Dimension-Reduced Second-Order Steepest Descent Methods for Optimization

ISE SEMINAR SERIES, LEHIGH U

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Today's Talk

(1) Motivation and Literature Review

(2) The Algorithm and Preliminary Convergence Analyses

(3) Computational Experiments

(4) Steepest Descent Integrating First and Second Order Information



Motivation and Literature Review

Part (1)

Early Complexity Analyses for Nonconvex Optimization

min $f(x), x \in X$ in \mathbb{R}^n ,

• where f is nonconvex and twice-differentiable,

$$g_k = \nabla f(x_k), H_k = \nabla^2 f(x_k)$$

• Goal: find x_k such that:

 $\|\nabla f(x_k)\| \le \epsilon$ (primary, first-order condition)

- For the ball-constrained nonconvex QP: min $c^T x + 0.5 x T Q x$ s.t. $\| x \|_2 \le 1$ $O(loglog(\epsilon^{-1}))$; see Y (1989,93), Vavasis&Zippel (1990)
- For nonconvex QP with polyhedral constraints: $O(\epsilon^{-1})$; see Interior-Trust-Region method Y (1998), Vavasis (2001)

- $\lambda_{min}(H_k) \ge -\sqrt{\epsilon}$ (in active subspace, secondary, second-order condition)

Standard methods for general nonconvex optimization I

First-order Method (FOM): Gradient-Type Methods

- Assume f has L-Lipschitz cont. gradient
- Global convergence by, e.g., linear-search (LS)
- No guarantee for the second-order condition
- Worst-case complexity, $O(\epsilon^{-2})$; see the textbook by Nesterov (2004)
- Each iteration requires $O(n^2)$ operations

Standard methods for general nonconvex optimization II

Second-order Method (SOM): Hessian-Type Methods

- Assume f has M-Lipschitz cont. Hessian
- Global convergence by, e.g., linear-search (LS), Trust-region (TR), or **Cubic Regularization**
- Convergence to second-order points
- No better than $O(\epsilon^{-2})$, for traditional methods (steepest descent and Newton); according to Cartis et al. (2010).

Each iteration requires O(n³) operations

Analyses of SOM for general nonconvex optimization since 2000

Variants of SOM

- since 20??
- Cubic regularization, $O(\epsilon^{-3/2})$, see Nesterov and Polyak (2006), Cartis, Gould, and Toint (2011)
- A new trust-region framework, $O(e^{-3/2})$, Curtis, Robinson, and Samadi (2017) With "slight" modification, complexity of SOM reduces from $O(\epsilon^{-2})$ to $O(\epsilon^{-\frac{3}{2}})!$

• Trust-region with the fixed-radius strategy, $O(\epsilon^{-3/2})$, see the lecture notes by Y

Other complexity analyses for some structural nonconvex optimization

- Ge, Jiang, and Y (2011), $O(\epsilon^{-1}\log(1/\epsilon))$, for L_p minimization arisen from Comp. Sensing. • Bian, Chen, and Y (2015), $O(\epsilon^{-3/2})$, for certain non-Lipschitz and nonconvex
- optimization.
- Chen et al. (2014) shows strongly NP-hardness for $L_2 L_p$ minimization; but later Ge, He, and He (2017) proposes a method with complexity of $O(\log(\epsilon^{-1}))$ to find a local minimum
- Haeser, Liu, and Y (2019) uses the first-order and second-order interior point trust-region method achieving first-order ϵ -KKT points with complexity of $O(\epsilon^{-2})$ and $O(\epsilon^{-3/2})$, respectively.





Recent efforts for general nonconvex optimization

FOM Improvements:

- FOM with Hessian negative curvature (NC) detections, $O(\epsilon^{-7/4}\log(1/\epsilon))$
 - Carmon et al. (2018), with Hessian-vector product (HVP) and Lanczos
 - cost $O(\epsilon^{-1/4})$ for each negative curvature request
 - Also, Carmon et al. (2017), does not require HVP (only first-order condition)
- Agarwal et al. (2016), also $O(\epsilon^{-7/4})$, using accelerated methods for fast approximate matrix inversion

They are hybrid and/or randomized methods and seem difficult to be implemented

Our approach: Reduce dimension in SOM

Part (2)

The Algorithm and Preliminary Convergence Analyses

Motivation from multi-directional FOM

• Two-directional FOM, with d_k being the momentum direction $(x_k - x_{k-1})$

$$x_{k+1} = x_k - \alpha_k^1 \nabla f(x_k) + \alpha_k^2 d_k = x_k \cdot$$

- In SOM, a method typically minimizes a full dimensional quadratic Taylor expansion to obtain direction vector d_{k+1} . For example, one TR step solves for d_{k+1} from $\min_{d} (g_k)^T d + 0.5 d^T H_k d \quad s.t. ||d||_2 \le \Delta_k$ where Δ_k is the trust-region radius.
- DRSOM: Dimension Reduced Second-Order Method **Motivation: using few directions in SOM**

- $+d_{k+1}$
- where step-sizes are constructed; including CG, PT, AGD, Polyak, and many others.

DRSOMI

- The DRSOM in general uses m-independent directions $d(\alpha) := D_k \alpha$, $D_k \in \mathbb{R}^{nm}$, $\alpha \in \mathbb{R}^m$

min
$$m_k^{\alpha}(\alpha) \coloneqq (c_k)^T \alpha + \frac{1}{2} \alpha^T Q_k \alpha$$

 $||\alpha||_{G_k} \le \Delta_k$

$$G_k = D_k^T D_k, Q_k = D_k^T H_k D$$

How to choose D_k ? How great would *m* be?

• Plug the expression into the full-dimension TR quadratic minimization problem, we minimize a m-dimension trust-region subproblem to decide "m stepsizes":

 $D_k, C_k = (g_k)^T D_k$

DRSOM II

In following DRSOM adopts two FOM directions

$$d = -\alpha^1 \nabla f(x_k) + \alpha^2 d_k := d(\alpha)$$

where $g_k = \nabla f(x_k), H_k = \nabla^2 f(x^k), d_k$

• Then we minimize a 2-D trust-region problem to decide "two step-sizes":

$$\min \ m_k^{\alpha}(\alpha) \coloneqq f(x_k) + (c_k)^T \alpha + \frac{1}{2} \alpha^T Q_k \alpha$$
$$||\alpha||_{G_k} \le \Delta_k$$
$$G_k = \begin{bmatrix} g_k^T g_k & -g_k^T d_k \\ -g_k^T d_k & d_k^T d_k \end{bmatrix}, Q_k = \begin{bmatrix} g_k^T H_k g_k & -g_k^T H_k d_k \\ -g_k^T H_k d_k & d_k^T H_k d_k \end{bmatrix}, c_k = \begin{bmatrix} -||g_k||^2 \\ g_k^T d_k \end{bmatrix}$$

$$_{k} = x_{k} - x_{k-1}$$

DRSOM III

DRSOM can be seen as:

- "Adaptive" Accelerated Gradient Method (Polyak's momentum 60)
- A second-order method minimizing quadratic model in the reduced 2-D

 $m_k(d) = f(x_k) + \nabla f(x_k)^T d + \frac{1}{2} d^T \nabla^2 f(x_k) d, d \in \text{span}\{-g_k, d_k\}$

compare to, e.g., Dogleg method, 2-D Newton Trust-Region Method

 $d \in \text{span}\{g_k, [H(x_k)]^{-1}g_k\} \text{ (e.g., Powell 70)}$

- A conjugate direction method for convex optimization exploring the Krylov **Subspace** (e.g., Yuan&Stoer 95)
- For convex quadratic programming with no radius limit, terminates in n steps

Computing Hessian-Vector Product in DRSOM is the Key

In the DRSOM with two directions:

$$Q_k = \begin{bmatrix} g_k^T H_k g_k & -g_k^T H_k d_k \\ -g_k^T H_k d_k & d_k^T H_k d_k \end{bmatrix}, c_k = \begin{bmatrix} -||g_k|| \\ g_k^T d_k \end{bmatrix}$$

How to "cheaply" obtain Q? Compute $H_k g_k, H_k d_k$ first.

Finite difference:

$$H_k \cdot v \approx \frac{1}{\epsilon} [g(x_k + \epsilon \cdot v) - g_k],$$

- Analytic approach to fit modern automatic differentiation, $H_k g_k = \nabla(\frac{1}{2}g_k^T g_k), H_k d_k = \nabla(d_k^T g_k),$
- or use Hessian if readily available !



Subproblem adaptive strategies in DRSOM I

Recall 2-D quadratic model:

$$\min m_k^{\alpha}(\alpha) \coloneqq f(x_k) + (c_k)^T \alpha + \frac{1}{2} \alpha^T Q_k \alpha$$

$$||\alpha||_{G_k} \le \Delta_k, G_k = \begin{bmatrix} g_k^T g_k & -g_k^T d_k \\ -g_k^T d_k & d_k^T d_k \end{bmatrix}, Q_k = \begin{bmatrix} g_k^T H_k g_k & -g_k^T H_k d_k \\ -g_k^T H_k d_k & d_k^T H_k d_k \end{bmatrix}, c_k = \begin{bmatrix} -||g_k||^2 \\ g_k^T d_k \end{bmatrix}$$

Apply two strategies that ensure global and convergence

• Trust-region: Adaptive radius

 $\min_{\alpha} m_k^{\alpha}(\alpha), \| \alpha \|_{G_k} \le \Delta_k, G_k = \begin{bmatrix} g_k^T g_k & -g_k^T g_k$

Radius-free: Apply Lagrangian multiplier λ_k lacksquare

 $\min_{\alpha} m_k^{\alpha}(\alpha) + \lambda_k \|\alpha\|_{G_k}^2$

• The subproblems can be solved efficiently.

$$-g_k^T d_k \\ d_k^T d_k \end{bmatrix}$$

Subproblem adaptive strategies in DRSOM II

At each iteration k, the DRSOM proceeds:

- Solving 2-D Quadratic trust-region model
- Computing quality of the approximation*

$$p^{k} := \frac{f(x^{k}) - f(x^{k} + d^{k+1})}{m_{p}^{k}(0) - m_{p}^{k}(d^{k+1})} = \frac{f(x^{k}) - f(x^{k} + d^{k+1})}{m_{\alpha}^{k}(0) - m_{\alpha}^{k}(\alpha)}$$

- If ρ is too small, increase λ (Radius-Free) or decrease Δ (trust-region)
- Otherwise, decrease λ or increase Δ

* Can be further improved by other acceptance criteria, e.g., Curtis et al. 2017

 $\left(\frac{k+1}{k}\right)$

DRSOM: key assumptions and theoretical results (Zhang at al. SHUFE)

Assumption. (a) f has Lipschitz continuous Hessian. (b) DRSOM iterates with a fixedradius strategy: $\Delta_k = \epsilon/\beta$ (c) If the Lagrangian multiplier $\lambda_k < \sqrt{\epsilon}$, assume $\| (H_k - \tilde{H}_k) d_{k+1} \| \le C \| d_{k+1} \|^2$ (Cartis et al.), where \tilde{H}_k is the projected Hessian in the subspace (commonly adopted for approximate Hessian)

