Convergence of the Randomized Kaczmarz Algorithm in Hilbert Space

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Outline

- The Classical Kaczmarz Algorithms
- Randomized Kaczmarz Algorithm in Hilbert Space
- Motivating Applications
- Convergence Analysis
- Summary and Future Works

The classical Kaczmarz algorithm

Consider a linear equation system Ax=y: $x\in\mathbb{R}^d$, $y\in\mathbb{R}^m$, and A is a matrix with dimension $m\times d$.

The classical Kaczmarz algorithm: $x_1=0$ and for $k\geq 1$,

$$x_{k+1} = x_k + (y_i - \langle a_i, x_k \rangle) \frac{a_i}{\|a_i\|^2},$$

- $i = 1 + ((k-1) \mod m)$
- a_1, \ldots, a_m : rows of A. So $\langle a_i, x \rangle = y_i$.
- The algorithm and its convergence: (Kaczmarz 1937).
- step size: 1
- projection of error

$$x_{k+1} - x = \left(I - \frac{a_i}{\|a_i\|} \otimes \frac{a_i}{\|a_i\|}\right)(x_k - x)$$

Randomized Kaczmarz algorithm

$$x_{k+1} = x_k + (y_k - \langle \varphi_k, x_k \rangle) \, \frac{\varphi_k}{\|\varphi_k\|^2}$$

- $\{\varphi_k\}_{k=1}^{\infty} \stackrel{iid}{\sim} (\mathbb{R}^d, \rho)$: random measures
- $y_k = \langle \varphi_k, x \rangle$
- A special example: ρ supported on the row vectors $\{a_1,\dots,a_m\}$ of the matrix A, with $\rho(a_i) \propto \|a_i\|^2$.

$$\mathbb{E}\left[\|x_{k+1}-x\|^2\right] \leq (1-\frac{1}{\|A\|_F^2\|A^{-1}\|_2^2})^k \|x\|^2,$$

Strohmer & Vershynin '09; for general ρ , Zouzias & Freris '13, Gower & Richtárik '15.

• For general $\rho,\, \lim_{k\to\infty}C^k\|x_k-x\|^2=0$ almost surely for some C>1 (Chen & Powell '12).

• Recall the definition:

$$x_{k+1} = x_k + (y_k - \langle \varphi_k, x_k \rangle) \, \frac{\varphi_k}{\|\varphi_k\|^2}.$$

Since $\frac{y_k}{\|\varphi_k\|} = \left\langle \frac{\varphi_k}{\|\varphi_k\|}, x \right\rangle$, it is convenient to assume $\|\varphi_k\| = 1$.

Relaxed randomized Kaczmarz algorithm

$$x_{k+1} = x_k + \eta_k(y_k - \langle \varphi_k, x_k \rangle) \varphi_k$$

- $y_k = \langle \varphi_k, x \rangle + \epsilon_k$, ϵ_k : centered independent noise, $\|\varphi_k\| = 1$
- $0 < \eta_k < 1$: necessary to guarantee a convergence
- Needell '10: With step size $\eta_k\equiv 1$, $\mathbb{E}[\|x_{T+1}-x\|]=O(\|A^{-1}\|\|A\|_F)$ as $T\to\infty.$
- (Bach & Moulines '13):

$$\mathbb{E}\left[\left\langle a, \frac{1}{k} \sum_{j=2}^{k+1} x_j - x \right\rangle^2\right] = O\left(\frac{\dim H}{n}\right)$$

• Lin & Zhou '15: $\lim_{k\to\infty}\mathbb{E}[\|x_{k+1}-x\|^2]=0$ if and only if $\lim_{k\to\infty}\eta_k=0$ and $\sum_{k=1}^\infty\eta_k=\infty$. In this case, one further has

$$\sum_{k=1}^{\infty} \sqrt{\mathbb{E}[\|x_{k+1} - x\|^2]} = \infty.$$

• Lin & Zhou '15: $\mathbb{E}[\|x_{k+1}-x\|^2]=O(k^{-\theta})$ for $\eta_k\sim k^{-\theta}$ and $\theta\in(0,1)$.

