Second-order methods for nonconvex optimization with complexity guarantees

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0. Complexity in Optimization

Complexity: Finding bounds on the amount of computation for an algorithm and / or problems in a certain class.

Computation can be measured in several ways, including

- Iterations (sometimes broken down into different levels of iteration: outer and inner);
- Oracle: how many queries for information about the functions are required to find an approximate solution. Sometimes separated into function evaluations, first-derivative, second-derivative information.

In this talk, we deal with upper bounds on the computation required by a given algorithm for all problems in a certain class.

(There's also interest in lower bounds.)

Complexity in Optimization: Nemirovski and Yudin

[Nemirovski and Yudin, 1983] is a founding document in complexity of continuous optimization problems and algorithms. Identified 3 ingredients:

- class of problems
- sources of information about the problem e.g. values of $f(x)$ and $\nabla f(x)$ for a given x: oracles (attributed to Bakhvalov)
- methods for definining error / solution accuracy.

Discusses different types of complexity:

- iterations ("laboriousness")
- elementary operations
- memory.

Complexity $N(\epsilon)$ depends on (relative) error ϵ in approximate solution.

Convex only: general, strongly convex, mirror descent, nonlinear conjugate gradient...

(They comment that global minimization of nonconvex functions is exponential in the dimension.)

Complexity in Optimization: Nonlinear

Complexity results in convex optimization.

- polynomial interior-point for LP, convex QP, feasible sets with self-concordant barriers (80s-90s).
- momentum methods for nonlinear convex (heavy ball, Nesterov): faster rates than steepest descent (80s, then 2010-)
- subgradient and stochastic subgradient: convergence rates for averaged iterates.

Interest in complexity for nonconvex optimization is more recent, and focuses on finding approximate second-order points (or higher-order), rather than global solutions.

- Enhances the theory, possibly the practice too.
- Nonconvex applications from machine learning (e.g. matrix optimization) have nice properties such as
  - all saddle points are strict, or
  - all local minima are global.

Philosophy

- There's a rich collection of practical algorithms for nonlinear nonconvex optimization — unconstrained, simple constraints, nonlinear constraints.
- Typical convergence theory is about *local convergence rates* or *accumulation points are stationary* or perhaps *accumulation points satisfy second-order necessary conditions*.
- Can we build on these algorithms, modifying to equip them with global complexity properties without sacrificing practical appeal?

Interested mostly in algorithms that find approximate second-order points but that don't require evaluation of second-derivative information (Hessians) explicitly.

Then can use computational differentiation to obtain Hessian-vector products, based on code for first derivatives: Apply computational differentiation to $\nabla f(x)^T d$ to get $\nabla^2 f(x) d$, for a given d.

1. Smooth Nonconvex Unconstrained Optimization

$\min_{x \in \mathbb{R}^n} f(x)$ where f is smooth and nonconvex.

Seek a second-order necessary (2oN) point:

$$\nabla f(x) = 0, \quad \nabla^2 f(x) \succeq 0.$$

Let $\mathcal{D}$ be an open set containing level set $\{x \mid f(x) \leq f(x^0)\}$. Assume

- f is bounded below: $f(x) \geq f_{\text{low}}$ for all x.
- Gradient and Hessian are Lipschitz continuous: For all $y, z \in \mathcal{D}$, have

$$\|\nabla f(y) - \nabla f(z)\| \leq L_g \|y - z\|, \quad \|\nabla^2 f(y) - \nabla^2 f(z)\| \leq L_H \|y - z\|.$$

At any x, have quadratic and cubic upper bounds on f over all $\mathcal{D}$:

$$f(x+p) \leq f(x) + \nabla f(x)^T p + \frac{L_g}{2}\|p\|^2,$$
$$f(x+p) \leq f(x) + \nabla f(x)^T p + \frac{1}{2} p^T \nabla^2 f(x) p + \frac{L_H}{6}\|p\|^3.$$

Approximate 2oN Points & Guarantees

Seek approximate 2oN points satisfying

$$\|\nabla f(x)\| \leq \epsilon_g, \quad \nabla^2 f(x) \succeq -\epsilon_H I,$$

where ϵ_g and ϵ_H are small positive tolerances.

Seek iteration complexities for finding such points. Also seek operation complexities in terms of the number of fundamental operations required. Bound these in terms of ϵ_g and ϵ_H. (Also L_g and L_H.)

We take the "fundamental operations" to be

- gradient evaluations $\nabla f(x)$, and
- Hessian-vector products $\nabla^2 f(x)d$ for arbitrary d.

whose cost is comparable — see earlier discussion about computational differentiation.

Explicit knowledge of $\nabla^2 f(x)$ is not required!

A Basic Algorithm with Pretty Good Complexity

When L_g and L_H are known, there is an elementary steepest-descent + negative curvature method that finds an approximate 2oN point in $O(\max(\epsilon_g^{-2}, \epsilon_H^{-3}))$ iterations.

For $k = 0, 1, 2, \ldots$:

- If $\|\nabla f(x^k)\| > \epsilon_g$, take a short steepest-descent step:

$$x^{k+1} = x^k - \tfrac{1}{L_g} \nabla f(x^k).$$

  Use quadratic upper bound to get a decrease of $\geq \epsilon_g^2/(2L_g)$.

- Otherwise, if $\nabla^2 f(x^k) \not\succeq -\epsilon_H I$, find direction d^k such that

$$\|d^k\| = 1, \quad (d^k)^T \nabla^2 f(x^k) d^k = \lambda_{\min}^k < -\epsilon_H, \quad \nabla f(x^k)^T d^k \leq 0.$$

  Take a step of length $2|\lambda_{\min}^k|/L_H$ along d^k to get decrease of $\geq \frac{2}{3}\epsilon_H^3/L_H^2$, using cubic upper bound.

