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

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Co-authors

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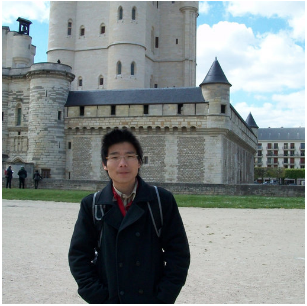

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Objective

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

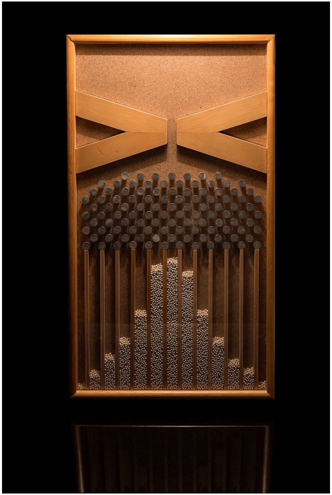
$$\mathbb{P}\left\{|U - \mathbb{E}(U)| \geq x\right\} \leq \frac{\mathrm{Var}(U)}{x^2}.$$

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

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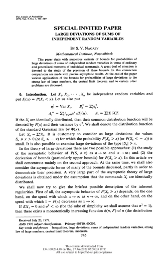
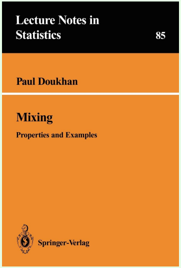
$$= e^{-sx}\prod_{t=1}^{n}\mathbb{E}\left(e^{\frac{s}{n}(X_t-\mu)}\right)$$

Deviation for time series : an active research field


The Annals of Probability 1979, Vol. 7, No. 5, 745–789

SPECIAL INVITED PAPER
LARGE DEVIATIONS OF SUMS OF INDEPENDENT RANDOM VARIABLES

By S. V. Nagaev
Mathematical Institute, Novosibirsk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Paul Doukhan
Mixing
Properties and Examples
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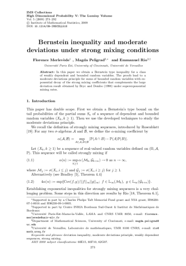
J Theor Probab (2009) 22: 146–163

Moment Inequalities for Sums of Dependent Random Variables under Projective Conditions

Emmanuel Rio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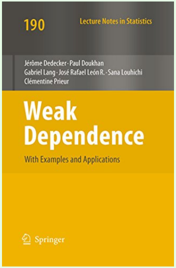
Bernstein inequality and moderate deviations under strong mixing conditions

Florence Merlevède, Magda Peligrad and Emmanuel Rio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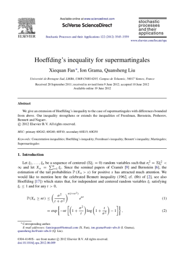
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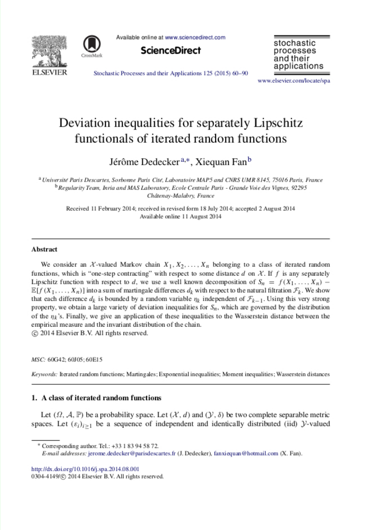
Stochastic Processes and their Applications 122 (2012) 3545–3559
stochastic processes and their applications

Hoeffding's inequality for supermartingales

Xiequan Fan, Ion Grama, Quansheng Liu

A remarkable result for Markov chains



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Stochastic Processes and their Applications 125 (2015) 60–90
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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 $X_1, X_2, \dots, X_n$ 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 $S_n = f(X_1, \dots, X_n) - \mathbb{E}[f(X_1, \dots, X_n)]$ 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

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

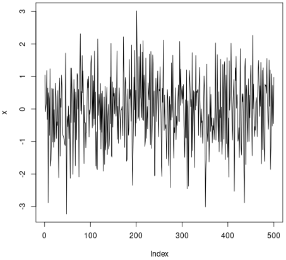
for some $\rho < 1$.

Example (1/2)

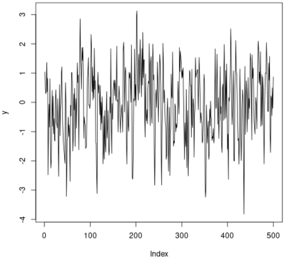
AR(1) process

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

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



$\rho = 0$



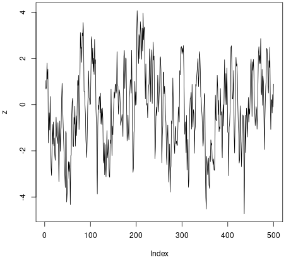
$\rho = 0.5$

Example (2/2)

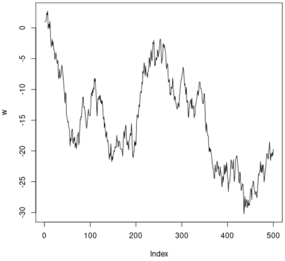
AR(1) process

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

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



$\rho = 0.8$

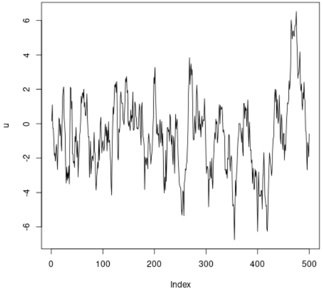


$\rho = 1$

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

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

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. $\mathbb{E}\left\{ d\Big(F_n(x, \varepsilon_n), F_n(x', \varepsilon_n)\Big) \right\} \leq \rho_n d(x, x')$.
3. $d\Big(F_n(x, y), F_n(x, y')\Big) \leq \tau_n \delta(y, y') + \xi_n$.

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) :

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

- Projected stochastic gradient Langevin descent (SGLD) :

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

Example : SGD

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

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

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

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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

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

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

Empirical risk minimization (2/2)

ERM

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

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

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

Application to SGLD (1/2)

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

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

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

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

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