Tensor methods for nonconvex optimization problems

Coralia Cartis (University of Oxford)

Joint with Nick Gould (Rutherford Appleton Laboratory, UK)
and Philippe Toint (University of Namur, Belgium)

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Standard methods for nonconvex optimization

$$\underset{x\in\mathbb{R}^n}{\text{minimize}} \quad f(x) \quad \text{where} \quad f \quad \text{is smooth.}$$

• f has gradient vector ∇f (first derivatives) and Hessian matrix $\nabla^2 f$ (second derivatives).

$\longrightarrow$ local minimizer x_* with $\nabla f(x_*) = 0$ (stationarity) and $\nabla^2 f(x_*) \succ 0$ (local convexity).

Derivative-based methods:

- user-given $x_0 \in \mathbb{R}^n$, generate iterates x_k, $k \geq 0$.
- $f(x_k + s) \approx \; m_k(s)$ simple model of f at x_k;
  m_k linear or quadratic Taylor approximation of f.
  $s_k \to \min_s \; m_k(s)$; $s_k \to x_{k+1} - x_k$
- terminate within ϵ of optimality (small gradient values).

Derivative-based local models

Choices of models

- linear : $m_k(s) = f(x_k) + \nabla f(x_k)^T s$

  $\longrightarrow$ s_k steepest descent direction.
- quadratic : $m_k(s) = f(x_k) + \nabla f(x_k)^T s + \frac{1}{2} s^T \nabla^2 f(x_k) s$

  $\longrightarrow$ s_k Newton-like direction.

Must safeguard s_k to ensure method converges globally, from an arbitrary starting point x_0, to first/second order critical points.

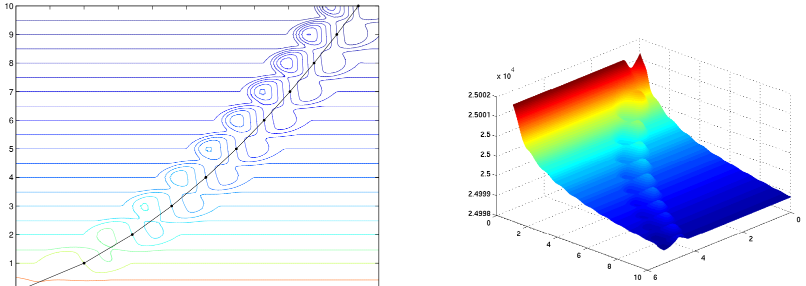
Adaptive 'globalization' strategies:

- Linesearch (Cauchy?, Armijo (1966))
- Trust region (Fletcher, Powell (1970s))
- Regularization (Levenberg-Marquardt ('44, '63), Griewank ('83), Nesterov & Polyak ('06), C, Gould & Toint ('11), ...)

Global efficiency of Newton's method

Newton's method: as slow as steepest descent

- may require $\lceil \epsilon^{-2} \rceil$ evaluations/iterations, same as steepest descent method



Globally Lipschitz continuous gradient and Hessian

But Regularized Newton (ie, ARC) has better/optimal complexity.

Worst-case evaluation complexity of methods

Global rates of convergence from any initial guess

Under sufficient smoothness assumptions on derivatives of f (Lipschitz continuity), for any $(\epsilon_1, \epsilon_2) > 0$, the algorithms generate $\|\nabla f(x_k)\| \leq \epsilon_1$ (and $\lambda_{\min}(\nabla^2 f(x_k)) \geq -\epsilon_2$) in at most $k_\epsilon^{\mathrm{alg}}$ iterations/evaluations:

1st, 2nd Criticality	SD	Newton/TR/LS	ARC	TR+/ LS+
$\|\nabla f(x_k)\|_2 \leq \epsilon_1$	$\mathcal{O}(\epsilon_1^{-2})$	$\mathcal{O}(\epsilon_1^{-2})$	$\mathcal{O}\left(\epsilon_1^{-\frac{3}{2}}\right)$	$\mathcal{O}\left(\epsilon_1^{-\frac{3}{2}}\right)$
$\lambda_{\min}(\nabla^2 f(x_k)) \geq -\epsilon_2$	–	$\mathcal{O}(\epsilon_2^{-3})$	$\mathcal{O}(\epsilon_2^{-3})$	$\mathcal{O}(\epsilon_2^{-3})$

