A Trust Region Algorithm with Improved Iteration Complexity for Nonconvex Smooth Optimization

Frank E. Curtis, Lehigh University

joint work with

Daniel P. Robinson, Johns Hopkins University
Mohammadreza Samadi, Lehigh University

University of Oxford, Mathematical Institute
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Outline

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Unconstrained (nonconvex) optimization

Given $f : \mathbb{R}^n \to \mathbb{R}$, consider the unconstrained optimization problem

$$\min_{x \in \mathbb{R}^n} f(x).$$

In this talk, we are primarily interested in

- solving nonconvex instances
- ... to find first- or second-order critical points;
- employing second-order methods;
- attaining global and fast local (i.e., quadratic) convergence;
- attaining good worst-case iteration (evaluation, etc.) complexity bounds.

Methods of interest in this talk

Trust region methods

- Decades of algorithmic development
- Levenberg (1944); Marquardt (1963); Powell (1970); many more!

Cubic regularization methods

- Relatively recent algorithmic development; fewer variants
- Griewank (1981); Nesterov & Polyak (2006); Cartis, Gould, & Toint (2011)

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Theoretical guarantees to assess a nonconvex optimization algorithm:

- Global convergence, i.e., $\nabla f(x_k) \to 0$ and maybe $\min(\text{eig}(\nabla^2 f(x_k))) \to \zeta > 0$
- Local convergence rate, i.e., $\|\nabla f(x_{k+1})\|_2 / \|\nabla f(x_k)\|_2 \to 0$ (or more)
- Worst-case complexity, i.e., upper bound on number of iterations[1] to achieve

$$\|\nabla f(x_k)\|_2 \leq \epsilon \quad \text{and perhaps} \quad \min(\text{eig}(\nabla^2 f(x_k))) \geq -\epsilon \quad \text{for some} \quad \epsilon > 0$$

[1] ...or function evaluations, subproblem solves, etc.

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- Decades of algorithmic development
- Levenberg (1944); Marquardt (1963); Powell (1970); many more!
- Global convergence, local quadratic rate when $\nabla^2 f(x_*) \succ 0$
- $\mathcal{O}(\epsilon^{-2})$ complexity to first-order ϵ-criticality

Cubic regularization methods

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- Griewank (1981); Nesterov & Polyak (2006); Cartis, Gould, & Toint (2011)
- Global convergence, local quadratic rate when $\nabla^2 f(x_*) \succ 0$
- $\mathcal{O}(\epsilon^{-3/2})$ complexity to first-order ϵ-criticality, $\mathcal{O}(\epsilon^{-3})$ to second-order

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Goals and contributions

What are our goals in this work?

- Question: Can we design a TR method with improved complexity?
- ...and does this lead to improved performance?

What are our contributions? A TR method that has

- global and quadratic local convergence rate guarantees;
- a worst-case iteration complexity of $\mathcal{O}(\epsilon^{-3/2})$ to first-order ϵ-criticality;
- ...and of $\mathcal{O}(\epsilon^{-3})$ to second-order ϵ-criticality.

How is this achieved?

- new step acceptance criteria;
- new mechanism for rejecting a step while expanding the TR radius;
- new updates that may involve sublinear TR radius decrease.

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- new mechanism for rejecting a step while expanding the TR radius;
- new updates that may involve sublinear TR radius decrease.

We discuss three algorithms:

- TTR: "Traditional" Trust Region algorithm
- ARC: Adaptive Regularisation algorithm using Cubics
  - Cartis, Gould, & Toint (2011)
- TRACE: Trust Region Algorithm with Contractions and Expansions
  - Curtis, Robinson, & Samadi (2014)

Outline

Algorithm basics

TTR	ARC
1: Solve to compute s_k:	1: Solve to compute s_k:
$\min_{s\in\mathbb{R}^n} \; q_k(s) := f_k + g_k^T s + \frac{1}{2} s^T H_k s$ s.t. $\|s\|_2 \leq \delta_k$ (dual: λ_k)	$\min_{s\in\mathbb{R}^n} \; c_k(s) := f_k + g_k^T s + \frac{1}{2} s^T H_k s + \frac{1}{3}\sigma_k \|s\|_2^3$
2: Compute ratio:	2: Compute ratio:
$\rho_k^q \leftarrow \frac{f_k - f(x_k+s_k)}{f_k - q_k(s_k)}$	$\rho_k^c \leftarrow \frac{f_k - f(x_k+s_k)}{f_k - c_k(s_k)}$
3: Update radius:	3: Update regularization:
$\rho_k^q \geq \eta$: accept and $\delta_k \nearrow$	$\rho_k^c \geq \eta$: accept and $\sigma_k \searrow$
$\rho_k^q < \eta$: reject and $\delta_k \searrow$	$\rho_k^c < \eta$: reject and $\sigma_k \nearrow$

