

SEGA: Variance Reduction via Gradient Sketching

Peter Richtárik

Joint work with Filip Hanzely (KAUST) and Konstantin Mishchenko (KAUST)



King Abdullah University
of Science and Technology



ICCOPT Summer School



SEGA: Variance Reduction via Gradient Sketching

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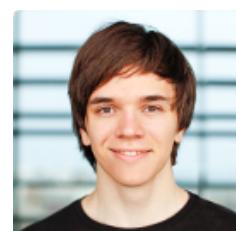
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Authors

- [Filip Hanzely](#)
- [Konstantin Mishchenko](#)
- [Peter Richtarik](#)

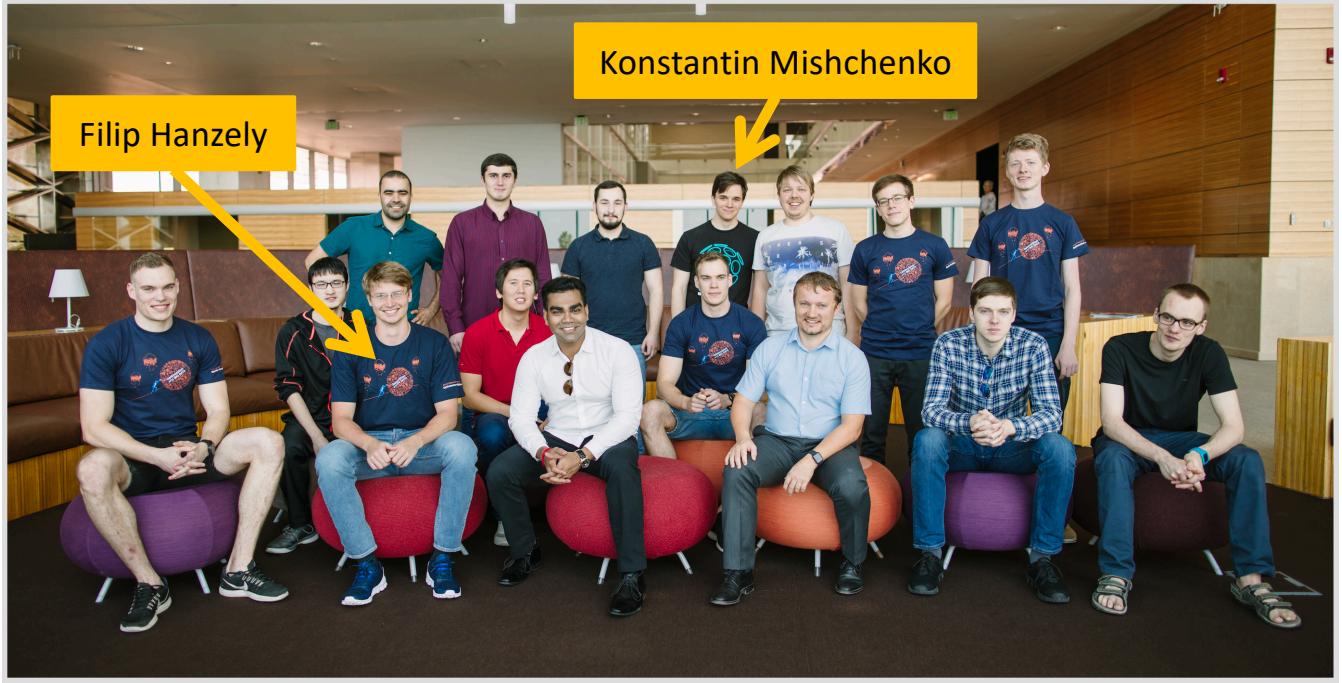


Filip Hanzely



Konstantin
Mishchenko

Optimization & Machine Learning Lab @ KAUST



SEGA: Variance Reduction via Gradient Sketching

Filip Hanzely¹ Konstantin Mishchenko¹ Peter Richtárik^{1,2,3}

¹KAUST ²University of Edinburgh ³Moscow Institute of Physics and Technology



Problem and Assumptions

Regularized Optimization

$$\min_{x \in \mathbb{R}^n} F(x) = f(x) + R(x) \quad (1)$$

- $f: \mathbf{M}$ smooth & μ -strongly convex/convex
- $f(x+h) \leq f(x) + (\nabla f(x), h) + \frac{L}{2}\|h\|^2$
- $f(x) + (\nabla f(x), h) + \frac{\mu}{2}\|h\|^2 \leq f(x+h)$ (natural assumptions for ERM with linear predictors)
- R non-smooth, convex & proximable

New Oracle: Gradient Sketch

We do not have direct access to $\nabla f(x)$. Instead, we have access to a random linear transformation of the gradient:

$$\mathbf{S}^\top \nabla f(x) \in \mathbb{R}^b, \quad \mathbf{S} \sim \mathcal{D} \quad (2)$$

- \mathbf{S} : random $n \times b$ matrix (b small)
- \mathcal{D} : distribution from which \mathbf{S} is drawn

Goal

Design a proximal stochastic gradient-type method for solving (1) using the gradient sketch oracle (2).

Simple Algorithmic Idea

$$x^{k+1} = \text{prox}_{\alpha R}(x^k - \alpha g^k), \quad (3)$$

α : stepsize; g^k is a “nice” estimator of $\nabla f(x^k)$.

How to design a good gradient estimator g^k ?

Key Challenges:

- In the case when \mathcal{D} is a distribution over standard basis vectors $e_1, \dots, e_n \in \mathbb{R}^n$, i.e., if we have access to random partial derivatives of f , then we can use

$$g^k = e_i^\top \nabla f(x^k) e_i,$$

and (3) reduces to proximal randomized coordinate descent (**CD**). However, **CD** does not work with non-separable regularizers R . So, we have an issue even in this simple case! How to resolve it?

- How to deal with gradient sketches coming from any distribution \mathcal{D} ?

Resolution: The **SEGA** estimator. We will iteratively learn an unbiased variance-reduced estimator g^k of the gradient $\nabla f(x^k)$ by incorporating the latest information provided by the gradient sketch.

Constructing the SEGA Estimator

SEGA Estimator

- Ask oracle for a gradient sketch at $x^k: \mathbf{S}_k^\top \nabla f(x^k)$
- Define h^{k+1} as the closest (in some norm) $\|h\|_B \leq h^k$ vector to h^k consistent with the gradient sketch:

$$h^{k+1} = \arg \min_{h \in \mathbb{R}^n} \|h - h^k\|_B^2 \quad \text{subject to } \mathbf{S}_k^\top h = \mathbf{S}_k^\top \nabla f(x^k) \quad (4)$$

Closed-form solution of (4):

$$h^{k+1} = h^k + \mathbf{B}^{-1} \mathbf{B}^\top (\nabla f(x^k) - h^k), \quad \mathbf{Z}_k \stackrel{\text{iid}}{\sim} \mathbf{S}_k (\mathbf{S}_k^\top \mathbf{S}_k)^{-1} \mathbf{S}_k^\top$$

- Define the **SEGA** estimator:

$$g^k = h^k + \theta_k \mathbf{B}^{-1} \mathbf{B}^\top (\nabla f(x^k) - h^k) \quad (5)$$

(θ_k is a random variable ensuring that g^k is unbiased)

Key property: As $x_k \rightarrow x^*$, we get $g^k \rightarrow 0$, and hence **SEGA** estimator is variance-reduced.

Variants:

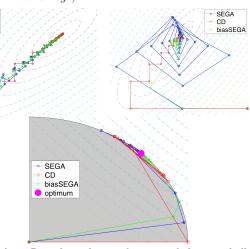
- **biasSEGA** estimator: use h^{k+1} instead of g^k
- **subspaceSEGA** estimator: If $f(x) = \phi(\mathbf{A}x)$ for some matrix $\phi \in \mathbb{R}^{d \times n}$, we can improve the **SEGA** estimator by exploiting the fact that ∇f lies in $\text{Range}(\mathbf{A}^\top)$. We do this by adding the constraint $h \in \text{Range}(\mathbf{A}^\top)$ to (4).

