The double descent phenomenon

Generalization of overparametrized models

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DSC291 Machine Learning — November 8, 2022

Review: classical statistical learning framework

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The model's ability to **generalize** is how well it accounts for out-of-sample data.

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3. Construct a **risk estimation** procedure that finds an estimate $\hat{R}(h)$ of $R(h)$.
4. **Minimize** the risk estimator:

$$\hat{h} := \arg\min_{h \in \mathcal{H}} \hat{R}(h).$$

Generalization theory through empirical risk minimization

We can decompose the risk $R(h)$ as:

$$R(h) = \underbrace{\hat{R}(h) - \hat{R}(h^*)}_{\text{estimated gap}} + \underbrace{\left(R(h) - \hat{R}(h)\right)}_{\text{estimation error for } h} + \underbrace{\left(\hat{R}(h^*) - R(h^*)\right)}_{\text{estimation error for } h^*} + \underbrace{R(h^*)}_{\text{model bias}}$$

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- For the empirical risk minimizer $\hat{h}$, the *estimated gap* term is non-positive, so:

$$R(\hat{h}) \leq \text{estimation error terms} + \text{model bias term}.$$

Results from classical generalization theory

Generalization theory tends to give us bounds on the estimation error term so that:

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- The **capacity** of $\mathcal{H}$ measures how many worlds $\mathcal{H}$ can explain.
- Generally, the bias of a model increases as its capacity shrinks.
  - This leads to the **bias-variance tradeoff**.

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Bias-variance tradeoff

Intuition: how the bias of $\mathcal{H}$ relate to the capacity of $\mathcal{H}$.

- **Small capacity:** if $\mathcal{H}$ cannot explain many worlds, it may poorly explain the one in which the learner lives. This leads to a large bias term.
- **Large capacity:** if many (very different) explanations account for what the learner sees, how to pick among these explanations? This leads to a large variance term.

Classical bias-variance tradeoff

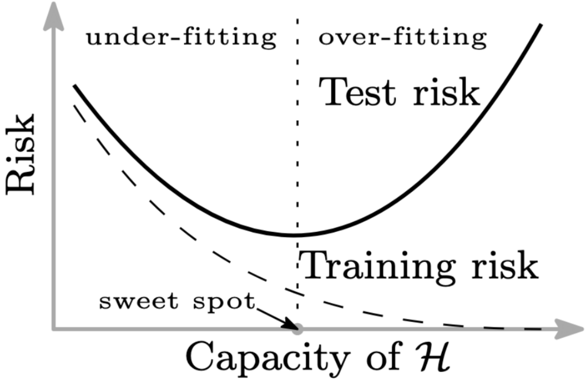

Figure 1: Belkin et al. (2018)

Model selection problem

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- Classical statistics says not too large: try to find the 'sweet spot'.
- However, in modern machine learning, we often fit very over-parameterized models and achieve good generalization.
  - The capacity of neural nets often allow for training loss to be driven down to zero (that is, the model *interpolates* the training data).

Double descent phenomenon

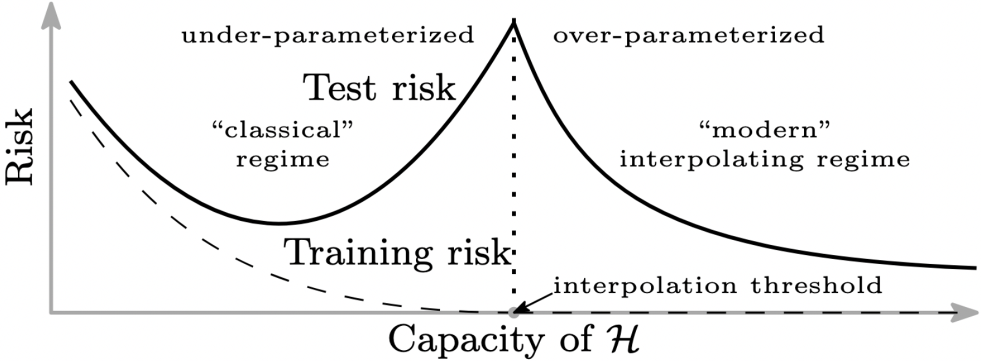

Figure 2: In the 'modern' interpolating regime, increasing model capacity often empirically leads to better generalization, Belkin et al. (2018).

