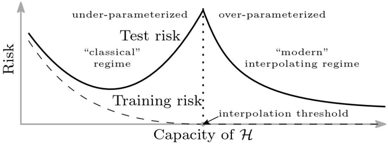

Yikun Zhang
Department of Statistics,
University of Washington
∗ Part of the slides were made when I was an
Advanced Algorithmic Engineer at Trip.com

Shall We Always Avoid Overfitting?

A generalized framework of the classical bias-variance trade-off in modern deep learning regime

November 4, 2021

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What is Overfitting?

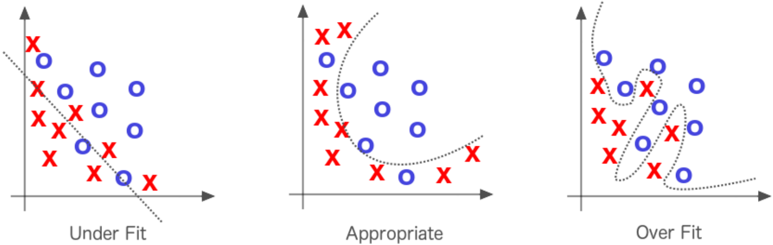

Figure 1: A binary classification problem with underfitting, just-right, and overfitting decision boundaries (or classifiers).

Survey: Is Overfitting Good or Bad?

How many of you think that overfitting is a *bad* phenomenon in machine learning practices and should be avoided?

[1] Cited from *The Element of Statistical Learning, Second Edition*, Hastie et al. (2009).

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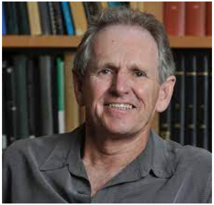
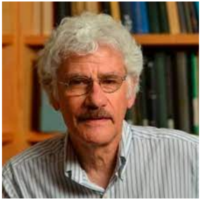


(a) Trevor Hastie

(b) Robert Tibshirani



(c) Jerome H. Friedman

- "...Fitting the training data too well can lead to overfitting, which degrades the risk on future prediction." [1]

[1] Cited from *The Element of Statistical Learning, Second Edition*, Hastie et al. (2009).

Survey: Is Overfitting Good or Bad?

- "...With so many candidate models, **overfitting is a real danger. Is the monkey who typed Hamlet actually a good writer?"** [2]

Figure 3: A typing monkey (Image source: iStock).

[2] Cited from *Model Selection and Model Averaging*, Claeskens et al. (2008).

A Central Tenet in Machine Learning: Bias-Variance Trade-off

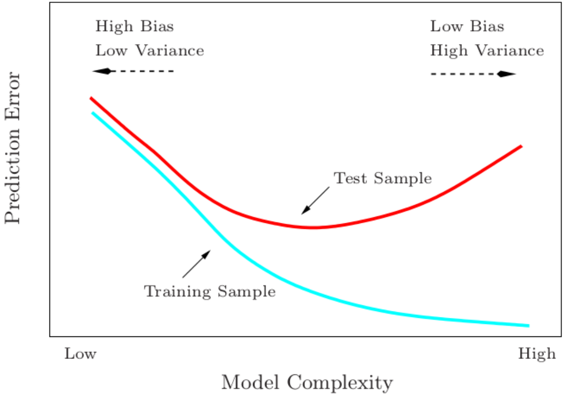


Figure 4: Training and test errors with respect to model complexity.

Practical Remedies for Overfitting

Take the neural network as an example:

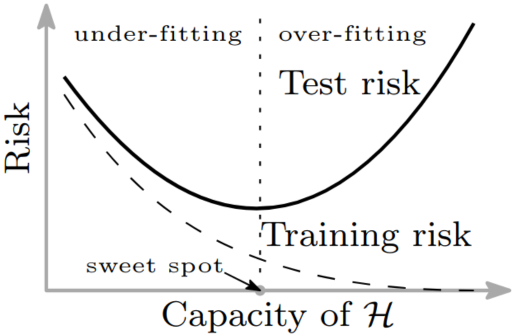
- Pick a simpler neural network architecture:
  1. Reducing the number of layers or neurons
  2. Dropout, weight decay, ...
- Regularization:
  1. Add penalized terms to the loss function

$$h_n = \arg\min_{h\in\mathcal{H}} \frac{1}{n}\sum_{i=1}^{n} \ell\left(h(x_i), y_i\right)$$

$$\Longrightarrow \quad h_n = \arg\min_{h\in\mathcal{H}} \left[\frac{1}{n}\sum_{i=1}^{n} \ell\left(h(x_i), y_i\right) + \lambda||h||_{\mathcal{H}}\right].$$