SEGA (SkEtched GrAdient descent)

- SEGA** = Method (3) + **SEGA** estimator (5)
biasSEGA = Method (3) + **biasSEGA** estimator (4)
subspaceSEGA = Method (3) + **subspaceSEGA** estimator

Iterates of SEGA (in 2D)

Iterates evolution of **SEGA**, **CD** and **biasSEGA** (updates made using h^{k+1} instead of g^k):



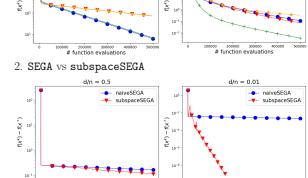
Bottom plot: R is the indicator function of the unit ball. While **CD** does not converge, **SEGA** does!

Experiments

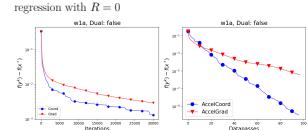
1. **SEGA** vs Random Direct Search (RDS) [2] (coordinate and Gaussian sketches) for derivative-free optimization



2. **SEGA** vs **subspaceSEGA**



3. **SEGA** vs Coordinate Descent (CD) [3] (left) and **ASEGA** [4, 5] (right) on ridge regression with $R = 0$



SEGA with Coordinate Sketches

Setup:

- S are column submatrices of the identity matrix
- Probability vector $p \in \mathbb{R}^n$; $p_i \stackrel{\text{def}}{=} \text{Prob}(e_i \in S)$
- Probability matrix $P \in \mathbb{R}^{n \times n}$; $P_{ij} \stackrel{\text{def}}{=} \text{Prob}(e_i \in S, e_j \in S)$
- ESO vector $v \in \mathbb{R}^n$ (for mini-batching) defined by:

$$P \bullet M \preceq \text{Diag}(p \bullet v)$$

Acceleration: For coordinate sketches we also designed an accelerated variant of **SEGA**:

Algorithm Accelerated SEGA (ASEGA)

```

1:  $x^0 = y^0 = z^0 \in \mathbb{R}^n$ ;  $h^0 \in \mathbb{R}^n$ ; params  $\alpha, \beta, \tau, \mu > 0$ 
2: for  $k = 1, 2, \dots$  do
3:    $z^k = (1 - \tau)y^{k-1} + \tau z^{k-1}$ 
4:   Sample  $\mathbf{S}_k \sim \mathcal{D}$ , and compute  $g^k$  and  $h^{k+1}$ 
5:    $y^k = x^k - \alpha p \bullet g^k$ 
6:    $z^k = \frac{1}{1 + \mu p} (z^k + \beta \mu x^k - \beta g^k)$ 
7: end for

```

Rates: We prove the following iteration complexity bounds of **SEGA** and **ASEGA** with coordinate sketches:

Method	Complexity
SEGA	$8.55 \cdot \frac{\text{Tr}(M)}{\mu} \log \frac{1}{\epsilon}$
importance sampling	$8.55 \cdot \left(\max_i \frac{p_i}{\mu p} \right) \log \frac{1}{\epsilon}$
SEGA	$8.55 \cdot \left(\max_i \frac{p_i}{\mu p} \right) \log \frac{1}{\epsilon}$
arbitrary sampling	$9.8 \cdot \frac{\sum \sqrt{M_i}}{\sqrt{\mu}} \log \frac{1}{\epsilon}$
ASEGA	$9.8 \cdot \sqrt{\max_i \frac{p_i}{\mu p}} \log \frac{1}{\epsilon}$
arbitrary sampling	$9.8 \cdot \sqrt{\max_i \frac{p_i}{\mu p}} \log \frac{1}{\epsilon}$

Up to the constant factors 8.55 and 9.5, these rates are exactly the same as the rates of coordinate descent [3] and accelerated coordinate descent [4, 5]. So, we extend the reach of coordinate descent methods to problem (1) with a non-separable regularizer (e.g., arbitrary convex constraint)

References

- [1] Filip Hanzely, Konstantin Mishchenko, and Peter Richtárik. SEGA: Variance reduction via gradient sketching. In *NewSPG 2018*.
- [2] El Houssine Bergou, Peter Richtárik, and Edouard Gorbunov. Stochastic three point method for minimizing nonconvex, convex and strongly convex functions. 2018.
- [3] Peter Richtárik and Martin Takáč. On optimal probabilities in stochastic coordinate descent methods. *Optimization Letters*, 10(6):1233–1243, 2016.
- [4] Zeyuan Allen-Zhu, Zheng Qu, Peter Richtárik, and Yang Yuan. Even faster accelerated coordinate descent using non-uniform sampling. In *ICML*, 2018.
- [5] Filip Hanzely and Peter Richtárik. Accelerated coordinate descent with arbitrary sampling and best rates for minibatches. *arXiv:1809.09354*, 2018.

Outline

1. Introduction
 - a) The problem
 - b) SEGA Oracle
 - c) A “Gutless” Method
2. SEGA Estimator
 - a) Sketch & Project
 - b) Correcting for Bias
 - c) Examples
3. SEGA Algorithm
 - a) Variants
 - b) Complexity
4. Experiments

1. Introduction

The Problem

Composite Minimization

Smoothness: $f(x + h) \leq f(x) + \langle \nabla f(x), h \rangle + \frac{1}{2} \langle \mathbf{L}h, h \rangle$

Strong convexity: $f(x) + \langle \nabla f(x), h \rangle + \frac{1}{2} \langle \mu \mathbf{I}h, h \rangle \leq f(x + h)$

$$\min_{x \in \mathbb{R}^n} F(x) := f(x) + R(x)$$

Dimension n :
very large

convex & closed
(and not necessarily separable)

New Stochastic First-Order Oracle

New Stochastic First Order Oracle

SkEtched GrAdient (SEGA) Oracle

Access to a random linear transformation (i.e., “sketch”) of the gradient:

$$\mathbf{S}^\top \nabla f(x)$$

$\mathbf{S} = [s_1, s_2, \dots, s_b] \in \mathbb{R}^{n \times b}$
 $\mathbf{S} \sim \mathcal{D}$

$$\mathbf{S}^\top \nabla f(x) = \begin{pmatrix} \langle \nabla f(x), s_1 \rangle \\ \langle \nabla f(x), s_2 \rangle \\ \vdots \\ \langle \nabla f(x), s_b \rangle \end{pmatrix} \in \mathbb{R}^b$$

Examples

1

Gaussian sketch

$$\mathbf{S} = \mathbf{s} \sim \mathcal{N}(0, \boldsymbol{\Omega})$$

$$\mathbf{S}^\top \nabla f(x) = \langle \nabla f(x), \mathbf{s} \rangle = \lim_{t \rightarrow 0} \frac{f(x + t\mathbf{s}) - f(x)}{t}$$

2

Coordinate sketch

$$\mathbf{S} = \mathbf{e}_i \text{ with probability } p_i > 0$$

$$\mathbf{S}^\top \nabla f(x) = \langle \nabla f(x), \mathbf{e}_i \rangle = (\nabla f(x))_i$$

A “Gutless” Method

Proximal Stochastic Gradient Descent

$$\text{prox}_{\alpha R}(z) \stackrel{\text{def}}{=} \arg \min_{x \in \mathbb{R}^n} \left(\alpha R(x) + \frac{1}{2} \|x - z\|^2 \right)$$

$$x^{k+1} = \text{prox}_{\alpha R}(x^k - \alpha g^k)$$

stepsize

“Good” estimator
of the gradient

Key question:

How to construct a “good” estimator
using the SkEtched GrAdient (SEGA)
oracle?

2. SEGA: The Estimator

What Do We Want?

What is a “Good” Estimator?

