From kernel methods to neural networks: double descent, function spaces, curse of dimensionality

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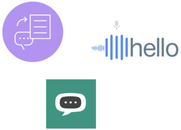
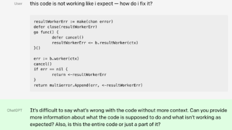
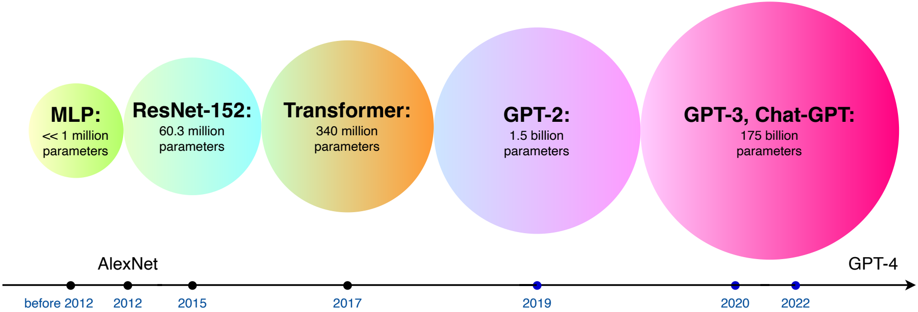
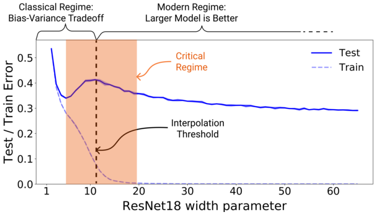
Over-parameterization: more parameters than training data



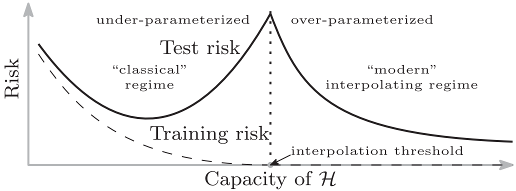




Surprises in modern neural networks: double descent



(a) Training and test error on ResNet18 [1]



(b) Double descent [2] (Belkin, Hsu, Ma, Mandal, 2019).

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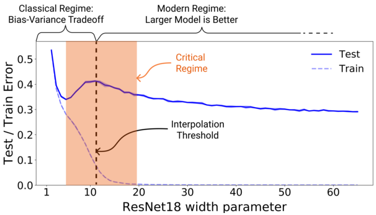

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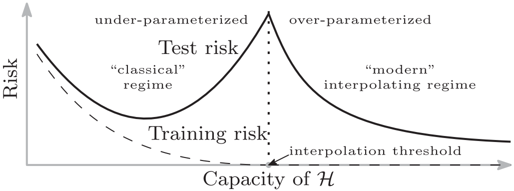


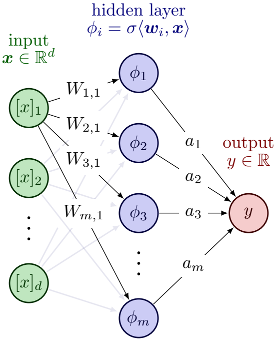
(b) Double descent [2] (Belkin, Hsu, Ma, Mandal, 2019).

Observations: beyond bias-variance trade-off

- 1) Monotonic decreasing in the overparameterized regime
- 2) Global minimum when #parameters is infinite
- 3) Peak at the interpolation thresholds

Background: Two-layer neural networks

kernel methods → **random features** → **neural networks**



$$f_m(\boldsymbol{x};\boldsymbol{\theta}) = \sum_{i=1}^{m} a_i \phi(\boldsymbol{x}, \boldsymbol{w}_i), \quad \boldsymbol{\theta} := \{(a_i, \boldsymbol{w}_i)\}_{i=1}^{m}$$

- $\phi : \mathcal{X} \times \mathcal{W} \to \mathbb{R}$, e.g., ReLU: $\phi(\boldsymbol{x}, \boldsymbol{w}) = \max(\langle \boldsymbol{x}, \boldsymbol{w}\rangle, 0)$

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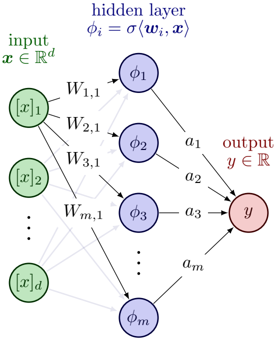

