Excess Risk Decomposition

David S. Rosenberg

New York University

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Excess Risk Decomposition
Error Decomposition

\[ f^* = \arg \min \mathbb{E} \ell(f(X), Y) \]
\[ f_{\mathcal{F}} = \arg \min_{f \in \mathcal{F}} \mathbb{E} \ell(f(X), Y) \]
\[ \hat{f}_n = \arg \min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) \]

- **Approximation Error** (of \( \mathcal{F} \)) = \( R(f_{\mathcal{F}}) - R(f^*) \)
- **Estimation error** (of \( \hat{f}_n \) in \( \mathcal{F} \)) = \( R(\hat{f}_n) - R(f_{\mathcal{F}}) \)
Excess Risk

Definition

The **excess risk** compares the risk of $f$ to the Bayes optimal $f^*$:

$$\text{Excess Risk}(f) = R(f) - R(f^*)$$

- Can excess risk ever be negative?
The excess risk of the ERM $\hat{f}_n$ can be decomposed:

$$\text{Excess Risk}(\hat{f}_n) = R(\hat{f}_n) - R(f^*)$$

$$= R(\hat{f}_n) - R(f_F) + R(f_F) - R(f^*)$$

- estimation error
- approximation error
Approximation error $R(f) - R(f^*)$ is

- a property of the class $\mathcal{F}$
- the penalty for restricting to $\mathcal{F}$ (rather than considering all possible functions)

_Bigger $\mathcal{F}$ mean smaller approximation error._

Concept check: Is approximation error a random or non-random variable?
Estimation Error

Estimation error $R(\hat{f}_n) - R(f_F)$

- is the performance hit for choosing $f$ using finite training data
- is the performance hit for minimizing empirical risk rather than true risk

With smaller $\mathcal{F}$ we expect smaller estimation error.

*Under typical conditions:* “With infinite training data, estimation error goes to zero.”

Concept check: Is estimation error a random or non-random variable?
ERM Overview

- Given a loss function $\ell: \mathcal{A} \times \mathcal{Y} \to \mathbb{R}$.
- Choose hypothesis space $\mathcal{F}$.
- Use an optimization method to find ERM $\hat{f}_n \in \mathcal{F}$:

  $$\hat{f}_n = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i).$$

- Data scientist’s job:
  - choose $\mathcal{F}$ to balance between approximation and estimation error.
  - as we get more training data, use a bigger $\mathcal{F}$
ERM in Practice

- We’ve been cheating a bit by writing “argmin”.
- In practice, we need a method to find $\hat{f}_n \in \mathcal{F}$.
- For nice choices of loss functions and classes $\mathcal{F}$, we can get arbitrarily close to a minimizer
  - But takes time – is it worth it?
- For some hypothesis spaces (e.g. neural networks), we don’t know how to find $\hat{f}_n \in \mathcal{F}$. 
Optimization Error

- In practice, we don’t find the ERM $\hat{f}_n \in \mathcal{F}$.
- We find $\tilde{f}_n \in \mathcal{F}$ that we hope is good enough.
- **Optimization error**: If $\tilde{f}_n$ is the function our optimization method returns, and $\hat{f}_n$ is the empirical risk minimizer, then
  \[
  \text{Optimization Error} = R(\tilde{f}_n) - R(\hat{f}_n).
  \]
- Can optimization error be negative? Yes!
- But
  \[
  \hat{R}(\tilde{f}_n) - \hat{R}(\hat{f}(n)) \geq 0.
  \]
Error Decomposition in Practice

- Excess risk decomposition for function $\tilde{f}_n$ returned by algorithm:

$$\text{Excess Risk}(\tilde{f}_n) = R(\tilde{f}_n) - R(f^*)$$

$$= R(\tilde{f}_n) - R(\hat{f}_n) + R(\hat{f}_n) - R(f_{\mathcal{F}}) + R(f_{\mathcal{F}}) - R(f^*)$$

- Optimization error
- Estimation error
- Approximation error

- Concept check: It would be nice to have a concrete example where we find an $\tilde{f}_n$ and look at it’s error decomposition. Why is this usually impossible?

