

# Batched Stochastic Gradient Descent with Weighted Sampling

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# Includes joint works with

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# Objective

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▶ Minimize:

$$F(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n f_i(\mathbf{x}) = \mathbb{E} f_i(\mathbf{x})$$

▶ Examples:

- ▶ Linear Feasibility ( $A\mathbf{x} \leq \mathbf{b}$ )
- ▶ Least Squares

$$\mathbf{x}_{LS} \stackrel{\text{def}}{=} \operatorname{argmin}_{\mathbf{x} \in \mathbb{R}^m} \frac{1}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2 = \operatorname{argmin}_{\mathbf{x} \in \mathbb{R}^m} \frac{1}{n} \sum_{i=1}^n \frac{n}{2} (\mathbf{b}_i - \langle \mathbf{a}_i, \mathbf{x} \rangle)^2 = \operatorname{argmin}_{\mathbf{x} \in \mathbb{R}^m} \mathbb{E} f_i(\mathbf{x})$$

- ▶ Hinge Loss

$$\mathbf{x}_{HL} \stackrel{\text{def}}{=} \operatorname{argmin}_{\mathbf{w} \in \mathbb{R}^m} \frac{1}{n} \sum_{i=1}^n [1 - y_i \langle \mathbf{w}, \mathbf{x}_i \rangle]_+ + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$



# Assumptions

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▶ Strong Convexity:

$$\langle \mathbf{x} - \mathbf{y}, \nabla F(\mathbf{x}) - \nabla F(\mathbf{y}) \rangle \geq \mu \|\mathbf{x} - \mathbf{y}\|_2^2$$

▶ Residual:

$$\frac{1}{n} \sum_{i=1}^n \|\nabla f_i(\mathbf{x}_*)\|_2^2 \leq \sigma^2$$

▶ Smoothness:

$$\|\nabla f_i(\mathbf{x}) - \nabla f_i(\mathbf{y})\|_2 \leq L_i \|\mathbf{x} - \mathbf{y}\|_2$$

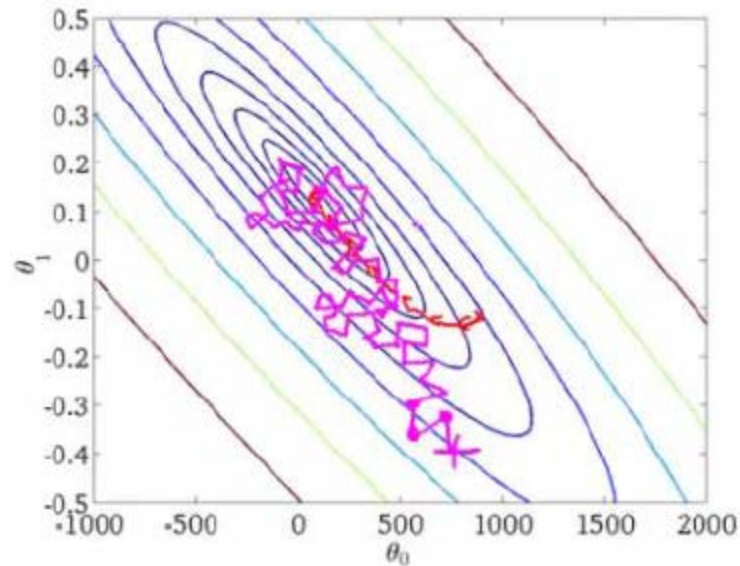
- ▶ -or- functionals themselves have bounded Lipschitz (later)



# Stochastic Gradient Descent

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$$\mathbf{x}_{k+1} \leftarrow \mathbf{x}_k - \gamma \nabla f_{i_k}(\mathbf{x}_k)$$



# Convergence Guarantees

---

▶ Can guarantee  $\mathbb{E} \|\mathbf{x}_k - \mathbf{x}_*\|_2^2 \leq \varepsilon$  after:

▶ [Bach & Moulines '11]:

$$k = 2 \log(\varepsilon_0 / \varepsilon) \left( \left( \frac{\sqrt{\frac{1}{n} \sum_i L_i^2}}{\mu} \right)^2 + \frac{\sigma^2}{\mu^2 \varepsilon} \right)$$

▶ [N & Srebro & Ward '16]:

$$k = 2 \log(\varepsilon / \varepsilon_0) \left( \frac{\sup_i L_i}{\mu} + \frac{\sigma^2}{\mu^2 \varepsilon} \right)$$



# Tightness

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▶ Can guarantee  $\mathbb{E} \|\mathbf{x}_k - \mathbf{x}_*\|_2^2 \leq \varepsilon$  after:

▶ [N & Srebro & Ward '16]:  $k = 2 \log(\varepsilon/\varepsilon_0) \left( \frac{\sup_i L_i}{\mu} + \frac{\sigma^2}{\mu^2 \varepsilon} \right)$

$$\begin{pmatrix} 1 & 0 \\ 0 & 1/\sqrt{n} \\ 0 & 1/\sqrt{n} \\ \vdots & \vdots \\ 0 & 1/\sqrt{n} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$\frac{\sup_i L_i}{\mu} = n \sup_i \|\mathbf{a}_i\|^2 \|\mathbf{A}^\dagger\|^2 = n$$



# Convergence Guarantees

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▶ [N & Srebro & Ward '16]:  $k = 2 \log(\varepsilon/\varepsilon_0) \left( \frac{\sup_i L_i}{\mu} + \frac{\sigma^2}{\mu^2 \varepsilon} \right)$

▶ *With weighted sampling (proportional to  $L_i$ ):*

$$k = 2 \log(\varepsilon/\varepsilon_0) \left( \frac{\frac{1}{n} \sum_i L_i}{\mu} + \frac{(\sum_i L_i)^2 \sigma^2}{n^2 L_{\min} \mu^2 \varepsilon} \right)$$

▶ *With partially weighted sampling (proportional to  $1/2 + 1/2 L_i$ ):*

$$k = 4 \log(\varepsilon_0/\varepsilon) \left( \frac{\frac{1}{n} \sum_i L_i}{\mu} + \frac{\sigma^2}{\mu^2 \varepsilon} \right)$$

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# Convergence – Other scenarios

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- ▶ Can guarantee  $\mathbb{E}\|\mathbf{x}_k - \mathbf{x}_*\|_2^2 \leq \varepsilon$  using partially weighted sampling after:

- ▶ In the smooth, non-strongly convex case:

$$k = O\left(\frac{\bar{L}\|\mathbf{x}_*\|_2^2}{\varepsilon} \cdot \frac{F(\mathbf{x}_*) + \varepsilon}{\varepsilon}\right)$$

- ▶ In the strongly convex, non-smooth case:

- Using subgradients, and assuming functionals have Lipschitz  $G_i$   
We have  $\mathbb{E}[F(\mathbf{x}_k) - F(\mathbf{x}_*)] \leq \varepsilon$  after:

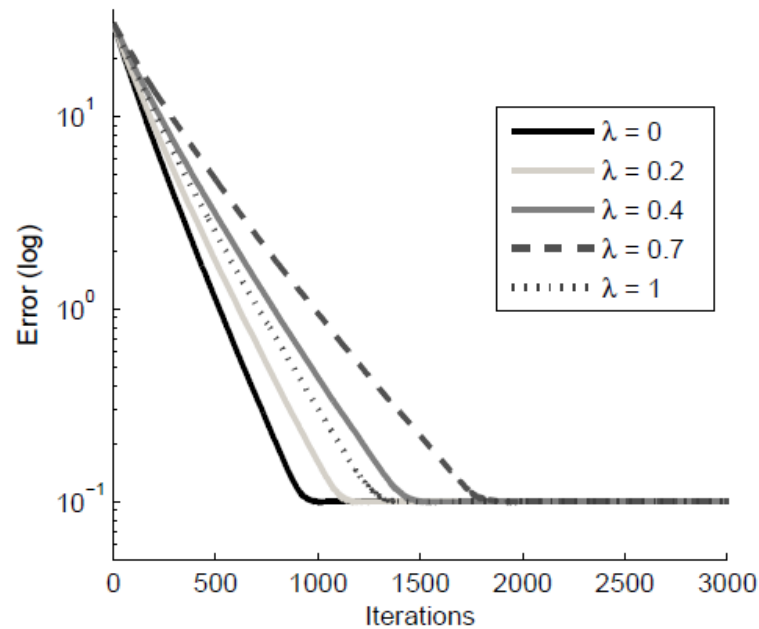
$$k = O\left(\frac{(\sum_i G_i)^2}{\mu\varepsilon}\right)$$