1. Implementable given the information provided by the gradient sketch oracle

2. Unbiased

$$\mathbb{E}_{\mathbf{S}_k \sim \mathcal{D}} [g^k \mid x^k] = \nabla f(x^k)$$

3. Diminishing variance

$$\mathbb{E} [\|g^k - \nabla f(x^k)\|^2] \rightarrow 0$$

Sketch & Project

Sketch & Project

New estimator of the gradient

Previous estimator of the gradient

$$h^{k+1} = \arg \min_{h \in \mathbb{R}^n} \|h - h^k\|^2$$

subject to $\mathbf{S}_k^\top h = \mathbf{S}_k^\top \nabla f(x^k)$

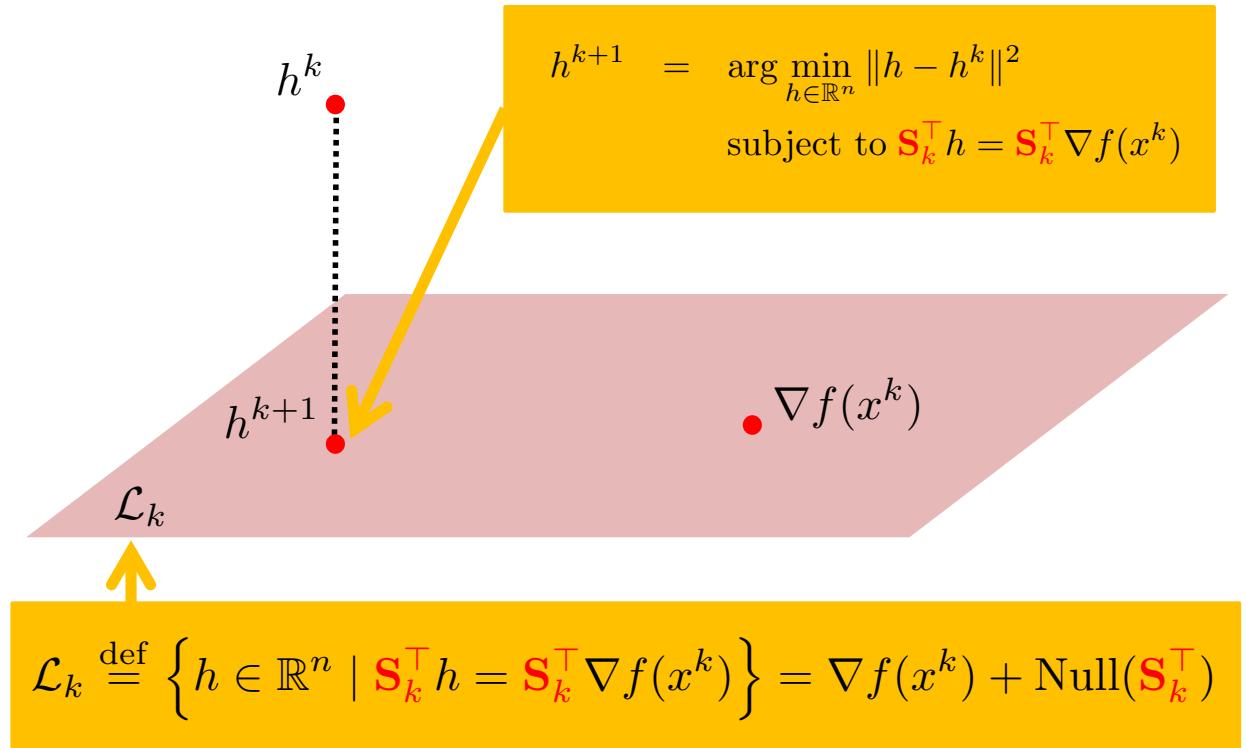
Closed-form solution:

$$h^{k+1} = h^k + \mathbf{Z}_k (\nabla f(x^k) - h^k)$$

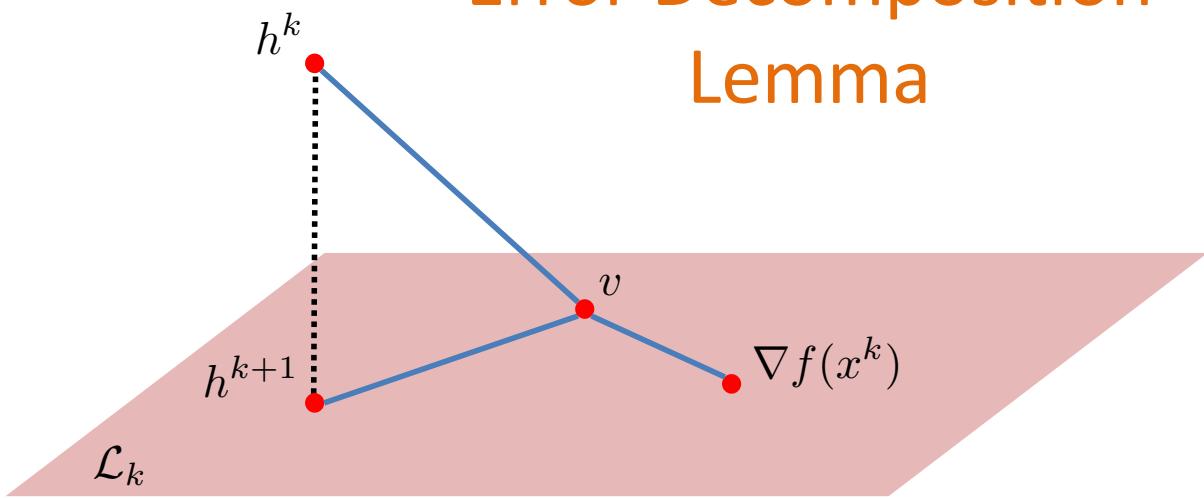
$$\mathbf{Z}_k \stackrel{\text{def}}{=} \mathbf{S}_k (\mathbf{S}_k^\top \mathbf{S}_k)^\dagger \mathbf{S}_k^\top$$

Sketched Gradient

Sketch & Project: Visualization



Error Decomposition Lemma



Lemma For any $v \in \mathbb{R}^n$

$$\mathbb{E}_{\mathcal{D}} [\|h^{k+1} - v\|_{\mathbf{I}}^2] = \|h^k - v\|_{\mathbf{I} - \mathbb{E}_{\mathcal{D}}[\mathbf{Z}]}^2 + \|\nabla f(x^k) - v\|_{\mathbb{E}_{\mathcal{D}}[\mathbf{Z}]}^2$$

Sketch and Project I

Original sketch and project



Robert Mansel Gower and P.R.
Randomized Iterative Methods for Linear Systems
SIAM J. Matrix Analysis and Applications 36(4):1660-1690, 2015

- 2017 IMA Fox Prize (2nd Prize) in Numerical Analysis
- Most downloaded SIMAX paper (2017)

Removal of full rank assumption + duality



Robert Mansel Gower and P.R.
Stochastic Dual Ascent for Solving Linear Systems
arXiv:1512.06890, 2015

Inverting matrices & connection to quasi-Newton updates



Robert Mansel Gower and P.R.
Randomized Quasi-Newton Methods are Linearly Convergent Matrix Inversion Algorithms
SIAM J. on Matrix Analysis and Applications 38(4), 1380-1409, 2017

New understanding
of Quasi-Newton
Rules

Computing the pseudoinverse



Robert Mansel Gower and P.R.
Linearly Convergent Randomized Iterative Methods for Computing the Pseudoinverse
arXiv:1612.06255, 2016

Application to machine learning



Robert Mansel Gower, Donald Goldfarb and P.R.
Stochastic Block BFGS: Squeezing More Curvature out of Data
ICML 2016

My course from
last week

Sketch and project revisited: stochastic reformulations of linear systems



P.R. and Martin Takáč
Stochastic Reformulations of Linear Systems: Algorithms and Convergence Theory
arXiv:1706.01108, 2017

Sketch and Project II

Linear convergence of the stochastic heavy ball method



Nicolas Loizou and P.R.
Momentum and Stochastic Momentum for Stochastic Gradient, Newton, Proximal Point and Subspace Descent Methods
arXiv:1712.09677, 2017

Stochastic projection methods for convex feasibility



Ion Necoara, Andrei Patrascu and P.R.
Randomized Projection Methods for Convex Feasibility Problems: Conditioning and Convergence Rates
arXiv:1801.04873, 2018

