Sketch-and-project and Kaczmarz

Iterative methods with corruptions

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Quantile-based Iterative Methods for Corrupted Systems of Linear Equations

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What do I do?

- Study the structure of large high-dimensional objects in the presence of randomness
- Use this understanding to develop (randomized) methods that work with complex data efficiently



Large high-dimensional objects:

- Sets
- Matrices
- Tensors
- Graphs
- Systems of linear equations
- Neural nets

High-dimensional probability helps revealing their structure:





Concentration of measure phenomenon

Intro 00●0 Sketch-and-project and Kaczmarz

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Solving linear systems

$A\mathbf{x} = \mathbf{b}$, find $\mathbf{x} \in \mathbb{R}^n$ given $A \in \mathbb{R}^{m \times n}$, $\mathbf{b} \in \mathbb{R}^m$.

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- Direct methods: $\mathbf{x} = A^{\dagger} \mathbf{b}$, LU, Cholesky, ...
- Methods exploiting the structure of A: H-, HSS solvers, ...
- Iterative methods: SGD, GMRES, projection based methods, ...
- Sketch-and-project (Gower and Richtarik, 2015)

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Disclaimer: I will focus on overdetermined full-rank systems $m \ge n$ either we assume that solution exists (redundant equations) or not (then we search for a least square solution)

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Model: overdetermined linear system



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Sketch-and-project

instead of
$$A\mathbf{x} = b$$
, solve $S^T A \mathbf{x} = S^T b$

 $S = m \times s$ sketch matrix, if $s \ll m$ (sketched system is easier) Iteration:

$$\mathbf{x}_{k} = \mathbf{x}_{k-1} + (S^{\mathsf{T}}A)^{\dagger}(S^{\mathsf{T}}\mathbf{b} - S^{\mathsf{T}}A\mathbf{x}_{k})$$



Discrete random sketches and Kaczmarz methods

$$A_i = (0, \ldots, 0, 1, 0, \ldots, 0) \cdot A$$

$$A_{\tau} = \begin{bmatrix} 0 & | & \mathrm{Id} & | & 0 \end{bmatrix} \cdot A = S^{T}A; \quad \mathbf{b}_{\tau} = S^{T}b$$



Sketch-and-project methods with S = (randomly placed identity completed by zeroes) are randomized Kaczmarz methods

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Randomized Kaczmarz (RK) method

Assume that for all the rows $\|\mathbf{A}_{\mathbf{i}}\| = 1$.

- 1. initialize x₀
- 2. project current iterate to \mathbf{A}_i : $\mathbf{x}_{k+1} = \mathbf{x}_k - (\langle \mathbf{A}_i, \mathbf{x}_k \rangle - \mathbf{b}_i)\mathbf{A}_i$, where $i \sim Unif\{1, \dots, m\}$



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Geometrically, each index *i* corresponds to a hyperplane in \mathbb{R}^n . RK projects orthogonally onto a randomly chosen hyperplane

Convegence theorem (Strohmer - Vershynin 2009)

For a system $A\mathbf{x}_* = b$, RK converges to \mathbf{x}_* linearly in expectation:

$$\mathbb{E}||\mathbf{x}_k - \mathbf{x}_*||_2^2 \leq \left(1 - \frac{\sigma_{\min}^2(A)}{\|A\|_F^2}\right)^k ||\mathbf{x}_0 - \mathbf{x}_*||_2^2$$

Block Kaczmarz Method

Starting at $\mathbf{x}_0 \in \mathbb{R}^n$:

- 1. Choose A_{τ} a block row subset at random, $\tau = \tau(k) \subset [m], |\tau| = s$
- 2. Define $\mathbf{x}_k := \mathbf{x}_{k-1} + (A_{\tau})^{\dagger} (\mathbf{b}_{\tau} A_{\tau} \mathbf{x}_k)$



Convegence theorem (Needell - Tropp 2012)