Iteration and Operation Complexity

Because of the lower bound f_{low}, the number of iterations is at most

$$\max\left(2L_g\epsilon_g^{-2}, \frac{3}{2}L_H^2\epsilon_H^{-3}\right)(f(x^0) - f_{\text{low}}).$$

Each iteration in this scheme requires gradient evaluation and (sometimes) cost of finding the most negative eigenvalue of $\nabla^2 f(x^k)$.

In fact, for the negative curvature direction, need only d such that

$$d^T\nabla^2 f(x^k)d \leq -\tfrac{1}{2}\epsilon_H\|d\|^2.$$

If $\lambda_{\min}(\nabla^2 f(x^k)) \leq -\epsilon_H$, this can be computed to probability $1-\delta$ using randomly-started Lanczos iteration at a cost of

$$\min\left\{n, O\left(\sqrt{\frac{L_g}{\epsilon_H}}|\log\delta|\right)\right\}$$

Hessian-vector products (without necessarily knowing $\nabla^2 f$ explicitly).

Operation complexity is a factor of $\epsilon_H^{-1/2}$ greater than iteration complexity.

Literature on Complexity for Second Order Points

[Nesterov and Polyak, 2006] proposed adding a cubic regularization term to the second-order Taylor-series model, to find approximate second-order points with complexity guarantees:

$$f(x+p) \leq f(x) + \nabla f(x)^T p + \frac{1}{2} p^T \nabla^2 f(x) p + \frac{M}{6} \|p\|^3.$$

(Cubic regularization previously proposed by [Griewank, 1981].)

Many later papers on iteration complexity for second-order points:

- Cubic regularization and trust-region methods
  [Nesterov and Polyak, 2006, Birgin and Martínez, 2017, Cartis et al., 2012, Curtis et al., 2017a, Curtis et al., 2017b, Martínez and Raydan, 2017, Cartis et al., 2019a]
- p-order necessary points ($p \geq 2$)
  [Cartis et al., 2020a, Cartis et al., 2020b]

Algorithms with good operation complexity described in

- Cubic regularization [Agarwal et al., 2017];
- Adapting accelerated gradient in various ways [Carmon et al., 2017a, Carmon et al., 2017b];
- Gradient descent (+ acceleration), with noise injection to escape from saddles [Jin et al., 2017a, Jin et al., 2017b].

1a. Line-Search Newton-CG Procedure

The method in [Royer et al., 2020] uses two kind of directions p_k:

- "sufficient" negative curvature for $\nabla^2 f(x_k)$;
- approximate (slightly) damped Newton $-(\nabla^2 f(x_k) + 2\epsilon_H I)^{-1} \nabla f(x_k)$ (provided it's a descent direction).

Does a backtracking line search along each such direction.

- CG is used to find damped Newton step OR detect and return a direction of "sufficient negative curvature"
- Monitor the CG procedure to ensure that no more than $O(\epsilon_H^{-1/2})$ steps are taken. (Requires some complicated termination tests.)
- As a backup to CG (rarely needed), use randomized Lanczos to search for the "sufficient negative curvature" direction for $\nabla^2 f(x_k)$.

Follows the traditional line-search Newton-CG approach, but the new features yield provable complexity, and exploit negative curvature explicitly.

Modified CG (Modifications in red)

Define

$$\bar{H} := H + 2\epsilon I,\ \kappa := \frac{M + 2\epsilon}{\epsilon},\ \ T := \frac{4\kappa^4}{(1-\sqrt{1-\tau})^2},\ \ \tau := \frac{1}{\sqrt{\kappa}+1};$$

$y_0 \leftarrow 0,\ r_0 \leftarrow g,\ p_0 \leftarrow -g,\ j \leftarrow 0;$
if $p_0^\top \bar{H} p_0 < \epsilon \|p_0\|^2$ **then**
  Set $d = p_0$ and terminate with d_type=NC;
end if
while TRUE **do**
  $\alpha_j \leftarrow r_j^\top r_j / p_j^\top \bar{H} p_j;$
  $y_{j+1} \leftarrow y_j + \alpha_j p_j;$
  $r_{j+1} \leftarrow r_j + \alpha_j \bar{H} p_j;$
  $\beta_{j+1} \leftarrow (r_{j+1}^\top r_{j+1})/(r_j^\top r_j);$
  $p_{j+1} \leftarrow -r_{j+1} + \beta_{j+1} p_j;$
  $j \leftarrow j + 1;$
  Perform Termination Tests;
end while

Modified CG Properties

Four Termination Tests!

- **1.** $\|r_j\| \leq \hat{\zeta}\|r_0\|$: approx damped Newton step.
- **2,3.** Either y_j or p_j has negative curvature, less than $-\epsilon$. Return it!
- **4.** "Residual norm $\|r_j\|$ is decreasing slowly and this is an indication that H has an eigenvalue less than $-\epsilon$." Moreover, a direction of negative curvature can be recovered by combining two of the iterates y_i encountered so far.

Case **4** uses an idea of [Carmon et al., 2017b] for accelerated gradient (but requires significant modification for CG). Based on an earlier argument of Bubeck (2014).

Complexity of Modified CG:

$$\min\left(n, \tilde{\mathcal{O}}\left(\sqrt{\frac{L_g}{\epsilon}}\right)\right).$$

(Similar to accelerated gradient.)

Since we usually set $\epsilon = \epsilon_H = \epsilon_g^{1/2}$, this is $O(\epsilon_g^{-1/4})$.

Minimum Eigenvalue Oracle (MEO)

Inputs: Symmetric $H \in \mathbb{R}^{n \times n}$, scalar M with $\lambda_{\max}(H) \leq M$, and $\epsilon > 0$; Set parameter $\delta \in [0, 1)$;
Outputs: Estimate λ of $\lambda_{\min}(H)$ such that $\lambda \leq -\epsilon/2$, and vector v with $\|v\| = 1$ such that $v^\top H v = \lambda$ OR certificate that $\lambda_{\min}(H) \geq -\epsilon$.

