# Newton-type methods with complexity guarantees for nonconvex data science

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## Collaborators



- Trust-region Newton-CG with strong second-order complexity guarantees for nonconvex optimization,
   F. E. Curtis, D. P. Robinson, C. W. Royer and S. J. Wright, SIAM Journal on Optimization, 2021.
- Newton-type methods for strict saddle problems F. Goyens and C. W. Royer, in preparation.

# The plan

## Our interests

- Nonconvex data science tasks.
- Algorithms with complexity guarantees.

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#### Our framework

- Newton-Conjugate Gradient + trust region, revisited.
- Complexity results + numerical relevance.

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- Newton-Conjugate Gradient + trust region, revisited.
- Complexity results + numerical relevance.

#### Our latest

- Manifold optimization.
- Strict saddle problems.

Nonconvex problems and algorithms

2 Newton-type framework



# Nonconvex problems and algorithms Nonconvexity in data science

Complexity bounds

Newton-type framework

## Extensions

#### Nonconvex ?

- Many data science problems are convex: linear classification, logistic regression,...
- Nonconvex instances: Deep/shallow neural networks, nonconvex regularization (SCAD,MDP),...

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- Many data science problems are convex: linear classification, logistic regression,...
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#### **Optimization** ?

- Those problems often come with structure.
- In many cases, global minima can be characterized (and found) in polynomial time!

## Definition (S. Wright, 2023)

A nonconvex optimization problem has **benign nonconvexity** if useful solutions (even global minima) can be found by optimization methods.

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#### Typical properties

- All local minima are global.
- All saddle points (zero derivative but not local minima) are strict.
- Algorithms can start close to a global minimum.

# Examples of benignly nonconvex problems (1/2)

Nonconvex factored matrix problems

• With two matrix variables:

$$\min_{U \in \mathbb{R}^{n \times r}, V \in \mathbb{R}^{m \times r}} f(U V^{\top}) \quad f \text{ smooth.}$$

 $\Rightarrow$  Nonconvex in *U* and *V* even when *f* convex, but second-order stationary points typically global minima (or close in function value).

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## Examples (Ge et al '17,Eftekhari '20)

• Low-rank matrix sensing :

$$f(UV^{\top}) = rac{1}{2s} \sum_{i=1}^{s} \left( \langle UV^{\top}, A_i \rangle - b_i 
ight)^2, \quad M \in \mathbb{R}^{m \times n}$$

• Deep linear networks :  $f(U_1, \ldots, U_r) = \frac{1}{2} ||U_r \cdots U_1 A - B||_F^2$ .

# Examples of benignly nonconvex problems (2/2)

#### Phase retrieval

Given  $A = [a_i]_{i=1}^m \in \mathbb{R}^{m \times n}$  and  $b \in \mathbb{R}^m$ , find  $x \in \mathbb{C}^n$  such that

$$|a_i^*x| = b_i \quad \forall i = 1, \ldots, n.$$

### Nonconvex optimization problem (Sun et al '18)

$$\min_{x\in\mathbb{C}^n}\frac{1}{2m}\sum_{i=1}^m(b_i^2-|a_i^*x|^2)^2$$

- All local minima are global.
- Saddle points are strict.



## What we have

- Classes of structured nonconvex problems.
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- Classes of structured nonconvex problems.
- Characterization of their solutions using second-order derivatives.

#### What we want

- Efficient algorithms to reach second-order necessary points;
- Efficiency measured by **complexity**, akin to theoretical CS/**convex** optimization.

Nonconvex problems and algorithms
 Nonconvexity in data science
 Complexity bounds

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## Extensions

# General problem and definitions

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

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## Definitions in smooth nonconvex minimization

- First-order stationary point:  $\|\nabla f(x)\| = 0$ ;
- Second-order stationary point:  $\|\nabla f(x)\| = 0, \nabla^2 f(x) \succeq 0^a$ .

$${}^{a}A \succeq \beta I \Leftrightarrow \lambda_{\min}(A) \geq \beta.$$

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If x does not satisfy these conditions,  $\exists d$  such that

- $d^{\top} \nabla f(x) < 0$ : gradient-related direction. and/or

 ${}^{a}A \succeq \beta I \Leftrightarrow \lambda_{\min}(A) \geq \beta.$ 

## Complexity in nonconvex optimization

**Setup:** Sequence of points  $\{x_k\}$  generated by an algorithm applied to  $\min_{x \in \mathbb{R}^n} f(x)$ .

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Given  $\epsilon \in (0, 1)$ :

- Worst-case cost to obtain an  $\epsilon$ -point  $x_K$  such that  $\|\nabla f(x_K)\| \leq \epsilon$ .
- Focus: Dependency on  $\epsilon$ .

