CME 307 / MS&E 311: Optimization

Low rank approximation for faster optimization

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   minimize $f(Ax) + g(x)$, e.g.,
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   - regularized logistic regression
   - support vector machine

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   - speed (vs other quasi-Newton methods)

   even works for deep learning!

Outline

Low rank approximation

Nyström PCG

SketchySGD

ADMM

NysADMM

Low rank approximation via eigenvalues

given $A \in \mathbf{S}_{+}^{n}$ (symmetric positive definite), find the best rank-s approximation:

- compute the eigenvalue decomposition ($O(n^3)$ flops)

$$A = U \Lambda U^T$$

with $\Lambda = \mathbf{diag}(\lambda_1, \ldots, \lambda_n)$, $\lambda_1 \geq \cdots \geq \lambda_n$,
$UU^T = U^T U = I_n$,

- truncate to top s eigenvector/value pairs:

$$\hat{A} = U_s \Lambda_s U_s^T$$

with $\Lambda_s = \mathbf{diag}(\lambda_1, \ldots, \lambda_s)$,
$U_s \in \mathbf{R}^{n \times s}$ is first s columns of $U \in \mathbf{R}^{n \times n}$ so $U_s^T U_s = I_s$

Nyström approximation

given $A \in \mathbf{S}_+^n$, approximate with the *Nyström method*:

- choose any test matrix $\Omega \in \mathbb{R}^{n \times s}$, $1 \le s \le n$
- *Nyström approximation* of A wrt Ω is [Tropp et al. (2017)]

$$A\langle\Omega\rangle = (A\Omega)(\Omega^T A\Omega)^\dagger (A\Omega)^T.$$

properties:

- $A\langle\Omega\rangle \in \mathbf{S}_+^n$
- $\mathbf{rank}(A\langle\Omega\rangle) \le s$
- $A\langle\Omega\rangle \preceq A$

Efficient eigs via randomized NLA

given $A \in \mathbf{S}_+^n$, find a good rank-s approximation:

- draw random Gaussian matrix $\Omega \in \mathbb{R}^{n \times s}$
- compute randomized linear sketch $Y = A\Omega$.
- form *Nyström approximation*

$$\hat{A}_{\text{nys}} = (A\Omega)(\Omega^T A\Omega)^\dagger (A\Omega)^T = Y(\Omega^T Y)^\dagger Y^T.$$

- in practice, construct apx eigs $\hat{A} = V\hat{\Lambda}V^T$ using tall-skinny QR, small SVD

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properties:

- requires only matvecs with A, streaming ok
- total computation: s matvecs + $O(ns^2)$
- total storage: $O(ns)$
- $\hat{A}_{\mathrm{nys}}$ is spd, $\mathbf{rank}(\hat{A}_{\mathrm{nys}}) \leq s$, and $\hat{A}_{\mathrm{nys}} \preceq A$

Randomized Nyström approximation: guarantees

define the *p-stable rank* $\mathrm{sr}_p(A) = \lambda_p^{-1} \sum_{j=p}^{n} \lambda_j$

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Theorem (Randomized Nyström approximation)

Let $A \in \mathbf{S}_+^n$ *with eigenvalues* $\lambda_1 \geq \cdots \geq \lambda_n$. *Pick any* $p \geq 2$ *and set sketch size* $s = 2p - 1$. *Draw a Gaussian random test matrix* $\Omega \in \mathbb{R}^{n \times s}$. *Then* $\hat{A}_{\mathrm{nys}}$ *satisfies*

$$\mathbb{E}\|A - \hat{A}_{\mathrm{nys}}\| \leq \left(3 + \frac{4e^2}{p}\mathrm{sr}_p(A)\right)\lambda_p.$$

- error of randomized rank-s approximation is comparable with best error of any rank-$p = \frac{s+1}{2}$ approximation

Outline

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Regularized linear system

find $x \in \mathbf{R}^n$ such that

$$(A + \mu I)x = b$$

where $A \in \mathbf{S}_+^n$ is symmetric psd and $\mu \geq 0$.

- eigenvalues of A $\lambda_1 \geq \cdots \geq \lambda_n$
- condition number $\kappa(A) = \lambda_1(A)/\lambda_n(A)$
- regularized matrix $A_\mu = A + \mu I$ has $\kappa(A_\mu) \leq \kappa(A)$
- matvec(A) time to compute matrix vector product Ax (often = nnz(A))

Sketch-and-solve

Given a rank-s (Nyström) approximation $A \approx \hat{A} = V\hat{\Lambda}V^T$, why not solve

$$(\hat{A} + \mu I)\hat{x} = b \qquad \text{instead of} \qquad (A + \mu I)x^\star = b?$$

- $(+)$ can apply inverse in $O(ns)$ time, since

$$(\hat{A} + \mu I)^{-1} = V(\hat{\Lambda} + \mu I)^{-1}V^T + \frac{1}{\mu}(I - VV^T)$$

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- $(+)$ works well if $b \in \mathbf{span}(V)$
- (-) high accuracy requires $s \to n$

Preconditioning CG

for any $P \succ 0$,

$$Ax = b \quad \Longleftrightarrow \quad \begin{aligned} P^{-1/2}Ax &= P^{-1/2}b \\ P^{-1/2}AP^{-1/2}z &= P^{-1/2}b \end{aligned}$$

where $x = P^{-1/2}z$.

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how to precondition?

- common heuristic: Jacobi preconditioning $P = \mathbf{diag}(A)$
- incomplete Cholesky (best for structured sparsity)

Sketch-and-precondition

Sketch-and-precondition [Avron, Maymounkov, and Toledo (2010), Martinsson and Tropp (2020), X. Meng, Saunders, and Mahoney (2014), and Rokhlin and Tygert (2008)]: for an overdetermined problem $A = X^T X$ where $X \in \mathbf{R}^{N \times n}$, $N \gg n$,

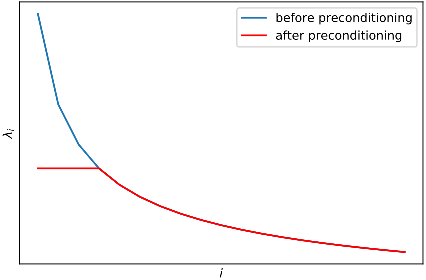
- pick *sketch size* $s = \Omega(n)$
- draw random matrix $S \in \mathbb{R}^{s \times n}$ (eg, iid normal entries)
- compute randomized *sketch* SX
- compute pivoted-QR factorization $SX = QR$
- precondition with $P = R^{-1}$