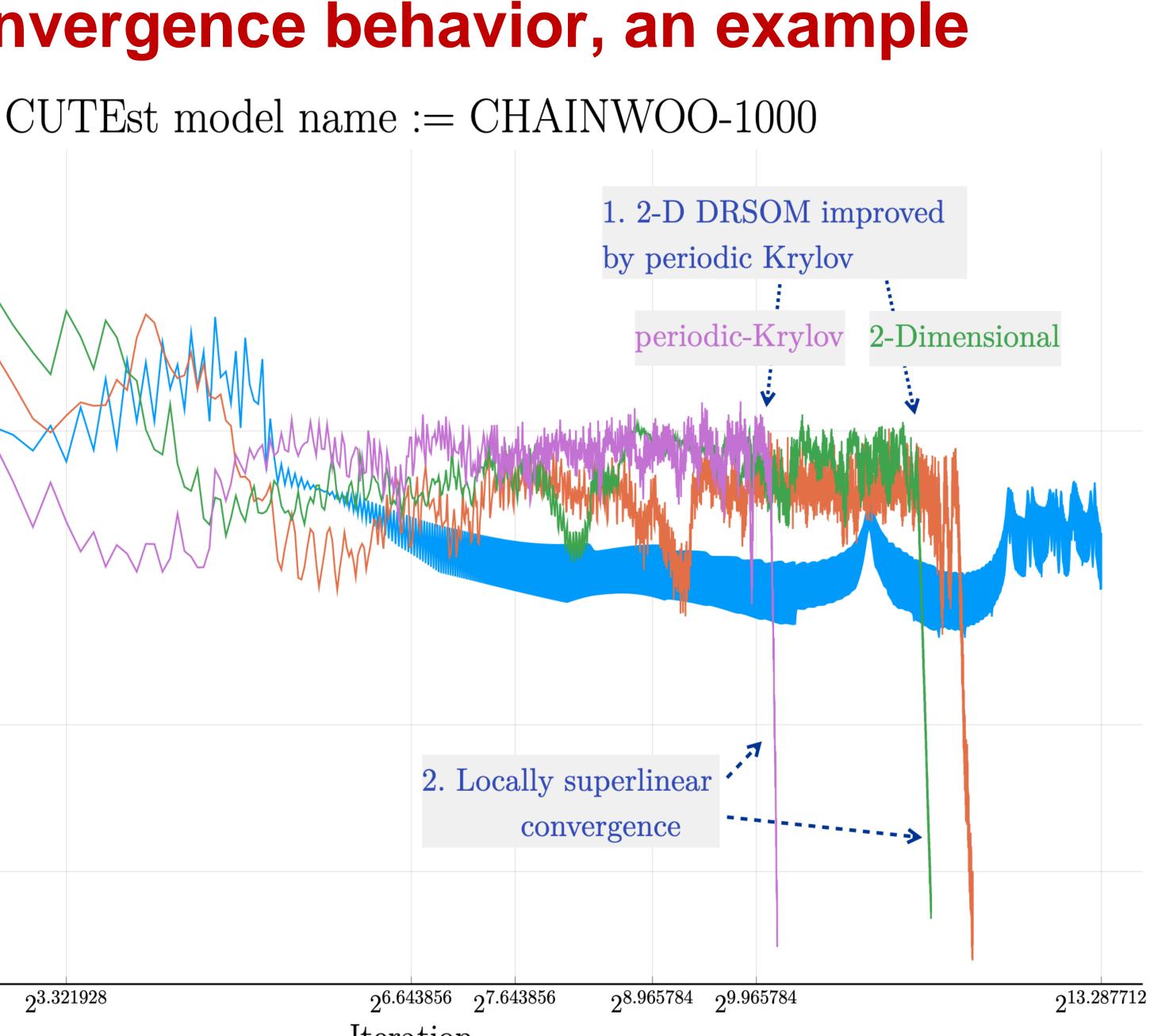
Theorem 1. If we apply DRSOM to QP, then the algorithms terminates in at most n steps to find a first-order stationary point

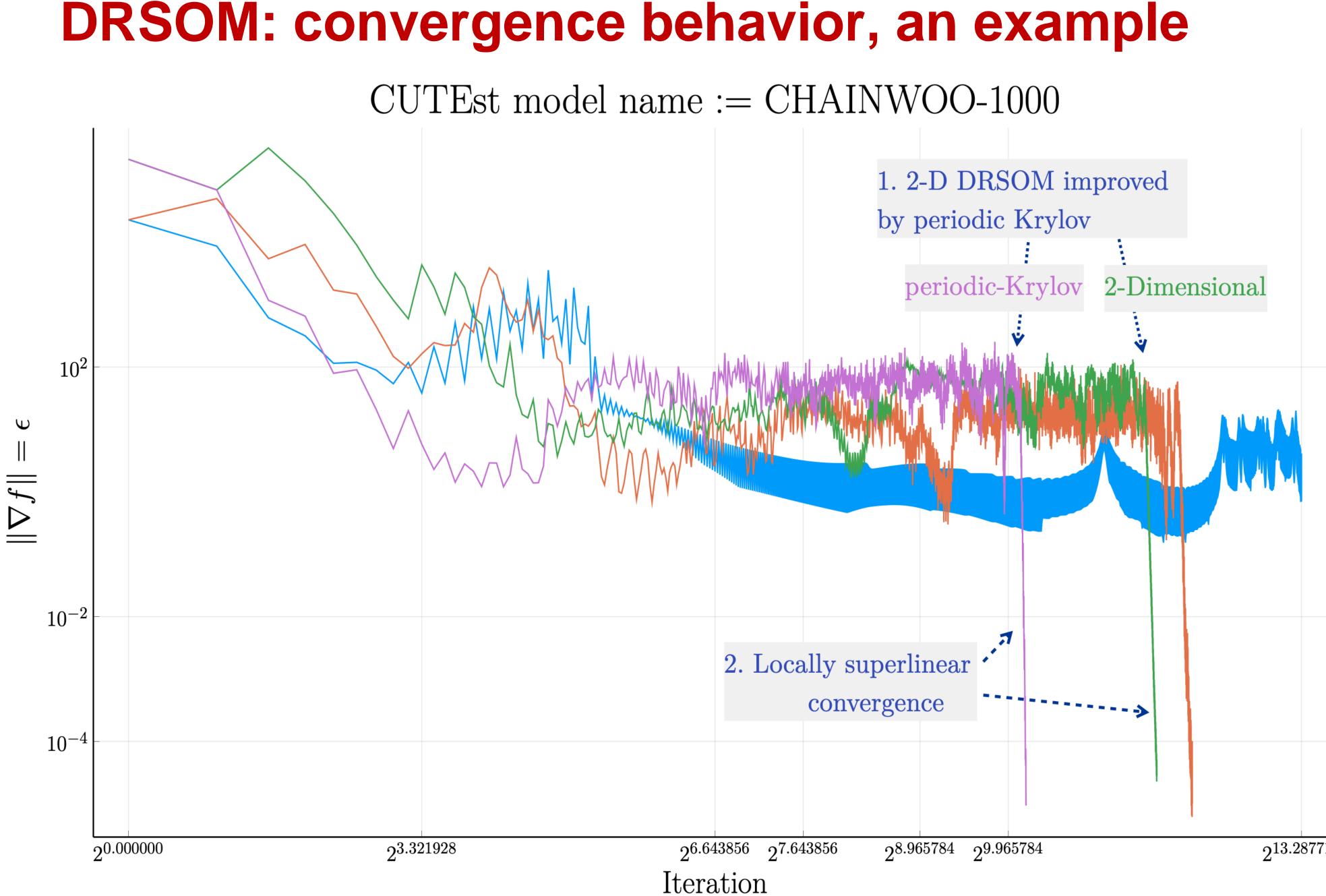
Theorem 2. (Global convergence rate) For f with second-order Lipschitz condition, DRSOM terminates in $O(e^{-3/2})$ iterations. Furthermore, the iterate x_k satisfies the firstgradient and momentum.

Theorem 3. (Local convergence rate) If the iterate x_k converges to a strict local optimum x^* such that $H(x^*) > 0$, and if **Assumption (c)** is satisfied as soon as $\lambda_k \leq C_{\lambda} \parallel d_{k+1} \parallel$, then DRSOM has a local superlinear (quadratic) speed of convergence, namely: $|| x_{k+1}$ $-x^* \parallel = O(\parallel x_k - x^* \parallel^2)$

- order condition, and the Hessian is positive semi-definite in the subspace spanned by the







GD+Wolfe LBFGS+Wolfe DRSOM-F(2-D)DRSOM-F(periodic-Krylov) **Example from the**

CUTEst dataset

• GD and LBFGS both

use a Line-search

(Hager-Zhang)

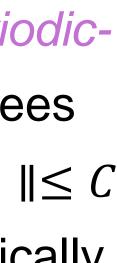
- *DRSOM-F (2-D)*: original 2-dimensional version with g_k and d_k
- DRSOM-F (periodic-*Krylov*), guarantees $\parallel (H_k - \widetilde{H}_k) d_{k+1} \parallel \leq C$ $|| d_{k+1} ||^2$ periodically.











Computational Experiments

Part (3)

Nonconvex L₂-L_p Minimization in Compressed Sensing

Consider nonconvex L2-Lp minimization, p < 1 $f(r) = ||Ar - b||_{2}^{2} \perp \lambda ||r||^{p}$

m	m	\sim	DRSOM		AGD		LBFGS			Newton TR			
11	116	k	$\ abla f\ $	time	k	$\ abla f\ $	time	k	$\ abla f\ $	time	k	$\ abla f\ $	time
100	10	28	5.8e-07	1.3e+00	58	8.5e-06	4.3e-01	21	8.9e-06	1.4e-01	10	7.1e-07	1.4e-02
100	20	47	6.0e-07	1.0e-03	150	8.2e-06	7.0e-03	35	6.2e-06	2.0e-03	9	4.9e-07	9.0e-03
p = 100	100	98	1.8e-06	1.1e-02	632	1.0e-05	4.6e-01	106	9.8e-06	7.3e-02	47	9.9e-07	$7.3e{+}00$
200	10	24	1.3e-06	1.0e-03	37	7.8e-06	1.0e-03	18	1.4e-06	1.0e-03	13	5.9e-10	4.0e-03
200	20	47	9.3 e-07	2.0e-03	115	9.4e-06	2.9e-02	33	6.2e-06	2.0e-03	17	6.7e-06	5.2e-02
200	100	107	4.3e-06	1.5e-02	814	9.9e-06	9.3e-01	85	6.2e-06	1.1e-01	36	1.1e-07	$7.6e{+}00$
1000	10	25	4.2e-06	3.0e-03	97	9.0e-06	3.6e-02	18	2.2e-06	5.0e-03	16	3.2e-07	5.4e-02
1000	20	27	5.8e-06	3.0e-03	68	7.6e-06	3.4e-02	27	4.5e-06	4.7e-02	13	7.8e-06	1.6e-01
1000	100	76	1.7e-05	2.6e-02	408	1.4e-05	$2.6e{+}00$	73	6.4e-06	6.1e-01	32	8.3e-07	$1.3e{+}01$
	n 100 100 100 200 200 200 1000 1000 1000	n m 100 10 100 20 100 20 200 10 200 20 200 100 1000 10 1000 20	$p = egin{array}{cccccc} n & m & k \ 100 & 10 & 28 \ 100 & 20 & 47 \ 100 & 100 & 98 \ 200 & 10 & 100 & 98 \ 200 & 10 & 24 \ 200 & 20 & 47 \ 200 & 100 & 107 \ 1000 & 100 & 107 \ 1000 & 10 & 25 \ 1000 & 20 & 27 \ \end{array}$	$p \begin{array}{c cccccccccc} n & m & & & & & & & & & & & & & & & & &$	$p \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$p \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$p \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$p \stackrel{n}{\longrightarrow} \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$

- DRSOM is comparable to full-dimensional SOM in iteration number
- DRSOM is much better in computation time !

