Overfitting and Generalization Performance

March 31, 2021

Main Papers

- *Reconciling modern machine-learning practice and the classical bias-variance trade-off*, Belkin et al
- *To undersand deep learning we need to understand kernel learning*, Belkin et al

General Aim

Given training sample

$$\{(x_1, y_1), ..., (x_n, y_n)\} \in \mathbb{R}^d \times \mathbb{R}$$

where (x_i, y_i) are i.i.d. variables drawn from probability distribution P, learn a predictor $h_n : \mathbb{R}^d \to \mathbb{R}$ that predicts y "well" given unseen x.

Loss function l

Minimize loss:
squared-loss function $l(y, \hat{y}) = (\hat{y} - y)^2$
0-1 loss/ classification loss: $l(\hat{y}, y) = 1_{\hat{y} \neq y}$

Generalization

- Find h_n that performs well on unseen data.
- Minimize true risk: $h^*(x) = \arg\min_h \mathbb{E}[\ell(h(x), y)]$ where (x, y) drawn independently from P.
- Empirical Risk Minimization (ERM) goal: Minimize training risk. $L_{emp}(h_n) = \frac{1}{n}\sum_{i=1}^{n} l(h_n(x_i), y_i)$.

$$\hat{h_n} = \arg\min_{h_n \in \mathcal{H}} L_{emp}(h_n).$$

- $\mathcal{H}$ is a function class that contains functions approximating h^*.
- Classically, we do not choose function h_n that reduces the empirical loss to near zero values, typically due to bounds on the generalization gap.

Bias Variance Tradeoff

- Finding a balance between underfitting and overfitting.
- "Bias-Variance Tradeoff"
- 0 training error does not tend to generalize well.

Generalization Error

Difference Between empirical and expected classifier loss:
$\mathbb{E}_{x,y}[l(\hat{h}_n(x), y)] \leq L_{emp}(\hat{h}_n) + O(\sqrt{c/n})$
where c is some measure of the complexity of $\mathcal{H}$, for example the fat-shattering dimension, VC-dimension, etc.

- To control L_{emp} and c, control $\mathcal{H}$ implicitly or explicitly.
- Examples: Changing NN architectures, regularization, early stopping.

Modern practice

- Modern ML methods such as large neural networks and other non-linear predictors have very low to no training risk
- NN architectures chosen such that interpolation can be achieved.
- Works even when training data have high levels of noise.

# params	random crop	weight decay	train accuracy	test accuracy
1,649,402	yes	yes	100.0	89.05
	yes	no	100.0	89.31
	no	yes	100.0	86.03
	no	no	100.0	85.75

Understanding Deep Learning Requires Rethinking Generalization, Zhang et al

Question

- Unanswered as to why these overparameterized data do not seem to cause high test loss due to overfitting.
- Papers discussed further show empirically that this property is not exclusive to deep learning, but also seems to appear in learning for kernel machines as well.

Short introduction to Kernels and RKHS

- Where $\mathbb{K}$ may refer to either $\mathbb{R}$ or $\mathbb{C}$.
- For kernel $k : X \times X \to \mathbb{K}$, there exists $\mathbb{K}$-Hilbert space $\mathcal{H}$ and map $\psi : X \to \mathcal{H}$ such that for all $x_1, x_2 \in X$,

$$k(x_1, x_2) = \langle \psi(x_2), \psi(x_1) \rangle.$$

- ψ is called a feature map of k.
- (Real) Gaussian RBF kernel with width γ:

$$k_\gamma(x, x') := e^{\frac{-\|x-x'\|_2^2}{\gamma^2}}.$$

where $x, x' \in \mathbb{R}^d$.

Positive Definite Functions

For a non-empty set X, a function $k : X \times X \to \mathbb{R}$ is said to be a positive definite if, for all $x_1, ..., x_n \in X$, for all $a_1, ..., a_n \in \mathbb{R}$, we have:

$$\sum_{j=1}^{n} \sum_{i=1}^{n} a_j a_i k(x_j, x_i) \geq 0.$$

Positive Definite Symmetric Functions are Kernels

A real function $k : X \times X \to \mathbb{R}$ is a kernel if and only if k is a positive definite symmetric function.

