Excess Risk Decomposition

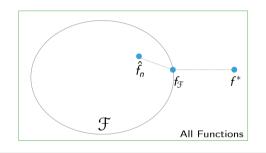
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Excess Risk Decomposition

Error Decomposition



$$f^* = \underset{f}{\arg\min} \mathbb{E}\ell(f(X), Y)$$

$$f_{\mathcal{F}} = \underset{f \in \mathcal{F}}{\arg\min} \mathbb{E}\ell(f(X), Y))$$

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

- Approximation Error (of \mathfrak{F}) = $R(f_{\mathfrak{F}}) R(f^*)$
- 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^* :

Excess
$$Risk(f) = R(f) - R(f^*)$$

• Can excess risk ever be negative?

Excess Risk Decomposition for ERM

• The excess risk of the ERM \hat{f}_n can be decomposed:

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

$$= \underbrace{R(\hat{f}_n) - R(f_{\mathcal{F}})}_{\text{estimation error}} + \underbrace{R(f_{\mathcal{F}}) - R(f^*)}_{\text{approximation error}}.$$

Approximation Error

Approximation error $R(f_{\mathcal{F}}) - R(f^*)$ is

- ullet a property of the class ${\mathcal F}$
- \bullet 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 $R(\hat{f}_n) - R(f_{\mathcal{F}})$

- 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 $\ell: \mathcal{A} \times \mathcal{Y} \to \mathbf{R}$.
- 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:
 - \bullet choose \mathcal{F} to balance between approximation and estimation error.
 - ullet 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 $\hat{f}_n \in \mathcal{F}$.
- ullet 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

Optimization Error =
$$R(\tilde{f}_n) - R(\hat{f}_n)$$
.

- Can optimization error be negative? Yes!
- But

$$\hat{R}(\tilde{f}_n) - \hat{R}(\hat{f}(n)) \geqslant 0.$$

Error Decomposition in Practice

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

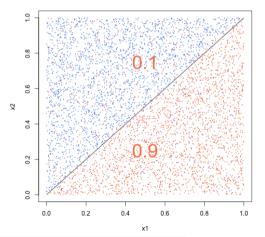
Excess Risk
$$(\tilde{f}_n) = R(\tilde{f}_n) - R(f^*)$$

$$= \underbrace{R(\tilde{f}_n) - R(\hat{f}_n)}_{\text{optimization error}} + \underbrace{R(\hat{f}_n) - R(f_{\mathcal{F}})}_{\text{estimation error}} + \underbrace{R(f_{\mathcal{F}}) - R(f^*)}_{\text{approximation error}}$$

- 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 constuct an artificial example, where we know $P_{\mathfrak{X} \times \mathfrak{Y}}$ and f^* and $f_{\mathfrak{F}}$...

Excess Risk Decomposition: Example

A Simple Classification Problem



$$\mathcal{Y} = \{\text{blue}, \text{orange}\}\$$

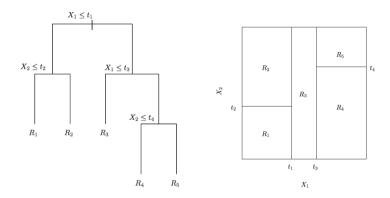
 $P_{\mathcal{X}} = \text{Uniform}([0, 1]^2)$

$$\begin{array}{lcl} \mathbb{P}(\mathsf{orange} \mid x_1 > x_2) & = & .9 \\ \mathbb{P}(\mathsf{orange} \mid x_1 < x_2) & = & .1 \end{array}$$

Bayes Error Rate = 0.1

Binary Decision Trees on \mathbb{R}^2

• Consider a binary tree on $\{(X_1, X_2) \mid X_1, X_2 \in \mathbb{R}\}$



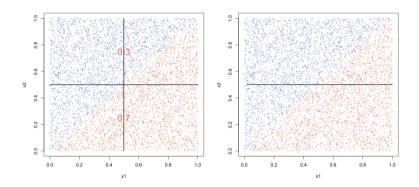
From An Introduction to Statistical Learning, with applications in R (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

Hypothesis Space: Decision Tree

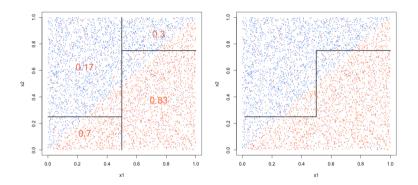
- $\mathcal{F} = \left\{ \text{all decision tree classifiers on } [0, 1]^2 \right\}$
- $\mathcal{F}_d = \left\{ \text{all decision tree classifiers on } [0,1]^2 \text{ with DEPTH} \leqslant d \right\}$
- We'll consider

$$\mathcal{F}_1 \subset \mathcal{F}_2 \subset \mathcal{F}_3 \subset \mathcal{F}_4 \cdots \subset \mathcal{F}_{15}$$

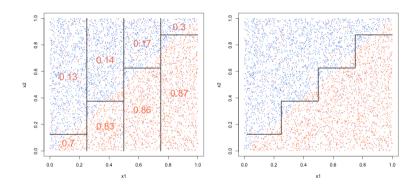
• Bayes error rate = 0.1



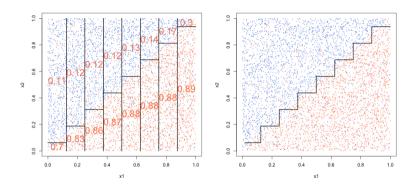
- Risk Minimizer in \mathcal{F}_1 has Risk = $\mathbb{P}(\text{error}) = 0.3$.
- Approximation Error = 0.3 0.1 = 0.2.