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- Random features models (RFMs) [3]:
  - $\{\boldsymbol{w}_i\}_{i=1}^{m} \overset{iid}{\sim} \mu$ for a given $\mu \in \mathcal{P}(\mathcal{W})$
  - only train the second layer

Recall RFMs in high-dimensional asymptotic setting (Mei and Montanari, 2022)

- random feature regression with $\widehat{\boldsymbol{a}}_\lambda = \arg\min_{\boldsymbol{a}} \widehat{\mathcal{E}}_\lambda(\boldsymbol{a})$

$$\widehat{\mathcal{E}}_\lambda(\boldsymbol{a}) = \frac{1}{n}\sum_{i=1}^{n}\left[y_i - \frac{1}{m}\sum_{j=1}^{m} a_j \sigma(\langle \boldsymbol{x}_i, \boldsymbol{w}_j \rangle)\right]^2 + \frac{\lambda m}{d}\|\boldsymbol{a}\|_2^2$$

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$$\mathcal{E}(\boldsymbol{a}, f_\rho) = \mathbb{E}_{\boldsymbol{x},y}\left[f_\rho(\boldsymbol{x}) - \frac{1}{m}\sum_{j=1}^{m} a_j \sigma(\langle \boldsymbol{x}_i, \boldsymbol{w}_j\rangle)\right]^2$$

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Theorem (double descent of RFMs [4])

Under proper assumptions, if target function is linear, under the high-dimensional setting

- $n, m, d \to \infty$, $m/d \to \psi_1$ *and* $n/d \to \psi_2$ *as* $d \to \infty$ *with* $\psi_1, \psi_2 \in (0, \infty)$

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$$\mathcal{E}(\widehat{\boldsymbol{a}}_\lambda, f_\rho) = \textit{Bias} + \textit{Variance} + o_{d,\mathbb{P}}(1)\,.$$

observations 1), 2), 3) for double descent can be theoretically proved.

Questions on high dimensional kernel methods

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◦ asymptotic expansion under high dimensions [6] (El Karoui, 2010)
under the setting of $n, d \to \infty$, $n/d \to \psi_1$ as $d \to \infty$ with $\psi_1 \in (0, \infty)$, we have

$$\|\boldsymbol{K} - (a\boldsymbol{X}\boldsymbol{X}^\top + b\boldsymbol{I})\|_2 \xrightarrow{\mathbb{P}} 0 \quad \text{when } d \to \infty \quad \text{for some parameters } a, b$$

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- $\|f\|_{\mathcal{H}} < \infty$ when $d \to \infty$?

Example (a linear function $f : \mathbb{S}^d \to \mathbb{R}$ such that $f(\boldsymbol{x}) = \boldsymbol{v}^\top \boldsymbol{x}$ for a certain $\boldsymbol{v} \in \mathbb{S}^d$)

- zero-order arc-cosine kernel $k(\boldsymbol{x}, \boldsymbol{x}') = \int_{\mathbb{S}^d} 1_{\{\boldsymbol{w}^\top \boldsymbol{x} \geq 0\}} 1_{\{\boldsymbol{w}^\top \boldsymbol{x}' \geq 0\}} \mathrm{d}\mu(\boldsymbol{w})$
  $\Rightarrow \|f\|_{\mathcal{H}} = \frac{2d\pi}{d-1}\pi < 4\pi$ [7] (Bach 2017)

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  $\Rightarrow \|f\|_{\mathcal{H}} = \frac{2d\pi}{d-1}\pi < 4\pi$ [7] (Bach 2017)
- first-order arc-cosine kernel, we have $\|f\|_{\mathcal{H}} \asymp C\sqrt{d}$ for some constant C independent of d.

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- high dimension vs. fixed dimension
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- SGD: implicit regularization $\rightarrow$ without λ
- dimension-free SGD bound
- multiple randomness sources
  - data sampling, label noise, Gaussian initialization, stochastic gradients