Iterations needed to reach $\varepsilon = 10e-6$

Compare DRSOM to Accelerated Gradient Descend (AGD), LBFGS, and Newton Trust-region

Sensor Network Location (SNL)

Consider Sensor Network Location (SNL) lacksquare

 $N_x = \{(i, j) : \|x_i - x_j\| = d_{ij} \le r_d\}, N_a$

where r_d is a fixed parameter known as the

The SNL problem considers the following QCQP feasibility problem:

$$||x_i - x_j||^2 = d_{ij}^2, \forall (i, j) \in$$

 $||x_i - a_k||^2 = \bar{d}_{ik}^2, \forall (i, k) \in$

We can solve SNL by the nonconvex nonlinear least square (NLS) problem

$$\min_{X} \sum_{(i < j, j) \in N_x} (\|x_i - x_j\|^2 - d_{ij}^2)^2 + \sum_{(k, j) \in N_a} (\|a_k - x_j\|^2 - \bar{d}_{kj}^2)^2.$$



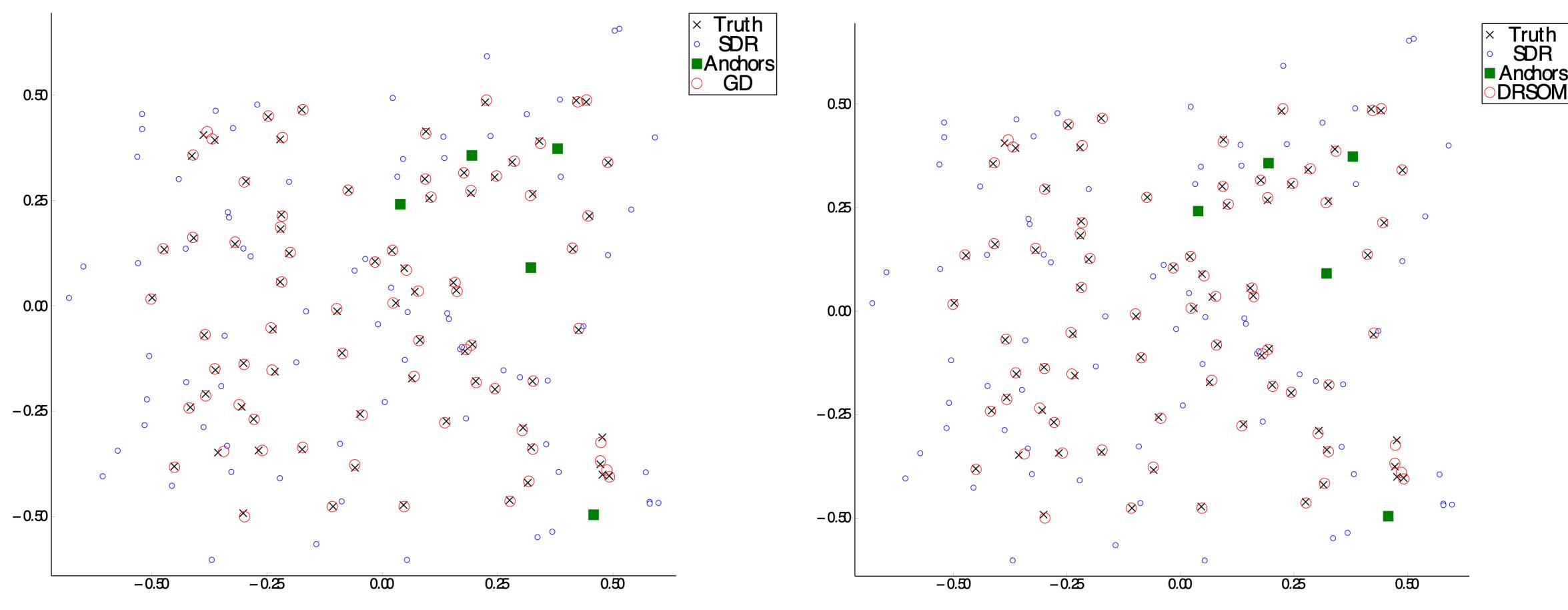
$$= \{(i,k): \|x_i - a_k\| = d_{ik} \leq r_d\}$$
radio range.

$$N_x$$

$$N_a$$

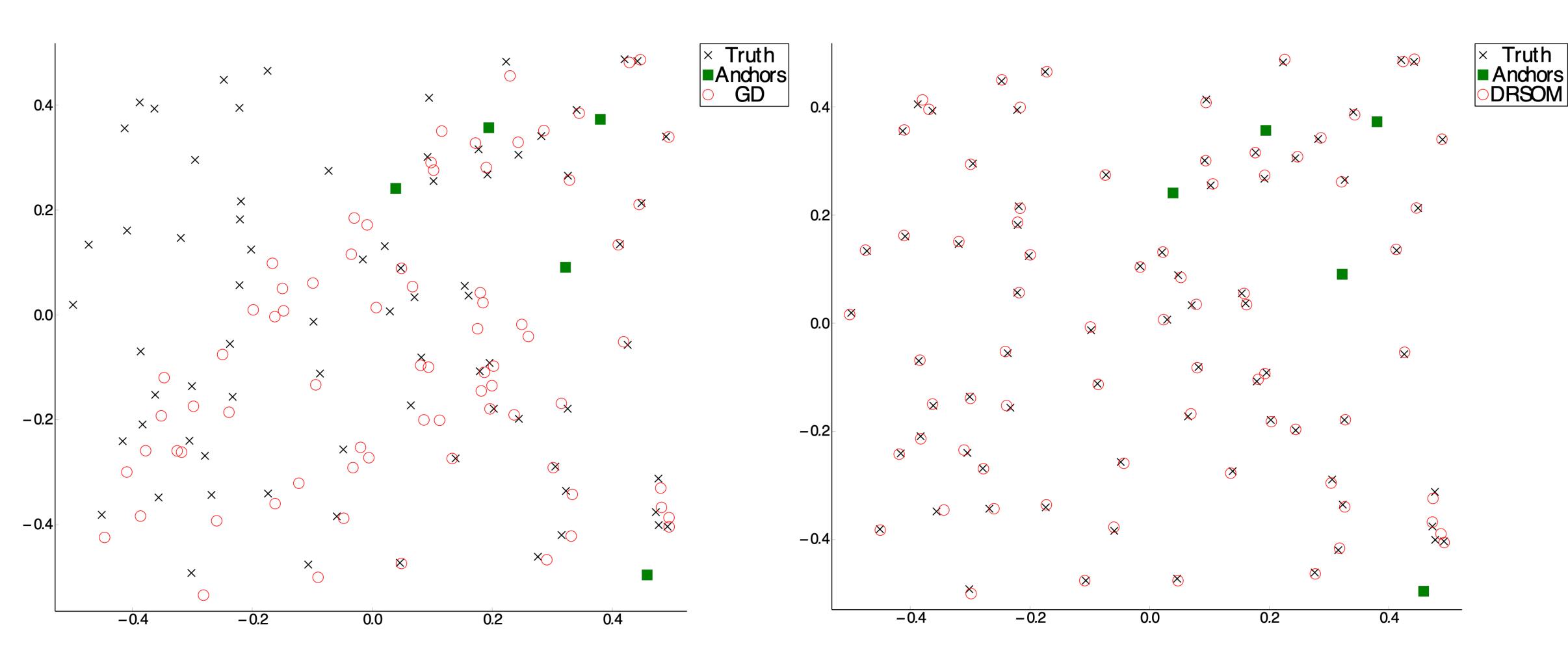
Sensor Network Location (SNL)

- Graphical results using SDP relaxation (Biswas et al. 2004) to initialize the NLS
- n = 80, m = 5 (anchors), radio range = 0.5, degree = 25, noise factor = 0.05
- Both Gradient Descent and DRSOM can find good solutions !



Sensor Network Location (SNL)

- Graphical results without SDP relaxation initialization
- DRSOM can still converge to optimal solutions





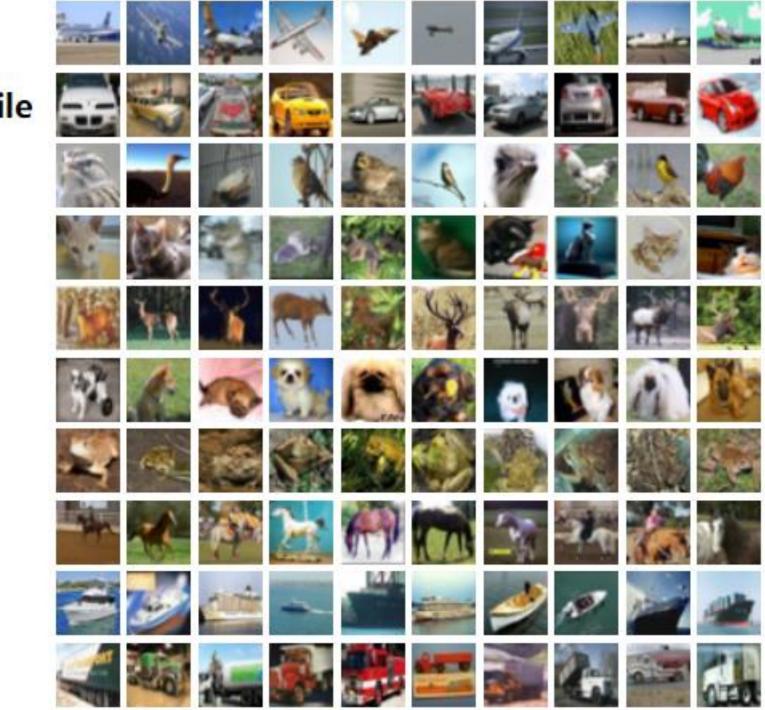


Neural Networks and Deep Learning

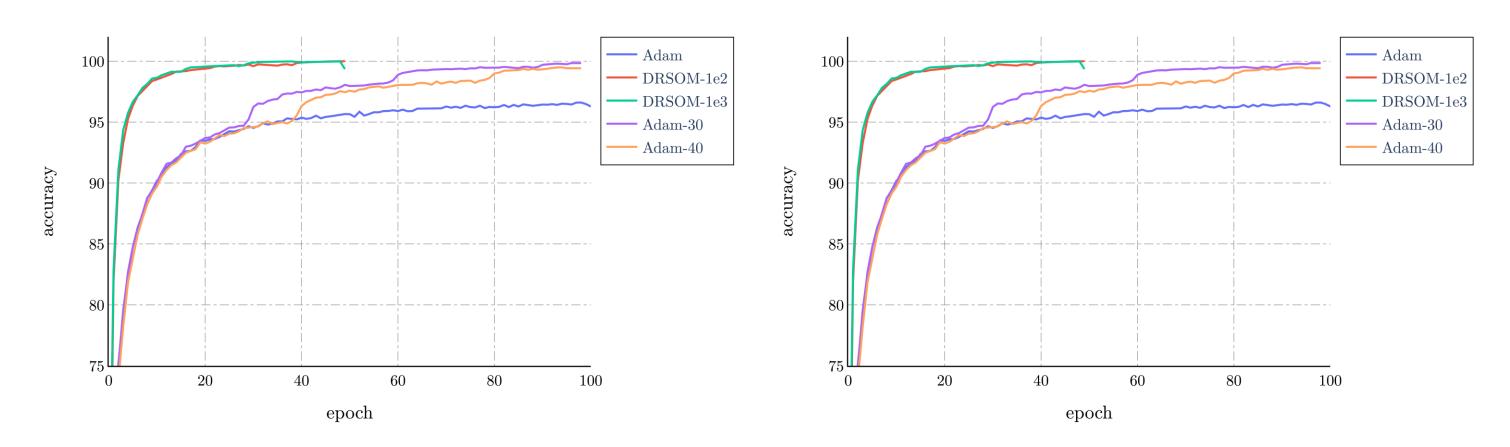
To use DRSOM in machine learning problems