Randomized Kaczmarz algorithm in Hilbert space

$$x_{k+1} = x_k + \eta_k(y_k - \langle \varphi_k, x_k \rangle) \varphi_k.$$

- $\{\varphi_k\}_{k=1}^{\infty} \stackrel{iid}{\sim} \rho$ on H, a general Hilbert space; $\|\varphi_k\| = 1$.
- $y_k = \langle \varphi_k, x \rangle$
- It is closely related to the online learning algorithms (online gradient descent algorithm): let $\{(w_k,y_k)\}_k$ be a sample of input-output pairs. Let $f_1=0$ and

$$f_{k+1} = f_k + \eta_k (y_k - \left\langle f_k, K_{w_k} \right\rangle_K) K_{w_k} - \eta_k \lambda f_k.$$

K: a Mercer kernel; $(\mathcal{H}_K, \left\langle \cdot, \cdot \right\rangle_K, \| \cdot \|_K)$ is the corresponding reproducing kernel Hilbert space; $K_w: u \mapsto K(w,u)$, a function in \mathcal{H}_K . Some Reference: Cesa-Bianchi & Long & Warmuth '96, Vapnik '98, Kivinen & Smola & Williamson '04, Pontil & Ying & Zhou '05, Smale & Yao '06, Ying & Zhou '06, ...

- It is understood that the regularization parameter λ is not necessary (Ying & Pontil 07).
- Usually the regularity assumption $f_{\rho}=L_{K}^{s}(\mathcal{H}_{K})$, s>0, is made.

Application to functional data analysis

• Functional linear models (β_0 : unknown slope function)

$$Y^* = \alpha_0 + \int_{\mathcal{T}} X^*(t) \beta_0(t) dt + \epsilon.$$

- \mathcal{T} : a compact domain, e.g., an interval or a square. $Y^* \in \mathbb{R}$.
- ullet $X^*(t)$: a square integrable stochastic process over ${\mathcal T}$ with covariance

$$C(s,t) = \mathbb{E}[(X(s) - \mathbb{E}[X(s)])(X(t) - \mathbb{E}[X(t)])].$$

- Data: $\{(X_k,Y_k)\}_k$, iid copies of (X^*,Y^*) .
- a large literature [James 2002, Cardot&Ferraty&Sarda 2003, Ramsay&Silverman 2005, Yao&Müller&Wang 2005, Ferraty&Vieu 2006, Cai&Hall 2006, Li&Hsing 2007, Hall&Horowitz 2007, ...]
- Reproducing kernel approaches [Yuan&Cai 2010, Cai&Yuan 2012]

$$(\hat{\alpha}_0, \hat{\beta}_0) = \arg \min_{\alpha \in \mathbb{R}, \beta \in \mathcal{H}_K} \left\{ \frac{1}{m} \sum_{i=1}^m \left(Y_i - F(X_i)\right)^2 + \lambda J(F) \right\},$$

where $F(X) = \alpha + \int_{\mathcal{T}} X(t) \beta(t) dt$, and $J(F) = \|\beta\|_K^2$.

- We assume $\alpha_0 = 0$ for simplicity
- ullet Consider the noise-free case $\epsilon=0$
- Apply randomized Kaczmarz algorithm with RKHS

$$x_{k+1} = x_k + \eta_k \left(Y_k^* - \int_{\mathcal{T}} x_k(t) X_k^*(t) dt \right) \frac{a_k^*}{\|a_k^*\|_K^2}.$$

- $\bullet \ a_k^* = \smallint_{\mathcal{T}} X_k^*(s) K_s ds$
- Write $\varphi_k = a_k^*/\|a_k^*\|_K$, $y_k = Y_k^*/\|a_k^*\|_K$. One has

$$x_{k+1} = x_k + \eta_k(y_k - \langle x_k, \varphi_k \rangle)\varphi_k.$$

The assumption $x \in L^s(H)$, s > 0

- $\bullet \ L:=\mathbb{E}[\varphi_k\otimes\varphi_k] \text{ where for any } u\in H\text{, } (\varphi_k\otimes\varphi_k)u:=\langle\varphi_k,u\rangle\,\varphi_k.$
- ullet L is symmetric, positive semi-definite, Hilbert-Schmidt, and of trace class.
- \bullet For online learning algorithms, $\varphi=K_X/\|K_X\|_K$ with X having some unknown distribution, and

$$L = \mathbb{E} \frac{K_X \otimes K_X}{\|K_X\|^2} = \mathbb{E} \frac{K_X \otimes K_X}{K(X,X)}.$$

When $K_X/\|K_X\|_K$ and $\|K_X\|_K$ are independent, for example when $K(x,x)\equiv 1$, L is the integral operator L_K that is widely used in literature, and $x\in L^s_K(\mathcal{H}_K)$ is a widely used assumption.

