Deviation inequalities for Markov chains, with applications to SGD and empirical risk minimization

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Center for
Advanced Intelligence Project

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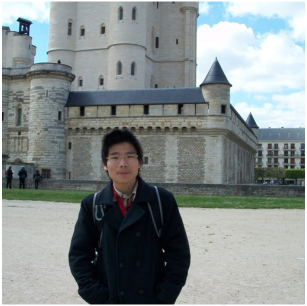

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Objective

General problem in probability and statistics

$$\mathbb{P}\left\{\left|\frac{1}{n}\sum_{i=1}^{n} X_i - \frac{1}{n}\mathbb{E}\left(\sum_{i=1}^{n} X_i\right)\right| \geq x\right\} \leq ?$$

What can we expect ? (1/2)

Chebyshev's inequality

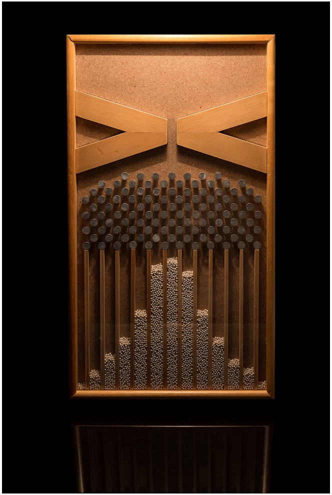
$$\mathbb{P}\left\{|U - \mathbb{E}(U)| \geq x\right\} \leq \frac{\mathrm{Var}(U)}{x^2}.$$

In a first time, assume the X_i's are independent, $\mathbb{E}(X_i) = \mu$ and $\mathrm{Var}(X_i) = \sigma^2$,

$$\mathbb{P}\left\{\left|\frac{1}{n}\sum_{i=1}^{n} X_i - \mu\right| \geq x\right\} = \frac{\mathrm{Var}\left(\sum_{i=1}^{n} X_i\right)}{n^2 x^2}$$

$$= \frac{\sigma^2}{n x^2}.$$

But...



(Photo : Wikipedia).

What can we expect ? (2/2)

$$\mathbb{P}\left\{\left|\frac{1}{n}\sum_{i=1}^{n} X_i - \mu\right| \geq x\right\} \leq \frac{\sigma^2}{n x^2}.$$

However, CLT :

$$\sqrt{\frac{n}{\sigma^2}}\left(\frac{1}{n}\sum_{i=1}^{n} X_i - \mu\right) \rightsquigarrow \mathcal{N}(0,1).$$

So, we expect :

$$\mathbb{P}\left\{\left|\frac{1}{n}\sum_{i=1}^{n} X_i - \mu\right| \geq x\right\} \simeq 2\Phi\left(\frac{x\sqrt{n}}{\sigma}\right) \sim \frac{2\mathrm{e}^{-\frac{x^2 n}{2\sigma^2}}}{\frac{x\sqrt{n}}{\sigma}\sqrt{2\pi}}.$$

Chernoff bound

Chernoff bound

$$\mathbb{P}\left\{U - \mathbb{E}(U) \geq x\right\} = \mathbb{P}\left\{\mathrm{e}^{s(U-\mathbb{E}(U))} \geq \mathrm{e}^{sx}\right\} \leq \frac{\mathbb{E}\left(\mathrm{e}^{s(U-\mathbb{E}(U))}\right)}{\mathrm{e}^{sx}}.$$

$$\mathbb{P}\left\{\frac{1}{n}\sum_{i=1}^{n} X_i - \mu \geq x\right\} \leq \frac{\mathbb{E}\left(\mathrm{e}^{\frac{s}{n}\sum_{i=1}^{n}(X_i-\mu)}\right)}{\mathrm{e}^{sx}}$$

$$= \mathrm{e}^{-sx}\prod_{i=1}^{n}\mathbb{E}\left(\mathrm{e}^{\frac{s}{n}(X_i-\mu)}\right).$$

