Localized Complexities for Transductive Learning

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Short Summary

Concentration inequalities

- For independent random variables see overview in [BLM13]:

	1st order	2nd order
Sum	**Hoeffding's**	**Bennett's** **Bernstein's**
Supremum of empirical process	**McDiarmid's**	**Talagrand's** **Bousquet's**

- For random variables *sampled without replacement* (**SWOR**):

	1st order	2nd order
Sum	**Serfling's**	[BM13]
Supremum of empirical process	[EYP09] [CMPR09]	(**New results**)

Application:

Local complexities (and fast rates) in statistical learning

- Inductive setting: [Mas00, BBM05, Kol06] and others.
- Transductive setting: (**New results**)

Concentration Inequalities: known results

Given:

random variables $\boldsymbol{X}_1^n = \{X_1, \dots, X_n\} \subset \mathcal{X}$

function $g\colon \mathcal{X}^n \to \mathbb{R}$

random variable $Q = g(X_1, \dots, X_n)$

Find: high-probability (over $X_1, \dots, X_n$) upper bounds on:

$$Q - \mathbb{E}[Q] \quad \text{and/or} \quad \mathbb{E}[Q] - Q.$$

Sums of random variables

For random variables $X_1, \dots, X_n$ *bounded in* $[0,1]$ consider:

$$S_n = \frac{1}{n}\sum_{i=1}^n X_i, \quad \sigma^2 = \frac{1}{n}\sum_{i=1}^n \mathrm{Var}[X_i]$$

$S_n - \mathbb{E}[S_n]$ and $\mathbb{E}[S_n] - S_n$ are upper bounded with prob. $\geq 1-\delta$ by:

	$\boldsymbol{X}_1^n$ are independent	$\boldsymbol{X}_1^n$ are SWOR from $\{c_1, \dots, c_N\}$
1st order	**Hoeffding** $\sqrt{\frac{\ln(1/\delta)}{2n}}$	**Serfling** $\sqrt{\frac{\ln(1/\delta)}{2n}\left(\frac{N-n+1}{N}\right)}$
2nd order	**Bernstein** $\sqrt{\frac{2\sigma^2 \ln\frac{1}{\delta}}{n}} + \frac{2\ln(1/\delta)}{3n}$	[BM13] $\sqrt{\frac{2\sigma^2 \ln\frac{1}{\delta}}{n}\left(\frac{N-n+1}{N}\right)} + O(n^{-1})$

Factor $\left(\frac{N-n+1}{N}\right)$ is a SWOR-specific improvement.

Suprema of empirical processes

For *identically distributed* random variables $X_1, \dots, X_n$ and countable class $\mathcal{F}$ of functions $f\colon \mathcal{X} \to [-1,1]$, such that $\mathbb{E}[f(X_1)] = 0$, consider:

$$Q_n = \sup_{f\in\mathcal{F}} \frac{1}{n}\sum_{i=1}^n f(X_i), \quad v_{\mathcal{F}} = \sup_{f\in\mathcal{F}} \mathrm{Var}[f(X_1)] + 2\mathbb{E}[Q_n]$$

$Q_n - \mathbb{E}[Q_n]$ and $\mathbb{E}[Q_n] - Q_n$ are upper bounded with prob. $\geq 1-\delta$ by:

	$\boldsymbol{X}_1^n$ are independent	$\boldsymbol{X}_1^n$ are SWOR from $\{c_1, \dots, c_N\}$
1st order	**McDiarmid** $\sqrt{\frac{2\ln(1/\delta)}{n}}$	[EYP09, CMPR09] $\sqrt{\frac{2\ln(1/\delta)}{n}\left(\frac{N-n}{N-1/2}\right)}$ (**EP**)
2nd order	**Talagrand** $\sqrt{\frac{2v_{\mathcal{F}} \ln\frac{1}{\delta}}{n}} + \frac{2\ln(1/\delta)}{3n}$ (*only for* $Q_n - \mathbb{E}[Q_n]$)	(**New results:**) $2\sqrt{\frac{2\sigma^2_{\mathcal{F}}\log(1/\delta)}{n}\cdot\left(\frac{N}{n}\right)}$ $\sqrt{\frac{2(\sigma^2_{\mathcal{F}} + 2\mathbb{E}[Q_n^{iid}])\log\frac{1}{\delta}}{n}} + O(n^{-1})$

Factor $\left(\frac{N-n}{N-1/2}\right)$ is a SWOR-specific improvement.