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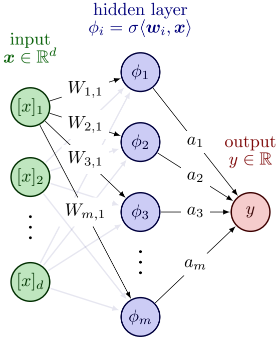
Problem settings: function space and SGD



random features mapping:

$$\varphi(\boldsymbol{x}) := \frac{1}{\sqrt{m}}\sigma\left(\frac{\boldsymbol{W}\boldsymbol{x}}{\sqrt{d}}\right) \quad W_{ij} \sim \mathcal{N}(0,1)$$

function space

$$\mathcal{H} := \left\{ f \in L^2_{\rho_X} \,\middle|\, f(\boldsymbol{x}) = \langle \boldsymbol{a}, \varphi(\boldsymbol{x})\rangle \right\}, \quad \boldsymbol{W}_{ij} \sim \mathcal{N}(0,1)$$

covariance operator: $\Sigma_m := \mathbb{E}_{\boldsymbol{x}}[\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})]$

expected covariance operator: $\widetilde{\Sigma}_m := \mathbb{E}_{\boldsymbol{x},\boldsymbol{W}}[\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})]$

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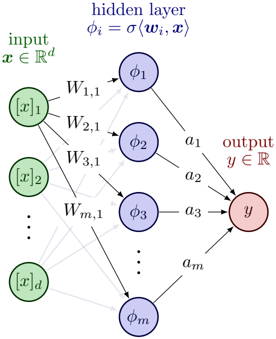

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Online SGD: one-pass, average output, adaptive step-size...

$$\boldsymbol{a}_t = \boldsymbol{a}_{t-1} + \gamma_t[y_t - \langle \boldsymbol{a}_{t-1}, \varphi(\boldsymbol{x}_t)\rangle]\varphi(\boldsymbol{x}_t), \qquad t = 1, 2, \ldots n\,.$$

- averaged output: $\bar{\boldsymbol{a}}_n := \frac{1}{n}\sum_{t=0}^{n-1} \boldsymbol{a}_t \Longrightarrow \bar{f}_n = \langle \varphi(\cdot), \bar{\boldsymbol{a}}_n \rangle$
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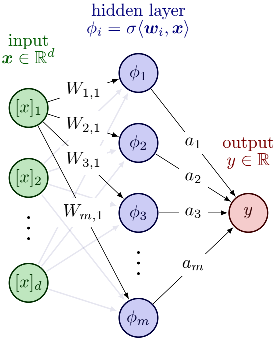

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Averaged expected risk

- optimal solution: $f^* = \arg\min_{f \in \mathcal{H}} \|f - f_\rho\|^2_{L^2_{\rho_X}}$ with $\|f^*\|_{\mathcal{H}} < \infty$
- averaged excess risk:
  $\mathbb{E}\|\bar{f}_n - f^*\|^2_{L^2_{\rho_X}} = \mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}} \langle \bar{f}_n - f^*, \Sigma_m (\bar{f}_n - f^*) \rangle$

Assumptions

Assumption (Basic assumptions)

- **non-asymptotic:** $\|\boldsymbol{x}\|_2^2 \leq \mathcal{O}(d)$, $\Sigma_d := \mathbb{E}_{\boldsymbol{x}}[\boldsymbol{x} \otimes \boldsymbol{x}]$ *with* $\|\Sigma_d\|_2 < \infty$
- **boundedness of f^*:** $\|f^*\|_{\mathcal{H}} < \infty$
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Assumption (Fourth moment condition)

for any PSD operator A, we assume

$$\mathbb{E}_{\boldsymbol{W}}[\Sigma_m A \Sigma_m] \preccurlyeq r' \mathbb{E}_{\boldsymbol{W}}[\mathrm{Tr}(\Sigma_m A)\Sigma_m] \preccurlyeq r \mathrm{Tr}(\widetilde{\Sigma}_m A)\widetilde{\Sigma}_m \,.$$

Remark:

- the special case $A := I$ can be proved.
- holds for sub-Gaussian data.
- widely used in SGD analysis [8, 9, 10]

Main results: bias-variance decomposition

Define $\eta_t := f_t - f^*$, we have

$$\eta_t = [I - \gamma_t \varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)](f_{t-1} - f^*) + \gamma_t \varepsilon_t \varphi(\boldsymbol{x}_t)\,,$$

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Theorem (Bias-variance decomposition)