[TR+:Curtis et al,'17]

[LS+:Royer et al'18]

- $\mathcal{O}(\cdot)$ contains $f(x_0) - f_{\mathrm{low}}$, L_{grad} or L_{Hessian} and algorithm parameters.
- all bounds are sharp, ARC bound is optimal for second-order methods [C, Gould & Toint,'10,'11, '17; Carmon et al ('18)]

Adaptive cubic regularization: ARC (=AR2)

[Griewank ('81, TR); Nesterov & Polyak ('06); Weiser et al ('07); C, Gould & Toint ('11)]

[Dussault ('15); Birgin et al ('17)]

- cubic regularization model at x_k

$$m_k(s) = \underbrace{f(x_k) + \nabla f(x_k)[s] + \tfrac{1}{2}\nabla f^2(x_k)[s]^2}_{T_2(x_k,s)} + \tfrac{1}{3}\sigma_k \|s\|_2^3$$

where $\sigma_k > 0$ is a regularization weight. [$B_k \approx \nabla f^2(x_k)$ allowed]

- compute s_k : $m_k(s_k) < f(x_k)$, $\|\nabla_s m_k(s_k)\| \leq \theta_1 \|s_k\|_2^2$ and $\lambda_{\min}(\nabla_s^2 m_k(s_k)) \geq -\theta_2 \|s_k\|_2^1$ [no global model minimization required, but possible]
- compute $\rho_k = \dfrac{f(x_k) - f(x_k + s_k)}{f(x_k) - T_2(x_k, s_k)}$
- set $x_{k+1} = \begin{cases} x_k + s_k & \text{if } \rho_k > \eta = 0.1 \\ x_k & \text{otherwise} \end{cases}$
- $\sigma_{k+1} = \dfrac{\sigma_k}{\gamma_1} = 2\sigma_k$ when $\rho_k < \eta$; else $\sigma_{k+1} = \max\{\gamma_2 \sigma_k, \sigma_{\min}\} = \max\{\tfrac{1}{2}\sigma_k, \sigma_{\min}\}$

Regularization methods with higher derivatives

Adaptive pth order regularization: ARp

[Birgin et al ('17), C, Gould, Toint('20)]

ARp proceeds similarly to ARC/AR2:

- pth order regularization model at x_k

$$m_k(s) = \underbrace{f(x_k) + \nabla f(x_k)[s] + \ldots + \frac{1}{p!}\nabla^p f(x^k)[s]^p}_{T_p(x_k,s)} + \frac{1}{(p+1)!}\sigma_k\|s\|_2^{p+1}$$

  where $\sigma_k > 0$ is a regularization weight.

- compute s_k : $m_k(s_k) < f(x_k)$, $\|\nabla_s m_k(s_k)\| \leq \theta_1\|s_k\|_2^p$ and $\lambda_{\min}(\nabla_s^2 m_k(s_k)) \geq -\theta_2\|s_k\|^{p-1}$ [no global model minimization required]
- compute $\rho_k = \dfrac{f(x_k) - f(x_k + s_k)}{f(x_k) - T_p(x_k, s_k)}$
- set $x_{k+1} = \begin{cases} x_k + s_k & \text{if } \rho_k > \eta = 0.1 \\ x_k & \text{otherwise} \end{cases}$
- $\sigma_{k+1} = \dfrac{\sigma_k}{\gamma_1} = 2\sigma_k$ when $\rho_k < \eta$; else $\sigma_{k+1} = \max\{\gamma_2\sigma_k, \sigma_{\min}\} = \max\{\frac{1}{2}\sigma_k, \sigma_{\min}\}$

Worst-case complexity of ARp for 1st/2nd-order criticality

[Birgin et al ('17), C, Gould, Toint('20)]

Theorem: Let $p \geq 2$, $f \in C^p(\mathbb{R}^n)$, bounded below by $f_{\rm low}$ and with the pth derivative Lipschitz continuous. Then ARp requires at most

$$\left\lceil \kappa_{1,2} \cdot (f(x_0) - f_{\rm low}) \cdot \max\left[\epsilon_1^{-\frac{p+1}{p}}, \epsilon_2^{-\frac{p+1}{p-1}}\right] + \kappa_{1,2} \right\rceil$$

function and derivatives' evaluations/iterations to ensure $\|\nabla f(x_k)\| \leq \epsilon_1$ and $\lambda_{\min}(\nabla^2 f(x_k)) \geq -\epsilon_2$.