Hoeffding's inequality

$$\mathbb{P}\left\{\frac{1}{n}\sum_{i=1}^{n} X_i - \mu \geq x\right\} \leq \mathrm{e}^{-sx}\prod_{i=1}^{n}\mathbb{E}\left(\mathrm{e}^{\frac{s}{n}(X_i-\mu)}\right).$$

Hoeffding's lemma - U bounded : $a \leq U \leq b$

$$\mathbb{E}\left(\mathrm{e}^{s[U-\mathbb{E}(U)]}\right) \leq \mathrm{e}^{\frac{s^2(b-a)^2}{8}}.$$

Hoeffding's inequality

Assume the X_i's are independent and $a \leq X_i \leq b$,

$$\mathbb{P}\left\{\left|\frac{1}{n}\sum_{i=1}^{n} X_i - \mu\right| \geq x\right\} \leq 2\mathrm{e}^{-\frac{2nx^2}{(b-a)^2}}.$$

McDiarmid's inequality

McDiarmid's inequality

Assume the X_i's are independent and $f : \mathcal{X}^n \to \mathbb{R}$ such that

$$|f(x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_n) - f(x_1, \dots, x_{i-1}, x_i', x_{i+1}, \dots, x_n)| \leq c.$$

then

$$\mathbb{P}\left\{ \left| \frac{f(X_1, \dots, X_n) - \mathbb{E}[f(X_1, \dots, X_n)]}{n} \right| \geq x \right\} \leq 2\mathrm{e}^{-\frac{2x^2 n}{c^2}}.$$

We recover Hoeffding for $f(x_1, \dots, x_n) = \sum_{i=1}^n x_i$, $c = (b - a)$.

Assumptions on moments

Hoeffding's lemma - U bounded : $a \leq U \leq b$

$$\mathbb{E}\left(\mathrm{e}^{s[U-\mathbb{E}(U)]}\right) \leq \mathrm{e}^{\frac{s^2(b-a)^2}{8}}.$$

In general, why not assuming U satisfies such an inequality ?

Definition - sub-Gaussian random variable U

$$\mathbb{E}\left(\mathrm{e}^{s[U-\mathbb{E}(U)]}\right) \leq \mathrm{e}^{s^2 C_0^2}$$

$$U \text{ sub-Gaussian } \Leftrightarrow \forall k \in \mathbb{N},\ \mathbb{E}(|U|^{2k}) \leq k! C_1^k.$$

Contents

Objective of this talk

Objective : for some time series $\{X_t, t = 0, \dots, \infty\}$

$$\mathbb{P}\left\{\left|\frac{1}{n}\sum_{t=1}^{n} X_t - \frac{1}{n}\mathbb{E}\Big(\sum_{t=1}^{n} X_t\Big)\right| \geq x\right\} \leq ?$$

$$\mathbb{P}\left\{\left|\frac{f(X_1,\dots,X_n) - \mathbb{E}[f(X_1,\dots,X_n)]}{n}\right| \geq x\right\} \leq ?$$

$$\mathbb{P}\left\{\frac{1}{n}\sum_{t=1}^{n} X_t - \mu \geq x\right\} \leq \frac{\mathbb{E}\left(\mathrm{e}^{\frac{s}{n}\sum_{t=1}^{n}(X_t-\mu)}\right)}{\mathrm{e}^{sx}}$$

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Objective of this talk

Objective : for some time series $\{X_t, t = 0, \dots, \infty\}$

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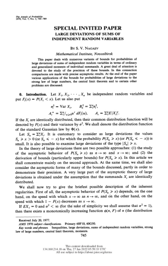
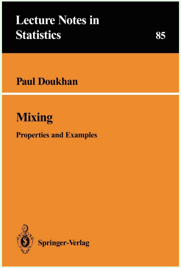
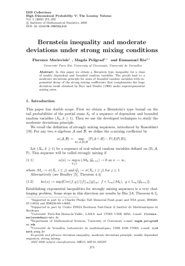
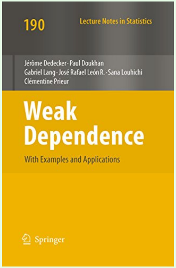
$$\mathbb{P}\left\{\frac{1}{n}\sum_{t=1}^{n} X_t \geq x\right\} \leq \frac{\mathbb{E}\left(e^{\frac{s}{n}\sum_{t=1}^{n}(X_t-\mu)}\right)}{e^{sx}} = e^{-sx}\prod_{t=1}^{n}\mathbb{E}\left(e^{\frac{s}{n}(X_t-\mu)}\right)$$

