Overparametrization and the bias-variance dilemma

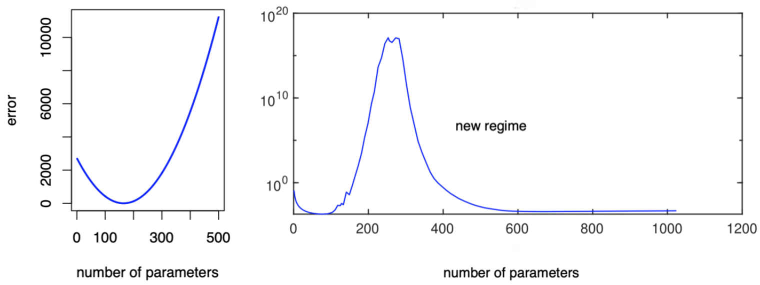
Johannes Schmidt-Hieber

joint work with Alexis Derumigny

https://arxiv.org/abs/2006.00278.pdf

feel free to ask questions during the talk!

double descent and implicit regularization



overparametrization generalizes well $\rightsquigarrow$ implicit regularization

can we defy the bias-variance trade-off?

Geman et al. '92: "the fundamental limitations resulting from the bias-variance dilemma apply to all nonparametric inference methods, including neural networks"

Because of the double descent phenomenon, there is some doubt whether this statement is true. Recent work includes

Statistics > Machine Learning

[Submitted on 28 Dec 2018 (v1), last revised 10 Sep 2019 (this version, v2)]

Reconciling modern machine learning practice and the bias-variance trade-off

Mikhail Belkin, Daniel Hsu, Siyuan Ma, Soumik Mandal

Computer Science > Machine Learning

[Submitted on 19 Oct 2018 (v1), last revised 18 Dec 2019 (this version, v4)]

A Modern Take on the Bias-Variance Tradeoff in Neural Networks

Brady Neal, Sarthak Mittal, Aristide Baratin, Vinayak Tantia, Matthew Scicluna, Simon Lacoste-Julien, Ioannis Mitliagkas

lower bounds on the bias-variance trade-off

Similar to minimax lower bounds we want to establish a general mathematical framework to derive lower bounds on the bias-variance trade-off that hold for all estimators.

given such bounds we can answer many interesting questions

- are there methods (e.g. deep learning) that can defy the bias-variance trade-off?
- lower bounds for the U-shaped curve of the classical bias-variance trade-off

related literature

- Low '95 provides complete characterization of bias-variance trade-off for functionals in the Gaussian white noise model
- Pfanzagl '99 shows that estimators of functionals satisfying an asymptotic unbiasedness property must have unbounded variance

No general treatment of lower bounds for the bias-variance trade-off yet.

overview

1. abstract lower bounds for bias-variance trade-off
2. applications to standard nonparametric and high-dimensional models

Cramér-Rao inequality

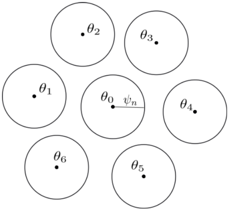
for parametric problems:

$$V(\theta) \geq \frac{(1 + B'(\theta))^2}{F(\theta)}$$

- $V(\theta)$ the variance
- $B'(\theta)$ the derivative of the bias
- $F(\theta)$ the Fisher information

abstract lower bounds on bias-variance trade-off

the well-known hypotheses testing reduction to prove lower bounds for the minimax risk relies on a careful selection of probability measures $P_0, \dots, P_M$ together with bounds on information distances such as KL, Hellinger, ...



- to prove lower bounds for the bias-variance trade-off, we want to follow a similar approach
- similar as for minimax lower bounds we need to distinguish the cases $M = 1$ (linear functionals) and $M > 1$

change of expectation inequalities

for two measures P, Q ($M = 1$), we derived inequalities for the most common information measures that link the change of expectation and the variance

Hellinger version: For all random variables X,

$$\frac{(E_P[X] - E_Q[X])^2}{4}\Big(\frac{1}{H(P,Q)} - H(P,Q)\Big)^2 \leq \mathrm{Var}_P(X) + \mathrm{Var}_Q(X)$$

with $H(P, Q)$ the Hellinger distance.