1st, 2nd Criticality	p=2	p=3	p=4	...p
$\|\nabla f(x_k)\|_2 \leq \epsilon_1$	$\mathcal{O}(\epsilon_1^{-3/2})$	$\mathcal{O}(\epsilon_1^{-4/3})$	$\mathcal{O}\left(\epsilon_1^{-5/4}\right)$	$\mathcal{O}\left(\epsilon_1^{-(p+1)/p}\right)$
$\lambda_{\min}(\nabla^2 f(x_k)) \geq -\epsilon_2$	$\mathcal{O}(\epsilon_2^{-3})$	$\mathcal{O}(\epsilon_2^{-2})$	$\mathcal{O}(\epsilon_2^{-5/3})$	$\mathcal{O}(\epsilon_2^{-(p+1)/(p-1)})$

All bounds are sharp, and ARp 1st-order bound is optimal for pth order mthds.

[C, Gould & Toint,'20 Carmon et al ('18)]

Worst-case complexity of ARp for 1st/2nd-order criticality

Sketch of Proof (Theorem): [Birgin et al ('17), C, Gould, Toint('20)]

- Sufficient decrease on successful steps

$$\begin{aligned} f(x_k) - f(x_{k+1}) &\geq \eta[f(x_k) - T_p(x_k, s_k)] \\ &= f(x_k) - m_k(s_k) + \tfrac{\sigma_k}{(p+1)!}\|s_k\|^{p+1} \\ &\geq \tfrac{\sigma_{\min}}{(p+1)!}\|s_k\|^{p+1} \\ &\geq c\min\{\epsilon_1^{(p+1)/p}, \epsilon_2^{(p+1)/(p-1)}\} \qquad (*) \end{aligned}$$

- Long steps: first-order

$$\|s_k\| \geq c_1 \left(\frac{\nabla f(x_k + s_k)}{L + \theta_1 + \sigma_{\max}}\right)^{1/p} \geq c_1 \epsilon_1^{1/p}$$

and second-order

$$\|s_k\| \geq c_2 \left(\frac{\lambda_{\min}(\nabla^2 f(x_k + s_k))}{L + \theta_2 + \sigma_{\max}}\right)^{1/(p-1)} \geq c_2 \epsilon_2^{1/(p-1)}$$

where $\sigma_k \leq \sigma_{\max} = C \cdot L$. Summing up (*) over successful iterations + counting unsuccessful iterations.

ARp for 3rd-order criticality

In the model minimization, require also the 3rd order approximate condition:

$$\max_{d \in \mathcal{M}_{k+1}} \left| \nabla_s^3 m_k(s_k)[d]^3 \right| \leq \|s_k\|^{p-2},$$

whenever

$$\mathcal{M}_{k+1} = \left\{ d \mid \|d\| = 1 \text{ and } |\nabla_s^2 m_k(s_k)[d]^2| \leq \|s_k\|^{p-1} \right\} \neq \emptyset.$$

Then under same conditions as Theorem, ARp takes at most

$$\left\lceil \kappa_{1,2,3} \cdot (f(x_0) - f_{\rm low}) \cdot \max\left[\epsilon_1^{-\frac{p+1}{p}}, \epsilon_2^{-\frac{p+1}{p-1}}, \epsilon_3^{-\frac{p+1}{p-2}} \right] + \kappa_{1,2,3} \right\rceil$$

function and derivatives' evaluations/iterations to ensure

$$\|\nabla f(x_k)\| \leq \epsilon_1, \; \lambda_{\min}(\nabla^2 f(x_k)) \geq -\epsilon_2$$

and $\left| \nabla^3 f(x_k)[d]^3 \right| \leq \epsilon_3$, $|\nabla^2 f(x_k)[d]^2| \leq \epsilon_2$, for all $d \in \mathcal{M}_k$.