Extension to
Convex
Feasibility

Stochastic spectral & conjugate descent



Dmitry Kovalev, Eduard Gorbunov, Elnur Gasanov and P.R.
Stochastic Spectral and Conjugate Descent Methods
NeurIPS 2018

Accelerated stochastic matrix inversion



Robert Mansel Gower, Filip Hanzely, P.R. and Sebastian Stich
Accelerated Stochastic Matrix Inversion: General Theory and Speeding up BFGS Rules for Faster Second-Order Optimization
NeurIPS 2018

SAGD: a “strange” special case of JacSketch



Adel Bibi, Alibek Sailanbayev, Bernard Ghanem, Robert Mansel Gower and P.R.
Improving SAGA via a Probabilistic Interpolation with Gradient Descent
arXiv:1806.05633, 2018

Acceleration

Unbiasedness: SEGA for Coordinate Sketches

$n = 2$
2D Example

$$\mathbf{S} = \begin{cases} e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \text{with probability } p_1 \in (0, 1) \\ e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} & \text{with probability } p_2 = 1 - p_1 \end{cases}$$

$$\mathbf{S}_k = e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \implies \mathcal{L}_k = \{h \in \mathbb{R}^2 \mid h_1 = (\nabla f(x^k))_1\}$$

$$\mathbf{S}_k = e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \implies \mathcal{L}_k = \{h \in \mathbb{R}^2 \mid h_2 = (\nabla f(x^k))_2\}$$

Case 1

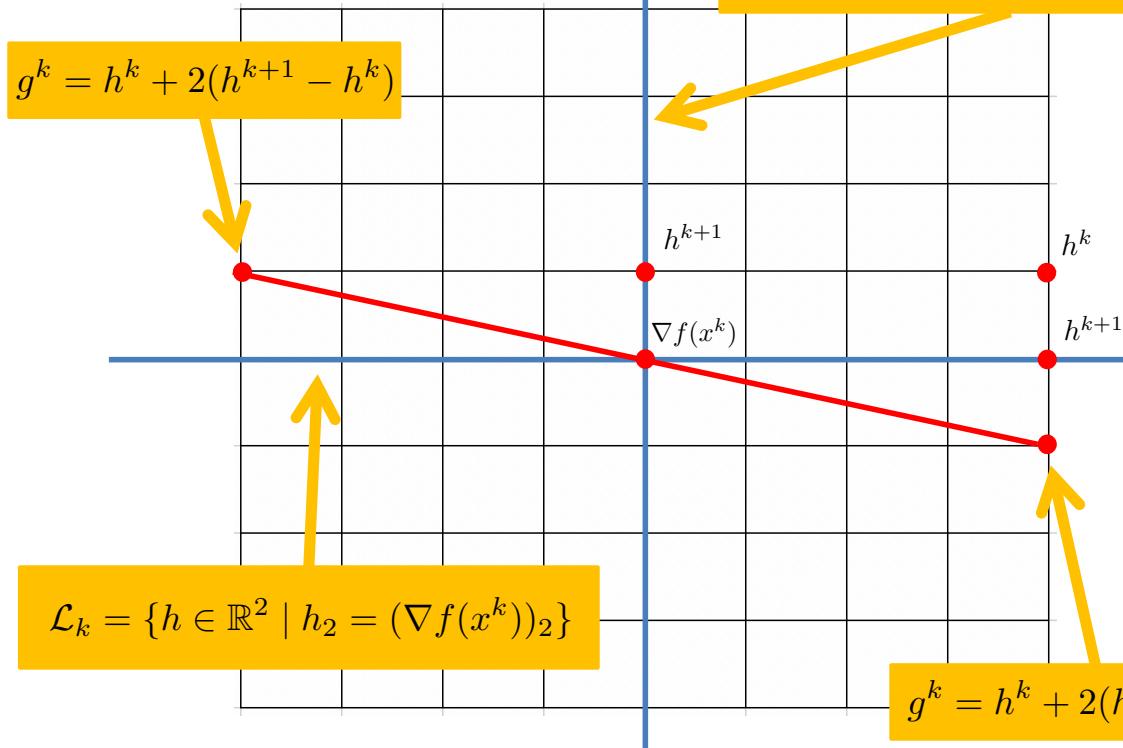
$$p_1 = \frac{1}{2} \quad p_2 = \frac{1}{2}$$

SEGA Estimator

$n = 2$

$$p_1 = \frac{1}{2} \quad p_2 = \frac{1}{2}$$

$$\mathcal{L}_k = \{h \in \mathbb{R}^2 \mid h_1 = (\nabla f(x^k))_1\}$$



Case 2

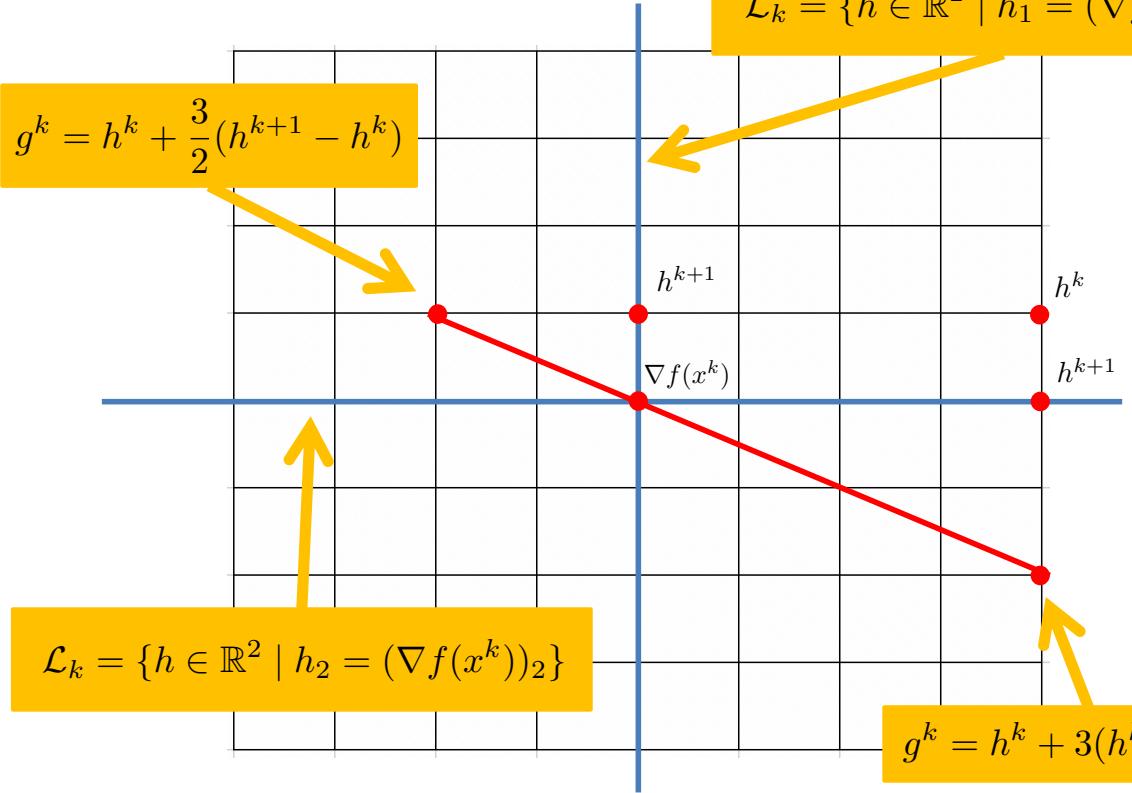
$$p_1 = \frac{2}{3} \quad p_2 = \frac{1}{3}$$