How can this be used to prove lower bounds for the bias-variance trade-off?

recovering the Cramér-Rao inequality

If $P = P_\theta$ and $Q = P_{\theta+\Delta}$, then, the inequality

$$\frac{(E_P[X] - E_Q[X])^2}{4}\Big(\frac{1}{H(P,Q)} - H(P,Q)\Big)^2 \leq \mathrm{Var}_P(X) + \mathrm{Var}_Q(X)$$

becomes (under suitable regularity conditions) the Cramér-Rao inequality as $\Delta \downarrow 0$

$$\frac{H(P_\theta, P_{\theta+\Delta})^2}{\Delta^2} = \frac{1}{8}\text{Fisher info}(\theta) + o(\Delta).$$

why we need to generalize

- with two measures, we can only study perturbation in one direction
- not enough to derive rate optimal lower bounds for bias-variance trade-off
- we derived two change of expectation inequalities to deal with multiple probability measures

change of expectation for multiple measures

χ^2-version:

- probability measures $P_0, \dots, P_M$
- $\chi^2(P_0, \dots, P_M)$ the matrix with entries

$$\chi^2(P_0, \dots, P_M)_{j,k} = \int \frac{dP_j}{dP_0} dP_k - 1$$

- any random variable X
- $\Delta := (E_{P_1}[X] - E_{P_0}[X], \dots, E_{P_M}[X] - E_{P_0}[X])^\top$

then,

$$\Delta^\top \chi^2(P_0, \dots, P_M)^{-1} \Delta \leq \mathrm{Var}_{P_0}(X)$$

some examples for χ^2-matrix

distribution	$\chi^2(P_0, \ldots, P_M)_{j,k}$
$P_j = \mathcal{N}(\theta_j, \sigma^2 I_d)$, $\theta_j \in \mathbb{R}^d$, I_d identity	$\exp\left(\frac{\langle \theta_j - \theta_0, \theta_k - \theta_0 \rangle}{\sigma^2}\right) - 1$
$P_j = \otimes_{\ell=1}^d \mathrm{Pois}(\lambda_{j\ell})$, $\lambda_{j\ell} > 0$	$\exp\left(\sum_{\ell=1}^d \frac{(\lambda_{j\ell} - \lambda_{0\ell})(\lambda_{k\ell} - \lambda_{0\ell})}{\lambda_{0\ell}}\right) - 1$
$P_j = \otimes_{\ell=1}^d \mathrm{Exp}(\beta_{j\ell})$, $\beta_{j\ell} > 0$	$\prod_{\ell=1}^d \frac{\beta_{j\ell}\beta_{k\ell}}{\beta_{0\ell}(\beta_{j\ell} + \beta_{k\ell} - \beta_{0\ell})} - 1$
$P_j = \otimes_{\ell=1}^d \mathrm{Ber}(\theta_{j\ell})$, $\theta_{j\ell} \in (0,1)$	$\prod_{\ell=1}^d \left(\frac{(\theta_{j\ell} - \theta_{0\ell})(\theta_{k\ell} - \theta_{0\ell})}{\theta_{0\ell}(1 - \theta_{0\ell})} + 1\right) - 1$

χ^2-matrix decodes a form of linear dependence of the measures $P_1 - P_0, \ldots, P_M - P_0$

overview

1. abstract lower bounds for bias-variance trade-off
2. applications

pointwise estimation

Gaussian white noise model: We observe $(Y_x)_x$ with

$$dY_x = f(x)\,dx + n^{-1/2}\,dW_x$$

- estimate $f(x_0)$ for a fixed x_0
- $\mathscr{C}^\beta(R)$ denotes ball of Hölder β-smooth functions
- for any estimator $\widehat{f}(x_0)$, we obtain the bias-variance lower bound

$$\inf_{\widehat{f}} \sup_{f\in\mathscr{C}^\beta(R)} \left|\operatorname{Bias}_f\left(\widehat{f}(x_0)\right)\right|^{1/\beta} \sup_{f\in\mathscr{C}^\beta(R)} \operatorname{Var}_f\left(\widehat{f}(x_0)\right) \gtrsim \frac{1}{n}$$

