

Characterizing the Worst-Case Performance of Algorithms for Nonconvex Optimization

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joint work with

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Outline

Motivation

Contemporary Analyses

Partitioning the Search Space

Behavior of Common Methods

Summary & Perspectives

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Problem

Consider the problem to minimize an objective function $f : \mathbb{R}^n \rightarrow \mathbb{R}$:

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

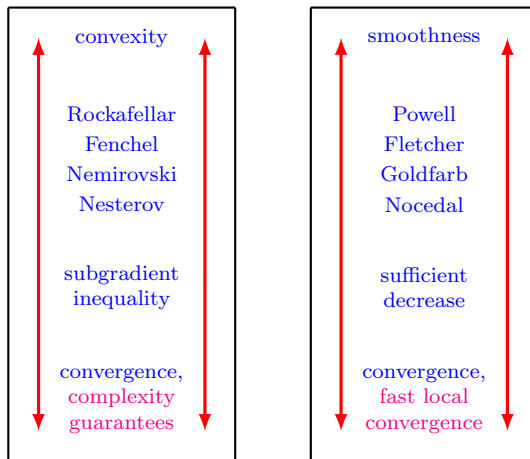
Various iterative algorithms have been proposed of the form

$$x_{k+1} \leftarrow x_k + s_k \quad \text{for all } k \in \mathbb{N},$$

where $\{x_k\}$ is the iterate sequence and $\{s_k\}$ is the step sequence.

History

Nonlinear optimization algorithm design has had parallel developments:



Worlds are finally colliding!

Worst-case complexity for convex optimization

Worst-case complexity:

Upper limit on the resources an algorithm will require to (approximately) solve a given problem

Worst-case complexity for convex optimization

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...for convex optimization: Bound on the number of iterations (or function or derivative evaluations) until

$$\begin{aligned} \|x_k - x_*\| &\leq \epsilon_x \\ \text{or } f(x_k) - f(x_*) &\leq \epsilon_f, \end{aligned}$$

where x_* is some global minimizer of f .

Worst-case complexity for convex optimization

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...for convex optimization: Bound on the number of iterations (or function or derivative evaluations) until

$$\|x_k - x_*\| \leq \epsilon_x$$

or $f(x_k) - f(x_*) \leq \epsilon_f,$

where x_* is some global minimizer of f .

Fact(?): Convex setting: better complexity *often* implies better performance.

(Really, need to consider work complexity, conditioning, structure, etc.)

Worst-case complexity for nonconvex optimization

...for **nonconvex optimization**: Here is how we do it now:

Since one generally cannot guarantee that $\{x_k\}$ converges to a minimizer, one asks for an upper bound on the number of iterations until

$$\|\nabla f(x_k)\| \leq \epsilon_g \quad (\text{first-order stationarity})$$

$$\text{and maybe also } \lambda(\nabla^2 f(x_k)) \geq -\epsilon_H \quad (\text{second-order stationarity})$$

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For example, it is known that for first-order stationarity we have the bounds...

Algorithm	until $\ \nabla f(x_k)\ _2 \leq \epsilon_g$
Gradient descent	$\mathcal{O}(\epsilon_g^{-2})$
Newton / trust region	$\mathcal{O}(\epsilon_g^{-2})$
Cubic regularization	$\mathcal{O}(\epsilon_g^{-3/2})$

Self-examination

But...

- ▶ Is this the best way to *characterize* our algorithms?
- ▶ Is this the best way to *represent* our algorithms?

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People listen! Cubic regularization...

- ▶ Griewank (1981)
- ▶ Nesterov & Polyak (2006)
- ▶ Weiser, Deufhard, Erdmann (2007)
- ▶ Cartis, Gould, Toint (2011), the ARC method

...is a framework to which researchers have been attracted...

- ▶ Agarwal, Allen-Zhu, Bullins, Hazan, Ma (2017)
- ▶ Carmon, Duchi (2017)
- ▶ Kohler, Lucchi (2017)
- ▶ Peng, Roosta-Khorasan, Mahoney (2017)

However, there remains a large gap between theory and practice!