Algorithm basics: Subproblem solution correspondence

TTR		ARC
1: Solve to compute s_k: $\min_{s\in\mathbb{R}^n} q_k(s) := f_k + g_k^T s + \frac{1}{2}s^T H_k s$ s.t. $\|s\|_2 \leq \delta_k$ (dual: λ_k)	$\sigma_k = \frac{\lambda_k}{\delta_k}$ →	1: Solve to compute s_k: $\min_{s\in\mathbb{R}^n} c_k(s) := f_k + g_k^T s + \frac{1}{2}s^T H_k s + \frac{1}{3}\sigma_k\|s\|_2^3$
2: Compute ratio: $\rho_k^q \leftarrow \frac{f_k - f(x_k+s_k)}{f_k - q_k(s_k)}$	← $\delta_k = \|s_k\|_2$	2: Compute ratio: $\rho_k^c \leftarrow \frac{f_k - f(x_k+s_k)}{f_k - c_k(s_k)}$
3: Update radius: $\rho_k^q \geq \eta$: accept and $\delta_k \nearrow$; $\rho_k^q < \eta$: reject and $\delta_k \searrow$		3: Update regularization: $\rho_k^c \geq \eta$: accept and $\sigma_k \searrow$; $\rho_k^c < \eta$: reject and $\sigma_k \nearrow$

Discussion

What are the similarities?

- algorithmic frameworks are almost identical
- one-to-one correspondence (except $\lambda_k = 0$) between subproblem solutions

What are the key differences?

- step acceptance criteria
- trust region vs. regularization coefficient updates

Discussion

What are the similarities?

- algorithmic frameworks are almost identical
- one-to-one correspondence (except $\lambda_k = 0$) between subproblem solutions

What are the key differences?

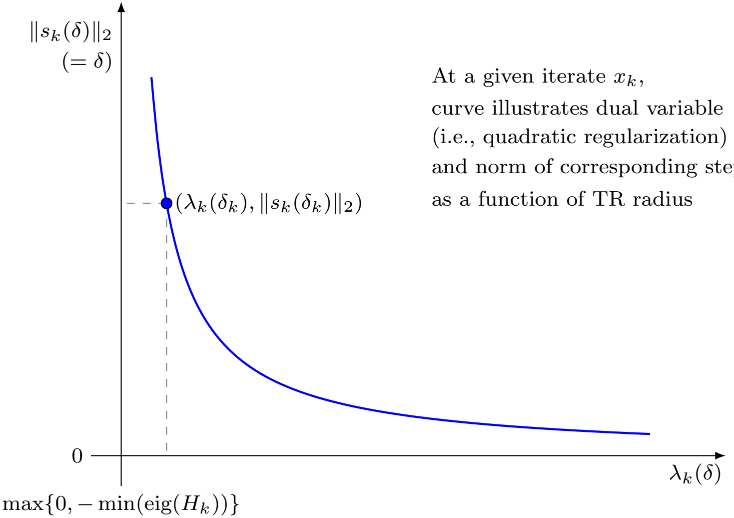
- step acceptance criteria
- trust region vs. regularization coefficient updates

Recall that a solution s_k of the TR subproblem is also a solution of

$$\min_{s \in \mathbb{R}^n} \; f_k + g_k^T s + \tfrac{1}{2} s^T (H_k + \lambda_k I) s,$$

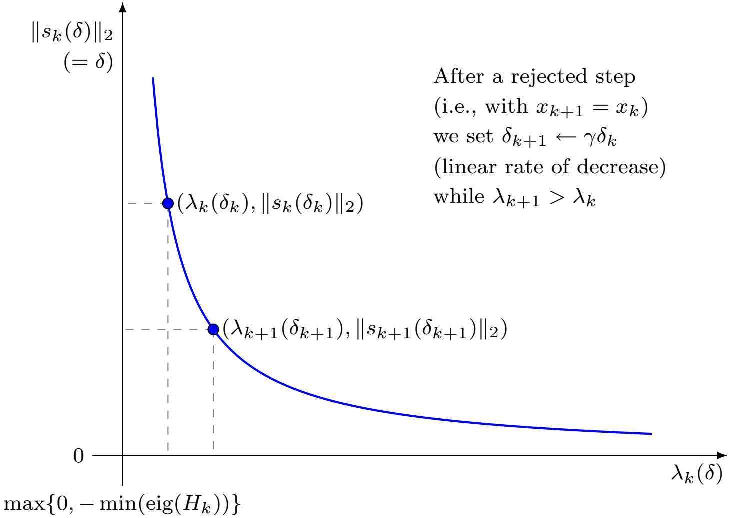
so the dual variable λ_k can be viewed as a quadratic regularization coefficient.

