

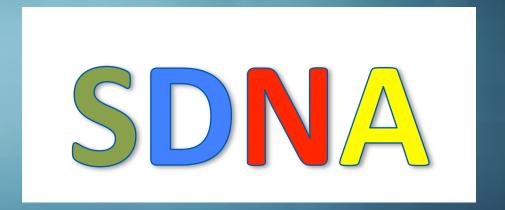


Lecture 4: Curvature

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Zheng Qu, P.R., Martin Takáč and Olivier Fercoq

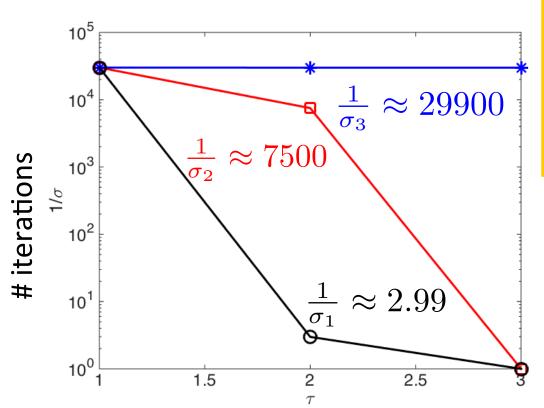
SDNA: Stochastic Dual Newton Ascent for empirical risk minimization

arXiv:1502.02268, 2015

Motivation

Why Curvature Is Cute

$$\min_{x \in \mathbb{R}^3} \left[f(x) = \frac{1}{2} x^T \mathbf{M} x + b^\top x + c \right]$$

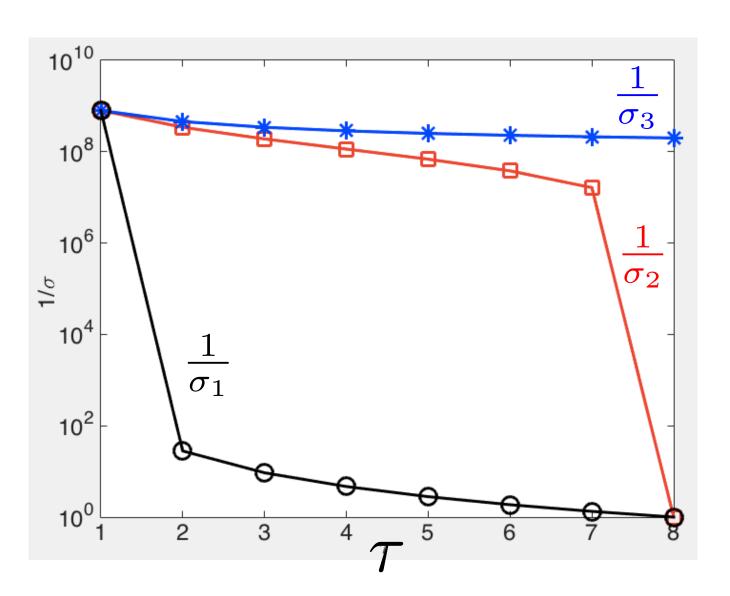


$$\mathbf{M} = \begin{pmatrix} 1.0000 & 0.9900 & 0.9999 \\ 0.9900 & 1.0000 & 0.9900 \\ 0.9999 & 0.9900 & 1.0000 \end{pmatrix}$$

condition number $\approx 3 \times 10^4$

- Phenomenon described in [Qu et al 15]
- Method 1: Two points of view: "Exact line search in higher dimensional subspaces" or "inversion of random submatrices of the Hessian"

8D Quadratic



Objectives

- Learn about one way of combining curvature information & randomization to get a faster optimization algorithm
- The basic idea is to extend the randomized Newton method (studied in Lecture 1) to nonquadratic functions
- Close links with the NSync method (studied in Lecture 2)
- Can also apply it to the ERM dual, obtaining the SDNA method (link to Lecture 3)