The block Kaczmarz converges to \boldsymbol{x}_* in expectation with accelerated rate

$$\mathbb{E}||\mathbf{x}_k - \mathbf{x}_*||_2^2 \leq \left(1 - c \frac{\sigma_{\min}^2(A)}{||A||^2 \log m}\right)^k ||\mathbf{x}_0 - \mathbf{x}_*||_2^2,$$

if all blocks are well-conditioned: for some $\delta \in (0, 1)$, number of blocks $\cdot \max_{\tau} \|A_{\tau}\|_2^2 \lesssim \|A\|_2^2 \log(m) \frac{1}{\delta^2} \cdot (1 + \delta)$.

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Gaussian sketching

$$A_{xi} := \xi^T \cdot A$$
, where $\xi \sim N(0, \mathrm{Id})$

 $A_S := S^T \cdot A$, where S is $m \times s$ gaussian random matrix

Gaussian sketch-and-project method takes gaussian random matrices S with i.i.d. entries as sketches. $(z) \in (z)$ $z \in S \setminus C$

BGK convergence rate

Convegence theorem (R. - Needell 2019)

The gaussian block Kaczmarz method converges to \boldsymbol{x}_* with the rate

$$\mathbb{E}\|\mathbf{x}_k - \mathbf{x}_*\|_2^2 \leq \left(1 - \frac{s\sigma_{\min}^2(A)}{(9\sqrt{s}\|A\| + C\|A\|_F)^2}\right)^k \|\mathbf{x}_0 - \mathbf{x}_*\|_2^2,$$

where $1 \le s \le m$ is the dimension of the gaussian sketch S.

- recovers "standard rate" $\sigma_{min}^2(A)/\|A\|_F^2$ for s=1
- per iteration performance improves with increasing s
- actually, cputime performance also improves with increasing s

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Better convergence for bigger sketch size

For $A = 50000 \times 500$ i.i.d. gaussian matrix:



Left: time(s) vs relative error for the varying sketch size s = 1, 10, 100, 500; right: block size vs average time until relative error 1e - 4

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Proof ideas: random matrices

$$\begin{aligned} \mathbf{x}_k &= \mathbf{x}_{k-1} + (S^T A)^{\dagger} (S^T \mathbf{b} - S^T A \mathbf{x}_k) \\ &= (\mathrm{Id} - (S^T A)^{\dagger} S^T A) \mathbf{x}_k + (S^T A)^{\dagger} S^T \mathbf{b}. \end{aligned}$$

1. We need to estimate $\mathbb{E} \| (S^T A)^{\dagger} \cdot S^T A \mathbf{x} \|_2^2$ from below - a product of two (dependent!) random matrices

Proof ideas: random matrices

$$\begin{aligned} \mathbf{x}_k &= \mathbf{x}_{k-1} + (S^T A)^{\dagger} (S^T \mathbf{b} - S^T A \mathbf{x}_k) \\ &= (\mathrm{Id} - (S^T A)^{\dagger} S^T A) \mathbf{x}_k + (S^T A)^{\dagger} S^T \mathbf{b}. \end{aligned}$$

- 1. We need to estimate $\mathbb{E} || (S^T A)^{\dagger} \cdot S^T A \mathbf{x} ||_2^2$ from below a product of two (dependent!) random matrices
- 2. S is $m \times s$ standard normal i.i.d. matrix.

$$\mathbb{E}\|\boldsymbol{S}^{\mathsf{T}}\boldsymbol{A}\mathbf{x}\|_{2}^{2} = \boldsymbol{s}\|\boldsymbol{A}\mathbf{x}\|_{2}^{2} \ge \boldsymbol{s}\sigma_{\min}^{2}(\boldsymbol{A})$$

But we need a high probability statement for any $s \ge 1$:

$$\mathbb{P}(\|S^{T}v\|_{2}^{2} > \|v\|^{2}s/10) \geq 0.5$$

for any $v \in \mathbb{R}^m$ and $s \ge 1$ - Cramér's concentration theorem.

