Excess Risk Decomposition

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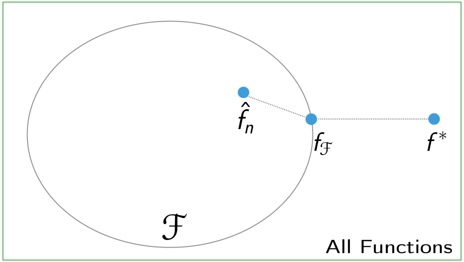
Error Decomposition



$$f^* = \arg\min_f \mathbb{E}\ell(f(x), y)$$

$$f_{\mathcal{F}} = \arg\min_{f \in \mathcal{F}} \mathbb{E}\ell(f(x), y))$$

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

- **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^*:

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

- Can excess risk ever be negative?

Excess Risk Decomposition for ERM

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

$$
\begin{aligned}
\textbf{Excess Risk}(\hat{f}_n) &= R(\hat{f}_n) - R(f^*) \\
&= \underbrace{R(\hat{f}_n) - R(f_{\mathcal{F}})}_{\text{estimation error}} + \underbrace{R(f_{\mathcal{F}}) - R(f^*)}_{\text{approximation error}}.
\end{aligned}
$$

Approximation Error

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

- 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 $\hat{f}_n \in \mathcal{F}$:

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

- 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

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

Error Decomposition in Practice

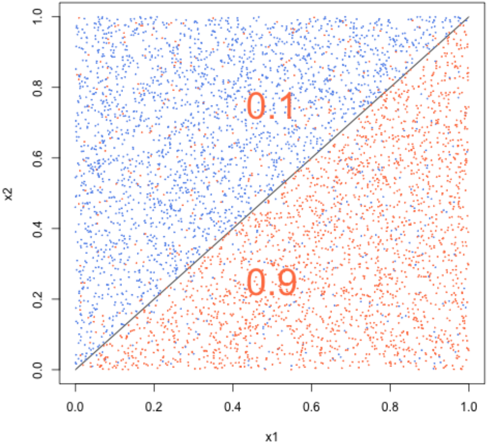
- Excess risk decomposition for function $\tilde{f}_n$ returned by algorithm:

$$\begin{aligned}\textbf{Excess Risk}(\tilde{f}_n) &= R(\tilde{f}_n) - R(f^*)\\ &= \underbrace{R(\tilde{f}_n) - R(\hat{f}_n)}_{\text{optimization error}} + \underbrace{R(\hat{f}_n) - R(f_{\mathcal{F}})}_{\text{estimation error}} + \underbrace{R(f_{\mathcal{F}}) - R(f^*)}_{\text{approximation error}}\end{aligned}$$

- 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 $P_{\mathcal{X}\times\mathcal{Y}}$ and f^* and $f_{\mathcal{F}}$...

Excess Risk Decomposition: Example

A Simple Classification Problem



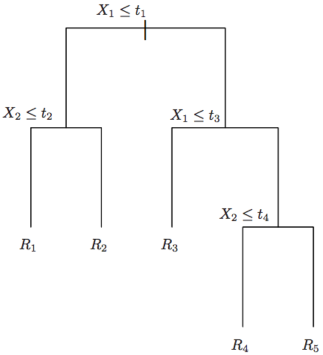
$$\begin{aligned}\mathcal{Y} &= \{\text{blue}, \text{orange}\} \\ P_{\mathcal{X}} &= \text{Uniform}([0,1]^2)\end{aligned}$$

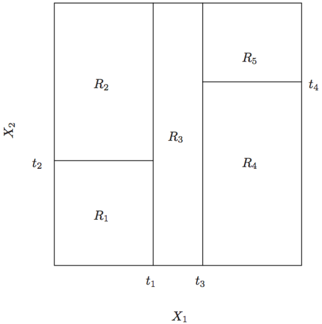
$$\begin{aligned}\mathbb{P}(\text{orange} \mid x_1 > x_2) &= .9 \\ \mathbb{P}(\text{orange} \mid x_1 < x_2) &= .1\end{aligned}$$

