ORIE 4741: Learning with Big Messy Data

Generalization

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October 9, 2020
Announcements

- section this week: trees, boosting, bagging
- hw2 due this morning 9:30am; hw3 out today
  - save slip days for emergencies
- quiz 5 today (Thursday) 6:15pm - Friday 11:59pm; set a reminder!
- peer reviews for project proposals due Sunday 11:59pm

(All times ET)
Generalization and Overfitting

- goal of model is **not** to predict well on $\mathcal{D}$
- goal of model is to predict well on **new data**

if the model has ____ training set error and ____ test set error, we say the model:

<table>
<thead>
<tr>
<th>low training set error</th>
<th>low test set error</th>
<th>high test set error</th>
</tr>
</thead>
<tbody>
<tr>
<td>generalizes</td>
<td>overfits</td>
<td></td>
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<tr>
<td>?!?!</td>
<td>underfits</td>
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</tbody>
</table>
Simplest case: generalizing from a mean

exit polling

- sample $n$ voters leaving polling places
- for each voter $i$, define the Boolean random variable

$$z_i = \begin{cases} 
1 & \text{if voter } i \text{ voted for Biden} \\
0 & \text{otherwise}
\end{cases}$$

- sample mean: $\nu = \frac{1}{n} \sum_{i=1}^{n} z_i$
- true mean: $\mu = \mathbb{E}_{i \sim \text{US electorate}} z_i$ is Biden’s expected vote share
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Q: When does sample mean $\nu$ estimate true mean $\mu$ well?
A: (1) sample voters uniformly from all voters (2) $n$ large!
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Q: When does sample mean $\nu$ estimate true mean $\mu$ well?
A: (1) sample voters uniformly from all voters (2) $n$ large!

Q: Why might these conditions fail to hold?
A: Absentee votes; failure to sample small or remote polling places; voters who refuse to answer; limited polling resources
Suppose voters in our polling sample are uniformly sampled from the set of all voters, and give truthful answers. The strong law of large numbers states that sample mean converges to the true mean

A. false
B. true
C. as the number of samples $n \to \infty$
D. as the number of voters in the US $\to \infty$
E. so long as the poll is conducted by a respectable nonpartisan organization
Hoeffding inequality

**Theorem (Hoeffding Inequality)**

Let $z_i \in \{0, 1\}, \ i = 1, \ldots, \ n$, be independent Boolean random variables with mean $\mathbb{E}z_i = \mu$. Define the sample mean $\nu = \frac{1}{n} \sum_{i=1}^{n} z_i$. Then for any $\epsilon > 0$,

$$\mathbb{P}[|\nu - \mu| > \epsilon] \leq 2 \exp \left(-2\epsilon^2 n\right).$$

an example of a concentration inequality
Hoeffding inequality

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\mathbb{P}[|\nu - \mu| > \epsilon] \leq 2 \exp \left(-2\epsilon^2 n\right).
\]

an example of a concentration inequality

- \( \mu \) can’t be much higher than \( \nu \)
- \( \mu \) can’t be much lower than \( \nu \)
- more samples \( n \) improve estimate exponentially quickly
Theorem (Strong Law of Large Numbers)

Let $z_i \in \mathbb{R}$, $i = 1, \ldots, n$, be independent random variables with mean $\mathbb{E}z_i = \mu$. Define the sample mean $\nu = \frac{1}{n} \sum_{i=1}^{n} z_i$. Then

$$\nu \to \mu \quad \text{as} \quad n \to \infty$$

compare with the Hoeffding bound:

- the Hoeffding bound provides \textbf{quantitative} predictions on how fast the sample mean $\nu$ \textbf{concentrates} near $\mu$.
- the Hoeffding bound only holds for Boolean random variables
- similar \textbf{concentration inequalities} (named, e.g., Azuma, McDiarmid, Bennet, Bernstein, Chernoff, \ldots) hold for other kinds of random variables
Back to the learning problem

fix a hypothesis $h : \mathcal{X} \rightarrow \mathcal{Y}$. take

$$z_i = \begin{cases} 1 & y_i = h(x_i) \\ 0 & \text{otherwise} \end{cases}$$

$$= 1(y_i = h(x_i))$$
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example. build a model of voting behavior:

