Learning curve in modern ML
The ”double descent” behavior

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Outline

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The classical learning curve

We all know the Bias-Variance Trade-Off:
The classical learning curve

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The common knowledge - very low training error $\rightarrow$ very high variance
The classical learning curve

We all know the Bias-Variance Trade-Off:

The common knowledge - very low training error → very high variance

One may think of some criteria for finding the optimal model
Is NN immune to variance?

On the other hand - very rich models such as NN are trained to exactly fit the train data, and yet they obtain high accuracy on test data.
Is NN immune to variance?

On the other hand - very rich models such as NN are trained to exactly fit the train data, and yet they obtain high accuracy on test data.

How can we reconcile the modern practice with the classical bias-variance trade-off?
A "jamming transition"

Spigler in mid 2018, argued that in fully-connected networks, a phase transition delimits the over and under-parametrized regimes where fitting can or cannot be achieved.

Background

A jamming transition from under- to over-parametrization affects loss landscape and generalization

N: degrees of freedom, P: training examples.
Reconciling the discrepancy

Just one year ago - Belkin et al first analyzed the behavior of rich models around the interpolation point

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Reconciling modern machine learning practice and the bias-variance trade-off

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Abstract

Breakthroughs in machine learning are rapidly changing science and society, yet our fun-
Reconciling the discrepancy

Just one year ago - Belkin et al first analyzed the behavior of rich models around the interpolation point

Since then many authors published results, that justified the innovative approach
Reconciling the discrepancy

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Since then many authors published results, that justified the innovative approach

Hastie, Rosset, and Tibshirani provided a precise quantitative explanation for the potential benefits of over-parametrization in linear regression
Empirical risk minimization

Given a training sample \((x_1, y_1), \cdots, (x_n, y_n)\), where \((x_i, y_i) \in \mathbb{R}^d \times \mathbb{R}\), we learn a predictor \(h_n : \mathbb{R}^d \rightarrow \mathbb{R}\).

In ERM, the predictor is taken to be

\[
h_n = \operatorname{argmin}_{h \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^{n} l(y_i, h(x_i)) \right\}
\]
Empirical risk minimization

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In ERM, the predictor is taken to be

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

- Empirical risk (train error): \(\frac{1}{n} \sum_{i=1}^{n} l(y_i, h_n(x_i))\)
  
  - *Interpolation*: \(l(y_i, h_n(x_i)) = 0 \quad \forall i\)

- True risk (test error): \(\mathbb{E}_{x,y} \left[ l(y_i, h_n(x_i)) \right]\)
Controlling $\mathcal{H}$

Conventional wisdom in machine learning suggests controlling the capacity of $\mathcal{H}$:

- $\mathcal{H}$ too small $\rightarrow$ under-fitting (large empirical and true risk)
- $\mathcal{H}$ too large $\rightarrow$ over-fitting (small empirical risk but large true risk)
Controlling $\mathcal{H}$

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Example (OLS)

$$\hat{\beta}_n = \arg\min_{\beta \in \mathbb{R}^p} \left\{ \frac{1}{n} \sum_{i=1}^{n} \left( y_i - x_i^T \beta \right)^2 \right\}$$

True risk $\propto \frac{p}{n-p}$
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True risk $\propto \frac{p}{n-p}$

Yet, best practice in DL: network should be large enough to permit effortless zero train-loss
The “double descent” risk curve

The main finding of Belkin’s work is summarized in the “double descent” risk curve:

![Diagram showing the double descent risk curve]

(a) U-shaped “bias-variance” risk curve

(b) “double descent” risk curve

This is demonstrated on important model classes including neural networks and a range of real data sets.
The “double descent” risk curve

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The “double descent” risk curve

The main finding of Belkin’s work is summarized in the “double descent” risk curve:

This is demonstrated on important model classes including neural networks and a range of real data sets.

The capacity of $\mathcal{H}$ is identified with the number of parameters needed to specify the function $h_n$. 