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

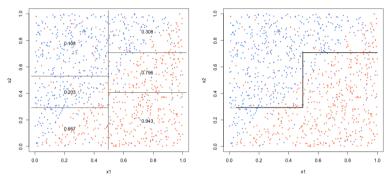


- Risk Minimizer in \mathcal{F}_3 has Risk = $\mathbb{P}(\text{error}) = 0.15$.
- Approximation Error = 0.15 0.1 = 0.05



- Risk Minimizer in \mathcal{F}_4 has Risk = $\mathbb{P}(\text{error}) = 0.125$.
- Approximation Error = 0.125 0.1 = 0.025

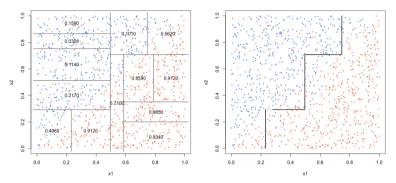
Decision Tree in \mathcal{F}_3 Estimated From Sample (n = 1024)



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

Estimation Error+Optimization Error =
$$\underbrace{0.176 \pm .004}_{R(\tilde{f})}$$
 - $\underbrace{0.150}_{\min_{f \in \mathcal{F}_3} R(f)}$ = .026 ± .004

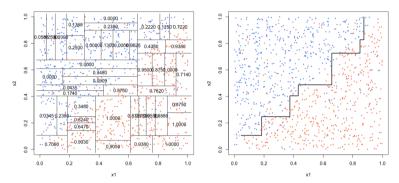
Decision Tree in \mathcal{F}_4 Estimated From Sample (n = 1024)



$$R(\tilde{f}) = \mathbb{P}(\text{error}) = 0.144 \pm .005$$

Estimation Error+Optimization Error =
$$\underbrace{0.144 \pm .005}_{R(\tilde{f})}$$
 - $\underbrace{0.125}_{\min_{f \in \mathcal{F}_4} R(f)}$ = .019 ± .005

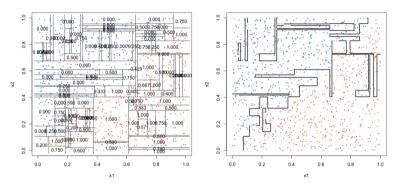
Decision Tree in \mathcal{F}_6 Estimated From Sample (n = 1024)



$$R(\tilde{f}) = \mathbb{P}(\mathsf{error}) = 0.148 \pm .007$$

Estimation Error+Optimization Error =
$$\underbrace{0.148 \pm .007}_{R(\tilde{f})}$$
 - $\underbrace{0.106}_{\min_{f \in \mathcal{F}_6} R(f)}$ = .042 ± .007

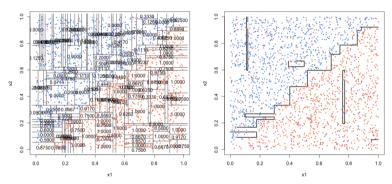
Decision Tree in \mathcal{F}_8 Estimated From Sample (n = 1024)



$$R(\tilde{f}) = \mathbb{P}(\mathsf{error}) = 0.162 \pm .009$$

Estimation Error+Optimization Error =
$$\underbrace{0.162 \pm .009}_{R(\tilde{f})}$$
 - $\underbrace{0.102}_{\min_{f \in \mathcal{F}_{\mathbf{B}}} R(f)}$ = .061 ± .009

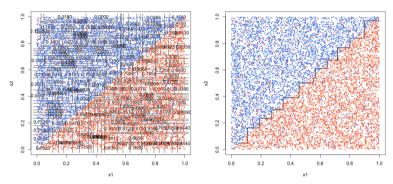
Decision Tree in \mathcal{F}_8 Estimated From Sample (n = 2048)



$$R(\tilde{f}) = \mathbb{P}(\mathsf{error}) = 0.146 \pm .006$$

Estimation Error+Optimization Error =
$$\underbrace{0.146 \pm .006}_{R(\tilde{f})}$$
 - $\underbrace{0.102}_{\min_{f \in \mathcal{F}_3} R(f)}$ = .045 ± .006

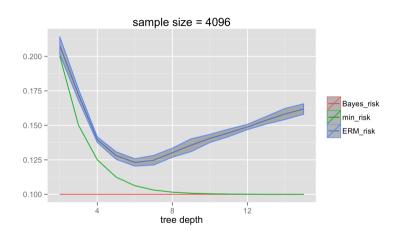
Decision Tree in \mathcal{F}_8 Estimated From Sample (n = 8192)



$$R(\tilde{f}) = \mathbb{P}(\text{error}) = 0.121 \pm .002$$

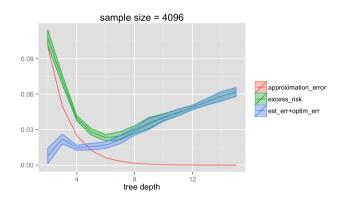
Estimation Error+Optimization Error =
$$\underbrace{0.121 \pm .002}_{R(\tilde{f})}$$
 - $\underbrace{0.102}_{\min_{f \in \mathcal{F}_3} R(f)}$ = .019 ± .002

Risk Summary



Why do some curves have confidence bands and others not?

Excess Risk Decomposition



Why do some curves have confidence bands and others not?