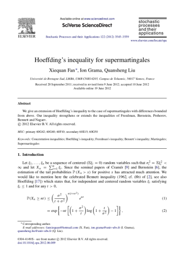
Deviation for time series : an active research field



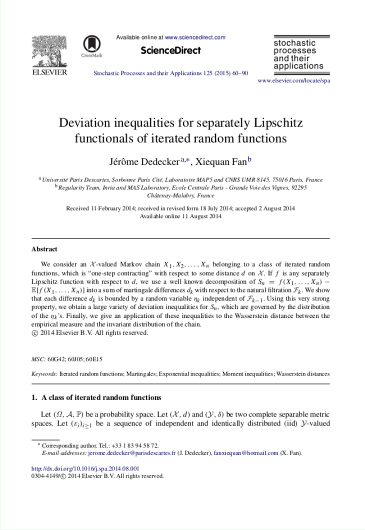








A remarkable result for Markov chains



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Deviation inequalities for separately Lipschitz functionals of iterated random functions

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Abstract

We consider an $\mathcal{X}$-valued Markov chain $X_1, X_2, \ldots, X_n$ belonging to a class of iterated random functions, which is "one-step contracting" with respect to some distance d on $\mathcal{X}$. If f is any separately Lipschitz function with respect to d, we use a well known decomposition of $S_n = f(X_1, \ldots, X_n) - \mathbb{E}[f(X_1, \ldots, X_n)]$ into a sum of martingale differences d_k with respect to the natural filtration $\mathcal{F}_k$. We show that each difference d_k is bounded by a random variable η_k independent of $\mathcal{F}_{k-1}$. Using this very strong property, we obtain a large variety of deviation inequalities for S_n, which are governed by the distribution of the η_k's. Finally, we give an application of these inequalities to the Wasserstein distance between the empirical measure and the invariant distribution of the chain.

MSC: 60G42; 60J05; 60E15

Keywords: Iterated random functions; Martingales; Exponential inequalities; Moment inequalities; Wasserstein distances

1. A class of iterated random functions

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a probability space. Let $(\mathcal{X}, d)$ and $(\mathcal{Y}, \delta)$ be two complete separable metric spaces. Let $(\varepsilon_i)_{i\geq 1}$ be a sequence of independent and identically distributed (iid) $\mathcal{Y}$-valued

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- study Markov chains of the form

$$X_n = F(X_{n-1}, \varepsilon_n)$$

- provide deviation inequalities when

$$\mathbb{E}\left\{ d\left(F(x, \varepsilon_n), F(x', \varepsilon_n) \right) \right\} \leq \rho d(x, x')$$

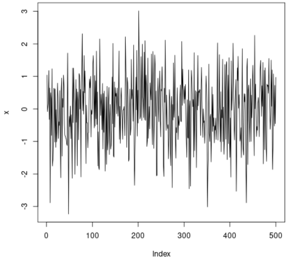
for some $\rho < 1$.