(If the certificate is output, it is false with probability δ.)

Need MEO, as Modified CG alone may not suffice to identify negative curvature directions, e.g. when $\nabla f(x_k) = 0$ (a possible saddle point).

Can be implemented with randomized Lanczos. Theory from [Kuczyński and Woźniakowski, 1992, Kuczyński and Woźniakowski, 1994] shows that this requires $\tilde{\mathcal{O}}((L_g/\epsilon)^{1/2})$ matrix-vector multiplications with H.

Line-Search Newton-CG (Step k)

if $\|\nabla f(x_k)\| > \epsilon_g$ **then**
  Call CG to obtain d and step type;
  if step type = "negative curvature" **then**
    Scale and flip sign of d to get d_k;
  else {step type is "approx damped Newton"}
    $d_k \leftarrow d$;
  end if
else
  Call MEO to output v;
  if MEO certifies that $\lambda_{\min}(\nabla^2 f(x_k)) \geq -\epsilon_H$ **then**
    Terminate;
  else
    Scale and flip sign of v to get d_k; (negative curvature direction)
  end if
end if
Backtrack to find α_k s.t. $f(x_k + \alpha_k d_k) < f(x_k) - \frac{\eta}{6}\alpha_k^3 \|d_k\|^3$;
$x_{k+1} \leftarrow x_k + \alpha_k d_k$;

Operation Complexity Result

If $\epsilon_H = \epsilon_g^{1/2}$, the method finds an approximate 2oN point in $\tilde{\mathcal{O}}(\epsilon_g^{-7/4}|\log\delta|)$ operations (with $\delta =$ probability of failure).

Also, $\tilde{\mathcal{O}}(\epsilon_g^{-7/4})$ operations needed to find a point satisfying approximate 1oN conditions $\|\nabla f(x)\| \leq \epsilon_g$, with no probability of failure: deterministic!

($\tilde{\mathcal{O}}$ hides log factors.)

Independent of dimension n, for large n. (But the constants in $\tilde{\mathcal{O}}$ depend on Lipschitz constants.)

1b. Trust-Region Newton-CG

Trust-region Newton methods for minimizing smooth f solve at k:

$$s^k = \arg \min_{\|s\| \le \delta_k} m_k(s) := \nabla f(x^k)^T s + \tfrac{1}{2} s^T \nabla^2 f(x^k) s,$$

where δ_k is the trust-region (TR) radius.

Define ratio ρ_k of actual to predicted decrease in f:

$$\rho_k := \frac{f(x^k) - f(x^k + s^k)}{m_k(0) - m_k(s^k)}.$$

If $\rho_k \ge \eta$ (for some small positive η), take step $x^{k+1} = x^k + s^k$ and choose $\delta_{k+1} > \delta_k$. Otherwise decrease δ_k and compute a new s^k.

- Line-search methods choose direction first, then steplength.
- Trust-region methods choose steplength bound first, then direction.

Steihaug's method (1980)

Steihaug (1980) applies CG to minimization of model $m_k(s)$.

- Start from $s = 0$;
- If it crosses the TR boundary, stop at the TR boundary and return;
- If negative curvature direction in $\nabla^2 f(x^k)$ is detected, move along that direction to the TR boundary, then return.
- If TR boundary does not interfere, keep iterating to the minimum of m_k. (At most n iterations.)

Properties:

- Popular and practical.
- First step of CG is to the "Cauchy point," which is enough to guarantee overall convergence to a first-order point.
- Each CG step reduces model m_k, and moves further away from 0.
- (No second-order guarantees; method does not move away from a saddle point.)
- No complexity guarantees.

TR Newton-CG: Modifying for Complexity Guarantees

[Curtis et al., 2019]: Keep the spirit of Steihaug's method, but modify to enable convergence guarantees.

- Add regularization term to model function:

$$m_k(s) := \nabla f(x^k)^T s + \tfrac{1}{2} s^T \nabla^2 f(x^k) s + \epsilon_H s^T s.$$

- Use the same CG method as in the line-search method, but with explicit cap on the number of iterations, and modified to stay inside the trust region.
- Add the minimum eigenvalue oracle (MEO) to check explicitly for negative curvature. Such directions are almost always found in CG, so in practice MEO is usually invoked only as a final check, at the last iteration.

Complexity Results

The approach broadly follows the line-search method:

- CG called at every iteration to compute a step s^k — either approx solution to the damped trust-region subproblem OR negative curvature direction.
- MEO called as check when CG does not return a useful result and gradient $\nabla f(x^k)$ is small (typically only at last iteration).

Complexity results are broadly the same as line-search too:

To find a point x with

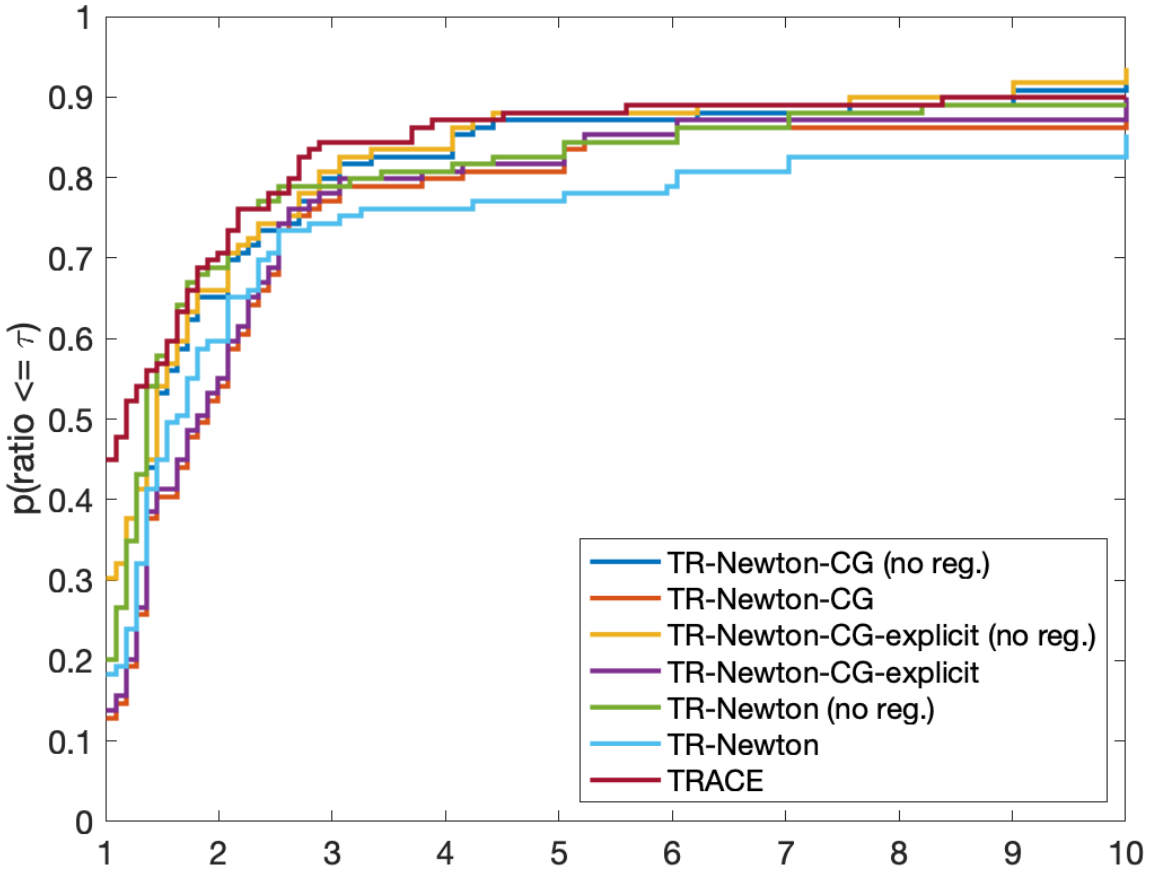
$$\|\nabla f(x)\| \leq \epsilon_g, \quad \nabla^2 f(x) \succeq -\epsilon_H I,$$

with $\epsilon_H = \sqrt{\epsilon_g}$, and with high probability, need $\tilde{\mathcal{O}}(\epsilon_g^{-3/2})$ iterations and $\tilde{\mathcal{O}}(\epsilon_g^{-7/4})$ operations.

Computational Results: Iterations

Problems from the CUTEst set with dimension $n \in [100, 1000]$ All variants solve $\geq 101/109$ problems within $10^4 n$ iterations. $\epsilon_g = 10^{-5}$, $\epsilon_H = 10^{-2.5}$.

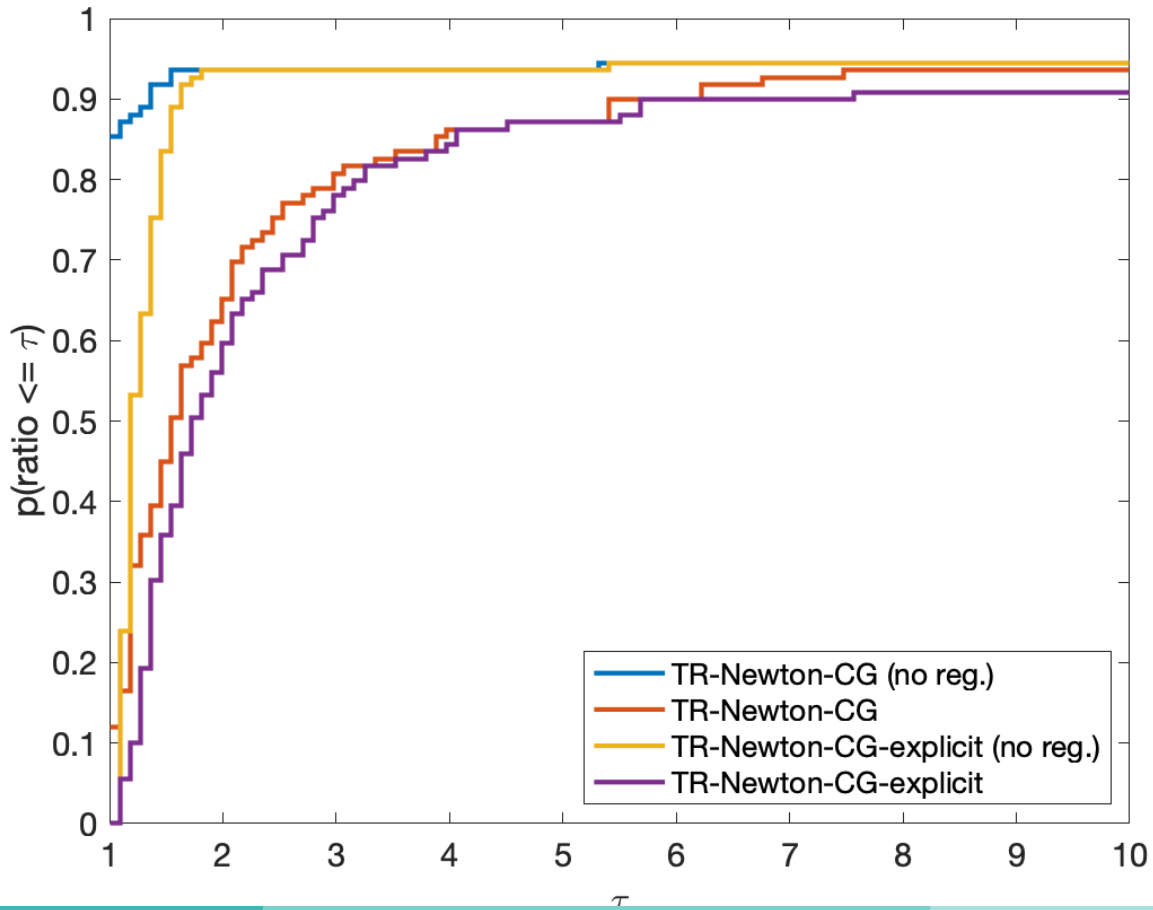
Variants include inexact (CG) and exact subproblems solution. (The analyzed method is TR-Newton-CG-explicit — purple line.)