- $y_i$ is 1 if voter $i$ voted for Biden, 0 otherwise
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- $z_i$ depends on $x_i$, $y_i$, and $h$
Adding in probability

make our model probabilistic:

- fix a probability distribution $P(x, y)$
- sample $(x_i, y_i)$ iid\(^1\) from $P(x, y)$
- form data set $\mathcal{D}$ by sampling:
  - for $i = 1, \ldots, n$
    - sample $(x_i, y_i) \sim P(x, y)$
  - set $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$

\(^1\)iid: independent and identically distributed
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make our model probabilistic:

- fix a probability distribution \( P(x, y) \)
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- form data set \( D \) by sampling:
  - for \( i = 1, \ldots, n \)
    - sample \((x_i, y_i)\) \(\sim P(x, y)\)
  - set \( D = \{(x_1, y_1), \ldots, (x_n, y_n)\} \)

**special case.** \( y = f(x) \) is deterministic conditioned on \( x \):

\[
P(y|x) = \begin{cases} 1 & y = f(x) \\ 0 & \text{otherwise} \end{cases}
\]

\[
P(x, y) = P(x)P(y|x) = \begin{cases} P(x) & y = f(x) \\ 0 & \text{otherwise} \end{cases}
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Hoeffding for the noisy learning problem

- fix a hypothesis $h : \mathcal{X} \rightarrow \mathcal{Y}$.
- draw samples $(x_i, y_i)$ iid from $P(x, y)$ to form $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$
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Q: Probability? Where's the randomness here?
A: The dataset \( \mathcal{D} \) is random, drawn iid according to \( P(x, y) \).

Q: Is \( \frac{1}{n} \sum_{i=1}^{n} z_i \) more like training set error or test set error?
A: It's more like test set error, since \( h \) is independent of \( \mathcal{D} \).
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so we can apply Hoeffding! for any $\epsilon > 0$,

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\Pr \left[ \left| \frac{1}{n} \sum_{i=1}^{n} z_i - \mathbb{E}z \right| > \epsilon \right] \leq 2 \exp \left( -2\epsilon^2 n \right)
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some new terminology:

► **in-sample error.**

\[ E_{\text{in}}(h) = \text{fraction of } \mathcal{D} \text{ where } y_i \text{ and } h(x_i) \text{ disagree} \]

\[ = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}(y_i \neq h(x_i)) \]

► **out-of-sample error.**

\[ E_{\text{out}}(h) = \text{probability that } y \text{ and } h(x) \text{ disagree} \]

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In-sample and out-of-sample error

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notice

\[ E_{\text{out}}(h) = \mathbb{E}[E_{\text{in}}(h)] \]
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apply Hoeffding: for any $\varepsilon > 0$,

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\mathbb{P}[|E_{in}(h) - E_{out}(h)| > \varepsilon] \leq 2 \exp \left(-2\varepsilon^2 n\right)
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Does Hoeffding work for our learned model?

two scenarios:

1. Without looking at any data, pick a model $h : \mathcal{X} \rightarrow \mathcal{Y}$ to predict who will vote for Biden. Then sample data $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$, and set $z_i = \mathbb{1}(y_i = h(x_i))$. 
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2. Sample the data $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$, and use it to develop a model $g : \mathcal{X} \rightarrow \mathcal{Y}$ to predict who will vote for Biden (e.g., using perceptron). Set $z_i' = \mathbb{1}(y_i = g(x_i))$.

Is the sample mean $\frac{1}{n} \sum_{i=1}^{n} z_i$ a good estimate for the expected performance $\mathbb{E}z$? Is $\frac{1}{n} \sum_{i=1}^{n} z_i'$ a good estimate for $\mathbb{E}z'$?
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Are the \( z_i \)'s iid?

A. yes
B. no
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A. yes  
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Are the \( z'_i \)'s iid?

