Spectrum-Dependent Learning Curves in Kernel Regression and Wide Neural Networks

Blake Bordelon, Abdulkadir Canatar, Cengiz Pehlevan

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- Data follows some distribution $\boldsymbol{x} \sim p$

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- Being RKHS means:
  $\exists!$ $K(\cdot, \cdot)$ symmetric, positive semi-definite fulfilling the reproducing property:

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- Equivalent to requiring that the evaluation functional $L_{\boldsymbol{x}}(f) = f(\boldsymbol{x})$ is continuous (which in turn is equivalent to boundedness of the linear functional):

$$\forall \boldsymbol{x} \;\; |L_{\boldsymbol{x}}(f)| \leq M ||f||_{\mathcal{H}}$$

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- **RKHS Magic**: $f(\boldsymbol{x}_i) = \langle f_{\mathbb{L}} + f_{\perp}, K(\cdot, \boldsymbol{x}_i) \rangle_{\mathcal{H}} = f_{\mathbb{L}}(\boldsymbol{x}_i)$

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- **Remember:** $f(\boldsymbol{x}) = \boldsymbol{y}^T \boldsymbol{\Theta}(\boldsymbol{X}, \boldsymbol{X})^{-1} \boldsymbol{\Theta}(\boldsymbol{x}, \boldsymbol{X})$

Predictive function of NTK

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- Sometimes, expectations will be denoted in physics-fashion:

$$\langle f(\boldsymbol{X})\rangle_{\boldsymbol{X}}=\mathbb{E}_{\boldsymbol{X}\sim p}[f(\boldsymbol{X})]$$

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- $E_g = \langle E_g(\boldsymbol{X}, f^*) \rangle_{\boldsymbol{X}, f^*}$ (Integrate over data and teacher)
- **Observe:** Fixed teacher f^* is included in this analysis by setting $p_{f^*} \sim \delta_{f^*}$
- **Goal:** Calculate E_g for any kernel $\boldsymbol{K}$ and any teacher distribution

Mercer Decomposition

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- Due to Mercer, we can decompose any kernel into a (possibly) infinite eigenbasis:

$\psi_i(x) = \sqrt{\lambda_i}\,\phi_i(x)$

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Feature representation of sample x

where ϕ_i fulfills $\int_{\mathcal{X}} K(\boldsymbol{x}, \boldsymbol{y}) \phi_i(\boldsymbol{y}) p(\boldsymbol{y}) d\boldsymbol{y} = \lambda_i \phi_i(\boldsymbol{x})$

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- Write $f^*(\boldsymbol{x}) = \sum_{i=1}^{M} \bar{w}_i \psi_i(\boldsymbol{x})$ and $f(\boldsymbol{x}) = \sum_{i=1}^{M} w_i \psi_i(\boldsymbol{x})$

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Lemma 1:
We have the following decompostion of the generalization error:

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This provides in some sense a **spectral decomposition** of the generalization error as each term is weighted by the corresponding eigenvalue of the kernel.

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$$E_g(\boldsymbol{X}, f^*) = \left\langle (f(\boldsymbol{x}) - f^*(\boldsymbol{x}))^2 \right\rangle_{\boldsymbol{x}} = (\boldsymbol{w} - \bar{\boldsymbol{w}})^T \boldsymbol{\Lambda} (\boldsymbol{w} - \bar{\boldsymbol{w}})$$

Let's recall the minimal solution (using $\boldsymbol{y} = f^*(\boldsymbol{x}) = \boldsymbol{\Psi}^T \bar{\boldsymbol{w}}$)

$$\boldsymbol{w} = \left(\boldsymbol{\Psi}\boldsymbol{\Psi}^T + \lambda \mathbb{1}\right)^{-1} \boldsymbol{\Psi}\boldsymbol{\Psi}^T \bar{\boldsymbol{w}} = \bar{\boldsymbol{w}} - \lambda \left(\boldsymbol{\Psi}\boldsymbol{\Psi}^T + \lambda \mathbb{1}\right)^{-1} \bar{\boldsymbol{w}}$$

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- Both approximations **agree**!