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#### Second-order complexity result

Given  $\epsilon, \epsilon_H \in (0, 1)$ :

• Worst-case cost to obtain an  $(\epsilon, \epsilon_H)$ -point  $x_K$  such that

$$\|
abla f(x_{\mathcal{K}})\| \leq \epsilon, \qquad 
abla^2 f(x_{\mathcal{K}}) \succeq -\epsilon_{\mathcal{H}}.$$

• Focus: Dependencies on  $\epsilon, \epsilon_H$ .

# Complexity results

## From nonconvex optimization (2006-)

- Cost measure: Number of iterations (but those may be expensive);
- Two types of guarantees:

$$\|\nabla f(x)\| \le \epsilon; \|\nabla f(x)\| \le \epsilon \text{ and } \nabla^2 f(x) \succeq -\epsilon_H I$$

• <u>Best methods</u>: Second-order methods, deterministic variations on Newton's iteration involving Hessians.

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## Influenced by convex optimization/learning (2016-)

- <u>Cost measure</u>: gradient evaluations+Hessian-vector products.
- Two types of guarantees:

$$\|\nabla f(x)\| \le \epsilon$$

$$\|\nabla f(x)\| \le \epsilon \text{ and } \nabla^2 f(x) \succeq -\epsilon^{1/2} I.$$

• <u>Best methods</u>: developed from accelerated gradient, assume knowledge of Lipschitz constants.

## Methods with good complexity

- Designed to get good guarantees;
- Sensitive to parameter choices;
- Not necessarily efficient in practice.

## Practical methods

- Efficient without convexity;
- Often scalable (e.g. matrix-free);
- No complexity guarantees.

## Nonconvex problems and algorithms

## 2 Newton-type framework

- Problem and exact method
- Inexact variants
- Numerics

## 3 Extensions

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Goal: Find approximate stationary points

Given  $\epsilon, \epsilon_H \in (0, 1)$ ,

• x is an 
$$(\epsilon, \epsilon_H)$$
-point if

$$\|\nabla f(x)\| \leq \epsilon$$
 and  $\nabla^2 f(x) \succeq -\epsilon_H I$ .

• Complexity: Given an algorithm, bound the cost of the method to find an  $(\epsilon, \epsilon_H)$ -point.

**Goal:** Find x such that  $\|\nabla f(x)\| \leq \epsilon$ ,  $\nabla^2 f(x) \succeq -\epsilon_H I$ .

Gradient-based line search/trust region (Cartis et al '12)

- Cost: Iterations, calls to  $f, \nabla f, \nabla^2 f$ ;
- Order: max{ $\epsilon^{-2}\epsilon_H^{-1}, \epsilon_H^{-3}$ };

• Newton steps not used/leveraged.

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#### Optimal Newton-type methods (Cartis et al '19, Curtis et al '17)

- Cost: Iterations, calls to  $f, \nabla f, \nabla^2 f$ ;
- Bound:  $\max\{\epsilon^{-3/2}, \epsilon_H^{-3}\} \Rightarrow \epsilon^{-3/2}$  when  $\epsilon_H = \sqrt{\epsilon}$ ;
- Optimal iteration complexity but expensive Newton steps.

## Newton-type methods

- Compute a Newton step or use negative curvature;
- Provide decrease guarantees (for complexity);
- Use inexact steps (for practicality).

## Specific features

- Trust region for globalization;
- Conjugate gradient (inexact version).

# Trust-region Newton-type method

Inputs: 
$$x_0 \in \mathbb{R}^n$$
,  $\delta_0 > 0$ ,  $\eta > 0$ .  
For k=0, 1, 2, ...  
Define  $m_k(x_k + s) := \nabla f(x_k)^T s + \frac{1}{2}s^T \nabla^2 f(x_k)s$  and compute  
 $s_k \in \underset{\|s\| \le \delta_k}{\operatorname{argmin}} m_k(x_k + s)$ .  
Scompute  $\rho_k = \frac{f(x_k) - f(x_k + s_k)}{m_k(x_k) - m_k(x_k + s_k)}$ .  
If  $\rho_k \ge \eta$ , set  $x_{k+1} = x_k + s_k$  and  $\delta_{k+1} = 2\delta_k$ .  
Otherwise, set  $x_{k+1} = x_k$  and  $\delta_{k+1} = 0.5\delta_k$ .