SEGA Estimator

$n = 2$

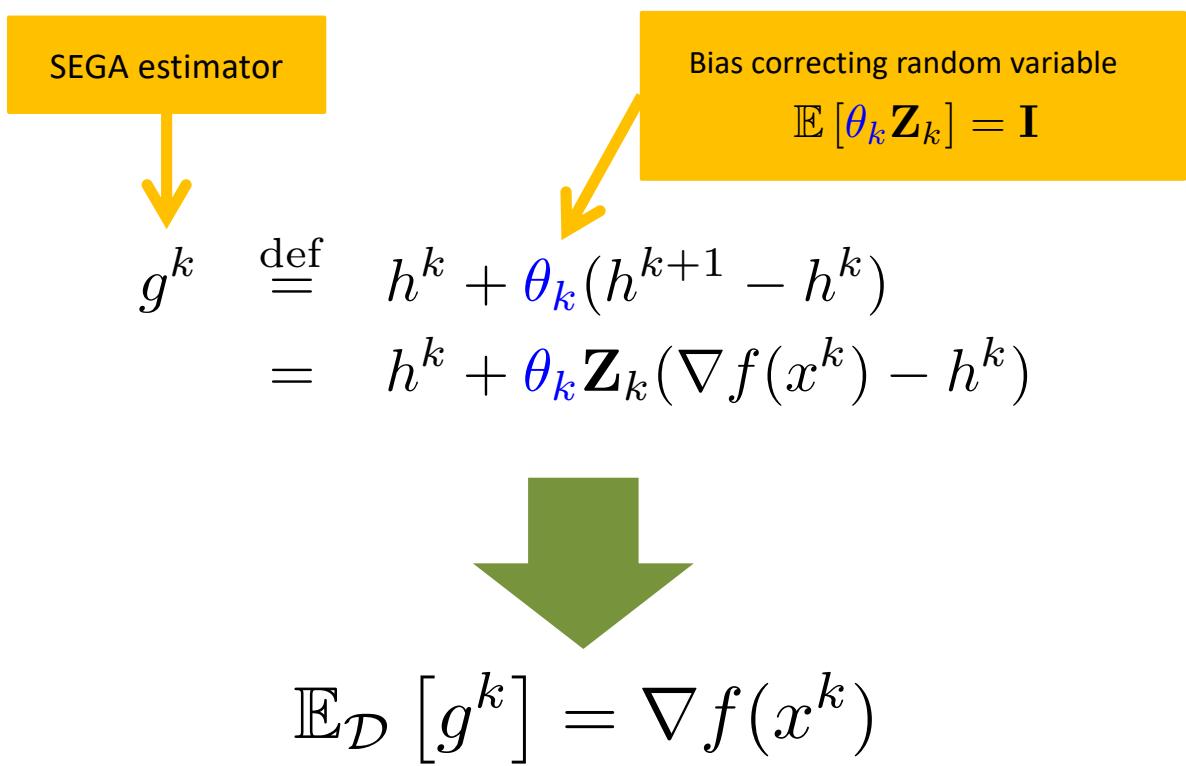
$$p_1 = \frac{2}{3} \quad p_2 = \frac{1}{3}$$

$$\mathcal{L}_k = \{h \in \mathbb{R}^2 \mid h_1 = (\nabla f(x^k))_1\}$$



SEGA for General Sketches

SEGA Estimator



3. SEGA: The Algorithm

The Algorithm

The SEGA Algorithm

$$\min_{x \in \mathbb{R}^n} F(x) := f(x) + R(x)$$

0 Choose $x^0, h^0 \in \text{dom}F$

For $k \geq 0$ **REPEAT**

1 Ask **SEGA Oracle** for $\mathbf{S}_k^\top \nabla f(x^k)$

Perform **Sketch & Project**

$$h^{k+1} = \arg \min_{h \in \mathbb{R}^n} \|h - h^k\|^2$$

$$\text{subject to } \mathbf{S}_k^\top h = \mathbf{S}_k^\top \nabla f(x^k)$$

Sketched Gradient

2 Compute the **SEGA Estimator**

$$g^k = h^k + \theta_k(h^{k+1} - h^k)$$

3 Perform **Proximal SGD** step

$$x^{k+1} = \text{prox}_{\alpha R}(x^k - \alpha g^k)$$

Variants of SEGA

$$x^{k+1} = \text{prox}_{\alpha R}(x^k - \alpha g^k)$$

$$\mathbb{E}_{\mathcal{D}} [\theta_k \mathbf{Z}_k] = \mathbf{I}$$

1. SEGA $g^k = h^k + \theta_k(h^{k+1} - h^k)$

2. Biased SEGA Use $\theta_k \equiv 1$ $\rightarrow g^k = h^{k+1}$

3. Subspace SEGA

$$f(x) = \phi(Ax) \rightarrow \nabla f(x) \in \text{Range}(A^\top)$$

$$h^{k+1} = \arg \min_{h \in \mathbb{R}^n} \|h - h^k\|^2$$

$$\text{subject to } \mathbf{S}_k^\top h = \mathbf{S}_k^\top \nabla f(x^k)$$

$$h \in \text{Range}(A^\top)$$

4. Accelerated SEGA

Complexity: General Sketch

Complexity for General Sketches

Strong convexity:

$$f(x) + \langle \nabla f(x), h \rangle + \frac{\mu}{2} \|h\|^2 \leq f(x + h)$$

Theorem

$$\mathbb{E} [\Phi^k] \leq (1 - \alpha\mu)^k \Phi^0$$

Lyapunov function: $x^0, h^0 \in \text{dom}F$

$$\Phi^k \stackrel{\text{def}}{=} \|x^k - x^*\|^2 + \sigma\alpha\|h^k - \nabla f(x^*)\|^2$$

Stepsize can't be too large:

$$\alpha(2(\mathbf{C} - \mathbf{I}) + \sigma\mu\mathbf{I}) \leq \sigma\mathbb{E}_{\mathbf{S} \sim \mathcal{D}} [\mathbf{Z}]$$

$$2\alpha\mathbf{C} + \sigma\mathbb{E}_{\mathbf{S} \sim \mathcal{D}} [\mathbf{Z}] \leq \mathbf{L}^{-1}$$

$$\mathbf{C} \stackrel{\text{def}}{=} \mathbb{E}_{\mathbf{S} \sim \mathcal{D}} [\theta^2 \mathbf{Z}]$$

Complexity: Coordinate Sketch

Coordinate Sketch: Arbitrary Sampling Setup

Random subset of $\{1, \dots, n\}$

- $\mathbf{S} = \mathbf{I}_{:\mathcal{C}}$ (random column submatrix of the identity matrix)
- Probability vector $p \in \mathbb{R}^n$: $p_i \stackrel{\text{def}}{=} \text{Prob}(i \in \mathcal{C})$
- Probability matrix $\mathbf{P} \in \mathbb{R}^{n \times n}$: $\mathbf{P}_{ij} \stackrel{\text{def}}{=} \text{Prob}(i \in \mathcal{C} \& j \in \mathcal{C})$
- ESO vector $v \in \mathbb{R}^n$ (for mini-batching) defined by:

$$\mathbf{P} \bullet \mathbf{M} \preceq \text{Diag}(p \bullet v)$$

↑
Hadamard product

Complexity Results

$$f(x + h) \leq f(x) + \langle \nabla f(x), h \rangle + \frac{1}{2} \langle \mathbf{L}h, h \rangle$$

$$f(x) + \langle \nabla f(x), h \rangle + \frac{1}{2} \langle \mu \mathbf{I}h, h \rangle \leq f(x + h)$$

$$R \equiv 0$$

Method	Complexity
SEGA importance sampling	$8.55 \cdot \frac{\text{Tr}(\mathbf{L})}{\mu} \log \frac{1}{\epsilon}$
SEGA arbitrary sampling	$8.55 \cdot \left(\max_i \frac{v_i}{p_i \mu} \right) \log \frac{1}{\epsilon}$
ASEGA importance sampling	$9.8 \cdot \frac{\sum_i \sqrt{\mathbf{L}_{ii}}}{\sqrt{\mu}} \log \frac{1}{\epsilon}$
ASEGA arbitrary sampling	$9.8 \cdot \sqrt{\max_i \frac{v_i}{p_i^2 \mu}} \log \frac{1}{\epsilon}$

Up to the constant factors 8.55 and 9.5, these rates are exactly the same as the rates of CD [R. & Takáč '16] and accelerated CD [Allen-Zhu et al '16, Hanzely & R. '19].