  2. Early stopping,
  3. Stochastic gradient descent (implicit regularization), ...

Pursue a “Sweet Spot” Model



Training Risk: $\frac{1}{n}\sum_{i=1}^{n} \ell\left(h(x_i), y_i\right).$

Test Risk: $\mathbb{E}_{(x,y)\sim P}\left[\ell(h(x), y)\right].$

Assume that the data samples are sampled randomly from a probability distribution P.

So Far So Good...

To be an artificial intelligence (AI) engineer, we only need to

1. Understand the bias-variance trade-off principle.
2. Know how to do computer programming.
3. Avoid overfitting with those standard techniques.

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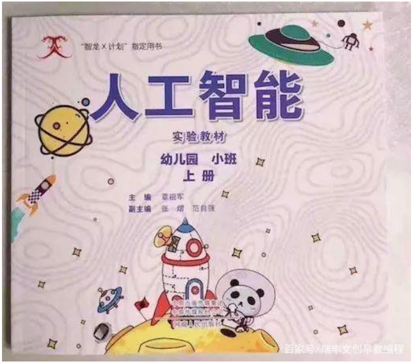

The picture is an AI textbook designed for children at the kindergarten level in China. There are some news saying that several kindergartens begin teaching computer programming to their 3-5 years-old kids.

Concerns

If a kindergarten kid is capable of tackling AI tasks, why do we need years of subsequent education and training?
A big waste of time?

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If a kindergarten kid is capable of tackling AI tasks, why do we need years of subsequent education and training?
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There is something weird happening in real-world applications...

Success of Deep Learning

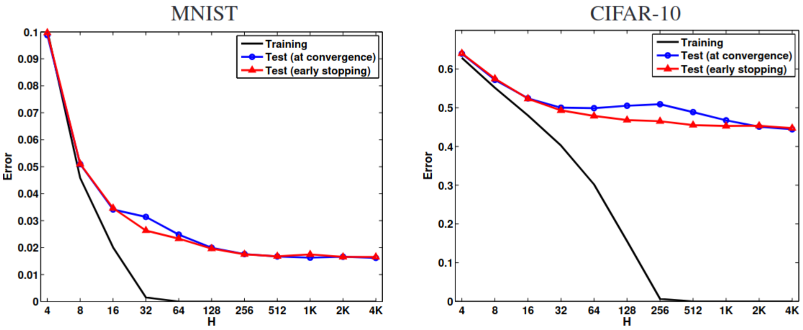
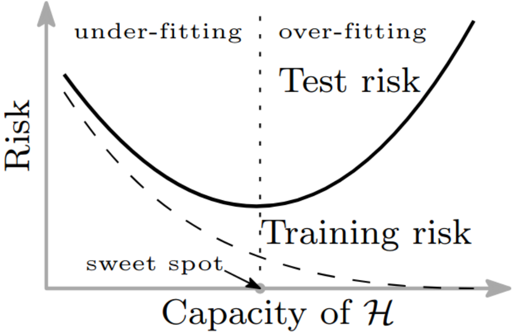


Figure 5: The training and test errors based on different stopping criteria when two-layer Neural Networks (NNs) with different number of hidden units H are trained on MNIST and CIFAR-10 data (Neyshabur et al., 2014).

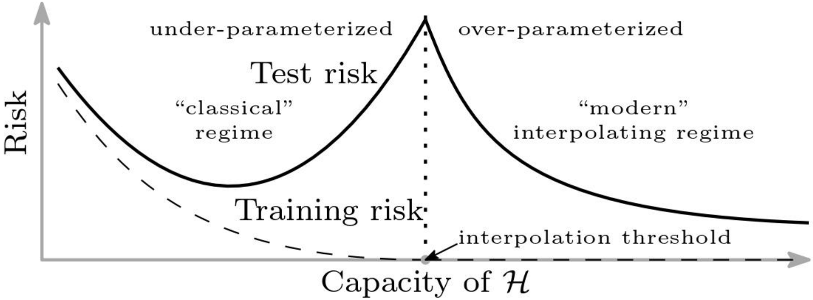
- Notes: The number of parameters/weights is $H(d+K)$ for each two-layer NN, where d is the number of features and K is the size of the output layer.