Regularization/stepsize trade-off: TTR

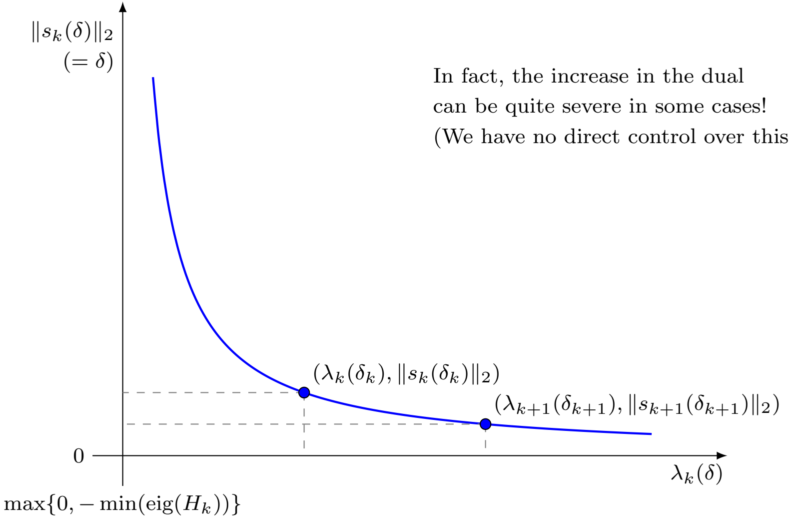


At a given iterate x_k,
curve illustrates dual variable
(i.e., quadratic regularization)
and norm of corresponding step
as a function of TR radius

Regularization/stepsize trade-off: TTR



Regularization/stepsize trade-off: TTR



In fact, the increase in the dual can be quite severe in some cases! (We have no direct control over this.)

Intuition, please!

Intuitively, what is so important about $\frac{\lambda_k}{\|s_k\|_2} = \frac{\lambda_k}{\delta_k}$?

- Large δ_k implies s_k may not yield objective decrease.
- Small δ_k prohibits long steps.
- Small λ_k suggests the TR is not restricting us too much.
- Large λ_k suggests more objective decrease is possible.

So what is so bad (for complexity's sake) with the following?

$$\frac{\lambda_k}{\delta_k} \approx 0 \quad \text{and} \quad \frac{\lambda_{k+1}}{\delta_{k+1}} \gg 0.$$

It's that we may go from a

- large, but unproductive step to a
- productive, but (too) short step!

ARC magic

So what's the magic of ARC?

- It's not the types of steps you compute (since TR subproblem gives the same).
- It's that a simple update for σ_k gives a good regularization/stepsize balance.

ARC magic

So what's the magic of ARC?

- It's not the types of steps you compute (since TR subproblem gives the same).
- It's that a simple update for σ_k gives a good regularization/stepsize balance.

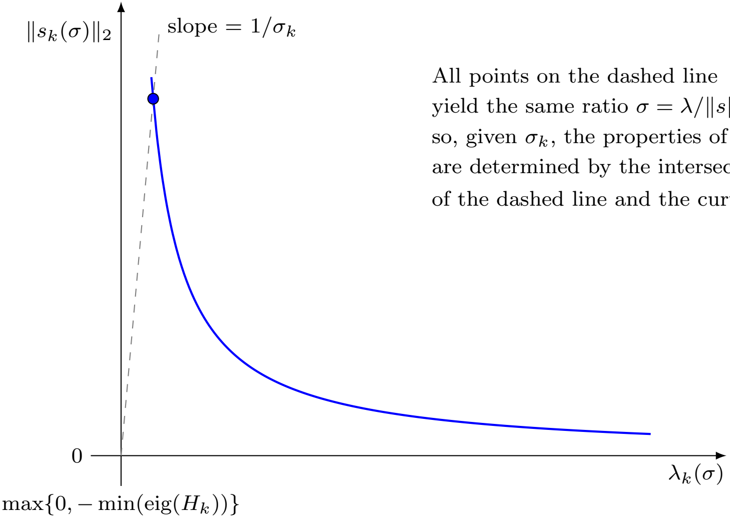
In ARC, restricting $\sigma_k \geq \sigma_{\min}$ for all k and proving that $\sigma_k \leq \sigma_{\max}$ for all k ensures that all accepted steps satisfy

$$f_k - f_{k+1} \geq c_1 \sigma_{\min} \|s_k\|_2^3 \quad \text{and} \quad \|s_k\|_2 \geq \left(\frac{c_2}{\sigma_{\max} + c_3} \right)^2 \|g_{k+1}\|_2^{1/2}.$$

One can also show that, at any point, the number of rejected steps that can occur consecutively is bounded above by a constant (independent of k and ϵ).