Motivation

Applications of sampling without replacement

- Cross-validation procedures
- Transductive learning
- Low rank matrix factorization (collaborative filtering,...)
- Randomized sequential algorithms (SGD,...)

Motivation of our work

McDiarmid-type concentration inequality (**EP**) for SWOR does not account for the variance. There are situations when variance $\sim O(n^{-1/2})$.

New concentration inequalities for SWOR

Arbitrary finite set $\mathcal{C} = \{c_1, \dots, c_N\}$

$Z_1, \dots, Z_n$ sampled uniformly *with replacement* from $\mathcal{C}$

$X_1, \dots, X_n$ sampled uniformly *without replacement* from $\mathcal{C}$

Countable class $\mathcal{F}$ of functions $f\colon \mathcal{C} \to [-1,1]$, such that $\mathbb{E}[f(X_1)] = 0$

$$Q_n^{iid} = \sup_{f\in\mathcal{F}} \frac{1}{n}\sum_{i=1}^n f(Z_i), \quad Q_n = \sup_{f\in\mathcal{F}} \frac{1}{n}\sum_{i=1}^n f(X_i), \quad \sigma^2_{\mathcal{F}} = \sup_{f\in\mathcal{F}} \mathrm{Var}[f(X_1)].$$

Theorem 1 ((**Sub-Gaussian concentr. ineq. for SWOR**)). *For any $\delta \in (0,1]$ with probability greater than $1-\delta$:*

$$Q_n - \mathbb{E}[Q_n] \leq 2\sqrt{\frac{2\sigma^2_{\mathcal{F}}\log(1/\delta)}{n}\cdot\left(\frac{N}{n}\right)}. \qquad \textbf{(New1)}$$

The same bound also holds for $\mathbb{E}[Q_n] - Q_n$.

Theorem 2 ((**Talagrand-type concentr. ineq. for SWOR**)). *For any $\delta \in (0,1]$ with probability greater than $1-\delta$:*

$$Q_n - \mathbb{E}[Q_n^{iid}] \leq \sqrt{\frac{2(\sigma^2_{\mathcal{F}} + 2\mathbb{E}[Q_n^{iid}])\log(1/\delta)}{n}} + \frac{\log(1/\delta)}{3n}. \qquad \textbf{(New2)}$$

Comparison with State-of-the-art

- (**EP**) does not account for $\sigma^2_{\mathcal{F}}$ while (**New1**) and (**New2**) do.
- Large N and $n = o(N)$: (**EP**) can outperform (**New1**).
- Large N and $n = \Omega(N)$: (**New1**) outperforms (**EP**) for $\sigma^2_{\mathcal{F}} < 1/16$.
- Shortcomings of the new results:

  (**New1**): factor of N/n which can be large;

  (**New2**): concentration not around $\mathbb{E}[Q_n]$ but around $\mathbb{E}[Q_n^{iid}]$.

Lemma. $$0 \leq \mathbb{E}[Q_n^{iid}] - \mathbb{E}[Q_n] \leq \frac{n^3}{N}.$$

- However, often $\mathbb{E}[Q_n^{iid}] \sim O(n^{-1/2})$ (e.g. finite $\mathcal{F}$ or VC-class $\mathcal{F}$)

Summary:

(**New1**) stays informative in all regimes of n and N.

(**New2**) can be preferable for $n = \Omega(N)$.

Both (**New1**) and (**New2**) account for the variance.