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 $s \in \mathbb{R}^n$   
 $\|s\| \le \delta_k$   
Compute  $\rho_k = \frac{f(x_k) - f(x_k + s_k)}{m_k(x_k) - m_k(x_k + s_k)}$ .  
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## • Standard version: Can get (suboptimal) iteration complexity.

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$$x_0 \in \mathbb{R}^n$$
,  $\delta_0 > 0$ ,  $\eta > 0$ ,  $\epsilon_H \in (0, 1)$ .  
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 $s_k \in \underset{\substack{s \in \mathbb{R}^n \\ \|s\| \le \delta_k}}{\operatorname{argmin}} m_k(x_k + s) + \frac{\epsilon_H}{2} \|s\|^2$ .  
Compute  $\rho_k = \frac{f(x_k) - f(x_k + s_k)}{m_k(x_k) - m_k(x_k + s_k)}$ .  
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Standard version: Can get (suboptimal) iteration complexity.
Our version: Regularization to improve complexity.
## Analysis of the exact method

**Goal:** Compute  $x_k$  such that  $\|\nabla f(x_k)\| \leq \epsilon$  and  $\nabla^2 f(x_k) \succeq -\epsilon_H I$ .

As long as  $x_k$  is not an  $(\epsilon, \epsilon_H)$ -point:

- $m_k(x_k) m_k(x_k + s_k) \ge \frac{\epsilon_H}{2} \|s_k\|^2$ ;
- $\delta_k \geq \mathcal{O}(\epsilon_H).$

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As long as  $x_k$  is not an  $(\epsilon, \epsilon_H)$ -point: •  $m_k(x_k) - m_k(x_k + s_k) \ge \frac{\epsilon_H}{2} ||s_k||^2$ ; •  $\delta_k \ge \mathcal{O}(\epsilon_H)$ .

For any successful iteration  $(x_{k+1} = x_k + s_k)$ , • If  $||s_k|| = \delta_k$ ,

$$f(x_k) - f(x_{k+1}) \ge \frac{\eta}{2} \epsilon_H \delta_k^2 \ge \mathcal{O}(\epsilon_H^3)$$

• If  $\|s_k\| < \delta_k$ ,

$$f(x_k) - f(x_{k+1}) \ge \mathcal{O}\left(\min\left\{\|\nabla f(x_{k+1})\|^2 \epsilon_H^{-1}, \epsilon_H^3\right\}\right)$$

#### Theorem

The trust-region algorithm reaches an  $(\epsilon, \epsilon_H)$ -point in at most

 $\mathcal{O}\left(\max\left\{\epsilon^{-2}\epsilon_{H},\epsilon_{H}^{-3}\right\}\right)$ 

successful iterations/calls to  $\nabla f / \nabla^2 f$  and

$$\mathcal{O}\left(\log(\epsilon_{H}^{-1})\max\left\{\epsilon^{-2}\epsilon_{H},\epsilon_{H}^{-3}\right\}\right) = \tilde{\mathcal{O}}\left(\max\left\{\epsilon^{-2}\epsilon_{H},\epsilon_{H}^{-3}\right\}\right)$$

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Order for classical method: max {ε<sup>-2</sup>ε<sub>H</sub><sup>-1</sup>, ε<sub>H</sub><sup>-3</sup>}.
ε<sub>H</sub> = ε<sup>1/2</sup> gives optimal O(ε<sup>-3/2</sup>) complexity.

### Nonconvex problems and algorithms

### 2 Newton-type framework

- Problem and exact method
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## Inexact trust-region Newton-type method

Inputs: 
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,  $\delta_0 > 0$ ,  $\zeta > 0$ ,  $\eta > 0$ .  
For k=0, 1, 2, ...  
Define  $m_k(x_k + s) := \nabla f(x_k)^T s + \frac{1}{2}s^T \nabla^2 f(x_k)s$  and compute  
 $s_k \approx \underset{\|s\| \leq \delta_k}{\operatorname{argmin}} m_k(x_k + s)$ .  
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• Standard version: Solve subproblem via Conjugate Gradient (CG);

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Standard version: Solve subproblem via Conjugate Gradient (CG);

### • Our approach:

- Regularization tailored to inexact setting.
- Extra stopping criteria on CG for complexity.