$$\text{Bayes Error Rate} = 0.1$$

Binary Decision Trees on $\mathbf{R}^2$

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

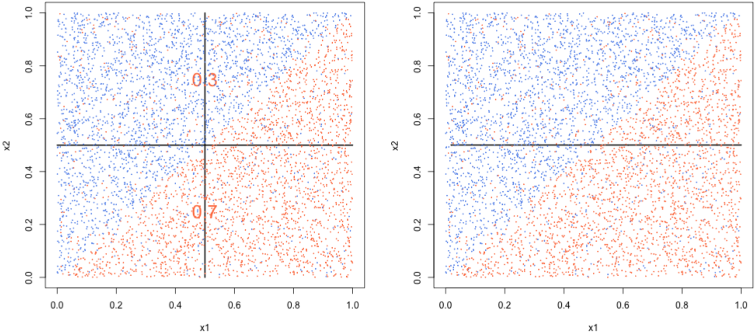




From *An Introduction to Statistical Learning, with applications in R* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

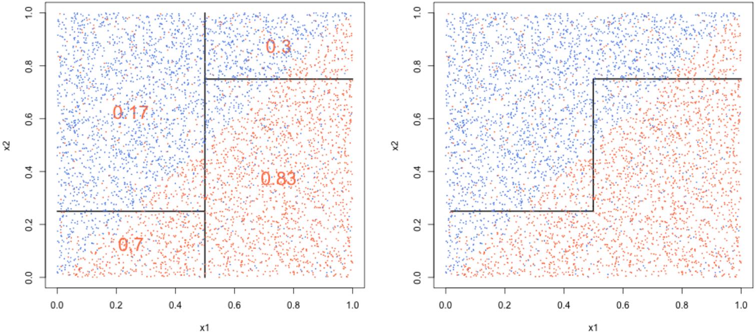
Hypothesis Space: Decision Tree

- $\mathcal{F} = \left\{ \text{all decision tree classifiers on } [0,1]^2 \right\}$
- $\mathcal{F}_d = \left\{ \text{all decision tree classifiers on } [0,1]^2 \text{ with DEPTH} \leqslant d \right\}$
- 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 $= 0.1$



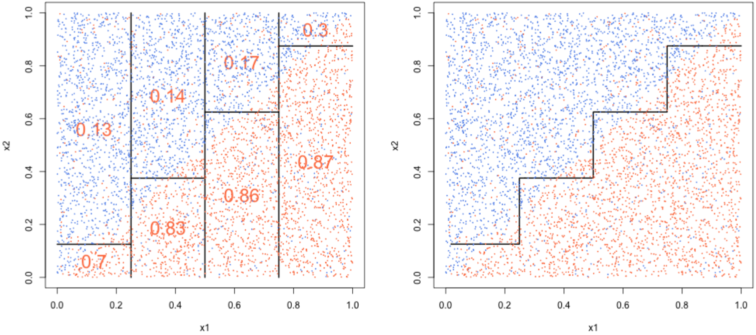
- Risk Minimizer in $\mathcal{F}_1$ has Risk $= \mathbb{P}(\text{error}) = 0.3$.
- Approximation Error $= 0.3 - 0.1 = 0.2$.

Theoretical Best in $\mathcal{F}_2$



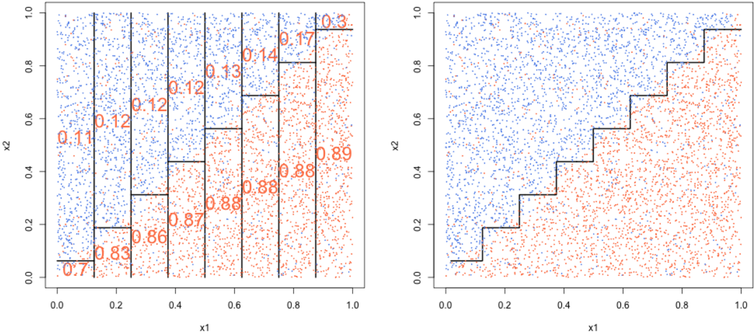
- Risk Minimizer in $\mathcal{F}_2$ has Risk $= \mathbb{P}(\text{error}) = 0.2$.
- Approximation Error = 0.2 - 0.1 = 0.1