Proof Idea

Chernoff's bounding method: for $\lambda > 0$

$$\mathbb{P}\{\xi \geq t\} = \mathbb{P}\left\{e^{\lambda\xi} \geq e^{\lambda t}\right\} \leq \frac{\mathbb{E}[e^{\lambda\xi}]}{e^{\lambda t}} \qquad (1)$$

Theorem 3 ([Bob04], simplified version). *Consider fixed finite set $\mathcal{C} = \{c_1, \dots, c_N\}$, a set $[\mathcal{C}]^n$ of all disjoint partitions $\mathcal{C} = \mathcal{C}' \cup \mathcal{C}''$ where $|\mathcal{C}'| = n$, and a function $g\colon [\mathcal{C}]^n \to \mathbb{R}$.*
If Euclidian norm of the discrete gradient $\|\nabla g(\mathcal{C}'\cup\mathcal{C}'')\|_2^2$ is bounded by Σ^2 and $(U \cup V)$ is sampled uniformly from $[\mathcal{C}]^n$ then the following upper bound on the MGF for $Q = g(U \cup V)$ holds:

$$\mathbb{E}\left[e^{\lambda(Q - \mathbb{E}[Q])}\right] \leq \exp\left(\frac{\Sigma^2\lambda^2}{N+2}\right), \quad \lambda \in \mathbb{R}. \qquad (2)$$

Theorem 4 ([Hoe63]). *Let $V_1, \dots, V_n$ and $U_1, \dots, U_n$ be sampled uniformly from a finite set $\{v_1, \dots, v_N\} \subset \mathbb{R}^d$ without and with replacements respectively. For any convex function $F\colon \mathbb{R}^d \to \mathbb{R}$:*

$$\mathbb{E}\left[F\left(\textstyle\sum_{i=1}^n V_i\right)\right] \leq \mathbb{E}\left[F\left(\textstyle\sum_{i=1}^n U_i\right)\right]. \qquad (3)$$

Proof sketch of Theorem 1: Use (1) for $\xi = Q_n - \mathbb{E}[Q_n^{iid}]$. Notice that $F\colon \boldsymbol{x} \to \exp\left(\sup_{i=1,\dots,d} x_i\right)$ for $\boldsymbol{x} = (x_1, \dots, x_d) \in \mathbb{R}^d$ is convex. Apply (3) and upper bound MGF using Talagrand's inequality.

Proof sketch of Theorem 2: Note that Q_n is a function over partitions of $\mathcal{C}$. Apply (1) and upper bound MGF using (2).

Application: Transductive Learning

Deterministic agnostic setting

Finite instance space $\boldsymbol{X}_n = \{X_1, \dots, X_N\} \subset \mathcal{X}$ and output space $\mathcal{Y}$

Class $\mathcal{H}$ of predictors $h\colon \mathcal{X} \to \mathcal{Y}$

Labelling function $\varphi\colon \mathcal{X} \to \mathcal{Y}$ (not necessarily in $\mathcal{H}$)

1. Sample $n \leq N$ inputs $\boldsymbol{X}_n \subseteq \boldsymbol{X}_N$ uniformly without replacement
2. Obtain outputs $\boldsymbol{Y}_n$ for $\boldsymbol{X}_n$ by applying function $\varphi\colon \mathcal{X} \to \mathcal{Y}$
3. Reveal training set $S_n = (\boldsymbol{X}_n, \boldsymbol{Y}_n)$ and $u = N - n$ test inputs $\boldsymbol{X}_u$

Goal of the learner: based on S_n and $\boldsymbol{X}_u$ find a predictor in hypothesis class $\mathcal{H} = \{h\colon \mathcal{X} \to \mathcal{Y}\}$ with minimal test error:

$$L_u(h) = \frac{1}{u}\sum_{X\in\boldsymbol{X}_u} \underbrace{\ell\big(h(X), \varphi(X)\big)}_{\ell_h(X)}$$

for *arbitrary bounded* loss function $\ell\colon \mathcal{Y}\times\mathcal{Y} \to [0,1]$.

Transductive learning: Notations

$L_N(h)$ and $\hat{L}_n(h)$ are errors over $\boldsymbol{X}_N$ and $\boldsymbol{X}_n$ respectively

$\hat{h}_n$, h_u^* and h_N^* minimize $\hat{L}_n(h)$, $L_u(h)$ and $L_N(h)$ respectively

Excess loss

$$\mathcal{E}_u(\hat{h}_n) = L_u(\hat{h}_n) - L_u(h_u^*)$$

measures how well ERM $\hat{h}_n$ approximates optimal h_u^* on $\boldsymbol{X}_u$.