Fitting beyond the interpolation point

When zero train error can be achieved, we choose $h_n$ as follows:

$$h_n = \arg\min_{h \in H} \left\{ \|h_n\| \quad s.t: \quad \frac{1}{n} \sum_{i=1}^{n} l(y_i, h(x_i)) = 0 \right\}$$
Fitting beyond the interpolation point

When zero train error can be achieved, we choose $h_n$ as follows:

$$h_n = \arg\min_{h \in \mathcal{H}} \left\{ ||h_n|| \; s.t: \frac{1}{n} \sum_{i=1}^{n} l(y_i, h(x_i)) = 0 \right\}$$

- Looking for the simplest/smoothelest function that explain the data
- By increasing the capacity of $\mathcal{H}$, we are able to find interpolating functions that have smaller norm
Why is the “double descent” important?

Stating that interpolation does not necessarily lead to poor generalization, as long as you “deep” enough in the interpolation regime.

Reconciling the modern practice with a statistical point-of-view.

Explicit analysis for Linear Models.

The true risk in the over-parameterized regime is typically lower!
Why is the “double descent” important?

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- Explicit analysis for Linear Models
- The true risk in the over-parameterized regime is typically lower!
Neural networks

- One Hidden layer with $N$ random features
- Minimizing squared loss or $||a||_2$ when $N \geq n$

\[ h(x) = \sum_{k=1}^{N} \tilde{x}_k a_k \]

\[ \tilde{x}_k = \varphi(x; v_k) = \varphi(<x, v_k>) , \quad v_k \sim MN(0, I_p) \]
Neural networks

Risk curve for RFF model on MNIST

- Near interpolation - parameters are "forced" to fit the training data
- Increasing $N$ results in decreasing the $l_2$ norm of the predictors
Neural networks

Fully connected two-layers network with $H$ hidden units

Optimizing the weight using SGD with up to $6 \cdot 10^3$ iterations:

- Interpolation is not assured even in the over-parameterized regime
- Automatically prefers minimal-norm solution

Sub-optimal behavior can lead to high variability in both the training and test risks that masks the double descent curve
Neural networks

Risk curves for two-Layers fully connected NN on MNIST

- Train risk may increase with increasing number of parameters
Decision trees

It was shown by Wyner et al (2017) that AdaBoost and Random-Forests perform better with large (interpolating) decision trees and are more robust to noise in the training data.

They questioned the conventional wisdom that suggests that boosting algorithms for classification requires regularization/early stopping/low complexity.

The effect of noise-point on a classifier: interpolating Vs non-interpolating
Decision trees

Risk curves for Random-Forests on MNIST

- The complexity is controlled by the size of a decision tree, and the number of trees
- Averaging of interpolating trees ensures substantially smoother function
Thinking about it...

The peak at the interpolation threshold is observed within a narrow range of parameters - sampling parameter-space out of that range may lead to the misleading (but conventional) conclusions.
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The peak at the interpolation threshold is observed within a narrow range of parameters - sampling parameter-space out of that range may lead to the misleading (but conventional) conclusions.

The understanding of the "double descent" behavior is important for practitioners to choose between models for optimal performance.
Why Least-Squares?

Theoretical analysis for Least-Squares

Easy to analyze
Easy to explain
Easy to simulate

Any non-linear model can be approximated by a linear one with large number of random features

\[ y|z = f(z; \theta) \approx \nabla_\theta f(z; \theta_0)^T \beta \]

There is a well known connection between the gradient descent and the minimum-norm Least-Squares solution
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$$\mathbb{E}[y|z] = f(z; \theta) \approx \nabla_{\theta} f(z; \theta_0)^T \beta$$
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\]

There is a well known connection between the gradient descent and the minimun-norm Least-Squares solution
The Linear model

\[ y_i = x_i^T \beta + \epsilon_i ; \quad i = 1, \cdots, n \]

\[ x_i \in \mathbb{R}^p, \quad \mathbb{E}[x_i] = 0, \quad \text{Cov}(x_i) = \Sigma \]

\[ \mathbb{E}[\epsilon_i] = 0, \quad \text{Var}(\epsilon_i) = \sigma^2 \]