Under the above-mentioned assumptions, if the step-size $\gamma_t := \gamma_0 t^{-\zeta}$ with $\zeta \in [0, 1)$ satisfies $\gamma_0 < C$, we have

$$\mathbb{E}\|\bar{f}_n - f^*\|^2_{L^2_{\rho_X}} = \underbrace{\mathbb{E}_{\boldsymbol{X},\boldsymbol{W}}\langle \bar{\eta}_n^{\texttt{bias}}, \Sigma_m \bar{\eta}_n^{\texttt{bias}} \rangle}_{:=\texttt{Bias}} + \underbrace{\mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\langle \bar{\eta}_n^{\texttt{var}}, \Sigma_m \bar{\eta}_n^{\texttt{var}} \rangle}_{:=\texttt{Variance}}\,.$$

Proof framework: randomness decoupling

- excess risk $\mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\langle \bar{\eta}_n, \Sigma_m \bar{\eta}_n \rangle$
  - $\texttt{Variance}$ $\mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\langle \bar{\eta}_n^{\texttt{var}}, \Sigma_m \bar{\eta}_n^{\texttt{var}} \rangle$
    - $\texttt{V1:}$ $\bar{\eta}_n^{\texttt{var}} - \bar{\eta}_n^{\texttt{vX}}$ $\begin{cases} \mathcal{O}(n^{\zeta-1}m) & \text{if } m \leqslant n \\ \mathcal{O}(1) & \text{if } m \geqslant n \end{cases}$
    - $\texttt{V2:}$ $\bar{\eta}_n^{\texttt{vX}} - \bar{\eta}_n^{\texttt{vXW}}$ $\begin{cases} \mathcal{O}(n^{\zeta-1}m) \\ \mathcal{O}(1) \end{cases}$
    - $\texttt{V3:}$ $\bar{\eta}_n^{\texttt{vXW}}$ $\begin{cases} \mathcal{O}(n^{\zeta-1}m) \\ \mathcal{O}(n^{\zeta-1} + \frac{n}{m}) \end{cases}$
  - $\texttt{Bias}$ $\mathbb{E}_{\boldsymbol{X},\boldsymbol{W}}\langle \bar{\eta}_n^{\texttt{bias}}, \Sigma_m \bar{\eta}_n^{\texttt{bias}} \rangle$
    - $\texttt{B1:}$ $\bar{\eta}_n^{\texttt{bias}} - \bar{\eta}_n^{\texttt{bX}}$ $\mathcal{O}(n^{\zeta-1})$
    - $\texttt{B2:}$ $\bar{\eta}_n^{\texttt{bX}} - \bar{\eta}_n^{\texttt{bXW}}$ $\begin{cases} \mathcal{O}(n^{2(\zeta-1)}m) \\ \mathcal{O}(\frac{1}{m}) \end{cases}$
    - $\texttt{B3:}$ $\bar{\eta}_n^{\texttt{bXW}}$ $\mathcal{O}(n^{\zeta-1})$

$$\texttt{Bias}: \quad \eta_t^{\texttt{bias}} = [I - \gamma_t \varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]\eta_{t-1}^{\texttt{bias}}$$

Proof framework: randomness decoupling

excess risk $\mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\langle \bar{\eta}_n, \Sigma_m \bar{\eta}_n \rangle$

- Variance $\mathbb{E}_{\boldsymbol{X},\boldsymbol{W},\boldsymbol{\varepsilon}}\langle \bar{\eta}_n^{\texttt{var}}, \Sigma_m \bar{\eta}_n^{\texttt{var}} \rangle$
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$$\texttt{Bias}: \quad \eta_t^{\texttt{bias}} = [I - \gamma_t \varphi(\boldsymbol{x}_t) \otimes \varphi(\boldsymbol{x}_t)]\eta_{t-1}^{\texttt{bias}}$$

Define "semi-stochastic" version: $\eta_t^{\texttt{bX}} = (I - \gamma_t \Sigma_m)\eta_{t-1}^{\texttt{bX}}, \quad \eta_t^{\texttt{bXW}} = (I - \gamma_t \widetilde{\Sigma}_m)\eta_{t-1}^{\texttt{bXW}},$

- $\texttt{B1} := \mathbb{E}_{\boldsymbol{X},\boldsymbol{W}}\left[\langle \bar{\eta}_n^{\texttt{bias}} - \bar{\eta}_n^{\texttt{bX}}, \Sigma_m(\bar{\eta}_n^{\texttt{bias}} - \bar{\eta}_n^{\texttt{bX}})\rangle\right]$
- $\texttt{B2} := \mathbb{E}_{\boldsymbol{W}}\left[\langle \bar{\eta}_n^{\texttt{bX}} - \bar{\eta}_n^{\texttt{bXW}}, \Sigma_m(\bar{\eta}_n^{\texttt{bX}} - \bar{\eta}_n^{\texttt{bXW}})\rangle\right]$
- $\texttt{B3} := \langle \bar{\eta}_n^{\texttt{bXW}}, \widetilde{\Sigma}_m \bar{\eta}_n^{\texttt{bXW}} \rangle$