Double descent a robust phenomenon

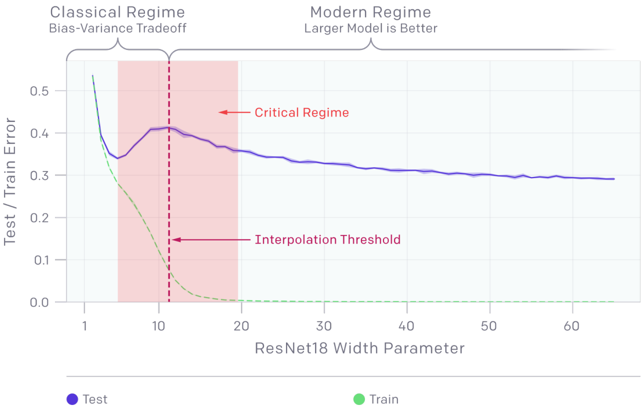

Figure 3: Double descent is observed across many models, tasks, optimizers, training time, and noise levels. Pictured is the train/test error for family of ResNet18 on CIFAR-10 (Nakkiran et al., 2021).

Generalization theory: what's missing?

- In an over-parameterized model where many explanations equally account for the training data, how does the learner select one?
  - Generalization also depends on how we regularize and optimize.

Algorithms without double descent?

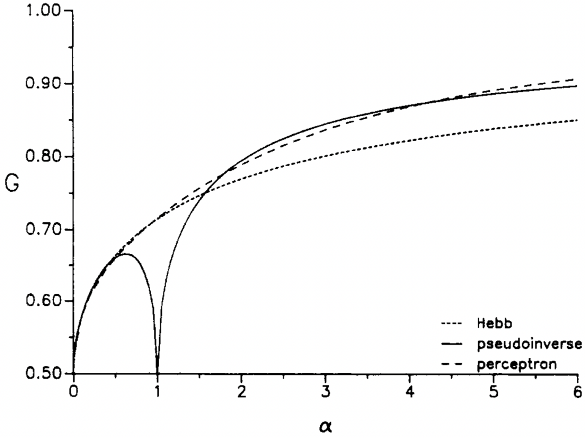

Figure 4: Generalization curves for different methods of learning a classifier on Boolean data $\{-1, +1\}^N$ using a dataset of size αN (Opper et al., 1990).

Double descent in ordinary least squares: warm-up

One explanation of double descent

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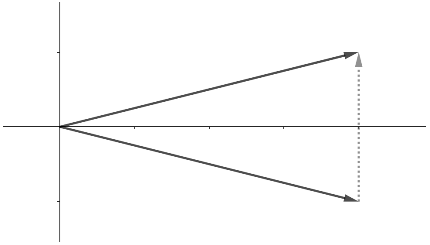

Figure 5: The instances x_1 and x_2 (black) provides good signal along the horizontal direction, but poor signal along the vertical direction.

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Goal. The goal of the learner is to use data to give an estimate $\hat{\beta}$ of β minimizing:

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Linear regression in the interpolating regime

When the number of parameters d is at least the number of data points n, we can always perfectly fit a linear regressor:

$$\mathbf{Y} = \mathbf{X}\hat{\beta},$$

where $\mathbf{X} \in \mathbb{R}^{n \times d}$, $\mathbf{Y} \in \mathbb{R}^{n}$, and $\hat{\beta} \in \mathbb{R}^{d}$.

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- In fact, if $d > n$, then there are infinitely many interpolating $\hat{\beta}$'s.
- If we fit $\hat{\beta}$ using OLS, we obtain a specific choice:

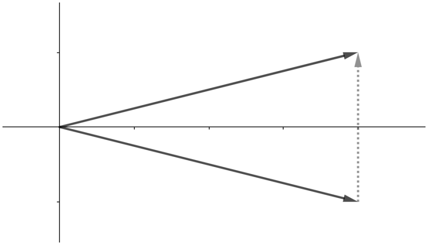
$$\hat{\beta} = \mathbf{X}^{+}\mathbf{Y},$$

where $\mathbf{X}^{+}$ is the Moore-Penrose pseudoinverse of $\mathbf{X}$. In this setting, $\mathbf{X}\mathbf{X}^{+} = \mathbf{I}_d$.

Linear regression in the interpolating regime

Question. How poorly can $\hat{\beta}$ estimate β in the interpolating regime?

A 2D example



Setting. Consider data in $\mathbb{R}^2$ generated by:

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where e_1 is the first basis direction and ε is Gaussian.