## Linear Conjugate Gradient (CG)

**Goal:** Solve Hs = -g with H symmetric matrix and  $g \in \mathbb{R}^n$ .

# Linear CG Init: Set $s_0 = 0_{\mathbb{R}^n}$ , $r_0 = g$ , $p_0 = -g$ , j = 0, $\xi \ge 0$ . For j = 0, 1, 2, ...• Compute $s_{j+1} = s_j + \frac{\|r_j\|^2}{p_j^T H p_j} p_j$ and $r_{j+1} = H s_{j+1} + g$ . • Set $p_{j+1} = -r_{j+1} + \frac{\|r_{j+1}\|^2}{\|r_j\|^2} p_j$ . • Set j = j + 1; terminate if $\|Hs_j + g\| \le \xi \|g\|$ .

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• Only requires  $v \mapsto Hv$  ("matrix-free");

• Terminates in at most *n* iterations when  $H \succ 0$ .

## The Steihaug-Toint approach

### TR subproblem

$$\min_{s \in \mathbb{R}^n} g^{\mathrm{T}} s + \frac{1}{2} s^{\mathrm{T}} H s \quad \text{s.t.} \quad \|s\| \leq \delta, \qquad H = H^{\mathsf{T}}.$$

- Apply conjugate gradient (CG) to the linear system Hs = -g;
- Stop when residual small enough  $||Hs + g|| \le \zeta ||g||$  or the boundary is reached;
- For H ≥ 0: if negative curvature is encountered in H, take a negative curvature step towards the boundary.

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#### Steihaug's approach within TR

- Optimal iteration complexity?
- Cost: Number of Hessian-vector products?

## Conjugate gradient method with explicit cap

Goal:  $\min_{s \in \mathbb{R}^n} g^{\mathrm{T}}s + \frac{1}{2}s^{\mathrm{T}}(H + 2\epsilon_H I)s$  s.t.  $||s|| \leq \delta$ .

## Conjugate gradient method with explicit cap

**Goal:** 
$$\min_{s \in \mathbb{R}^n} g^{\mathrm{T}}s + \frac{1}{2}s^{\mathrm{T}}(H + 2\epsilon_H I)s$$
 s.t.  $||s|| \leq \delta$ .

#### Key differences

Stop after J iterations of CG if one of the following conditions holds:

- Convergence:  $||(H+2\epsilon_H I)s+g|| \leq \zeta \min\{||g||, \epsilon_H ||s||\};$
- Boundary reached;

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Stop after J iterations of CG if one of the following conditions holds:

- Convergence:  $||(H + 2\epsilon_H I)s + g|| \le \zeta \min\{||g||, \epsilon_H ||s||\};$
- Boundary reached;
- Small curvature: A vector *u* is found such that

$$u^{\mathrm{T}}(H+2\epsilon_{H}I)u \leq \epsilon_{H}\|u\|^{2} \Rightarrow u^{\mathrm{T}}Hu \leq -\epsilon_{H}\|u\|^{2}$$

Explicit iteration cap: J ≤ Ĵ := min{n, Õ(ϵ<sub>H</sub><sup>-1/2</sup>)} iterations
 If H + 2ϵ<sub>H</sub>I ≽ ϵ<sub>H</sub>I, convergence (case 1) occurs in less than Ĵ iterations!

### CG with explicit cap

- Good steps when converged and  $\|\nabla f(x_k)\| \ge \epsilon$ ;
- Or when negative curvature is detected;
- But may not converge/miss negative curvature information!

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### Our approach

At iteration  $x_k$ ,

- Q Run CG on the regularized problem first;
- If the cap is triggered (Ĵ) or ||∇f(x<sub>k</sub>)|| ≤ ε and the convergence criterion is met, call a minimum eigenvalue oracle to check whether ∇<sup>2</sup>f(x<sub>k</sub>) ≥ -ε<sub>H</sub>I.