# Experiments – Least Squares

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- ▶ Consider sampling with weights  $\lambda$  proportion of the time



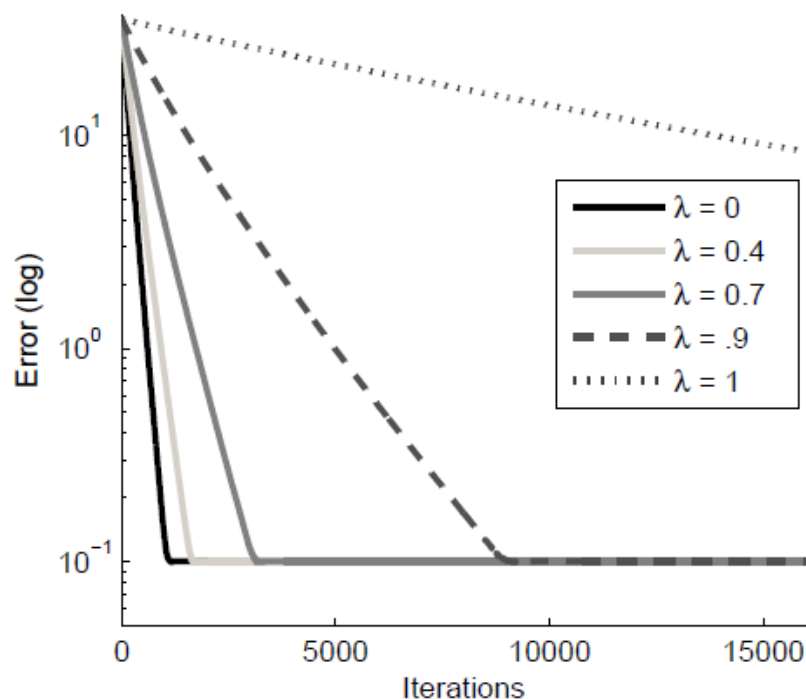
Gaussian Matrix  $\sim N(0, I)$

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# Experiments – Least Squares

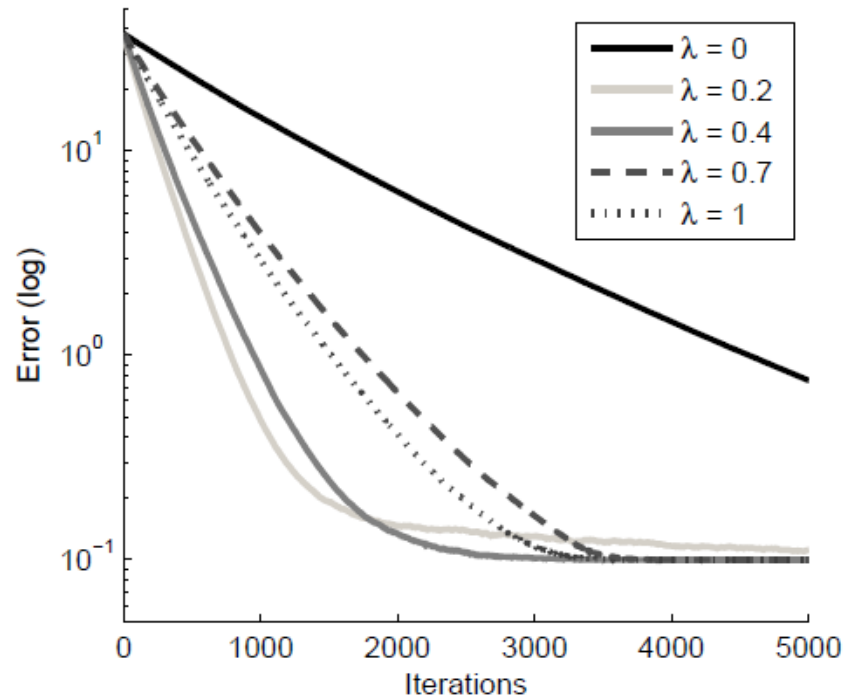
- ▶ Consider sampling with weights  $\lambda$  proportion of the time



Gaussian Matrix  $\sim N(0, I)$ , last row  $N(0, 100)$

# Experiments – Least Squares

- ▶ Consider sampling with weights  $\lambda$  proportion of the time

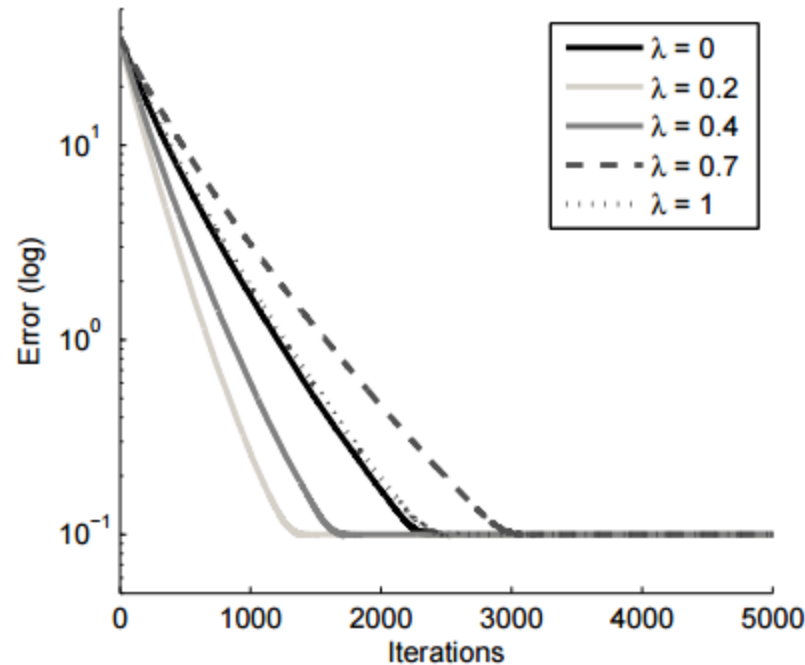


Gaussian Matrix,  $A_{ij} \sim N(0,j)$ , large residual

# Experiments – Least Squares

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- ▶ Consider sampling with weights  $\lambda$  proportion of the time