Coordinate Descent



P.R. and Martin Takáč

On optimal probabilities in stochastic coordinate descent methods

Optimization Letters 10(6), 1223-1243, 2016



Zeyuan Allen-Zhu, Zheng Qu, P.R. and Yang Yuan

Even faster accelerated coordinate descent using non-uniform sampling

ICML 2016



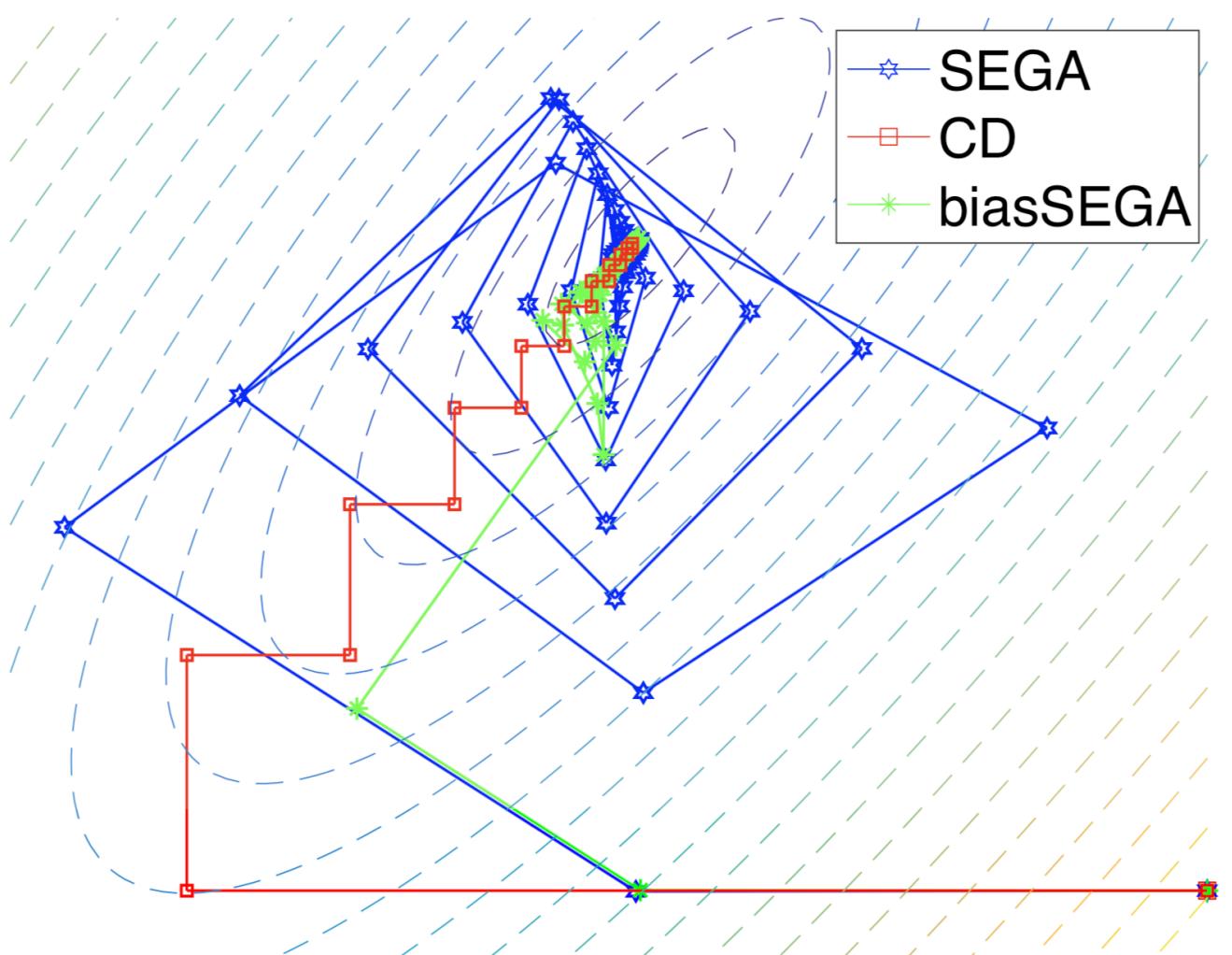
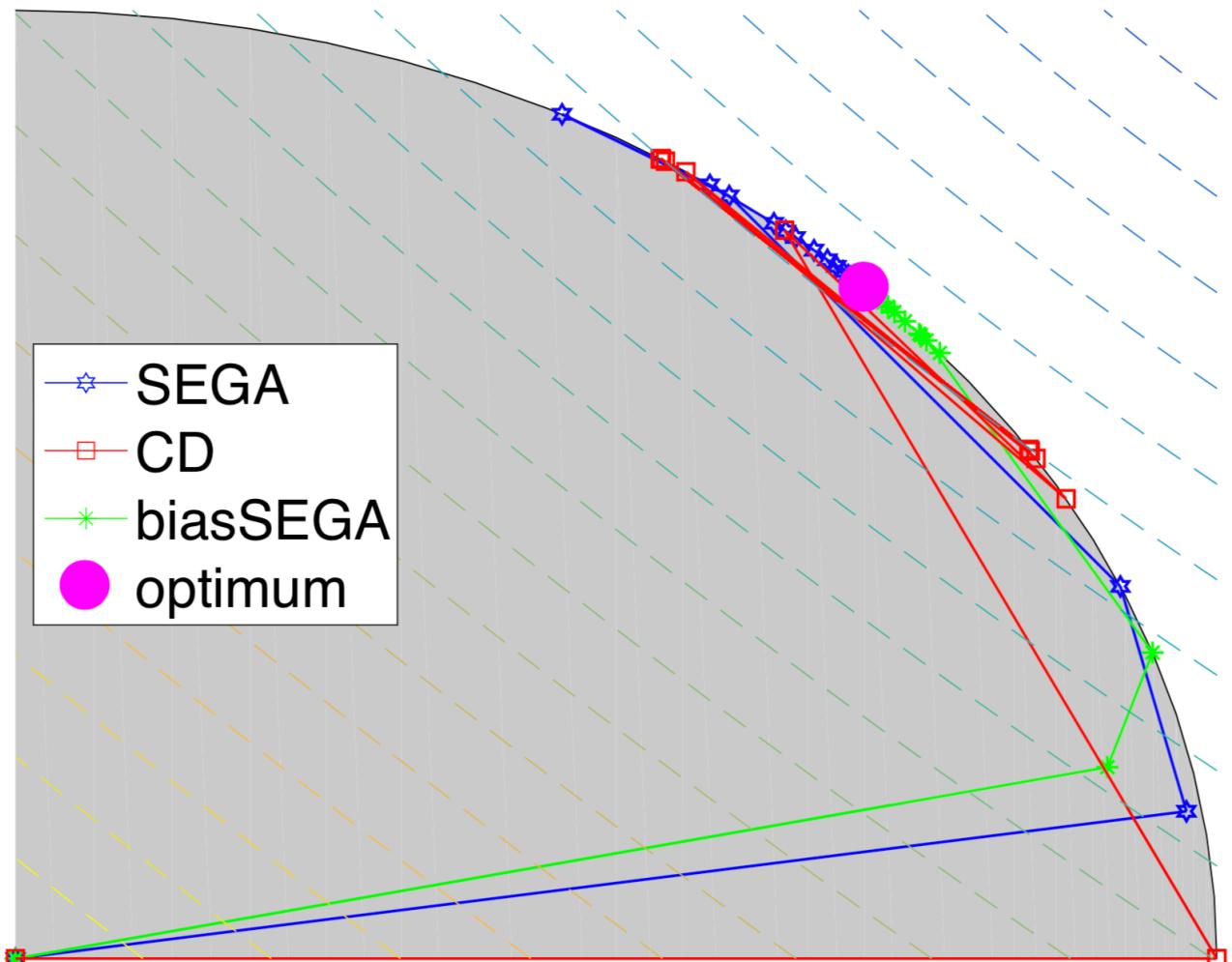
Filip Hanzely and P.R.