Theoretical Best in $\mathcal{F}_3$



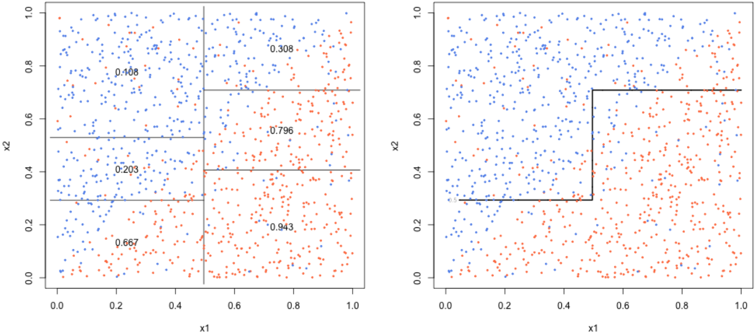
- Risk Minimizer in $\mathcal{F}_3$ has Risk $= \mathbb{P}(\text{error}) = 0.15$.
- Approximation Error = 0.15 - 0.1 = 0.05

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

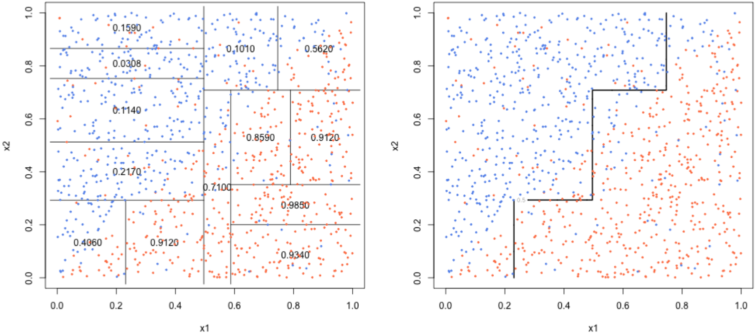
Decision Tree in $\mathcal{F}_3$ Estimated From Sample ($n = 1024$)



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

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

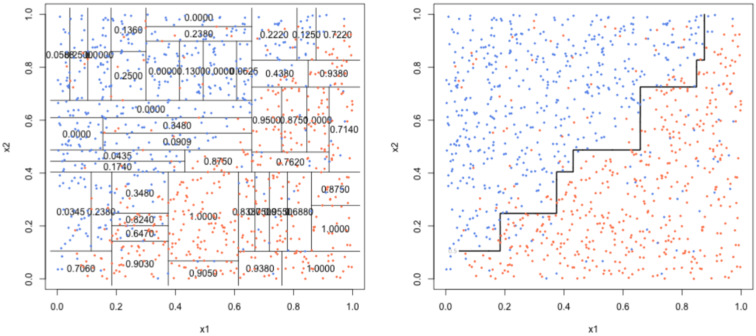
Decision Tree in $\mathcal{F}_4$ Estimated From Sample ($n = 1024$)



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

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

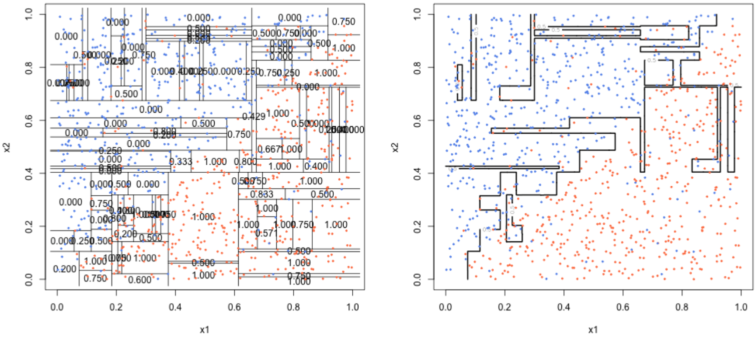
Decision Tree in $\mathcal{F}_6$ Estimated From Sample ($n = 1024$)