(Trust region methods arguably perform better in general.)

Example: Matrix factorization

Symmetric low-rank matrix factorization problem:

$$\min_{X \in \mathbb{R}^{d \times r}} \frac{1}{2} \|XX^T - M\|_F^2,$$

where $M \in \mathbb{R}^{d \times d}$ with $\text{rank}(M) = r$.

- ▶ Nonconvex, but...
- ▶ Global minimum value is known (it's zero)
- ▶ All local minima are global minima

Jin, Ge, Netrapalli, Kakade, Jordan (2017)

Example: Dictionary learning

Learning a representation of input data in the form of linear combinations of some (unknown) basic elements, called *atoms*, which compose a *dictionary*:

$$\begin{aligned} \min_{X \in \mathcal{X}, Y \in \mathbb{R}^{n \times n}} \quad & \|Z - XY\|^2 + \phi(Y) \\ \text{s.t. } \mathcal{X} := \quad & \{X \in \mathbb{R}^{d \times n} : \|X_i\|_2 \leq 1 \text{ for all } i \in \{1, \dots, n\}\}, \end{aligned}$$

where $Z \in \mathbb{R}^{d \times n}$ is a given input.

Nonconvex, but, under some conditions, all saddle points can be “escaped”.

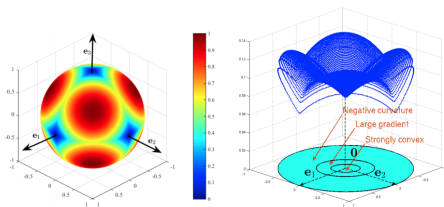
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Sun, Qu, Wright (2016)

Other examples

- ▶ Phase retrieval
- ▶ Orthogonal tensor decomposition
- ▶ Deep linear learning
- ▶ ...

Pedagogical example

But if we're talking about nonconvex optimization, we also could have...

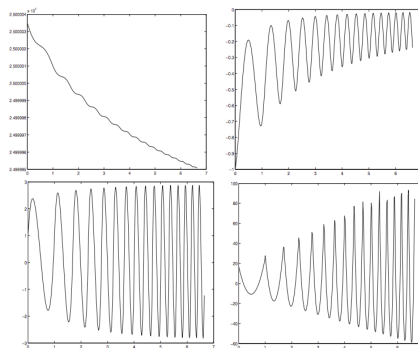


FIG. 2.1. The function $f^{(1)}$ (top left) and its derivatives of order one (top right), two (bottom left), and three (bottom right) on the first 16 intervals.

What *real* problem exhibits this behavior? (I don't know!)

More on this example later...

Purpose of this talk

Our goal: A *complementary* approach to characterize algorithms.

- ▶ global convergence
- ▶ worst-case complexity, contemporary type + **our approach**
- ▶ local convergence rate

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Our goal: A *complementary* approach to characterize algorithms.

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We're admitting: Our approach *does not always* give the complete picture.

But we believe it *is* useful.

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Simple setting

Suppose the gradient $g := \nabla f$ is Lipschitz continuous with constant $L > 0$.

Consider the iteration

$$x_{k+1} \leftarrow x_k - \frac{1}{L} g_k \quad \text{for all } k \in \mathbb{N}.$$

A contemporary complexity analysis considers the set

$$\mathcal{G}(\epsilon_g) := \{x \in \mathbb{R}^n : \|g(x)\|_2 \leq \epsilon_g\}$$

and aims to find an upper bound on the cardinality of

$$\mathcal{K}_g(\epsilon_g) := \{k \in \mathbb{N} : x_k \notin \mathcal{G}(\epsilon_g)\}.$$

$$g_k := \nabla f(x_k)$$

Upper bound on $|\mathcal{K}_g(\epsilon_g)|$

Using $s_k = -\frac{1}{L}g_k$ and the upper bound

$$f_{k+1} \leq f_k + g_k^T s_k + \frac{1}{2}L\|s_k\|_2^2,$$

one finds with $f_{\inf} := \inf_{x \in \mathbb{R}^n} f(x)$ that

$$\begin{aligned} f_k - f_{k+1} &\geq \frac{1}{2L}\|g_k\|_2^2 \\ \implies (f_0 - f_{\inf}) &\geq \frac{1}{2L}|\mathcal{K}_g(\epsilon_g)|\epsilon_g^2 \\ \implies |\mathcal{K}_g(\epsilon_g)| &\leq 2L(f_0 - f_{\inf})\epsilon_g^{-2}. \end{aligned}$$