Example (1/2)

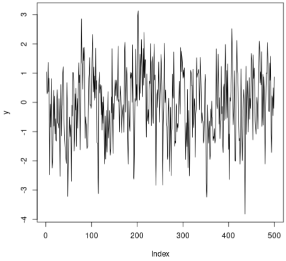
AR(1) process

$$X_n = F(X_{n-1}, \varepsilon_n) := \rho X_{n-1} + \varepsilon_n$$

$$|F(x, \varepsilon_n) - F(x', \varepsilon_n)| \leq \rho |x - x'|$$



$\rho = 0$



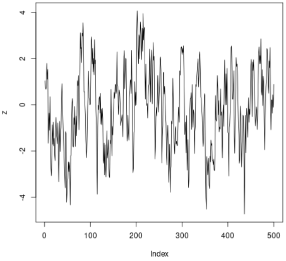
$\rho = 0.5$

Example (2/2)

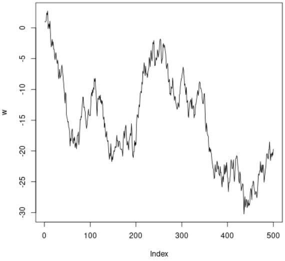
AR(1) process

$$X_n = F(X_{n-1}, \varepsilon_n) := \rho X_{n-1} + \varepsilon_n$$

$$|F(x, \varepsilon_n) - F(x', \varepsilon_n)| \leq \rho |x - x'|$$



$\rho = 0.8$

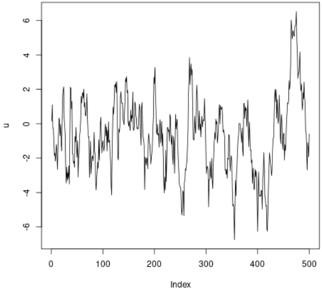


$\rho = 1$

What happens for non-homogeneous chains ?

AR(1) process with varying coefficients

$$X_n = F_n(X_{n-1}, \varepsilon_n) := \rho_n X_{n-1} + \varepsilon_n$$



$$\rho_n = \left(1 - \frac{1}{\sqrt{n}}\right).$$

Inequalities for non-homogeneous Markov chains

A class of non-homogeneous Markov chains

- X_n takes values in $(\mathcal{X}, d)$. Example : $\mathcal{X} = \mathbb{R}^d$, d large.
- (ε_n) are i.i.d random variables in $(\mathcal{Y}, \delta)$.

Definition

1. $X_n = F_n(X_{n-1}, \varepsilon_n)$.
2. $\mathbb{E}\left\{ d\left(F_n(x, \varepsilon_n), F_n(x', \varepsilon_n) \right) \right\} \leq \rho_n d(x, x')$.
3. $d\left(F_n(x, y), F_n(x, y') \right) \leq \tau_n \delta(y, y') + \xi_n$.

VAR with variying coefficients

Phillips, P.C.B. (1988). Regression theory for near integrated time series. *Econometrica*.

- $X_n \in \mathbb{R}^d$.
- (ε_n) are i.i.d $\mathcal{N}(0, \sigma^2 I_d)$.

1. $X_n = F_n(X_{n-1}, \varepsilon_n) = A_n X_{n-1} + \varepsilon_n$.
2. $\rho_n = \|A_n\|_{\mathrm{op}} = \sup_{x \neq 0} \frac{\|A_n x\|}{\|x\|} \xrightarrow[n\to\infty]{<} 1$.
3. $\tau_n = 1$, $\xi_n = 0$.

Example : stochastic optimization

$$\text{Minimize } L(x) = \sum_{i=1}^{N} \ell_i(x)$$

For I drawn uniformly in $\{1, \dots, N\}$ with M elements,

$$\hat{\nabla}_n L(x) := \frac{1}{M} \sum_{i \in I} \nabla \ell_i(x).$$

- Projected tochastic gradient descent (SGD) :

$$X_n = \Pi_{\mathcal{C}} \left[X_{n-1} - \frac{\gamma}{n^\alpha} \hat{\nabla}_n L(X_{n-1}) \right]$$

- Projected stochastic gradient Langevin descent (SGLD) :

$$X_n = \Pi_{\mathcal{C}} \left[X_{n-1} - \frac{\gamma}{n^\alpha} \hat{\nabla}_n L(X_{n-1}) + \frac{\eta}{n^\beta} \varepsilon_n \right]$$

Example : SGD

Assume L is m-strongly convex, M-Lipschitz and ∇L is ℓ-Lipschitz.