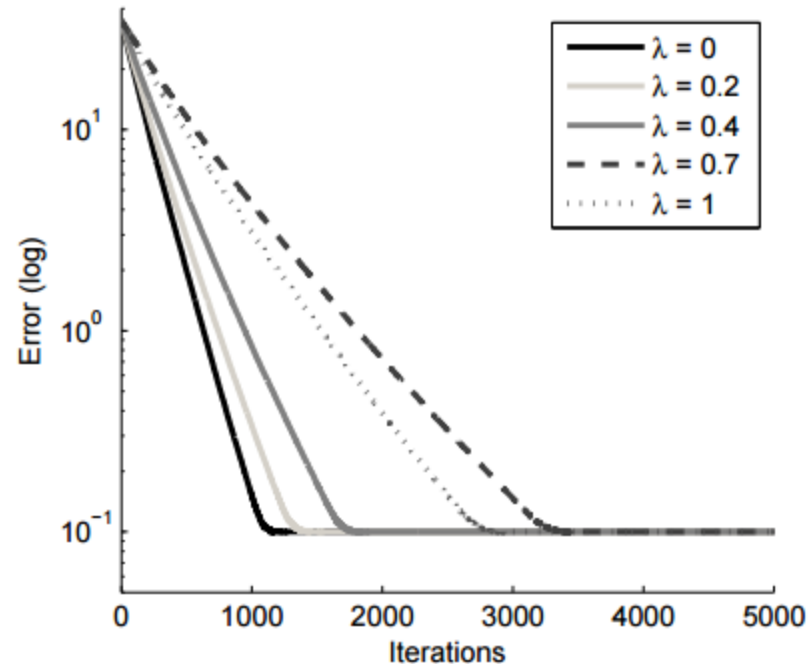
Gaussian Matrix,  $A_{ij} \sim N(0,j)$ , medium residual

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# Experiments – Least Squares

- ▶ Consider sampling with weights  $\lambda$  proportion of the time



Gaussian Matrix,  $A_{ij} \sim N(0,j)$ , small residual



# SGD with batching and weighting

---

- ▶ Batch functionals into  $d$  batches of size  $b$  ( $b$  cores)

$$F(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n f_i(\mathbf{x}) = \mathbb{E} f_i(\mathbf{x}) \rightarrow F(\mathbf{x}) = \frac{1}{d} \sum_{i=1}^d g_{\tau_i}(\mathbf{x}) = \mathbb{E} g_{\tau_i}(\mathbf{x})$$



# SGD with batching and weighting

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- The strong convexity parameter  $\mu$  for the function  $F$  remains invariant to the batching rule.
- The residual error  $\sigma_\tau^2$  such that  $\frac{1}{d} \sum_{i=1}^d \|\nabla g_{\tau_i}(x_*)\|_2^2 \leq \sigma_\tau^2$  can only **decrease** with increasing batch size, since

$$\sigma_\tau^2 = \frac{1}{d} \sum_{k=1}^d \left\| \frac{1}{b} \nabla \left( \sum_{k \in \tau_i} f_k(\mathbf{x}) \right) \right\|_2^2 \leq \frac{1}{n} \sum_{i=1}^n \|\nabla f_i(\mathbf{x})\|_2^2 \leq \sigma^2.$$



# SGD with batching and weighting

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- The strong convexity parameter  $\mu$  for the function  $F$  remains invariant to the batching rule.
- The residual error  $\sigma_\tau^2$  such that  $\frac{1}{d} \sum_{i=1}^d \|\nabla g_{\tau_i}(x_*)\|_2^2 \leq \sigma_\tau^2$  can only **decrease** with increasing batch size, since

$$\sigma_\tau^2 = \frac{1}{d} \sum_{k=1}^d \left\| \frac{1}{b} \nabla \left( \sum_{k \in \tau_i} f_k(\mathbf{x}) \right) \right\|_2^2 \leq \frac{1}{n} \sum_{i=1}^n \|\nabla f_i(\mathbf{x})\|_2^2 \leq \sigma^2.$$

- The average Lipschitz constant  $\bar{L}_\tau = \frac{1}{d} \sum_{i=1}^d L_{\tau_i}$  of the gradients of the batched functions  $g_{\tau_i}$  can only **decrease** with increasing batch size, since by the triangle inequality,  $L_{\tau_i} \leq \frac{1}{b} \sum_{k \in \tau_i} L_k$ , and thus

$$\frac{1}{d} \sum_{i=1}^d L_{\tau_i} \leq \frac{1}{n} \sum_{k=1}^n L_k = \bar{L}.$$



# SGD with batching and weighting

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**Theorem** Assume that the convexity and smoothness conditions on  $F(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n f_i(\mathbf{x})$  are in force. Consider the  $d = n/b$  batches  $g_{\tau_i}(\mathbf{x}) = \frac{1}{b} \sum_{k \in \tau_i} f_k(\mathbf{x})$ , and the batched weighted SGD iteration

$$\mathbf{x}_{k+1} \leftarrow \mathbf{x}_k - \frac{\gamma}{d \cdot p(\tau_{i_k})} \nabla g_{\tau_{i_k}}(\mathbf{x}_k)$$

where batch  $\tau_i$  is selected at iteration  $k$  with probability

$$p(\tau_i) = \frac{1}{2d} + \frac{1}{2d} \cdot \frac{L_{\tau_i}}{\bar{L}_\tau}. \quad (3.1)$$

For any desired  $\varepsilon$ , and using a stepsize of

$$\gamma = \frac{\mu\varepsilon}{4(\varepsilon\mu\bar{L}_\tau + \sigma_\tau^2)},$$

we have that after a number of iterations

$$k = 4 \log(2\varepsilon_0/\varepsilon) \left( \frac{\bar{L}_\tau}{\mu} + \frac{\sigma_\tau^2}{\mu^2\varepsilon} \right),$$

the following holds in expectation with respect to the weighted distribution (3.1):  $\mathbb{E}^{(p)} \|\mathbf{x}_k - \mathbf{x}_*\|_2^2 \leq \varepsilon$ .

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# Least Squares Case

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▶ **Non-batched:**  $f_i(\mathbf{x}) = \frac{n}{2}(b_i - \langle \mathbf{a}_i, \mathbf{x} \rangle)^2$

- (1) The individual Lipschitz constants are bounded by  $L_i = n\|\mathbf{a}_i\|_2^2$ , and the average Lipschitz constant by  $\frac{1}{n}\sum_i L_i = \|\mathbf{A}\|_F^2$  (where  $\|\cdot\|_F$  denotes the Frobenius norm),
- (2) The strong convexity parameter is  $\mu = \frac{1}{\|\mathbf{A}^{-1}\|^2}$  (where  $\|\mathbf{A}^{-1}\| = \sigma_{\min}^{-1}(\mathbf{A})$  is the reciprocal of the smallest singular value of  $\mathbf{A}$ ),
- (3) The residual is  $\sigma^2 = n\sum_i \|\mathbf{a}_i\|_2^2 |\langle \mathbf{a}_i, \mathbf{x}_* \rangle - a_i|^2$ .

▶ **Batched:**  $g_{\tau_i}(\mathbf{x}) = \frac{d}{2} \|\mathbf{A}_{\tau_i} \mathbf{x} - \mathbf{b}_{\tau_i}\|_2^2$

▶ 
$$L_{\tau_i} = \sup_{\mathbf{x}, \mathbf{y}} \frac{\|\nabla g_{\tau_i}(\mathbf{x}) - \nabla g_{\tau_i}(\mathbf{y})\|_2}{\|\mathbf{x} - \mathbf{y}\|_2} = \frac{n}{b} \|\mathbf{A}_{\tau_i}^* \mathbf{A}_{\tau_i}\|$$

▶ 
$$\sigma_{\tau}^2 = d \sum_{i=1}^d \|\mathbf{A}_{\tau_i}^* (\mathbf{A}_{\tau_i} \mathbf{x}_* - \mathbf{b}_{\tau_i})\|_2^2 \leq d \sum_{i=1}^d \|\mathbf{A}_{\tau_i}\|^2 \|\mathbf{A}_{\tau_i} \mathbf{x}_* - \mathbf{b}_{\tau_i}\|_2^2$$



# Examples in Least Squares

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- ▶ Orthonormal systems:  $\bar{L}_\tau = \sum_{i=1}^d \|A_{\tau_i}^* A_{\tau_i}\| = \frac{n}{b} = \frac{1}{b} \bar{L}$