Computational Results: Hessian-vector products

- Two variants have damped subproblems, consistent with our analysis; the others omit the damping.
- Two variants have explicit caps on CG iterations; the other two don't.

The damped variants use slightly more CG iterations.



1c. Matrix Optimization with Strict Saddles

Low-Rank Matrix Problems: Want to find a rank r solution to the matrix optimization problem:

$$\min_{X \in \mathbb{R}^{n \times m}} f(X), \quad \text{subject to } \mathrm{rank}(X) = r,$$

Matrix completion:

$$\min_X \frac{1}{2} \|(X - X^*)_\Omega\|_F^2, \quad \text{subject to } X \text{ low-rank},$$

where Ω is the set of observed entries and X^*_Ω are given.

Matrix sensing:

$$\min_X \frac{1}{2} \|\mathcal{A}(X - X^*)\|^2, \quad \text{subject to } X \text{ low-rank},$$

where $\mathcal{A} : \mathbb{R}^{n \times m} \to \mathbb{R}^p$ is a known linear measurement operator and $\mathcal{A}(X^*) \in \mathbb{R}^p$ is given.

Reformulation and Strict Saddle Property

Commonly reformulated in terms of $U \in \mathbb{R}^{n\times r}$ and $V \in \mathbb{R}^{m\times r}$:

$$\min_W F(W) := f(UV^T) \quad \text{where} \quad W = \begin{bmatrix} U \\ V \end{bmatrix} \in \mathbb{R}^{(n+m)\times r}.$$

Add a regularization term to eliminate scaling ambiguity:

$$G(W) = F(W) + \tfrac{1}{8}\|U^T U - V^T V\|_F^2.$$

While nonconvex, this formulation satisfies the robust strict saddle property: For any $W \in \mathbb{R}^{(n+m)\times r}$ at least one of the following holds:

1. W is in the neighborhood of a local minimizer W^* and $G(W)$ obeys a regularity condition for all W in this neighborhood (for $\alpha, \beta > 0$):

$$\langle \nabla G(W), W - W^* \rangle \geq \alpha \,\mathrm{dist}(W, W^*)^2 + \beta \|\nabla G(W)\|_F^2.$$

2. $\lambda_{\min}(\nabla^2 G(W)) \leq -\gamma$; or
3. $\|\nabla G(W)\|_F \geq \rho$.

Related Work

We use the global geometry of [Zhu et al., 2017].

Spectral Initialization: Specialized initialization followed by gradient descent. Overall complexity is cost of initialization (e.g. a rank r SVD) plus $\mathcal{O}(\log \max\{\epsilon_g^{-1}, \epsilon_H^{-1}\})$ iterations of gradient descent.

Nonconvex Optimization: Descent method with a saddle point escaping mechanism. When the strict saddle parameters are known at runtime, complexity of gradient descent with occasional perturbations is $\mathcal{O}(\log \max\{\epsilon_g^{-1}, \epsilon_H^{-1}\})$.

Issue: Strict saddle parameters for low-rank matrix problems depend on the singular values of the optimal solution — so we can't realistically assume advance knowledge.

Question: Can we design an algorithm without expensive initialization that does not depend on the strict saddle parameters with a worst case complexity of $\mathcal{O}(\log \max\{\epsilon_g^{-1}, \epsilon_H^{-1}\})$?

Approach

- Maintain γ_k as an upper estimate of strict saddle parameter γ (separation of $\lambda_{\min}\nabla^2 G(W)$ from 0 around strict saddles).
- Define estimates of the regularity parameters α_k and β_k (used in Local Phase) in terms of γ_k.
- Use these estimates to check the large gradient condition **3** and the large negative curvature condition **2**.
- If either of these are satisfied, the appropriate type of step is taken.
- Otherwise, we enter the Local Phase, within which gradient descent on G converges at a linear rate.
- (If we entered the local phase prematurely — because our estimate γ_k was too large — we return to the main algorithm expeditiously.)

Line-Search Algorithm

initial point W^0; initial guess $\gamma_0 \geq \sigma_r(X^*)$;
Iteration k:
if $\|\nabla G(W^k)\|_F \geq \gamma_k^{3/2}$ **then** {Large Gradient; Steepest Descent}
  Find W^{k+1} by backtracking on $-\nabla G(W^k)$; $\gamma_{k+1} \leftarrow \gamma_k$;
else
  Call MEO to approximate $\lambda_{\min}(\nabla^2 G(W^k))$;
  if MEO certifies $\lambda_{\min}(\nabla^2 G(W^k)) \geq -\gamma_k$ **then** {Local Phase}
    if Local Phase successful **then**
      TERMINATE;
    else
      $\gamma_{k+1} \leftarrow \gamma_k/2$;
    end if
  else {MEO Found Negative Curvature Direction D_k}
    Find W^{k+1} by backtracking on D^k;
    $\gamma_{k+1} \leftarrow \gamma_k$;
  end if
end if

MEO: A Complication?

The usual MEO implementation based on randomized Lanczos introduces a term $O(\epsilon^{-1/2})$ into the complexity (for finding a direction with curvature less than $-\epsilon$ in $\nabla^2 G(W)$).

This seems to destroy our hope of $\log \epsilon$ operation complexity!

But we note two things:

1. We can bound the curvature below in terms of easily evaluated terms:

$$\lambda_{\min}(\nabla^2 G(W)) \geq -2\|\nabla f(X)\|_F - \tfrac{1}{2}\|U^T U - V^T V\|_2,$$

   and use this to monitor convergence.