Our goal: obtain tight high-probability upper bounds on $\mathcal{E}(\hat{h}_n)$.

State-of-the-art transductive bounds

Algo. stability: $\sim 1/\sqrt{n}$

Global Rademacher: $\sim 1/\sqrt{n}$

L_2-loss: $\sim \sqrt{\hat{L}_n(\hat{h}_n)\frac{\log(n+u)}{n}}$

Binary loss and $\varphi \in \mathcal{H}$: $\sim 1/n$

Summary: Without restrictive assumptions all bounds $\sim 1/\sqrt{n}$

Localized transductive bounds

Let $\hat{L}_n^{iid}(h) = \frac{1}{n}\sum_{i=1}^n \ell_h(Z_i)$, where $Z_1, \dots, Z_n \sim$ i.i.d. from $\boldsymbol{X}_N$.

Consider the local neighbourhood of h_N^* in $\mathcal{H}$:

$$\mathcal{H}(r) = \left\{h \in \mathcal{H}\colon \mathbb{E}\left[\left(\ell_h(X) - \ell_{h_N^*}(X)\right)^2\right] \leq r\right\}.$$

Theorem 5 ((**Localized transductive excess risk bound**)). *Assume that there is a constant $B > 0$ such that for every $h \in \mathcal{H}$:*

$$\mathbb{E}\left[\left(\ell_h(X) - \ell_{h_N^*}(X)\right)^2\right] \leq B\cdot\left(L_N(h) - L_N(h_N^*)\right). \qquad \textbf{(C1)}$$

Assume there is a sub-root function $\psi_n(r)$, such that:

$$B\cdot\mathbb{E}\left[\sup_{h\in\mathcal{H}(r)} L_N(h) - \hat{L}_n^{iid}(h) - \left(L_N(h_N^*) - \hat{L}_n^{iid}(h_N^*)\right)\right] \leq \psi_n(r).$$

Let r_n^* be a fixed point of $\psi_n(r)$. Then with prob. greater than $1-\delta$:

$$L_N(\hat{h}_n) - L_N(h_N^*) \leq 901\frac{r_n^*}{B} + (16+25B)\frac{\log(1/\delta)}{3n} = \Delta_n(\delta). \qquad \textbf{(New3)}$$

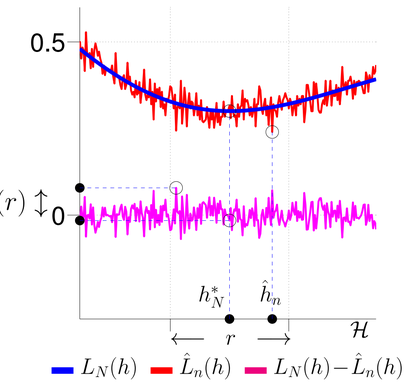
Also

$$\mathcal{E}_u(\hat{h}_n) \leq N\left(\frac{\Delta_n(\delta)}{u} + \frac{\Delta_u(\delta)}{n}\right). \qquad \textbf{(New4)}$$

Discussion:

"Order of the excess risk is related to the fixed point r_n^* of the modulus of continuity of the empirical process".

[Mas00, BBM05, Kol06]



Message: Theorem 5 recovers it in the transductive setting.

Condition (**C1**) is satisfied for:

- L_2-loss and *uniformly bounded convex* class $\mathcal{H}$ with $B = 1$;
- binary loss and VC-class $\mathcal{H}$ if $\varphi \in \mathcal{H}$ with $B = 8$.

Important: Fixed point r_n^* can be of the order $\sim o(n^{-1/2})$:

- For binary loss and VC-classes: $r_n^* \sim \frac{\mathrm{VC}(\mathcal{H})\log n}{n}$ [Mas00].
- For Lipschitz losses and balls in RKHS [Men03].

Future Work

1. Close the gap in concentration inequalities (**New1**) and (**New2**).
2. SWOR-specific improvements for Talagrand's inequality?
3. Local transductive Rademacher complexities.
4. Other applications: Cross-Validation, ...

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