# Examples in Least Squares

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- ▶ Orthonormal systems:  $\bar{L}_\tau = \sum_{i=1}^d \|A_{\tau_i}^* A_{\tau_i}\| = \frac{n}{b} = \frac{1}{b} \bar{L}$
- ▶ Incoherent (nearly) normalized systems:  $\bar{L}_\tau = \sum_{i=1}^d \|A_{\tau_i}^* A_{\tau_i}\| \leq C \frac{n}{b} \leq \frac{C}{C'} \frac{\bar{L}}{b}$



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- ▶ Incoherent (nearly) normalized systems:  $\bar{L}_\tau = \sum_{i=1}^d \|A_{\tau_i}^* A_{\tau_i}\| \leq C \frac{n}{b} \leq \frac{C}{C'} \frac{\bar{L}}{b}$
- ▶ Incoherent non-normalized systems:  $\bar{L}_\tau = \sum_{i=1}^d \|A_{\tau_i}^* A_{\tau_i}\| \leq C \sum_{i=1}^d \max_{k \in \tau_i} \|a_k\|_2^2$



# Examples in Least Squares

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- ▶ Orthonormal systems:  $\bar{L}_\tau = \sum_{i=1}^d \|A_{\tau_i}^* A_{\tau_i}\| = \frac{n}{b} = \frac{1}{b} \bar{L}$
- ▶ Incoherent (nearly) normalized systems:  $\bar{L}_\tau = \sum_{i=1}^d \|A_{\tau_i}^* A_{\tau_i}\| \leq C \frac{n}{b} \leq \frac{C}{C'} \frac{\bar{L}}{b}$
- ▶ Incoherent non-normalized systems:  $\bar{L}_\tau = \sum_{i=1}^d \|A_{\tau_i}^* A_{\tau_i}\| \leq C \sum_{i=1}^d \max_{k \in \tau_i} \|a_k\|_2^2$ 
  - ▶ Batching in decreasing arrangement of row norms:

$$\begin{aligned} \bar{L}_\tau &\leq C \sum_{i=1}^d \|a_{((i-1)b+1)}\|_2^2 \\ &\leq \frac{C}{b-1} \sum_{i=1}^n \|a_i\|_2^2 \\ &\leq \frac{C'}{b} \bar{L}. \end{aligned}$$

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# Practical Considerations

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- ▶ How to compute the Lipschitz constants  $L_{\tau_i}$  ?
  - ▶ Use upper bound: maximum row norm in batch
  - ▶ Power method:
    - ▶ After  $T \geq \varepsilon^{-1} \log(\varepsilon^{-1} b)$  iterations, one obtains approximation  $\hat{Q}_{\tau_i}$  s.t.

$$\|A_{\tau_i}^* A_{\tau_i}\| \geq \hat{Q}_{\tau_i} \geq \frac{\|A_{\tau_i}^* A_{\tau_i}\|}{1 + \varepsilon}$$

which yields

$$\bar{L}_{\tau} \geq \frac{b}{n} \sum_{i=1}^d \frac{n}{b} \hat{Q}_{\tau_i} \geq \frac{\bar{L}_{\tau}}{1 + \varepsilon}$$

at a computational cost (over  $b$  cores) of just  $b\varepsilon^{-1} \log(\varepsilon^{-1} \log(b))$

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# Non-smooth Hinge Loss

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**Corollary 4.3.** Consider  $P(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n [y_i \langle \mathbf{x}, \mathbf{a}_i \rangle]_+ + \frac{\lambda}{2} \|\mathbf{x}\|_2^2$ . Consider the batched weighted SGD iteration

$$\mathbf{x}_{k+1} \leftarrow \mathbf{x}_k - \frac{1}{\mu k p(\tau_i)} \left( \lambda \mathbf{x}_k + \frac{1}{b} \sum_{j \in \tau_i} \chi_j(\mathbf{x}_k) y_j \mathbf{a}_j \right), \quad (4.5)$$

where  $\chi_j(\mathbf{x}) = 1$  if  $y_j \langle \mathbf{x}, \mathbf{a}_j \rangle < 1$  and 0 otherwise. Let  $\mathbf{A}_\tau$  have rows  $y_j \mathbf{a}_j$  for  $j \in \tau$ . For any desired  $\varepsilon$ , we have that after

$$k = \frac{C \min(\alpha, 1 - \alpha) \left( \lambda + \frac{\sqrt{b}}{n} \sum_{i=1}^d \|\mathbf{A}_{\tau_i}\| \right)^2}{\lambda \varepsilon} \quad (4.6)$$

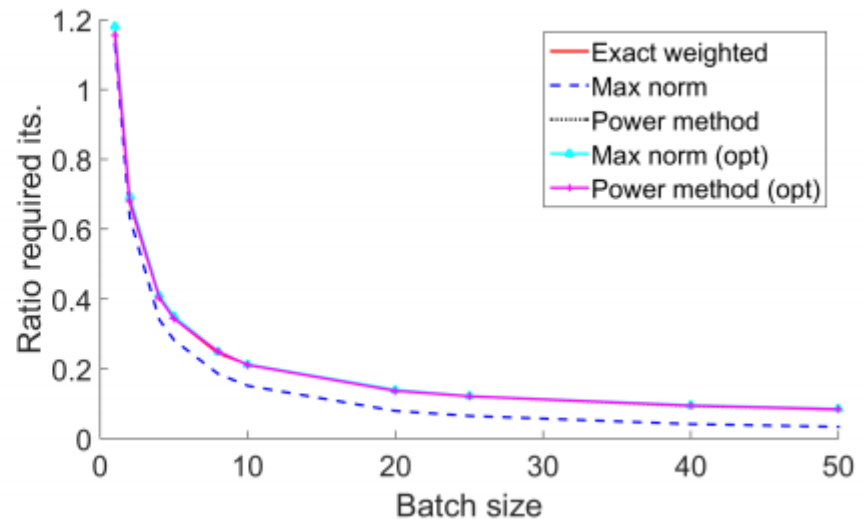
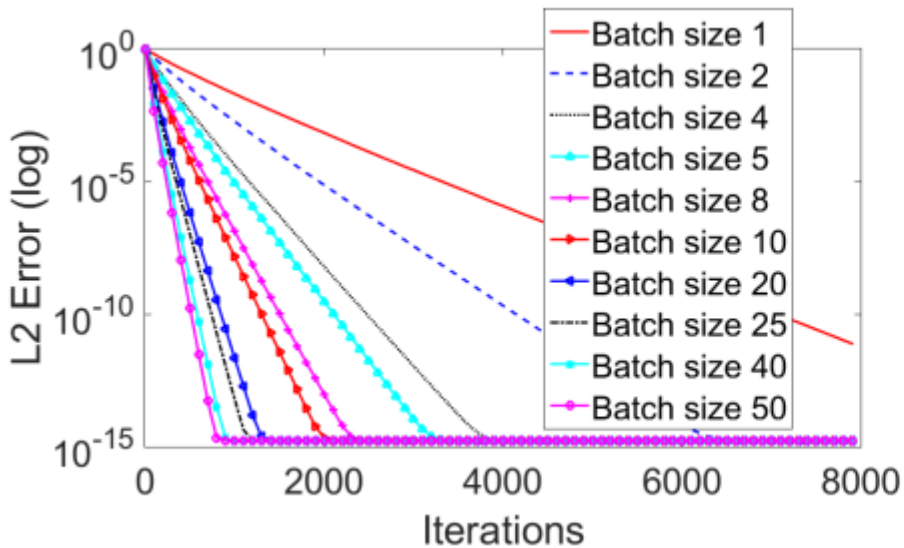
iterations of (4.5) with weights

$$p(\tau_i) = \frac{\|\mathbf{A}_{\tau_i}\| + \lambda \sqrt{b}}{\frac{n}{\sqrt{b}} \lambda + \sum_j \|\mathbf{A}_{\tau_j}\|}, \quad (4.7)$$

it holds that  $\mathbb{E}^{(p)}[P(\mathbf{x}_k) - P(\mathbf{x}_*)] \leq \varepsilon$ .