$O(n^3)$ flops, so only useful for moderate n

An optimal low-rank preconditioner

- suppose $\lfloor A \rfloor_s = V_s \Lambda_s V_s^T$ is a best rank-s apx to $A \in \mathbf{S}_+^n$.
- the best preconditioner using this information is

$$P_\star = \frac{1}{\lambda_{s+1}} V_s(\Lambda_s) V_s^T + (I - V_s V_s^T)$$



Nyström preconditioner

Given a rank-s Nyström approximation

$$\hat{A}_{\text{nys}} = V\hat{\Lambda}V^T \qquad \approx \qquad A \in \mathbf{S}_+^n,$$

the *Nyström preconditioner* for $(A + \mu I)x = b$ is

$$P_{\text{nys}} = \frac{1}{\hat{\lambda}_s + \mu} V(\hat{\Lambda} + \mu I)V^T + (I - VV^T)$$

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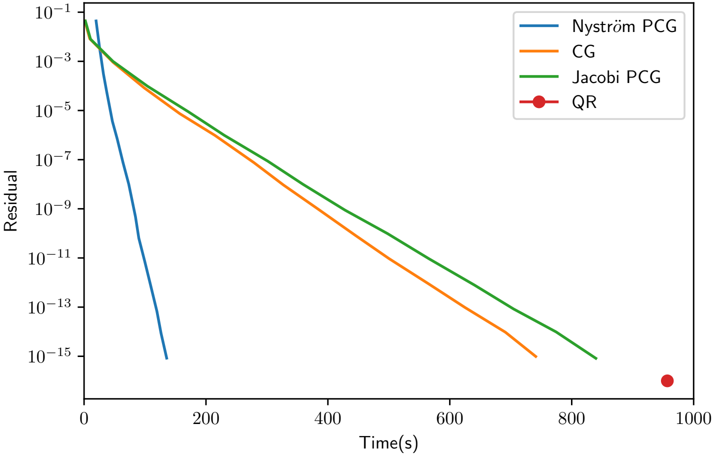
inverse can be applied in $O(ns)$:

$$P^{-1} = (\hat{\lambda}_s + \mu) V(\hat{\Lambda} + \mu I)^{-1} V^T + (I - VV^T)$$

Source: Frangella, Tropp, and Udell, 2023

Nyström preconditioner is fast!



Random features regression on YearMSD dataset ($463,715 \times 15,000$).
Regularization $\mu = 10^{-5}$; sketch size $s = 500$.

Nyström PCG controls the condition number

Theorem (Nyström condition number bound)

Let P be the Nyström preconditioner with regularization parameter $\mu \geq 0$ and let $M = P^{-1/2} A_\mu P^{-1/2}$ be the preconditioned matrix. Define the error $E = A - \hat{A}_{\mathrm{nys}}$. Then

$$\kappa(M) \leq \min \left\{ \frac{\hat{\lambda}_s + \mu + \|E\|}{\mu},\ 1 + \frac{\|E\|}{\hat{\lambda}_s + \mu} + \frac{\hat{\lambda}_s + \mu + \|E\|}{\lambda_n + \mu} \right\}.$$

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corollary: for large enough s, $\hat{\lambda}_s \leq \mu$ and $\|E\| \leq \mu$, so

$$\kappa_2(P^{-1/2} A_\mu P^{-1/2}) \leq 3.$$

How to choose sketch size?

how to get $\|E\| \sim \mu$?

- fixed sketch size $s = 50$ (works surprisingly well!)
- adaptive: increase sketch size until (estimated) error is small enough
  - $\|E\| \approx \hat{\lambda}_\ell$
  - add one dimension to sketch for a-posteriori error guarantee [Tropp et al. (2019)]
- a priori, bound sketch size needed to ensure $\|E\| \sim \mu$

A priori bound via the effective dimension

the *effective dimension* at μ is a smoothed count of evs $\geq \mu$:

$$d_{\mathsf{eff}}(\mu) = \sum_{j=1}^{n} \frac{\lambda_j}{\lambda_j + \mu}.$$

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the effective dimension bounds sketch size required for constant condition number

Theorem

Construct the randomized Nyström preconditioner P with rank $s = 2\lceil 1.5 d_{\text{eff}}(\mu) \rceil + 1$. Then

$$\mathbb{E}\left[\kappa(P^{-1/2} A_\mu P^{-1/2})\right] < 28.$$

So whp relative error is $< \epsilon$ after $T \leq \lceil 2.7 \log(\frac{2}{\epsilon}) \rceil$ iterations.

PCG converges fast when $s \sim d_{\text{eff}}$

plug in bound on condition number to CG convergence theory:

Corollary

Let $M = P^{-1/2} A_\mu P^{-1/2}$, and suppose

$$\kappa(M) < 28.$$

Then relative error $\delta_t := \|x_t - x_\star\|_M / \|x_\star\|_M$ of PCG iterate x_t, initialized with $x_0 = 0$, satisfies

$$\delta_t < 2\,(0.69)^t$$

and PCG attains relative error $\delta_t < \epsilon$ after $T \leq \lceil 2.7 \log(\frac{2}{\epsilon}) \rceil$ iterations.

Experimental results

Dataset	Method	# iterations	Runtime (s)
Higgs-rf	AdaIHS	55	$1,052.7$
	R&T	53	607.4
	Adaptive Nyström	**28**	**91.26**
YearMSD-rf	AdaIHS	44	$1,327.3$
	R&T	49	766.5
	Adaptive Nyström	**22**	**209.7**
EMNIST	Random features PCG	154	635.2
	Nyström	**32**	**268.4**
Santander	Random features PCG	160	810.4
	Nyström	**31**	**164.8**

Table: Nyström PCG is faster than other randomized preconditioners.