Short introduction to Kernels and RKHS

Reproducing kernel Hilbert spaces have many applications in the fields such as Statistical Learning and complex analysis. An RKHS is a K-Hilbert function space where point evaluation is continuous linear funcitonal.

Reproducing Kernel Hilbert Spaces (**RKHS**) Definition

Let $\mathcal{H}$ be a $\mathbb{K}$-Hilbert space of functions over a non-empty set X. $\mathcal{H}$ is called an RKHS over X if the Dirac function $\delta_x : \mathcal{H} \to \mathbb{K}$ defined as:

$$\delta_x(f) := f(x), \ x \in X, \ f \in \mathcal{H}$$

is continuous.

Reproducing Kernels

For a non-empty set X and a function $k : X \times X \to \mathbb{K}$ k is called a reproducing kernel of $\mathcal{H}$ (a Hilbert function space) if $k(\cdot, x) \in \mathcal{H}$ for all $x \in X$ and the following property hold for all $x \in X$ and $f \in \mathcal{H}$:

$$f(x) = \langle f, k(\cdot, x) \rangle$$

This condition is also known as the reproducing property.

- It can be shown that k is a kernel.
- $\mathcal{H}$ is then an RKHS.

Representer Theorem

Representer Theorem ensures that the argmin of an empirical risk expression involving a function over an RKHS can be expressed as a linear combination of kernels applied on the training data points as proven in Scholkopf et al.

Representer Theorem

Training data $(x_1, y_1), ...(x_n, y_n) \in X \times \mathbb{R}$, and RKHS $\mathcal{H}$ a $\mathbb{R}$-Hilbert function space over X with reproducing kernel $k : X \times X \to \mathbb{R}$.
Let g be a strictly increasing function $g : [0, \infty] \to \mathbb{R}$, and $I : (X \times \mathbb{R}^2)^n \to \mathbb{R} \cup \{\infty\}$ be an arbitrary loss function.
We want to minimize the following empirical risk term:
$L_{emp}(f, (x_1, y_1), ..., (x_n, y_n)) := I((x_1, y_1, f(x_1)), ..., (x_n, y_n, f(x_n))) + g(\|f\|)$
For $\hat{f} = \arg\min_{f \in \mathcal{H}} L_{emp}(f, (x_1, y_1), ..., (x_n, y_n))$, $\hat{f}$ can be represented in the form:

$$\hat{f}(\cdot) = \sum_{i=1}^{n} a_i k(\cdot, x_i)$$

with $a_i \in \mathbb{R}$ for $1 \leq i \leq n$.

Proof Sketch

- Let $\Phi(x)(\cdot) = k(\cdot, x)$.
- $f = \sum_{i=1}^{n} a_i \Phi(x_i) + \gamma$, where $\langle \Phi(x_i), \gamma \rangle = 0$
- $f(x_j) = \sum_{i=1}^{n} a_i \langle \Phi(x_i), \Phi(x_j) \rangle$
- So $f(x_j)$ is unaffected by γ.
- $\|f\|^2 = \|\sum_{i=1}^{n} a_i \Phi(x_i) + \gamma\|^2 \geq \|\sum_{i=1}^{n} a_i \Phi(x_i)\|^2$
- $g(\|f\|) \geq g(\|\sum_{i=1}^{n} a_i \Phi(x_i)\|)$
- So $\gamma = 0$ and $\hat{f} = \sum_{i=1}^{n} a_i k(\cdot, x_i)$

Random Fourier Features

Let the function class $\mathcal{H}_\infty$ be the Reproducing Kernel Hilbert Space (RKHS) corresponding to the Gaussian kernel.
We consider the following non-linear parametric model:

Random Fourier Features (RFF)

Random Features for Large-Scale Kernel Machines (Rahimi et al)