Three Methods

The Problem & Assumptions



Large dimension

Strong convexity

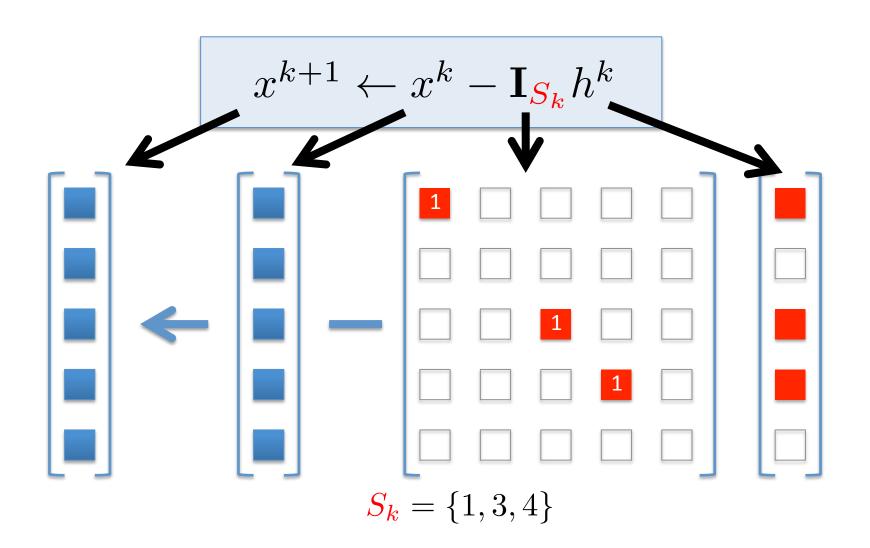
$$f(x) + (\nabla f(x))^{\top} h + \frac{1}{2} h^{\top} \mathbf{G} h \le f(x+h)$$

Positive definite matrices

Smoothness

$$f(x+h) \le f(x) + (\nabla f(x))^{\top} h + \frac{1}{2} h^{\top} \mathbf{M} h$$

Randomized Update



Method 3





P.R. and Martin Takáč

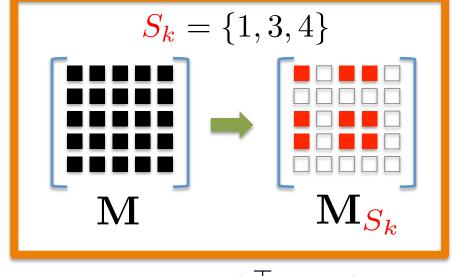
On optimal probabilities in stochastic coordinate descent methods In NIPS Workshop on Optimization for Machine Learning, 2013 Optimization Letters 2015 (arXiv:1310.3438)

Key Inequality

$$f(x+h) \le f(x) + (\nabla f(x))^{\top} h + \frac{1}{2} h^{\top} \mathbf{M} h$$



$$h \leftarrow \mathbf{I}_{S_k} h = \sum_{i \in S_k} h_i e_i$$





$$f(x^k + \mathbf{I}_{S_k}h) \le f(x^k) + (\nabla f(x^k))^\top (\mathbf{I}_{S_k}h) + \frac{1}{2}(\mathbf{I}_{S_k}h)^\top \mathbf{M} (\mathbf{I}_{S_k}h)$$



Method 3

$$f(x^k + \mathbf{I}_{S_k}h) \le f(x^k) + \left(\mathbf{I}_{S_k}\nabla f(x^k)\right)^\top h + \frac{1}{2}h^\top \mathbf{M}_{S_k}h$$



$$\mathbb{E}[f(x^k + \mathbf{I}_{S_k}h)] \le f(x^k) + (\mathbf{Diag}(p)\nabla f(x^k))^{\top}h + \frac{1}{2}h^{\top}\mathbb{E}[\mathbf{M}_{S_k}]h$$

2. diagonalize



$$\mathbb{E}[\mathbf{M}_{S_k}] \leq \mathbf{Diag}(p \circ v)$$

$$\mathbb{E}[f(x^k + \mathbf{I}_{S_k}h)] \le f(x^k) + (\mathbf{Diag}(p)\nabla f(x^k))^{\top}h + \frac{1}{2}h^{\top}\mathbf{Diag}(p \circ v)h$$

3. minimize the RHS in h



$$x^{k+1} \leftarrow x^k - \mathbf{I}_{S_k}(\mathbf{Diag}(v))^{-1} \nabla f(x^k)$$



Method 3

i.i.d. (with arbitrary distribution) and proper

Choose a random set S_k of coordinates

For $i \in S_k$ do

$$x_{i}^{k+1} \leftarrow x_{i}^{k} - \frac{1}{v_{i}} (\nabla f(x^{k}))^{\top} e_{i}$$

For $i \notin S_k$ do

$$x_{i}^{k+1} \leftarrow x_{i}^{k}$$



Convergence

Theorem (RT'13)

$$\mathbb{E}[f(x^k) - f(x^*)] \le (1 - \sigma_3)^k (f(x^0) - f(x^*))$$

$$\sigma_3 = \lambda_{\min} \left(\mathbf{G}^{1/2} \mathbf{Diag}(p \circ v^{-1}) \mathbf{G}^{1/2} \right)$$

Alternative formulation:

$$k \ge \frac{1}{\sigma_3} \log \left(\frac{f(x^0) - f(x^*)}{\epsilon} \right) \quad \Rightarrow \quad \mathbb{E}[f(x^k) - f(x^*)] \le \epsilon$$