SGD - $\alpha \in [0,1]$, $\gamma > 0$

1. $X_n = F_n(X_{n-1}, \varepsilon_n) = \Pi_{\mathcal{C}} \left[X_{n-1} - \frac{\gamma}{n^\alpha} \hat{\nabla}_n L(X_{n-1}) \right].$
2. - $\rho_n \sim 1 - \frac{m\gamma}{n^\alpha}$ for $\alpha > 0$,
   - $\rho_n = 1 - 2m\gamma + \ell^2\gamma^2$ if $\alpha = 0$.
3. $\xi_n = \frac{2\gamma M}{n^\alpha}, \tau_n = 0.$

Example : SGLD

Assume L is m-strongly convex, M-Lipschitz and ∇L is ℓ-Lipschitz.

SGLD - $\alpha, \beta \in [0,1]$, $\gamma, \eta > 0$, $\varepsilon_n \sim \mathcal{N}(0,1)$

1. $X_n = F_n(X_{n-1}, \varepsilon_n) = \Pi_{\mathcal{C}} \left[X_{n-1} - \frac{\gamma}{n^\alpha} \hat{\nabla}_n L(X_{n-1}) + \frac{\eta}{n^\beta} \varepsilon_n \right].$
2.
   - $\rho_n \sim 1 - \frac{m\gamma}{n^\alpha}$ for $\alpha > 0$,
   - $\rho_n = 1 - 2m\gamma + \ell^2\gamma^2$ if $\alpha = 0$.
3. $\xi_n = \frac{2\gamma M}{n^\alpha}, \tau_n = \frac{\eta}{n^\beta}$.

Deviation inequality

Theorem (Proposition 3.1 in the paper) - $p \in [1, +\infty], d \in \mathbb{N}$

Assume $f : \mathcal{X}^n \to \mathbb{R}^d$ such that

$$|f(x_1, \dots, x_i, \dots, x_n) - f(x_1, \dots, x_i', \dots, x_n)| \leq d(x_i, x_i'),$$

$\mathbb{E}_{\varepsilon_n}([\mathbb{E}_{\varepsilon_n'} \delta(\varepsilon_n, \varepsilon_n')]^k) \leq C_1^k k!$ and a similar condition for X_1,

$$\mathbb{P}\left\{ \left\| \frac{f(X_1, \dots, X_n) - \mathbb{E}[f(X_1, \dots, X_n)]}{n} \right\|_p \geq x \right\}$$

$$\leq \begin{cases} e^{-c_{p,d} n x} & \rho_n \leq 1 - \rho < 1,\ \tau_n + \xi_n \leq \frac{\tau}{n^\alpha},\ \alpha \in (0,1] \\ e^{-c_{p,d} n (x \mathbf{1}_{x>1} + x^2 \mathbf{1}_{x \leq 1})} & \rho_n \leq 1 - \frac{\rho}{n^\alpha},\ \tau_n + \xi_n \leq \frac{\tau}{n^\alpha},\ \alpha \in [0,1), \\ e^{-c_{p,d} n^{1-2\alpha} x^2} & \rho_n \leq 1 - \frac{\rho}{n^\alpha},\ \tau_n + \xi_n \leq \tau, \alpha \in (0, 1/2). \end{cases}$$

Proof technique

The proof technique relies on martingale decomposition :

$$f(X_1,\dots,X_n) - \mathbb{E}[f(X_1,\dots,X_n)] = \sum_{t=1}^{n} M_t$$

where

$$M_t = \mathbb{E}[f(X_1,\dots,X_n)|X_1,\dots,X_t] - \mathbb{E}[f(X_1,\dots,X_n)|X_1,\dots,X_{t-1}].$$

Conditional Chernoff :

$$\frac{\mathbb{E}\left(\mathrm{e}^{\frac{s}{n}\sum_{t=1}^{n} M_t}\right)}{\mathrm{e}^{sx}} = \frac{\mathbb{E}\left[\mathrm{e}^{\frac{s}{n}\sum_{t=1}^{n-1} M_t}\mathbb{E}\left(\mathrm{e}^{\frac{s}{n}M_n}|X_1,\dots,X_{n-1}\right)\right]}{\mathrm{e}^{sx}}.$$

Here the study of $\mathbb{E}\left(\mathrm{e}^{\frac{s}{n}M_n}|X_1,\dots,X_{n-1}\right)$ requires some care...