# Least Squares Experiments

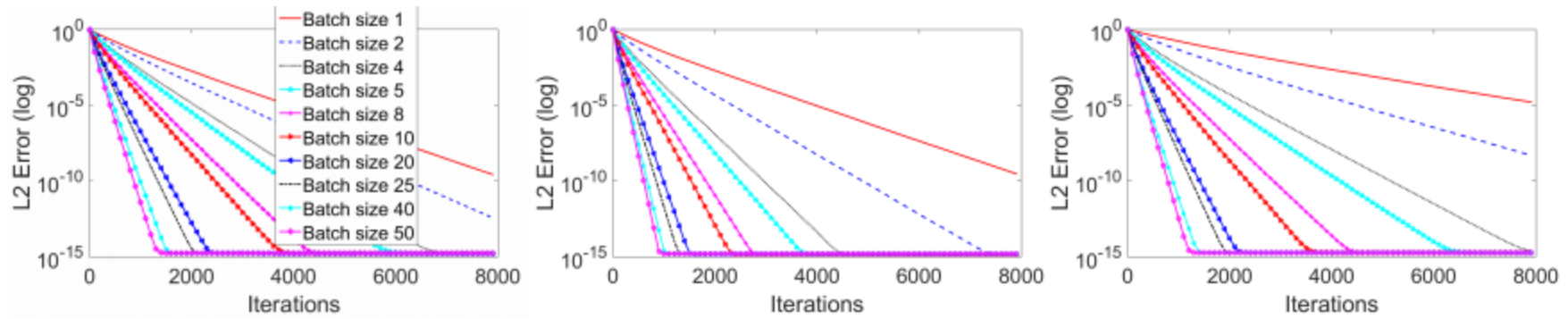


Gaussian systems. Right: Ratio of required iterations to reach error tolerance for batched SGD with weighting compared to classical SGD. "(opt)" denotes optimal step size was used.



# Least Squares Experiments

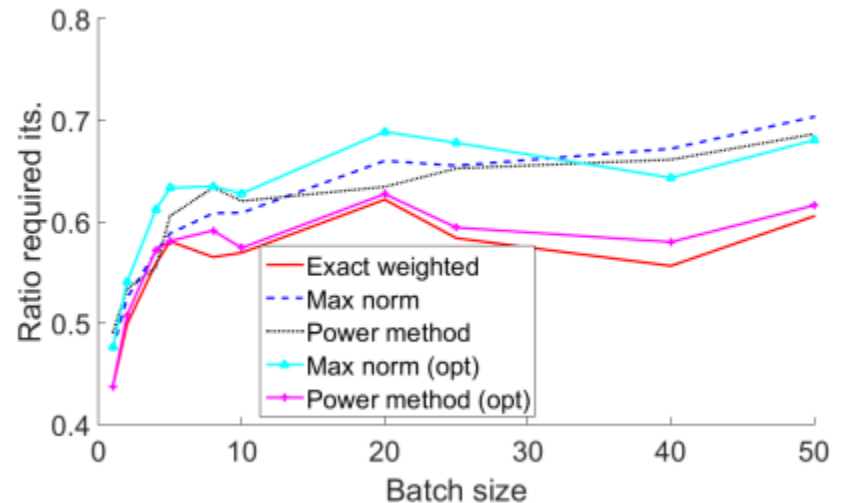
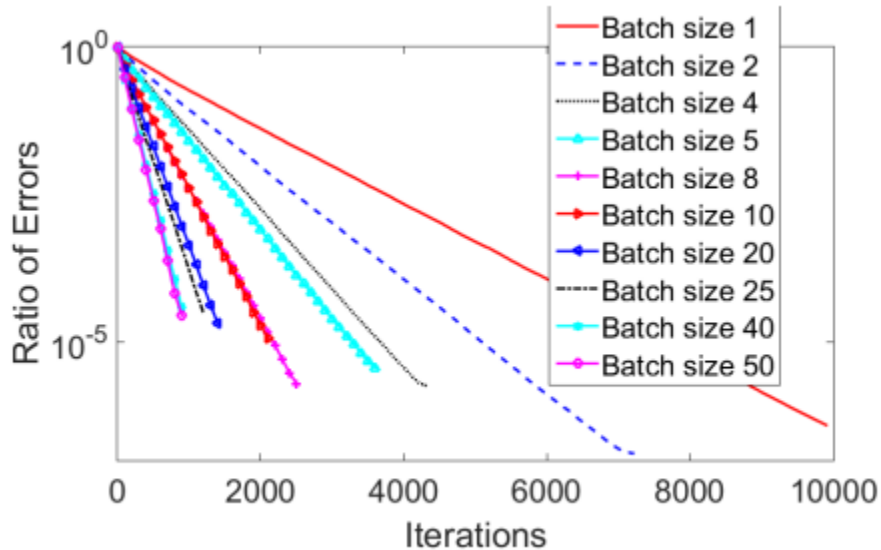
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Gaussian systems with varying row norms. Left: Random batches, weighted sampling. Center: Sequential batches, weighted SGD. Right: Sequential batched, unweighted SGD.

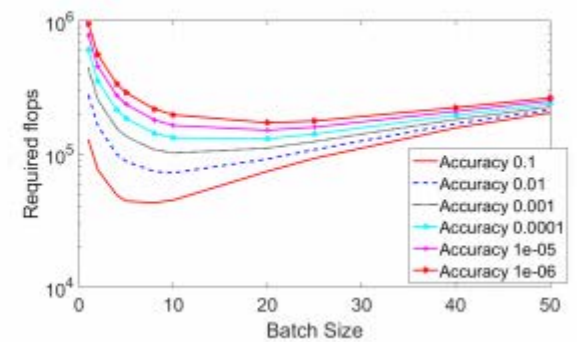
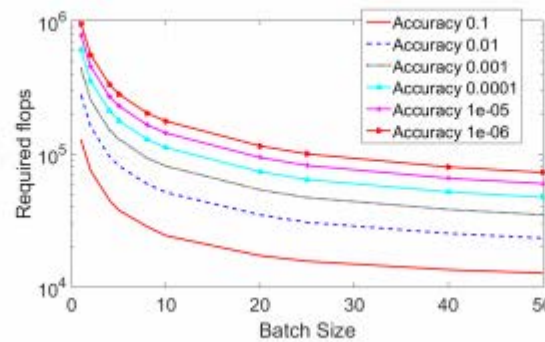
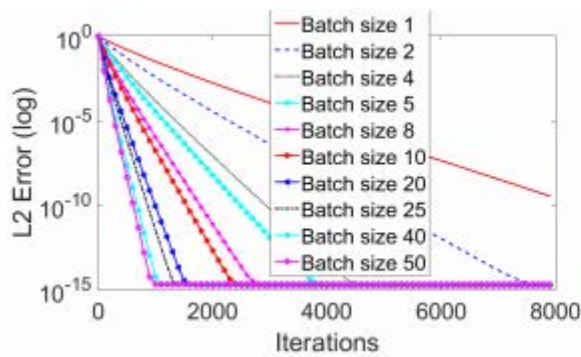