Given  $H = H^{\mathrm{T}} \in \mathbb{R}^{n \times n}$ ,  $\epsilon_H \in (0, 1)$ , and  $\xi \in (0, 1)$ , output A vector s such that  $s^{\mathrm{T}}Hs \leq -\frac{\epsilon_H}{2} \|s\|^2.$ 

**2** OR a certificate that  $H \succeq -\epsilon_H I$ , valid with probability  $1 - \xi$ .

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$$s^{\mathrm{T}}Hs \leq -rac{\epsilon_{H}}{2}\|s\|^{2}.$$

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#### An example of MEO

Run CG on Hs = b, b uniform on the unit sphere.

- Produces output in min $\{n, \tilde{\mathcal{O}}(\epsilon_H^{-1/2})\}$  iterations;
- Same order than the cap  $\hat{J}$  on CG earlier!

## Analysis of the *inexact* method

**Goal:** Compute  $x_k$  such that  $\|\nabla f(x_k)\| \leq \epsilon$  and  $\nabla^2 f(x_k) \succeq -\epsilon_H I$ .

For any realization, as long as  $x_k$  is not an  $(\epsilon, \epsilon_H)$ -point:

• 
$$m_k(x_k) - m_k(x_k + s_k) \ge \frac{\epsilon_H}{4} \|s_k\|^2;$$

• 
$$\delta_k \geq \mathcal{O}(\epsilon_H)$$

For any realization and any successful iteration (x<sub>k+1</sub> = x<sub>k</sub> + s<sub>k</sub>),
If ||s<sub>k</sub>|| = δ<sub>k</sub>,

$$f(x_k) - f(x_{k+1}) \ge \frac{\eta}{4} \epsilon_H \delta_k^2 \ge \mathcal{O}(\epsilon_H^3)$$

• If  $\|s_k\| < \delta_k$ ,

$$f(x_k) - f(x_{k+1}) \ge \mathcal{O}\left(\min\left\{\|\nabla f(x_{k+1})\|^2 \epsilon_H^{-1}, \epsilon_H^3\right\}\right)$$

## Iteration complexity of the inexact method (1/2)

#### Theorem

The trust-region algorithm reaches an  $(\epsilon, \epsilon_H)$ -point in at most

$$\mathcal{O}\left(\max\left\{\epsilon^{-2}\epsilon_{H},\epsilon_{H}^{-3}\right\}\right)$$

successful iterations/calls to  $\nabla f$  and

$$\tilde{\mathcal{O}}\left(\max\left\{\epsilon^{-2}\epsilon_{H},\epsilon_{H}^{-3}\right\}\right)$$

total iterations/calls to f with probability  $(1-\xi)^{\mathcal{O}\left(\max\left\{\epsilon^{-2}\epsilon_{H},\epsilon_{H}^{-3}\right\}\right)}$ .

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total iterations/calls to f with probability  $(1 - \xi)^{\mathcal{O}(\max\{\epsilon^{-2}\epsilon_{H}, \epsilon_{H}^{-3}\})}$ .

• Same order of complexity than before;

• With small probability, the method terminates at  $x_k$  where  $\|\nabla f(x_k)\| \le \epsilon$  but  $\nabla^2 f(x_k) \prec -\epsilon_H I$ .

## Computational complexity of the inexact method (2/2)

Matrix-free variant: Can we quantify the cost of computing the trust-region step?

#### Theorem

For any realization of the inexact algorithm, the number of Hessian-vector products used in CG+MEO is

$$\tilde{\mathcal{O}}\left(\min\{n,\epsilon_{H}^{-1/2}\} \times \max\left\{\epsilon^{-2}\epsilon_{H},\epsilon_{H}^{-3}\right\}\right).$$

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$$ilde{\mathcal{O}}\left(\min\{n,\epsilon_{H}^{-1/2}\}\, imes\,\max\left\{\epsilon^{-2}\epsilon_{H},\epsilon_{H}^{-3}
ight\}
ight).$$

• Deterministic result (covers early termination).

•  $\epsilon_H = \epsilon^{1/2}$  and large *n* gives best known  $\tilde{\mathcal{O}}(\epsilon^{-7/4})$  complexity.

### Nonconvex problems and algorithms

### 2 Newton-type framework

- Problem and exact method
- Inexact variants
- Numerics

### 3 Extensions

### Test problems

- CUTEst smooth unconstrained problems with  $n \ge 100$  (109 problems);
- Performance profiles for  $\epsilon_H = \epsilon^{1/2}$ ,  $\epsilon = 10^{-5}$ .

