Double Descent
The Success Recipe Behind Large Neural Networks

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- This contradicts the classical **bias–variance trade-off**

Bias–Variance Trade-Off

For regression:

$$\mathrm{MSE} = \mathbb{E}(Y - \hat{f}(X))^2$$

$$= \underbrace{\mathrm{Var}(\hat{f}(X))}_{\text{Variance}} + \underbrace{\mathrm{Bias}^2(\hat{f}(X))}_{\text{Bias}} + \underbrace{\mathrm{Var}(\varepsilon)}_{\text{Irreducible}}$$

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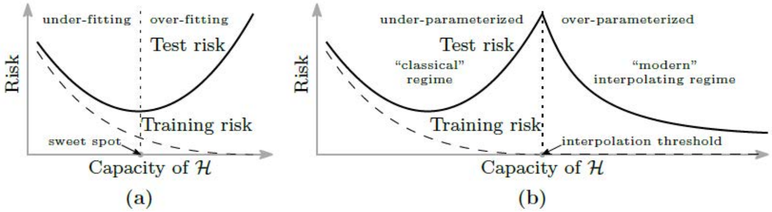
- The goal has been to find the optimal point where both training and test error are simultaneously minimized: **bias–variance sweet spot**

Double Descent Curve



Train and test error vs model complexity [Belkin et al., 2019]

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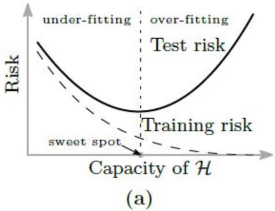

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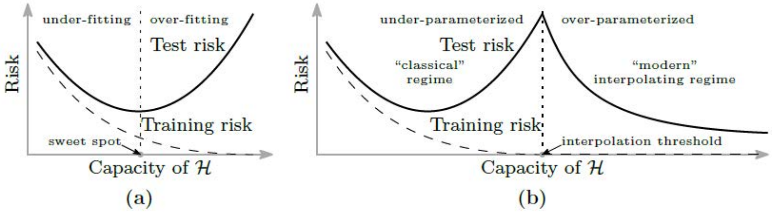

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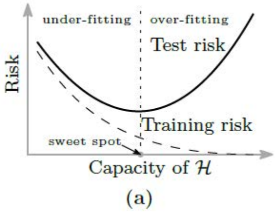

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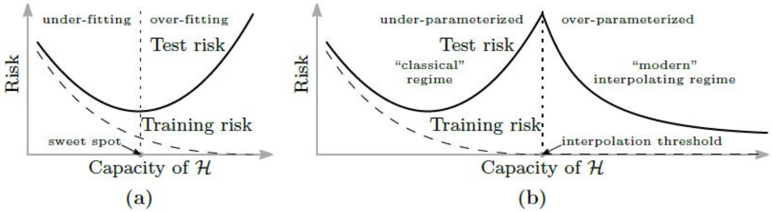

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  - Model fits training data perfectly and even beyond

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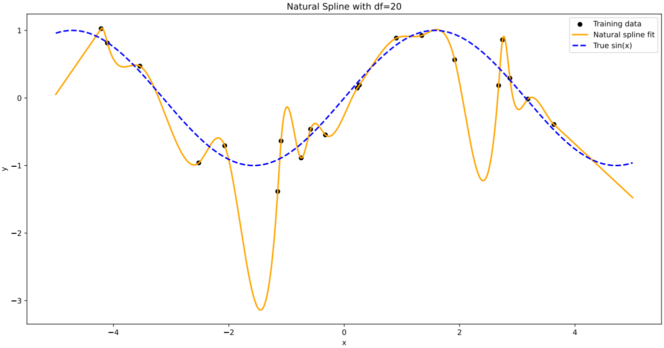
- Fit a spline regression model with d degrees of freedom,

$$f(x_i) = \sum_{j=1}^{d} \hat{\beta}_j \, N_j(x_i),$$

where $N_j(\cdot)$ are cubic spline basis functions and the coefficients $\hat{\beta}_j$ are estimated from the data.