# Least Squares Experiments: weighting



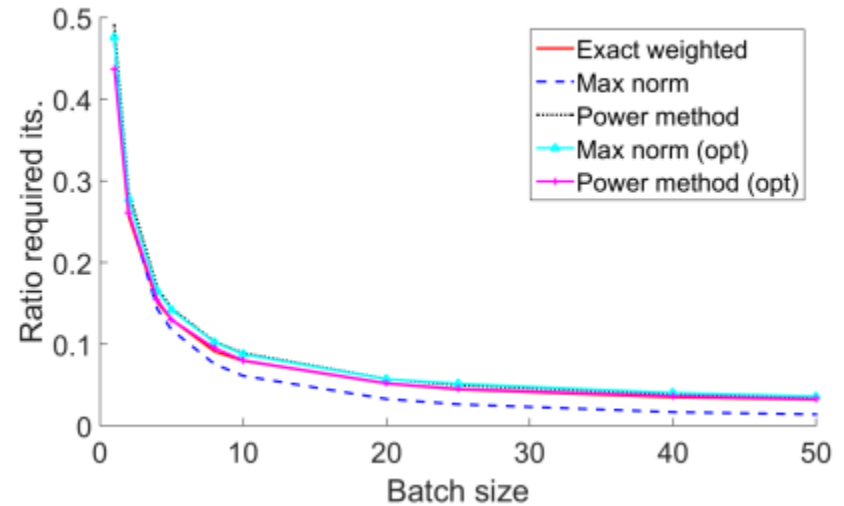
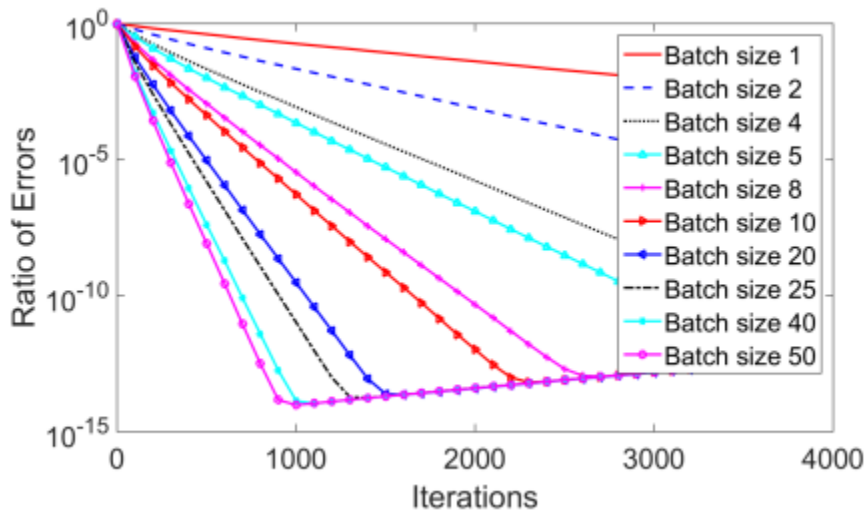
Gaussian systems with varying row norms. Left: Error ratios for weighted vs. unweighted SGD. Right: Ratio of required iterations to reach error tolerance for weighted versus unweighted SGD. “(opt)” denotes optimal step size was used.

# Least Squares Experiments: batching



Gaussian systems with varying row norms. Left: Error ratios for batched weighted SGD versus classical. Right: Ratio of required iterations to reach error tolerance for batched weighted SGD versus classical. “(opt)” denotes optimal step size was used.

# Least Squares Experiments: power method



Gaussian systems with varying row norms. Left: Convergence. Center: Flops versus batch size to achieve error tolerance, shared over  $b$  cores. Right: Flops versus batch size to achieve error tolerance (single core).

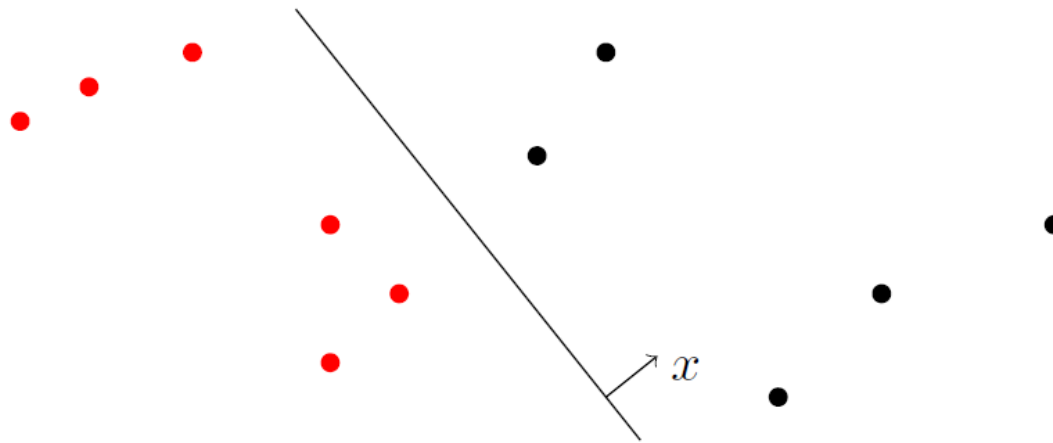


# Linear Feasibility

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## ► SVM Classification

Given binary classified training data,  $\{(a_i, y_i)\}_{i=1}^m$  where  $a_i \in \mathbb{R}^{n-1}$  and

$$y_i = \begin{cases} 1 & \text{if } a_i \in \text{class 1} \\ -1 & \text{if } a_i \in \text{class 2} \end{cases}$$


find a linear classifier  $F(a_i) = x^T a_i + z$  so that

$$y_i F(a_i) \geq 0 \text{ for all } i = 1, \dots, m.$$





# Linear Feasibility

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- ▶ Method of Motzkin [54] to find point in polytope  $P$  given by  $Ax < b$ :

Given  $x_0 \in \mathbb{R}^n$ , fix  $0 < \lambda \leq 2$  and iteratively construct approximations to  $P$ :

1. If  $x_k$  is feasible, stop.

2. Choose  $i_k \in [m]$  as  $i_k := \operatorname{argmax}_{i \in [m]} a_i^T x_{k-1} - b_i$ .

3. Define  $x_k := x_{k-1} - \lambda \frac{a_{i_k}^T x_{k-1} - b_{i_k}}{\|a_{i_k}\|^2} a_{i_k}$ .

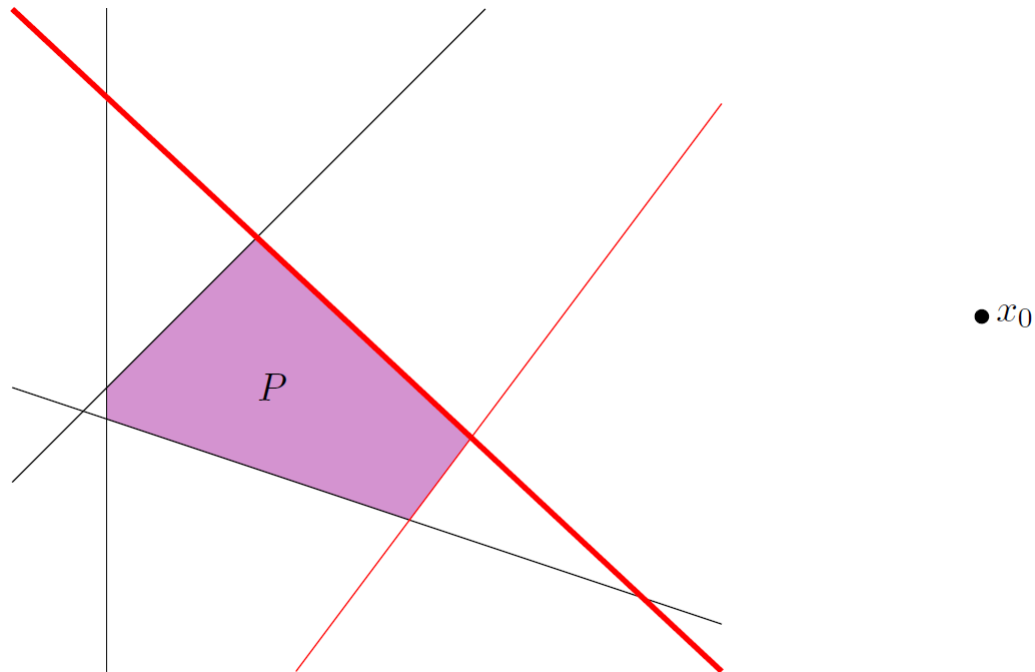
4. Repeat.