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3.

$$\mathbb{E}\sup_{\mathbf{x}\in S^{n-1}}\|S^{\mathsf{T}}A\mathbf{x}\|_2 \leq \sqrt{m}\|A\|_2$$

Can we get a better estimate? Yes!

$$\mathbb{E}\sup_{\mathbf{x}\in S^{n-1}}\|S^{\mathsf{T}}A\mathbf{x}\|_2=\mathbb{E}\sup_{w\in AS^{n-1}}\|S^{\mathsf{T}}w\|_2\leq \sqrt{s}\|A\|+C\|A\|_F.$$

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To show 3.: apply matrix deviation inequality:

$$\mathbb{E} \sup_{w \in U} \|S^{\mathsf{T}}w\|_2 \leq \sqrt{s} \sup_{w \in U} \|w\|_2 + C\gamma(U),$$

to the ellipse $U := AS^{n-1}$. Here, $\gamma(U)$ is gaussian complexity of the set U:

$$\gamma(U) := \mathbb{E} \sup_{w \in U} |\langle \xi, w \rangle|$$
, where $\xi \sim N(0, I_n)$

Sampling sketches from finite collection

We could select sketches from the pre-sampled collection of gaussian random matrices

Theorem (R. - Needell)

Let $S = \{S_1, \ldots, S_N\}$ be a set of $m \times s$ random matrices with *i.i.d.* standard normal entries, $m^{2.5} \leq N \leq e^{m/3}$. Then, with probability at least 1 - 3/m, for any initial estimate \mathbf{x}_0 , finite block gaussian Kaczmarz method converges with the rate

$$\mathbb{E}\|\mathbf{x}_k - \mathbf{x}_*\|_2^2 \leq \left(1 - \frac{s}{36m\kappa^2(A)}\right)^k \|\mathbf{x}_0 - \mathbf{x}_*\|_2^2$$

In practice, the collection ${\cal S}$ can be much smaller, about $|{\cal S}| \sim m/s$

Solving noisy systems

If the system is inconsistent, we can search for least-squares problem solution with gaussian block Kaczmarz method:

$$\mathbf{x}_* = rgmin_{\mathbf{x}} \|A\mathbf{x} - b\|_2^2$$

and the error (noise) $e := A\mathbf{x}_* - b$.

Theorem (R - Needell)

The gaussian block Kaczmarz method converges to \mathbf{x}_* with the rate:

$$\mathbb{E}\|\mathbf{x}_{k} - \mathbf{x}_{*}\|_{2}^{2} \leq r^{k}\|\mathbf{x}_{0} - \mathbf{x}_{*}\|_{2}^{2} + \frac{\|e\|_{2}^{2}}{s_{min}^{4}(A)} \cdot \left[\frac{(9\sqrt{s}\|A\| + C\|A\|_{F})^{2}}{(\sqrt{n} - \sqrt{s})^{2}}\right]$$

Structurally differs from the noiseless case: diverges when $s \sim n$

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Dependence on the block size in the noisy case

 $A = 50000 \times 500$ i.i.d. gaussian matrix, e = random gaussian noise, normalized: $||e||_2 = 0.05 * ||b||_2$



Left: iteration vs relative error for the sketch size s = 1, 10, 100, 490; right: block size vs average time until relative error 1e - 2; 70 sec is max allowed time

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Is gaussian sketching practical?

 $A = 50000 \times 500$ i.i.d. matrix: N(0, 1) model (thin) and Unif[0.8, 1] model (bold lines)



Left: s = 1, right: s = 223; blue = with gaussian sketching, red = without it

Gaussian sketching improves regular Kaczmarz for highly coherent systems when s = 1, but loses the advantage on bigger block sizes

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Gaussian sketching reduces variance

 $A = 50000 \times 500$ i.i.d. matrix, e = spiky noise, 10 random spikes of size 50.