#### Algorithms (trust-region type)

- TRACE (Curtis, Robinson, Samadi '17);
- TR-Newton (Moré, Sorensen '83);
- TR-Newton-CG (Steihaug '83);
- TR-Newton-CG-explicit (ours with capped CG+MEO).

TR-Newton methods tested with/without regularization.

## Performance profile: Iterations



### Performance profile: Hessian-vector products



### Matrix completion

$$\min_{X\in\mathbb{R}^{n\times m}, \operatorname{rank}(X)=r} \|\mathcal{P}_{\Omega}(X-M)\|_{F}^{2}, \quad M\in\mathbb{R}^{n\times m}, \ \Omega\subset[n]\times[m].$$

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Nonconvex factored reformulation (Burer & Monteiro, '03)

$$\min_{U\in\mathbb{R}^{m\times r}, V\in\mathbb{R}^{m\times r}}\left\|\mathcal{P}_{\Omega}(UV^{\top}-M)\right\|_{F}^{2},$$

 $\Rightarrow$  Nonconvex in U and V.

### Matrix problem

$$\min_{U,V}\frac{1}{2}\left\|P_{\Omega}(UV^{\top}-M)\right\|_{F}^{2},$$

with  $M \in \mathbb{R}^{m \times n}$ ,  $U \in \mathbb{R}^{m \times r}$ ,  $V \in \mathbb{R}^{n \times r}$ ,  $|\Omega| \approx \{5\%, 15\%\} \times mn$ .

• Synthetic data: 
$$(n, m) = (500, 499)$$
.

### Comparison

- Our Newton+Conjugate Gradient (CG) technique;
- Nonlinear CG (Polak-Ribière);
- Dedicated solvers (Alternating methods):
  - Alternated gradient descent (Tanner and Wei 2016);
  - LMaFit (Wen et al. 2012).

## Matrix completion (synthetic data, rank 5)



## Matrix completion (synthetic data, rank 15)



## In short: Newton-Capped Conjugate Gradient

#### Our changes to Steihaug's method

- Regularization to get decrease guarantees;
- MEO to get second-order probabilistic results;
- Extra checks in (linear) conjugate gradient.

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- Regularization to get decrease guarantees;
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### The (typical) cost of complexity

- More iterations of Conjugate Gradient;
- Eigenvalue oracle typically triggered once!

Nonconvex problems and algorithms

### 2 Newton-type framework



### Extensions

- Manifold optimization
- Strict saddle problems
#### Our problems of interest

- Could involve complex variables (e.g. phase retrieval).
- Matrix completion/factorization: Variables naturally in matrix form.
- Additional constraints: Orthogonal columns, e.g. in phase retrieval.

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#### Manifold optimization

- Solve problems on a Riemannian manifold, i.e. a space that can be mapped to ℝ<sup>n</sup>.
- Preserve feasibility throughout.
- Examples:

```
1 Vectors : \mathbb{R}^n, \mathbb{C}^n, \S^{n-1};
```

Matrices : R<sup>n×m</sup>, Grassmann (subspaces), Stiefel (orthogonal matrices).

# Manifold optimization

# **Problem:** $\min_{x \in \mathcal{M}} f(x)$ , $\mathcal{M}$ Riemannian manifold.

#### Algorithmic blocks

- Riemannian gradient and Hessian :
  - Counterparts of gradient and Hessian in Euclidean  $(\mathbb{R}^n)$  setting.
  - Formulas depending on  $\mathcal{M}, \nabla f(x), \nabla^2 f(x)$  can be derived by hand or using toolboxes (Manopt).

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- Retraction :
  - Operator that "projects" back onto the manifold.
  - $\bullet\,$  Depends solely on  $\mathcal{M},$  formulas available in toolboxes.
- With these operations, can adapt most algorithms to the Riemannian setting.
- Complexity guarantees are preserved but now apply to finding Riemannian stationary points.