We consider an asymptotic setup where \( n, p \to \infty \) and \( p/n \to \gamma \in (0, \infty) \)

We also assume that \( \|\beta\|_2^2 = r^2 \) - constant "signal"
The Linear model

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Some assumptions over the distribution of \( x \) may be taken:
- \( x \sim MN(0, \Sigma) \)
- \( x = \Sigma^{1/2} z, \ z_j \sim (0, 1) \)
  - Isotropic features: \( \Sigma = I_p \)
- \( x = \varphi(Wz), \text{where} \ W \in \mathbb{R}^{p \times d} \text{a random matrix with i.i.d. entries} \)
The Linear model

Assuming that the model is well-specified, the out-of-sample prediction risk is:

\[ R(\hat{\beta}; \beta) = \mathbb{E}_{XYx_0} \left( x_0^T \hat{\beta} - x_0^T \beta \right)^2 \]
The Linear model

Assuming that the model is well-specified, the out-of-sample prediction risk is:

\[
R(\hat{\beta}; \beta) = \mathbb{E}_{X,Y|X_0} \left( x_0^T \hat{\beta} - x_0^T \beta \right)^2
\]

Assuming isotropic features, we can decompose the risk to bias and variance terms:

\[
R(\hat{\beta}; \beta) = \mathbb{E}_X \left[ \| \mathbb{E}[\hat{\beta}|X] - \beta \|^2 \right] + \mathbb{E}_X \left[ \text{tr}[\text{Cov}(\hat{\beta}|X)] \right] := B(\hat{\beta}; \beta) + V(\hat{\beta})
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The Linear model

Assuming that the model is well-specified, the out-of-sample prediction risk is:

$$ R(\hat{\beta}; \beta) = \mathbb{E}_{X|Y_{x_0}} \left( x_0^T \hat{\beta} - x_0^T \beta \right)^2 $$

Assuming isotropic features, we can decompose the risk to bias and variance terms:

$$ R(\hat{\beta}; \beta) = \mathbb{E}_{X} \left[ ||\mathbb{E}[\hat{\beta}|X] - \beta||_2^2 \right] + \mathbb{E}_{X} \left[ \text{tr}[\text{Cov}(\hat{\beta}|X)] \right] := B(\hat{\beta}; \beta) + V(\hat{\beta}) $$

Taking $\hat{\beta} = (X^TX)^{-1}X^T Y$, we get:

$$ \mathbb{E}[\hat{\beta}|X] = \beta \; ; \; \text{Cov}(\hat{\beta}|X) = \sigma^2(X^TX)^{-1} \rightarrow \frac{\sigma^2}{n-p} I_p $$

and therefore $R(\hat{\beta}; \beta) \rightarrow \frac{\sigma^2 \gamma}{1-\gamma}$
When $\gamma > 1$, the empirical risk $|| Y - X \beta ||_2^2$ can be eliminated, and we are looking for the minimum $l_2$ norm estimator:

$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^p} \{ ||\beta||_2 \ s.t: || Y - X \beta ||_2^2 = 0 \}$$
High dimensional Least-Squares

When $\gamma > 1$, the empirical risk $\|Y - X\beta\|^2_2$ can be eliminated, and we are looking for the minimum $l_2$ norm estimator:

$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^p} \{ \|\beta\|_2 \text{ s.t.: } \|Y - X\beta\|^2_2 = 0 \}$$

Solving with Lagrange multipliers:

$$\arg\min_{\beta, \lambda} \left\{ \beta^T \beta + \lambda^T (Y - X\beta) \right\}$$

We get:

$$\hat{\beta} = X^T \hat{\lambda} ; \hat{\lambda} = (XX^T)^{-1} Y \implies \hat{\beta} = X^T (XX^T)^{-1} Y$$
High dimensional Least-Squares

When $\gamma > 1$, the empirical risk $||Y - X\beta||^2_2$ can be eliminated, and we are looking for the *minimum $l_2$ norm estimator*:

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Solving with Lagrange multipliers:

$$\arg\min_{\beta, \lambda} \left\{ \beta^T \beta + \lambda^T (Y - X\beta) \right\}$$

We get:

$$\hat{\beta} = X^T \hat{\lambda} ; \quad \hat{\lambda} = (XX^T)^{-1}Y \quad \Rightarrow \quad \hat{\beta} = X^T(XX^T)^{-1}Y$$

One can write: $\hat{\beta} = (X^TX)^+X^TY$
Computing the bias term

Now we have:

$$E[\hat{\beta}|X] = X^T(XX^T)^{-1}X\beta \neq \beta$$

and therefore the bias term is:

$$B(\hat{\beta}; \beta) = E_X \left[ \|E[\hat{\beta}|X] - \beta\|_2^2 \right] = \beta^T(I_p - E_X[X^T(XX^T)^{-1}X])\beta$$
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We can show that \( \mathbb{E}_X[X^T (XX^T)^{-1}X] \rightarrow \frac{n}{p} I_p \), and therefore:

\[ B(\hat{\beta}; \beta) = \beta^T \beta - \frac{n}{p} \beta^T \beta = r^2 (1 - \frac{1}{\gamma}) \]
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and therefore the bias term is:

$$B(\hat{\beta}; \beta) = E_X \left[ \left| \left| E[\hat{\beta}|X] - \beta \right| \right|^2 \right] = \beta^T(I_p - E_X[X^T(XX^T)^{-1}X])\beta$$

We can show that $E_X[X^T(XX^T)^{-1}X] \to \frac{n}{p}I_p$, and therefore:

$$B(\hat{\beta}; \beta) = \beta^T\beta - \frac{n}{p}\beta^T\beta = r^2(1 - \frac{1}{\gamma})$$

Note that:

$$E_X \left[ \left| \left| E[\hat{\beta}|X] \right| \right|^2 \right] \to \frac{n}{p}r^2 = \frac{r^2}{\gamma}$$
Computing the variance term

Recall that:

\[ V(\hat{\beta}) = \mathbb{E}_X \left[ \text{tr}[\text{Cov}(\hat{\beta}|X)] \right] \]

Now we have:

\[ \text{Cov}(\hat{\beta}|X) = \sigma^2 (XX^T)^{-1} XX^T (XX^T)^{-1} = \sigma^2 (XX^T)^{-1} \rightarrow \frac{\sigma^2}{p - n} I_n \]

and therefore:

\[ V(\hat{\beta}) \rightarrow \frac{\sigma^2}{\gamma - 1} \]
Limiting Risk

For the asymptotic setting, we can obtain the following formula:

\[
R(\gamma) = \begin{cases} 
\sigma^2 \frac{\gamma}{1-\gamma} & \text{for } \gamma < 1 \\
 r^2 \left(1 - \frac{1}{\gamma}\right) + \sigma^2 \frac{1}{\gamma-1} & \text{for } \gamma > 1 
\end{cases}
\]

- A new bias-variance trade-off in the over-parameterized regime
- The behavior can be controlled by the \( SNR = \frac{r^2}{\sigma^2} \)
- If \( SNR > 1 \), there is a local min at \( \gamma = \frac{\sqrt{SNR}}{\sqrt{SNR} - 1} \)
- As \( \gamma \to \infty \), the estimator \( \hat{\beta} \) converge to the null estimator \( \tilde{\beta} = 0 \), and the total risk is \( r^2 \)
Empirical results

Figure: $\sigma^2 = 1$, $r^2$ varies from 1 to 5
Misspecified model

\[ y_i = x_i^T \beta + \omega_i^T \theta + \epsilon_i \; ; \; i = 1, \cdots, n \]

\[ x_i \in \mathbb{R}^p, \; \omega_i \in \mathbb{R}^d, \; E[(x_i, \omega_i)] = 0, \; E[\epsilon_i] = 0, \; \text{Var}(\epsilon_i) = \sigma^2 \]

For simplicity, we assume that \( \text{Cov}((x_i, \omega_i)) = I_{p+d} \)
Misspecified model