A. yes  
B. no  

the \( z'_i \)'s depend on \( g \), which depends on the whole data set \( \mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\} \).
Does Hoeffding work for our learned model?

two scenarios:

1. Without looking at any data, pick a model \( h : \mathcal{X} \to \mathcal{Y} \) to predict who will vote for Biden. Then sample data \( \mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\} \), and set \( z_i = \mathbb{1}(y_i = h(x_i)) \).

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Does the Hoeffding bound apply to the sample mean of the (iid) \( z_i \)'s?

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B. no

Does the Hoeffding bound apply to the sample mean of the (not iid) $z_i'$s?

A. yes
B. no
Does Hoeffding work for our learned model?

two scenarios:

1. Without looking at any data, pick a model $h : \mathcal{X} \rightarrow \mathcal{Y}$ to predict who will vote for Biden. Then sample data $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$, and set $z_i = 1(y_i = h(x_i))$.

2. Sample the data $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$, and use it to develop a model $g : \mathcal{X} \rightarrow \mathcal{Y}$ to predict who will vote for Biden (e.g., using perceptron). Set $z'_i = 1(y_i = g(x_i))$.

Is the sample mean $\frac{1}{n} \sum_{i=1}^{n} z_i$ a good estimate for the expected performance $\mathbb{E}z$? Is $\frac{1}{n} \sum_{i=1}^{n} z'_i$ a good estimate for $\mathbb{E}z'$?

Q: Are the $z_i$s iid? What about the $z'_i$s?
A: $z_i$s are iid. $z'_i$s are not independent: they depend on $g$, which depends on the whole data set $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$.

Q: Does Hoeffding apply to the first? the second?
A: Hoeffding applies to first, not to second.

Extreme case for second scenario: model memorizes the data.
Recall validation procedure

how to decide which model to use?

- split data into training set $\mathcal{D}_{\text{train}}$ and test set $\mathcal{D}_{\text{test}}$
- pick $m$ different interesting model classes e.g., different $\phi$s: $\phi_1, \phi_2, \ldots, \phi_m$
- fit (“train”) models on training set $\mathcal{D}_{\text{train}}$
  get one model $h : \mathcal{X} \to \mathcal{Y}$ for each $\phi$s, and set
  $$\mathcal{H} = \{h_1, h_2, \ldots, h_m\}$$
- compute error of each model on test set $\mathcal{D}_{\text{test}}$ and choose lowest:
  $$g = \arg\min_{h \in \mathcal{H}} E_{\mathcal{D}_{\text{test}}} (h)$$
Recall validation procedure

how to decide which model to use?

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e.g., different $\phi$s: $\phi_1$, $\phi_2$, $\ldots$, $\phi_m$
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  $\mathcal{H} = \{h_1, h_2, \ldots, h_m\}$

- compute error of each model on test set $\mathcal{D}_{\text{test}}$ and choose lowest:

  $$g = \arg\min_{h \in \mathcal{H}} E_{\mathcal{D}_{\text{test}}}(h)$$

Q: Are \{\(z_i = \mathbb{1}(y_i = g(x_i)) : (x_i, y_i) \in \mathcal{D}_{\text{test}}\)\} independent?
Recall validation procedure

how to decide which model to use?

▶ split data into training set $D_{\text{train}}$ and test set $D_{\text{test}}$
▶ pick $m$ different interesting model classes
e.g., different $\phi$s: $\phi_1$, $\phi_2$, ..., $\phi_m$
▶ fit ("train") models on training set $D_{\text{train}}$
  get one model $h: \mathcal{X} \rightarrow \mathcal{Y}$ for each $\phi$s, and set

$$\mathcal{H} = \{h_1, h_2, \ldots, h_m\}$$

▶ compute error of each model on test set $D_{\text{test}}$ and choose lowest:

$$g = \arg\min_{h \in \mathcal{H}} E_{D_{\text{test}}}(h)$$

Q: Are $\{z_i = \mathbb{1}(y_i = g(x_i)) : (x_i, y_i) \in D_{\text{test}}\}$ independent?

A: No; $g$ was trained on $D_{\text{test}}$!