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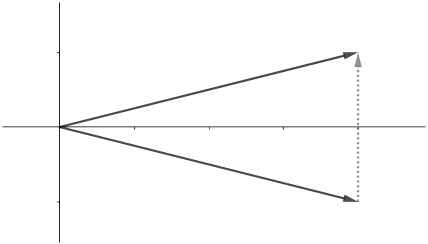

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$$x_A = \begin{bmatrix} 1 \\ -\delta \end{bmatrix} \qquad x_B = \begin{bmatrix} 1 \\ +\delta \end{bmatrix}$$

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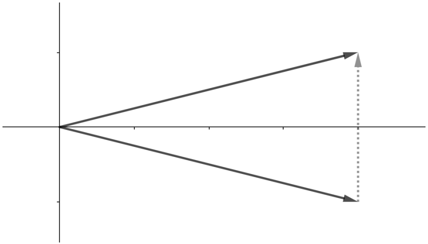

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Solution. OLS estimate $\hat{\beta}$ is:

$$\hat{\beta}_1 = 1 + \frac{\varepsilon_A + \varepsilon_B}{2} \qquad \hat{\beta}_2 = \frac{1}{\delta}\frac{\varepsilon_B - \varepsilon_A}{2}.$$

Computation of 2D example

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- But, the small vector δe_2 also has to explain a (relatively large) part of the noise:

$$\frac{y_B - y_A}{2} = \frac{\varepsilon_B - \varepsilon_A}{2}.$$

Double descent from 2D example

Suppose instead that x_A and x_B were actually $(d+1)$-dimensional vectors:

$$
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x_A &= \begin{bmatrix} 1 & -\delta/\sqrt{d} & \cdots & -\delta/\sqrt{d} \end{bmatrix}^\top \\
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- The same part of the noise $\frac{\varepsilon_B - \varepsilon_A}{2}$ needs to be explained by a vector:

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which has norm δ, as before. But, the same noise is spread out across d directions:

$$\hat{\beta}_j = \frac{1}{\delta d} \frac{\varepsilon_B - \varepsilon_A}{2} \qquad j > 1.$$

Double descent from 2D example

We can now compute the generalization error:

$$\mathbb{E}\left[\left\|\hat{\beta}-\beta\right\|^2\right]=\mathbb{E}\left[\left(\frac{\varepsilon_A+\varepsilon_B}{2}\right)^2\right]+\sum_{j>1}\mathbb{E}\left[\left(\frac{1}{\delta d}\frac{\varepsilon_B-\varepsilon_A}{2}\right)\right]=\frac{1}{2}+\frac{1}{d}\frac{1}{2\delta^2}.$$

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- The $\frac{1}{2}$ terms comes from the noise explained by the first term.
- The $\frac{1}{d}\frac{1}{2\delta^2}$ goes to zero as d goes to infinity.

Double descent in ordinary least squares: Gaussian model

Linear regression problem

Problem. Suppose nature generates data as follows:

$$y = x^\top \beta + \varepsilon,$$

- the covariates $x \in \mathbb{R}^d$ are d dimensional standard Gaussians, $x \sim \mathcal{N}\left(0, \frac{1}{d}\mathbf{I}_d\right)$
- the noise $\varepsilon \in \mathbb{R}$ is drawn from $\mathcal{N}(0, \sigma^2)$
- there is a true regressor β, but it is unknown to the learner

Goal. The goal of the learner is to use data to give an estimate $\hat{\beta}$ of β minimizing:

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Linear regression on a single data point

Data. Let $y = x^\top \beta + \varepsilon$ where:

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where Π_x is the projection operator onto $\mathrm{span}(x)$.

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where Π_x is the projection operator onto $\mathrm{span}(x)$.

- Note that $\hat{\beta}$ satisfies: $x^\top \hat{\beta} = \dfrac{x^\top xy}{\|x\|^2} = y$

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Denote $\beta_x = \Pi_x \beta$ and $\beta_x^\perp = \beta - \beta_x$ its orthogonal complement.