- For Higgs and YearMSD, s uses a posteriori error estimation.
- For EMNIST and Santander, $s = 1,000$
- R&T: sketch-and-precondition method [Rokhlin and Tygert (2008)]
- AdaIHS: Adaptive iterative Hessian sketch [Lacotte and Pilanci (2020)]
- Random features PCG [Avron, Clarkson, and Woodruff (2017)] uses $s = 1000$

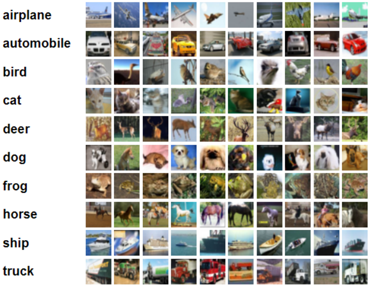
Numerics: details

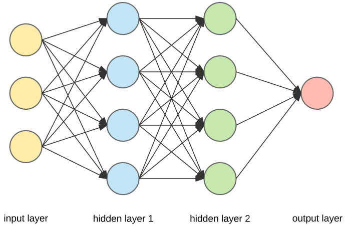
Dataset	n	d	# classes	μ	σ	PCG tolerance
Higgs-rf	800,000	10,000	2	1e-4	5	1e-10
YearMSD-rf	463,715	15,000	NA	1e-5	8	1e-10
EMNIST	105,280	784	47	1e-6	8	1e-3
Santander	160,000	200	2	1e-6	7	1e-3

Table: Datasets: statistics and parameters.

Outline

Classification with neural network

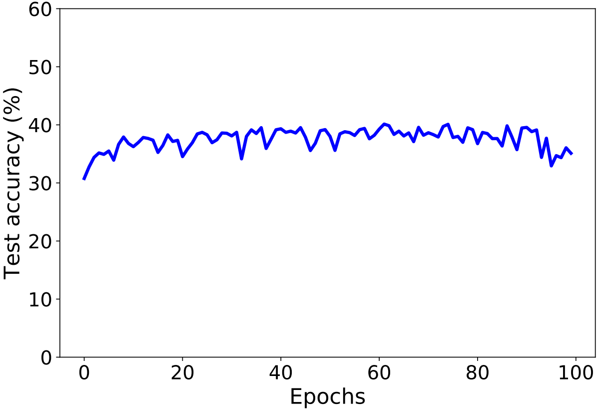




- CIFAR-10 dataset, tabular version
- basic MLP network
- use Adam to train the neural network

Adam needs babysitting

Adam is sensitive to hyperparameter settings



learning rate 0.005

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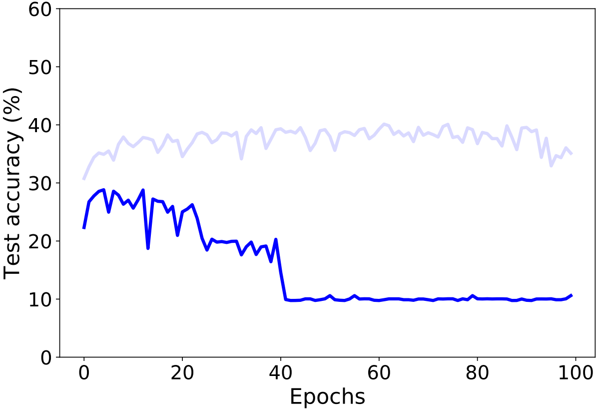

learning rate 0.01

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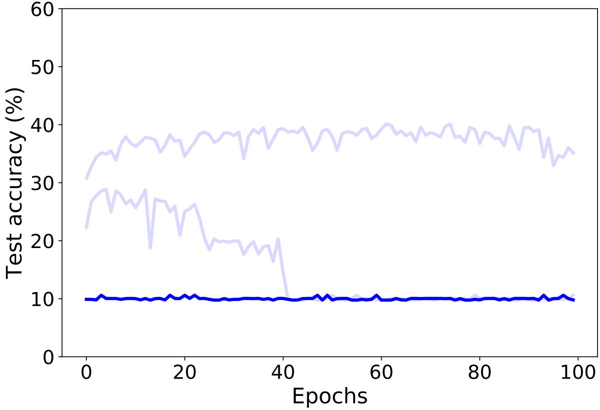
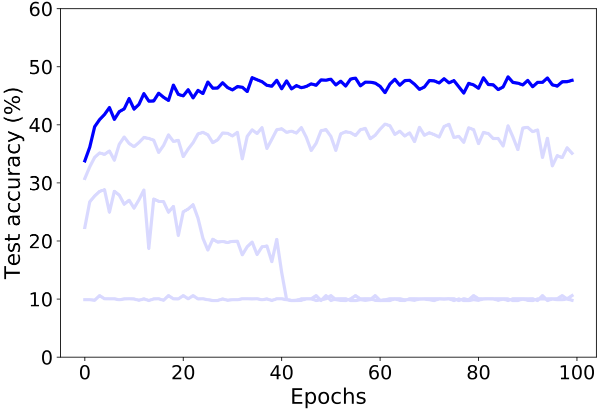


learning rate 0.02

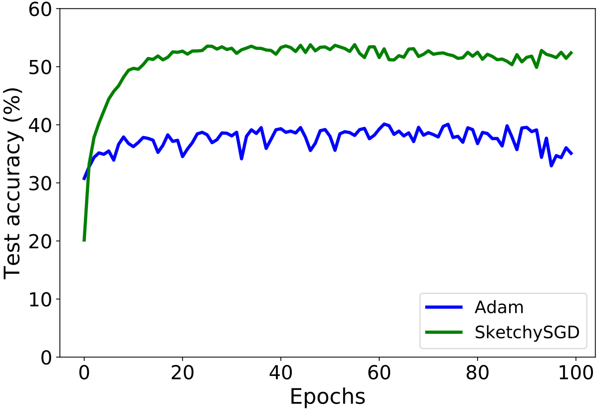
Adam needs babysitting

Adam is sensitive to hyperparameter settings



learning rate 0.001

Preconditioning improves robustness



learning rate 0.005

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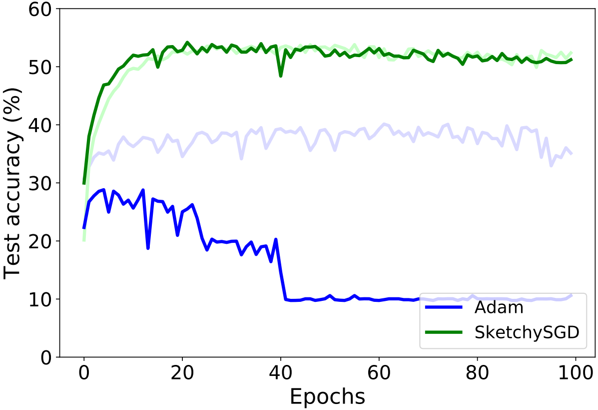