“Nice” f

But what if f is “nice”?

e.g., satisfying the Polyak-Łojasiewicz condition for $c \in (0, \infty)$, i.e.,

$$f(x) - f_{\inf} \leq \frac{1}{2c} \|g(x)\|_2^2 \quad \text{for all } x \in \mathbb{R}^n.$$

Now consider the set

$$\mathcal{F}(\epsilon_f) := \{x \in \mathbb{R}^n : f(x) - f_{\inf} \leq \epsilon_f\}$$

and consider an upper bound on the cardinality of

$$\mathcal{K}_f(\epsilon_f) := \{k \in \mathbb{N} : x_k \notin \mathcal{F}(\epsilon_f)\}.$$

Upper bound on $|\mathcal{K}_f(\epsilon_f)|$

Using $s_k = -\frac{1}{L}g_k$ and the upper bound

$$f_{k+1} \leq f_k + g_k^T s_k + \frac{1}{2}L\|s_k\|_2^2,$$

one finds that

$$\begin{aligned} f_k - f_{k+1} &\geq \frac{1}{2L}\|g_k\|_2^2 \\ &\geq \frac{c}{L}(f_k - f_{\inf}) \\ \implies (1 - \frac{c}{L})(f_k - f_{\inf}) &\geq f_{k+1} - f_{\inf} \\ \implies (1 - \frac{c}{L})^k(f_0 - f_{\inf}) &\geq f_k - f_{\inf} \\ \implies |\mathcal{K}_f(\epsilon_f)| &\leq \log\left(\frac{f_0 - f_{\inf}}{\epsilon_f}\right) \left(\log\left(\frac{L}{L-c}\right)\right)^{-1}. \end{aligned}$$

For the first step...

In the “general nonconvex” analysis...

...the expected decrease for the first step is much more pessimistic:

$$\text{general nonconvex:} \quad f_0 - f_1 \geq \frac{1}{2L} \epsilon_g^2$$

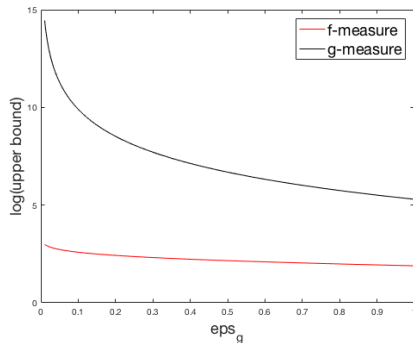
$$\text{PL condition:} \quad (1 - \frac{c}{L})(f_0 - f_{\inf}) \geq f_1 - f_{\inf}$$

...and it remains more pessimistic throughout!

Upper bounds on $|\mathcal{K}_f(\epsilon_f)|$ versus $|\mathcal{K}_g(\epsilon_g)|$

Let $f(x) = \frac{1}{2}x^2$, meaning that $g(x) = x$.

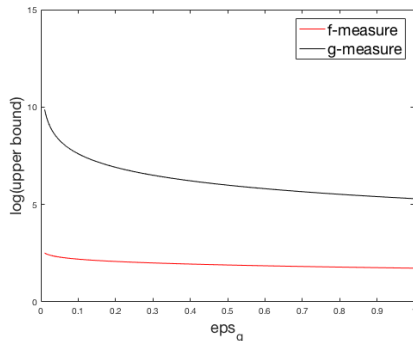
- ▶ Let $\epsilon_f = \frac{1}{2}\epsilon_g^2$, meaning that $\mathcal{F}(\epsilon_f) = \mathcal{G}(\epsilon_g)$.
- ▶ Let $x_0 = 10$, $c = 1$, and $L = 2$. (Similar pictures for any $L > 1$.)