Iteration vs relative error (median and range over 10 runs). Left: gaussian model, right: coherent model; blue = with gaussian sketching, red = without it.

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Noise vs corruptions

Noise:
$$A\mathbf{x} = \mathbf{\tilde{b}}$$
 and $\|\mathbf{\tilde{b}} - \mathbf{b}\| \le \mathbf{e}$

 E.g., for RK: [Needell '10], [Needell, Tropp '12], [R., Needell '19] The result contains convergence horizon depending on the size of noise, ||e|| or ||e||∞.

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Corruptions: **b** is obtained by large changes on some of the entries of $\hat{\mathbf{b}}$

Convergence horizon can be huge... Idea: look at the residual (distances from an iterate to the equation hyperplanes) to detect suspicious candidates.
 [Haddock, Needell '18] - run RK for several iterations to approach x_{*}, then examine the residual and remove the equations with the largest. This works with few corruptions only (up to 5 - 10%).

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Model: overdetermined linear system



- b_C ∈ ℝⁿ has at most βm nonzero entries (β is the fraction of corrupted entries)
- Given knowledge of A and the corrupted measurements $\tilde{b} := Ax_{\mathbf{x}} * + b_{C}$, we would like an algorithm to recover $\mathbf{x}_{\mathbf{x}} * .$

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RK on corrupted systems



Relative error as a function of iteration count plotted for a 50000×100 Gaussian and coherent model with a 0.2 corruption rate. The coherent system was generated by sampling entries uniformly in [0, 1) and then normalizing the rows of the resulting matrix.

QuantileRK algorithm

Idea: If a sampled hyperplane looks corrupted, don't project!

1: sample several hyperplanes: $i_1, \ldots, i_T \sim \text{Uniform}(1, \ldots, m)$ 2: select a random next direction: $i \sim \text{Uniform}(1, \ldots, m)$ 3: if distance to the *i*-th hyperplane is at most 4: $|\langle \mathbf{A}_i, \mathbf{x}_k - b_i \rangle| \leq q$ -Quantile $(|\langle \mathbf{A}_{i_\ell}, \mathbf{x}_k \rangle - b_{i_\ell}| : \ell \in [T])$ then 5: project: $\mathbf{x}_{k+1} = \mathbf{x}_k - (\langle \mathbf{A}_i, \mathbf{x}_k \rangle - b_i \rangle \mathbf{A}_i,$ 6: else 7: hold: $\mathbf{x}_{k+1} = \mathbf{x}_k$



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QuantileSGD algorithm

Idea: Adjust the step size of the "projection" according to the quantile.

- 1: sample several hyperplanes: $i_1, \ldots, i_T \sim \text{Uniform}(1, \ldots, m)$
- 2: select a random next direction: $i \sim \text{Uniform}(1, \ldots, m)$
- 3: define step size by $\gamma := q$ -Quantile ($|\langle \mathbf{A}_{i_{\ell}}, \mathbf{x}_{k} \rangle b_{i_{\ell}}| : \ell \in [T]$)
- 4: project cautiously:

5:
$$\mathbf{x}_{k+1} = \mathbf{x}_k - \gamma \operatorname{sign}(\langle \mathbf{A}_i, \mathbf{x}_k \rangle - b_i) \mathbf{A}_i$$

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 L_1 -SGD

• Another approach is to minimize

$$\mathbf{x}_* = \underset{\mathbf{x}}{\arg\min} \|A\mathbf{x} - b\|_1^2.$$

This is a standard relaxation of the minimization of L_0 -norm ([Candes, Tao, '05], [Candes, Rudelson, Tao, Vershynin, '05])

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• Stochastic Gradient Descent with L_1 loss has iteration