2. When we call MEO, we seek negative curvatures of $-\frac{1}{2}\gamma_k$, which is independent of ϵ_H! Thus the cost of MEO is bounded by $\log \gamma^{-1}$.

Conclusion: MEO does not mess up the operation complexity after all.

Complexity Results

- When a large gradient or large negative curvature step is taken, get

$$G(W^{k+1}) \leq G(W^k) - \mathcal{O}(\gamma_k^3).$$

- γ_k never gets reduced below $\frac{1}{2}\gamma$.

Theorem [O'Neill and Wright, 2020]

W.h.p. the algorithm terminates in at most

$$\mathcal{O}\left(\sigma_r(X^*)^{-3} + \frac{\log \max\{\epsilon_g^{-1}, \epsilon_H^{-1}\}}{\log(1/(1-\sigma_r(X^*)/L_g))}\right)$$

iterations at an approximate second-order point, where $\sigma_r(X^*)$ is the r-th singular value at the optimal solution X^* and L_g is the Lipschitz constant of $\nabla F(W)$. Operation complexity is

$$\mathcal{O}\left(\min\left\{(n+m)r\sigma_r(X^*)^{-3}, \sigma_r(X^*)^{-7/2}\right\} + \frac{\log \max\{\epsilon_g^{-1}, \epsilon_H^{-1}\}}{\log(1/(1-\sigma_r(X^*)/L_g))}\right).$$

2. Nonnegativity Bounds: Optimality Conditions

The most elementary inequality constrained problem.

$$\min_{x \geq 0} f(x)$$

First-order conditions: $0 \leq x \perp \nabla f(x) \geq 0$.

Less tersely: Can partition $\{1, 2, \ldots, n\} = \mathcal{A} \cup \mathcal{I} \cup \mathcal{D}$ such that

- $x_i = 0$, $\nabla_i f(x) > 0$ for $i \in \mathcal{A}$ (active);
- $x_i > 0$, $\nabla_i f(x) = 0$ for $i \in \mathcal{I}$ (inactive);
- $x_i = 0$, $\nabla_i f(x) = 0$ for $i \in \mathcal{D}$ (degenerate).

The strongest 2oN conditions are that $v^T \nabla^2 f(x^*) v \geq 0$ for v such that

$$\mathcal{S}_2 = \{v_i = 0,\ i \in \mathcal{A};\ \ v_i \geq 0,\ i \in \mathcal{D}\}.$$

But it can be NP-hard to check this condition. e.g. $f(x) := x^T Q x$ for symmetric Q. Satisfies first-order conditions with $\mathcal{D} = \{1, 2, \ldots, n\}$. But in this case 2oN conditions = copositivity of Q.

The standard "cop-out" is to aim for a weaker form of 2oN conditions:

$$[\nabla^2 f(x^*)]_{\mathcal{I}\mathcal{I}} \succeq 0.$$

2a. Log-Barrier Method: Approximate Optimality

Define $\bar{x} = \min(x, \mathbf{1})$ and $\bar{X} = \mathrm{diag}(\bar{x})$.

We work with the following approximate 2oN conditions (similar to [Haeser et al., 2018], except that they use X instead of $\bar{X}$).

Approx first-order: $x > 0, \quad \nabla f(x) > -\epsilon \mathbf{1}, \quad \|\bar{X} \nabla f(x)\|_\infty \leq \epsilon,$

Approx second-order: $\bar{X} \nabla^2 f(x) \bar{X} \succeq -\sqrt{\epsilon} I.$

Log-Barrier Approximation

We reduce the bound-constrained problem to unconstrained minimization of the log-barrier function:

$$\phi_\mu(x) := f(x) - \mu \sum_{i=1}^{n} \log(x_i)$$

for some $\mu > 0$. Only defined on the interior of the set $x \geq 0$.

We minimize this for a single (small) value of μ, chosen so that near-optimal second-order points for ϕ_μ satisfy the approximate second-order conditions for the bound-constrained problem.

Approach [O'Neill and Wright, 2019]: Use the Newton-CG approach for unconstrained minimization — modified to ensure positivity of all iterates x^k and well conditioned linear systems — to minimize this function.

Modifying Newton-CG for the Log-Barrier Function

Gradient and Hessian of the log-barrier function are:

$$\nabla \phi_\mu(x) = \nabla f(x) - \mu X^{-1} e \quad \text{and} \quad \nabla^2 \phi_\mu(x) = \nabla^2 f(x) + \mu X^{-2}.$$

Modify Newton-CG as follows:

- Fix $\mu = \frac{1}{4}\epsilon$.
- Precondition / scale the Newton equations with the diagonal $\bar{X}$.
- Keep iterates interior to the nonnegative orthant with a "fraction-to-the-boundary" rule:

$$x^k + d^k \geq (1-\beta)x^k, \quad \text{for fixed } \beta \in [\sqrt{\epsilon}, 1).$$

- Decrease in terms of optimality conditions: Add extra termination test to Modified CG ($\|r^j\|_\infty \leq \bar{\zeta}\mu$).

Log-Barrier Newton-CG

if Not first-order optimal **then**
  Call Modified CG with $H = \bar{X}_k \nabla^2 \phi_\mu(x^k) \bar{X}_k$ and $g = \bar{X}_k \nabla \phi_\mu(x^k)$;
  if step type = "negative curvature" **then**
    Scale d to stay interior and flip sign to get d^k;
  else {step type is "damped Newton"}
    Scale d to stay interior to get d^k
  end if
else
  Call MEO with $H = \bar{X}_k \nabla^2 f(x^k) \bar{X}_k$ to output v;
  if MEO certifies that $\lambda_{\min}(\bar{X}_k \nabla^2 f(x^k) \bar{X}_k) \geq -\sqrt{\epsilon}$ **then**
    Terminate;
  else {direction of sufficient negative curvature found}
    Scale v to stay interior and flip sign to get d^k;
  end if
end if
Line Search: Require $\phi_\mu(x^k + \alpha_k \bar{X}_k d^k) < \phi_\mu(x^k) - \frac{\eta}{6} \alpha_k^3 \|d^k\|^3$;
$x^{k+1} \leftarrow x^k + \alpha_k \bar{X}_k d^k$;

Theorem [O'Neill and Wright, 2019]

Assume f smooth and bounded below, and we use Log-Barrier Newton-CG to seek an approximate second-order point.