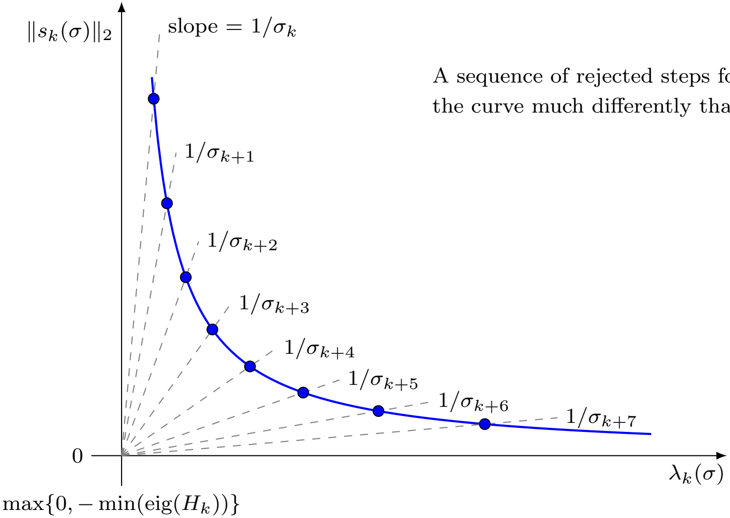
- Important to note that ARC always has the regularization "on."

Regularization/stepsize trade-off: ARC



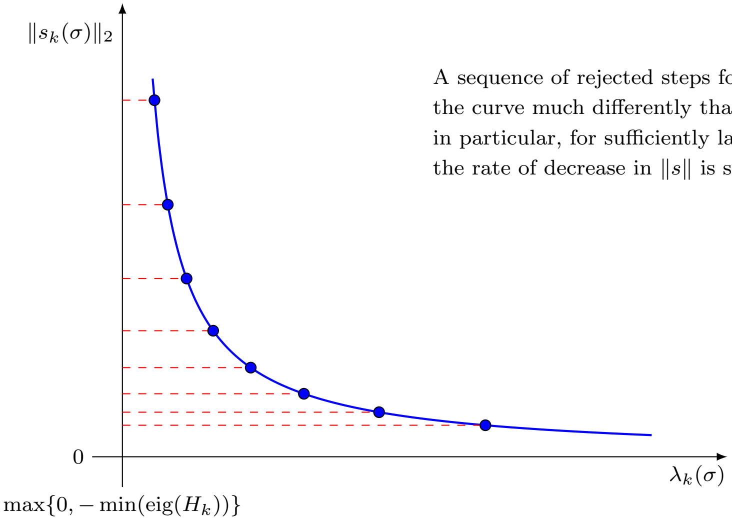
All points on the dashed line yield the same ratio $\sigma = \lambda/\|s\|_2$ so, given σ_k, the properties of s_k are determined by the intersection of the dashed line and the curve

Regularization/stepsize trade-off: ARC



A sequence of rejected steps follow the curve much differently than TTR;

Regularization/stepsize trade-off: ARC



A sequence of rejected steps follow the curve much differently than TTR; in particular, for sufficiently large σ, the rate of decrease in $\|s\|$ is sublinear

Outline

From TTR to TRACE

TRACE involves three key modifications of TTR.