Deep Learning Paradox

The preceding evidence in modern deep learning regime indicates a contradiction to the classical bias-variance trade-off.



“Double-Descent“ Curve



An extension of the classical bias-variance trade-off.

Illustration of Interpolation

- Data: $Y_i = \sin(X_i) + \epsilon_i$ with $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$ for $i = 1, ..., 20$.
- Model (*cubic spline*): $h(X) = \sum_{k=0}^{3} a_k X^k + \sum_{j=1}^{N-3} b_j (X - \xi_j)_+^3$

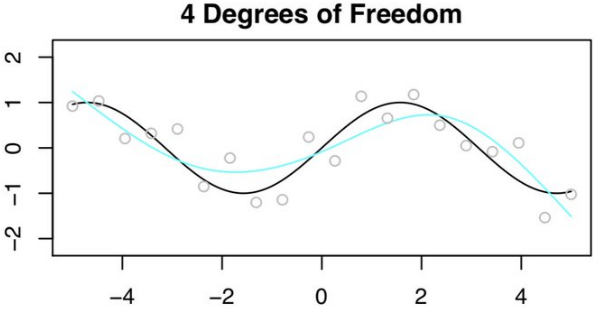


Figure 6: Fitting the true sine function (black) with cubic spline (cyan) (Image source: *Prof. Daniela Witten*'s Twitter).

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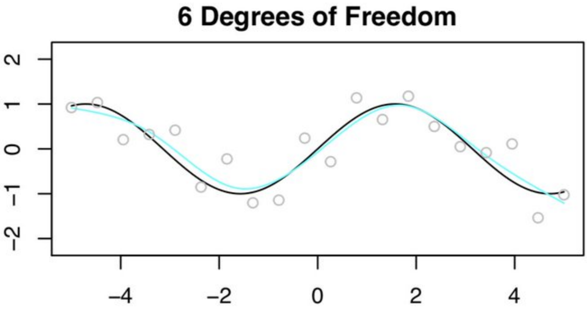

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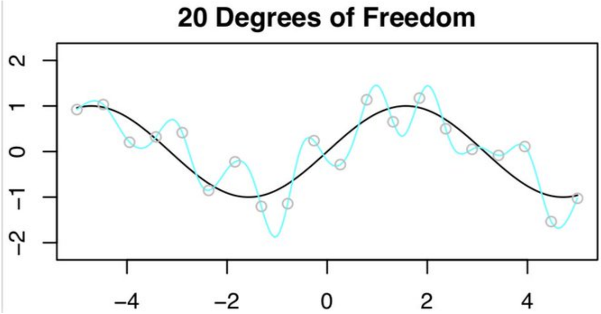

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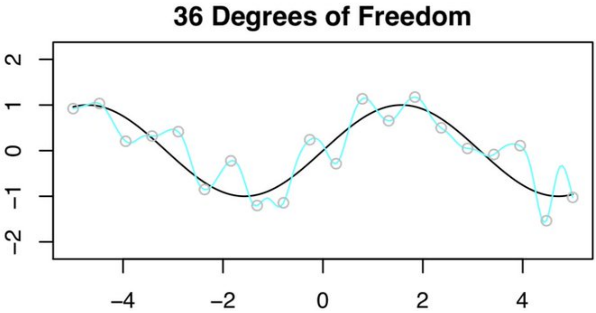

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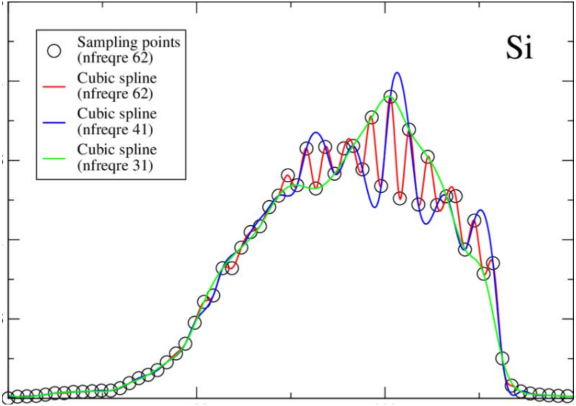
Over-Parameterization Regime

Problem: Among all the interpolating models in a function class, which one should we choose?