Hoeffding does not directly apply:
$E_{D_{\text{test}}}(g)$ may not accurately estimate $E_{\text{out}}(g)$
The union bound

recall the **union bound**: for two random events $A$ and $B$,

$$\Pr(A \cup B) \leq \Pr(A) + \Pr(B)$$
Poll: the union bound

In Ithaca, the probability of rain on any given day is 30%. The probability of sun on any given day is 50%. What is the probability \( p \) that there will be sun or rain on any given day?

A. \( \leq 30\%: \ p \leq .30 \)
B. between 30\% and 50\%: \( p \in (.30, .50] \)
C. between 50\% and 80\%: \( p \in (.50, .80] \)
D. > 80\%: \ p > .80 \)
In some other hypothetical city, the probability of rain on any given day is 30%; the probability of sun on any given day is 50%; and the probability of sun or rain on any given day is 80%. What can we say about the probability $p$ that it will be sunny and rain on the same day?

A. $p = 0$
B. $p \in (0, .30]$
C. $p \in (.30, .50]$
D. $p \in (.50, .80]$
E. $p > .80$
Poll: when is the union bound tight?

In some other hypothetical city, the probability of rain on any given day is 30%; the probability of sun on any given day is 50%; and the probability of sun or rain on any given day is 80%. What can we say about the probability $p$ that it will be sunny and rain on the same day?

A. $p = 0$
B. $p \in (0, .30]$
C. $p \in (.30, .50]$
D. $p \in (.50, .80]$
E. $p > .80$

Q: More generally, when is the union bound tight? i.e., when is $\mathbb{P}(A \cup B) = \mathbb{P}(A) + \mathbb{P}(B)$?
Poll: when is the union bound tight?

In some other hypothetical city, the probability of rain on any given day is 30%; the probability of sun on any given day is 50%; and the probability of sun or rain on any given day is 80%. What can we say about the probability $p$ that it will be sunny and rain on the same day?

A. $p = 0$
B. $p \in (0, .30]$
C. $p \in (.30, .50]$
D. $p \in (.50, .80]$
E. $p > .80$

Q: More generally, when is the union bound tight? i.e., when is $P(A \cup B) = P(A) + P(B)$?
A: When $A \cap B = \emptyset$
Rescuing Hoeffding: the union bound

- let’s suppose $\mathcal{H}$ is finite, with $m$ hypotheses in it
- the hypothesis $g$ is one of those $m$ hypotheses
- so if (given a data set $D$)

\[ |E_{\text{in}}(g) - E_{\text{out}}(g)| > \varepsilon, \]

then for some $h \in \mathcal{H}$, \[ |E_{\text{in}}(h) - E_{\text{out}}(h)| > \varepsilon \]

- ($g$ depends on the data set; we might choose different $h$s for different data sets)
Rescuing Hoeffding: the union bound

- let’s suppose $\mathcal{H}$ is finite, with $m$ hypotheses in it
- the hypothesis $g$ is one of those $m$ hypotheses
- so if (given a data set $\mathcal{D}$)

$$|E_{\text{in}}(g) - E_{\text{out}}(g)| > \varepsilon,$$

then for some $h \in \mathcal{H}$, $|E_{\text{in}}(h) - E_{\text{out}}(h)| > \varepsilon$

- ($g$ depends on the data set; we might choose different $h$s for different data sets)

So

$$\mathbb{P}[|E_{\text{in}}(g) - E_{\text{out}}(g)| > \varepsilon] \leq \sum_{h \in \mathcal{H}} \mathbb{P}[|E_{\text{in}}(h) - E_{\text{out}}(h)| > \varepsilon]$$

$$\leq \sum_{h \in \mathcal{H}} 2 \exp \left( -2\varepsilon^2 n \right)$$

$$= 2m \exp \left( -2\varepsilon^2 n \right)$$
we just proved that our learning algorithm generalizes!

**Theorem (Generalization bound for learning)**

*Let $g$ be a hypothesis chosen from among $m$ different hypotheses. Then*

$$\mathbb{P}[|E_{in}(g) - E_{out}(g)| > \varepsilon] \leq 2m \exp \left(-2\varepsilon^2 n\right).$$
we just proved that our learning algorithm generalizes!