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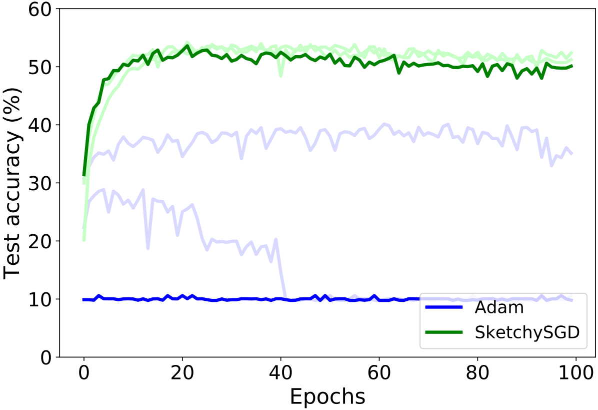

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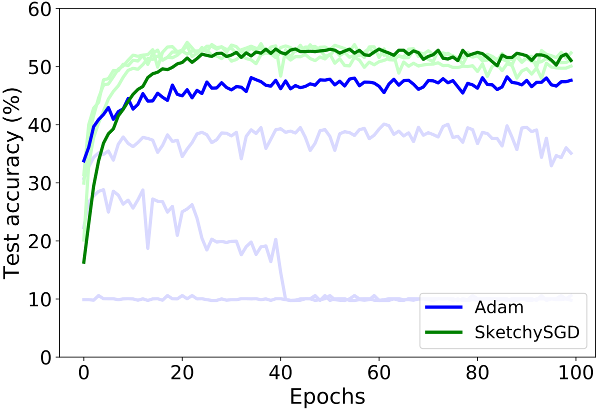

learning rate 0.001

Bad tuning $\implies$ slow convergence

how does initial learning rate affect performance?

- ResNet-20 architecture
- CIFAR-10 dataset
  ($m_{\mathrm{tr}} = 50,000$, $m_{\mathrm{tst}} = 10,000$, $n = 3,072$)
- SGD and Adam optimizers
- initialize learning rate η at

  $$\{10^{-4}, 3{\cdot}10^{-4}, 10^{-3}, 3{\cdot}10^{-3}, 10^{-2}, 3{\cdot}10^{-2}, 10^{-1}, 3{\cdot}10^{-1}, 10^{0}, 3{\cdot}10^{0}\}$$

- follow best practices to decay η throughout training

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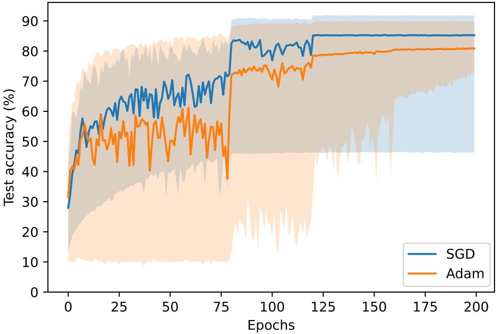

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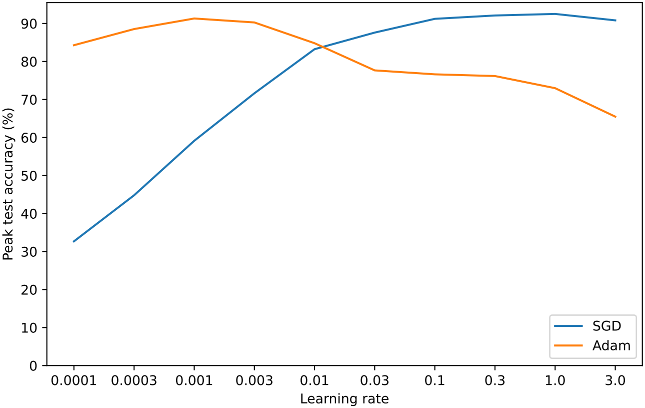
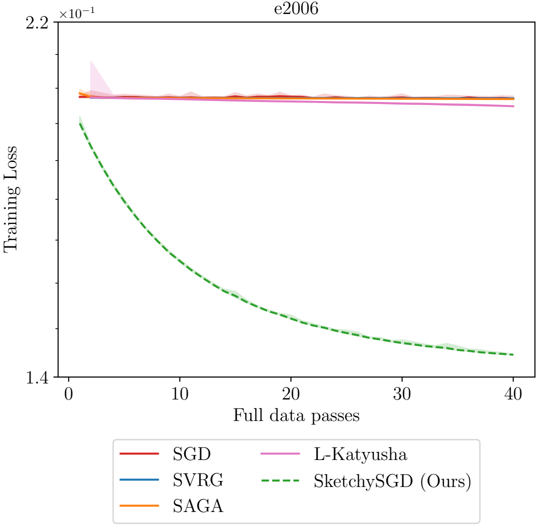


Ill-conditioning $\implies$ slow convergence

experiment on ill-conditioned dataset

- ridge regression on E2006-dataset ($m = 16,087, p = 150,360$)
- (small) l_2-regularization $\nu = \frac{10^{-2}}{m}$
- state of the art first order methods for this problem: SGD, SVRG, SAGA, L-Katyusha, tuned for best performance
- SketchySGD with default parameters

Ill-conditioning $\Longrightarrow$ slow convergence



Stochastic optimization

consider the empirical risk minimization problem for $w \in \mathbf{R}^p$

$$\text{minimize} \quad \frac{1}{n}\sum_{i=1}^{n} f_i(w)$$

stochastic gradient method (SGD):

$$w \leftarrow w - \eta g \quad \text{where} \quad g \approx \nabla f(w)$$

works if $\mathbf{E}\, g = \nabla f(w)$

Preconditioned stochastic optimization

stochastic quasi-Newton method:

$$w \leftarrow w - \eta H^{-1} g \quad \text{where} \quad g \approx \nabla f(w),\; H \approx \nabla^2 f(w)$$

pros:

- faster convergence
- more robust to ill-conditioned problems (= all ML problems)
- easier to choose hyperparameters (learning rate η)

cons:

- $\nabla^2 f(x)$ is expensive to compute and apply

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Q: Why not use Quasi-Newton methods like (L-)BFGS?