- It is an interesting open problem that under which (all?) circumstance would one get a better kernel simply by normalization.
- In functional linear regression problems,

$$L = \mathbb{E}\frac{a^* \otimes a^*}{\|a^*\|_K^2} = \mathbb{E}\frac{\int_{\mathcal{T}} \int_{\mathcal{T}} X^*(t) X^*(r) (K_t \otimes K_r) dt dr}{\int_{\mathcal{T}} \int_{\mathcal{T}} X^*(t) X^*(r) K(t,r) dt dr}.$$

when $\|a^*\|_K$ and $a^*/\|a^*\|_K$ are independent, L is the operator $L_{K^{1/2}CK^{1/2}}$ studied in literature (Yuan-Cai 2010, Cai-Yuan 2012), where $C(t,r)=\mathbb{E}[X^*(t)X^*(r)].$

Consider the noise-free model $y_k = \langle \varphi_k, x \rangle$ with $\{\varphi_k\}_{k=1}^{\infty} \stackrel{iid}{\sim} \rho$ and $\|\varphi_k\| = 1$. Let $L = \mathbb{E}[\varphi_k \otimes \varphi_k]$.

Theorem (rate of weak convergence, G-Lin-Zhou)

Let $\eta_k=\eta\in(0,1].$ For any $x\in L^{s_1}(H)$ and $u\in L^{s_2}(H)$ with some $s_1,s_2\in[0,1/4],$ we have

$$\mathbb{E}[\langle u, x_{k+1} - x \rangle^2] \leq \|L^{-s_2}u\|^2 \|L^{-s_1}x\|^2 (\eta k)^{-2s_1 - 2s_2};$$

If instead of a fixed u, $x_{k+1}-x$ is measured by an independent random vector $\alpha \sim (H,\rho)$, one has

$$\mathbb{E}[\langle \alpha, x_{k+1} - x \rangle^2] \leq \mathrm{Tr}(L) \|L^{-s_1} x\|^2 (\eta k)^{-2s_1 - \frac{1}{2}}.$$

 \bullet Remark: when $H=\mathcal{H}_K$ and $\alpha=K_X$ with X being random,

$$\mathbb{E}[\left<\alpha, x_{k+1} - x\right>^2] = \mathbb{E}[\|x_{k+1} - x\|_{L^2}^2].$$

• Example: suppose ρ is concentrated on only one point φ^* , then $L=\varphi^*\otimes\varphi^*$, and $\varphi_k=\pm\varphi^*$ for all k. So the randomized Kaczmarz algorithm converges if and only if $x=C\varphi^*$ for some constant C. Even if $x\perp\varphi^*$, $\langle u,x_{k+1}-x\rangle$ still converges if $u=C'\varphi^*$.

Outline of the proof.

$$\begin{split} x_{k+1} &= x_k + (y_k - \langle \varphi_k, x_k \rangle) \varphi_k, \\ x_{k+1} - x &= x_k - x + \langle \varphi_k, x - x_k \rangle \, \varphi_k \\ &= (I - \varphi_k \otimes \varphi_k) (x_k - x). \end{split}$$

Let $P_k=I-\varphi_k\otimes\varphi_k$, then P_1,\dots,P_k,\dots is a sequence of i.i.d. random orthogonal projections, and

$$\begin{split} \mathbb{E}[\|x_{k+1} - x\|^2] = & \mathbb{E}[(x_k - x)^T P_k^2(x_k - x)] \\ = & \mathbb{E}[(x_{k-1} - x)^T P_{k-1} P_k^2 P_{k-1}(x_{k-1} - x)] \\ = & \cdots \cdots \\ = & \mathbb{E}[(0 - x)^T P_1 \cdots P_k^2 \cdots P_1(0 - x)]. \end{split}$$

Strong convergence is not expected.

