Recent results in worst-case evaluation complexity for smooth and non-smooth, exact and inexact, nonconvex optimization

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Virtual 111 Seminar 2020, July 2020

The problem (again)

We consider the unconstrained nonlinear programming problem:

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

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

For now, focus on the

unconstrained case

but we are also interested in the case featuring

inexpensive constraints

Adaptive regularization

Adaptive regularization methods iteratively compute steps by mimizing

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

until an approximate first-order minimizer is obtained:

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

Note: no global optimization involved.

Second-order Adaptive Regularization (AR2)

Algorithm 1.1: The AR2 Algorithm

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

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

Step 2: Step computation:

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

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:

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

Evaluation complexity: an important result

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

$$\|g_k\| \le \epsilon?$$

If H is globally Lipschitz and the s-rule is applied, the AR2 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.

"Nesterov & Polyak",

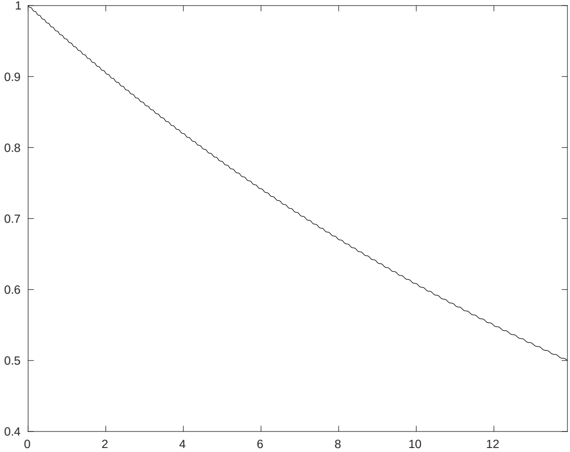
Cartis, Gould, T., 2011, Birgin, Gardenghi, Martinez, Santos, T., 2017

Note:

- The above result is sharp (in order of ϵ)!
- An $O(\epsilon^{-3})$ bound holds for convergence to second-order critical points.

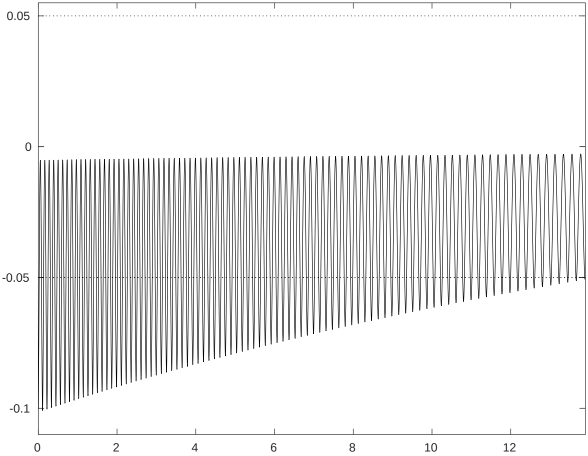
Evaluation complexity: sharpness

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



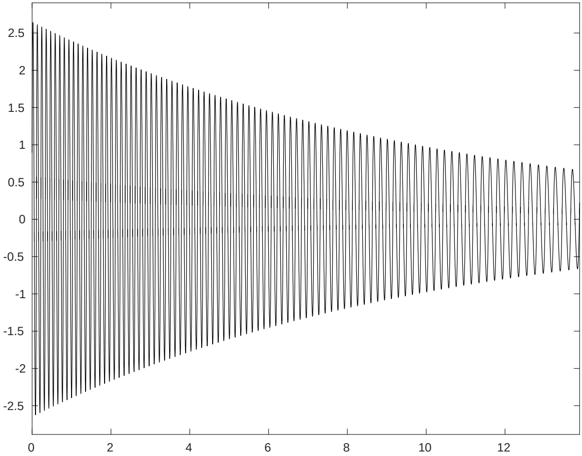
The objective function

An example of slow AR2 (2)



