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Risk bounds for linear regression

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Ordinary least squares and empirical risk minimization

- Let $\hat{f}^{(\text{ols})} \in \operatorname{argmin}_{f \in \mathcal{F}_{\text{lin}}} \frac{1}{n} \sum_{i=1}^{n} [Y_i f(X_i)]^2$.
- $\mathbb{E}R(\hat{f}^{(\text{ols})}) R(f^*_{\text{lin}}) = \mathbb{E}[\hat{f}^{(\text{ols})}(X) f^*_{\text{lin}}(X)]^2.$
- if $\sup_{x \in \mathcal{X}} \operatorname{Var}(Y|X = x) = \sigma^2 < +\infty$ and $f^{(\operatorname{reg})} = f^*_{\operatorname{lin}}$, we have

$$\mathbb{E}\left\{\frac{1}{n}\sum_{i=1}^{n}\left[\hat{f}^{(\text{ols})}(X_{i})-f^{*}_{\text{lin}}(X_{i})\right]^{2}\right\}\leq\sigma^{2}\frac{d}{n}$$

• It does not imply a $\frac{d}{n}$ upper bound on $\mathbb{E}R(\hat{f}^{(ols)}) - R(f^*_{lin})$.

New results

Ordinary least squares and empirical risk minimization

New results

Theorem (Györfi, Kohler, Krzyżak, Walk, 2004)

If $\sup_{x \in \mathcal{X}} Var(Y|X = x) = \sigma^2 < +\infty$ and

$$\|f^{(\mathsf{reg})}\|_{\infty} = \sup_{x \in \mathcal{X}} |f^{(\mathsf{reg})}(x)| \le H$$

for some H > 0, then the truncated estimator $\hat{f}_{H}^{(ols)} = (\hat{f}^{(ols)} \land H) \lor -H$ satisfies

$$\mathbb{E}R(\hat{f}_{H}^{(\text{ols})}) - R(f^{(\text{reg})}) \\ \leq 8[R(f_{\text{lin}}^{*}) - R(f^{(\text{reg})})] + \kappa \frac{(\sigma^{2} \vee H^{2})d\log n}{n}$$

for some numerical constant κ .

Ordinary least squares and empirical risk minimization

Theorem (Catoni, 2004)

Let $\mathcal{F}' \subset \mathcal{F}_{\mathsf{lin}}$ satisfying for some positive constants a, M, M' :

• there exists $f_0 \in \mathcal{F}'$ s.t. for any $x \in \mathcal{X}$,

$$\mathbb{E}\Big\{\exp\Big[a\big|Y-f_0(X)\big|\Big]\,\Big|\,X=x\Big\}\leq M.$$

• for any
$$f_1, f_2 \in \mathcal{F}', \sup_{x \in \mathcal{X}} |f_1(x) - f_2(x)| \leq M'$$
.

Let $Q = \mathbb{E}[\varphi(X)\varphi(X)^T]$ and $\hat{Q} = [\frac{1}{n}\sum_{i=1}^n \varphi(X_i)\varphi(X_i)^T]$. If det $Q \neq 0$, then there exist positive constants C_1 and C_2 s.t. with probability at least $1 - \epsilon$, as soon as

$$\left\{ f \in \mathcal{F}_{\mathsf{lin}} : r(f) \leq r(\hat{f}^{(\mathsf{ols})}) + C_1 \frac{d}{n} \right\} \subset \mathcal{F}',$$

we have

$$R(\hat{f}^{(\mathrm{ols})}) - R(f^*_{\mathrm{lin}}) \leq C_2 \frac{d + \log(\epsilon^{-1}) + \log(\frac{\det Q}{\det Q})}{n}.$$

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New results

Theorem (Alquier, 2008)

Let q_{\min} be the smallest eigenvalue of $Q = \mathbb{E}[\varphi(X)\varphi(X)^T]$. Let f_0 and H such that $||f_{\lim}^* - f_0||_{\infty} \leq H$. Assume that there exists C > 0 such that $|Y| \leq C$. Then for an appropriate randomized estimator requiring the knowledge of f_0 , H and C, for any $\epsilon > 0$ with probability at least $1 - \epsilon$, we have

$$R(\widehat{f}) - R(f^*_{\mathsf{lin}}) \leq \kappa (H^2 + C^2) rac{d \log(3q_{\mathsf{min}}^{-1}) + \log(\epsilon^{-1})}{n}.$$

