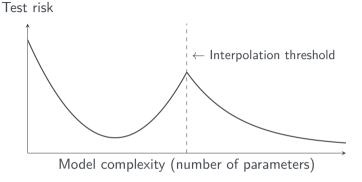


On the Universality of the Double Descent Peak in Ridgeless Regression ICLR 2021 22nd March 2021





Double Descent: Main message



Every interpolating linear model is sensitive to label noise around the interpolation threshold.

Setting (slightly simplified)

'Ridgeless' linear regression in feature space with p features and n samples:

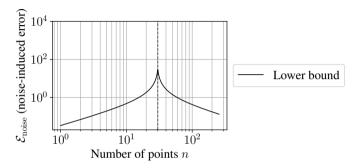
- Inputs $x_1, \ldots, x_n \in \mathbb{R}^d$ i.i.d., $y_i = f(x_i) + \varepsilon_i$ with centered i.i.d. label noise ε_i
- Given a feature map $\phi: \mathbb{R}^d \to \mathbb{R}^p$, compute

$$\hat{f}_{\boldsymbol{X}_{\mathsf{train}},\boldsymbol{y}_{\mathsf{train}}}(\boldsymbol{x}) = \widehat{\boldsymbol{\beta}}^{\top} \phi(\boldsymbol{x}), \qquad \widehat{\boldsymbol{\beta}} = \underbrace{\phi(\boldsymbol{X}_{\mathsf{train}})^{+}}_{\mathsf{pseudoinverse}} \boldsymbol{y}_{\mathsf{train}} \;.$$

- $\bullet \ \ \mathsf{Expected} \ \ \mathsf{excess} \ \mathsf{risk} \colon \, \mathcal{E}(f) \coloneqq \mathbb{E}_{X_{\mathsf{train}}, \varepsilon, x_{\mathsf{test}}} \left(f(x_{\mathsf{test}}) \hat{f}_{X_{\mathsf{train}}, f(X_{\mathsf{train}}) + \varepsilon}(x_{\mathsf{test}}) \right)^2$
- $\bullet \quad \text{Lower bound:} \ \mathcal{E}_{\text{noise}} \coloneqq \mathcal{E}(0) = \min_{f:\mathbb{R}^d \to \mathbb{R}} \mathcal{E}(f)$



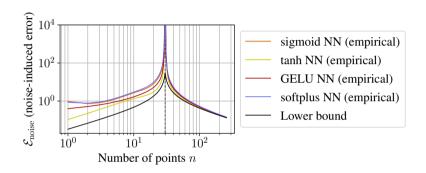
A lower bound (simplified)



Assume that $Var(\varepsilon_i) \geq \sigma^2$ and that p points can be interpolated almost surely. Then:

- Underparameterized case $p \le n$: $\mathcal{E}_{\text{noise}} \ge \sigma^2 \frac{p}{n+1-p}$
- $\bullet \ \ \text{Overparameterized case} \ p \geq n \text{:} \ \mathcal{E}_{\text{noise}} \geq \sigma^2 \frac{n}{p+1-n}$

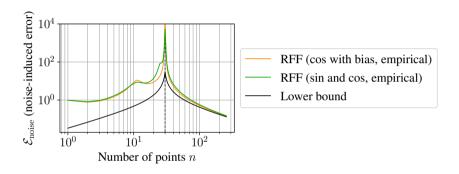
When are the assumptions satisfied? (1)



- Random deep NN feature map with non-polynomial analytic activation function
- ullet Input x with non-atomic distribution (every point has probability zero)



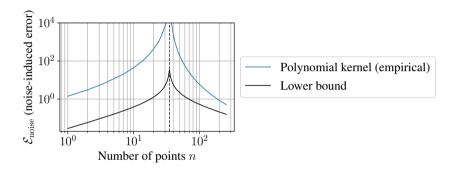
When are the assumptions satisfied? (2)



- Random Fourier features for kernel with continuous spectrum
- Input x with non-atomic distribution (every point has probability zero)



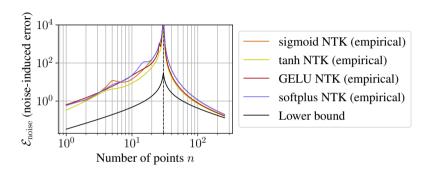
When are the assumptions satisfied? (3)



- Polynomial kernel $k(x, \tilde{x}) = (\langle x, \tilde{x} \rangle + c)^m$, c > 0, with $p \coloneqq \binom{m+d}{m}$
- Input x with (Lebesgue) density



When are the assumptions satisfied? (4)



- Simple computational verification for analytic random feature maps
- ullet Here: Finite-width NTK, input x with (Lebesgue) density





Remarks

- Lower bound is asymptotically sharp for $n, p \to \infty$, $p/n \to \gamma \in (0, \infty)$
- Key takeaway: Cannot prevent Double Descent by engineering the feature map