Uniform vs Optimal Sampling

Special case:

al case:
$$\mathbf{G} = \lambda \mathbf{I} \quad \Rightarrow \quad \frac{1}{\sigma_3} = \max_i \frac{v_i}{\lambda p_i}$$
 $\mathbb{P}\left(|S_{k}| = 1\right) = 1 \quad \Rightarrow \quad v_i = \mathbf{M}_{ii}$

$$\mathbb{P}\left(|S_k|=1\right)=1 \quad \Rightarrow \quad v_i=\mathbf{M}_{ii}$$

$$p_{\pmb{i}} = rac{1}{n}$$

$$\frac{1}{\sigma_3} = \frac{n \max_i \mathbf{M}_{ii}}{\lambda}$$

$$p_i = rac{\mathbf{M}_{ii}}{\sum_i \mathbf{M}_{ii}}$$



$$\frac{1}{\sigma_3} = \frac{\sum_{i=1}^n \mathbf{M}_{ii}}{\lambda}$$

Method 2

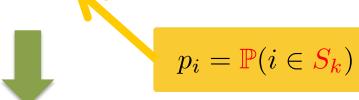
Method 2

$$f(x^k + \mathbf{I}_{S_k}h) \le f(x^k) + \left(\mathbf{I}_{S_k}\nabla f(x^k)\right)^{\top}h + \frac{1}{2}h^{\top}\mathbf{M}_{S_k}h$$

1. take expectations on both sides



$$\mathbb{E}[f(x^k + \mathbf{I}_{S_k}h)] \le f(x^k) + (\mathbf{Diag}(p)\nabla f(x^k))^{\top}h + \frac{1}{2}h^{\top}\mathbb{E}[\mathbf{M}_{S_k}]h$$



2. minimize the RHS in h

$$x^{k+1} \leftarrow x^k - \mathbf{I}_{S_k}(\mathbb{E}[\mathbf{M}_{S_k}])^{-1}\mathbf{Diag}(p)\nabla f(x^k)$$

Convergence of Method 2

Theorem (QRTF'15)

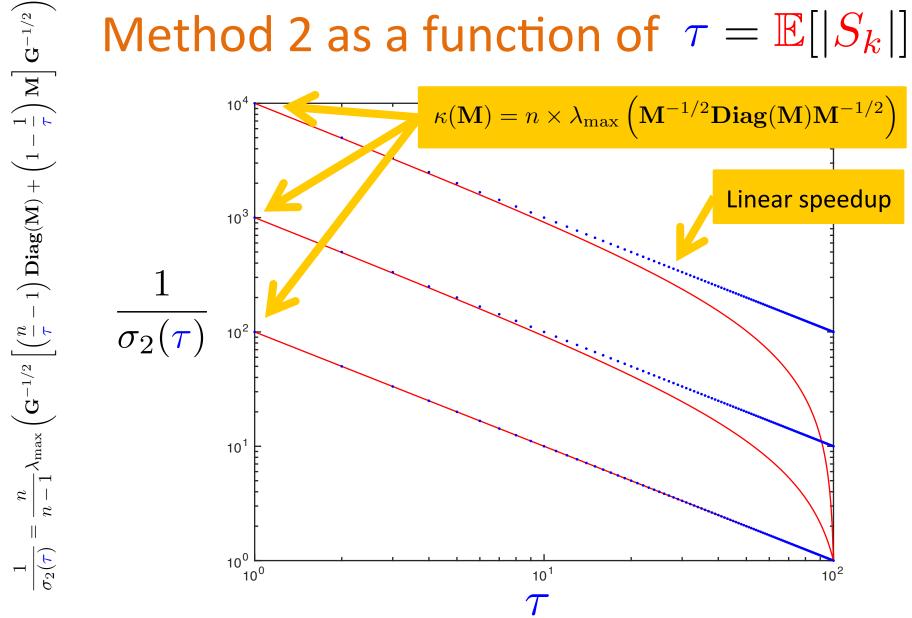
$$\mathbb{E}[f(x^k) - f(x^*)] \le (1 - \sigma_2)^k (f(x^0) - f(x^*))$$

$$\sigma_2 = \lambda_{\min} \left(\mathbf{G}^{1/2} \mathbf{Diag}(p) \left(\mathbb{E} \left[\mathbf{M}_{S_k} \right] \right)^{-1} \mathbf{Diag}(p) \mathbf{G}^{1/2} \right)$$

Alternative formulation:

$$k \ge \frac{1}{\sigma_2} \log \left(\frac{f(x^0) - f(x^*)}{\epsilon} \right) \quad \Rightarrow \quad \mathbb{E}[f(x^k) - f(x^*)] \le \epsilon$$

Leading term in the complexity of Method 2 as a function of $au = \mathbb{E}[|S_k|]$