Proof framework: properties of covariance operators

Properties of $\widetilde{\Sigma}_m$

- the diagonal elements are the same $a := [\widetilde{\Sigma}_m]_{ii}, \forall i \in [m]$
- the non-diagonal elements are the same $b := [\widetilde{\Sigma}_m]_{ij}, \forall i, j \in [m], i \neq j$

$$\widetilde{\Sigma}_m = (a-b)\boldsymbol{I}_m + b\mathbf{1}\mathbf{1}^\top$$

- two distinct eigenvalues: $\widetilde{\lambda}_1 = a - b + bm \sim \mathcal{O}(1)$, $\widetilde{\lambda}_2 = \cdots = \widetilde{\lambda}_m = a - b \sim \mathcal{O}(1/m)$

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$$\widetilde{\Sigma}_m = (a-b)\boldsymbol{I}_m + b\mathbf{1}\mathbf{1}^\top$$

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Example (ReLU activation)

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Proof framework: properties of covariance operators

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sub-exponential random variables

$\|\Sigma_m\|_2$, $\|\Sigma_m - \widetilde{\Sigma}_m\|_2$, $\mathrm{Tr}(\Sigma_m)$, and $\left\|\widetilde{\Sigma}_m^{-1}\mathbb{E}_{\boldsymbol{W}}(\Sigma_m^2)\right\|_2$ with $\mathcal{O}(1)$ sub-exponential norm order

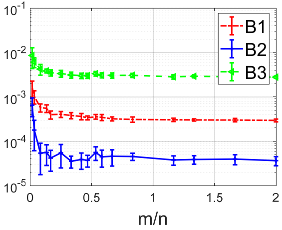
Main theorem

Theorem (Liu, Suykens, Volkan, NeurIPS 2022)

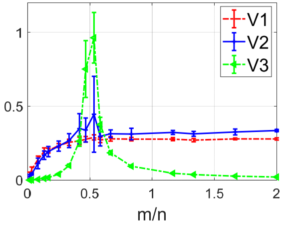
Under the above-mentioned assumptions, if the step-size $\gamma_t := \gamma_0 t^{-\zeta}$ *with* $\zeta \in [0,1)$ *satisfies* $\gamma_0 < C$, *we have*

$$\texttt{Bias} \lesssim \gamma_0 r' n^{\zeta-1} \|f^*\|^2 \sim \mathcal{O}\left(n^{\zeta-1}\right) .$$

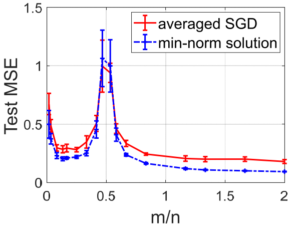
$$\texttt{Variance} \lesssim \gamma_0 r' \tau^2 \begin{cases} m n^{\zeta-1}, & \text{if } m \leqslant n \\ 1 + n^{\zeta-1} + \frac{n}{m}, & \text{if } m > n \end{cases}$$



(c) bias



(d) variance



(e) excess risk

Discussion

Constant step-size SGD doesn't hurt the convergence rate.

- under-parameterized regime (by taking $m = \mathcal{O}(\sqrt{n})$)

$$\mathbb{E}\|\bar{f}_n - f^*\|^2_{L^2_{\rho_X}} = \underbrace{\texttt{Bias}}_{\mathcal{O}(\frac{1}{n})} + \underbrace{\texttt{Variance}}_{\mathcal{O}(\frac{1}{\sqrt{n}})} \leq \mathcal{O}\left(\frac{1}{\sqrt{n}}\right),$$

  matches [11] (Carratino, Rudi, Rosasco, 2018) under one-pass, one-batch, SGD...[1]
- over-parameterized regime: matches [12] (Belkin, Hsu, Xu, 2020)

∘ no lower bound: $\texttt{Bias} \leqslant 3(\texttt{B1} + \texttt{B2} + \texttt{B3})$ based on Minkowski inequality

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Do you believe double descent?