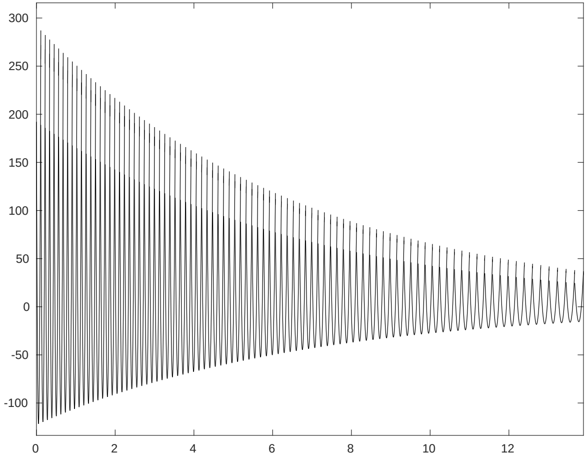
The first derivative

An example of slow AR2 (3)



The second derivative

An example of slow AR2 (4)



The third derivative

Slow steepest descent (1)

The steepest descent method with requires at most

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

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

Nesterov

Sharp??? YES

Newton's method (when convergent) requires at most

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

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

High-order models for first-order points (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

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

High-order models for first-order points (2)

unconstrained ϵ-approximate 1rst-order-necessary minimizer after at most

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

function and gradient evaluations

Birgin, Gardhenghi, Martinez, Santos, T., 2017

One then wonders. . .

If one uses a model of degree p ($T_{f,p}(x,s)$), why be satisfied with first- or second-order critical points???

What do we mean by critical points of order larger than 2 ???

What are necessary optimality conditions for order larger than 2 ???

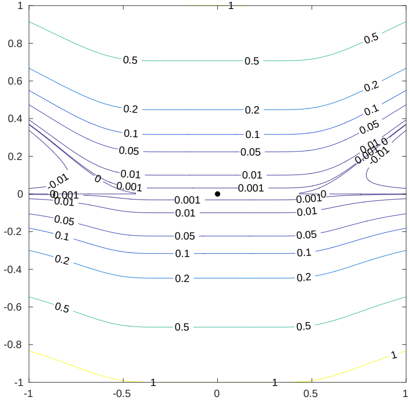
Not an obvious question!

A sobering example (1)

Consider the unconstrained minimization of

$$f(x_1, x_2) = \begin{cases} x_2 \left(x_2 - e^{-1/x_1^2} \right) & \text{if } \ x_1 \neq 0, \\ x_2^2 & \text{if } \ x_1 = 0, \end{cases}$$

Peano (1884), Hancock (1917)



A sobering example (2)

Conclusions:

- looking at optimality along straight lines is not enough
- depending on Taylor's expansion for necessary conditions is not always possible

Even worse:

$$f(x_1, x_2) = \begin{cases} x_2 \left(x_2 - \sin(1/x_1) e^{-1/x_1^2} \right) & \text{if } x_1 \neq 0, \\ x_2^2 & \text{if } x_1 = 0, \end{cases}$$

(no continuous descent path from 0, although not a local minimizer!!!)

Hopeless?

A new (approximate) optimality measure

Define, for some small $\delta > 0$, ($\mathcal{F} = \mathbb{R}^n$)

$$\phi_{f,q}^{\delta}(x) \stackrel{\rm def}{=} f(x) - \text{globmin}_{\substack{x+d\in\mathcal{F}\\ \|d\|\leq\delta}} T_{f,q}(x,d).$$

x is a strong (ϵ,δ)-approximate qth-order-necessary minimizer

$$\Leftrightarrow$$

$$\phi_{f,j}^{\delta}(x) \leq \epsilon \frac{\delta^j}{j!} \quad (j = 1,\ldots,q)$$

- $\phi_{f,q}^{\delta}(x)$ is continuous as a function of x for all q.
- $\phi_{f,j}^{\delta}(x) = o(\delta^j))$ is a necessary optimality condition

Approximate unconstrained optimality

Familiar results for low orders: when $q = 1$

$$\frac{\phi^{\delta}_{f,1}(x)}{\delta} = \|\nabla_x f(x)\|$$

while, for $q = 2$,

$$\frac{\phi^{\delta}_{f,2}(x)}{\delta^2} \le \epsilon \Rightarrow \max\left[0, -\lambda_{\min}(\nabla_x^2 f(x))\right] \le \epsilon$$

Introducing inexpensive constraints

Constraints are inexpensive

$\Leftrightarrow$

their evaluation/enforcement has negligible cost
(compared with that of evaluating f)

- evaluation complexity for the constrained problem well measured in counting evaluations of f and its derivatives
- many well-known and important examples
  - bound constraints
  - convex constraints with cheap projections
  - sparse sets
  - manifold with known retraction, ...