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Just the basis matrix from Mercer

- **Recall**: $\boldsymbol{\Phi} = \boldsymbol{\Lambda}^{-\frac{1}{2}}\boldsymbol{\Psi} \in \mathbb{R}^{M\times p}$. Add a sample: $\tilde{\boldsymbol{\Phi}} \in \mathbb{R}^{M\times(p+1)}$

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$$\tilde{\boldsymbol{\Phi}}\tilde{\boldsymbol{\Phi}}^T = \begin{bmatrix} | & & | & | \\ \phi_1 & \dots & \phi_p & \phi_{p+1} \\ | & & | & | \end{bmatrix} \begin{bmatrix} — & \phi_1^T & — \\ & \vdots & \\ — & \phi_p^T & — \\ — & \phi_{p+1}^T & — \end{bmatrix}$$

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$(A+\underline{u}\underline{v}^T)^{-1} = A^{-1} + \frac{A^{-1}\underline{u}\underline{v}^T A^{-1}}{1+\underline{v}^T A^{-1}\underline{u}}$

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\tilde{\boldsymbol{G}}(p+1, v) &= \left(\frac{1}{\lambda}\tilde{\boldsymbol{\Phi}}\tilde{\boldsymbol{\Phi}}^T + \boldsymbol{\Lambda}^{-1} + v\mathbb{1}\right)^{-1} \\
&= \left(\frac{1}{\lambda}\boldsymbol{\Phi}\boldsymbol{\Phi}^T + \frac{1}{\lambda}\phi_{p+1}\phi_{p+1}^T + \boldsymbol{\Lambda}^{-1} + v\mathbb{1}\right)^{-1} \\
&= \left(\tilde{\boldsymbol{G}}(p, v)^{-1} + \frac{1}{\lambda}\phi_{p+1}\phi_{p+1}^T\right)^{-1} \\
&= \tilde{\boldsymbol{G}}(p, v) - \frac{\tilde{\boldsymbol{G}}(p, v)\frac{1}{\lambda}\phi_{p+1}\phi_{p+1}^T\tilde{\boldsymbol{G}}(p, v)}{1 + \phi_{p+1}^T\tilde{\boldsymbol{G}}(p, v)\phi_{p+1}}
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- Taking the expectation over the data $\boldsymbol{X}$:

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\end{aligned}
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- Taking the expectation over the data $\boldsymbol{X}$:

$$
\langle \tilde{\boldsymbol{G}}(p+1, v) \rangle_{\tilde{\boldsymbol{\Phi}}} = \langle \tilde{\boldsymbol{G}}(p, v) \rangle_{\boldsymbol{\Phi}} - \left\langle \frac{\tilde{\boldsymbol{G}}(p, v) \phi_{p+1} \phi_{p+1}^T \tilde{\boldsymbol{G}}(p, v)}{\lambda + \phi_{p+1}^T \tilde{\boldsymbol{G}}(p, v) \phi_{p+1}} \right\rangle_{\tilde{\boldsymbol{\Phi}}}
$$

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$$\langle \tilde{\boldsymbol{G}}(p+1, v) \rangle_{\tilde{\boldsymbol{\Phi}}} \approx \langle \tilde{\boldsymbol{G}}(p, v) \rangle_{\boldsymbol{\Phi}} - \frac{\left\langle \tilde{\boldsymbol{G}}(p, v) \phi_{p+1} \phi_{p+1}^T \tilde{\boldsymbol{G}}(p, v) \right\rangle_{\tilde{\boldsymbol{\Phi}}}}{\left\langle \lambda + \phi_{p+1}^T \tilde{\boldsymbol{G}}(p, v) \phi_{p+1} \right\rangle_{\tilde{\boldsymbol{\Phi}}}}$$

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$$
\begin{aligned}
\left\langle \tilde{\boldsymbol{G}}(p+1, v) \right\rangle_{\tilde{\boldsymbol{\Phi}}} &\approx \left\langle \tilde{\boldsymbol{G}}(p, v) \right\rangle_{\boldsymbol{\Phi}} - \frac{\left\langle \tilde{\boldsymbol{G}}(p, v) \phi_{p+1} \phi_{p+1}^T \tilde{\boldsymbol{G}}(p, v) \right\rangle_{\tilde{\boldsymbol{\Phi}}}}{\left\langle \lambda + \phi_{p+1}^T \tilde{\boldsymbol{G}}(p, v) \phi_{p+1} \right\rangle_{\tilde{\boldsymbol{\Phi}}}} \\
&= \left\langle \tilde{\boldsymbol{G}}(p, v) \right\rangle_{\boldsymbol{\Phi}} - \frac{\left\langle \tilde{\boldsymbol{G}}(p, v) \left\langle \phi_{p+1} \phi_{p+1}^T \right\rangle_{\phi_{p+1}} \tilde{\boldsymbol{G}}(p, v) \right\rangle_{\boldsymbol{\Phi}}}{\lambda + \left\langle \operatorname{tr}\left(\left\langle \phi_{p+1} \phi_{p+1}^T \right\rangle_{\phi_{p+1}} \tilde{\boldsymbol{G}}(p, v) \right) \right\rangle_{\boldsymbol{\Phi}}}
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&= \langle \tilde{\boldsymbol{G}}(p,v)\rangle_{\boldsymbol{\Phi}} - \frac{\left\langle \tilde{\boldsymbol{G}}(p,v)\left\langle \phi_{p+1}\phi_{p+1}^T\right\rangle_{\phi_{p+1}}\tilde{\boldsymbol{G}}(p,v)\right\rangle_{\boldsymbol{\Phi}}}{\lambda + \left\langle \operatorname{tr}\left(\left\langle \phi_{p+1}\phi_{p+1}^T\right\rangle_{\phi_{p+1}}\tilde{\boldsymbol{G}}(p,v)\right)\right\rangle_{\boldsymbol{\Phi}}} \\
&= \langle \tilde{\boldsymbol{G}}(p,v)\rangle_{\boldsymbol{\Phi}} - \frac{\left\langle \tilde{\boldsymbol{G}}(p,v)^2\right\rangle_{\boldsymbol{\Phi}}}{\lambda + \left\langle \operatorname{tr}\left(\tilde{\boldsymbol{G}}(p,v)\right)\right\rangle_{\boldsymbol{\Phi}}}
\end{aligned}
$$