1: Different step acceptance ratio

2: New expansion step: May reject step while increasing TR radius

3: New contraction procedure: Explicit or implicit (through update of λ)

Step acceptance ratio

1: Different step acceptance ratio

$$\text{TTR: } \rho_k^q = \frac{f_k - f(x_k + s_k)}{f_k - q_k(s_k)} \quad \Rightarrow \quad \text{TRACE: } \rho_k = \frac{f_k - f(x_k + s_k)}{\|s_k\|_2^3}$$

Motivations:

- With second-order model, error is third-order.
- Recall the first guarantee of accepted steps in ARC:

$$f_k - f_{k+1} \geq c_1 \sigma_{\min} \|s_k\|_2^3.$$

Expansion steps

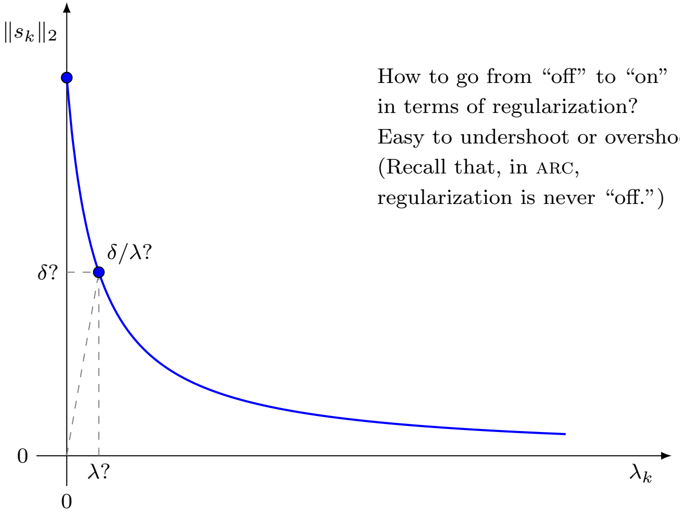
2: New expansion step: May reject step while increasing TR radius

- We define a monotonically increasing sequence $\{\sigma_k\}$.
- (Plays a similar theoretical role as the regularization coefficients in ARC.)
- If objective decrease is good, but dual suggests more decrease is possible, i.e.,

$$\rho_k \geq \eta \quad \text{but} \quad \lambda_k > \sigma_k \|s_k\|_2,$$

  then reject the step and increase the TR radius to allow more decrease.
- With $\delta_{k+1} \leftarrow \lambda_k / \sigma_k$, need at most one expansion between accepted steps.

Regularization/stepsize trade-off: "Off" to "on"



How to go from "off" to "on"
in terms of regularization?
Easy to undershoot or overshoot!
(Recall that, in ARC,
regularization is never "off.")

Contraction steps

3: New contraction procedure: Explicit or implicit (through update of λ)

$\lambda_k < \underline{\sigma}\|s_k\|_2$

- set $\lambda_{k+1} \leftarrow \lambda_k + (\underline{\sigma}\|g_k\|_2)^{1/2}$, or
- set $\lambda_{k+1} \in (\lambda_k, \lambda_k + (\underline{\sigma}\|g_k\|_2)^{1/2})$ so $\underline{\sigma} \leq \lambda_{k+1}/\|s_{k+1}\|_2 \leq \overline{\sigma}$

$\lambda_k \geq \underline{\sigma}\|s_k\|_2$

- set $\lambda_{k+1} \leftarrow \gamma_\lambda \lambda_k$ (with $\gamma_\lambda > 1$), or
- set $\delta_{k+1} \leftarrow \gamma_c \delta_k$ (with $\gamma_c \in (0, 1)$)

Update based on dual variable only requires a linear system solve!

$$(H_{k+1} + \lambda_{k+1} I)s = -g_{k+1}$$

Main algorithm

Algorithm 1 Trust Region Algorithm with Contraction and Expansion (TRACE)

Require: an acceptance constant $\eta \in \mathbb{R}_{++}$ with $0 < \eta < 1/2$
Require: update constants $\{\gamma_c, \gamma_e, \gamma_\lambda\} \subset \mathbb{R}_{++}$ with $0 < \gamma_c < 1 < \gamma_e$ and $\gamma_\lambda > 1$
Require: bound constants $\{\underline{\sigma}, \overline{\sigma}\} \subset \mathbb{R}_{++}$ with $0 < \underline{\sigma} \leq \overline{\sigma}$