From now on: $\mathcal{F} \stackrel{\text{def}}{=}$ (inexpensive) feasible set

A very general optimization problem

Our aim:

Compute an (ϵ, δ)-approximate qth-order-necessary minimizer for the problem

$$\min_{x \in \mathcal{F}} f(x)$$

where

- $p \geq q \geq 1$,
- $\nabla_x^p f(x)$ is β-Hölder continuous ($\beta \in (0, 1]$)
- $\mathcal{F}$ is an inexpensive feasible set

Note:

1. no convexity assumption of f
2. no convexity assumption on $\mathcal{F}$ (not even connectivity)
3. reduces to Lipschitz continuous $\nabla_x^p f(x)$ when $\beta = 1$.

A (theoretical) regularization algorithm

Algorithm 3.1: The ARqp algorithm for qth-order optimality

Step 0: Initialization: x_0, δ_{-1} and $\sigma_0 > 0$ given. Set $k = 0$

Step 1: Termination: If $\phi_{f,j}^{\delta_{k-1,j}}(x_k) \leq \epsilon \delta_{k-1,j}^{j}/j!$ for $j = 1, \ldots, q$, stop.

Step 2: Step computation:

Compute* s_k such that $x_k + s_k \in \mathcal{F}$, $m_k(s_k) < m_k(0)$ and

$$\|s_k\| \geq \kappa_s \, \epsilon^{\frac{1}{p-q+\beta}} \quad \text{or} \quad \phi_{m_k,j}^{\delta_{k,j}}(x_k + s_k) \leq \theta \epsilon_j \delta_{k,j}^{j}/j! \; (j = 1, \ldots, q)$$

Step 3: Step acceptance:

$$\text{Compute } \rho_k = \frac{f(x_k) - f(x_k + s_k)}{f(x_k) - T_{f,p}(x_k, s_k)}$$

and set $x_{k+1} = x_k + s_k$ if $\rho_k > 0.1$ or $x_{k+1} = x_k$ otherwise.

Step 4: Update the regularization parameter:

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

The main result

The ARp algorithm is well-defined and

The ARp algorithm finds an (ϵ,δ)-approximate qth-order-necessary minimizer for the problem

$$\min_{x\in\mathcal{F}} f(x)$$

in at most

$$O\left(\epsilon^{-\frac{p+\beta}{p-q+\beta}}\right) \quad (q=1,2) \quad \text{or} \quad O\left(\epsilon^{-\frac{q(p+\beta)}{p}}\right) \quad (q>2)$$

iterations and evaluations of the objective function and its p first derivatives. Moreover, this bound is sharp.

What this theorem does

1. generalizes ALL known complexity results for regularization methods to

   arbitrary degree p, arbitrary order q and arbitrary smoothness $p+\beta$

2. applies to very general constrained problems
3. generalizes the lower complexity bound of Carmon at al., 2018, to arbitrary dimension, arbitrary order and to constrained problems
4. provides a considerably better complexity order than the bound

   $$O\left(\epsilon^{-(q+1)}\right)$$

   known for unconstrained trust-region algorithms (Cartis, Gould, T., 2017)

   Note: linesearch methods all fail for $q > 3$!
5. is provably optimal within a wide class of algorithms (Cartis, Gould, T., 2018 for $p \leq 2$)

Moving on: allowing inexact evaluations

A common observation:

In many applications, it is necessary/useful to evaluate $f(x)$ and/or $\nabla_x^j f(x)$ inexactly

1. complicated computations involving truncated iterative processes
2. variable accuracy schemes
3. sampling techniques (machine learning)
4. noise
5. ...