- But we could construct an artificial example, where we know $P_{X \times Y}$ and $f^*$ and $f_{\mathcal{F}}$...
Excess Risk Decomposition: Example
A Simple Classification Problem

\[ y = \{\text{blue, orange}\} \]

\[ P_X = \text{Uniform}([0, 1]^2) \]

\[ P(\text{orange} \mid x_1 > x_2) = 0.9 \]

\[ P(\text{orange} \mid x_1 < x_2) = 0.1 \]

Bayes Error Rate = 0.1
Consider a binary tree on \( \{(X_1, X_2) \mid X_1, X_2 \in \mathbb{R}\} \)
Hypothesis Space: Decision Tree

- $\mathcal{F} = \left\{ \text{all decision tree classifiers on } [0, 1]^2 \right\}$

- $\mathcal{F}_d = \left\{ \text{all decision tree classifiers on } [0, 1]^2 \text{ with DEPTH } \leq d \right\}$

- We’ll consider $\mathcal{F}_1 \subset \mathcal{F}_2 \subset \mathcal{F}_3 \subset \mathcal{F}_4 \cdots \subset \mathcal{F}_{15}$

- Bayes error rate = 0.1
Theoretical Best in $\mathcal{F}_1$

- Risk Minimizer in $\mathcal{F}_1$ has Risk $= \mathbb{P}(\text{error}) = 0.3$.
- Approximation Error $= 0.3 - 0.1 = 0.2$. 

David S. Rosenberg (New York University)
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Theoretical Best in $\mathcal{F}_2$

- Risk Minimizer in $\mathcal{F}_2$ has Risk $= \mathbb{P}(\text{error}) = 0.2$.
- Approximation Error $= 0.2 - 0.1 = 0.1$
Theoretical Best in $\mathcal{F}_3$

- Risk Minimizer in $\mathcal{F}_3$ has Risk $= \mathbb{P}(\text{error}) = 0.15$.
- Approximation Error $= 0.15 - 0.1 = 0.05$
Theoretical Best in $\mathcal{F}_4$

- Risk Minimizer in $\mathcal{F}_4$ has Risk $= \mathbb{P}(\text{error}) = 0.125$.
- Approximation Error $= 0.125 - 0.1 = 0.025$
Decision Tree in $\mathcal{F}_3$ Estimated From Sample ($n = 1024$)

$$R(\tilde{f}) = \mathbb{P}(\text{error}) = 0.176 \pm .004$$

$$\text{Estimation Error + Optimization Error} = 0.176 \pm 0.004 - 0.150 = 0.026 \pm 0.004$$
Decision Tree in $\mathcal{F}_4$ Estimated From Sample ($n = 1024$)

\[ R(\tilde{f}) = P(\text{error}) = 0.144 \pm 0.005 \]

Estimation Error + Optimization Error = \[ \underbrace{0.144 \pm 0.005}_{R(\tilde{f})} - \underbrace{0.125}_{\min_{f \in \mathcal{F}_4} R(f)} = 0.019 \pm 0.005 \]
Decision Tree in $\mathcal{F}_6$ Estimated From Sample ($n = 1024$)

$$R(\tilde{f}) = \mathbb{P}(\text{error}) = 0.148 \pm 0.007$$

Estimation Error + Optimization Error

$$\underbrace{R(\tilde{f})}_{\text{Estimation Error}} + \underbrace{\min_{f \in \mathcal{F}_6} R(f)}_{\text{Optimization Error}} = 0.148 \pm 0.007 - 0.106 = 0.042 \pm 0.007$$
Decision Tree in $\mathcal{F}_8$ Estimated From Sample ($n = 1024$)

$$R(\tilde{f}) = \mathbb{P}(\text{error}) = 0.162 \pm 0.009$$

Estimation Error + Optimization Error = \underbrace{0.162 \pm 0.009}_{R(\tilde{f})} - \underbrace{0.102}_{\min_{f \in \mathcal{F}_8} R(f)} = 0.061 \pm 0.009
Decision Tree in $\mathcal{F}_8$ Estimated From Sample ($n = 2048$)

\[
R(\tilde{f}) = \mathbb{P}(\text{error}) = 0.146 \pm 0.006
\]

\[
\text{Estimation Error} + \text{Optimization Error} = 0.146 \pm 0.006 - 0.102 = 0.045 \pm 0.006
\]
Decision Tree in $\mathcal{F}_8$ Estimated From Sample ($n = 8192$)

$$R(\tilde{f}) = \mathbb{P}(\text{error}) = 0.121 \pm 0.002$$

Estimation Error + Optimization Error = \underbrace{0.121 \pm 0.002 - 0.102}_{R(\tilde{f})} = 0.019 \pm 0.002$$
Why do some curves have confidence bands and others not?
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