- bound is attained by most estimators
- generates U-shaped curve

pointwise estimation (ctd.)

for any estimator satisfying

$$\sup_{f \in \mathscr{C}^\beta(R)} |\operatorname{Bias}_f(\widehat{f}(x_0))| \lesssim n^{-\beta/(2\beta+1)}$$

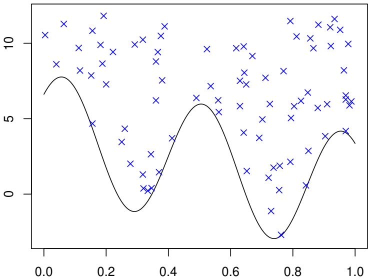
we also have that

$$\inf_{\widehat{f}} \sup_{f \in \mathscr{C}^\beta(R)} \left|\operatorname{Bias}_f\left(\widehat{f}(x_0)\right)\right|^{1/\beta} \inf_{f \in \mathscr{C}^\beta(R)} \operatorname{Var}_f\left(\widehat{f}(x_0)\right) \gtrsim \frac{1}{n}$$

- much stronger bias-variance trade-off
- sup over bias can never be replaced by inf!

pointwise estimation of the boundary

For an example of an irregular nonparametric problem consider support boundary recovery



$\rightsquigarrow$ we observe Poisson point process with intensity n on the epigraph of an unknown function f and want to recover f

pointwise estimation of the boundary (ctd.)

the minimax estimation rate in this model is $n^{-2\beta/(\beta+1)}$

For any estimator $\widehat{f}$ with

$$\sup_{f \in \mathscr{C}^\beta(R)} \mathrm{MSE}_f\left(\widehat{f}(x_0)\right) \lesssim n^{-\frac{2\beta}{\beta+1}},$$

we have

$$\sup_{f \in \mathscr{C}^\beta(R)} \mathrm{Bias}_f\left(\widehat{f}(x_0)\right)^2 \gtrsim n^{-\frac{2\beta}{\beta+1}}$$

and for all f in the interior of the Hölder ball

$$\mathrm{Var}_f\left(\widehat{f}(x_0)\right) \gtrsim n^{-\frac{2\beta}{\beta+1}}$$

high-dimensional models

Gaussian sequence model:

- observe independent $X_i \sim \mathcal{N}(\theta_i, 1)$, $i = 1, \ldots, n$
- $\Theta(s)$ the space of s-sparse vectors (here: $s \leq \sqrt{n}/2$)
- bias-variance decomposition

$$E_\theta[\|\widehat{\theta} - \theta\|^2] = \underbrace{\|E_\theta[\widehat{\theta}] - \theta\|^2}_{B^2(\theta)} + \sum_{i=1}^n \mathrm{Var}_\theta(\widehat{\theta}_i)$$

- **bias-variance lower bound:** if $B^2(\theta) \leq \gamma s \log(n/s^2)$, then,

$$\sum_{i=1}^{n} \mathrm{Var}_0\left(\widehat{\theta}_i\right) \gtrsim n\Big(\frac{s^2}{n}\Big)^{4\gamma}$$

- bound is matched (up to a factor in the exponent) by soft thresholding
- bias-variance trade-off more extreme than U-shape
- results also extend to high-dimensional linear regression