Upper bounds on $|\mathcal{K}_f(\epsilon_f)|$ versus $|\{k \in \mathbb{N} : \frac{1}{2}\|g_k\|_2^2 > \epsilon_g\}|$

Let $f(x) = \frac{1}{2}x^2$, meaning that $\frac{1}{2}g(x)^2 = \frac{1}{2}x^2$.

- ▶ Let $\epsilon_f = \epsilon_g$, meaning that $\mathcal{F}(\epsilon_f) = \mathcal{G}(\epsilon_g)$.
- ▶ Let $x_0 = 10$, $c = 1$, and $L = 2$. (Similar pictures for any $L > 1$.)



Bad worst-case!

Worst-case complexity bounds in the general nonconvex case are very pessimistic.

- ▶ The analysis immediately admits a large gap when the function is nice.
- ▶ The “essentially tight” examples for the worst-case bounds are... weird.¹

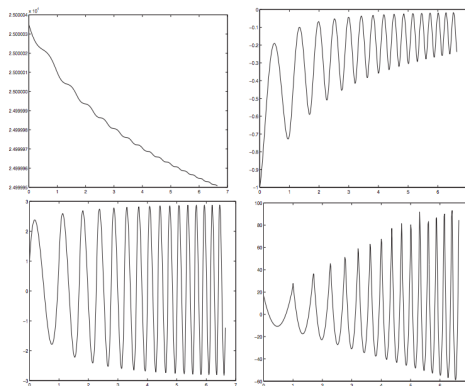


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¹Cartis, Gould, Toint (2010)

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Motivation

We want a characterization strategy that

- ▶ attempts to capture behavior in *actual practice*
- ▶ i.e., is not “bogged down” by pedagogical examples
- ▶ can be applied consistently across different classes of functions
- ▶ shows more than just the worst of the worst case

Motivation

We want a characterization strategy that

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Our idea is to

- ▶ partition the search space (dependent on f and x_0)
- ▶ analyze how an algorithm behaves over different regions
- ▶ characterize an algorithm’s behavior *by region*

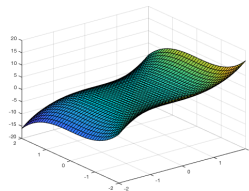
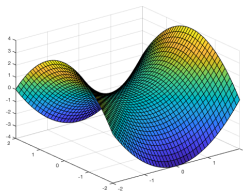
For some functions, there will be holes, but for some of interest there are none!

Intuition

Think about an arbitrary point in the search space, i.e.,

$$\mathcal{L} := \{x \in \mathbb{R}^n : f(x) \leq f(x_0)\}.$$

- ▶ If $\|g(x)\|_2 \gg 0$, then “a lot” of progress can be made.
- ▶ If $\min(\text{eig}(\nabla^2 f(x))) \ll 0$, then “a lot” of progress can also be made.



Assumption

Assumption 1

- ▶ f is $\bar{p}$ -times continuously differentiable
- ▶ f is bounded below by $f_{\inf} := \inf_{x \in \mathbb{R}^n} f(x)$
- ▶ for all $p \in \{1, \dots, \bar{p}\}$, there exists $L_p \in (0, \infty)$ such that

$$f(x+s) \leq f(x) + \underbrace{\sum_{j=1}^p \frac{1}{j!} \nabla^j f(x)[s]^j}_{t_p(x,s)} + \frac{L_p}{p+1} \|s\|_2^{p+1}$$

p th-order term reduction

Definition 2

For each $p \in \{1, \dots, \bar{p}\}$, define the function

$$m_p(x, s) = \frac{1}{p!} \nabla^p f(x)[s]^p + \frac{r_p}{p+1} \|s\|_2^{p+1}.$$

Letting $s_{m_p}(x) := \arg \min_{s \in \mathbb{R}^n}$, the *reduction in the p th-order term from x* is