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where we used that $\frac{\partial}{\partial v}\left\langle \tilde{\boldsymbol{G}}(p, v) \right\rangle_{\boldsymbol{\Phi}} = \left\langle \tilde{\boldsymbol{G}}(p, v)^2 \right\rangle_{\boldsymbol{\Phi}}$

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PDE Formulation (V)

- **Observe:** This is a matrix PDE
- We have the initial condition $\tilde{\boldsymbol{G}}(0, v) = (\boldsymbol{\Lambda}^{-1} + v\mathbb{1})^{-1}$
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- We can form the **normal vector** $\boldsymbol{n}(p,v) = \left(-1, \frac{\partial t}{\partial p}, \frac{\partial t}{\partial v}\right)$

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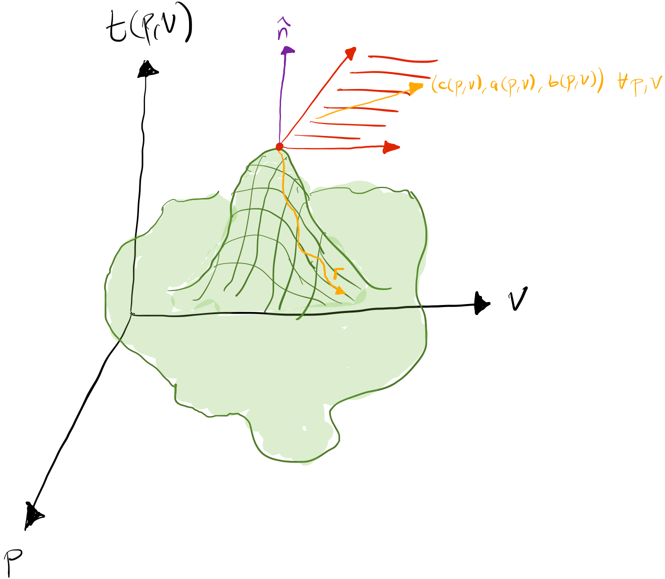
- Its solution is called **characteristic curve**, taking the unions of all such curves constructs entire S

Visualization



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- $$\begin{aligned}(z(s), p(s), v(s)) &= \left(c_1(v_0), s + c_2(v_0), -\frac{s}{\lambda+t} + c_3(v_0)\right)\\ &= (\mathrm{f}(\mathrm{v}_0), s, -\frac{s}{\lambda+t} + v_0)\end{aligned}$$

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$$t(p,v) = f\left(v + \frac{p}{\lambda + t}\right) = \mathrm{tr}\left(\left(\mathbf{\Lambda}^{-1} + (v + \frac{p}{\lambda + t(p,v)})\mathbb{1}\right)^{-1}\right)$$

$\implies$ Still an implicit equation

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Theorem 3:
The average generalization error can be approximated like

$$E_i(p) = \frac{\langle \bar{w}_i^2 \rangle}{\lambda_i} \left(\frac{1}{\lambda_i} + \frac{p}{\lambda + t(p)} \right)^{-2} \left(1 - \frac{p\gamma(p)}{(\lambda + t(p))^2} \right)^{-1}$$

where $\gamma(p) = \sum_{i=1}^{M} \left(\frac{1}{\lambda_i} + \frac{p}{\lambda + t(p)} \right)^{-2}$

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Algorithm 1 Computing Theoretical Learning Curves