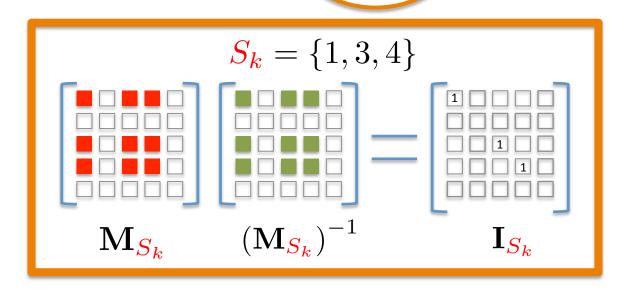
Method 1 Randomized Newton Method

Method 1: Randomized Newton

$$f(x^k + \mathbf{I}_{\mathbf{S}_k}h) \le f(x^k) + \left(\mathbf{I}_{\mathbf{S}_k}\nabla f(x^k)\right)^{\top}h + \frac{1}{2}h^{\top}\mathbf{M}_{\mathbf{S}_k}h$$



$$x^{k+1} \leftarrow x^k - (\mathbf{M}_{S_k})^{-1} \nabla f(x^k)$$



Convergence of Method 1 (Randomized Newton Method)

Theorem (QRTF'15)

$$\mathbb{E}[f(x^k) - f(x^*)] \le (1 - \sigma_1)^k (f(x^0) - f(x^*))$$

$$\sigma_1 = \lambda_{\min} \left(\mathbf{G}^{1/2} \mathbb{E} \left[\left(\mathbf{M}_{S_k} \right)^{-1} \right] \mathbf{G}^{1/2} \right)$$

Alternative formulation:

$$k \ge \frac{1}{\sigma_1} \log \left(\frac{f(x^0) - f(x^*)}{\epsilon} \right) \quad \Rightarrow \quad \mathbb{E}[f(x^k) - f(x^*)] \le \epsilon$$

Three Convergence Rates

3 Convergence Rates

Theorem [QRTF'15]

$$0 < \sigma_3 \le \sigma_2 \le \sigma_1 \le 1$$

$$\sigma_1(1) = \sigma_2(1) = \sigma_3(1)$$

$$\sigma_1(n) = \sigma_2(n) = \frac{1}{\kappa_f}$$

$$\sigma_2(\tau) \ge \tau \sigma_2(1)$$

$$\sigma_3(\tau) \leq \tau \sigma_3(1)$$

$$\kappa_f = \lambda_{\text{max}} \left(\mathbf{G}^{-1/2} \mathbf{M} \mathbf{G}^{-1/2} \right)$$

The 3 methods coincide if we update 1 coordinate at a time

Methods 1 and 2 coincide if we update all coordinates

Randomized Newton: superlinear speedup

Randomized Coordinate Descent: sublinear speedup

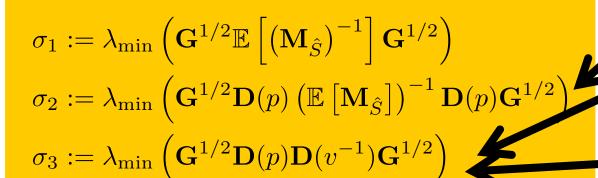
Proofs

Theorem 1
$$f$$
 is G-strongly convex & $\mathbf{G} \succ 0$ $S_k \stackrel{\text{i.i.d.}}{\sim} \hat{S}$ f is M-smooth & $\mathbf{M} \succ 0$ \hat{S} is proper



Method m (for m = 1, 2, 3) converges linearly:

$$\mathbb{E}[f(x^{k+1}) - f(x^*)] \le (1 - \sigma_m)\mathbb{E}[f(x^k) - f(x^*)]$$



Definition of *p*

$$p = (p_1, \dots, p_n) \in \mathbb{R}^n$$

 $p_i = \mathbb{P}(i \in \hat{S})$

Definition of v

$$\mathbb{E}\left[\mathbf{M}_{\hat{S}}\right] \leq \mathbf{D}(p)\mathbf{D}(v)$$

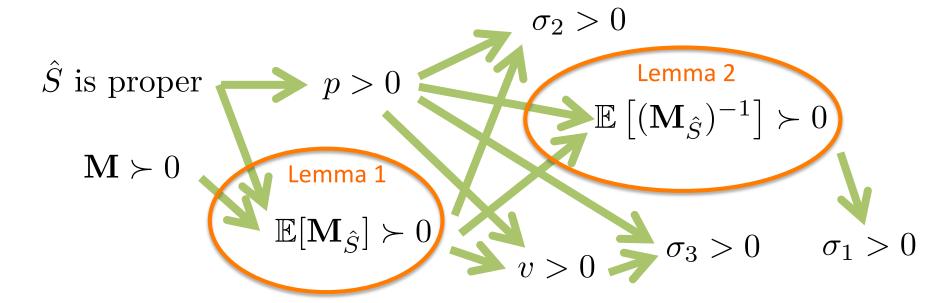
Sanity Check

Let us verify that the rates asserted by the theorem make sense (well defined & positive)

$$\sigma_{1} := \lambda_{\min} \left(\mathbf{G}^{1/2} \mathbb{E} \left[\left(\mathbf{M}_{\hat{S}} \right)^{-1} \right] \mathbf{G}^{1/2} \right)$$

$$\sigma_{2} := \lambda_{\min} \left(\mathbf{G}^{1/2} \mathbf{D}(p) \left(\mathbb{E} \left[\mathbf{M}_{\hat{S}} \right] \right)^{-1} \mathbf{D}(p) \mathbf{G}^{1/2} \right)$$

$$\sigma_{3} := \lambda_{\min} \left(\mathbf{G}^{1/2} \mathbf{D}(p) \mathbf{D}(v^{-1}) \mathbf{G}^{1/2} \right)$$