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Q: Why not use Quasi-Newton methods like (L-)BFGS?
A: Classical QN requires full gradient evaluations

How to approximate $\nabla^2 f(x)$?

- from a data subsample
- from stale data
- by the secant condition (BFGS, l-BFGS)
- by diagonal approximation (adaHessian)
- by block-diagonal kronecker approximation (Shampoo, KFAC, SENG, K-BFGS)
- by low rank approximation (sketchySGD)

Source: Erdogdu and Montanari, 2015, Shampoo Gupta, Koren, and Singer, 2018, Roosta-Khorasani and Mahoney, 2019, Bollapragada, Byrd, and Nocedal, 2019, AdaHessian Yao et al., 2021, R-SSN S. Y. Meng et al., 2020, KFAC Grosse and Martens, 2016, SENG Yang et al., 2020, Goldfarb, Ren, and Bahamou, 2020

Subsampling the Hessian

Hessian of $f(w) = \frac{1}{n}\sum_{i=1}^{n} f_i(w)$ is

$$\nabla^2 f(w) = \frac{1}{m}\sum_{i=1}^{m} \nabla^2 f_i(w)$$

Subsampled Hessian is

$$\widehat{\nabla}^2 f(w) = \frac{1}{|S|}\sum_{i\in S} \nabla^2 f_i(w),$$

where $S \subseteq \{1, \cdots, m\}$ is chosen uniformly at random.

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where $S \subseteq \{1, \cdots, m\}$ is chosen uniformly at random.

Subsampled Newton method:

$$w_{k+1} = w_k - \eta_k \left(\widehat{\nabla}^2 f(x_k)\right)^{-1} \widehat{\nabla} f(w_k)$$

More approximations, more problems

1. *complexity.* Hessian of single loss $f_i : \mathbf{R}^p \to \mathbf{R}$ costs p^2 to compute and to store
2. *invertibility.* Hessian approximation may not be invertible $\widehat{\nabla}^2 f(w_k)$
3. *descent.* (stochastic quasi-)Newton search direction

$$\left(\widehat{\nabla}^2 f(x_k)\right)^{-1} \widehat{\nabla} f(w_k)$$

may not be a descent direction

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   may not be a descent direction

solutions:

1. *complexity.* automatic differentiation
2. *invertibility.* use regularized Hessian approx $\widehat{\nabla}^2 + \rho I$
3. *descent.* harder ...

Complexity: how to access $\nabla^2 f(w)$?

our oracle: stochastic Hessian-vector products (HVPs)

1. minibatch loss $\tilde{f}(w) = \sum_{i \in S} f_i(w)$ for $S \subset \{1, \ldots, n\}$
2. compute minibatch gradient with automatic differentiation (AD) $\tilde{g}(w) = \nabla \tilde{f}(w)$
3. define minibatch Hessian vector product with vector v

$$(\nabla^2 \tilde{f}(w))v = \nabla(\tilde{g}(w) \cdot v)$$

   and compute using AD on $\tilde{g}(w) \cdot v$ (Pearlmutter's trick)

cost: two passes of AD $\approx 4\times$ cost of function evaluation

HVPs to find (stochastic quasi)-Newton direction

- CG (or MINRES, for indefinite $\widehat{\nabla}^2 f(x)$) to compute search direction
$$\left(\widehat{\nabla}^2 f(x_k)\right)^{-1} \widehat{\nabla} f(w_k)$$
uses only HVPs
  - problem: bad conditioning $\implies$ slow convergence of CG
- Nystrom approximation for regularized Hessian $\widehat{\nabla}^2 + \rho I$ uses only HVPs

SketchySGD

every now and then (e.g., each epoch),

- sample data batch S_k to sketch subsampled Hessian
$$H_{S_k}(w_k) = \frac{1}{|S_k|} \sum_{j \in S_k} \nabla^2 f_j(w_k)$$
- form rank r approximation $\hat{H}_{S_k}$

at each iteration k,

- sample data batch B_k
- form gradient estimate
$$g_{B_k}(w_k) = \frac{1}{|B_k|} \sum_{j \in B_k} g_j(w_k)$$
- take step
$$w_{k+1} = w_k - \eta_k (\hat{H}_{S_k} + \rho_k I)^{-1} g_{B_k}(w_k)$$

SketchySGD is fast

computing search direction v_k requires $O(pr)$ flops:

$$v_k = \hat{V}\left(\hat{\Lambda} + \rho_k I\right)^{-1} \hat{V}^T g_{B_k} + \frac{1}{\rho_k}(g_{B_k} - \hat{V}\hat{V}^T g_{B_k})$$

- the cost of a fresh low-rank Hessian approximation is $O((b_{h_k} + r^2)p)$.
- given Hessian approximation, per-iteration cost is $O\left((b_{g_k} + r)p\right)$.

Relative condition number

the *relative condition number* is $\hat{\kappa} = \hat{L}/\hat{\mu}$ where $\hat{L} \geq \hat{\mu} > 0$ are defined such that for all $w, w' \in \mathcal{X}$

$$f(w') \leq f(w) + \langle g(w), w' - w \rangle + \frac{\hat{L}}{2} \|w' - w\|_{H(w)}^2,$$
$$f(w') \geq f(w) + \langle g(w), w' - w \rangle + \frac{\hat{\mu}}{2} \|w' - w\|_{H(w)}^2.$$

(The condition number $\kappa = L/\mu$ is defined similarly, replacing $H(w)$ by I.)

Theory: convex

Suppose f_i are all smooth and convex and f is L-smooth and μ-strongly convex. Define

$$\lambda_{r+1}^{\star} = \sup_{w \in \mathcal{X}} \lambda_{r+1}(H(w)).$$

Observe $\lambda_{r+1}^{\star} \leq L$ and is often significantly smaller.