Over-parameterization Regime

Solution: Choose the *smoothest* one, i.e,

$$\arg\min_{h \in \mathcal{H}'} ||h||_{\mathcal{H}},$$

where $\mathcal{H}' \subset \mathcal{H}$ denotes the collection of all interpolating models. This principle is known as **Occam's razor** (Blumer et al., 1987).

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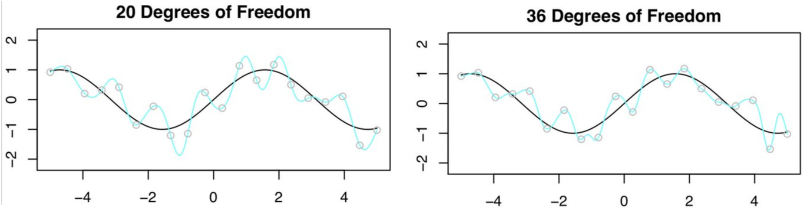

Experiment (I): Random Fourier Features (RFF)

The model family:

$$\mathcal{H}_N = \left\{ h : \mathbb{R}^d \to \mathbb{C} : h(x) = \sum_{i=1}^{N} a_k \phi(x; v_k) \text{ with } \phi(x; v) := e^{\sqrt{-1}\langle v_k, x\rangle} \right\},$$

where $v_1, ..., v_N \overset{i.i.d.}{\sim} \mathcal{N}(\mathbf{0}, I_d)$ and $\mathcal{H}_N$ is a class of real-valued functions with $2N$ parameters.

- Notes: As $N \to \infty$, $\mathcal{H}_N$ approximates the reproducing kernel Hilbert space (RKHS) using the Gaussian kernel.

Experiment (I): Random Fourier Features (RFF)

Optimization details on RFF:

1. Find $h_{n,N} \in \mathcal{H}_N$ via Empirical Risk Minimization (ERM):

$$h_{n,N} = \arg\min_{h \in \mathcal{H}_N} \frac{1}{n} \sum_{i=1}^{n} (h(x_i) - y_i)^2 .$$

2. When the minimizer is not unique (as is always the case when $N > n$), choose the one with minimal

$$||h_{n,N}||_2 := \sqrt{\sum_{i=1}^{n} |a_i|^2}.$$

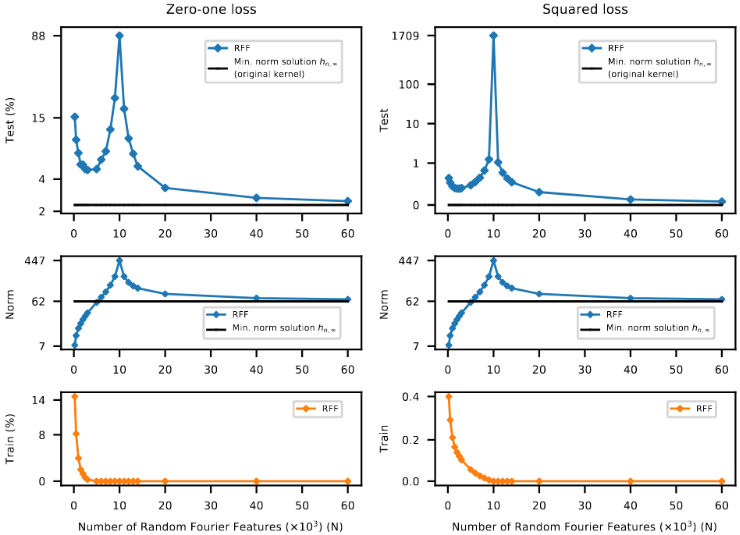

Figure 8: RFF on MNIST ($n = 10^4$, 10 classes). The interpolation threshold is achieved at $N = 10^4$.