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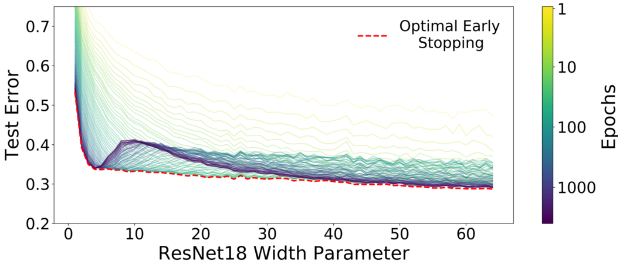

Figure: Optimal early stopping on ResNet18 [1]

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- Complexity of a prediction rule, e.g.,
  - number of parameters
  - norm of functions in RKHS
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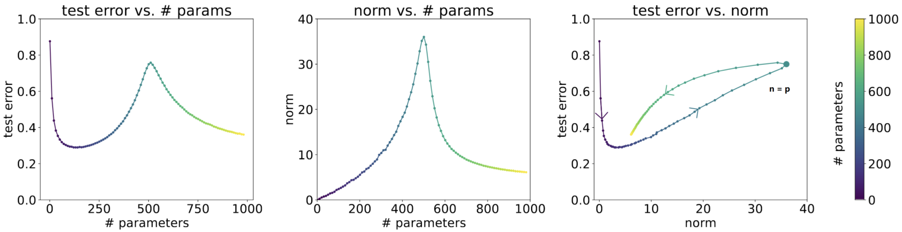

Figure: Source from lectures [Stanford CS229].

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- not data-adaptive
- RKHS is too small: curse of dimensionality [7, 13, 14]

From RKHS to Barron space

- RKHS of RFMs:

$$\hat{k}_m(\boldsymbol{x}, \boldsymbol{x}') = \frac{1}{m} \sum_{i=1}^{m} \phi(\boldsymbol{x}, \boldsymbol{w}_i) \phi(\boldsymbol{x}', \boldsymbol{w}_i) \;\; \rightarrow \;\; k_\mu(\boldsymbol{x}, \boldsymbol{x}') = \int_{\mathcal{W}} \phi(\boldsymbol{x}, \boldsymbol{w}) \phi(\boldsymbol{x}', \boldsymbol{w}) \mathrm{d}\mu(\boldsymbol{w})$$

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$$\mathcal{B} = \cup_{\mu \in \mathcal{P}(\mathcal{W})} \mathcal{H}_{k_\mu}\,, \quad \|f\|_{\mathcal{B}} = \inf_{\mu \in \mathcal{P}(\mathcal{W})} \|f\|_{\mathcal{H}_{k_\mu}}$$

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◦ parameter space vs. measure space
e.g., [7] (Bach, 2017), [16] (Bartolucci, Vito, Rosasco, Vigogna, 2022).

Our results: Learning with norm-constrained neural networks in Barron spaces

For the class of two-layer neural networks $\mathcal{F}_m$

$$\boldsymbol{\theta}^\star = \operatorname*{arg\,min}_{f_{\boldsymbol{\theta}} \in \mathcal{F}_m} \frac{1}{n} \sum_{i=1}^{n} (y_i - f_{\boldsymbol{\theta}}(\boldsymbol{x}_i))^2 + \lambda \|\boldsymbol{\theta}\|_{\mathcal{P}} \,.$$

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- [17] (Siegel, Xu, 2022) on metric entropy

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Optimization in Barron spaces is difficult: curse of dimensionality!

	approximation	generalization	optimization
RKHS	CoD	$\mathcal{O}(n^{-\frac{1}{d}})$	-
Barron spaces	$\mathcal{O}(m^{-\frac{2d}{d+3}})$	$\mathcal{O}(n^{-\frac{d+3}{2d+3}})$?	CoD

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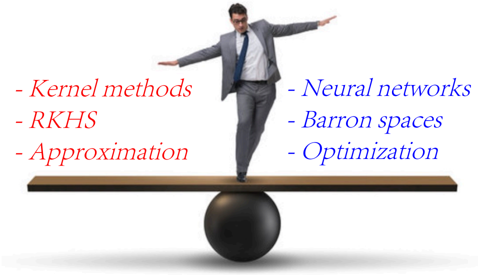

What is the suitable function space of NNs, both statistically and computationally efficient?

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Thanks for your attention!

Q & A

my homepage www.lfhsgre.org for more information!

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