procedure TRACE
  choose $x_0 \in \mathbb{R}^n$, $\{\delta_0, \Delta_0\} \subset \mathbb{R}_{++}$ with $\delta_0 \leq \Delta_0$, and $\sigma_0 \in \mathbb{R}_{++}$ with $\sigma_0 \geq \underline{\sigma}$
  compute (s_0, λ_0) by TR subproblem, then compute ρ_0
  for $k = 0, 1, 2, \ldots$ **do**
    if $\rho_k \geq \eta$ and either $\lambda_k \leq \sigma_k \|s_k\|_2$ or $\|s_k\|_2 = \Delta_k$ **then**
      set $x_{k+1} \leftarrow x_k + s_k$
      set $\Delta_{k+1} \leftarrow \max\{\Delta_k, \gamma_e \|s_k\|_2\}$
      set $\delta_{k+1} \leftarrow \min\{\Delta_{k+1}, \max\{\delta_k, \gamma_e \|s_k\|_2\}\}$
      set $\sigma_{k+1} \leftarrow \max\{\sigma_k, \lambda_k / \|s_k\|_2\}$
    else if $\rho_k < \eta$ **then**
      set $x_{k+1} \leftarrow x_k$
      set $\Delta_{k+1} \leftarrow \Delta_k$
      set $\delta_{k+1} \leftarrow \text{contract}(x_k, \delta_k, \sigma_k, s_k, \lambda_k)$
    else (i.e., **if** $\rho_k \geq \eta$, $\lambda_k > \sigma_k \|s_k\|_2$, and $\|s_k\|_2 < \Delta_k$)
      set $x_{k+1} \leftarrow x_k$
      set $\Delta_{k+1} \leftarrow \Delta_k$
      set $\delta_{k+1} \leftarrow \min\{\Delta_{k+1}, \lambda_k / \sigma_k\}$
      set $\sigma_{k+1} \leftarrow \sigma_k$
    compute (s_{k+1}, λ_{k+1}) by TR subproblem, then compute ρ_{k+1}
    if $\rho_k < \eta$ **then**
      set $\sigma_{k+1} \leftarrow \max\{\sigma_k, \lambda_{k+1} / \|s_{k+1}\|_2\}$

Contraction subroutine

Algorithm 2 Trust Region Contraction Subroutine

procedure CONTRACT$(x_k, \delta_k, \sigma_k, s_k, \lambda_k)$
  if $\lambda_k < \underline{\sigma}\|s_k\|_2$ **then**
    set $\lambda \leftarrow \lambda_k + (\underline{\sigma}\|g_k\|_2)^{1/2}$
    set s as the solution of $(H_k + \lambda I)s = -g_k$
    set $\delta \leftarrow \|s\|_2$
    if $\lambda/\delta \leq \overline{\sigma}$ **then**
      return $\delta_{k+1} \leftarrow \delta$
    else
      compute $\hat{\lambda} \in (\lambda_k, \lambda)$ so $(H_k + \hat{\lambda} I)\hat{s} = -g_k$ yields $\underline{\sigma} \leq \hat{\lambda}/\|\hat{s}\|_2 \leq \overline{\sigma}$
      set $\hat{\delta} \leftarrow \|\hat{s}\|_2$
      return $\delta_{k+1} \leftarrow \hat{\delta}$
  else (i.e., **if** $\lambda_k \geq \underline{\sigma}\|s_k\|_2$)
    set $\lambda \leftarrow \gamma_\lambda \lambda_k$
    set s as the solution of $(H_k + \lambda I)s = -g_k$
    set $\delta \leftarrow \|s\|_2$
    if $\delta \geq \gamma_c \|s_k\|_2$ **then**
      return $\delta_{k+1} \leftarrow \delta$
    else
      return $\delta_{k+1} \leftarrow \gamma_c \|s_k\|_2$

Global and local quadratic convergence

Assumption 1

- *f twice continuously differentiable and bounded below by $f_{\min}$*
- *g Lipschitz continuous in open convex set containing $\{x_k\}$ and $\{x_k + s_k\}$*
- *$\{g_k\}$ has nonzero elements and bounded above*
- *$\{H_k\}$ bounded above*

Theorem 2

$\|g_k\|_2 \to 0$

Assumption 3 (in addition to Assumption 1)

$\{x_k\}_{\mathcal{S}} \to x_*$ *around which H is positive definite and locally Lipschitz*

Theorem 4

$\{x_k\} \to x_*$ *with $g(x_*) = 0$ and, for sufficiently large k,*

$$\|g_{k+1}\|_2 = \mathcal{O}(\|g_k\|_2^2) \quad \text{and} \quad \|x_{k+1} - x_*\|_2 = \mathcal{O}(\|x_k - x_*\|_2^2)$$

Worst-case iteration complexity to first-order ϵ-criticality

Assumption 5 (in addition to Assumption 1)

H Lipschitz continuous in open convex set containing $\{x_k\}$ and $\{x_k + s_k\}$

Lemma 6

- $f_k - f_{k+1} \geq \eta \|s_k\|_2^3$ *for all accepted steps*
- $\{\sigma_k\}$ *bounded by* $\sigma_{\max} > 0$
- $\|s_k\|_2 \geq (H_{Lip} + \sigma_{\max})^{-1/2} \|g_{k+1}\|_2^{1/2}$

Theorem 7

Total number of iterations with $\|g_k\|_2 > \epsilon$ is

$$\mathcal{O}\left(\left\lfloor \frac{f_0 - f_{\min}}{\eta \Delta_0^3} \right\rfloor + \left\lfloor \left(\frac{f_0 - f_{\min}}{\eta (H_{Lip} + \sigma_{\max})^{-3/2}} \right) \epsilon^{-3/2} \right\rfloor \right)$$

Worst-case iteration complexity to second-order ϵ-criticality

Under the same assumptions...