Shameless name-dropping

In the paper, we provide an exhaustive list of inequalities, under various moment assumptions :

- exponential inequalities :
  - McDiarmid,
  - Hoeffding,
  - Bernstein.
- semi-exponential inequalities :
  - Fuk-Nagaev,
  - von Bahr-Esseen.
- moment inequalities :
  - Marcinkiewicz-Zygmund,
  - von Bahr-Esseen.

Applications

1. Deviation inequalities for time series : introduction
   - Why deviation inequalities ?
   - Deviation inequalities for time series
2. Non-homogeneous Markov chains
   - Inequalities for non-homogeneous Markov chains
   - Applications in machine learning

Empirical risk minimization (1/2)

In the stationary case,

$$f(X_1, \dots, X_n) = \frac{1}{n} \sum_{t=1}^{n} \ell(\theta, X_i) = R_n(\theta)$$

then

$$\mathbb{E}\left[f(X_1, \dots, X_n)\right] = \mathbb{E}\left[\ell(\theta, X)\right] = R(\theta).$$

$$\mathbb{P}\left\{ \left| R(\theta) - R_n(\theta) \right| \geq x \right\} \leq \begin{cases} \mathrm{e}^{-cnx}, \\ \mathrm{e}^{-cn(x \mathbf{1}_{x>1} + x^2 \mathbf{1}_{x \leq 1})}, \\ \mathrm{e}^{-cn^{1-2\alpha} x^2}. \end{cases}$$

Empirical risk minimization (2/2)

ERM

$$\hat{\theta} = \arg\min_{\theta \in \Theta} R_n(\theta).$$

Say $\mathrm{Card}(\Theta) = N$ is finite,

$$\mathbb{P}\left\{ R(\hat{\theta}) \geq R_n(\hat{\theta}) + x \right\} \leq \left\{ \begin{array}{l} N \mathrm{e}^{-cnx}, \\ N \mathrm{e}^{-cn(x 1_{x>1} + x^2 1_{x \leq 1})}, \\ N \mathrm{e}^{-c n^{1-2\alpha} x^2}. \end{array} \right.$$

Application to SGLD (1/2)

L is m-strongly convex, M-Lipschitz and ∇L is ℓ-Lipschitz.

SGLD - $\alpha \in (0,1)$, $\beta < \alpha$, $\gamma > 0$, $\eta \geq 0$

$$X_n = \Pi_{\mathcal{C}} \left[X_{n-1} - \frac{\gamma}{n^\alpha} \hat{\nabla}_n L(X_{n-1}) + \frac{\eta}{n^\beta} \varepsilon_n \right], \quad \bar{X}_n = \frac{1}{n} \sum_{t=1}^{n} X_t.$$

For some $c_{p,d} = c_{p,d}(\ell, m, M)$,

$$\mathbb{P}\left\{ \left\| \bar{X}_n - \mathbb{E}(\bar{X}_n) \right\|_p \geq x \right\} \leq \mathrm{e}^{-c_{p,d} n (x 1_{x>1} + x^2 1_{x \leq 1})}.$$

Application to SGLD (2/2)

Theorem - Moulines and Bach 2011

$$\mathbb{E}\|\bar{X}_n - x^*\|_2 \leq \frac{C_0}{n}.$$

Moulines, E. and Bach, F. (2011). Non-asymptotic analysis of stochastic approximation algorithms for machine learning. *NIPS*.

Combine with our inequality

$$\mathbb{P}\left\{ \left\|\bar{X}_n - x^*\right\|_2 \leq \sqrt{\frac{C_0 + \frac{1}{c_{2,d}} \log\left(\frac{1}{\delta}\right)}{n}} \right\} \geq 1 - \delta.$$