- We apply the mini-batch strategy to a vanill
- Use Automatic Differentiation to compute g
- Train ResNet18 Model with CIFAR 10
- Set Adam with initial learning rate 1e-3

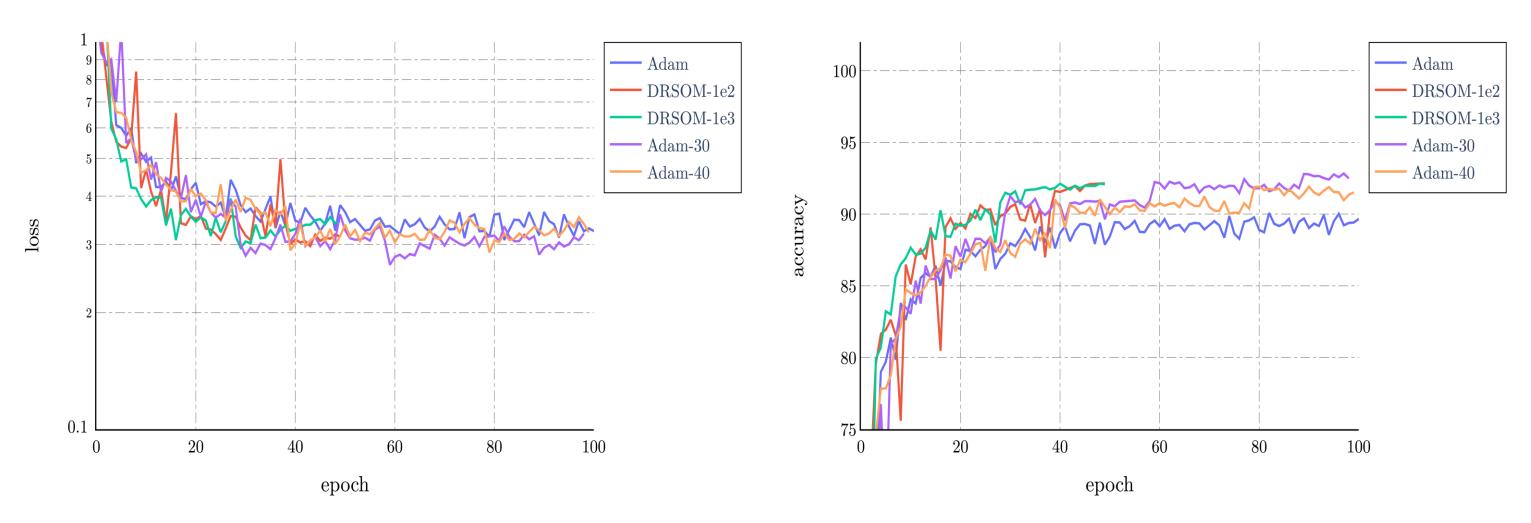
S	airplane			
	automobile			
lla DRSOM	bird			
	cat			
gradients	deer			
	dog			
	frog			
	horse			
	ship			
	truck			



Neural Networks and Deep Learning



Training results for ResNet18 with DRSOM and Adam



Test results for ResNet18 with DRSOM and Adam



Pros

- DRSOM has rapid convergence \bullet (30 epochs)
- DRSOM needs little tuning \bullet

Cons

- DRSOM may overfit the models
- Needs 4~5x time than Adam to run same number of epoch

Good potential to be a standard optimizer for deep learning!



DRSOM for Policy Gradient (PG) (Liu et al. SHUFE)

• As mentioned above, the goal is to maximize the expected discounted trajectory reward:

$$\max_{\theta \in \mathbb{R}^d} J(\theta) := \mathbb{E}_{\tau \sim p(\tau \mid \theta)} [\mathcal{R}(\tau)] = \int \mathcal{R}(\tau) p(\tau \mid \theta) d\tau$$

• The gradient can be estimated by:

$$\hat{\nabla} J(\theta) = \frac{1}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \nabla I(\theta)$$

• With the estimated gradient, we can apply DRSOM to get the step size α , and update the parameter by:

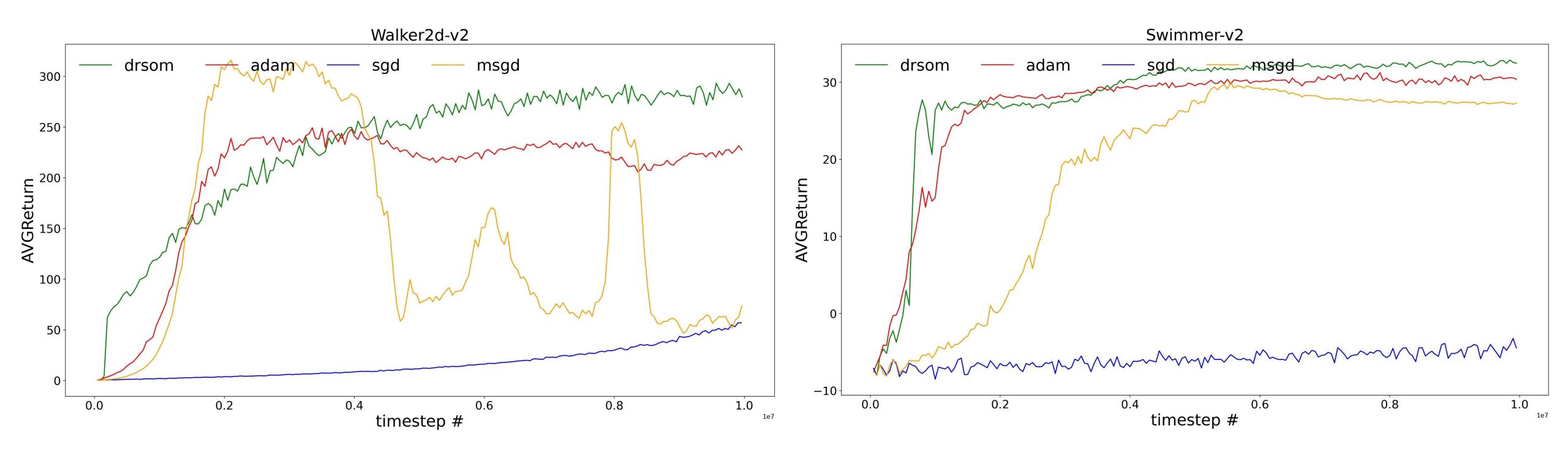
$$\theta_{t+1} = \theta_t + \alpha_t^1 \hat{\nabla} J(\theta_t) + \alpha_t^2 d_t$$

where d_t is the momentum direction.

$\log p\left(\tau_{i} \mid \theta\right) \mathcal{R}\left(\tau_{i}\right)$

DRSOM/ADAM/SGD Preliminary Results I

We compare the performance of DRSOM-based Reinforce with Adam-based reinforce and SGD-based reinforce(with(msgd) and without(sgd) momentum) on several GYM environments. We set the learning rate of Adam and SGD both as 1e-3, and momentum of MSGD as 0.99

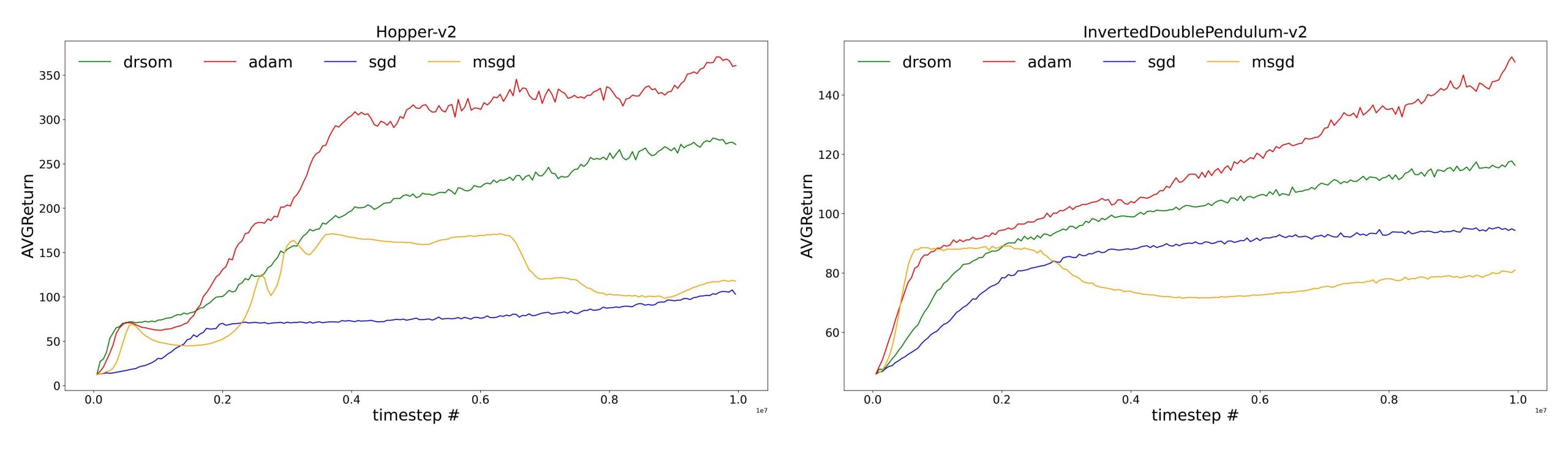


In these two cases, DRSOM converges faster and gain higher return than other algorithms. And also DRSOM seems to be more steady.





DRSOM/ADAM/SGD Preliminary Results II



In these two cases, DRSOM performs better than SGD but worse than ADAM.

DRSOM for TRPO I (Xue et al. SHUFE)

objective function while keep a KL divergence constraint

$$\max_{\theta} \quad L_{\theta_k}(\theta) \\ s.t. \quad \mathrm{KL}\left(\mathrm{Pr}_{\mu}^{\pi_{\theta_k}} \| \mathrm{Pr}_{\mu}^{\pi_{\theta}}\right) \leq \delta$$

$$\max_{\theta} \quad g_k^T (\theta - \theta_k) \\ \text{s.t.} \quad \frac{1}{2} (\theta - \theta_k)^T F_k (\theta - \theta_k) \leq \delta$$

where F_k is the Hessian of the KL divergence.