Corollary

Let $T_{\text{SketchySGD}}$ denote the iteration complexity of SketchySGD and T_{SGD} denote the iteration complexity of SGD given from Theorem 4.6 in Gower, Sebbouh, and Loizou, 2021. Then

$$\frac{T_{\text{SGD}}}{T_{\text{SketchySGD}}} \geq \frac{\hat{\mu}}{\hat{\kappa}} \frac{L}{30\lambda_{r+1}^{\star}}.$$

In particular, in the case of the least-squares loss we have

$$\frac{T_{\text{SGD}}}{T_{\text{SketchySGD}}} \geq \frac{L}{30\lambda_{r+1}^{\star}} = \frac{\lambda_1(H)}{30\lambda_{r+1}(H)}.$$

Theory: nonconvex

assumptions

- f and each f_i are twice differentiable and smooth
- f satisfies PL condition:

$$\|g(w)\|^2 \geq 2\theta(f(w) - f(w_\star)), \ \forall w$$

- interpolation: optimizer $w_\star \in \mathcal{W}_\star$ satisfies $\|g_i(w_\star)\| = 0$ for each $i \in \{1, \ldots n\}$

the SketchySGD iterate w_t after $t > 0$ iterations satisfies

$$\mathbb{E}[f(w_t)] - f(w_\star) \leq (1 - h(\theta))^t \, (f(w_0) - f(w_\star)).$$

- constant $h(\theta)$ has explicit analytical form
- linear convergence (optimality gap drops exponentially)

SketchySGD: simple parameter selection

For convex problems:

- Batch sizes set equal $b_g = b_h$. We used 256 in these examples.
- Fixed rank $r = 50$.
- Fixed regularization $\rho \in \{10^{-1}, 10^{-2}, 10^{-3}\}$ at every iteration. Here, $\rho = 10^{-3}$.
- Learning rate $\eta = \frac{1}{1+100\hat{\lambda}_r}$, where $\hat{\lambda}_r$ is the rth eigenvalue of the current subsampled Hessian approximation $\hat{H}$.
- Compute a fresh approximation $\hat{H}$ after each epoch or two.

For deep learning:

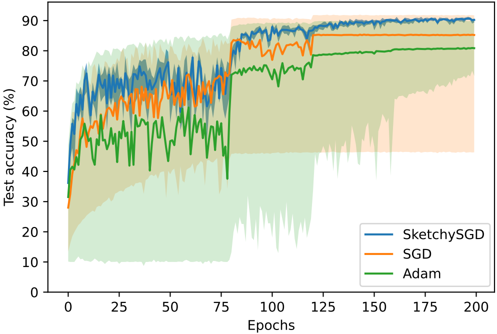
- Batch sizes set equal $b_g = b_h$. We used 128 in this paper.
- Fixed rank $r = 100$.
- Fixed learning rate $\eta = 10^{-2}$.
- Fixed regularization $\rho = \eta$ at every iteration.
- Compute a fresh approximation $\hat{H}$ after each epoch or two.

SOTAish results in deep learning

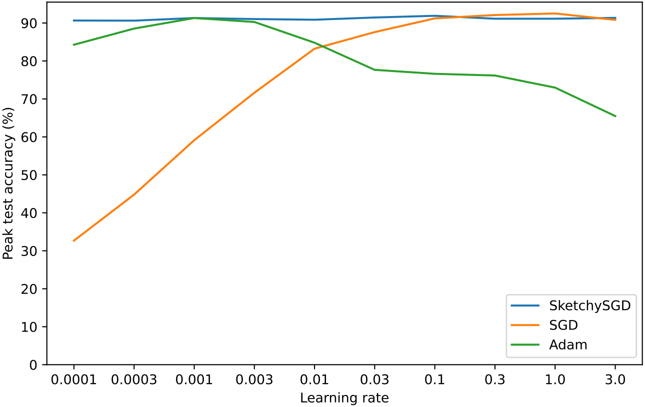
- SketchySGD uses the default parameter choices
- preconditioner is updated every 2 epochs
- all optimizers use the same learning rate decay

SketchySGD is reliable (CIFAR-10)

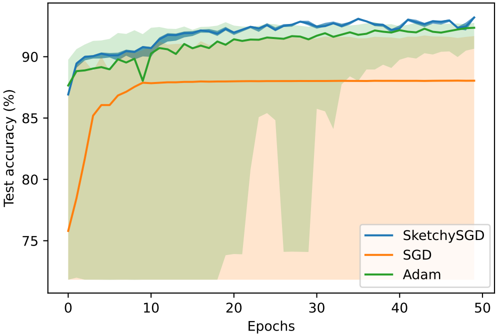
back to ResNet-20 on CIFAR-10



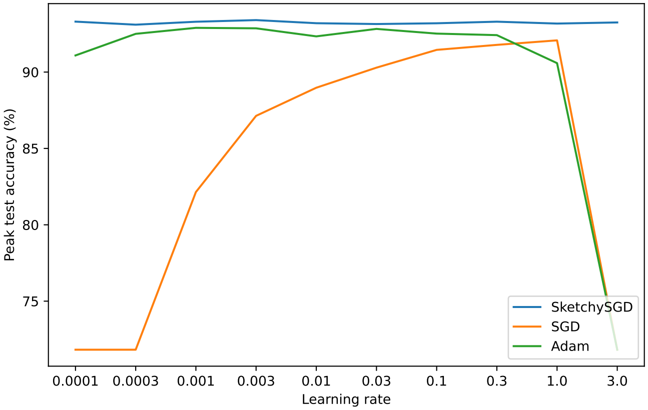
SketchySGD is near-optimal (CIFAR-10)



SketchySGD is reliable (Miniboone)

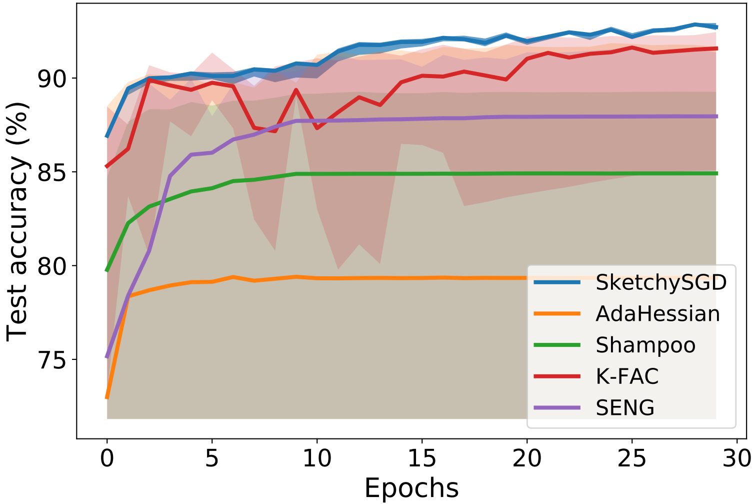


SketchySGD is near-optimal (Miniboone)