# Linear Feasibility

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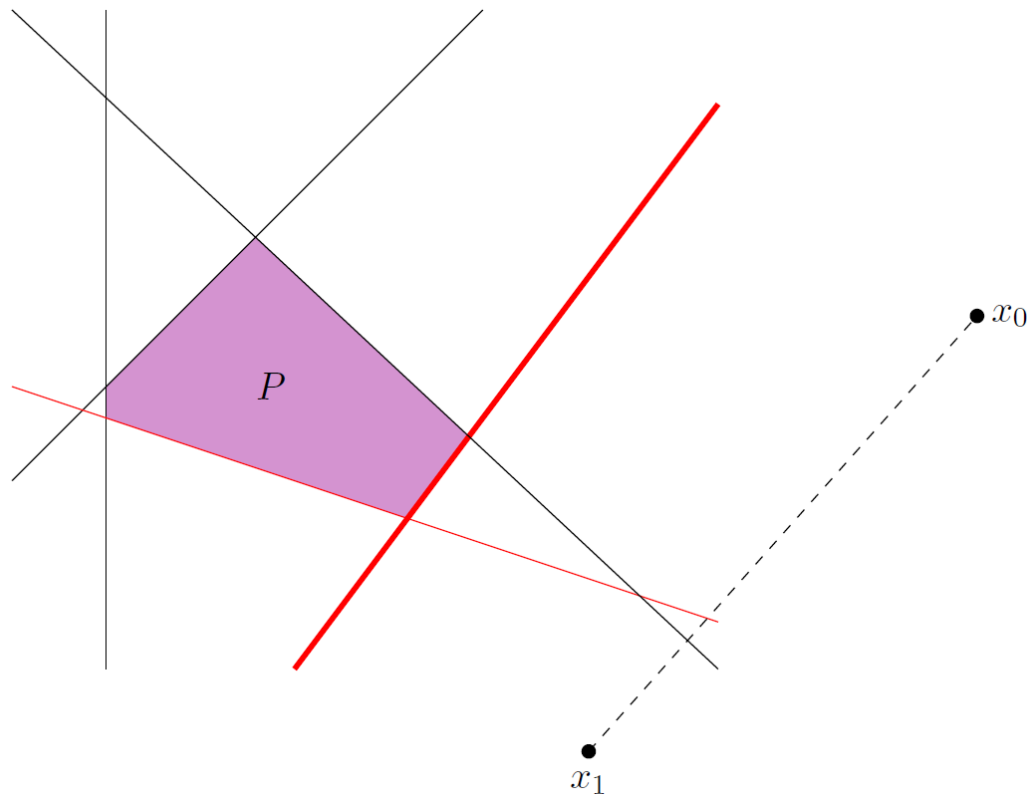
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# Linear Feasibility

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# Linear Feasibility

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- ▶ Method of Motzkin [54] to find point in polytope  $P$  given by  $Ax < b$ :
  - ▶ Pros: Monotonically decreasing, accelerated convergence
  - ▶ Cons: Computationally expensive
- ▶ Motivation: Use batched version of Motzkin's Method



# Batched Motzkin's Method

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Given  $x_0 \in \mathbb{R}^n$ , fix  $0 < \lambda \leq 2$  and iteratively construct approximations to  $P$  in the following way:

1. If  $x_k$  is feasible, stop.
2. Choose  $\tau_k \subset [m]$  to be a sample of size  $\beta$  constraints chosen uniformly at random from among the rows of  $A$ .
3. From among these  $\beta$  rows, choose
$$i_k := \operatorname{argmax}_{i \in \tau_k} a_i^T x_{k-1} - b_i.$$
4. Define  $x_k := x_{k-1} - \lambda \frac{(a_{i_k}^T x_{k-1} - b_{i_k})^+}{\|a_{i_k}\|^2} a_{i_k}.$
5. Repeat.



# Batched Motzkin's Method

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Let  $H$  denote the Hoffman constant ( $\sim$  conditioning) of the system. Then:

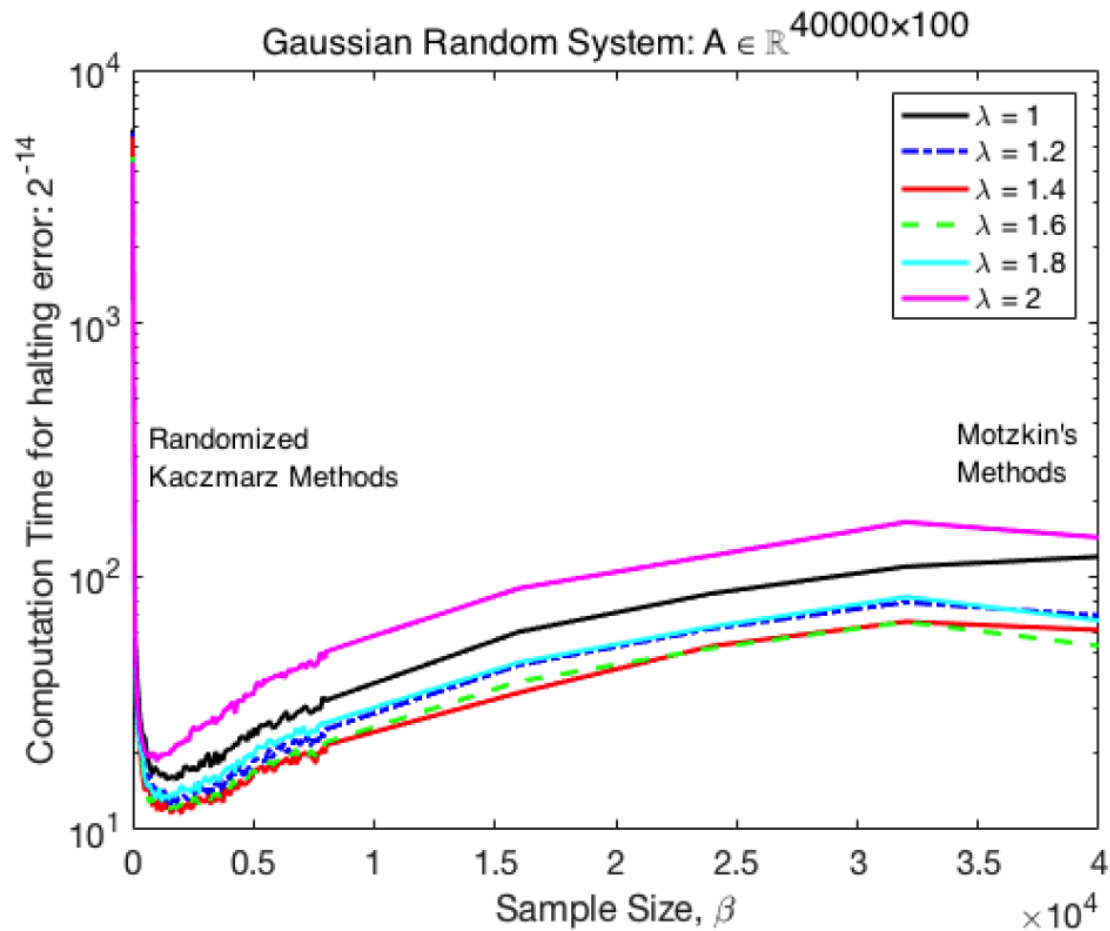
*If the feasible region (for normalized  $A$ ) is nonempty, then the SKM methods with samples of size  $\beta$  converge at least linearly in expectation:*

*Let  $s_{k-1}$  be the number of constraints satisfied by  $x_{k-1}$  and  $V_{k-1} := \max\{m - s_{k-1}, m - \beta + 1\}$ . Then, in the  $k$ th iteration,*