$$\Delta m_p(x) = m_p(x, 0) - m_p(x, s_{m_p}(x)) \geq 0.$$

*Exact definition of r_p is not complicated, but we'll skip it here

1st-order and 2nd-order term reductions

Theorem 3

For $\bar{p} \geq 2$, the following hold:

$$\Delta m_1(x) = \frac{1}{2r_1} \|\nabla f(x)\|_2^2$$

and $\Delta m_2(x) = \frac{1}{6r_2^2} \max\{-\lambda(\nabla^2 f(x_k)), 0\}^3.$

Regions

We propose to partition the search space, given $(\kappa, f_{\text{ref}}) \in (0, 1) \times [f_{\text{inf}}, f(x_0)]$, into

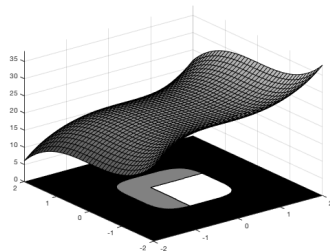
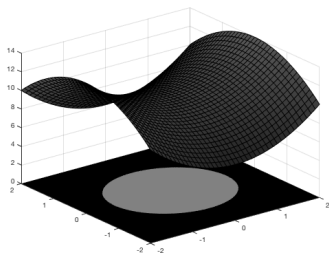
$$\mathcal{R}_1 := \{x \in \mathcal{L} : \Delta m_1(x) \geq \kappa(f(x) - f_{\text{ref}})\},$$

$$\mathcal{R}_p := \{x \in \mathcal{L} : \Delta m_p(x) \geq \kappa(f(x) - f_{\text{ref}})\} \setminus \left(\bigcup_{j=1}^{p-1} \mathcal{R}_j \right) \quad \text{for all } p \in \{2, \dots, \bar{p}\},$$

$$\text{and } \overline{\mathcal{R}} := \mathcal{L} \setminus \left(\bigcup_{j=1}^{\bar{p}} \mathcal{R}_j \right).$$

*We don't need $f_{\text{ref}} = f_{\text{inf}}$, but, for simplicity, think of it that way here

Illustration



$(\bar{p} = 2)$ $\mathcal{R}_1$: black $\mathcal{R}_2$: gray $\overline{\mathcal{R}}$: white

Functions satisfying Polyak-Łojasiewicz

Theorem 4

A continuously differentiable f with a Lipschitz continuous gradient satisfies the Polyak-Łojasiewicz condition if and only if $\mathcal{R}_1 = \mathcal{L}$ for any $x_0 \in \mathbb{R}^n$.

Hence, if we prove something about the behavior of an algorithm over $\mathcal{R}_1$, then

- ▶ we know how it behaves if f satisfies PL *and*
- ▶ we know how it behaves *at any point* satisfying the PL inequality.

Functions satisfying a strict-saddle-type property

Theorem 5

If f is twice-continuously differentiable with Lipschitz continuous gradient and Hessian functions such that, at all $x \in \mathcal{L}$ and for some $\zeta \in (0, \infty)$, one has

$$\max\{\|\nabla f(x)\|_2^2, -\lambda_{\min}(\nabla^2 f(x))^3\} \geq \zeta(f(x) - f_{\inf}),$$

then $\mathcal{R}_1 \cup \mathcal{R}_2 = \mathcal{L}$.

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Linearly convergent behavior over $\mathcal{R}_p$

Let $s_{w_p}(x)$ be a minimum norm global minimizer of the regularized Taylor model

$$w_p(x, s) = t_p(x, s) + \frac{l_p}{p+1} \|s\|_2^{p+1}$$

Theorem 6

If $\{x_k\}$ is generated by the iteration

$$x_{k+1} \leftarrow x_k + s_{w_p}(x),$$

then, with $\epsilon_f \in (0, f(x_0) - f_{ref})$, the number of iterations in

$$\mathcal{R}_p \cap \{x \in \mathbb{R}^n : f(x) - f_{ref} \geq \epsilon_f\}$$

is bounded above by

$$\left\lceil \log \left(\frac{f(x_0) - f_{ref}}{\epsilon_f} \right) \left(\log \left(\frac{1}{1 - \kappa} \right) \right)^{-1} \right\rceil = \mathcal{O} \left(\log \left(\frac{f(x_0) - f_{ref}}{\epsilon_f} \right) \right)$$