**Problem:**  $\min_{x \in \mathbb{R}^n} f(x)$ . Inputs:  $x_0 \in \mathbb{R}^n$ ,  $\delta_0 > 0$ , n > 0. For k=0, 1, 2, ... • Define  $m_k(x_k + s) := \nabla f(x_k)^T s + \frac{1}{2}s^T \nabla^2 f(x_k)s$  and compute  $s_k \in \operatorname*{argmin}_{s \in \mathbb{R}^n} m_k(x_k + s) + rac{\epsilon_H}{2} \|s\|^2.$  $\|s\| < \delta_k$ 2 Compute  $\rho_k = \frac{f(x_k) - f(x_k + s_k)}{m_k(x_k) - m_k(x_k + s_k)}$ . If  $\rho_k > \eta$ , set  $x_{k+1} = x_k + s_k$  and  $\delta_{k+1} = 2\delta_k$ . • Otherwise, set  $x_{k+1} = x_k$  and  $\delta_{k+1} = 0.5\delta_k$ .

# Illustration: Trust-Region Newton

**Problem:**  $\min_{x \in \mathcal{M}} f(x)$ ,  $\mathcal{M}$  Riemannian manifold.

Inputs: 
$$x_0 \in M$$
,  $\delta_0 > 0$ ,  $\eta > 0$ ,  $\epsilon_H \in (0, 1)$ .  
For k=0, 1, 2, ...

- Compute the Riemannian gradient  $g_{f,\mathcal{M}}(x_k)$  and Riemannian Hessian  $H_{f,\mathcal{M}}(x_k)$ .
- **3** Define  $m_k(x_k + s) := g_{f,\mathcal{M}}(x_k)^{\mathrm{T}}s + \frac{1}{2}s^{\mathrm{T}}H_{f,\mathcal{M}}(x_k)s$  and compute

$$s_k \in \operatorname*{argmin}_{\substack{s \in \mathbb{R}^n \\ \|s\| \leq \delta_k}} m_k(x_k + s) + rac{\epsilon_H}{2} \|s\|^2.$$

• Define  $x_k^{\mathcal{M}}$  as the retraction of  $x_k + s_k$  onto  $\mathcal{M}$ .

• Compute  $\rho_k = \frac{f(x_k) - f(x_k^{\mathcal{M}})}{m_k(x_k) - m_k(x_k^{\mathcal{M}})}$ .

- $If \rho_k \ge \eta, \text{ set } x_{k+1} = x_k^{\mathcal{M}} \text{ and } \delta_{k+1} = 2\delta_k.$
- Otherwise, set  $x_{k+1} = x_k$  and  $\delta_{k+1} = 0.5\delta_k$ .



#### Extensions

- Manifold optimization
- Strict saddle problems

## What are those?

- Special nonconvex functions;
- Various definitions exist.

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- Various definitions exist.

#### An informal definition

Given  $\alpha > 0, \beta > 0, \gamma > 0$ , a function  $f : \mathbb{R}^n \to \mathbb{R}$  is  $(\alpha, \beta, \gamma)$ -strict saddle if for any  $x \in \mathbb{R}^n$ , one of these properties holds:

$$\|\nabla f(x)\| \geq \alpha;$$

$$2 \nabla^2 f(x) \not\geq -\beta I;$$

**3** There exists  $x^* \in \operatorname{argmin}_x f(x)$  such that  $||x - x^*|| \le \gamma$ .

# Strict saddle functions (2)

#### Why are strict saddle functions interesting?

- Second-order methods will converge near a global minimum.
- Convergence will be driven by problem-dependent quantities  $(\alpha, \beta, \gamma)$ .

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#### Phase retrieval (Sun et al '18)

$$\min_{x\in\mathbb{C}^n}\frac{1}{2m}\sum_{i=1}^m(b_i^2-|a_i^*x|^2)^2.$$

• Manifold optimization problem  $(\mathbb{C}^n)$ .

• Under certain assumptions and for *m* large enough, the objective is  $\left(c, \frac{c}{n\log(m)}, \frac{c}{n\log(m)}\right)$ -strict saddle for some absolute constant c > 0.

# Our approach

#### Algorithm

- Newton trust-region (+manifold if needed).
- Assuming  $(\alpha, \beta, \gamma)$  are known, take different steps at every iteration.
- Promote Newton steps, especially for the third case (close to global minimum).

# Our approach

#### Algorithm

- Newton trust-region (+manifold if needed).
- $\bullet$  Assuming  $(\alpha,\beta,\gamma)$  are known, take different steps at every iteration.
- Promote Newton steps, especially for the third case (close to global minimum).