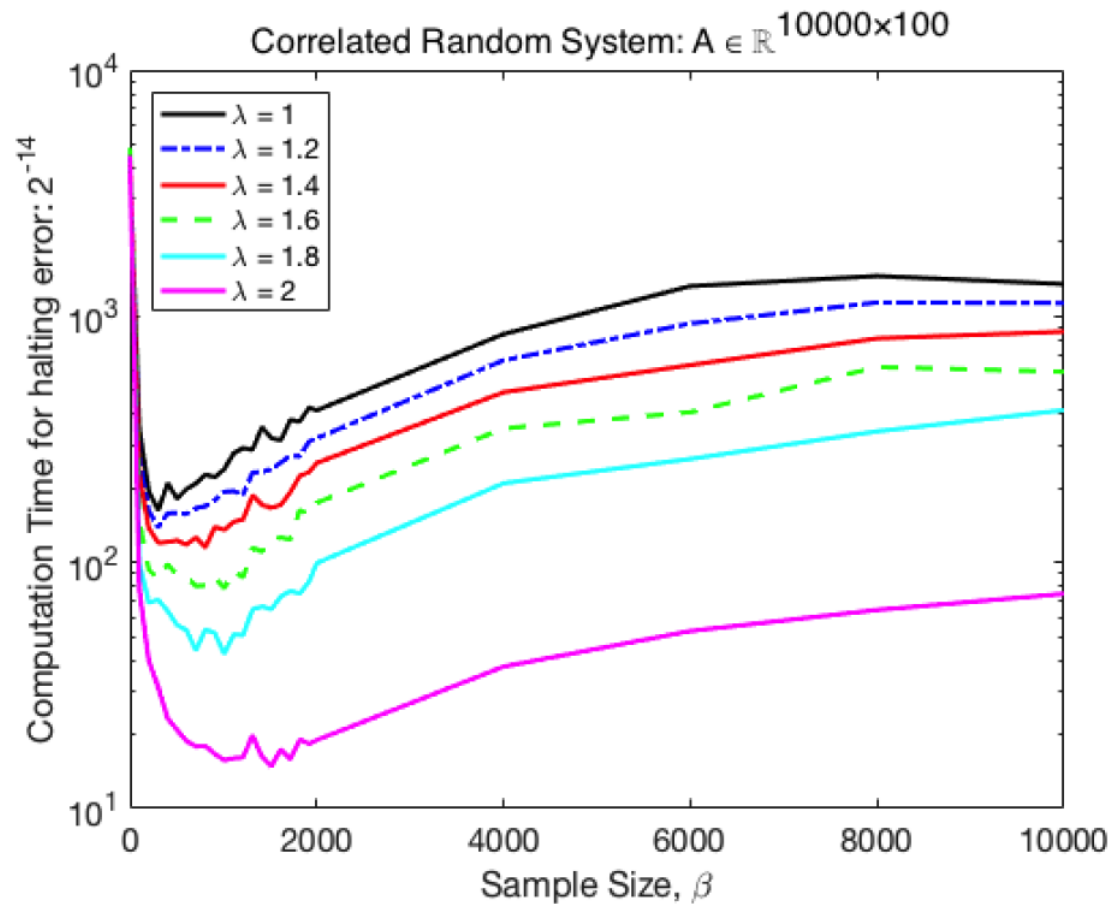
$$\mathbb{E} \left[ d(x_k, P)^2 \right] \leq \left( 1 - \frac{2\lambda - \lambda^2}{V_{k-1} H_2^2} \right) d(x_{k-1}, P)^2$$



# Batched Motzkin's Method

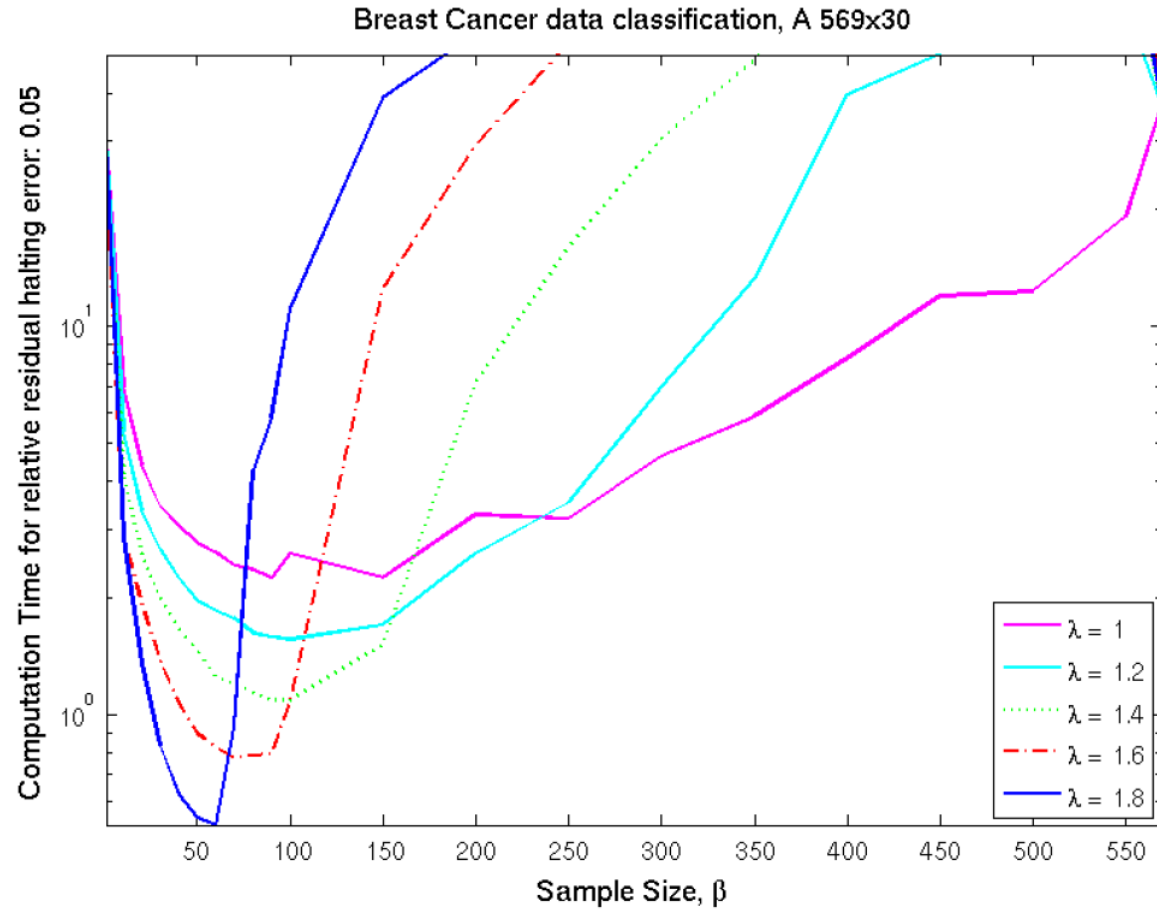


# Batched Motzkin's Method





# Batched Motzkin's Method



# Thank you!

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"Batched Stochastic Gradient Descent with Weighted Sampling"  
by D. Needell and R. Ward.  
Submitted.

"A Sampling Kaczmarz-Motzkin Algorithm for Linear Feasibility"  
by J.A. De Loera, J. Haddock, D. Needell.  
Submitted.

"Stochastic Gradient Descent and the Randomized Kaczmarz algorithm"  
by D. Needell, N. Srebro, R. Ward.  
*Mathematical Programming Series A*, vol. 155, num. 1, 549 - 573, 2016.

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[www.cmc.edu/pages/faculty/DNeedell](http://www.cmc.edu/pages/faculty/DNeedell)

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