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For simplicity, we assume that \( \text{Cov}((x_i, \omega_i)) = I_{p+d} \)

In this case we can write:

\[ y_i = x_i^T \beta + \delta_i ; \quad i = 1, \ldots, n \]

\( \mathbb{E}[\delta_i] = 0, \text{Var}(\delta_i) = \sigma^2 + ||\theta||_2^2 \)
Misspecified model

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\[ \mathbb{E}[\delta_i] = 0, \; Var(\delta_i) = \sigma^2 + ||\theta||_2^2 \]

We also assume that \( ||\beta||_2^2 + ||\theta||_2^2 = r^2 \) - constant "signal"
Misspecified model

The risk is:

\[ R(\hat{\beta}; \beta, \theta) = \mathbb{E}_X \left[ ||\mathbb{E}[\hat{\beta}|X] - \beta||_2^2 \right] + \mathbb{E}_X \left[ tr[Cov(\hat{\beta}|X)] \right] + ||\theta||_2^2 \]

\[ := B(\hat{\beta}; \beta) + V(\hat{\beta}; \theta) + M(\beta, \theta) \]
**Misspecified model**

The risk is:

\[ R(\hat{\beta}; \beta, \theta) = \mathbb{E}_X \left[ ||\mathbb{E}[\hat{\beta}|X] - \beta||_2^2 \right] + \mathbb{E}_X \left[ \text{tr}[\text{Cov}(\hat{\beta}|X)] \right] + ||\theta||_2^2 \]

\[ := B(\hat{\beta}; \beta) + V(\hat{\beta}; \theta) + M(\beta, \theta) \]

For the variance term we have:

- \( V(\hat{\beta}; \theta) = (\sigma^2 + ||\theta||_2^2)^\frac{\gamma}{1-\gamma}, \) for \( \gamma < 1 \)
- \( V(\hat{\beta}; \theta) = (\sigma^2 + ||\theta||_2^2)^\frac{1}{\gamma-1}, \) for \( \gamma > 1 \)
Misspecified model

The total risk for $\gamma < 1$:

$$\|\theta\|^2_2 + (\sigma^2 + \|\theta\|^2_2) \frac{\gamma}{1 - \gamma}$$

The total risk for $\gamma > 1$:

$$\|\theta\|^2_2 + \|\beta\|^2_2 (1 - \frac{1}{\gamma}) + (\sigma^2 + \|\theta\|^2_2) \frac{1}{\gamma - 1}$$
Misspecified model

The total risk for $\gamma < 1$:

$$||\theta||_2^2 + (\sigma^2 + ||\theta||_2^2) \frac{\gamma}{1 - \gamma}$$

The total risk for $\gamma > 1$:

$$||\theta||_2^2 + ||\beta||_2^2(1 - \frac{1}{\gamma}) + (\sigma^2 + ||\theta||_2^2) \frac{1}{\gamma - 1}$$

What can be a conventional connection between $\gamma$ and $||\theta||_2^2$?

How the signal is distributed over $\gamma$?
Polynomial decay of the signal

We now assume that:

\[ ||\theta||_2^2 = r^2 (1 + \gamma)^{-a} \]
\[ ||\beta||_2^2 = r^2 (1 - (1 + \gamma)^{-a}) \]

for some \( a > 0 \)

Figure: \( ||\theta||_2^2 = ((1 + \gamma)^{-a}, a \in \{0.5, 1, 2, 5\} \)
Polynomial decay of the signal

We now obtain the following formula:

\[
R_a(\gamma) = \begin{cases} 
    r^2 (1 + \gamma)^{-a} + (r^2 (1 + \gamma)^{-a} + \sigma^2) \frac{\gamma}{1 - \gamma} & \text{for } \gamma < 1 \\
    r^2 (1 + \gamma)^{-a} + r^2 (1 - (1 + \gamma)^{-a}) (1 - \frac{1}{\gamma}) + (r^2 (1 + \gamma)^{-a} + \sigma^2) \frac{1}{\gamma - 1} & \text{for } \gamma > 1 
\end{cases}
\]

- We can see that \( R(\gamma = 0) = R(\gamma = \infty) = r^2 \) (the null risk)
- For \( a \leq 1 + \frac{1}{SNR} \), \( R_a(\gamma) \) is a monotonically increasing function in the under-parameterized regime
- If \( SNR \leq 1 \), the risk in the over-parameterized regime always worse than the null risk
- If \( SNR > 1 \), there is a local minimum in the over-parameterized regime, and it is **global** for small enough \( a \)
Empirical results

The "double descent" behavior achieved...
Thinking about it...