Lemma 8

$$\liminf_{k\to\infty} \min(\text{eig}(H_k)) \geq 0$$

Theorem 9

Total number of iterations with

$$\|g_k\|_2 > \epsilon \quad or \quad \min(\text{eig}(H_k)) < -\epsilon$$

is

$$\mathcal{O}\left(\left\lfloor \frac{f_0 - f_{\min}}{\eta\Delta_0^3} \right\rfloor + \left\lfloor \left(\frac{f_0 - f_{\min}}{\eta(H_{Lip} + \sigma_{\max})^{-3/2}}\right) \epsilon^{-3/2} \right\rfloor\right) + \mathcal{O}\left(\left\lceil \left(\frac{f_0 - f_{\min}}{\eta\sigma_{\max}^{-3}}\right) \epsilon^{-3} \right\rceil\right)$$

Outline

Implementation

Implemented TRACE, TTR, and ARC together in MATLAB

- "Same" subproblem solver for all algorithms; Conn, Gould, Toint (2000)
- MATLAB's `eigs` for leftmost eigenvalues
- Radius and regularization updates:

$$(\text{TTR}) \qquad \delta_{k+1} \leftarrow \begin{cases} \max\{\delta_k, 2\|s_k\|_2\} & \text{if } \rho_k^q \geq \eta_2 \\ \delta_k & \text{if } \rho_k^q \in [\eta_1, \eta_2) \\ \delta_k/2 & \text{if } \rho_k^q < \eta_1 \end{cases}$$

$$(\text{ARC}) \qquad \sigma_{k+1} \leftarrow \begin{cases} \sigma_k/2 & \text{if } \rho_k^c \geq \eta_2 \\ \sigma_k & \text{if } \rho_k^c \in [\eta_1, \eta_2) \\ 2\sigma_k & \text{if } \rho_k^c < \eta_1 \end{cases}$$

- Termination criterion:

$$\|g_k\|_\infty \leq 10^{-6} \cdot \max\{\|g_0\|_\infty, 1\}$$

TRACE implementation details

- Reduction ratio:

$$\rho_k = \frac{f_k - f(x_k + s_k)}{\min\{\|s_k\|_2^3, f_k - c_k(s_k; \underline{\sigma})\}}$$

- Radius and regularization updates:

$$(\textsc{trace}) \qquad \delta_{k+1} \leftarrow \begin{cases} \max\{\delta_k, 2\|s_k\|_2\} & \text{if } \rho_k \geq \eta_2 \\ \delta_k & \text{if } \rho_k \in [\eta_1, \eta_2) \\ \textsc{contract} & \text{if } \rho_k < \eta_1 \end{cases}$$

where CONTRACT uses

$$\underline{\sigma} = 10^{-10}, \quad \overline{\sigma} = 10^{10}, \quad \gamma_\lambda = 2, \quad \gamma_c = 10^{-2}$$

Test set

Unconstrained problems from the CUTEr collection

- Removed 9 problems due to memory or decoding errors
- Removed 21 problems on which all algorithms failed
- Remaining set includes 130 problems

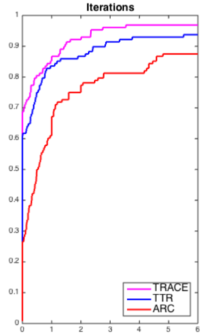
Step types taken (normalized by iterations per problem):

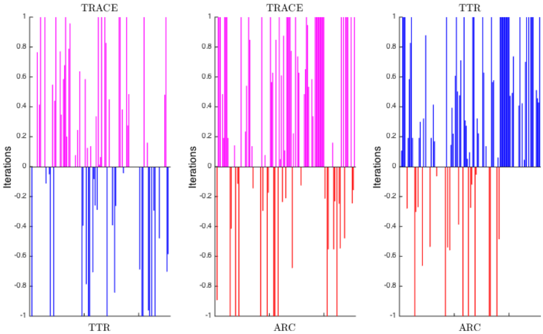
Accepted	Contraction	Expansion
60.07%	39.11%	0.82%