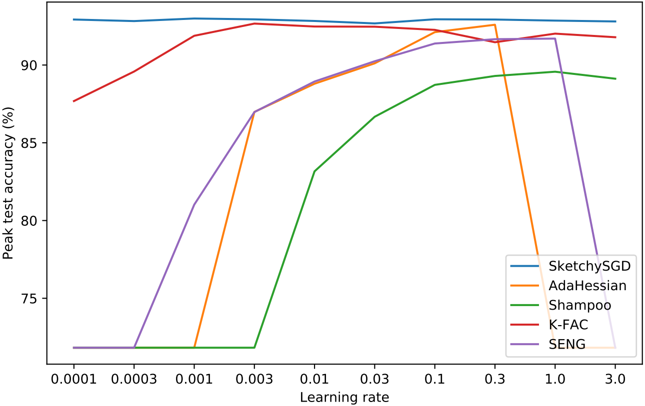


SketchySGD is more reliable than SQN competitors

stochastic quasi-Newton methods for DL on MiniBoone



SketchySGD outperforms SQN competitors



Outline

Composite optimization

$$\text{minimize} \quad \ell(Ax) + r(x)$$

- $A : \mathbf{R}^n \to \mathbf{R}^m$ linear
- $\ell : \mathbf{R}^m \to \mathbf{R}$ smooth
- $r : \mathbf{R}^n \to \mathbf{R}$ proxable
  - easy (often closed form) solution to $\mathbf{prox}_r(x) = \mathrm{argmin}_y \, r(y) + \frac{1}{2}\|x - y\|^2$
  - e.g., for $r(x) = \|x\|_1$, $\mathbf{prox}_r(x)$ is soft-thresholding operator

Example: Lasso

$$\text{minimize} \quad \frac{1}{2}\|Ax - b\|_2^2 + \gamma\|x\|_1$$

- $\ell(Ax) = \frac{1}{2}\|Ax - b\|_2^2$ smooth
- $r(x) = \gamma\|x\|_1$ proxable
- parameter $\gamma > 0$ controls strength of regularization

Example: Lasso

$$\text{minimize} \quad \frac{1}{2}\|Ax - b\|_2^2 + \gamma\|x\|_1$$

- $\ell(Ax) = \frac{1}{2}\|Ax - b\|_2^2$ smooth
- $r(x) = \gamma\|x\|_1$ proxable
- parameter $\gamma > 0$ controls strength of regularization

other examples: regularized logistic regression, SVM, ...

ADMM

consider the problem

$$\begin{array}{ll} \text{minimize} & f(x) + g(z) \\ \text{subject to} & Ax + Bz = c \end{array}$$

Augmented Lagrangian for this problem (with dual variable y) is

$$L_t(x, z, y) = f(x) + g(z) + y^T(Ax + Bz - c) + t/2\|Ax + Bz - c\|^2$$

Alternating Directions Method of Multipliers (ADMM) iteration is

$$\begin{aligned} x^{(k+1)} &= \operatorname*{argmin}_x L_t(x, z^{(k)}, y^{(k)}) \\ z^{(k+1)} &= \operatorname*{argmin}_z L_t(x^{(k+1)}, z, y^{(k)}) \\ y^{(k+1)} &= y^{(k)} + \frac{1}{t}(Ax^{(k+1)} + Bz^{(k+1)} - c) \end{aligned}$$

ADMM

properties:

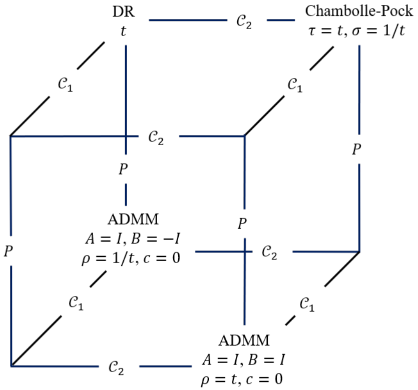
- converges for any $t > 0$ (but can be very slow)
- letting $y = tu$, equivalent to the iteration

$$\begin{aligned} x^{(k+1)} &= \underset{x}{\operatorname{argmin}}\, f(x) + t/2\|Ax + Bz^{(k)} - c + u^{(k)}\|^2 \\ z^{(k+1)} &= \underset{z}{\operatorname{argmin}}\, g(z) + t/2\|Ax^{(k+1)} + Bz - c + u^{(k)}\|^2 \\ u^{(k+1)} &= u^{(k)} + Ax^{(k+1)} + Bz^{(k+1)} - c \end{aligned}$$

- frequently used for distributed optimization:
  problems decouple if A or B is diagonal

Equivalence between iterative algorithms for optimization

Figure: relations between DR, ADMM, and Chambolle-Pock.



Source: [Zhao, Lessard, and Udell (2021)]

ADMM for statistical learning

Algorithm ADMM

Input: loss function $\ell \circ A$, regularization r, stepsize ρ,
initial z^0, $u^0 = 0$
for $k = 0, 1, \ldots$ **do**
    $x^{k+1} = \text{argmin}_x \{\ell(Ax) + \frac{\rho}{2}\|x - z^k + u^k\|_2^2\}$
    $z^{k+1} = \textbf{prox}_{\frac{2}{\rho} r(z)}(x^{k+1} + u^k)$
    $u^{k+1} = u^k + x^{k+1} - z^{k+1}$
return $x_\star$ (nearly) minimizing $\ell(Ax) + r(x)$

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ADMM for statistical learning