Focus on the case where f and all its derivatives are inexact

The dynamic accuracy framework

Suppose that

- the absolute accuracy of f
- the relative accuracy of the Taylors' model ΔT

can be specified by the algorithm before their computation

(all examples cites above)

Note: relative accuracy of ΔT controlled via absolute accuracy of the derivatives!

Denote inexact quantities with overbars.

The ARpDA algorithm

Algorithm 4.1: The ARpDA algorithm for qth-order optimality

Step 0: Initialization: x_0, δ_{-1} and $\sigma_0 > 0$ given. Set $k = 0$

Step 1: Termination: If $\overline{\phi}_{f,j}^{\delta_{k-1,j}}(x_k) \leq \frac{1}{2}\epsilon_j \delta_{k-1,j}^j / j!$ for $j = 1, \ldots, q$, terminate.

Step 2: Step computation:

Compute* s_k such that $x_k + s_k \in \mathcal{F}$, $m_k(s_k) < m_k(0)$ and

$$\|s_k\| \geq \kappa_s \, \epsilon^{\frac{1}{p-q+\beta}} \quad \text{or} \quad \overline{\phi}_{m_k,q}^{\delta_{k,j}}(x_k + s_k) \leq \theta \epsilon_j \frac{\delta_{k,j}^j}{j!}$$

Step 3: Step acceptance:

$$\text{Compute } \rho_k = \frac{\overline{f}(x_k) - \overline{f}(x_k + s_k)}{\overline{\Delta T}_{f,p}(x_k, s_k)}$$

and set $x_{k+1} = x_k + s_k$ if $\rho_k > 0.1$ or $x_{k+1} = x_k$ otherwise.

Step 4: Update the regularization parameter:

(as in ARp)

Evaluation complexity for the ARpDA algorithm

And then (sweeping some dust under the carpet)...

The ARpDA algorithm finds an (ϵ,δ)-approximate qth-order-necessary minimizer for the problem

$$\min_{x\in\mathcal{F}} f(x)$$

in at most

$$O\left(\epsilon^{-\frac{p+\beta}{p-q+\beta}}\right) \;\text{ or }\; O\left(\epsilon^{-\frac{q(p+\beta)}{p}}\right)$$

iterations (inexact) evaluations of the objective function, and at most

$$O\left(|\log(\epsilon)| + \epsilon^{-\frac{p+\beta}{p-q+\beta}}\right) \;\text{ or }\; O\left(|\log(\epsilon)| + \epsilon^{-\frac{q(p+\beta)}{p}}\right)$$

(inexact) evaluations of its p first derivatives.

A probabilistic complexity bound

Suppose that absolute evaluation errors are random and independent, $q \in \{1,2\}$ and that, for given ε,

$$Pr\left[\| \overline{\nabla_x^j f}\,(x_k) - \nabla_x^j f(x_k)\| \leq \varepsilon\right] \geq 1 - t \quad (j \in \{1,\ldots,p\})$$

where

$$t = O\left(\frac{t_{\rm final}\,\epsilon^{\frac{p+1}{p-q+\beta}}}{p+q+2}\right)$$

Then the ARpDA algorithm finds an (ϵ,δ)-approximate qth-order-necessary minimizer for the problem $\min_{x\in\mathcal{F}} f(x)$ in at most $O\left(\epsilon^{-\frac{p+\beta}{p-q+\beta}}\right)$ iterations and (inexact) evaluations of the objective function, and at most $O\left(|\log(\epsilon)| + \epsilon^{-\frac{p+\beta}{p-q+\beta}}\right)$ (inexact) evaluations of its p first derivatives, with probability $1 - t_{\rm final}$.