Lemma 1

Lemma 1

Α

$$\mathbf{M} \succeq 0$$
 & \hat{S} is any sampling \Rightarrow $\mathbb{E}\left[\mathbf{M}_{\hat{S}}\right] \succeq 0$

В

$$\mathbf{M} \succ 0$$
 & \hat{S} is a proper sampling \Rightarrow $\mathbb{E}\left[\mathbf{M}_{\hat{S}}\right] \succ 0$

Α

The first claim follows from:

- $\mathbf{M}_S \succeq 0$ for all subsets S of $[n] = \{1, 2, \dots, n\}$
- average of PSD matrices is a PSD matrix

В

Denote $supp\{x\} = \{i \in [n] : x_i \neq 0\}$. Since $\mathbf{M} \succ 0$, any principal submatrix of \mathbf{M} is also positive definite. Hence, for any $x \in \mathbb{R}^n \setminus \{0\}$, $x^{\top} \mathbf{M}_S x = 0$ implies that $supp\{x\} \cap S = \emptyset$ for all $S \subseteq [n]$. If $x \in \mathbb{R}^n$ is such that

$$x^{\top} \mathbb{E}\left[\mathbf{M}_{\hat{S}}\right] x = \sum_{S \subseteq [n]} \mathbb{P}(\hat{S} = S) x^{\top} \mathbf{M}_{S} x = 0,$$

then $\mathbb{P}(supp\{x\} \cap \hat{S} = \emptyset) = 1$. Since \hat{S} is proper, this only happens when x = 0. Therefore, $\mathbb{E}[\mathbf{M}_{\hat{S}}] \succ 0$.

Lemma 2

Lemma 2

 $\mathbf{M} \succ 0$, \hat{S} is proper, and $\mathbb{P}(\hat{S} = \emptyset) = 0$



 $\prec \mathbf{D}(p) \left(\mathbb{E} \left[\mathbf{M}_{\hat{S}} \right] \right)^{-1} \mathbf{D}(p) \leq \mathbb{E} \left[\left(\mathbf{M}_{\hat{S}} \right)^{-1} \right]$

Follows from

- Lemma 1, and
- the fact that for proper \hat{S} we have p > 0 and hence $\mathbf{D}(p) \succ 0$.

Proof of Lemma 2 B

Fix $h \in \mathbb{R}^n$. For arbitrary $\emptyset \neq S \subseteq [n]$ and $y \in \mathbb{R}^n$ we have:

$$\frac{1}{2}h^{\top} (\mathbf{M}_S)^{-1} h = \frac{1}{2}h_S^{\top} (\mathbf{M}_S)^{-1} h_S$$

$$= \max_{x \in \mathbb{R}^n} \langle x, h_S \rangle - \frac{1}{2}x^{\top} \mathbf{M}_S x$$

$$\geq \langle y, h_S \rangle - \frac{1}{2}y^{\top} \mathbf{M}_S y.$$

Proof of Lemma 2 B

Substituting $S = \hat{S}$ and taking expectations, we obtain

$$\frac{1}{2}\mathbb{E}\left[h^{\top}\left(\mathbf{M}_{\hat{S}}\right)^{-1}h\right] \geq \mathbb{E}\left[\langle y, h_{\hat{S}}\rangle - \frac{1}{2}y^{\top}\mathbf{M}_{\hat{S}}y\right] \\
= y^{\top}\mathbf{D}(p)h - \frac{1}{2}y^{\top}\mathbb{E}\left[\mathbf{M}_{\hat{S}}\right]y.$$

Finally, maximizing in y gives:

$$\frac{1}{2}h^{\top}\mathbb{E}\left[\left(\mathbf{M}_{\hat{S}}\right)^{-1}\right]h \geq \max_{y \in \mathbb{R}^{n}} y^{\top}\mathbf{D}(p)h - \frac{1}{2}y^{\top}\mathbb{E}\left[\mathbf{M}_{\hat{S}}\right]y$$

$$= \frac{1}{2}h^{\top}\mathbf{D}(p)\left(\mathbb{E}\left[\mathbf{M}_{\hat{S}}\right]\right)^{-1}\mathbf{D}(p)h.$$