- Iteration complexity is $\bar{K}_2 = \tilde{\mathcal{O}}\left(n\epsilon^{-1/2} + \epsilon^{-3/2}\right)$ with probability at least $(1-\delta)^{\bar{K}_2}$.
- Operation complexity is $\tilde{\mathcal{O}}(n\epsilon^{-3/4} + \epsilon^{-7/4})$ for large n and $\tilde{\mathcal{O}}(n\epsilon^{-3/2})$ for smaller n.

- The "n" term seems to be an unavoidable consequence of using the log-barrier function. Best previous result is $\tilde{\mathcal{O}}(n\epsilon^{-3/2})$ — we do better in the "large n" case.
- If we assume a priori that $\{x^k\}$ is bounded, get $\tilde{\mathcal{O}}(\epsilon^{-7/4})$ operation complexity.
- Complexities to get an approximate first-order point are the same, but without the possibility of failure in MEO.

2b. Projected Newton-CG

Bounds on a subset $\mathcal{I} \subset \{1, 2, \ldots, n\}$ of the components of x:

$$\min f(x) \text{ subject to } x_i \geq 0 \text{ for all } i \in \mathcal{I}.$$

For feasible x and small positive threshold ϵ, define *active set* $I^{\text{active}}(x)$ and *free set* $I^{\text{free}}(x)$:

$$I^{\text{active}}(x) := \{i \in \mathcal{I} \,|\, 0 \leq x_i \leq \sqrt{\epsilon}\}$$
$$I^{\text{free}}(x) := \{i \in \mathcal{I} \,|\, x_i > \sqrt{\epsilon}\} \cup \mathcal{I}^c$$

Define diagonal scaling matrix $S(x)$ to have ith diagonal 1 when $i \in I^{\text{free}}(x)$ and x_i when $i \in I^{\text{active}}(x)$.

Approx first-order conditions at feasible x:

$$\begin{aligned} \|S(x)\nabla f(x)\| &\leq 2\epsilon, \\ \nabla_i f(x) &\geq -\epsilon, \qquad i \in I^{\text{free}}(x), \\ \nabla_i f(x) &\geq -\epsilon^{3/4}, \quad i \in I^{\text{active}}(x). \end{aligned}$$

Approx second-order condition: $S(x)\nabla^2 f(x) S(x) \succeq -\sqrt{\epsilon} I$.

Projected Newton-CG: Details

Use $g^k = \nabla f(x^k)$, $H^k = \nabla^2 f(x^k)$, $S_k = S(x^k)$;
g^k_{active}, H^k_{active}, $S_{k,\text{active}}$ are the parts corresponding to $I^{\text{active}}(x^k)$.

1. If $\|g^k_{\text{free}}\| > \epsilon$, apply Modified CG to $(H^k_{\text{free}} + 2\sqrt{\epsilon} I)d = -g^k_{\text{free}}$ to obtain either an approximate reduced Newton direction or negative curvature direction d_{free}. Fill out with zeros to get $d^k \in \mathbb{R}^n$.
2. Else If $g^k_i < -\epsilon^{3/4}$ for some $i \in I^{\text{active}}(x^k)$ or $\|S_{k,\text{active}} g^k_{\text{active}}\| > \epsilon$, set $d^k = -g^k$ (negative gradient).
3. Else call MEO with $S_k H^k S_k$. If a direction d found with $d^T(S_k H^k S_k)d < -(\sqrt{\epsilon}/2)\|d\|^2$, search along $S^k d$ (scaled negative curvature).

For each direction d^k, obtain steplength α by backtracking along the projected path: $P(x^k + \alpha d^k)$, where $P(\cdot)$ is projection onto feasibility.

An approach like this investigated for convex QP in [Wright, 1990] and general nonconvex in [Lin and Moré, 1999].

Projected Newton-CG: Result

Theorem [Xie and Wright, 2020]

The algorithm will terminate at a point satisfying the approximate first-order conditions in $O(\epsilon^{-3/2})$ iterations. With high probability, the same iteration complexity holds for the approximate second-order conditions.

Operation complexity (gradients and Hessian-vector products) is a factor of $O(\epsilon^{-1/4})$ greater.

No explicit dependence on dimension n. (But there is dependence on Lipschitz constants.)

Similar results as for the unconstrained case!

3. Nonconvex Optimization with Equality Constraints

$$\min f(x) \quad \text{s.t. } c(x) = 0,$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is smooth, and $c : \mathbb{R}^n \to \mathbb{R}^m$ $(m \leq n)$ is a smooth vector function of equality constraints.

$\nabla c(x) \in \mathbb{R}^{n \times m}$ is the matrix of first partial derivatives of c.

Approx first-order (ϵ-1o):

$$\|\nabla f(x) + \nabla c(x)\lambda\| \leq \epsilon, \quad \|c(x)\| \leq \epsilon.$$

Approx second-order (ϵ-2o):

$$d^T \left(\nabla^2 f(x) + \sum_{i=1}^{m} \lambda_i \nabla^2 c_i(x) \right) d \geq -\epsilon \|d\|^2,$$

for any $d \in \mathbb{R}^n$ such that $\nabla c(x)^T d = 0$.

3a. Proximal Augmented Lagrangian (PAL) algorithm

The augmented Lagrangian is

$$\mathcal{L}_\rho(x,\lambda) \triangleq f(x) + \lambda^T c(x) + \frac{\rho}{2}\|c(x)\|^2,$$

where $\rho > 0$ and $\lambda \triangleq (\lambda_1, \ldots, \lambda_m)^T$.