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

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

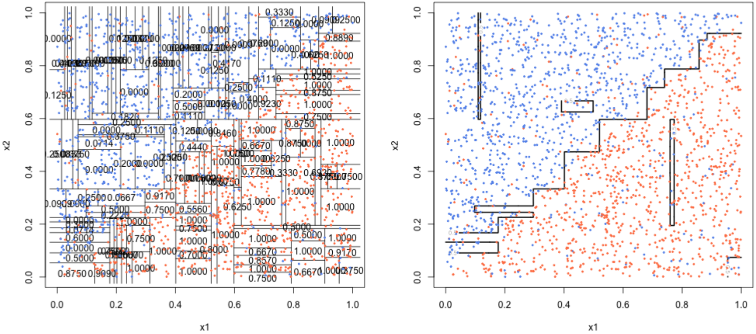
Decision Tree in $\mathcal{F}_8$ Estimated From Sample ($n = 1024$)



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

$$\text{Estimation Error+Optimization Error} = \underbrace{0.162 \pm .009}_{R(\tilde{f})} - \underbrace{0.102}_{\min_{f \in \mathcal{F}_8} R(f)} = .061 \pm .009$$

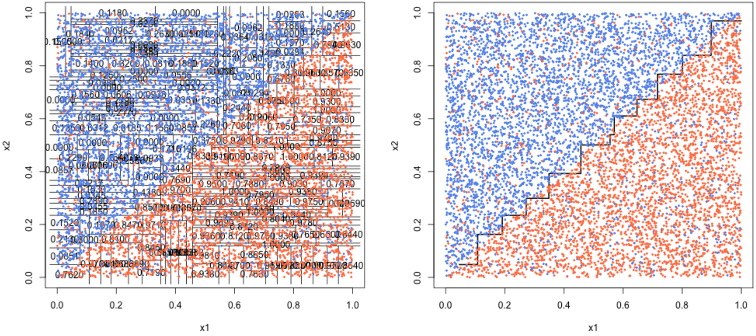
Decision Tree in $\mathcal{F}_8$ Estimated From Sample ($n = 2048$)



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

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

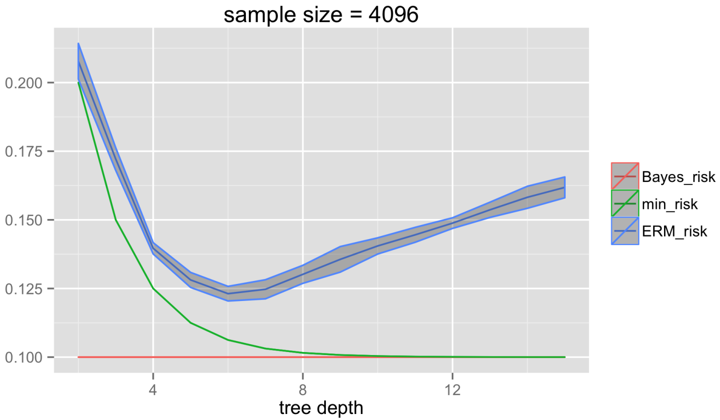
Decision Tree in $\mathcal{F}_8$ Estimated From Sample ($n = 8192$)



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

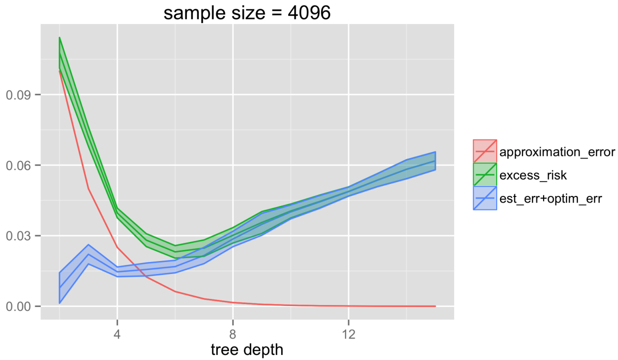
$$\text{Estimation Error} + \text{Optimization Error} = \underbrace{0.121 \pm .002}_{R(\tilde{f})} - \underbrace{0.102}_{\min_{f \in \mathcal{F}_3} R(f)} = .019 \pm .002$$

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?