Proof of Theorem 1: First Steps

• From G-strong convexity of f (by minimizing both sides in h) we get:

$$f(x) - f(x^*) \le \frac{1}{2} \langle \nabla f(x), \mathbf{G}^{-1} \nabla f(x) \rangle, \quad \forall x \in \mathbb{R}^n$$
 (*)

• From M-smoothness of f we get:

$$f(x^k + \mathbf{I}_{S_k}h) \le f(x^k) + \langle \nabla f(x^k), \mathbf{I}_{S_k}h \rangle + \frac{1}{2} \langle \mathbf{M}_{S_k}h, h \rangle, \quad \forall h \in \mathbb{R}^n \quad (**)$$

Proof of Theorem 1: Method 1

• Use (**) with $h \leftarrow h^k := -(\mathbf{M}_{S_k})^{-1} \nabla f(x^k)$:

$$f(x^{k+1}) \le f(x^k) - \frac{1}{2} \langle \nabla f(x^k), (\mathbf{M}_{S_k})^{-1} \nabla f(x^k) \rangle$$

• Taking conditional expectations on both sides:

$$\mathbb{E}[f(x^{k+1}) \mid x^{k}] - f(x^{k}) \leq -\frac{1}{2} \langle \nabla f(x^{k}), \mathbb{E}[(\mathbf{M}_{\hat{S}})^{-1}] \nabla f(x^{k}) \rangle$$

$$\stackrel{\text{def of } \sigma_{1}}{\leq} -\frac{\sigma_{1}}{2} \langle \nabla f(x^{k}), \mathbf{G}^{-1} \nabla f(x^{k}) \rangle$$

$$\stackrel{(*)}{\leq} -\sigma_{1} \left(f(x^{k}) - f(x^{*}) \right)$$

• Rearrange the inequality and take expectation to get:

$$\mathbb{E}[f(x^{k+1}) - f(x^*)] \le (1 - \sigma_1)\mathbb{E}[f(x^k) - f(x^*)]$$

Proof of Theorem 1: Method 2

• Let $\mathbf{D} = \mathbf{D}(p)$ and take expectations on both sides of (**):

$$\mathbb{E}[f(x^k + \mathbf{I}_{S_k}h) \mid x^k] \le f(x^k) + \langle \mathbf{D}\nabla f(x^k), h \rangle + \frac{1}{2} \langle \mathbb{E}[\mathbf{M}_{S_k}]h, h \rangle$$

• Note that the choice $\tilde{h}^k := -(\mathbb{E}[\mathbf{M}_{\hat{S}}])^{-1} \mathbf{D} \nabla f(x^k)$ minimizes the RHS of the inequality in h. Since $h^k = \mathbf{I}_{S_k} \tilde{h}^k$,

$$\mathbb{E}[f(x^{k+1}) \mid x^{k}] - f(x^{k}) \leq -\frac{1}{2} \langle \nabla f(x^{k}), \mathbf{D} \left(\mathbb{E}[\mathbf{M}_{\hat{S}}] \right)^{-1} \mathbf{D} \nabla f(x^{k}) \rangle$$

$$\stackrel{\text{def of } \sigma_{2}}{\leq} -\frac{\sigma_{2}}{2} \langle \nabla f(x^{k}), \mathbf{G}^{-1} \nabla f(x^{k}) \rangle$$

$$\stackrel{(*)}{\leq} -\sigma_{2} \left(f(x^{k}) - f(x^{*}) \right)$$

• Rearrange the inequality and take expectation to get:

$$\mathbb{E}[f(x^{k+1}) - f(x^*)] \le (1 - \sigma_2) \mathbb{E}[f(x^k) - f(x^*)]$$

Proof of Theorem 1: Method 3

Same as for Method 2, except in the first inequality replace $\mathbb{E}[\mathbf{M}_{S_k}]$ by the upper bound:

$$\mathbb{E}[\mathbf{M}_{S_k}] \leq \mathbf{D}(p)\mathbf{D}(v)$$

Ordering Theorem

Theorem 2
$$\sigma_3 \leq \sigma_2 \leq \sigma_1$$

Proof:
$$\mathbf{D}(p)\mathbf{D}(v^{-1}) = \mathbf{D}(p)\mathbf{D}(p^{-1})\mathbf{D}(v^{-1})\mathbf{D}(p)$$

$$\stackrel{\mathrm{ESO}}{\preceq} \mathbf{D}(p) \left(\mathbb{E}\left[\mathbf{M}_{\hat{S}}\right]\right)^{-1}\mathbf{D}(p)$$

$$\stackrel{\mathrm{Lemma 2}}{\preceq} \mathbb{E}\left[\left(\mathbf{M}_{\hat{S}}\right)^{-1}\right]$$

