

# Excess Risk Decomposition

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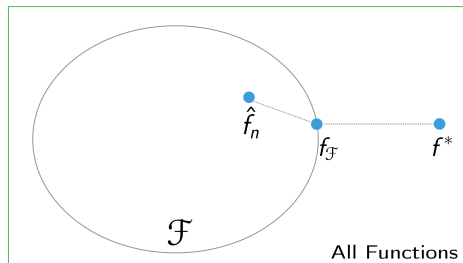
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## Excess Risk Decomposition

# 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  $\mathcal{F}$ ) =  $R(\hat{f}_n) - R(f_{\mathcal{F}})$

## 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?

# Excess Risk Decomposition for ERM

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

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

# 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  $R(\hat{f}_n) - R(f_{\mathcal{F}})$

- 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?

- Given a loss function  $\ell : \mathcal{A} \times \mathcal{Y} \rightarrow \mathbf{R}$ .
- 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:
  - choose  $\mathcal{F}$  to balance between approximation and estimation error.
  - as we get more training data, use a bigger  $\mathcal{F}$



- 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

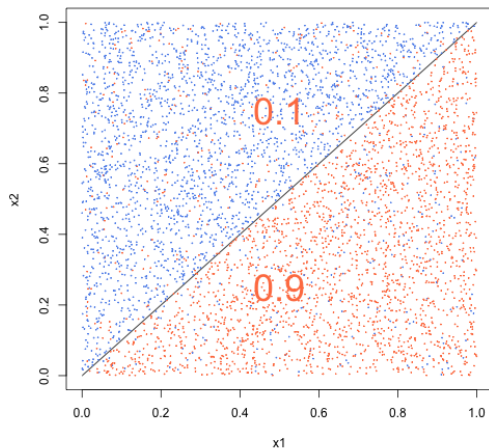
- Excess risk decomposition for function  $\tilde{f}_n$  returned by algorithm:

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

- Concept check: It would be nice to have a concrete example where we find an  $\tilde{f}_n$  and look at its error decomposition. Why is this usually impossible?
- But we could construct an artificial example, where we know  $P_{\mathcal{X} \times \mathcal{Y}}$  and  $f^*$  and  $f_{\mathcal{F}} \dots$

## Excess Risk Decomposition: Example

# A Simple Classification Problem



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

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

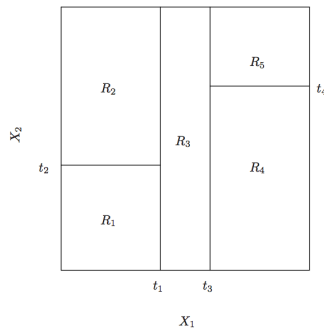
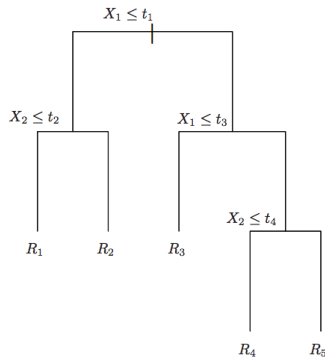
$$\mathbb{P}(\text{orange} \mid x_1 > x_2) = .9$$

$$\mathbb{P}(\text{orange} \mid x_1 < x_2) = .1$$

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

# 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

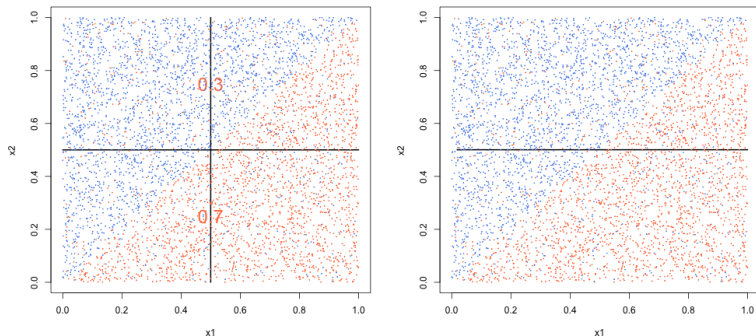
- $\mathcal{F} = \left\{ \text{all decision tree classifiers on } [0, 1]^2 \right\}$
- $\mathcal{F}_d = \left\{ \text{all decision tree classifiers on } [0, 1]^2 \text{ with DEPTH} \leq d \right\}$