Selecting a sample size in subsampling methods (1)

Now consider $p = 2,\ \beta = 1,\ \mathcal{F} = \mathbb{R}^n$ and (as in machine learning)

$$f(x) = \frac{1}{N}\sum_{i=1}^{N} \psi_i(x)$$

Estimating the values of $\{\nabla_x^j f(x_k)\}_{j=0}^2$ by sampling:

$$\overline{f}\,(x_k) = \frac{1}{|\mathcal{D}_k|}\sum_{i\in\mathcal{D}_k} \psi_i(x_k), \quad \overline{\nabla_x^1 f}\,(x_k) = \frac{1}{|\mathcal{G}_k|}\sum_{i\in\mathcal{G}_k} \nabla_x^1\psi_i(x_k),$$

$$\overline{\nabla_x^2 f}\,(x_k) = \frac{1}{|\mathcal{H}_k|}\sum_{i\in\mathcal{H}_k} \nabla_x^2\psi_i(x_k),$$

and applying the Operator-Bernstein matrix concentration inequality...

Selecting a sample size in subsampling methods (2)

Suppose that $\beta = 1 \le q \le 2 = p$, that, for all k and $j \in \{0,1,2\}$,

$$\max_{i \in \{1,\ldots,N\}} \|\nabla_x^j \psi_i(x_k)\| \le \kappa_j(x_k)$$

and that, for given ε,

$$|\mathcal{D}_k| \ge \vartheta_{0,k}(\varepsilon) \log\left(2/t\right), \qquad |\mathcal{G}_k| \ge \vartheta_{1,k}(\varepsilon) \log\left((n+1)/t\right),$$

$$|\mathcal{H}_k| \ge \vartheta_{2,k}(\varepsilon) \log\left(2n/t\right),$$

where

$$\vartheta_{j,k}(\varepsilon) \stackrel{\rm def}{=} \frac{4\kappa_j(x_k)}{\varepsilon}\left(\frac{2\kappa_j(x_k)}{\varepsilon} + \frac{1}{3}\right) \quad \text{and} \quad t = O\left(\frac{t_{\rm final}\,\epsilon^{\frac{3}{3-q}}}{4+q}\right).$$

Then the AR2DA algorithm finds an ϵ-approximate qth-order-necessary minimizer for the problem $\min_{x \in \mathbb{R}^n} f(x)$ in at most $O\left(\epsilon^{-\frac{3}{3-q}}\right)$ iterations and subsampled evaluations of f, and at most $O\left(|\log(\epsilon)| + \epsilon^{-\frac{3}{3-q}}\right)$ subsampled evaluations $\nabla_x^1 f$ and $\nabla_x^2 f$, with probability $1 - t_{\rm final}$.

Non-smooth Lipschitzian composite problems

Finally, consider

$$\min_x w(x) = f(x) + h(c(x))$$

where f and c have Lipschitz p-th derivative but are inexact, and h is subadditive, $h(0) = 0$, Lispchitz and exact (lots of examples: norms...)

- not a special case of smooth inexact case because $\overline{\Delta f}$ now involves h as well as $\overline{\nabla_x^j f}$ and $\overline{\nabla_x^j c}$
- allows high-order minimizers for non-smooth problem by using

$$\phi_{w,q}^{\delta}(x) = w(x) - \operatorname*{globmin}_{x+d\in\mathcal{F};\|d\|\leq\delta} \left[T_{f,q}(x,d) - h(T_{c,q}(x,d))\right]$$

$O\left(\epsilon^{-\frac{p+1}{p}}\right)$ $(q = 1, \mathcal{F}$ convex), or $O\left(\epsilon^{-(q+1)}\right)$ otherwise

evaluations of f, h, c and derivatives.

Also for problems with inexpensive constraints

Tentative new results

1. for inexpensively constrained problems:

$$\begin{array}{lll} O\left(\epsilon^{-(p+1)/(p-q+1)}\right) & [sharp] & \text{for } q \in \{1,2\} \text{ and } \mathcal{F} \text{ convex,} \\ O\left(\epsilon^{-q(p+1)/p}\right) & [sharp] & \text{otherwise.} \end{array}$$

2. for inexpensively constrained composite problems:

$$\begin{array}{lll} O\left(\epsilon^{-(p+1)/p}\right) & [sharp] & \text{for } q = 1 \text{ and } \mathcal{F} \text{ convex,} \\ O\left(\epsilon^{-(q+1)}\right) & [?] & \text{otherwise.} \end{array}$$

A weaker approximate optimality measure. . .