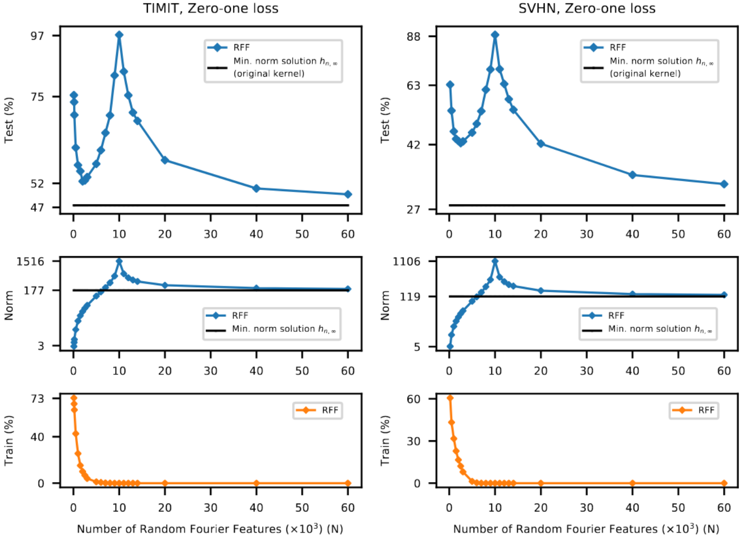

Figure 9: RFF on TIMIT ($n = 1.1 \times 10^6$, 48 classes) and SVHN ($n = 7.3 \times 10^4$, 10 classes).

Experiment (II): Fully Connected Two-Layer Neural Networks

Setup:

- Given a $(n \times d)$ training set with K classes, a fully connected neural network with a single layer of H hidden units has the number of parameters $H(d+K)$.
- It can be trained via stochastic gradient descent (SGD)

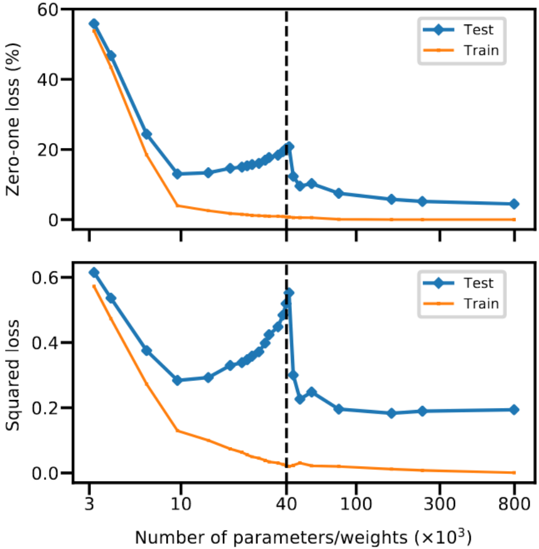

Figure 10: A fully connected neural network on a subset of MNIST ($n = 4 \times 10^3$, $d = 784$, $K = 10$ classes). The interpolation threshold is achieved at $N = 4 \times 10^4$.

Experiment (III): Random Forests

- In order to interpolate a $(n \times d)$ training set, a tree with n leaves (or fewer) will be learned.
- Beyond the interpolation threshold, the number of such trees will be increased.

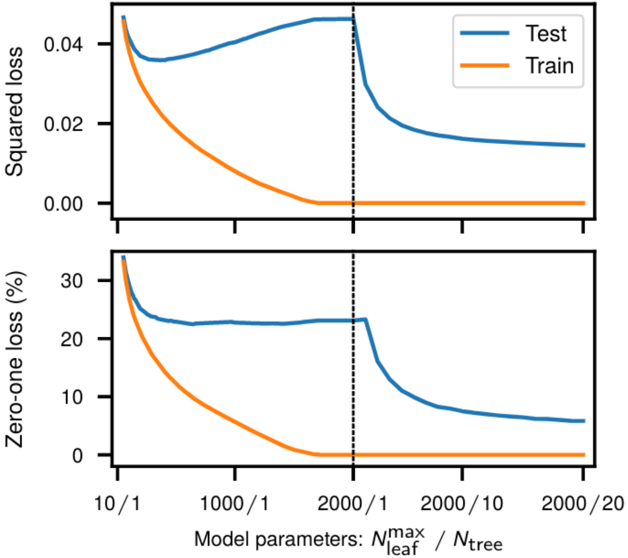

Figure 11: Random Forests on a subset of MNIST ($n = 10^4$, 10 classes).

“Double Descent” in Linear Regression

Consider the model:

$$Y_i = \boldsymbol{\beta}^T X_i + \epsilon_i, \quad (X_i, \epsilon_i) \sim P_X \times P_\epsilon,$$

where $\mathbb{E}(X_i) = \mathbf{0}$, Cov$(X_i) = \Sigma$, $\mathbb{E}(\epsilon_i) = 0$, and Var$(\epsilon_i) = \sigma^2$.