- 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

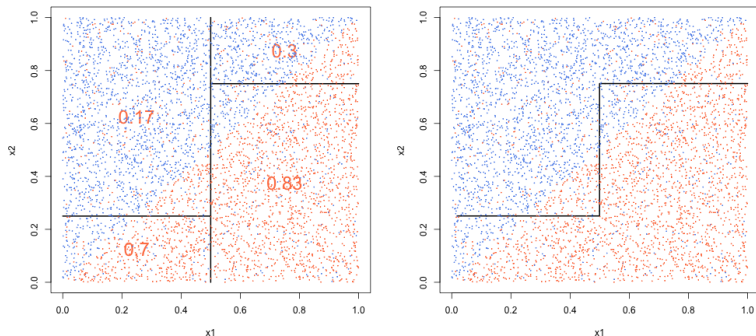
# Theoretical Best in $\mathcal{F}_1$



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

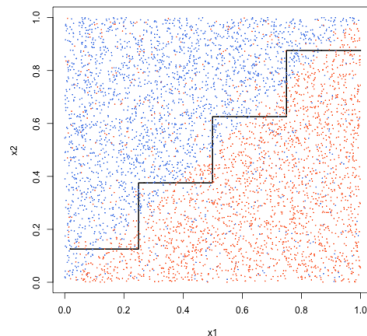
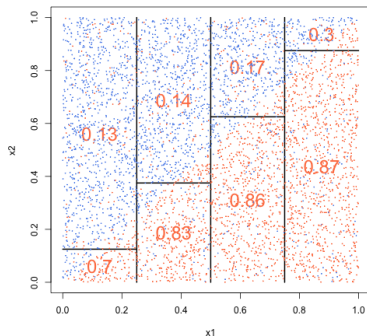


## Theoretical Best in $\mathcal{F}_2$



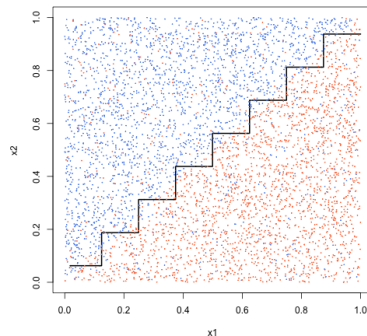
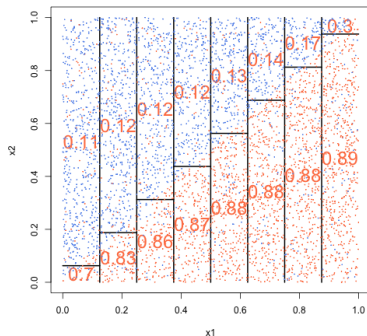
- Risk Minimizer in  $\mathcal{F}_2$  has Risk =  $\mathbb{P}(\text{error}) = 0.2$ .
- Approximation Error =  $0.2 - 0.1 = 0.1$