- $\mathcal{M}_k$ includes approximate objective's Hessian null space if subproblem is solved to local ϵ accuracy.

Regularization methods for high order optimality

Beyond 3rd order: high(er)-order optimality conditions

[C, Gould, Toint('18, J FoCM)]

Let x_* be a local minimizer of $f \in C^q(\mathbb{R}^n)$. Consider (feasible) descent arcs $x(\alpha) = x_* + \sum_{i=1}^q \alpha^i s_i + o(\alpha^q)$ where $\alpha > 0$. Derive necessary (and sometimes sufficient) optimality conditions.

[Hancock, Peano example of non-Taylor based arcs along which descent happens!]

For $j \in \{1, \ldots, q\}$, the inequality

$$\sum_{k=1}^{j} \frac{1}{k!} \left(\sum_{(\ell_1,\ldots,\ell_k)\in\mathcal{P}(j,k)} \nabla_x^k f(x_*)[s_{\ell_1}, \ldots, s_{\ell_k}] \right) \geq 0$$

holds for all $(s_1, \ldots, s_j)$ such that, for $i \in \{1, \ldots, j-1\}$,

$$\sum_{k=1}^{i} \frac{1}{k!} \left(\sum_{(\ell_1,\ldots,\ell_k)\in\mathcal{P}(i,k)} \nabla_x^k f(x_*)[s_{\ell_1}, \ldots, s_{\ell_k}] \right) = 0,$$

where the index sets $\mathcal{P}(j,k) = \{(\ell_1, \ldots, \ell_k) \in \{1, \ldots, j\}^k \mid \sum_{i=1}^k \ell_i = j\}$.

Beyond 3rd order: high(er)-order optimality conditions

[C, Gould, Toint('18, J FoCM)]

- Convex constraints (and suitable constraint qualifications) can be incorporated.
- Usual first, second and third order optimality conditions can be derived.
- But, starting at fourth-order and beyond, necessary conditions above involve a mixture of derivatives of different orders and cannot/should not be separated/disentangled.

Example: Peano variant: $\min_{x\in\mathbb{R}^2} f(x) = x_2^2 - \kappa_1 x_1^2 x_2 + \kappa_2 x_1^4$,

where κ_1 and κ_2 are specified parameters.

Fourth-order condition (κ_1 large):

$\ker^1[\nabla_x^1 f(0)] = \Re^2$, $\ker^2[\nabla_x^2 f(0)] = e_1$, $\ker^3[\nabla_x^3 f(0)] = e_1 \cup e_2$.

$$\tfrac{1}{2}\nabla_x^2 f(0)[s_2]^2 + \tfrac{1}{2}\nabla_x^3 f(0)[s_1, s_1, s_2] + \tfrac{1}{24}\nabla_x^4 f(0)[s_1]^4 \geq 0$$

implies the much weaker $\nabla_x^4 f(x_*)[s_1]^4 \geq 0$ on $\cap_{i=1}^3 \ker^i[\nabla_x^i f(x_*)]$.

Beyond 3rd order: high(er)-order optimality conditions

[C, Gould, Toint('20, arXiv)]

Challenge: find a (necessary) optimality measure for qth order criticality for f that is sufficiently accurate and useful in ARp ?
For $j \in \{1, \ldots, q\}$, a jth order criticality measure for f is: for some $\delta \in (0, 1]$, let

$$\phi^{\delta}_{f,j}(x) = f(x) - \text{globmin}_{\|d\| \leq \delta} T_j(x, d).$$

$\longrightarrow$ a robust notion of criticality.

- $\phi^{\delta}_{f,j}(x)$ is continuous in x and δ for all orders q.
- $\phi^{\delta}_{f,1}(x) = \|\nabla f(x)\| \delta$
- $\phi^{\delta}_{f,2}(x) = \max\{0, -\lambda_{\min}(\nabla^2 f(x))\} \delta^2$.

If x is a local minimizer of f, then for $j \in \{1, \ldots, q\}$,

$$\lim_{\delta \to 0} \frac{\phi^{\delta}_{f,j}(x)}{\delta^j} = 0,$$

and this limit also implies the involved necessary conditions before.