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$\Longrightarrow$

Least square regression estimator:

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta} \in \mathbb{R}^p} \|\boldsymbol{Y} - \boldsymbol{\beta}^T \boldsymbol{X}\|_2 = \left(\boldsymbol{X}^T \boldsymbol{X}\right)^+ \boldsymbol{X}\boldsymbol{Y},$$

where $\boldsymbol{X} = (X_1, ..., X_n)^T \in \mathbb{R}^{n \times p}$, $\boldsymbol{Y} = (Y_1, ..., Y_n)^T \in \mathbb{R}^n$, and $(\boldsymbol{X}^T \boldsymbol{X})^+$ is the pseudoinverse of $\boldsymbol{X}^T \boldsymbol{X}$.

“Double Descent” in Linear Regression

- $\gamma := \frac{p}{n}$ is the overparametrization ratio (as $n, p \to \infty$).
- SNR $= \frac{\|\boldsymbol{\beta}\|_2^2}{\sigma^2}$ is the signal-to-noise ratio.

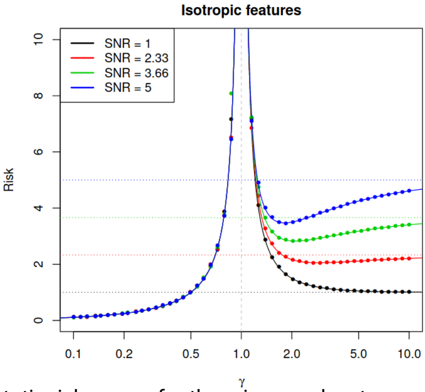

Figure 12: Asymptotic risk curves for the min-norm least square estimator (Hastie et al., 2019).

“Multiple Descent” in Linear Regression

Minimum ℓ_1-norm interpolation (Li and Wei, 2021):

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}\in\mathbb{R}^p} ||\boldsymbol{\beta}||_1 \quad \text{subject to } Y_i = \boldsymbol{\beta}^T X_i, i = 1, ..., n.$$

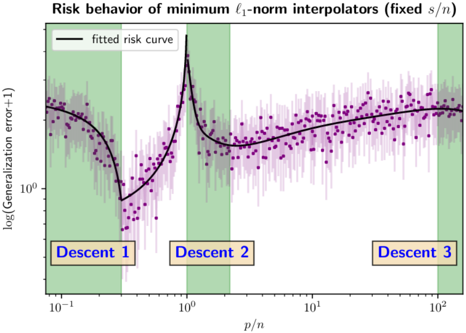

Figure 13: Triple descent in sparse linear regression. Here, s is the ratio of sparsity in the true signal.

Why are linear models are informative? (Neural Tangent Kernel Theory)

When the number of parameter p is very large, we approximate the model $\boldsymbol{z} \mapsto f(\boldsymbol{z}; \boldsymbol{\theta})$ by

$$\boldsymbol{z} \mapsto \nabla_{\boldsymbol{\theta}} f(\boldsymbol{z}; \boldsymbol{\theta}_0)^T \boldsymbol{\beta},$$

where we suppose that $f(\boldsymbol{z}; \boldsymbol{\theta}_0) \approx 0$ and let $\boldsymbol{\theta} = \boldsymbol{\theta}_0 + \boldsymbol{\beta}$.

This argument can be made rigorous via **Neural Tangent Kernel** theory (Jacot et al., 2018), especially when $p > n$. See, for instance, Allen-Zhu et al. (2019):

- Allen-Zhu, Zeyuan, Yuanzhi Li, and Zhao Song. *"A convergence theory for deep learning via over-parameterization."* International Conference on Machine Learning. PMLR, 2019.

Conclusion Thoughts

- Shall we always avoid overfitting?

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- Shall we always avoid overfitting? The answer is “NOT Necessarily”!
- The classical bias-variance trade-off is still useful when
    1. The training set is of large scale.
    2. An interpolating class cannot be fitted.

A Final Reflection

Is the interpolation or overparametrization theory correct?

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The interpolation point of view does not seem to be right!

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However, in my opinion, an overparametrized model is still effective in practice! Why?

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- Fefferman, Charles, Sanjoy Mitter, and Hariharan Narayanan. ”*Testing the manifold hypothesis*.” Journal of the American Mathematical Society 29.4 (2016): 983-1049.

Thank You

Comments or Questions?

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