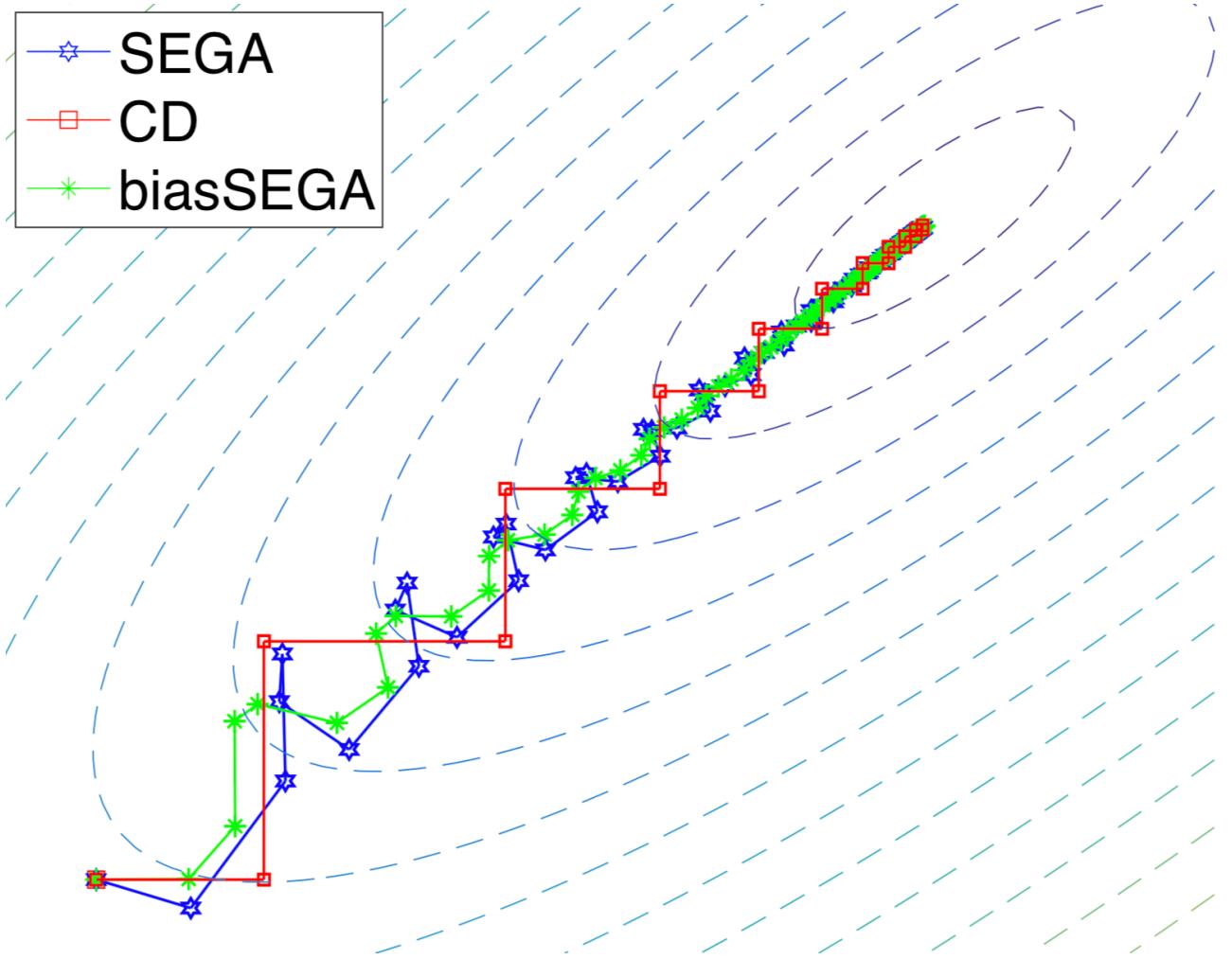
Accelerated coordinate descent with arbitrary sampling and best rates for minibatches

AISTATS 2019

4. Experiments

Illustration in 2D

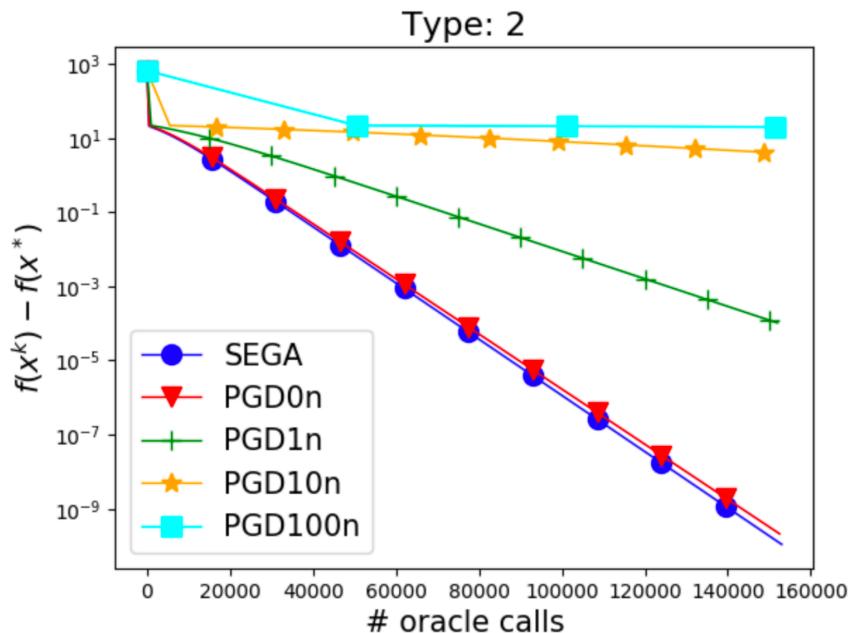




SEGA vs
Projected Gradient
Descent

Gaussian Sketch, Ball Constraint

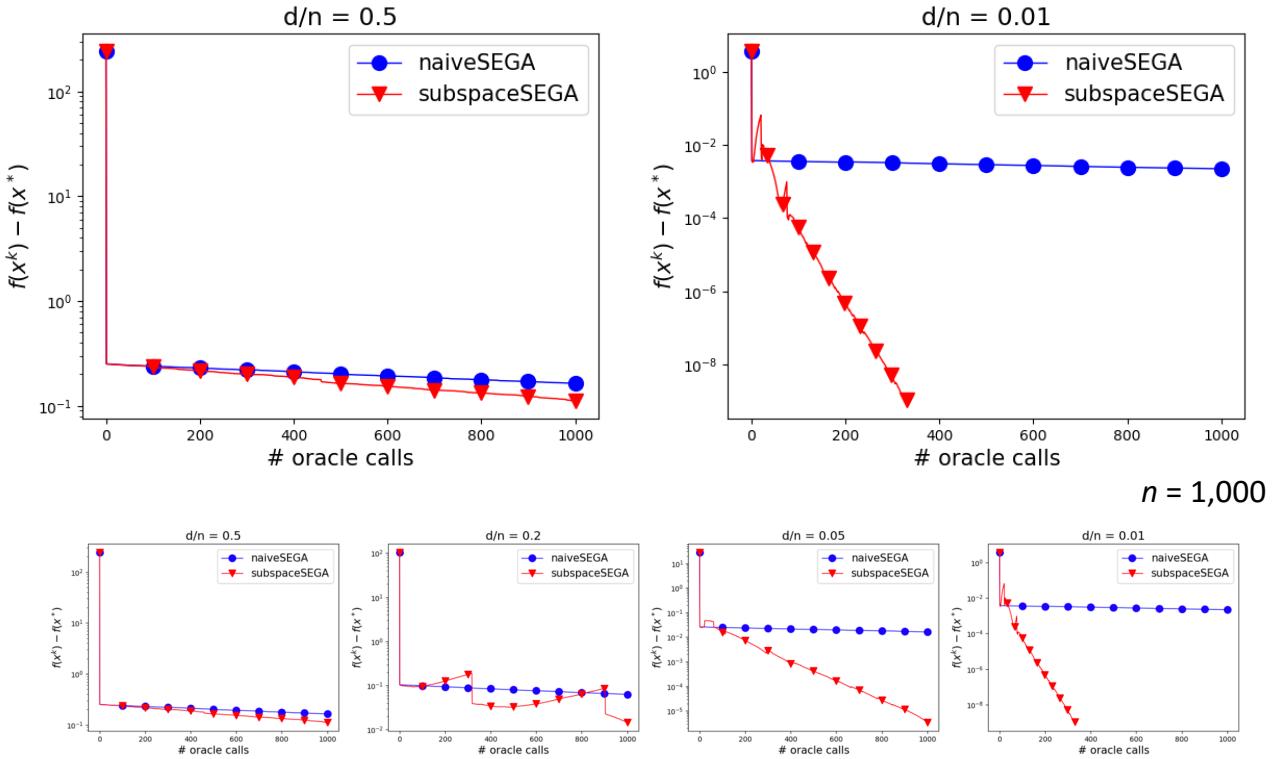
\mathbf{S} = Gaussian vector $R(x) = 1_{\mathcal{B}(0,1)}(x)$