Let the function class $\mathcal{H}_N$ consist of functions $h_n : \mathbb{R}^d \to \mathbb{C}$ of the form:

$$h(\cdot) = \sum_{k=1}^{N} a_k \phi(\cdot, v_k)$$

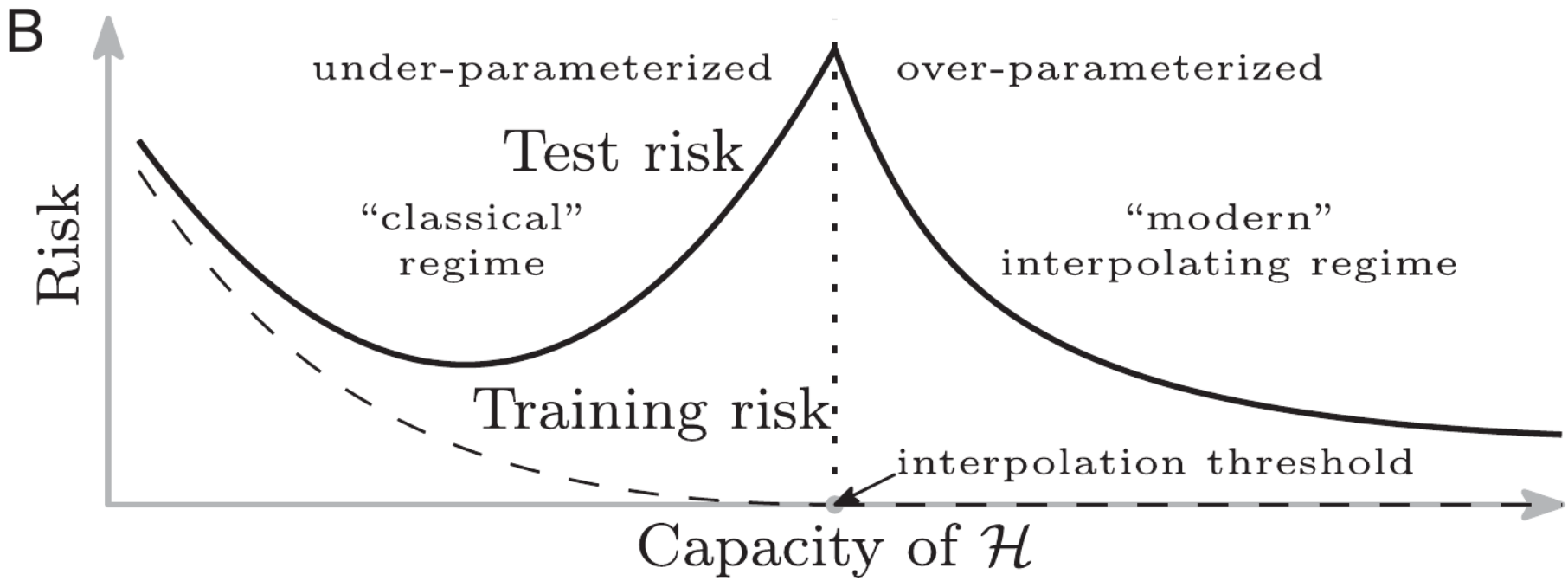
where $\phi(\cdot, v_k) := e^{i\langle v_k, \cdot \rangle}$ vectors $v_1, ..., v_N$ are sampled independently from the standard normal distribution in $\mathbb{R}^d$.

H_N has N parameters in $\mathbb{C}$, $\{ a_1, ..., a_N \}$.
As $N \to \infty$, H_N becomes a closer approximation to $\mathcal{H}_\infty$

"Double Descent"

- "Double Descent" curve proposed and empirically observed to some extent.
- Curve the extends beyond the point of interpolation
- Risk decreases beyond this point, typically surpassing performance of classical stopping point.

Double Descent Curve



Explanations on Double Descent

Why should the test risk decrease even when empirical risk stays the same?

- Capacity of function class needs not suit the appropriate inductive bias for the problem.
- By having a larger function class, may find a function that matches the inductive bias better.
- Eg., smoother function, smaller norm, larger margin.

Empirical Evidence - Learning Procedure

- Given training sample $(x_1, y_1), ..., (x_n, y_n) \in \mathbb{R}^d \times \mathbb{R}$.
- Minimize empirical risk: $\frac{1}{n} \sum_{j=1}^{n} (h(x_j) - y_j)^2$ for $h \in \mathcal{H}_N$.
- When minimizer not unique ($N > n$), choose the minimizer with the coefficients $(a_1, ..., a_N)$ that have the smallest ℓ_2 norm.
- Let this predictor be: $h_{n,N} \in \mathcal{H}_N$.

