(x) - t)^2 \quad \text{such that} \quad x \in \mathcal{F}$$

- decrease t (proportionally to the decrease in $\phi(x)$)

at most $O(\epsilon_P^{-1/2}\epsilon_D^{-3/2})$ evaluations

A view of Algorithm ARC2CC





First-order complexity for general NLO (2)

Under the "conditions stated above", the ARC2CC algorithm takes at most

$$O(\epsilon_P^{-1/2}\epsilon_D^{-3/2}) \text{ evaluations}$$

to find an iterate x_k with either

$$\|c(x_k)\| \leq \delta\epsilon_P \quad \text{and} \quad \chi_{\mathcal{L}} \leq \|(y,1)\|\epsilon_D$$

for some Lagrange multiplier y and where

$$\mathcal{L}(x,y) = f(x) + \langle y, c(x)\rangle,$$

or

$$\|c(x_k)\| > \delta\epsilon \quad \text{and} \quad \chi_{\|c\|} \leq \epsilon.$$

Conclusions

- Complexity analysis for first-order points using second-order methods

$$O(\epsilon^{-3/2}) \quad \text{(unconstrained, convex constraints)}$$
$$O(\epsilon_p^{-1/2}\epsilon_d^{-3/2}) \quad \text{(equality and general constraints)}$$

- Available also for p-th order methods :

$$O(\epsilon^{-(p+1)/(p+1-q)}) \quad \text{(unconstrained, convex constraints)}$$
$$\left[O(\epsilon_p^{-1/p}\epsilon_d^{-(p+1)/p}) \quad \text{(equality and general constraints)} \right]$$

- Jarre's example $\Rightarrow$ global optimization much harder
- ARC2 is optimal amongst second-order method
- More also known (DFO, non-smooth, etc)

Many thanks for your attention!