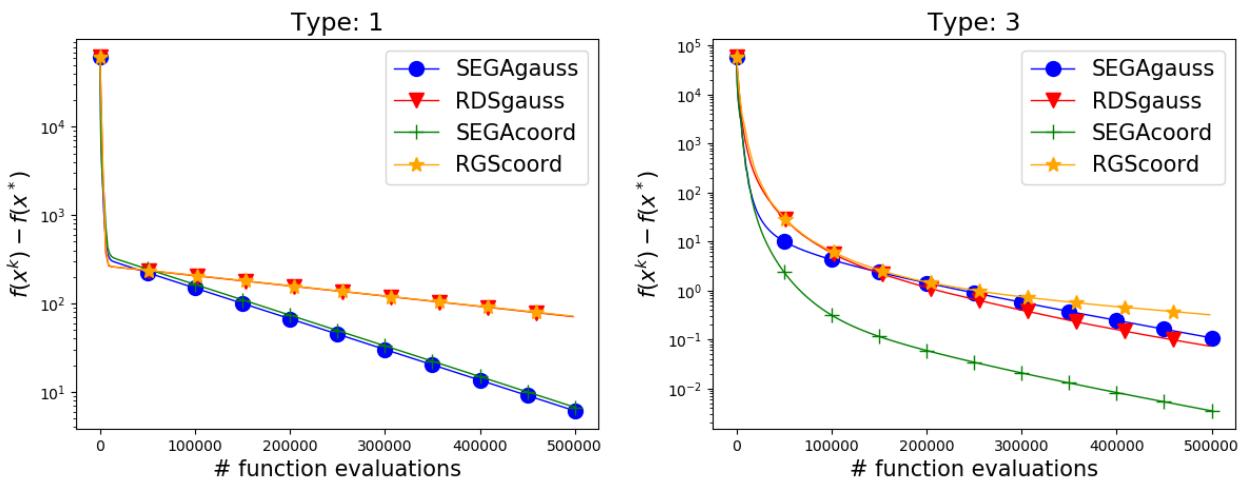
SEGA vs
Subspace SEGA

SEGA vs Subspace SEGA

$$f(x) = \phi(Ax) \rightarrow \nabla f(x) \in \text{Range}(A^\top)$$

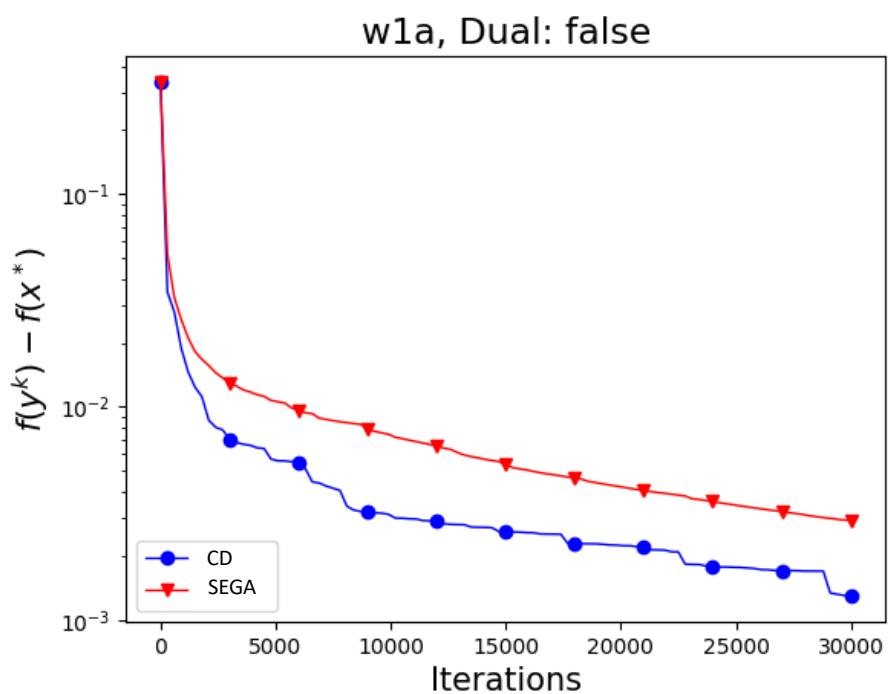


SEGA vs Random Direct Search

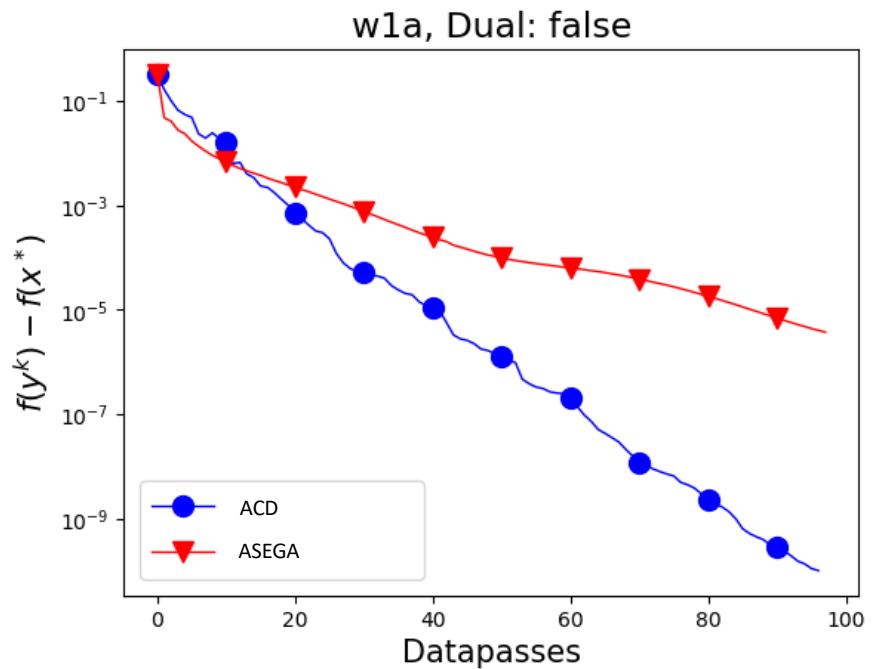


SEGA vs Coordinate Descent

SEGA vs CD



Accelerated SEGA vs Accelerated CD



5. Summary

Summary

- New Stochastic First-Order Oracle:
SkEtched GrAident (SEGA)
- New Stochastic Proximal SGD method.
Comes in several variants:
 - SEGA (based on the **SEGA Estimator**)
 - Biased SEGA
 - Subspace SEGA
 - Accelerated SEGA
- Coordinate sketches:
 - Same complexity as state-of-the art CD methods
 - Can handle non-separable regularizer R

The End