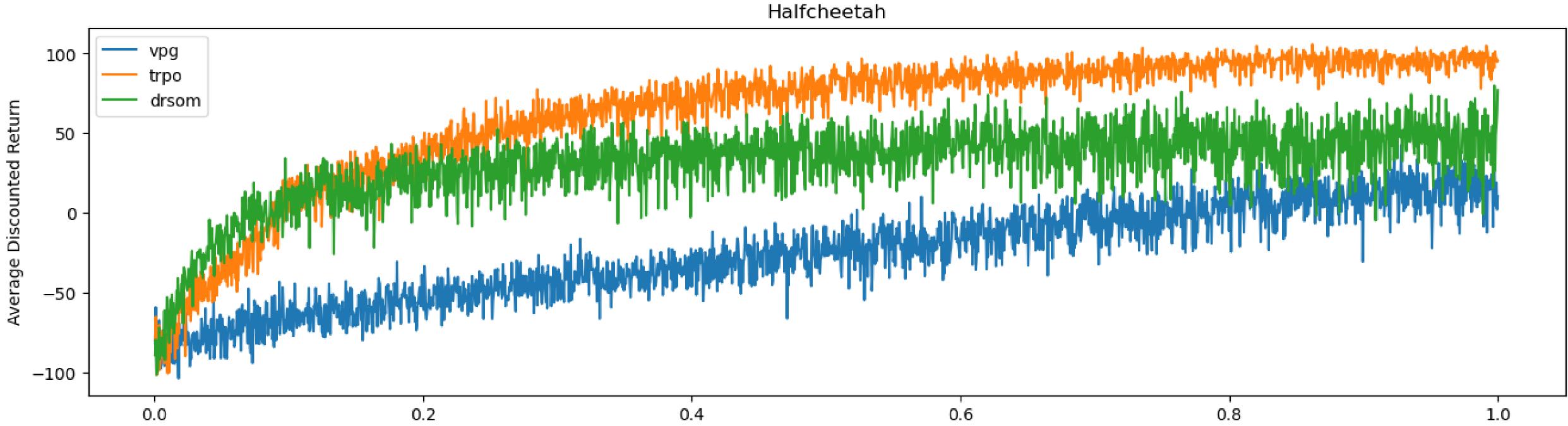
• **TRPO** attempts to optimize a surrogate function (based on the current iterate) of the

• In practice, it linearizes the surrogate function, quadratizes the KL constraint, and obtain



DRSOM/TRPO Preliminary Results I

algorithm works well in some RL environments



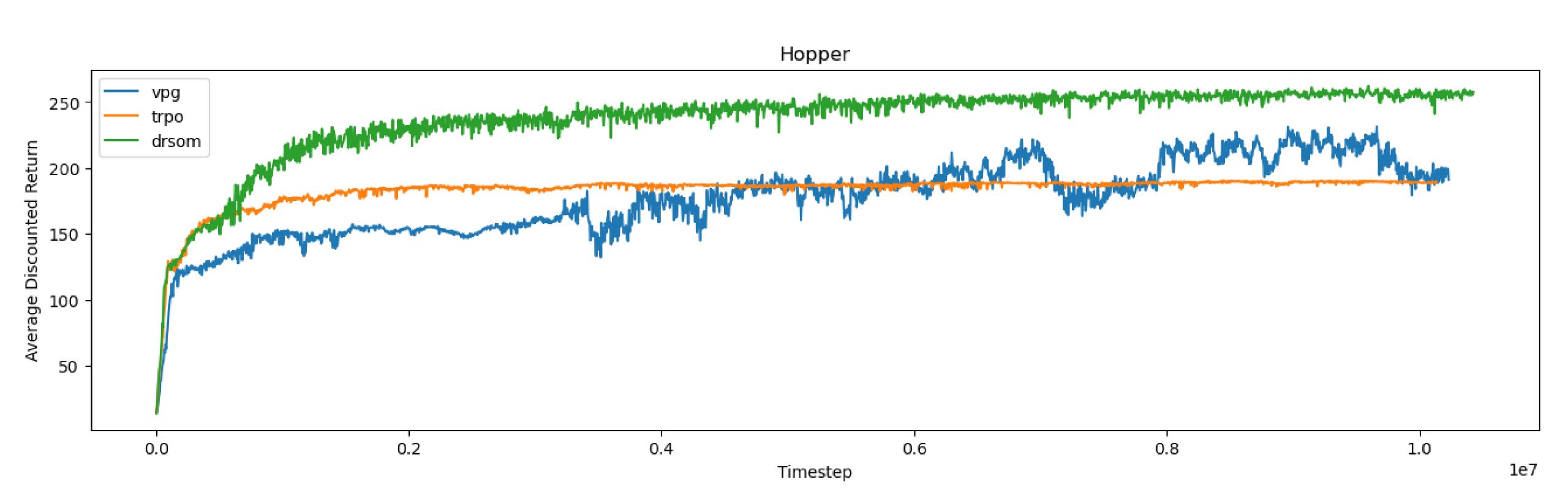
• Although we only maintain the linear approximation of the surrogate function, surprisingly the

Timestep

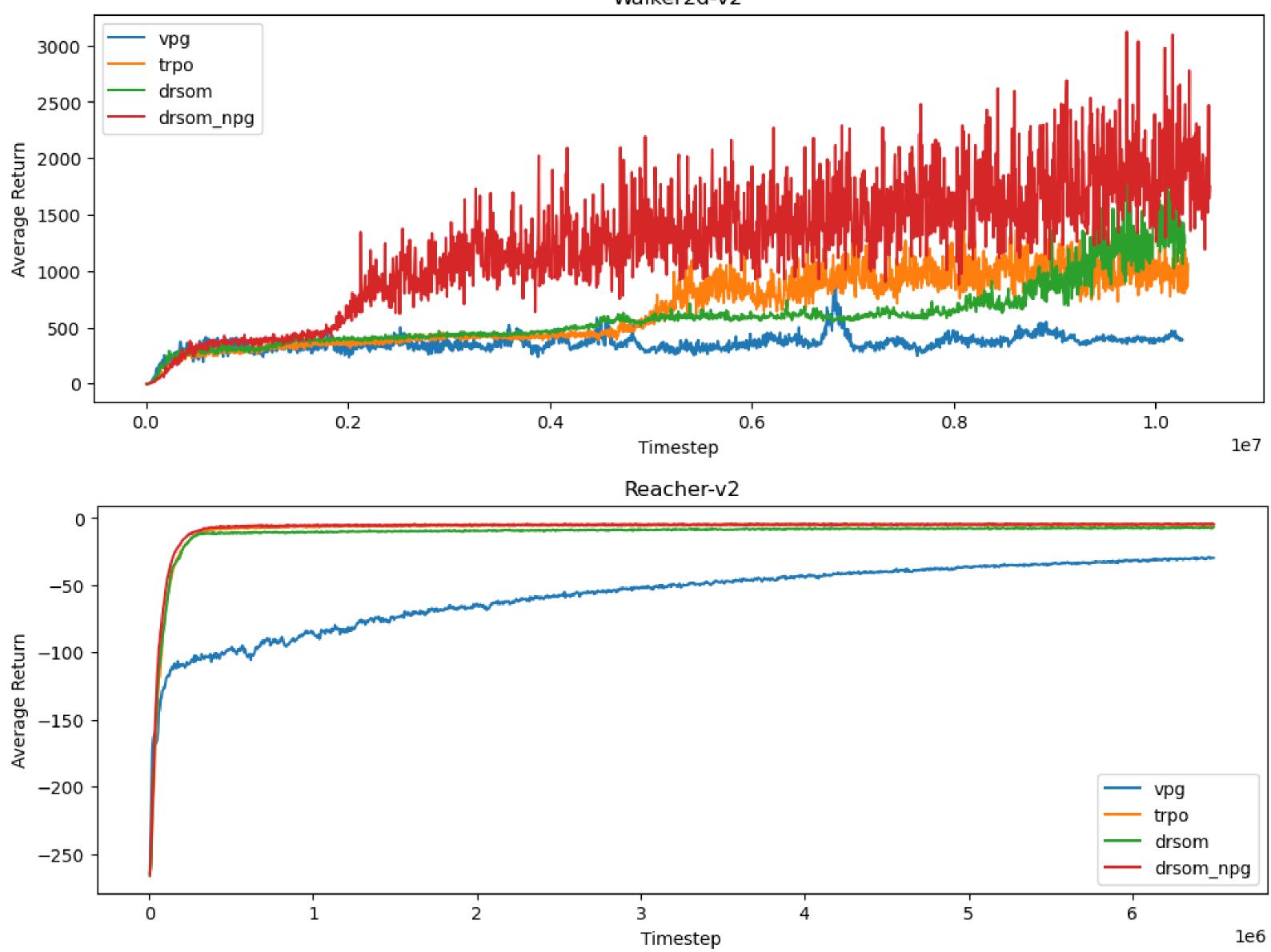


DRSOM/TRPO Preliminary Results II

• Sometimes even better than TRPO !