Min Norm RKHS solution $h_{n,\infty}$

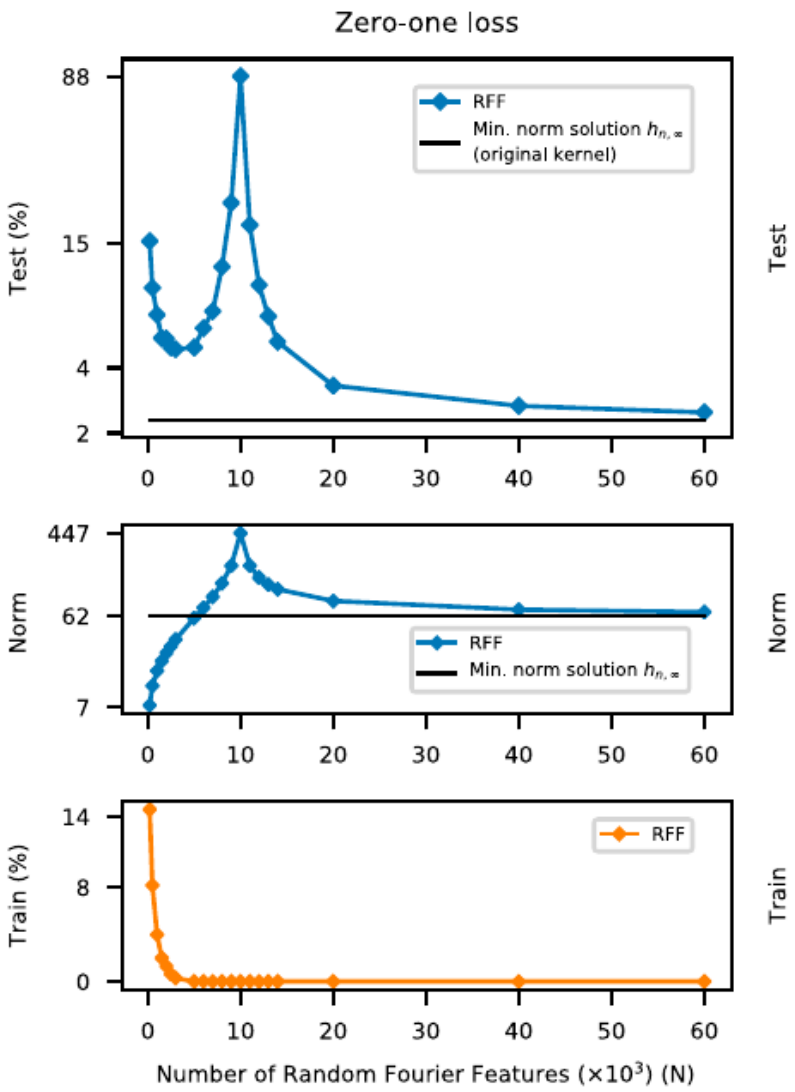
- $f^* = \arg\min_{f \in \mathcal{H}_\infty, f(x_i)=y_i} \|f\|_{\mathcal{H}_\infty}$
- $f^*(\cdot) = \sum_{i=1}^n \alpha_i k(\cdot, x_i)$ (Representer theorem)
- Since f^* interpolates, $(\alpha_1, ..., \alpha_n)^\mathsf{T} = K^{-1}(y_1, ..., y_n)^\mathsf{T}$
- $\|f\|^2_{\mathcal{H}_\infty} = \sum_{i,j} \alpha_i \alpha_j K(x_i, x_j)$