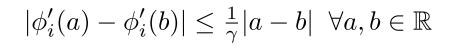
$$\sigma_{1} := \lambda_{\min} \left(\mathbf{G}^{1/2} \mathbb{E} \left[\left(\mathbf{M}_{\hat{S}} \right)^{-1} \right] \mathbf{G}^{1/2} \right)$$

$$\sigma_{2} := \lambda_{\min} \left(\mathbf{G}^{1/2} \mathbf{D}(p) \left(\mathbb{E} \left[\mathbf{M}_{\hat{S}} \right] \right)^{-1} \mathbf{D}(p) \mathbf{G}^{1/2} \right)$$

$$\sigma_{3} := \lambda_{\min} \left(\mathbf{G}^{1/2} \mathbf{D}(p) \mathbf{D}(v^{-1}) \mathbf{G}^{1/2} \right)$$

Application to Empirical Risk Minimization

Primal Problem



P = Regularized Empirical Risk

 $1/\gamma$ - smooth & convex functions ("risk")

positive regularization parameter

$$\min_{w \in \mathbb{R}^d} \left[P(w) \equiv \frac{1}{n} \sum_{i=1}^n \phi_i(A_i^\top w) + \lambda g(w) \right]$$

w = linear predictor

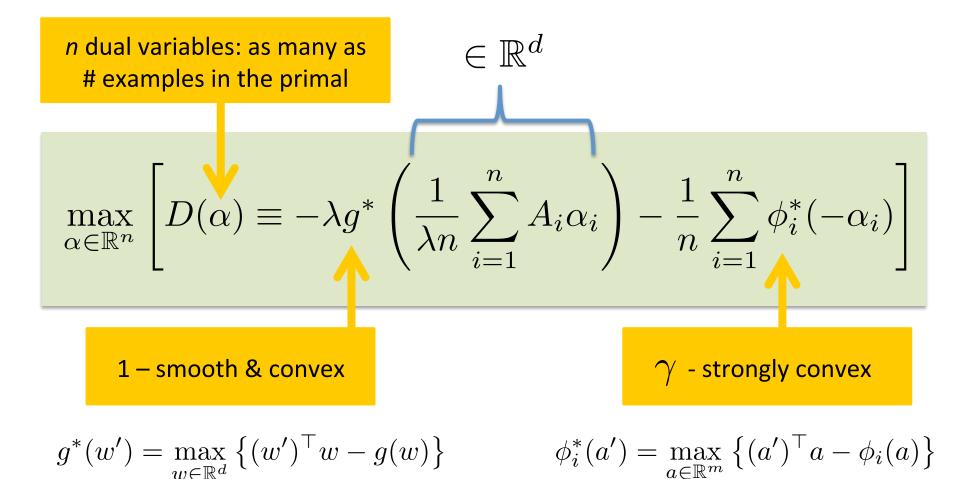
n data vectors
 ("examples")

d = # features
(parameters)

1 - strongly convex function ("regularizer")

$$g(w) \ge g(w') + \langle \nabla g(w'), w - w' \rangle + \frac{1}{2} ||w - w'||^2, \quad w, w' \in \mathbb{R}^d$$

Dual Problem



 $\phi_i^*(a') = \max_{a \in \mathbb{R}^m} \{(a')^\top a - \phi_i(a)\}$

Initialization:
$$\alpha^0 \in \mathbb{R}^n \ \bar{\alpha}^0 = \frac{1}{\lambda n} \mathbf{A} \alpha^0$$

Iterate:

Primal update: $w^k = \nabla g^*(\bar{\alpha}^k)$

Generate a random set S_k

Compute:

$$\mathbf{A} = [A_1, A_2, \dots, A_n] \in \mathbb{R}^{d \times n}$$

$$\mathbf{X} = \frac{1}{\lambda n} \mathbf{A}^{\top} \mathbf{A}$$

$$h^k = \arg\min_{h \in \mathbf{R}^n} \left((\mathbf{A}^\top w^k)_{\mathbf{S}_k} \right)^\top h + \frac{1}{2} h^\top \mathbf{X}_{\mathbf{S}_k} h + \sum_{i \in \mathbf{S}_k} \phi_i^* (-\alpha_i^k - h_i)$$

Dual update: $\alpha^{k+1} \leftarrow \alpha^k + \sum_{i \in S_k} h_i^k e_i$

Maintain average: $\bar{\alpha}^{k+1} = \bar{\alpha}^k + \frac{1}{\lambda_n} \sum_{i \in S_k} h_i^k A_i$

Convergence of SDNA

Theorem (QRTF'15)

Assume that S_k is uniform

$$\mathbb{E}[P(w^k) - D(\alpha^k)] \le (1 - \sigma_1^{prox})^k \frac{D(\alpha^*) - D(\alpha^0)}{\theta(S_k)}$$