Regularized gradient and Newton methods

- ▶ Regularized gradient method: Computes s_k by solving

$$\min_{s \in \mathbb{R}^n} f(x_k) + \nabla f(x_k)^T s + \frac{l_1}{2} \|s\|_2^2 \implies s_k = -\frac{1}{l_1} \nabla f(x_k)$$

- ▶ Regularized Newton method: Computes s_k by solving

$$\min_{s \in \mathbb{R}^n} f(x_k) + \nabla f(x_k)^T s + \frac{1}{2} s^T \nabla^2 f(x_k) s + \frac{l_2}{3} \|s\|_2^3,$$

also known as cubic regularization (mentioned earlier)

Characterization: Contemporary

Let RG and RN represent regularized gradient and Newton, respectively.

Theorem 7

With $\bar{p} \geq 2$, let

$$\mathcal{K}_1(\epsilon_g) := \{k \in \mathbb{N} : \|\nabla f(x_k)\|_2 > \epsilon_g\}$$

$$\text{and } \mathcal{K}_2(\epsilon_H) := \{k \in \mathbb{N} : \lambda_{\min}(\nabla^2 f(x_k)) < -\epsilon_H\}.$$

Then, the cardinalities of $\mathcal{K}_1(\epsilon_g)$ and $\mathcal{K}_2(\epsilon_H)$ are of the order...

Algorithm	$ \mathcal{K}_1(\epsilon_g) $	$ \mathcal{K}_2(\epsilon_H) $
RG	$\mathcal{O}\left(\frac{l_1(f(x_0)-f_{\inf})}{\epsilon_g^2}\right)$	∞
RN	$\mathcal{O}\left(\frac{l_2^{1/2}(f(x_0)-f_{\inf})}{\epsilon_g^{3/2}}\right)$	$\mathcal{O}\left(\frac{l_2^2(f(x_0)-f_{\inf})}{\epsilon_H^3}\right)$

Characterization: Our approach

Theorem 8

The numbers of iterations in $\mathcal{R}_1$ and $\mathcal{R}_2$ with $f_{\text{ref}} = f_{\text{inf}}$ are of the order...

Algorithm	$\mathcal{R}_1$	$\mathcal{R}_2$
RG	$\mathcal{O}\left(\log\left(\frac{f(x_0) - f_{\text{inf}}}{\epsilon_f}\right)\right)$	∞
RN	$\mathcal{O}\left(\frac{l_2^2(f(x_0) - f_{\text{inf}})}{r_1^3}\right) + \mathcal{O}\left(\log\left(\frac{f(x_0) - f_{\text{inf}}}{\epsilon_f}\right)\right)$	$\mathcal{O}\left(\log\left(\frac{f(x_0) - f_{\text{inf}}}{\epsilon_f}\right)\right)$

There is an **initial phase**, as seen in Nesterov & Polyak (2006)

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There is an **initial phase**, as seen in Nesterov & Polyak (2006)

A ∞ can appear, but one could consider probabilistic bounds, too

Trust region method: Gradient-dependent radii

$$\min_{s \in \mathbb{R}^n} f(x_k) + \nabla f(x_k)^T s + \frac{1}{2} s^T \nabla^2 f(x_k) s \quad \text{s.t.} \quad \|s\|_2 \leq \delta_k$$

- ▶ Set $\delta_k \leftarrow \nu_k \|\nabla f(x_k)\|_2$
- ▶ Initialize $\nu_0 \in [\underline{\nu}, \bar{\nu}]$
- ▶ For some $(\eta, \beta) \in (0, 1) \times (0, 1)$, if

$$\rho_k = \frac{f(x_k) - f(x_k + s_k)}{t_2(x_k, 0) - t_2(x_k, s_k)} \geq \eta,$$

then $x_{k+1} \leftarrow x_k + s_k$ and $\nu_{k+1} \in [\underline{\nu}, \bar{\nu}]$; else, $x_{k+1} \leftarrow x_k$ and $\nu_{k+1} \leftarrow \beta \nu_k$.