Contraction types taken (normalized by contractions per problem):

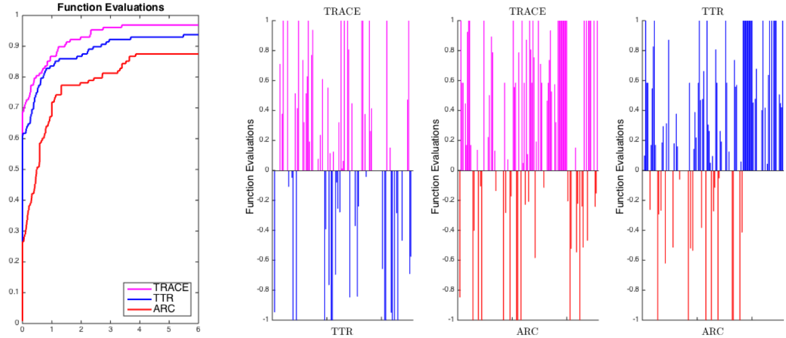
$\lambda_k + (\underline{\sigma}\|g_k\|_2)^{1/2}$	$\underline{\sigma} \leq \lambda/\|s\|_2 \leq \overline{\sigma}$	$\gamma_\lambda \lambda_k$	$\delta \leftarrow \gamma_c \|s_k\|_2$
5.43%	0.00%	84.43%	10.14%

Performance profiles: Iterations

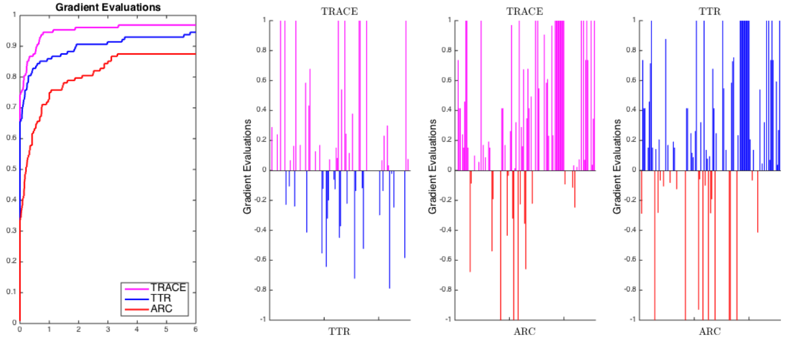




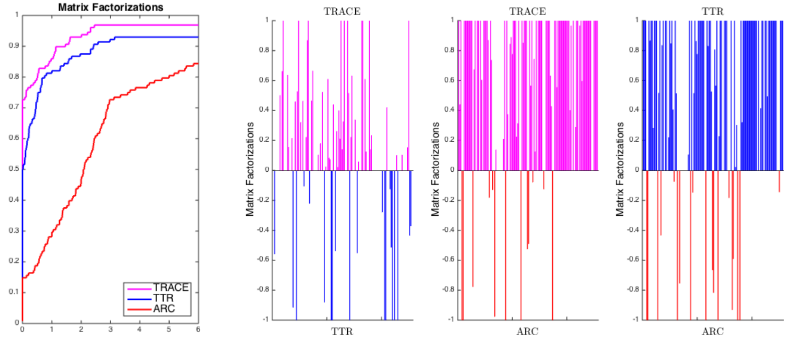
Performance profiles: Function evaluations



Performance profiles: Gradient evaluations



Performance profiles: Matrix factorizations



Outline

Contributions

Question: Can we design a TR method with improved complexity?

- Yes, TRACE achieves the same convergence/complexity guarantees as ARC
- New step acceptance criteria
- New mechanism for rejecting a step while expanding the TR radius
- New updates that may involve sublinear TR radius decrease

Numerical experiments show algorithm is at least competitive with TTR and ARC

F. E. Curtis, D. P. Robinson, and M. Samadi, "A Trust Region Algorithm with a Worst-Case Iteration Complexity of $\mathcal{O}(\epsilon^{-3/2})$ for Nonconvex Optimization," COR@L Laboratory, Department of ISE, Lehigh University, 14T-009, 2014.

Future work

Next questions: Does TRACE offer new insights for improved performance?

- Competitive performance is not surprising, but can it be better?
- Note that an iteration of TRACE may only need a linear system solve!
- One may imagine algorithms like TRACE and ARC that achieve the same convergence/complexity guarantees and never fully solve a subproblem
- ...worst-case (approximate) linear system solve complexity?
- Does TRACE offer new insights for constrained optimization?