ARqp: a high order regularization and criticality framework

[C, Gould, Toint('20, arXiv)]

- Let $q \leq p$. The pth order regularization model at x_k

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

- compute (s_k, δ_s): $m_k(s_k) < f(x_k)$,

$$\phi_{m_k,j}^{\delta_s}(s_k) \leq \theta \epsilon_j \delta_s^j, \quad j \in \{1, \ldots, q\}.$$

- compute $\rho_k = \dfrac{f(x_k) - f(x_k + s_k)}{f(x_k) - T_p(x_k, s_k)}$
- set $x_{k+1} = x_k + s_k$ and $\delta_{k+1} = \delta_s$ if $\rho_k > \eta = 0.1$; else $x_{k+1} = x_k$ and $\delta_{k+1} = \delta_k$.
- $\sigma_{k+1} = \dfrac{\sigma_k}{\gamma_1} = 2\sigma_k$ when $\rho_k < \eta$; else $\sigma_{k+1} = \max\{\gamma_2 \sigma_k, \sigma_{\min}\} = \max\{\frac{1}{2}\sigma_k, \sigma_{\min}\}$

ARqp: a high order regularization and criticality framework

[C, Gould, Toint('20, arXiv)]

Theorem: Let $p \geq q \geq 1$, $f \in C^p(\mathbb{R}^n)$, bounded below by $f_{\rm low}$ and with derivatives $\nabla^j f$ Lipschitz continuous for $j \in \{1, \ldots, p\}$. Terminate ARqp when

$$\phi_{f,j}^{\delta_k}(x_k) \leq \epsilon_j \delta_k^j \quad \text{for all } j \in \{1, \ldots, q\}$$

for some δ_k that is either 1 ($q = 1, 2$) or at least $C\epsilon = C(\epsilon_i)_{i=\overline{1,q}}$ [achievable for ARqp]. Until termination, ARqp requires at most

- $q = 1, 2$: $\quad \left\lceil \kappa_{1,2} \cdot (f(x_0) - f_{\rm low}) \cdot \max_{j=\overline{1,q}} \epsilon_j^{-\frac{p+1}{p-j+1}} + \kappa_{1,2} \right\rceil$

  [same as ARp]
- $q > 2$: $\quad \left\lceil \kappa_q \cdot (f(x_0) - f_{\rm low}) \cdot \max_{j=\overline{1,q}} \epsilon_j^{-\frac{q(p+1)}{p}} + \kappa_q \right\rceil$

function and derivatives' evaluations/iterations.

All bounds are sharp [C, Gould, Toint,'20]

ARqp: a high order regularization and criticality framework

[C, Gould, Toint('20, arXiv)]

Sketch of Proof (Theorem): Same ingredients as for ARp complexity proof:

Sufficient decrease on successful steps

$$f(x_k) - f(x_{k+1}) \geq \frac{\sigma_{\min}}{(p+1)!} \|s_k\|^{p+1}$$

Long steps: much more challenging when $q > 2$!

$$\|s_k\| \geq c_q \left(\frac{1-\theta}{L+\sigma_{\max}} \right)^{1/p} \epsilon_j^{j/p}$$

for some $j \in \{1, \ldots, q\}$, where $\sigma_k \leq \sigma_{\max} = C \cdot L$.

Lower bound on s_k: $(1-\theta)\epsilon_j \delta_k^j \leq (L+\sigma_{\max}) \sum_{l=1}^{j} \delta_k^l \|s_k\|^{p-l+1}$

Summing up (*) over successful iterations + counting unsuccessful iterations.

Higher order methods

A few remarks...

- ARqp with weaker optimality condition: $\phi_{f,j}^{\delta_k} \leq \epsilon_j \delta_k$, $j = \overline{1,q}$, satisfies complexity bound $\mathcal{O}\left(\max_{j=\overline{1,q}} \epsilon_j^{-\frac{p+1}{p-j+1}}\right)$.
- TRq (Trust-region detecting qth order criticality) satisfies the weaker complexity bound: $\mathcal{O}(\max_{j=\overline{1,q}} \epsilon_j^{-(q+1)})$.
- Convex constraints can be incorporated into ARp and ARqp without affecting the complexity.