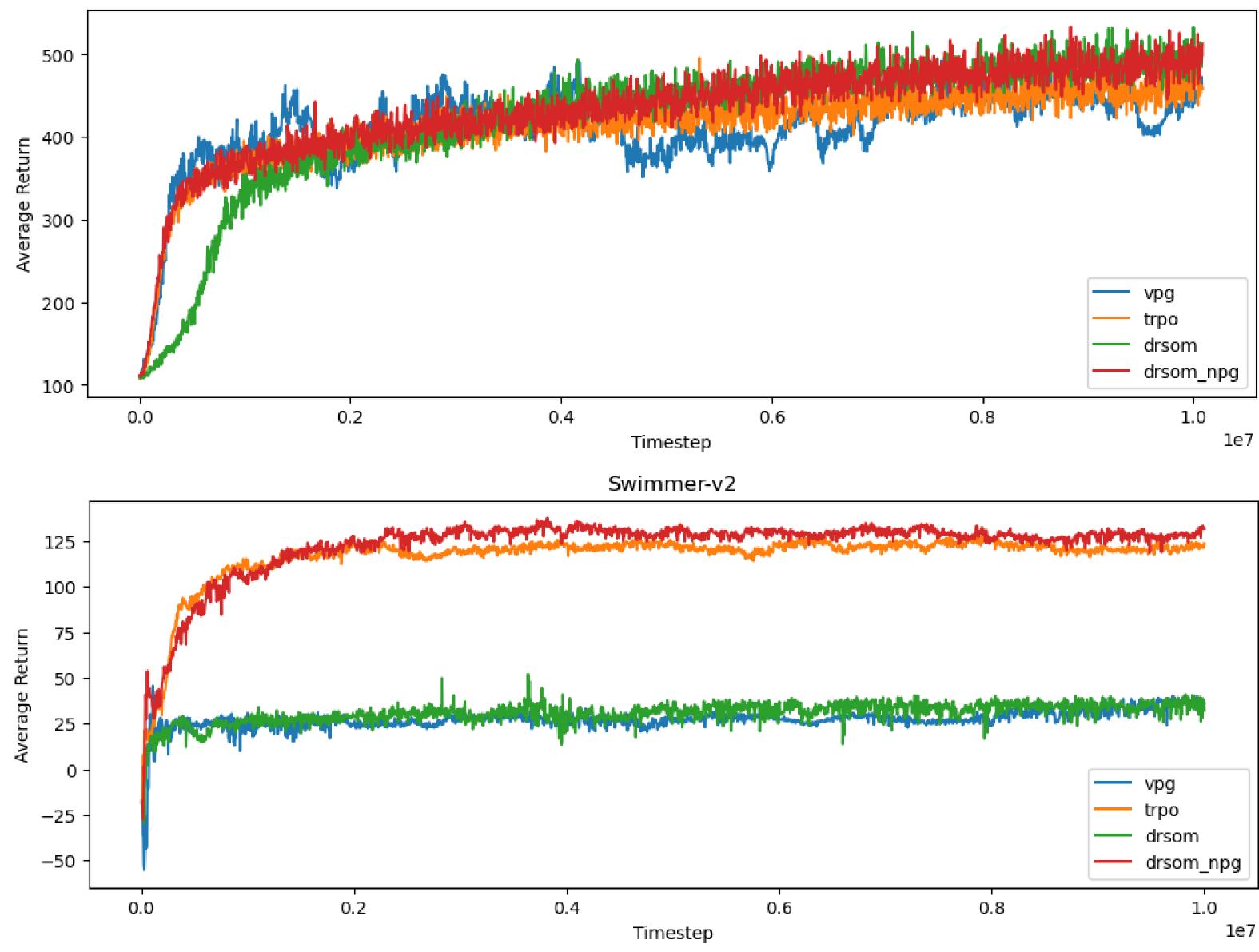


DRSOM/TRPO Preliminary Results III



Walker2d-v2

DRSOM/TRPO Preliminary Results IV



Humanoid-v2

DRSOM for Riemannian Optimization (Tang et al. NUS) $\min_{x\in\mathcal{M}} f(x)$ (ROP)

- \mathcal{M} is a Riemannian manifold embeded in Euclidean space \mathbb{R}^n .
- bounded in \mathcal{M} .

R-DRSOM: Ch for k Step $H_k d_k$

Step

(SOM: Choose an initial point
$$x_0 \in \mathcal{M}$$
, set $k = 0$, $p_{-1} = 0$;
 $= 0, 1, ..., T$ do
1. Compute $g_k = \operatorname{grad} f(x_k)$, $d_k = \operatorname{T}_{x_k \leftarrow x_{k-1}}(p_{k-1})$, $H_k g_k = \operatorname{Hess} f(x_k)[g_k]$ and
 $= \operatorname{Hess} f(x_k)[d_k]$;
2. Compute the vector $c_k = \begin{bmatrix} -\langle g_k, g_k \rangle_{x_k} \\ \langle g_k, d_k \rangle_{x_k} \end{bmatrix}$ and the following matrices
 $Q_k = \begin{bmatrix} \langle g_k, H_k g_k \rangle_{x_k} & \langle -d_k, H_k g_k \rangle_k \\ \langle -d_k, H_k g_k \rangle_{x_k} & \langle d_k, H_k d_k \rangle_{x_k} \end{bmatrix}$, $G_k := \begin{bmatrix} \langle g_k, g_k \rangle_{x_k} & -\langle d_k, g_k \rangle_{x_k} \\ -\langle d_k, g_k \rangle_{x_k} & \langle d_k, d_k \rangle_{x_k} \end{bmatrix}$.

Step 3. Solve the following 2 by 2 trust region subproblem with radius $\Delta_k > 0$

$$egin{aligned} lpha_k &:= rg \min_{\|lpha_k\|_{G_k} \leq riangle_k} f(x_k) + c_k^ op lpha + rac{1}{2} lpha^ op Q_k lpha; \ &ig(x_k - lpha_k^1 g_k + lpha_k^2 d_kig); \end{aligned}$$

Step 4. $x_{k+1} := \mathcal{R}_{x_k}$ end Return x_k .

• $f: \mathbb{R}^n \to \mathbb{R}$ is a second-order continuously differentiable function that is lower

Max-CUT SDP

Max-Cut: min
$$\{-\langle L, X \rangle : \operatorname{diag}(X) = e, X \in \mathbb{S}^n_+\}$$
.
min $\{-\langle L, RR^\top \rangle : \operatorname{diag}(RR^\top) = e, R \in \mathbb{R}^{n \times r}\}$.

g67	Fval	-30977.7	-30977.7	-30977.7	-30977.7	-30977.7
n=10000	Residue	1.3e-10	2.4e-10	9.7e-10	2.6e-10	8.3e-09
m=20000	Time [s]	131.0	1371.4	177.8	1114.4	356.9
g70	Fval	-39446.1	-39446.1	-39446.1	-39446.1	-39446.1
n=10000	Residue	2.2e-10	3.7e-12	1.6e-09	2.3e-10	3.4e-09
m=9999	Time [s]	36.2	288.4	63.5	250.8	100.7
g72	Fval	-31234.2	-31234.2	-31234.2	-31234.2	-31234.2
n=10000	Residue	8.2e-11	1.8e-12	5.8e-10	2.0e-10	1.1e-08
m=20000	Time [s]	110.4	881.2	191.9	907.5	359.2
g77	Fval	-44182.7	-44182.7	-44182.7	-44182.7	-44182.7
n=14000	Residue	7.8e-11	1.4e-10	7.1e-10	1.2e-10	1.0e-08
m=28000	Time [s]	268.3	1576.9	450.4	2402.6	603.8
g81	Fval	-62624.8	-62624.8	-62624.8	-62624.8	-62624.8
n=20000	Residue	4.6e-11	1.3e-10	1.4e-09	7.9e-11	2.0e-08
m=40000	Time [s]	650.1	4283.9	1219.0	6087.4	1062.1

1D-Kohn-Sham Equation

$$\min\left\{\frac{1}{2}\operatorname{tr}(R^{\top}LR)+\frac{\alpha}{4}\operatorname{diag}(RR^{\top})^{\top}L^{-1}\operatorname{diag}(RR^{\top}): R^{\top}R=I_{p}, R\in\mathbb{R}^{n\times r}\right\}, \quad (3)$$

where L is a tri-diagonal matrix with 2 on its diagonal and -1 on its subdiagonal and $\alpha > 0$ is a parameter. We terminate algorithms when $\|\operatorname{grad} f(R)\| < 10^{-4}$.

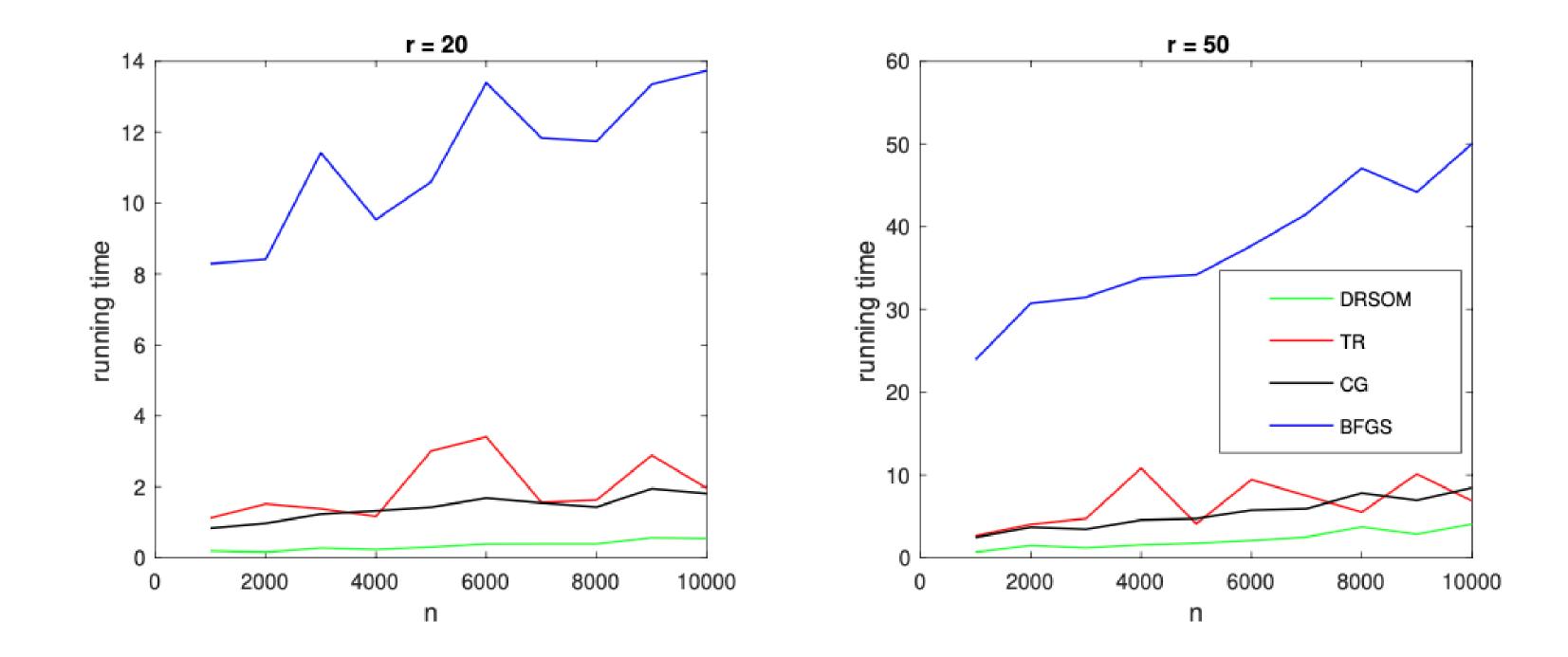


Figure 1: Results for Discretized 1D Kohn-Sham Equation. $\alpha = 1$.

DRSOM for LP Potential Reduction (Gao et al. SHUFE)

We consider a simplex-constrained QP model

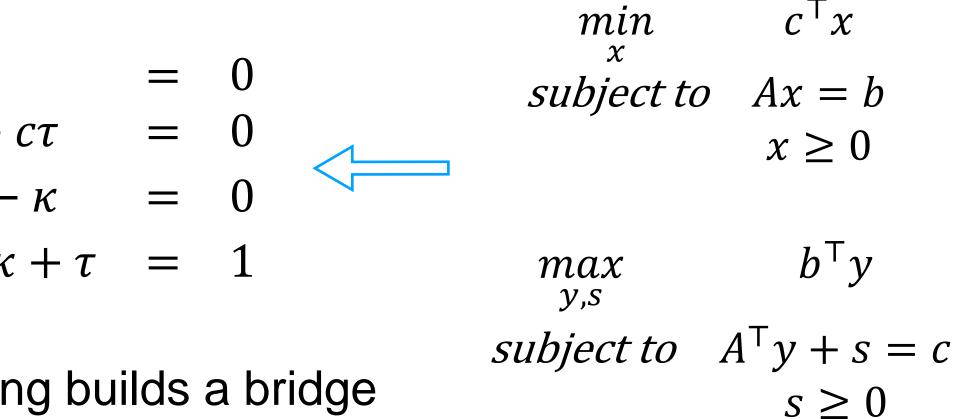
The self-dual embedding builds a bridge

•The here designentereu (an On Concerns) potential function and apply DRSOM to it

• How to solve much more general LPs?