PAL Algorithm:

0. Initialize x_0, λ_0 and fix $\rho > 0$, $\beta > 0$; Set $k := 0$;
1. Update x_k: Find approximate solution x_{k+1} to

$$\text{argmin } \mathcal{L}_\rho(x,\lambda_k) + \frac{\beta}{2}\|x - x_k\|^2;$$

2. Update λ_k: $\lambda_{k+1} := \lambda_k + \rho c(x_{k+1})$;
3. If termination criterion is satisfied, STOP; otherwise, $k := k+1$ and go to Step 1.

[Xie and Wright, 2019]

Complexities and Assumptions

PAL involves two levels of iteration: the outer iteration, and the inner iterations to solve the nonconvex unconstrained subproblem.

Three types of complexity:

- Outer iteration complexity
- Total iteration complexity: total number of iterations of the inner loop. (a.k.a. "evaluation complexity")
- Operation complexity: bound on number of gradient evaluations / Hessian-vector products.

The assumptions vary between results, but include the following:

- f and c are twice Lipschitz continuously differentiable.
- $f(x) + (\rho_0/2)\|c(x)\|_2^2$ has compact level sets, for some $\rho_0 \geq 0$.
- $\nabla c(x)$ has uniformly full rank m for all x in a compact level set.

Note: We *don't* assume that β is large enough to make the subproblem convex i.e. swamp out the negative curvature in $\mathcal{L}_\rho$.

PAL Outer Iteration Complexity

For any $\epsilon > 0$ and $\eta \in [0, 2]$, choose

- Prox parameter $\beta = \epsilon^\eta/2$ (small)
- Penalty parameter $\rho = O(\epsilon^{-\eta})$ and above some threshold.

Outer iterations for ϵ-1o: Assume that an approx first-order point is found for each subproblem with gradient $\leq \frac{1}{2}\epsilon$, and $\|c(x_0)\| = O(\epsilon^{\eta/2})$. Then an ϵ-1o solution is found in $O(\epsilon^{\eta-2})$ outer iterations.

$\eta = 2$: need only $O(1)$ outer iterations! (But then the subproblems are extremely ill conditioned.)

$\eta = 0$: (settings of β and ρ are independent of ϵ), get $O(\epsilon^{-2})$ outer iterations.

Outer iterations for ϵ-2o: Require $\eta \in [1, 2]$, and additionally that subproblem solutions have Hessian $\succeq -\frac{1}{2}\epsilon I$. Then an ϵ-2o point is found in $O(\epsilon^{\eta-2})$ outer iterations.

PAL Total Iteration and Operation Complexity

Use line-search Newton-CG to solve the subproblems inexactly. Then get estimates of total iteration complexity and operation complexity. Require

$$\nabla_x \mathcal{L}_\rho(x_{k+1}, \lambda_k) + \beta(x_{k+1} - x_k) = \tilde{r}_{k+1},$$
$$\nabla^2_{xx} \mathcal{L}_\rho(x_{k+1}, \lambda_k) + \beta I \succeq -\tfrac{1}{2}\epsilon I,$$

with $\|\tilde{r}_k\| \leq \min(1/k, \frac{1}{2}\epsilon)$.

Total Iter Complexity: $\eta \in [1, 2]$, ϵ-2o point w.h.p.:

Constraints	Total Iter.	Optimal	
nonlinear	$\mathcal{O}(\epsilon^{-2\eta-5})$	$\mathcal{O}(\epsilon^{-7})$	$(\eta = 1)$
linear	$\mathcal{O}(\epsilon^{\eta-5})$	$\mathcal{O}(\epsilon^{-3})$	$(\eta = 2)$

Operation Complexity: $\eta \in [1, 2]$, ϵ-2o point w.h.p.:

Constraints	Operations	Optimal	
nonlinear	$\mathcal{O}(\epsilon^{-5\eta/2-11/2})$	$\mathcal{O}(\epsilon^{-8})$	$(\eta = 1)$
linear	$\mathcal{O}(\epsilon^{\eta/2-11/2})$	$\mathcal{O}(\epsilon^{-9/2})$	$(\eta = 2)$

PAL: Choosing ρ

Recall that $\rho = O(\epsilon^{-\eta})$, but it also has to be above a certain threshold (depending on many problem-dependent parameters).

Can wrap an outer loop around PAL in which ρ is increased by a constant factor on each loop.

For each ρ, run PAL for the # of outer iterations predicted by the theory. If an ϵ-2o point is not found by then, increase ρ and try again.

Increases total iteration complexity by a factor of only $\log \epsilon$.

Related Work

There are many related works on nonconvex constrained optimization, with complexity analyses of various types. See [Xie and Wright, 2020].

Often in more limited settings (e.g. linear constraints, approximate first-order optimality, iteration / evaluation complexity only, explicit second derivatives, use original feasible set in subproblems).

- Augmented Lagrangian type: [Grapiglia and Yuan, 2019], [Birgin and Martínez, 2019]
- (Modified) Proximal AL (linear constraints): [Zhang and Luo, 2020], [Hajinezhad and Hong, 2019]
- Other algorithms: Exact penalty [Cartis et al., 2011], two-phase target-following [Cartis et al., 2014, Cartis et al., 2019b] and others.
- Methods that use the original feasible set in the subproblems: SQP [Nouiehed et al., 2018], cubic regularization [Cartis et al., 2015, Cartis et al., 2020a], active set [Birgin and Martínez, 2018], interior-point [Haeser et al., 2018].

Conclusions

- Second-order necessary points are of interest in some new applications
- Complexity analysis of (nearly) practical methods for finding such points is interesting too
- Significant open questions, particularly surrounding nonconvex nonlinear constrained:
  - primal-dual interior-point methods;
  - exact penalty functions;
  - can some "impractial" methods with good complexity inspire "practical" methods?

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