Algorithm ADMM

```
Input: loss function ℓ ∘ A, regularization r, stepsize ρ,
initial z^0, u^0 = 0
for k = 0, 1, ... do
    x^{k+1} = argmin_x {ℓ(Ax) + ρ/2 ‖x − z^k + u^k‖_2^2}
    z^{k+1} = argmin_z {r(z) + ρ/2 ‖x^{k+1} − z + u^k‖_2^2}
    u^{k+1} = u^k + x^{k+1} − z^{k+1}
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solution: inexact ADMM

- solve x-min approximately with error ε^k
- converges if $\sum_k \varepsilon^k < \infty$ [Eckstein and Bertsekas (1992)]

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add randNLA: use Nyström PCG to speed up x-min

Quadratic approximation

if ℓ is twice diffable, approximate obj near prev iterate x^k

$$\ell(Ax) \approx \ell(Ax^k) + (x - x^k)^T A^T \nabla \ell(Ax^k) + \frac{1}{2}(x - x^k)^T A^T H_\ell(Ax^k) A(x - x^{k}$$

where H_ℓ is the Hessian of ℓ.

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where H_ℓ is the Hessian of ℓ.

with this approximation, x-min becomes linear system: find x so

$$(A^T H_\ell(Ax^k) A + \rho I)x = r^k$$

where $r^k = \rho z^k - \rho u^k + A^T H_\ell(Ax^k) A x^k - A^T \nabla \ell(Ax^k)$

Nyström PCG to solve ADMM subproblem

$$(A^T H_\ell(x^k)A + \rho I)x = r^k$$

- $A^T H_\ell(x^k)A$ has data in it $\implies$ fast spectral decay
- stepsize ρ regularizes linear system
- if ℓ is quadratic (e.g., lasso and SVM), $H_\ell(x^k) = H_\ell$ is constant, so only need to sketch $A^T H_\ell A$ once

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in theory:

- solve to tolerance ϵ^k at iteration k, where $\sum_k \epsilon^k < \infty$
- if sketch size $s \approx d_{\text{eff}}(\rho)$, need $\leq O(\log(1/\epsilon^k))$ CG steps

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- solve to tolerance ϵ^k at iteration k, where $\sum_k \epsilon^k < \infty$
- if sketch size $s \approx d_{\text{eff}}(\rho)$, need $\leq O(\log(1/\epsilon^k))$ CG steps

in practice:

- set $\epsilon^k = \text{geomean}(\text{primal resid}, \text{dual resid})$
- set sketch size $s = 50$

NysADMM algorithm

Algorithm NysADMM

input loss function $\ell \circ A$, regularization r, stepsize ρ, positive summable sequence $\{\varepsilon^k\}_{k=0}^{\infty}$, initial z^0, $u^0 = 0$

for $k = 0, 1, \ldots$ **do**

  compute $r^k = \rho z^k - \rho u^k + A^T H_\ell(Ax^k)Ax^k - A^T \nabla \ell(Ax^k)$

  use Nyström PCG to find ε^k-apx solution x^{k+1} to

$$(A^T H_\ell(Ax^k)A + \rho I)x^{k+1} = r^k$$

  $z^{k+1} = \text{argmin}_z \{r(z) + \frac{\rho}{2}\|x^{k+1} - z + u^k\|_2^2\}$

  $u^{k+1} = u^k + x^{k+1} - z^{k+1}$

return $x_\star$ (nearly) minimizing $\ell(Ax) + r(x)$

Source: Zhao, Frangella, and Udell, 2022

The competition

lasso:

- SSNAL, a Newton augmented Lagrangian method [Li, Sun, and Toh (2018)]
- mfIPM, a matrix-free interior point method [Fountoulakis, Gondzio, and Zhlobich (2014)]
- glmnet, a coordinate-descent method [Friedman, Hastie, and Tibshirani (2010)]

logistic regression:

- SAGA, a stochastic average gradient method [Defazio, Bach, and Lacoste-Julien (2014)]

SVM:

- LIBSVM, a sequential minimal optimization (pairwise coordinate descent) method [Chang and Lin (2011)]

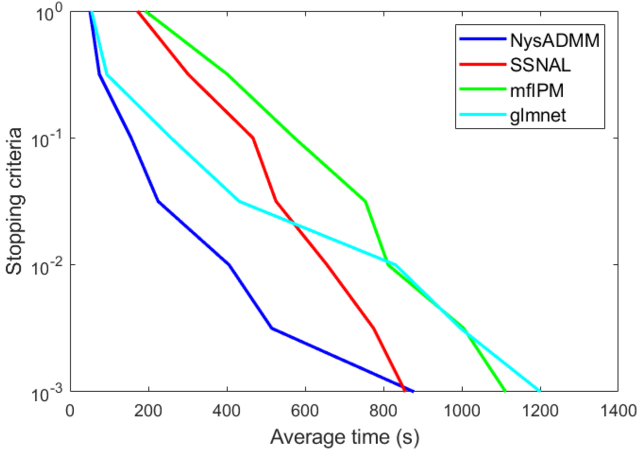
Numerical experiments: settings

- pick datasets with $n > 10,000$ or $d > 10,000$ from LIBSVM, UCI, and OpenML.
- use random feature map to generate more features
- use same stopping criterion and parameter settings as the standard solver for each problem class
- constant sketch size $s = 30$

Lasso results

stl10 dataset. stop iteration when

$$\frac{\|x - \mathrm{prox}_{\gamma\|\cdot\|_1}(x - A^T(Ax - b))\|}{1 + \|x\| + \|Ax - b\|} \leq \epsilon.$$



Lasso results

Task	Time for $\epsilon = 10^{-1}$ (s)			
	NysADMM	mfIPM	SSNAL	glmnet
STL-10	**165**	573	467	278
CIFAR-10-rf	**251**	655	692	391
smallNorb-rf	**219**	552	515	293
E2006.train	**313**	875	903	554
sector	**235**	678	608	396
realsim-rf	**193**	–	765	292
rcv1-rf	**226**	563	595	273
cod-rna-rf	**208**	976	865	324

ℓ_1-regularized logistic regression results

Table: Results for ℓ_1-regularized logistic regression experiment.

Task	NysADMM time (s)	SAGA (sklearn) time (s)
STL-10	**3012**	6083
CIFAR-10-rf	**7884**	21256
p53-rf	**528**	2116
connect-4-rf	**866**	4781
smallnorb-rf	**1808**	6381
rcv1-rf	**1237**	3988
con-rna-rf	**7528**	21513

Support vector machine results

NysADMM is $\geq 5\times$ faster, although code is pure python!

Table: Results of SVM experiment.

Task	NysADMM time (s)	LIBSVM time (s)
STL-10	**208**	11573
CIFAR-10	**1636**	8563
p53-rf	**291**	919
connect-4-rf	**7073**	42762
realsim-rf	**17045**	52397
rcv1-rf	**564**	32848
cod-rna-rf	**4942**	36791

What approximations are allowed?

Source: Frangella et al., 2023

Conclusion

low rank structure is everywhere! use it to accelerate

- top-k eigenvalue decomposition
- (regularized) linear system solve: $(A + \mu I)x = b$
- composite optimization: minimize $\ell(x) + r(x)$
- stochastic gradient descent
- ... your favorite problem ... ?