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Ordinary least squares and empirical risk minimization

New results

Theorem (Bartlett, Bousquet, Mendelson, 2005)

Assume that for some positive constants H and C,

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\sup_{\theta \in \Theta} \|\theta\| \le 1,\|\varphi(x)\| \le H, \qquad \forall x \in \mathcal{X}
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$$|Y| \leq C.$$

Let $\nu_1 \geq \cdots \geq \nu_d$ be the eigenvalues of $Q = \mathbb{E}[\varphi(X)\varphi(X)^T]$. With probability at least $1 - \epsilon$, we have

$$egin{aligned} & \min_{0\leq h\leq d} \left(h+\sqrt{rac{n}{(H+C)^2}\sum_{i>h}
u_i}
ight) + \log(\epsilon^{-1}) \ & n \ & \leq \kappa(H+C)^2rac{d+\log(\epsilon^{-1})}{n}, \end{aligned}$$

where κ is a numerical constant.

New results

Ordinary least squares and empirical risk minimization

Theorem (Birgé, Massart, 1998)

Assume that for any f_1,f_2 in $\mathcal{F},\,\|f_1-f_2\|_\infty\leq H$ and $\exists f_0\in\mathcal{F}$ satisfying

for any
$$x \in \mathcal{X}, \quad \mathbb{E}\Big\{ \exp\Big[A^{-1} \big| \, Y - f_0(X) \big| \Big] \, \Big| \, X = x \Big\} \leq M,$$

for some positive constants A and M. Let

$$\tilde{B} = \inf_{\phi_1, \dots, \phi_d} \sup_{\theta \in \mathbb{R}^d - \{0\}} \frac{\|\sum_{j=1}^d \theta_j \phi_j\|_{\infty}^2}{\|\theta\|_{\infty}^2}$$

where the infimum is taken w.r.t. all possible orthonormal basis of \mathcal{F} for $\langle f_1, f_2 \rangle = \mathbb{E} f_1(X) f_2(X)$. Then, with probability at least $1 - \epsilon$:

$$R(\hat{f}^{(ext{erm})}) - R(f^*) \leq \kappa (A^2 + H^2) rac{d \log[2 + (ilde{B}/n) \wedge (n/d)] + \log(\epsilon^{-1})}{n},$$

where κ is a positive constant depending only on M.

Projection estimator

New results

Theorem (Tsybakov, 2003)

Let ϕ_1, \ldots, ϕ_d be an o.n.b. of \mathcal{F}_{lin} for $\langle f_1, f_2 \rangle = \mathbb{E}f_1(X)f_2(X)$. The projection estimator on this basis is $\hat{f}^{(\text{proj})} = \sum_{j=1}^d \hat{\theta}_j^{(\text{proj})} \phi_j$, with

$$\hat{\theta}^{(\mathsf{proj})} = rac{1}{n} \sum_{i=1}^{n} Y_i \phi_i(X_i).$$

lf

$$\sup_{x\in\mathcal{X}} \operatorname{Var}(Y|X=x) = \sigma^2 < +\infty$$

and

$$\|f^{(\operatorname{reg})}\|_{\infty} = \sup_{x \in \mathcal{X}} |f^{(\operatorname{reg})}(x)| \le H < +\infty,$$

then we have

$$\mathbb{E}R(\hat{f}^{(\text{proj})}) - R(f_{\text{lin}}^*) \le (\sigma^2 + H^2)\frac{d}{n}.$$

Theorem (Caponnetto, De Vito, 2007)

$$\hat{f}_{\lambda}^{(\mathsf{ridge})} \in \operatorname*{argmin}_{\{f_{ heta}; \, heta \in \mathbb{R}^d\}} rac{1}{n} \sum_{i=1}^n [Y_i - f_{ heta}(X_i)]^2 + \lambda \| heta\|^2.$$