# Theoretical Best in $\mathcal{F}_3$



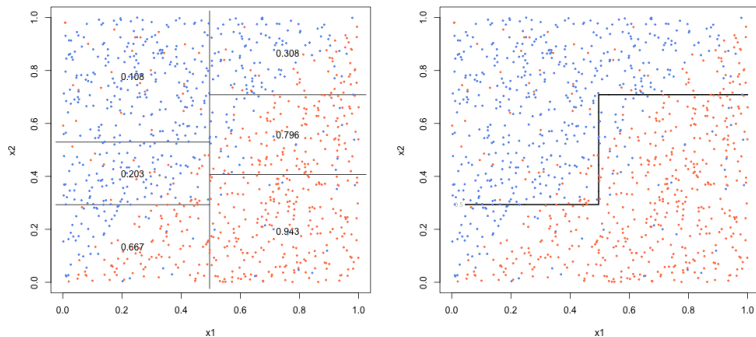
- Risk Minimizer in  $\mathcal{F}_3$  has Risk =  $\mathbb{P}(\text{error}) = 0.15$ .
- Approximation Error =  $0.15 - 0.1 = 0.05$

# Theoretical Best in $\mathcal{F}_4$



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

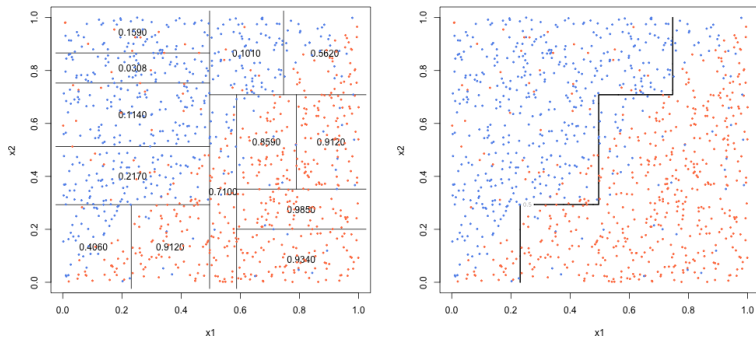
## Decision Tree in $\mathcal{F}_3$ Estimated From Sample ( $n = 1024$ )



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

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

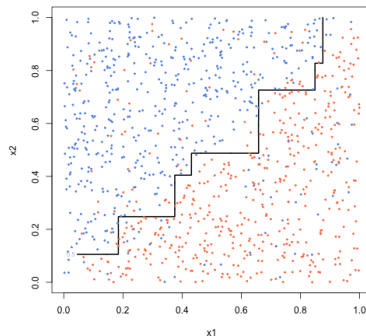
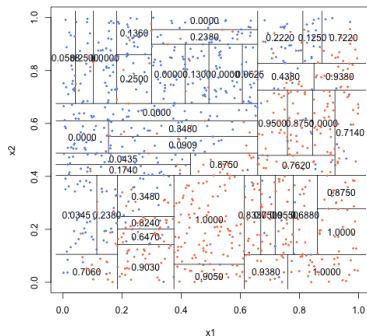
# Decision Tree in $\mathcal{F}_4$ Estimated From Sample ( $n = 1024$ )



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

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

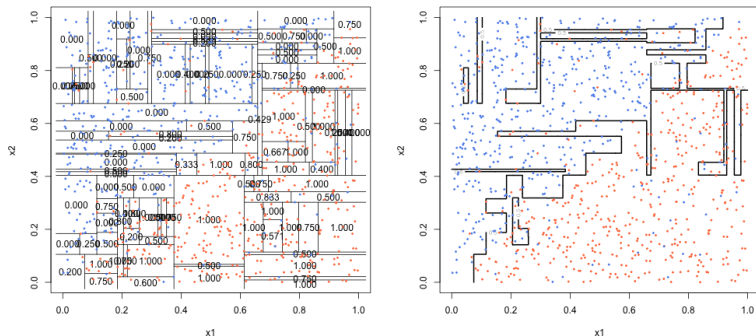
# Decision Tree in $\mathcal{F}_6$ Estimated From Sample ( $n = 1024$ )



