Excess Risk Decomposition

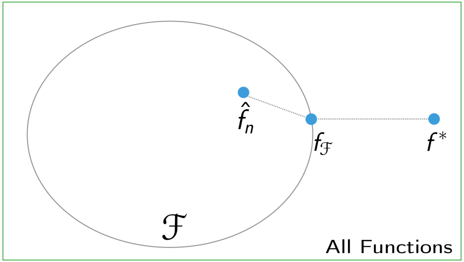
Julia Kempe & David S. Rosenberg

NYU CDS

January 29, 2019

Excess Risk Decomposition

Error Decomposition

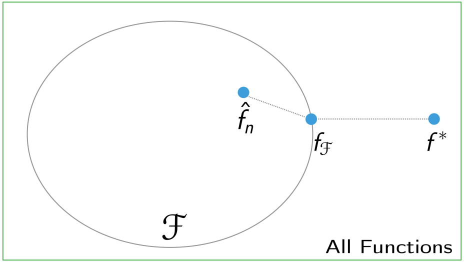


$$f^* = \arg\min_f \mathbb{E}\ell(f(x), y)$$

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

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

Error Decomposition



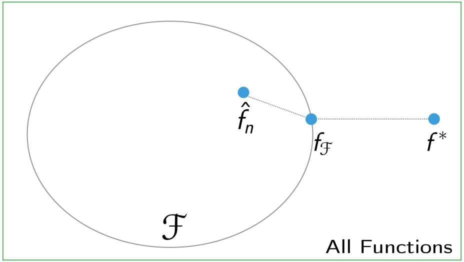
$$f^* = \underset{f}{\arg\min}\, \mathbb{E}\ell(f(x), y)$$

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

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

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

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^*:

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

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:

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

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 $\mathcal{F}$

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)

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.

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

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

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.

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."

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".

ERM in Practice

- We've been cheating a bit by writing "argmin".
- In practice, we need a method to find $\hat{f}_n \in \mathcal{F}$.

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?

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

- 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

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

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?

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:

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

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?

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 $f_{\mathcal{F}}$...