Example

Let $\{e_i\}_{i=1}^{\infty}$ be an orthonormal basis of H. Let $q_1 \geq q_2 \geq ... > 0$ and $\sum_{i=1}^{\infty} q_i = 1$. Let ρ be a discrete probability distribution such that $\rho(e_i) = q_i$. Assume $\mathrm{Var}(\epsilon) = \sigma^2 > 0$ the model $y = \langle \varphi, x \rangle + \epsilon$ and set $\eta_k \equiv \eta \in (0,1]$ for Algorithm

$$x_{k+1} = x_k + \eta_k (y_k - \langle \varphi_k, x_k \rangle) \varphi_k.$$

Then $\lim_{k\to\infty} \mathbb{E}[\|x_{k+1}-x\|^2] = \infty$. Note that if $x\in L^{s_1}(H)$ and $u\in L^{s_2}(H)$ with some $s_1,s_2\in [0,\frac{1}{4}]$, we still have $\mathbb{E}[\langle u,x_{k+1}-x\rangle^2] = \mathcal{O}((\eta k)^{-2s_1-2s_2}+\sigma^2\eta^{1-2s_2})$.

Recall [Needell 2010]: In the finite dimensional case with step sizes $\eta_k \equiv 1$, $\mathbb{E}[\|x_{k+1} - x\|] \sim \|A^{-1}\| \|A\|_F$ as $k \to \infty$.

Regularization by relaxation

If we allow that η_k be small enough, we can obtain strong convergence in H.

Theorem (G-Lin-Zhou)

Let M be a positive integer or infinity. Suppose the step sizes satisfy $\sum_{j=1}^M \eta_j^2 = \eta_{2,M} < 1$ and the slope vector satisfies $x \in L^{s_1}(H)$. Then for $1 \le k \le M$, one has

$$\begin{split} \mathbb{E}[\|x_{k+1} - x\|^2] &\leq \frac{2\|x\|^2 \|L^{-s_1}x\|^2 s_1^{2s_1}}{\|L^{-s_1}x\|^2 s_1^{2s_1} + \|x\|^2 e^{2s_1} \left(\sum_{j=1}^k \eta_j\right)^{2s_1}} \\ &+ \frac{\|x\|^2 + \sigma^2 \mathrm{Tr}(L)}{1 - \eta_{2,M}} \sum_{j=1}^k \eta_j^2. \end{split}$$

Theorem (G & Lin & Zhou)

Suppose $x_{\rho} \in L^{s_1}(H)$ for some $s_1 > 0$, and $\mathrm{Tr}(L^{s_*}) < \infty$ for some $0 < s_* < 1$. Let $2 \leq T < \infty$ be the number of iterations with constant step size

$$\eta_k \equiv \eta = \left\{ \begin{array}{ll} T^{-(2s_1+s_*)/(1+2s_1+s_*)}, & s_1+s_* \geq 1, \\ T^{-(1+s_1)/(2+s_1)}, & s_1+s_* < 1. \end{array} \right.$$

Then

$$\mathbb{E}[\|x_{T+1} - x_{\rho}\|^2] \leq C_1 \left\{ \begin{array}{l} T^{-2s_1/(1 + 2s_1 + s_*)}, & s_1 + s_* \geq 1, \\ T^{-2s_1/(2 + s_1)}, & s_1 + s_* < 1, \end{array} \right.$$

where C_1 is independent of T.

Note: the error estimate in this theorem is much better than the bound given in Ying & Pontil '07, and is arbitrarily close to the minimax optimal convergence rate given by G & Fan & Zhou '16.

Summary, and Future Work

- The classical randomized Kaczmarz algorithm is generalized to Hilbert space inspired by the "regularity" assumption from learning theory.
- Polynomial convergence is obtained regardless of the minimum eigenvalue of the coefficient matrix, for classical Kaczmarz algorithm;
- Future works: minimax rates; a better connection and understanding of the applications in functional data; mini-batch; averaging; Kaczmarz in Banach space; ...
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THANK YOU!