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

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

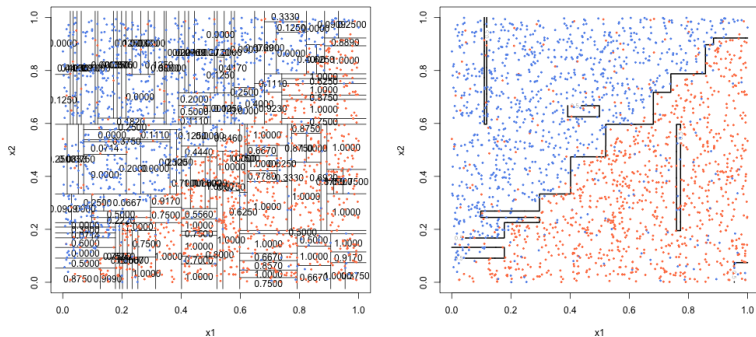
# Decision Tree in $\mathcal{F}_8$ Estimated From Sample ( $n = 1024$ )



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

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

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

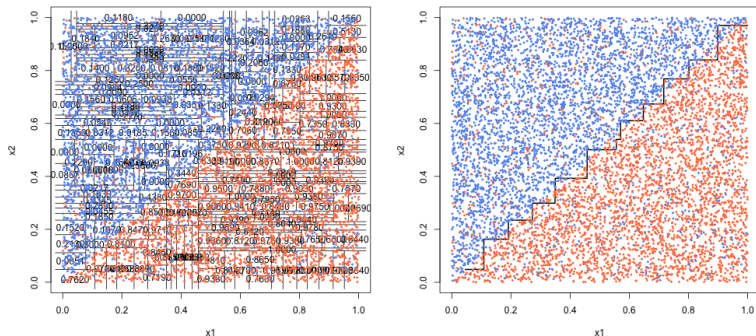


$$R(\tilde{f}) = \mathbb{P}(\text{error}) = 0.146 \pm .006$$

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



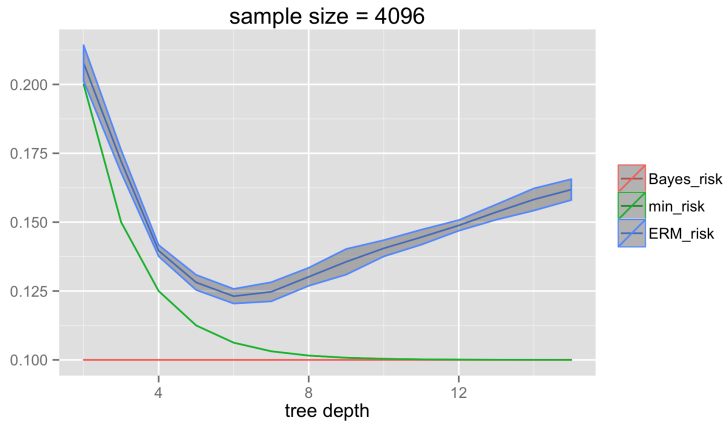
# Decision Tree in $\mathcal{F}_8$ Estimated From Sample ( $n = 8192$ )



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

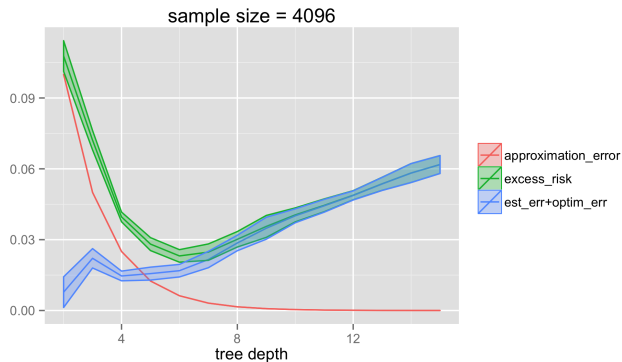
$$\text{Estimation Error} + \text{Optimization Error} = \underbrace{0.121 \pm .002}_{R(\tilde{f})} - \underbrace{0.102}_{\min_{f \in \mathcal{F}_3} R(f)} = .019 \pm .002$$

# 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?