Combined with scaled gradient(Hessian) projection, the method solves LPs

We wish to solve a standard LP (and its dual)



DR-Potential Reduction: Preliminary Results

One feature of the DR-Potential reduction is the use of negative curvature of

- $\nabla^2 \phi(x) = -\frac{\rho \nabla f(x)}{f(x)}$
- Computable using Lanczos iteration
- Getting LPs to high accuracy $10^{-6} \sim 10^{-8}$ if negative curvature is efficiently computed

Problem	PInfeas	DInfeas.	Compl.	Problem	PInfeas	DInfeas.	Compl.
ADLITTLE	1.347e-10	2.308e-10	2.960e-09	KB2	5.455e-11	6.417e-10	7.562e-11
AFIRO	7.641e-11	7.375e-11	3.130e-10	LOTFI	2.164e-09	4.155e-09	8.663e-08
AGG2	3.374e-08	4.859e-08	6.286e-07	MODSZK1	1.527e-06	5.415e-05	2.597e-04
AGG3	2.248e-05	1.151e-06	1.518e-05	RECIPELP	5.868e-08	6.300e-08	1.285e-07
BANDM	2.444e-09	4.886e-09	3.769e-08	SC105	7.315e-11	5.970e-11	2.435e-10
BEACONFD	5.765e-12	9.853e-12	1.022e-10	SC205	6.392e-11	5.710e-11	2.650e-10
BLEND	2.018e-10	3.729e-10	1.179e-09	SC50A	1.078e-05	6.098e-06	4.279e-05
BOEING2	1.144e-07	1.110e-08	2.307e-07	SC50B	4.647e-11	3.269e-11	1.747e-10
BORE3D	2.389e-08	5.013e-08	1.165e-07	SCAGR25	1.048e-07	5.298e-08	1.289e-06
BRANDY	2.702e-05	7.818e-06	1.849e-05	SCAGR7	1.087e-07	1.173e-08	2.601e-07
CAPRI	7.575e-05	4.488e-05	4.880e-05	SCFXM1	4.323e-06	5.244e-06	8.681e-06
E226	2.656e-06	4.742e-06	2.512e-05	SCORPION	1.674e-09	1.892e-09	1.737e-08
FINNIS	8.577e-07	8.367e-07	1.001e-05	SCTAP1	5.567e-07	8.430e-07	5.081e-06
FORPLAN	5.874e-07	2.084e-07	4.979e-06	SEBA	2.919e-11	5.729e-11	1.448e-10
GFRD-PNC	4.558e-05	1.052e-05	4.363e-05	SHARE1B	3.367e-07	1.339e-06	3.578e-06
GROW7	1.276e-04	4.906e-06	1.024e-04	SHARE2B	2.142e-04	2.014e-05	6.146e-05
ISRAEL	1.422e-06	1.336e-06	1.404e-05	STAIR	5.549e-04	8.566e-06	2.861e-05
STANDATA	5.645e-08	2.735e-07	5.130e-06	STANDGUB	2.934e-08	1.467e-07	2.753e-06
STOCFOR1	6.633e-09	9.701e-09	4.811e-08	VTP-BASE	1.349e-10	5.098e-11	2.342e-10
				•	•		

$$\frac{f(x)\nabla f(x)^{\top}}{f(x)^{2}} + \rho \frac{A^{\top}A}{f(x)} + X^{-2}$$

Now solving small and medium Netlib instances in 10 seconds

within 1000 iterations

In MATLAB and getting transferred into C for acceleration



Steepest Descent Integrating First and Second Order Information (Zhang et al. SHUFE)

Part (4)

A Descent Direction Using Homogenized Quadratic Model

Big Question: How to drop Assumption (c) in DRSOM analyses? \bullet Recall the classical trust-region method minimizes the quadratic model

$$\min_{d \in \mathbb{R}^n} m_k(d) := g_k^T d$$
$$s.t. \|d\|$$

• $-g_k$ is the first-order steepest descent direction but ignores Hessian; the direction of H_k negative curvature v meets Assumption (c) and also enables $O(\epsilon^{1.5})$ decrease if $R(H_k, v) = v^T H_k v / \|v\|^2 < -\sqrt{\epsilon},$

but such direction does not exist if it becomes nearly convex...

Could we construct a direction integrating both? \bullet Answer: Use the homogenized quadratic model!

$$d + \frac{1}{2} d^T H_k d$$
$$\| \leq \Delta_k.$$

A Descent Direction Using the Homogenized Quadratic Model

Using the homogenization trick by lifting with extra scalar t: \bullet

$$\psi_k\left(\xi_0,t\right) := \frac{1}{2} \begin{bmatrix} \xi_0 \\ t \end{bmatrix}^T \begin{bmatrix} H_k & g_k \\ g_k^T & 0 \end{bmatrix} \begin{bmatrix} \xi_0 \\ t \end{bmatrix} = \frac{t^2}{2} \begin{bmatrix} \xi_0/t \\ 1 \end{bmatrix}^T \begin{bmatrix} H_k & g_k \\ g_k^T & 0 \end{bmatrix} \begin{bmatrix} \xi_0/t \\ 1 \end{bmatrix}$$

- The homogeneous model is equivalent to m_k up to scaling: \bullet $\psi_k(\xi_0, t) = t^2 \cdot m_k(\xi_0/t)$
- Find a good direction $\xi = \xi_0/t$ (if t = 0 then set t=1) by the leftmost eigenvector:

$$\min_{\substack{|[\xi_0;t]| \le 1}} \psi_k(\xi_0,t)$$

Accessible at the cost of $O(\epsilon^{-1/4})$ v

 \bullet

via the randomized Lanczos method.

This is the Classical Homogenization Trick in QCQP via SDP

• For inhomogeneous QP (and QCQP):

$$\min x^{T}Q_{0}x - 2b_{0}^{T}x$$

s.t. $x^{T}Q_{i}x - 2b_{i}^{T}x + c_{i} \le 0, \quad i = 1, ..., m$

Used with SDP relaxation:

min
$$M_0 \bullet X$$

s.t. $M_i \bullet X \le 0$, $i = 1, ..., m$
 $X_{00} = 1, X \ge 0$

 Homogenized QCQP and SDP relaxation enables strong performance and theoretical analysis, and it guarantees a rank-one solution if m=1. * Rojas and Sorensen 2001

min
$$x^{T}Q_{0}x - 2b_{0}^{T}xt$$

s.t. $x^{T}Q_{i}x - 2b_{i}^{T}xt + c_{i}t^{2} \le 0$, $i = 1,...,$
 $t^{2} = 1$

$$M_i = \begin{bmatrix} c_i & b_i^T \\ b_i & Q_i \end{bmatrix}, X = \begin{bmatrix} 1 & x^T \\ x^T & X_0 \end{bmatrix}$$



The Homogenization Trick was Also Successful in LP

 $\min c^{\mathrm{T}}x$

- s.t. Ax + s = b $(x,s) \in \mathbb{R}^n \times \mathcal{K},$
- Homogenize to: lacksquare $\begin{bmatrix} r \\ s \\ \kappa \end{bmatrix} = \begin{bmatrix} 0 & A^{\mathrm{T}} \\ -A & 0 \\ -c^{\mathrm{T}} & -b^{\mathrm{T}} \end{bmatrix}$
- Introduced for solving linear programs and later widely used in general linear conic programs and MCPs (Andersen et al. 1999)

The homogeneous self-dual embedding (HSD) for the linear conic program:

$$\max - b^{\mathrm{T}}y$$

s.t.
$$-A^{\mathrm{T}}y + r = c$$

$$(r, y) \in \{0\}^n \times \mathscr{K}^*$$

$$\begin{bmatrix} T & c \\ b & b \\ b & T & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ \tau \end{bmatrix}$$

 $(x, s, r, y, \tau, \kappa) \in \mathbb{R}^n \times \mathscr{K} \times \{0\}^n \times \mathscr{K}^* \times \mathbb{R}_+ \times \mathbb{R}_+$

A Descent Direction Using the Homogenized Quadratic Model

Coming back to the homogenized quadratic model at x_k : \bullet

$$\psi_k\left(\xi_0,t\right) := \frac{1}{2} \begin{bmatrix} \xi_0 \\ t \end{bmatrix}^T \begin{bmatrix} H_k & g_k \\ g_k^T & 0 \end{bmatrix} \begin{bmatrix} \xi_0 \\ t \end{bmatrix} = \frac{t^2}{2} \begin{bmatrix} \xi_0/t \\ 1 \end{bmatrix}^T \begin{bmatrix} H_k & g_k \\ g_k^T & 0 \end{bmatrix} \begin{bmatrix} \xi_0/t \\ 1 \end{bmatrix}$$

- The "un-homogenized vector" $\xi = \xi_0/t$ can be found by the leftmost eigenvalue computation and scaling

eigenvalue of
$$\begin{bmatrix} H_k & g_k \\ g_k^T & 0 \end{bmatrix}$$
, then $\lambda_1 < 0$

• The motivates us to use ξ as a descent direction Alone or in DRSOM.

(if
$$t = 0$$
 then set $t=1$);

• Lemma 1 (strict negative curvature) : if $g_k \neq 0, H_k \neq 0$, let λ_1 be the leftmost

< 0.

Algorithm Frameworks Utilizing the Homogeneous Direction

- Compute the "homogeneous vector" $\xi = \xi_0/t$ at x_k **DRSOM + homogeneous direction**
- Use ξ in the subspace of DRSOM
- If we construct DRSOM subspace using $\{\xi, g_k\}$, then Assumption (c) holds SOSDM: A second-order steepest descent method – a single loop method
- Use ξ alone just like a "**steepest descent**" direction
- Line-search and rescaling can be used for practical adaptive implementation. Both frameworks will have first and second-order complexity guarantees:
- complexity of $O(\epsilon^{-3/2})$ in iterations
- complexity of $O(\epsilon^{-7/4})$ in function and gradient evaluations using the randomized

Lanczos method for eigenvector comput

tation in
$$O\left(\epsilon^{-1/4}\log(\frac{1}{\epsilon})\right)$$

Theoretical Guarantees of SOSDM

- Consider use Homogenized Direction only, and the length of each step $\|\eta\xi\|$ is fixed: $\|\eta\xi\| \leq \Delta_k = \frac{2\sqrt{\epsilon}}{M}$ where f(x) has L-Lipschitz gradient and M-Lipschitz Hessian.
- Previous Assumption (c): $\| (H_k \tilde{H}_k) d_{k+1} \| \le C \| d_{k+1} \|^2$ is not needed! • Theorem 1 (Global convergence rate) : if f(x) satisfies the Lipchitz Assumption and the iterate moves along homogeneous vector ξ : $x_{k+1} = x_k$ $+\eta_k \xi$, then, if we choose $\eta_k = \Delta_k / \|\xi\|$, and terminate at $\|\xi\| < \Delta_k$, then algorithm has $O(\epsilon^{-3/2})$ iteration complexity. Furthermore, x_{k+1} satisfies approximate first-order and second-order conditions.