Let q_{\min} be the smallest eigenvalue of $Q = \mathbb{E}[\varphi(X)\varphi(X)^T]$. Let $\mathcal{K} = \sup_{x \in \mathcal{X}} \sum_{j=1}^d \varphi_j(x)^2 = \|\|\varphi\|^2\|_{\infty}$. Recall $f_{\lim}^* = \sum_{j=1}^d \theta_j^* \varphi_j$. Let $0 < \epsilon < 1/2$ and $\mathcal{L}_{\epsilon} = \log^2(\epsilon^{-1})$. Assume that for any $x \in \mathcal{X}$,

$$\mathbb{E}(e^{|Y-f_{\rm lin}^*(X)|/A}|X=x)\leq M.$$

For $\lambda = (\mathcal{K} d\mathcal{L}_{\epsilon})/n$, if $\lambda \leq q_{\min}$, with probability at least $1 - \epsilon$:

$$R(\hat{f}^{(\mathsf{ridge})}_{\lambda}) - R(f^*_{\mathsf{lin}}) \leq \kappa \mathcal{L}_\epsilon rac{d}{n} igg(A^2 + rac{\lambda}{q_{\mathsf{min}}} \mathcal{KL}_\epsilon \| heta^* \|^2 igg)$$

for some positive constant κ depending only on M.

Penalized least squares estimator

$$\hat{f}_{\lambda}^{(\text{lasso})} \in \operatorname*{argmin}_{\{f_{\theta};\,\theta \in \mathbb{R}^{d}\}} \frac{1}{n} \sum_{i=1}^{n} \left(Y_{i} - f_{\theta}(X_{i})\right)^{2} + \lambda \|\theta\|_{1}.$$

- As the L^2 penalty, the L^1 penalty shrinks the coefficients.
- It allows to select relevant variables (i.e., find the j's such that θ_i^{*} ≠ 0).
- Assume that f^(reg) is a linear combination of only d^{*} ≪ d variables/functions φ_j's, then under strong conditions on the eigenvalues of submatrices of Q, the risk of the Lasso estimator for λ of order √(log d)/n is of order (d^{*} log d)/n.
- From a model selection approach, the assumptions can be weakened.

- $R(\hat{f}^{(\text{erm})}) R(f^*) = O(\frac{d \log(2+n/d) + \log(e^{-1})}{n})$ for L_{∞} -bounded \mathcal{F} and exponential moments
- There is no simple *d*/*n* which does not require strong assumptions
- Degraded convergence rate when Q is ill-conditioned ?

Ridge regression and empirical risk minimization

Theorem

Let
$$\lambda \geq 0$$
 and $\tilde{f} \in \arg \min_{f_{\theta} \in \mathcal{F}} \{ R(f_{\theta}) + \lambda \|\theta\|^2 \}$.
Assume $\mathbb{E}[\|\varphi(X)\|^4] < +\infty$ and $\mathbb{E}\{\|\varphi(X)\|^2[\tilde{f}(X) - Y]^2\} < +\infty$.
Let ν_1, \ldots, ν_d be the eigenvalues of Q , and $Q_{\lambda} = Q + \lambda I$. Let

$$D = \sum_{i=1}^{d} \frac{\nu_i}{\nu_i + \lambda} \mathbf{1}_{\nu_i > 0} = \operatorname{Tr} \left[(Q + \lambda I)^{-1} Q \right] = \mathbb{E} \left\{ \|Q_{\lambda}^{-1/2} \varphi(X)\|^2 \right\}.$$

For any $\epsilon > 0$, there is n_{ϵ} s.t. for any $n \ge n_{\epsilon}$, with proba. at least $1 - \epsilon$,

$$\begin{split} & \mathcal{R}(\hat{f}_{\lambda}^{(\mathsf{ridge})}) + \lambda \| \hat{\theta}^{(\mathsf{ridge})} \|^{2} \leq \min_{f_{\theta} \in \mathcal{F}} \left\{ \mathcal{R}(f_{\theta}) + \lambda \| \theta \|^{2} \right\} \\ & \quad + \frac{30 \,\mathbb{E} \left\{ \| Q_{\lambda}^{-1/2} \varphi(X) \|^{2} [\tilde{f}(X) - Y]^{2} \right\}}{\mathbb{E} \left\{ \| Q_{\lambda}^{-1/2} \varphi(X) \|^{2} \right\}} \, \frac{D}{n} \\ & \quad + 1000 \sup_{v \in \mathbb{R}^{d}} \frac{\mathbb{E} \left[\langle v, \varphi(X) \rangle^{2} [\tilde{f}(X) - Y]^{2} \right]}{\mathbb{E} (\langle v, \varphi(X) \rangle^{2}) + \lambda \| v \|^{2}} \frac{\log(3\epsilon^{-1})}{n}. \end{split}$$

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Ridge regression and empirical risk minimization