Expected duality gap after *k* iterations

$$\sigma_1^{prox} = \frac{\tau}{n} \min\{1, s_1\}$$

Better rate than SDCA

$$au = \mathbb{E}[|S_k|] \quad s_1 = \lambda_{\min}\left[\left(rac{1}{ au\gamma\lambda}\mathbb{E}[(\mathbf{A}^{ op}\mathbf{A})_{S_k}] + \mathbf{I}
ight)^{-1}
ight]$$

Experiments

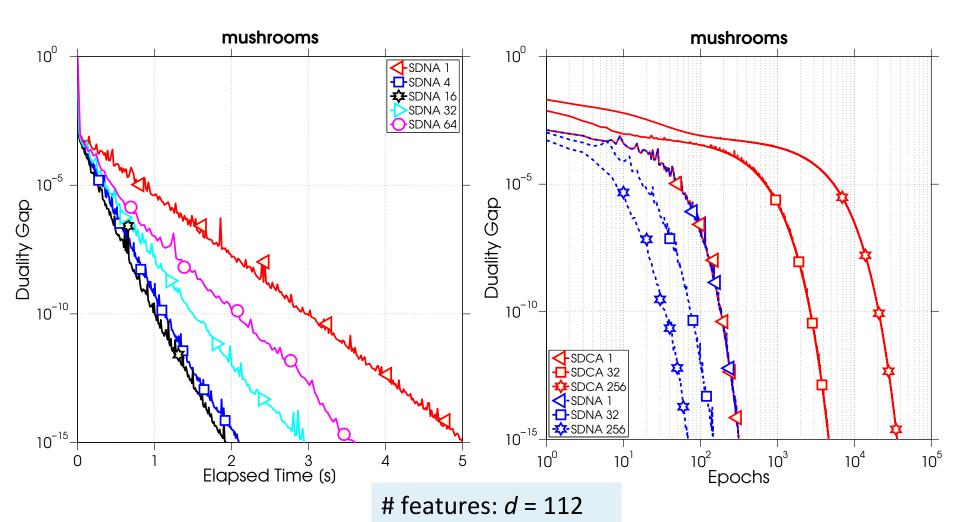
Real Dataset:

mushrooms

$$d = 112$$
 $n = 8,124$



Sampling "Smallish" Submatrices of the Hessian Helps



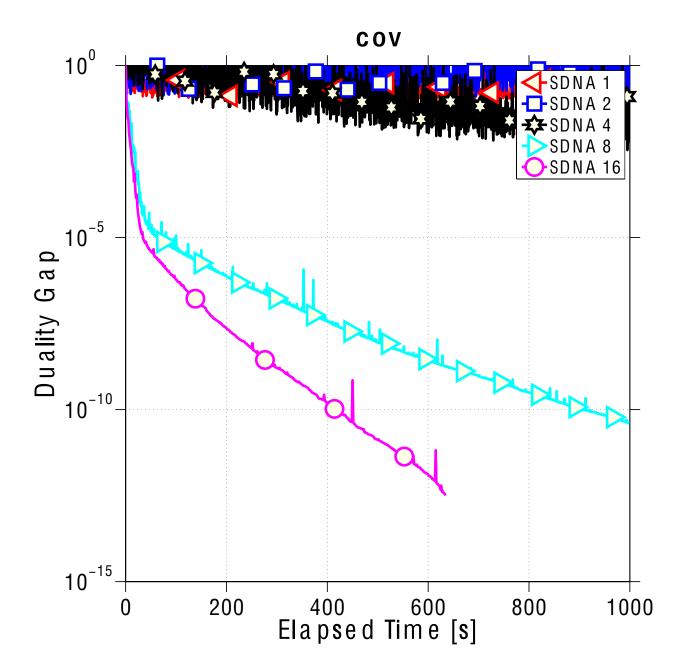
examples: n = 8124

Real Dataset:

COV

$$d = 54$$
 $n = 581,012$





Summary

Summary

- Can combine curvature & randomization and get complexity rates
- Curvature is utilized by doing exact computations in small but multidimensional subspaces
- Randomized "Newton" (Method 1):
 - Superlinear speedup (always)
 - Expensive iterations: Needs to solve a "small" but potentially dense linear system in each step
- Randomized Coordinate Descent (Method 3):
 - Sublinear speedup (gets better with sparsity or good spectral properties)
 - Cheap iterations: Needs to solve a small diagonal linear system in each step
- Can apply to the dual of ERM: SDNA
 - Coincides with SDCA if minibatch size = 1
 - Improves on SDCA when minibatch size is larger, but not too large
 - New effect: # passes over data decreases as minibatch size increases
- Further reading: Stochastic quasi-Newton [Schraudolph, Yu, Gunter '07] [Bordes, Bottou, Gallinari '09] [Byrd, Hansen, Nocedal, Singer '14] Newton sketch [Pilanci & Wainwright '15]