L^2-loss

Gaussian white noise model: We observe $(Y_x)_x$ with

$$dY_x = f(x)\,dx + n^{-1/2}\,dW_x$$

- bias-variance decomposition

$$\begin{aligned}\mathrm{MISE}_f\left(\widehat{f}\right) &:= E_f\left[\left\|\widehat{f} - f\right\|_{L^2[0,1]}^2\right] \\ &= \int_0^1 \mathrm{Bias}_f^2\left(\widehat{f}(x)\right)dx + \int_0^1 \mathrm{Var}_f\left(\widehat{f}(x)\right)dx \\ &=: \mathrm{IBias}_f^2(\widehat{f}) + \mathrm{IVar}_f\left(\widehat{f}\right).\end{aligned}$$

- is there a bias-variance trade-off between $\mathrm{IBias}_f^2(\widehat{f})$ and $\mathrm{IVar}_f\left(\widehat{f}\right)$?
- turns out to be a very hard problem

reductions for L^2-loss

- direct application of abstract lower bound does not seem to work
- we propose a two-fold reduction scheme
  - reduction to a simpler model
  - reduction to a smaller class of estimators

first reduction for L^2-loss

Consider the Gaussian sequence model

$$X_i = \theta_i + \frac{1}{\sqrt{n}}\varepsilon_i, \quad i = 1, \ldots, m$$

- $S^\beta(R)$ Sobolev space of β-smooth functions
- $\Theta_m^\beta(R) := \{\theta : \|\theta\|_2 \le R/(\Gamma_\beta m^\beta)\}$, Γ_β a suitable constant

Reduction: For any estimator $\widehat{f}$, there exists estimator $\widehat{\theta}$, s.t.

$$\sup_{\theta \in \Theta_m^\beta(R)} \left\| E_\theta\left[\widehat{\theta}\right] - \theta \right\|_2^2 \le \sup_{f \in S^\beta(R)} \mathrm{IBias}_f^2(\widehat{f}),$$

and

$$\sup_{\theta \in \Theta_m^\beta(R)} \sum_{i=1}^m \mathrm{Var}\left(\widehat{\theta}_i\right) \le \sup_{f \in S^\beta(R)} \mathrm{IVar}_f\left(\widehat{f}\right).$$

second reduction for L^2-loss

- a function is spherically symmetric if for any x and any orthogonal matrix D, $f(x) = D^{-1}f(Dx)$.
- estimator $\widehat{\theta} = \widehat{\theta}(X)$ is spherically symmetric if $X \mapsto \widehat{\theta}(X)$ is spherically symmetric

in the second reduction step we show that the best bias-variance trade-off is attained for spherically symmetric estimators

- argument in Stein '56 shows that $\widehat{\theta}$ is of the form $r(\|X\|_2)X$

L^2-loss (ctd.)

Bias-variance lower bound: For any estimator $\widehat{f}$,

$$\inf_{\widehat{f}} \sup_{f \in S^\beta(R)} \left| \mathrm{IBias}_f(\widehat{f}) \right|^{1/\beta} \sup_{f \in S^\beta(R)} \mathrm{IVar}_f \left(\widehat{f}\right) \geq \frac{1}{8n},$$

- many estimators $\widehat{f}$ can be found with upper bound $\lesssim 1/n$

summary

- general framework to derive bias-variance lower bounds
- leads to matching bias-variance lower bounds for standard models in nonparametric and high-dimensional statistics
- different types of the bias-variance trade-off occur
- can machine learning methods defy the bias-variance trade-off? **No, there are universal lower bounds that no method can avoid**

for details and more results consult the preprint

`https://arxiv.org/abs/2006.00278.pdf`

Open problems

mean absolute deviation

- several extensions of the bias-variance trade-off have been proposed in the literature, e.g. for classification
- the mean absolute deviation (MAD) of an estimator $\widehat{\theta}$ is

$$E_\theta[|\widehat{\theta} - m|]$$

with m either the mean or the median of $\widehat{\theta}$

can the general framework be extended to lower bounds on the trade-off between bias and MAD?

- derived change of expectation inequality
- this can be used to obtain a partial answer for pointwise estimation in the Gaussian white noise model

double descent