## Complexity (Goyens and R., '23)

The method reaches an  $(\epsilon, \epsilon_H)$ -point in

$$\mathcal{O}\left(\max\left\{\alpha^{-2},\beta^{-3}\right\}\right) + \log_2\log_2\left[\mathcal{O}\left(\max\{\epsilon^{-1},\epsilon_H^{-1}\}\right)\right]$$

- Dependencies in  $\epsilon/\epsilon_H$  are "log-log" thanks to Newton.
- Improves over existing results (O'Neill and Wright '23).
- Key: Dependencies in  $\alpha/\beta!$

#### Nonconvex optimization problems

- Tractable formulations ubiquitous in data science.
- Interest in fast algorithms (in a complexity sense).

#### Our approach

- Revisit popular frameworks in nonlinear optimization (Newton-CG);
- Get optimal complexity + good numerical performance.

### Going further

- Handle constraints/matrix variables using manifold optimization.
- Tailor the method to specific structures (strict saddle).

## References

- S. Burer and R. D. C. Monteiro, A nonlinear programming algorithm for solving semidefinite programs via low-rank factorization, Mathematical Programming, 2003.
- C. Cartis, N. I. M. Gould and Ph. L. Toint, Complexity bounds for second-order optimality in unconstrained optimization, Journal of Complexity, 2012.
- C. Cartis, N. I. M. Gould and Ph. L. Toint, Worst-case evaluation complexity and optimality of second-order methods for nonconvex smooth optimization, International Congress of Mathematicians (ICM), 2019.
- F. E. Curtis, D. P. Robinson and M. Samadi, A trust region Algorithm with a worst-case iteration complexity of O (e<sup>-3/2</sup>) for nonconvex optimization, Mathematical Programming, 2017.
- F. E. Curtis, D. P. Robinson, C. W. Royer and S. J. Wright. Trust-region Newton-CG with strong second-order complexity guarantees for nonconvex optimization, SIAM Journal on Optimization, 2021.
- A. Eftekhari, Training linear neural networks: Non-local convergence and complexity results, International Conference on Machine Learning, 2020.
- R. Ge, C. Jin and Y. Zheng, No spurious local minima in nonconvex low rank problems: A unified geometric analysis, International Conference on Machine Learning, 2017.
- R. Ge and T. Ma, On the optimization landscape of tensor decompositions, Advances in Neural Information Processing Systems, 2017.
- F. Goyens and C. W. Royer. Newton-type methods for strict saddle problems, in preparation, 2023.
- J. J. Moré and D. C. Sorensen, Computing a trust-region step, SIAM Journal on Scientific Computing, 1983.
- M. O'Neill and S. J. Wright. A line-search descent algorithm for strict saddle functions with complexity guarantees, Journal of Machine Learning Research, 2023.
- T. Steihaug. The conjugate gradient method and trust regions in large scale optimization, SIAM Journal on Numerical Analysis, 1983.
- J. Sun, Q. Qu and J. Wright. A geometric analysis of phase retrieval, Found. Comput. Math., 2018.

## References

- S. Burer and R. D. C. Monteiro, A nonlinear programming algorithm for solving semidefinite programs via low-rank factorization, Mathematical Programming, 2003.
- C. Cartis, N. I. M. Gould and Ph. L. Toint, Complexity bounds for second-order optimality in unconstrained optimization, Journal of Complexity, 2012.
- C. Cartis, N. I. M. Gould and Ph. L. Toint, Worst-case evaluation complexity and optimality of second-order methods for nonconvex smooth optimization, International Congress of Mathematicians (ICM), 2019.
- F. E. Curtis, D. P. Robinson and M. Samadi, A trust region Algorithm with a worst-case iteration complexity of O (e<sup>-3/2</sup>) for nonconvex optimization, Mathematical Programming, 2017.
- F. E. Curtis, D. P. Robinson, C. W. Royer and S. J. Wright. Trust-region Newton-CG with strong second-order complexity guarantees for nonconvex optimization, SIAM Journal on Optimization, 2021.
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- T. Steihaug. The conjugate gradient method and trust regions in large scale optimization, SIAM Journal on Numerical Analysis, 1983.
- J. Sun, Q. Qu and J. Wright. A geometric analysis of phase retrieval, Found. Comput. Math., 2018.

#### Thank you!

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