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Theorem 9

of iterations in $\mathcal{R}_1$ is at most $\mathcal{O}\left(\chi \log\left(\frac{f(x_0) - f_{\text{ref}}}{\epsilon_f}\right)\right)$. For $\mathcal{R}_2$, no guarantee.

Trust region method: Gradient- and Hessian-dependent radii

$$\min_{s \in \mathbb{R}^n} f(x_k) + \nabla f(x_k)^T s + \frac{1}{2} s^T \nabla^2 f(x_k) s \quad \text{s.t.} \quad \|s\|_2 \leq \delta_k$$

- Set

$$\delta_k \leftarrow \nu_k \begin{cases} \|\nabla f(x_k)\|_2 & \|\nabla f(x_k)\|_2^2 \geq |\lambda(\nabla^2 f(x_k))|^3 \\ |\lambda(\nabla^2 f(x_k))| & \text{otherwise} \end{cases}$$

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- For some $(\eta, \beta) \in (0, 1) \times (0, 1)$, if

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$$\min_{s \in \mathbb{R}^n} f(x_k) + \nabla f(x_k)^T s + \frac{1}{2} s^T \nabla^2 f(x_k) s \quad \text{s.t.} \quad \|s\|_2 \leq \delta_k$$

- Set

$$\delta_k \leftarrow \nu_k \begin{cases} \|\nabla f(x_k)\|_2 & \|\nabla f(x_k)\|_2^2 \geq |\lambda(\nabla^2 f(x_k))|^3 \\ |\lambda(\nabla^2 f(x_k))| & \text{otherwise} \end{cases}$$

- Initialize $\nu_0 \in [\underline{\nu}, \bar{\nu}]$
- For some $(\eta, \beta) \in (0, 1) \times (0, 1)$, if

$$\rho_k = \frac{f(x_k) - f(x_k + s_k)}{t_2(x_k, 0) - t_2(x_k, s_k)} \geq \eta,$$

then $x_{k+1} \leftarrow x_k + s_k$ and $\nu_{k+1} \in [\underline{\nu}, \bar{\nu}]$; else, $x_{k+1} \leftarrow x_k$ and $\nu_{k+1} \leftarrow \beta \nu_k$.

Theorem 10

of iterations in $\mathcal{R}_1$ is at most $\mathcal{O}\left(\chi \log\left(\frac{f(x_0) - f_{ref}}{\epsilon_f}\right)\right)$.

of iterations in $\mathcal{R}_2$ is at most $\mathcal{O}\left(\chi_2 \log\left(\frac{f(x_0) - f_{ref}}{\epsilon_f}\right)\right)$.

Trust region method: Always good?

What about the classical update?

$$\delta_{k+1} \leftarrow \begin{cases} \geq \delta_k & \text{if } \rho_k \geq \eta \\ < \delta_k & \text{otherwise.} \end{cases}$$

Two challenges:

- ▶ Proving a uniform upper bound on number of consecutive rejected steps
- ▶ Proving that accepted steps yield sufficient decrease in $\mathcal{R}_1$ and $\mathcal{R}_2$

Outline

Motivation

Contemporary Analyses

Partitioning the Search Space

Behavior of Common Methods

Summary & Perspectives

Summary & Perspectives

Our goal: A *complementary* approach to characterize algorithms.

- ▶ global convergence
- ▶ worst-case complexity, contemporary type + **our approach**
- ▶ local convergence rate

Our idea is to

- ▶ partition the search space (dependent on f and x_0)
- ▶ analyze how an algorithm behaves over different regions
- ▶ characterize an algorithm's behavior *by region*

For some functions, there are holes, but for others the characterization is complete.

F. E. Curtis and D. P. Robinson, “How to Characterize the Worst-Case Performance of Algorithms for Nonconvex Optimization,” Lehigh ISE/COR@L Technical Report 18T-003, submitted for publication, 2018.