Interpolation - Illustration



Exact fit of 20 points (interpolation)

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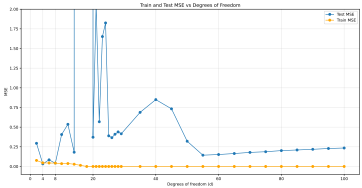
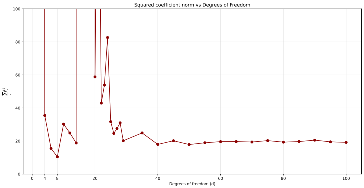
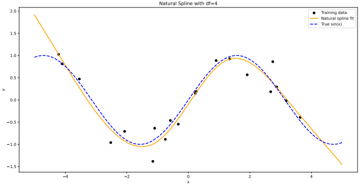


Training and test mean squared error versus model complexity

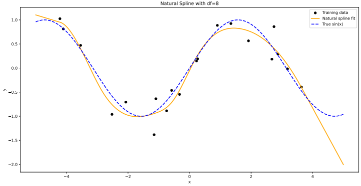


ℓ_2 norm of spline coefficients

Natural Spline Fits for Increasing Degrees of Freedom



df = 4



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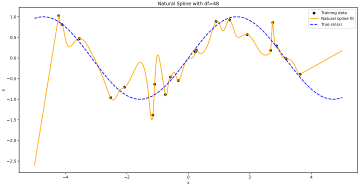

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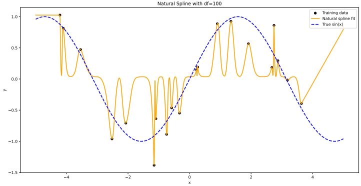

df = 100

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- Least squares (and various other algorithms that solve optimization problems) selects the **minimum** ℓ_2-norm solution
- The solution with the least absolute coefficient value
- This results in jiggly functions (equations) that tend to *approach* reality through many different angles as demonstrated above

Example II: Random Fourier Features

- We demonstrate double descent on a real-world application using the MNIST dataset, using Random Fourier Features:

$$f(x) = \sum_{k=1}^{N} a_k \phi(x; v_k), \qquad \phi(x, v) := e^{i\langle v, x\rangle}$$

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- Inner products $z(x)^\top z(x')$ approximate the Gaussian kernel

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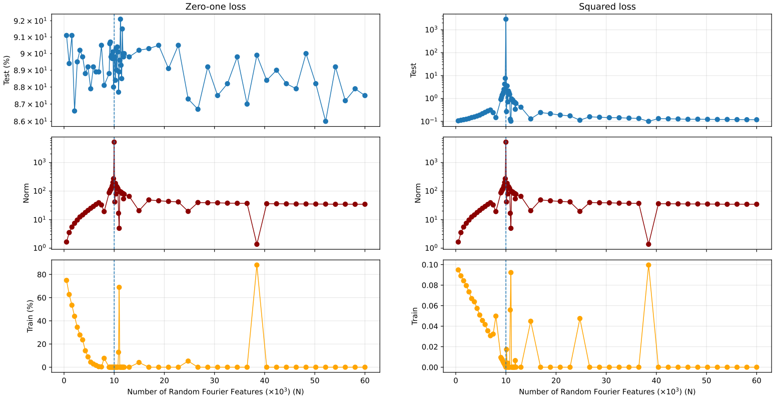
- In the classification setting, we additionally report the zero–one loss, which equals 1 for an incorrect prediction and 0 for a correct one.

RFF Results



Training/test error and coefficient norms vs N

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- Minimum-norm solutions play a crucial role as the key requirement to yield such results
- SGD acts as an implicit regularizer and is widely used to estimate the parameters of neural networks
- The examples share a common approach to neural networks, essentially estimating a function f through the sum of multiple simpler functions

Conclusion

- Double **describes/illustrates** why modern large (to the point of over-parameterization) models perform exceptionally
- The main idea is that, by using too many parameters, selecting the minimum-norm solution leads to predictors that approximate the true underlying behavior well.
- This is what Large Language Models essentially are, over-fitted models that have been trained on the whole internet with billions of parameters and are able to **approximate** the truth (with a pinch of randomness)
- Full theoretical understanding is yet to be found

References

Belkin, M., Hsu, D., Ma, S., and Mandal, S. (2019).
Reconciling modern machine-learning practice and the classical bias–variance trade-off.
Proceedings of the National Academy of Sciences, 116(32):15849–15854.