Can one generalize the good complexity orders for $q = 1, 2$ to higher order?
Yes, if one settles for a weaker notion of approximate optimality:

x is a weak (ϵ, δ)-approximate qth-order-necessary minimizer

$$\Leftrightarrow$$

$$\phi^{\delta}_{f,q}(x) \le \epsilon\, \chi_q(\delta)$$

where $\chi_j(\delta) = \sum_{\ell=1}^{j} \frac{\delta^\ell}{\ell!}$.

(weak vs strong approximate minimizers)

$O\left(\epsilon^{-\frac{p+\beta}{p-q+\beta}}\right)$ evaluations of f and its derivatives

Turning to non-smooth problems: non-Lipschitzian singularities 1

Now consider

$$\min_{x\in\mathcal{F}} f(x) + \sum_{i\in\mathcal{H}} |x_i|^a, \qquad a \in (0,1)$$

with $\mathcal{F}$ convex and "kernel centered"
Define

$$\mathcal{C}(x) = \{ i \in \mathcal{H} \mid x_i = 0 \} \;\text{ and }\; \mathcal{R}(x) = \bigcap_{i\in\mathcal{H}\setminus\mathcal{R}(x)} \text{span}\,\{e_i\}$$

Criticality measure

$$\phi^{\delta}_{f,q}(x) = f(x) - \underset{\substack{x+d\in\mathcal{F}\\ \|d\|\leq\delta,\, d\in\mathcal{R}(x)}}{\text{globmin}} T_{f,q}(x,d)$$

Non-Lipschitzian singularities 2

- define a Lipschitzian model of the non-Lipschitzian singularities based on inherent symmetry
- prove that the related Lipschitz constant is independent of ϵ
- assemble the singular and non-singular complexity estimates

For weak q-th order:

$O\left(\epsilon^{-\frac{p+\beta}{p-q+\beta}}\right)$ evaluations of f and its derivatives

Conclusions

A global view (also tentative)

		weak minimizers		strong minimizers				
	inexpensive constraints	non-composite ($h = 0$)		non-composite ($h = 0$)		composite h convex		composite h non-convex
$q = 1$	none	$\mathcal{O}\left(\epsilon^{-\frac{p+1}{p}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-\frac{p+1}{p}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-\frac{p+1}{p}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-2}\right)$
	convex	$\mathcal{O}\left(\epsilon^{-\frac{p+1}{p}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-\frac{p+1}{p}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-\frac{p+1}{p}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-2}\right)$
	non-convex	$\mathcal{O}\left(\epsilon^{-\frac{p+1}{p}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-\frac{p+1}{p}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-2}\right)$		$\mathcal{O}\left(\epsilon^{-2}\right)$
$q = 2$	none	$\mathcal{O}\left(\epsilon^{-\frac{p+1}{p-1}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-\frac{p+1}{p-1}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-3}\right)$		$\mathcal{O}\left(\epsilon^{-3}\right)$
	convex	$\mathcal{O}\left(\epsilon^{-\frac{p+1}{p-1}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-\frac{p+1}{p-1}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-3}\right)$		$\mathcal{O}\left(\epsilon^{-3}\right)$
	non-convex	$\mathcal{O}\left(\epsilon^{-\frac{p+1}{p-1}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-\frac{2(p+1)}{p}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-3}\right)$		$\mathcal{O}\left(\epsilon^{-3}\right)$
$q > 2$	none, or general	$\mathcal{O}\left(\epsilon^{-\frac{p+1}{p-q+1}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-\frac{q(p+1)}{p}}\right)$	sharp	$\mathcal{O}\left(\epsilon^{-(q+1)}\right)$		$\mathcal{O}\left(\epsilon^{-(q+1)}\right)$

Perspectives

Complexity for expensive constraints for $q > 1$?

A purely probabilistic approach of inexact evaluation (partly done)

Optimization in variable arithmetic precision

etc., etc., etc.

Thank you for your attention!

Some references

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See also http://perso.fundp.ac.be/~phtoint/toint.html