Yet, we did not see the same behavior as in the NN simulations...

The reason may be - the distribution of the signal over the parameters space
Thinking about it...

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The reason may be - the distribution of the signal over the parameters space

What if - the majority of the signal is located within some range in the over-parameterized regime?

\[
\|\theta\|_2^2 = g(\gamma)
\]

**Figure:** \(\|\theta\|_2^2 = g(\gamma)\)
Model evaluation

For the task of models evaluation and selection we may use the *leave-one-out cross-validation* estimator (CV for short):

\[
CV_n = \frac{1}{n} \sum_{i=1}^{n} \left( y_i - \hat{f}_{n-i}(x_i) \right)^2
\]

where \( S \) is the linear smoother matrix.
Model evaluation

For the task of models evaluation and selection we may use the *leave-one-out cross-validation* estimator (CV for short):

$$CV_n = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{f}_n^{-i}(x_i))^2$$

We may also want use the ”shortcut formula”:

$$CV_n = \frac{1}{n} \sum_{i=1}^{n} \left( \frac{y_i - \hat{f}_n(x_i)}{1 - S_{ii}} \right)^2 = \frac{1}{n} \sum_{i=1}^{n} \left( \frac{y_i - [SY]_i}{1 - S_{ii}} \right)^2$$

where $S$ is the linear smoother matrix.
Model evaluation

For any linear interpolator:

$$SY = Y \implies S = I_n \implies \frac{y_i - [SY]_i}{1 - S_{ii}} = \frac{0}{0}$$

in particular for the min-norm interpolator: $$S = XX^T(XX^T)^{-1} = I_n$$
Model evaluation

For any linear interpolator:

\[ SY = Y \implies S = I_n \implies \frac{y_i - [SY]_i}{1 - S_{ii}} = 0 \]

in particular for the min-norm interpolator: \( S = XX^T(XX^T)^{-1} = I_n \)

Fortunately, we can solve this problem! Rewrite \( S \) to be:

\[ S = XX^T(XX^T + \lambda I_n)^{-1}, \quad \lambda \to 0^+ \]
Now we can apply L’Hopital’s rule by with derivative at $\lambda = 0$

$$\frac{(y_i - [SY]_i)'}{(1 - S_{ii})'} = \frac{[XX^T(XX^T + \lambda I_n)^{-2} Y]_i}{[XX^T(XX^T + \lambda I_n)^{-2}]_{ii}} \bigg|_{\lambda=0} = \frac{[(XX^T)^{-1} Y]_i}{[(XX^T)^{-1}]_{ii}}$$
Model evaluation

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\[
\frac{(y_i - [SY]_i)'}{(1 - S_{ii})'} = \frac{[XX^T(XX^T + \lambda I_n)^{-2}Y]_i}{[XX^T(XX^T + \lambda I_n)^{-2}]_{ii}} \bigg|_{\lambda=0} = \frac{[(XX^T)^{-1}Y]_i}{[(XX^T)^{-1}]_{ii}}
\]

Finally, the CV estimator can be calculated with the following formula:

\[
CV_n = \frac{1}{n} \sum_{i=1}^{n} \left( \frac{[(XX^T)^{-1}Y]_i}{[(XX^T)^{-1}]_{ii}} \right)^2
\]
Ridge regression