Universal regularization methods

Universal ARp for first order criticality

[C, Gould, Toint ('19)]

Universal ARp (U-ARp) employs regularized local models

$$m_k(s) = T_p(x_k, s) + \frac{\sigma_k}{r}\|s\|_2^r,$$

where $r > p \geq 1$, r real, and $T_p(x_k, s)$ as in ARp.

U-ARp proceeds similarly to ARp:

- compute s_k: $m_k(s_k) < f(x_k)$ and $\|\nabla_s m_k(s_k)\| \leq \theta \|s_k\|^{r-1}$
- $\rho_k = \dfrac{f(x_k) - f(x_k + s_k)}{f(x_k) - T_p(x_k, s_k)}$
- update σ_k

But U-ARp has an additional crucial ingredient: if $\rho_k \geq \eta$ [i.e., k successful], check whether

$$\sigma_k \|s_k\|^{r-1} \geq \alpha \epsilon_1 \qquad (*)$$

where $\alpha \in (0, \frac{1}{3}]$ is a user-chosen constant.

U-ARp allows $x_{k+1} = x_k + s_k$ (and σ_k decrease) only when both $\rho_k \geq \eta$ and (*) hold. Else, σ_k is increased.

Beyond Lipschitz continuity, towards non-smoothness

$f \in C^{p,\beta_p}(\mathbb{R}^n)$: $f \in C^p(\mathbb{R}^n)$ and $\nabla^p f$ is Hölder continuous on the path of the iterates (and trial points), namely,

$$\|\nabla^p f(y) - \nabla^p f(x_k)\| \leq L\|y - x_k\|^{\beta_p}$$

holds for all $y \in [x_k, x_k + s_k]$, $k \geq 0$.
$L_p > 0$ and $\beta_p \in [0, 1]$ for any $p \geq 1$.

- $\beta_p = 0$: $\nabla^p f$ uniformly bounded.
- $\beta_p \in (0, 1)$: $\nabla^p f$ continuous but not differentiable.
- $\beta_p = 1$: $\nabla^p f$ Lipschitz continuous (and differentiable).
- $\beta_p > 1$: f reduces to polynomials.

$\longrightarrow$ Hölder continuity : a bridging case between smooth and non-smooth problems [Nemirovskii & Yudin ('83), Nesterov ('13), Devolder ('13), Grapiglia & Nesterov ('16)]

Worst-case complexity of UARp

Let $r \geq p \geq 1$, r real and p integer.
Let $f \in C^{p,\beta_p}(\mathbb{R}^n)$.
If $r \geq p + \beta_p$ [e.g., $r = p + 1$], then U-ARp requires at most

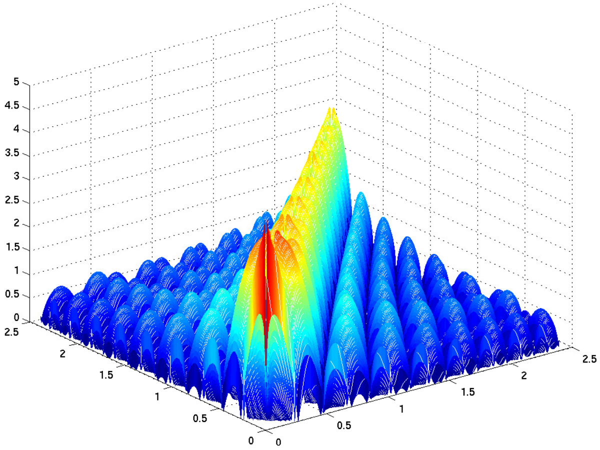
$$\left\lceil \kappa_1 \cdot (f(x_0) - f_{\text{low}}) \cdot \epsilon_1^{-\frac{p+\beta_p}{p+\beta_p-1}} \right\rceil$$

function/derivative evaluations and iterations to ensure $\|\nabla f(x_k)\| \leq \epsilon_1$.

$r \geq p + \beta_p$ [e.g., $r = p + 1$]: the bound is 'universal', adapting to landscape smoothness without knowing β_p/smoothness of f, independent of r.

Smooth or nonsmooth?

Sharpness example: the ragged landscape of a $f \in C^{1,\beta_1}$



Ratio of $|\nabla f(x) - \nabla f(y)|/|x-y|^{\beta}$