Input: RKHS spectrum $\{\lambda_\rho\}$, target function weights $\{\overline{w}_\rho\}$, regularizer λ, sample sizes $\{p_i\}$, $i = 1, ..., m$;

for $i = 1$ **to** m **do**

Solve numerically $t_i = \sum_\rho \left(\frac{1}{\lambda_\rho} + \frac{p_i}{\lambda + t_i}\right)^{-1}$

Compute $\gamma_i = \sum_\rho \left(\frac{1}{\lambda_\rho} + \frac{p_i}{\lambda + t_i}\right)^{-2}$

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This allows one to plot learning curves with the sample size as the varying parameter

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- As usual the calculations are **very bizarre**, order parameter definitions are enforced via Dirac deltas, those get replaced by their Fourier integral representation and then the whole thing simplifies somehow...
- Using a saddle point approximation they finally find the same solution as with the PDE approach

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- Assume target is given by $f^*(\boldsymbol{x}) = \sum_{i=1}^{p'} \bar{\alpha}_i \boldsymbol{\Theta}(\boldsymbol{x}, \bar{\boldsymbol{x}}_i)$, $\bar{\alpha}_i \sim$ Bernoulli($\frac{1}{2}$) and $\boldsymbol{x} \sim \mathbb{S}^{d-1}$

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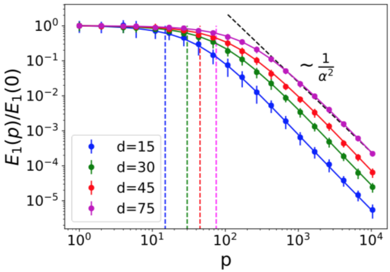
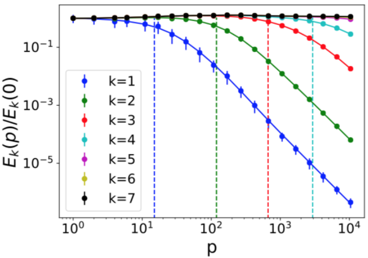


(b) 3-layer NTK $k = 1$ $\lambda = 1$



(a) 3-layer NTK $d = 15$ $\lambda = 0$

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- f^* is hence composed of harmonics belonging to the same eigenvalue

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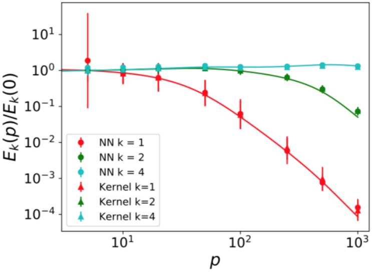

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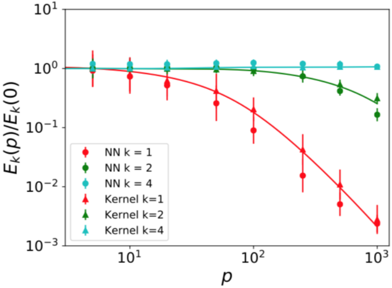

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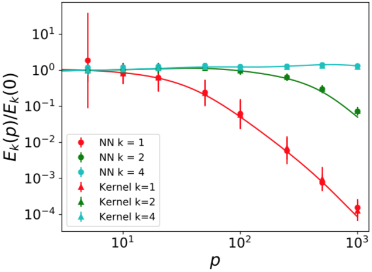

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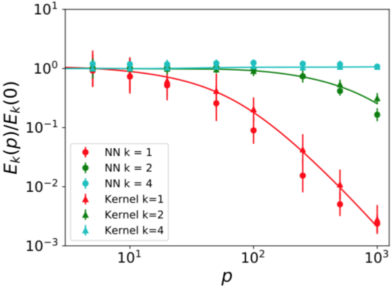

(b) 4-layer NN $N = 500$

- Good agreement for two layer network, but seems to get worse with depth. No deeper depth experiments included.

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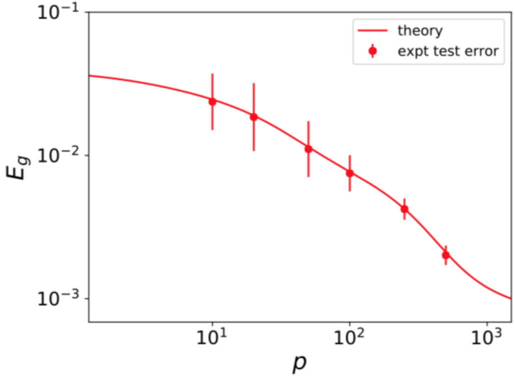

(c) 2-Layer NN Student-Teacher; $N = 8000$

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- Would also have been nicer to have an **analytical** expression (instead of these implicit equations) but probably hard to do
- Nice that the same solution pops out under two different approximations. But maybe they are **more similar** than one can see at first glance. In both cases, two integer parameters are **made continuous** and limits are taken