Approximation theorem

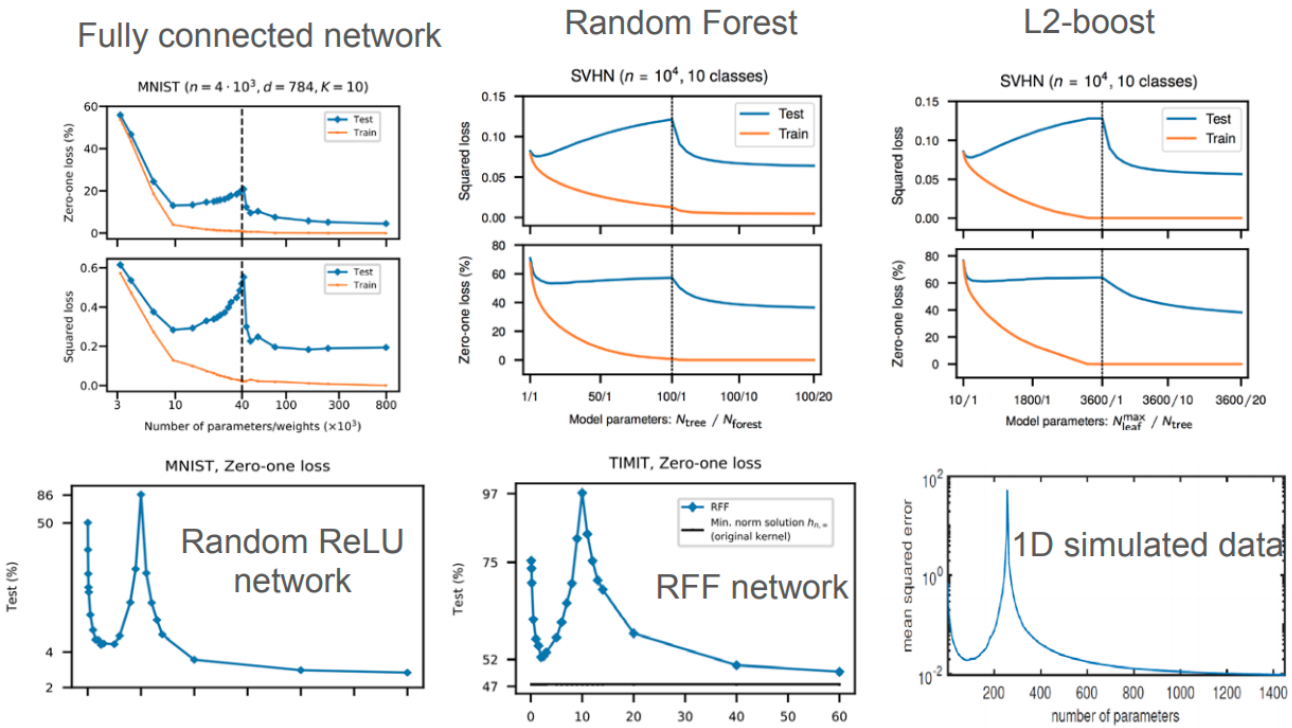
Fix $h^* \in \mathcal{H}_\infty$. Let $(x_1, y_1), ..., (x_n, y_n)$ be i.i.d. random variables where x_i drawn randomly from a compact cube $\Omega \subset \mathbb{R}^d$, $y_i = h^*(x_i)\, \forall i$. There exists $A, B > 0$ such that for any interpolating $h \in \mathcal{H}_\infty$ with high probability

$$\sup_{x \in \Omega} |h(x) - h^*(x)| < A e^{-B(n/\log n)^{1/d}} (\|h^*\|_{\mathcal{H}_\infty} + \|h\|_{\mathcal{H}_\infty})$$

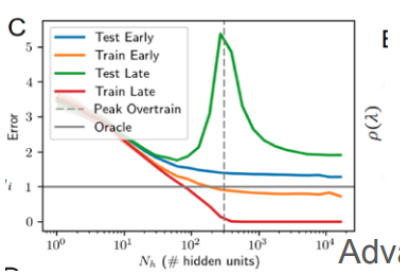
Empirical Evidence - Results



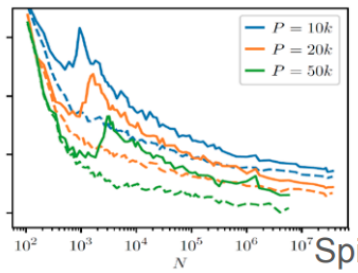
Empirical Evidence - Other Examples



[B., Hsu, Ma, Mandal, 18]



Advani, Saxe, 2017



Spigler, et al, 2018