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \eta_k \operatorname{sign}(\langle \mathbf{A}_i, \mathbf{x}_k \rangle - b_i) \mathbf{A}_i$$

with randomly sampled $i \in [m]$ and some step size schedule η_k

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with randomly sampled $i \in [m]$ and some step size schedule η_k

• Note that RK can be viewed as SGD with L₂ loss and correct step size:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - (\langle \mathbf{A}_i, \mathbf{x}_k \rangle - \mathbf{b}_i) \mathbf{A}_i,$$

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Optimal step size

• An optimal choice for η_k is such that

$$\mathbb{E}(\|\mathbf{e}_{k+1}\|_2^2) = \mathbb{E}(\|\mathbf{x}_{k+1} - \mathbf{x}_*\|_2^2) \quad \text{minimized}$$

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• Can be computed analytically:

$$\eta_k^* = rac{1}{m} \sum_{j=1}^m \mathrm{sign}(\langle \mathbf{A_i}, \mathbf{x}_k
angle - \mathbf{b}_i) \langle \mathbf{e}_k, \mathbf{a}_i
angle$$

and also

$$\mathbb{E}(\|\mathbf{e}_{k+1}\|_2^2) = \left(1 - \left(\frac{\eta_k^*}{\|\mathbf{e}_k\|}\right)^2\right) \|\mathbf{e}_k\|^2$$

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The last quantity \$\begin{pmatrix} \frac{\pi_k^*}{\|\mbox{e}_k\|} \begin{pmatrix}^2 \ge 1 \n n & \text{subgaussian matrices} \$\$ (which gives standard "Kaczmarz" linear convergence rate)\$
 Clearly, \$\mbox{e}_k = \mmox{k}_k - \mmox^*\$ is not known.

Approximating optimal step size

Two key facts:

• Step sizes of similar order lead to similar convergence:

L₁-SGD with the stepsize η_k , satisfying $0 < c_1 \le \frac{\eta_k}{\eta_k^*} \le c_2 < 2$ at each iteration, converges with

$$\mathbb{E}(\|\mathbf{e}_{k+1}\|_2^2) \leq \left(1 - \frac{C}{n}\right) \|\mathbf{e}_k\|^2$$

Residual quantiles: q-quantile $(|\langle \mathbf{A}_{i_{\ell}}, \mathbf{x}_{k} \rangle - \mathbf{b}_{i_{\ell}}| : \ell \in [T]) \approx$ Uncorrupted quantiles: q-quantile $\{|\langle \mathbf{A}_{i_{\ell}}, \mathbf{x}_{k} - \mathbf{x}^{*} \rangle| : \ell \in [T]\} \approx$

Empirical mean :
$$\frac{1}{m} \sum_{i=1}^{m} |\langle \mathbf{x}_{\mathbf{k}} - \mathbf{x}^*, \mathbf{A}_i \rangle| \approx \text{Optimal step size } \eta^*.$$

Convergence Theorem

Theorem (Haddock, Needell, R., Swartworth, 2020)

Let an $m \times n$ matrix A have subgaussian isotropic rows, and its entries have centered and bounded density functions. Then with probability $1 - ce^{-c_q m}$, QuantileRK(q) and QuantileSGD(q) on the full residual converge with the standard convergence rate

$$\mathbb{E}||x_k - x_*||_2^2 \le \left(1 - C_q \frac{\sigma_{min}^2(A)}{\|A\|_F^2}\right)^k ||x_0 - x_*||_2^2$$

if β is smaller than some positive constant, $q \leq 0.5 - \beta$, and n and m/n are larger than fixed constants.

- The same order as standard RK rate for uncorrupted systems.
- Result essentially holds with subsampling as well.
- The corrupted entries and values may be chosen adversarially.

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Model

Assumption

All the rows \mathbf{A}_i of the matrix A have unit norm and are independent. Additionally, for all $i \in [m]$, $\sqrt{n}\mathbf{A}_i$ is mean zero isotropic and has uniformly bounded subgaussian norm $\|\sqrt{n}\mathbf{A}_i\|_{\psi_2} \leq K$.