Global Convergence Rate: Outline of Analysis

• A concise analysis using fixed radius Δ

Let $x_{k+1} = x_k + \eta \xi$, $R(H_k, \xi) = \xi^T H_k \xi / \|\xi\|^2$ • (sufficient decrease in large step) If $\|\xi\| \ge \Delta$, we choose $\eta = \Delta / \|\xi\|$ If $R(H_k,\xi) \leq -\sqrt{\epsilon}, f(x_{k+1}) - f(x_k) \leq -O(\epsilon^{1.5})$ i. ii. If $R(H_k,\xi) \ge +\sqrt{\epsilon}$, the same order reduction. which yields the same order reduction o (small step means convergence) Otherwise $\|\xi\| < \Delta$, then we choose step-size $\eta = 1$ and have $||g_{k+1}|| \leq \epsilon$ and $R(H_k, \xi) > -\sqrt{\epsilon}$

- iii. Otherwise we perturb the Hessian by $2\sqrt{\epsilon}$ and compute the eigenvector

Theoretical Guarantees of SOSDM (cont.)

- Theorem 2 (Local convergence rate): If the iterate x_k of SOSDM converges to a strict local optimum x^* such that $H(x^*) > 0$, then step-size $\eta_k = 1$ in the following iterations and SOSDM has a local superlinear (quadratic) speed of convergence, namely: $||x_{k+1} - x^*|| = O(||x_k - x^*||^2)$
- The local convergence property of SOSDM is very similar to classical trust-region method when the iterate becomes unconstrained Newton steps





Comparison Summary to Other Recent Algorithms Again

Second-order algorithms: $O(\epsilon^{-3/2})$ iteration complexity

- Satisfy first and second-order conditions
- Each iteration takes $O(n^3)$ to run a Lanczos-like algorithm
- Including: Ye 2005, Cartis et al., 2011; Curtis et al., 2017; Royer et al., 2018;

First-order hybrid algorithms: $O(\epsilon^{-\frac{7}{4}}\log(\frac{1}{\epsilon}))$ gradient and function evaluations*

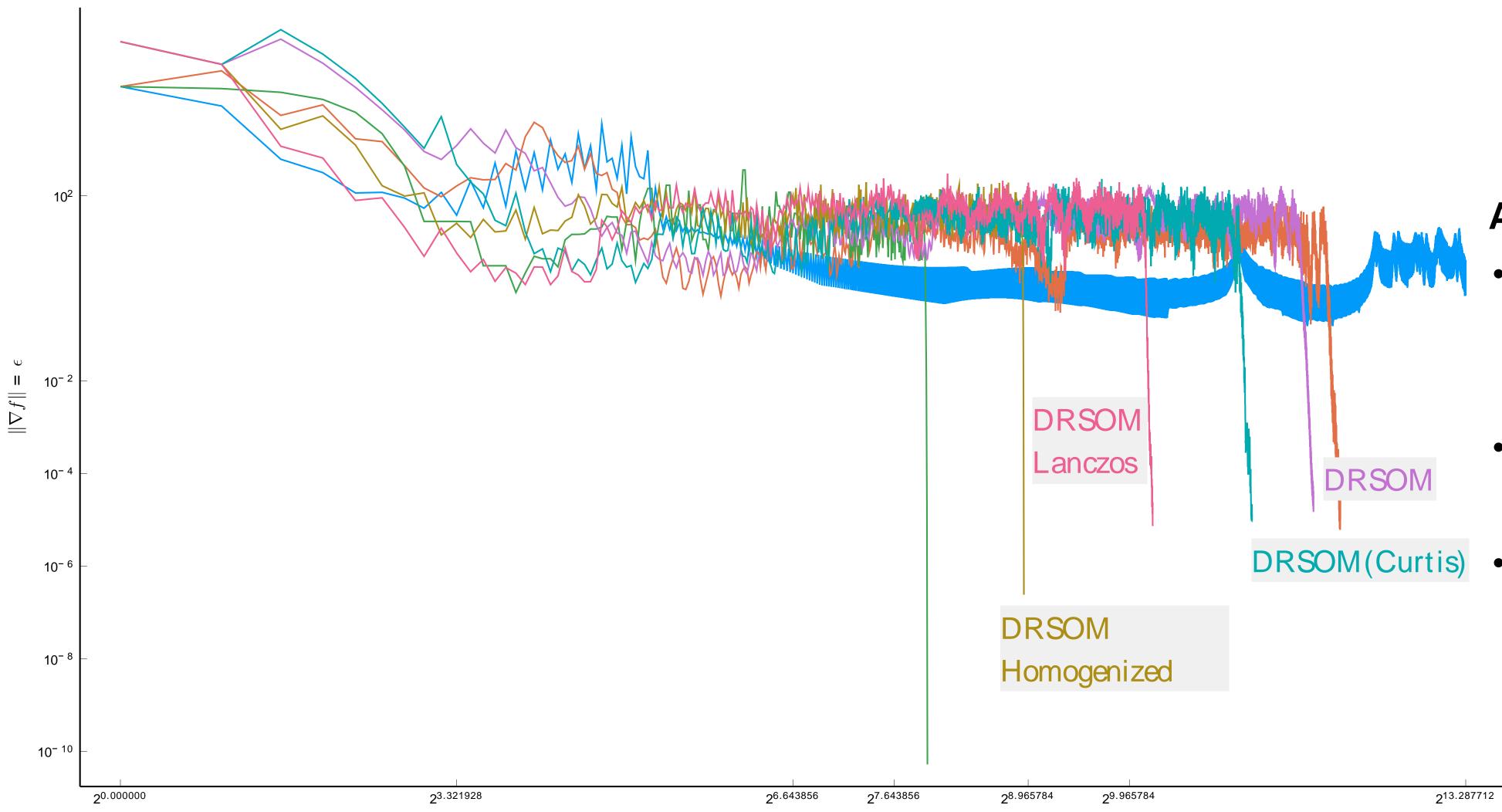
- Satisfy first-order conditions, some of them has second-order guarantees.
- Extra $O(\epsilon^{-\frac{1}{4}}\log(\frac{1}{\epsilon}))$ comes from eigenvector, perturbation, and so on.
- Including: Carmon et al., 2018; Agarwal et al., 2017; Carmon & Duchi, 2020; Jin et al., 2018.

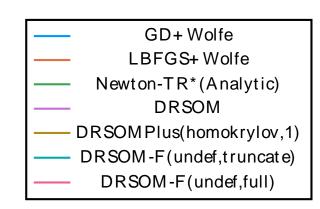
Our work: a single-looped (easy-to-implement) method with the same complexity as the hybrid ones but guarantee to first and second-order points

* Recently, Li and Lin (2022) drops the "log $\left(\frac{1}{\epsilon}\right)$ " term to satisfy first-order conditions, but not for second-order points.

Preliminary results: DRSOM + Homogenized Quadratic Model

CUTEst model name := CHAINWOO-1000





An example of CUTEst

• GD and LBFGS both use

a Line-search (Hager-Zhang)

• DRSOM, DRSOM(Curtis)

use 2-D subspace

DRSOM Homogenized is

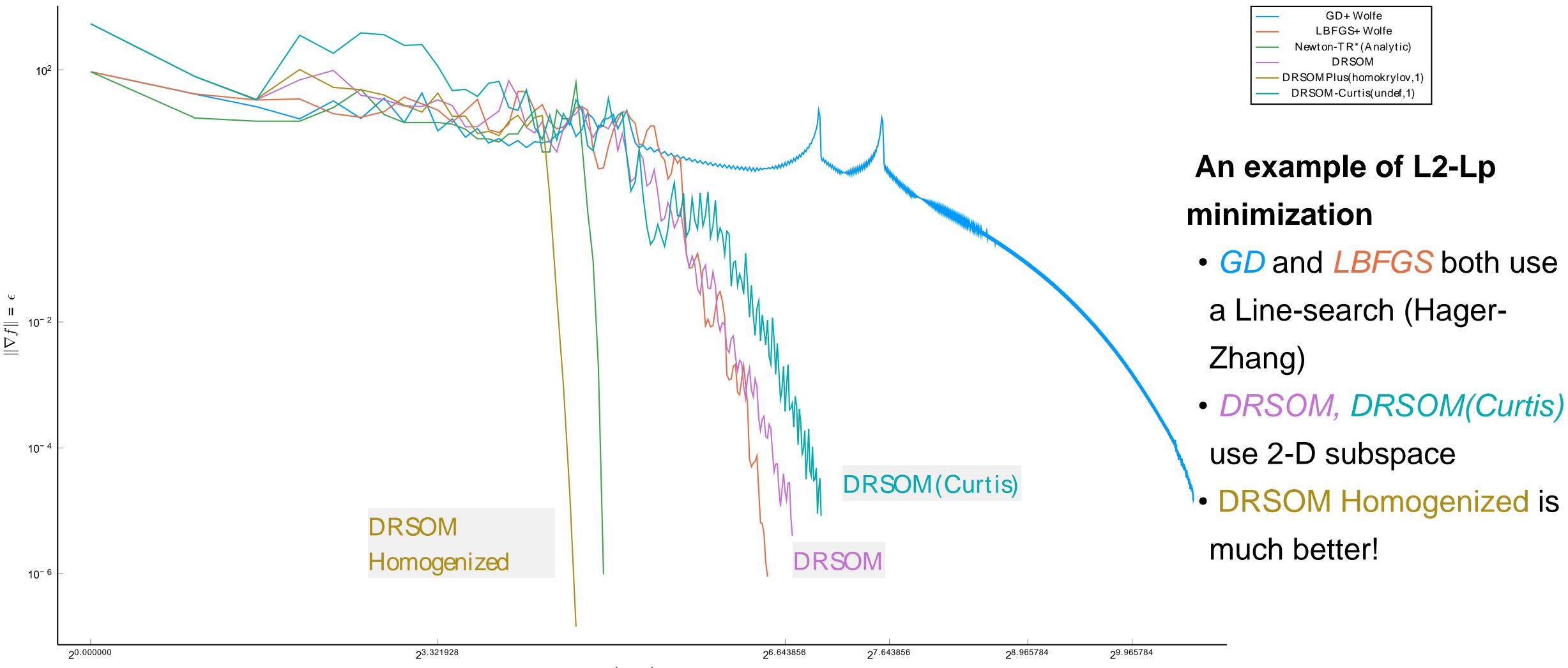
much better!





Preliminary results: DRSOM + Homogenized Quadratic Model

 $\frac{1}{2} ||Ax - b||^2 + ||x||_p^p, p = 0.5, A \in \mathbb{R}^{100 \times 50}, nnz = 0.5$



Iteration

Ongoing Research and Future Directions

- Are there other alternatives to remove Assumption c) in DRSOM analyses?
- Low-rank approximation of the homogenized matrix $\begin{vmatrix} H_k & g_k \\ a_{\nu}^T & \mathbf{0} \end{vmatrix}$ (+µ•I, that is, adding sufficiently large scalar µ so that it is positive definite if necessary) to make the leftmost eigenvector computing easier (Randomized rank reduction of a symmetric matrix to log(n), So et al. 08) and "Hot-Start" eigenvector computing by Power Methods (linear convergence of Liu et al. 2017)?
- Indefinite and Randomized Hessian rank-one updating via BFGS/SR1
- **Dimension Reduced Non-Smooth/Semi-Smooth Newton**
- Dimension Reduced Second-Order Methods for optimization with more complicated constraints

THANK YOU