The min-norm estimator is related to the Ridge regression estimator as follows:

\[ \hat{\beta} = \lim_{\lambda \to 0^+} \hat{\beta}_\lambda \]

where \( \hat{\beta}_\lambda \) is the Ridge regression estimator:

\[ \hat{\beta}_\lambda = \arg\min_{\beta \in \mathbb{R}^p} \left\{ \frac{1}{n} \left\| Y - X\beta \right\|^2_2 + \lambda \left\| \beta \right\|^2_2 \right\} = \left( X^T X + n\lambda I_p \right)^{-1} X^T Y \]

Thus, an optimal tune \( \hat{\beta}_\lambda \) should be better than \( \hat{\beta} \)
Ridge regression

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Thus, an optimal tune $\hat{\beta}_\lambda$ should be better than $\hat{\beta}$

The limiting risk for the optimal $\hat{\beta}_\lambda$ can be written explicitly as:

$$\sigma^2 - \frac{1 - (1 + \sigma^2/r^2)\gamma + \sqrt{(1 - (1 + \sigma^2/r^2)\gamma)^2 - 4\sigma^2\gamma^2/r^2}}{2\gamma}$$
Ridge regression

In overview looking we can simplify the optimal risk into:

\[ R(\hat{\beta}_{\lambda^*}; \beta, \theta) \approx ||\theta||_2^2 + f(\sigma^2; \gamma) + g(||\beta||_2^2; \gamma) \]

where \( f(z; \gamma) \to 0, g(z; \gamma) \to z \) as \( \gamma \to \infty \)

and \( g(z; 0) = f(z; 0) = 0 \)
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Looks like trade-off between observed and unobserved signals
Ridge regression

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and $g(z; 0) = f(z; 0) = 0$

Looks like trade-off between observed and unobserved signals

Again, the distribution of the signal over $\gamma$ may play a role...
Ridge regression - optimal risk curves

Min-norm versus ridge, well-specified

Min-norm versus ridge, misspecified
Optimal risk curves - misspecified model

\[ R(\hat{\beta}_\lambda^*; \beta, \theta) \approx ||\theta||^2 + f(\sigma^2; \gamma) + g(||\beta||^2; \gamma) \]

Optimal risk curves with
\[ ||\theta||^2 = (1 + \gamma)^{-a}, \quad a = 2 \]

Why is the minimum risk around \( \gamma = 1 \)?

"... it seems we want the complexity of the feature space to put us as close to the interpolation boundary as possible..."
Theoretical analysis for Least-Squares

Optimal risk curves - misspecified model

\[ R(\hat{\beta}_\lambda^*; \beta, \theta) \approx \|\theta\|_2^2 + f(\sigma^2; \gamma) + g(\|\beta\|_2^2; \gamma) \]

Optimal risk curves with:

- \( \sigma^2 = 1, r^2 = 5 \)
- \( \|\theta\|_2^2 = (1 + \gamma)^{-a} \), \( a \in \{1, 2, 4\} \)

Curves get steeper as \( r^2 \) grows

What conclusions can we draw regarding Neural Networks?

Oren Yuval

Learning curve in modern ML, The "double descent" behavior
Additional results - nonlinear features

Asymptotic variance in a nonlinear feature model, $x = \varphi(Wz)$
Additional results - correlated features

Asymptotic variance and bias for auto-regressive structure, $\Sigma_{ij} = \rho|i-j|$

Reminder:

$$B(\hat{\beta}; \beta) = \beta^T(I_p - \mathbb{E}_X[X^T(XX^T)^{-1}X])\beta$$
Additional results - correlated features

Asymptotic risk for auto-regressive structure, $\Sigma_{ij} = \rho^{|i-j|}$
CV-tuned Ridge regression

Finite-sample risks for CV-tuned ridge regression estimator compared to Asymptotic risk (20 independent training samples)
Summary

There is a growing interest in Interpolators in ML. The double descent phenomenon must be well understood and taken into account for model optimization. The linear model analysis explains the bias-variance trade-off in the interpolation regime. The real-life trade-off: balance between signal, bias-variance, controlled by complexity-regularization/early stopping.
Summary

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The real-life trade-off:
- Balance between signal\textsubscript{obs}-bias-variance
- Controlled by complexity-regularization/early stopping
Thank you for listening😊