Assumption

Each entry A_{ij} of A has probability density function ϕ_{ij} which satisfies $\phi_{ij}(t) \leq D\sqrt{n}$ for all $t \in \mathbb{R}$. (The quantity D is a constant which we will use throughout when referring to this assumption.)

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Proof sketch for QuantileRK

1. Concentration of the residual quantiles $(|\langle \mathbf{A}_i, \mathbf{x}_k \rangle - \mathbf{b}_i| : i \in [m])$:

For *n* large enough, with probability at least $1 - e^{-cn}$, for every $\mathbf{x} \in \mathbb{R}^n$ for all but $\beta'm$ indices *i* the following holds $|\langle \mathbf{A}_i, \mathbf{x} \rangle| \leq C/(\beta'\sqrt{n}) ||\mathbf{x}||$.

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 Condition on choosing a row from the uncorrupted sub-matrix A'. Known RK rate holds here, since the condition number of A' is of the same order as of A by a non-trivial high probability uniform lower bound for the singular values of submatrices:

$$\Pr\left(\inf_{\substack{T \subseteq [m]:\\|T| \ge \alpha m}} \sigma_{\min}(\mathbf{A}_T) \gtrsim \frac{\alpha^{3/2}}{24D} \sigma_{\min}(\mathbf{A})\right) \ge 1 - 3e^{-c_2 \alpha m}$$

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3. Condition on choosing a corrupted row. This does not hurt too much by 1., since the step size is bounded by the quantile.

Concentration of the quantiles

Theorem

For n large enough, with probability at least $1 - e^{-cn}$, for every $\mathbf{x} \in \mathbb{R}^n$ for all but $\beta'm$ indices i the following holds $|\langle \mathbf{A}_i, \mathbf{x} \rangle| \leq C/(\beta'\sqrt{n}) ||\mathbf{x}||$.

• Enough to show that with probability $1 - 2e^{-t^2m}$ for every unit x

$$\frac{1}{m}\sum_{i=1}^m |\langle \mathbf{x}, \mathbf{A}_i \rangle| \leq \frac{1}{\sqrt{n}} + K\left(\frac{c_1}{\sqrt{m}} + \frac{c_2 t}{\sqrt{n}}\right)$$

- This follows from uniform concentration of *M*(**x**) := ¹/_m ∑^m_{i=1} |⟨**x**, **A**_i⟩| on the sphere (chaining + Dudley's inequality)
- And noticing that $(\mathbb{E}M(\mathbf{x}))^2 \leq \mathbb{E}(M(\mathbf{x}))^2 \sim \frac{1}{n}$, so there exists \mathbf{x} at least that small.

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Various quantiles



 $\log(||\mathbf{x}_{2000} - \mathbf{x}^*|| / ||\mathbf{x}_0 - \mathbf{x}^*||)$ for (a) QuantileRK and (b) QuantileSGD run on 50000 × 100 Gaussian system, with various corruption rates β and quantile choices.

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Arbitrarily large corruptions



(a) Log relative error for QuantileSGD and QuantileRK after 1000 iterations on a $100a \times 100$ Gaussian system with a 0.2 corruption rate, where a = m/n is the aspect ratio of the matrix.

(b) Log relative error for QuantileSGD and QuantileRK after 2000 iterations, as a function of corruption size. We use a 50000×100 Gaussian system and corrupt our system by adding a uniform value in $[-10^x, 10^x]$.

Iterative methods with corruptions

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Future directions

- More general corruption models: byzantine corruptions, errors on the left hand side, mix of noise and corruptions
- More general methods: block methods for corrupted systems (with Ben Jarman, Deanna Needell)
- More general problems: randomized iterative methods for optimization problems beyond solving linear systems (with Will Swartworth, Han Lyu, Deanna Needell)

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Thanks for your attention!