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\mathbb{E}\left[\|\hat{\beta} - \beta\|^2\right] &= \mathbb{E}\left[\left\|\Pi_x \beta + \frac{x\varepsilon}{\|x\|^2} - \beta\right\|^2\right] \\
&= \mathbb{E}\left[\left\|\beta_x^\perp + \frac{x\varepsilon}{\|x\|^2}\right\|^2\right] \\
&= \underbrace{\mathbb{E}\left[\|\beta_x^\perp\|^2\right]}_{\text{error from unseen directions}} + \underbrace{\mathbb{E}\left[\frac{\varepsilon^2}{\|x\|^2}\right]}_{\text{error from explaining noise}} .
\end{aligned}$$

Generalization error

Denote $\beta_x = \Pi_x \beta$ and $\beta_x^\perp = \beta - \beta_x$ its orthogonal complement.

$$
\begin{aligned}
\mathbb{E}\left[\|\hat{\beta} - \beta\|^2\right] &= \mathbb{E}\left[\left\|\Pi_x \beta + \frac{x\varepsilon}{\|x\|^2} - \beta\right\|^2\right] \\
&= \mathbb{E}\left[\left\|\beta_x^\perp + \frac{x\varepsilon}{\|x\|^2}\right\|^2\right] \\
&= \underbrace{\mathbb{E}\left[\|\beta_x^\perp\|^2\right]}_{\text{error from unseen directions}} + \underbrace{\mathbb{E}\left[\frac{\varepsilon^2}{\|x\|^2}\right]}_{\text{error from explaining noise}} .
\end{aligned}
$$

Notice that the last term is related to the signal-to-noise ratio.

Generalization error

Because x is isotropic Gaussian, the error from unseen directions is:

$$\underbrace{\mathbb{E}\left[\|\beta_x^{\perp}\|^2\right]}_{\text{error from unseen directions}} = \frac{d}{d-1}\|\beta\|^2.$$

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- Note that when x is standard normal, $1/\|x\|^2$ follows an **inverse Wishart distribution** (and $\|x\|^2$ follows a χ^2-distribution with degree of freedom d).
- If $d = 1$ or $d = 2$, then the expected generalization error is infinite.

χ^2-distribution

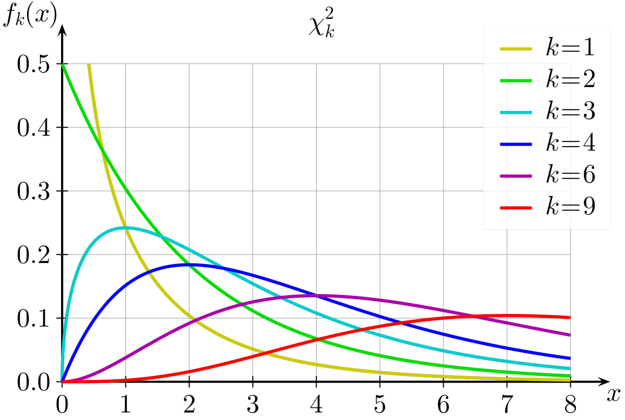

Figure 6: χ^2-distributions where k is the degree of freedom, from *Wikipedia*.

Main result from Belkin et al. (2020)

Setting. Their setting extends this setting of linear regression on single point $x \in \mathbb{R}^d$.

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Theorem (Belkin et al. (2020))

Let $\hat{\beta}$ be the OLS regressor in this setting. Then its expected risk is:

$$\mathbb{E}\left[\left(y - x^\top \hat{\beta}\right)^2\right] = \begin{cases} \left(\left(1 - \frac{p}{d}\right) \cdot \|\beta\|^2 + \sigma^2\right) \cdot \left(1 + \frac{p}{n-p-1}\right) & p \leq n-2 \\ \infty & p = n, n+1 \\ \|\beta\|^2 \cdot \left(1 - \frac{n}{d} \cdot \left(2 - \frac{d-n-1}{p-n-1}\right)\right) + \sigma^2 \cdot \left(1 + \frac{n}{p-n-1}\right) & p \geq n+2 \end{cases}$$

Main result from Belkin et al. (2020)

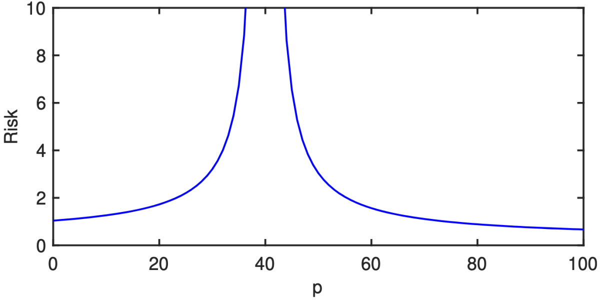

Figure 7: Visualization of the double descent curve from previous theorem(Belkin et al., 2020).

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