Corollary

For any $\epsilon > 0$, there is n_{ϵ} s.t. for any $n \ge n_{\epsilon}$, with proba. at least $1 - \epsilon$, $R(\hat{t}_{\lambda}^{(\text{ridge})}) \le R(f_{\text{lin}}^*) + \lambda \|\theta^*\|^2$ $+ \operatorname{ess\,sup} \mathbb{E}\{[Y - \tilde{f}(X)]^2 | X\} \frac{30D + 1000 \log(3\epsilon^{-1})}{n}$

$$D = \sum_{i=1}^{d} \frac{\nu_i}{\nu_i + \lambda} \mathbf{1}_{\nu_i > 0} = \operatorname{Tr} \left[(Q + \lambda I)^{-1} Q \right] = \text{ effective ridge dimension}$$

Ridge regression and empirical risk minimization

Theorem

Let
$$d' = \operatorname{rank}(Q)$$
. Assume $\mathbb{E}\left\{[Y - f^*(X)]^4\right\} < +\infty$ and

$$B = \sup_{f \in \operatorname{span}\{\varphi_1, \dots, \varphi_d\} - \{0\}} \|f\|_{\infty}^2 / \mathbb{E}[f(X)^2] < +\infty.$$

Consider the (unique) function $\hat{f}^{(\text{erm})} : x \mapsto \langle \hat{\theta}^{(\text{erm})}, \varphi(x) \rangle$ on \mathcal{F} for which $\hat{\theta}^{(\text{erm})} \in \text{span}\{\varphi(X_1), \dots, \varphi(X_n)\}$. For any values of ϵ and n such that $2/n \le \epsilon \le 1$ and

$$n > 1280B^2 \left[3Bd' + \log(2\epsilon^{-1}) + \frac{16B^2{d'}^2}{n} \right],$$

with probability at least $1 - \epsilon$,

$$R(\hat{f}^{(\text{erm})}) - R(f^*)$$

$$\leq 1920 B \sqrt{\mathbb{E}[Y - f^*(X)]^4} \left[\frac{3Bd' + \log(2\epsilon^{-1})}{n} + \left(\frac{4Bd'}{n}\right)^2 \right].$$

A simple tight risk bound for a sophisticated PAC-Bayes algorithm

Let

- ⊖ bounded
- π uniform distribution on \mathcal{F}
- λ > 0

•
$$W_i(f, f') = \lambda \{ [Y_i - f(X_i)]^2 - [Y_i - f'(X_i)]^2 \}$$

•
$$\hat{\mathcal{E}}(f) = \log \int \frac{\pi(df')}{\prod_{i=1}^{n} [1 - W_i(f, f') + \frac{1}{2} W_i(f, f')^2]}$$

 $\hat{\mathcal{E}}(f) \approx \lambda \sum_{i=1}^{n} [Y_i - f(X_i)]^2 + \log \int \pi(df') \exp\left\{-\lambda \sum_{i=1}^{n} [Y_i - f'(X_i)]^2\right\},$ We consider the "posterior" distribution $\hat{\pi}$ on the set \mathcal{F} with density:

$$\frac{d\hat{\pi}}{d\pi}(f) = \frac{\exp[-\hat{\mathcal{E}}(f)]}{\int \exp[-\hat{\mathcal{E}}(f')]\pi(df')}.$$

$$\frac{d\hat{\pi}}{d\pi}(f) \approx \frac{\exp\{-\lambda \sum_{i=1}^{n} [Y_i - f(X_i)]^2\}}{\int \exp\{-\lambda \sum_{i=1}^{n} [Y_i - f'(X_i)]^2\} \pi(df')}.$$

New results

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A simple tight risk bound for a sophisticated PAC-Bayes algorithm

Theorem

Assume $\sup_{f_1, f_2 \in \mathcal{F}} \|f_1 - f_2\|_{\infty} \leq H$ and, for some $\sigma > 0$,

$$\sup_{\mathbf{X}\in\mathcal{X}}\mathbb{E}\big\{[\mathbf{Y}-f^*(\mathbf{X})]^2\big|\mathbf{X}=\mathbf{X}\big\}\leq\sigma^2<+\infty.$$

Let $\lambda = \frac{1}{3(2\sigma+H)^2}$ and \hat{f} be a prediction function drawn from the distribution $\hat{\pi}$. Then for any $\epsilon > 0$, with probability at least $1 - \epsilon$, we have

$$R(\hat{f}) - R(f^*) \le 17(2\sigma + H)^2 \, rac{d + \log(2\epsilon^{-1})}{n}.$$