**Theorem (Generalization bound for learning)**

Let \( g \) be a hypothesis chosen from among \( m \) different hypotheses. Then

\[
\mathbb{P}[|E_{in}(g) - E_{out}(g)| > \varepsilon] \leq 2m \exp \left(-2\varepsilon^2 n\right).
\]

**Q:** do you think this bound is tight?
Hoeffding for learning

we just proved that our learning algorithm generalizes!

Theorem (Generalization bound for learning)

Let \( g \) be a hypothesis chosen from among \( m \) different hypotheses. Then

\[
P[|E_{in}(g) - E_{out}(g)| > \varepsilon] \leq 2m \exp (-2\varepsilon^2 n).
\]

Q: do you think this bound is tight?

A: no, it can overcount badly. for random events \( A \) and \( B \), if \( P(A \cap B) \) is large, then \( P(A \cup B) \ll P(A) + P(B) \)
we just proved that our learning algorithm generalizes!

**Theorem (Generalization bound for learning)**

Let $g$ be a hypothesis chosen from among $m$ different hypotheses. Then

$$
P[|E_{in}(g) - E_{out}(g)| > \varepsilon] \leq 2m \exp\left(-2\varepsilon^2 n\right).$$

**Q:** do you think this bound is tight?

**A:** no, it can overcount badly. for random events $A$ and $B$, if $P(A \cap B)$ is large, then $P(A \cup B) \ll P(A) + P(B)$

**more information.** look up the Vapnik-Chervonenkis (VC) dimension, e.g., in *Learning from Data*, by Abu-Mostafa, Magdon-Ismail, and Lin.
A tradeoff for learning

- we want $\mathcal{H}$ to be **big** to make $E_{in}$ small
- we want $\mathcal{H}$ to be **small** to ensure $E_{out}$ is close to $E_{in}$
A tradeoff for learning

- we want $\mathcal{H}$ to be **big** to make $E_{in}$ small
- we want $\mathcal{H}$ to be **small** to ensure $E_{out}$ is close to $E_{in}$

what does this tell us about the difficulty of learning complicated functions $f$?
Generalization for regression

**Theorem (Generalization bound for learning)**

Let $g$ be a hypothesis chosen from among $m$ different hypotheses. Then

$$
\mathbb{P}[|E_{in}(g) - E_{out}(g)| > \varepsilon] \leq 2m \exp (-2\varepsilon^2 n).
$$

to apply Hoeffding to real-valued outputs:

- pick some small $\varepsilon > 0$
- $1((y_i - h(x_i))^2 \leq \varepsilon))$ is 0 if hypothesis $h$ predicts well, 1 if hypothesis $h$ predicts poorly
- define error of hypothesis $h$ on data set $\mathcal{D}$ as

$$
E_{\mathcal{D}}(h) = \frac{1}{|\mathcal{D}|} \sum_{(x,y)\in\mathcal{D}} 1((y - h(x))^2 \leq \varepsilon)
$$
Recap

- we introduced a probabilistic framework for generating data
- we showed that the in-sample error predicts the out-of-sample error for a single hypothesis
- we showed that the in-sample error predicts the out-of-sample error for a learned hypothesis, when $\mathcal{H}$ is finite
- we stopped there, because the math gets much more complicated — but indeed, generalization is possible!
- the practical lesson: (especially for complex models), don’t learn and estimate your error on the same data set
the in-sample error and training error do **not** obey the Hoeffding inequality (without using, e.g., a union bound)

- if test set is **only** used for testing (not for model selection), the test error **does** obey the Hoeffding inequality

\[
P[|E_{\text{test}}(g) - E_{\text{out}}(g)| > \varepsilon] \leq 2 \exp \left(\frac{-2\varepsilon^2|D_{\text{test}}|}{n}\right).
\]

so we can use the test error to predict generalization
Overfitting to the test set

If test set is used for model selection, the test error obeys the Hoeffding inequality with the union bound

- For each model family, optimal model trained on $\mathcal{D}$ is a hypothesis $h$
- So finite number of models $m \implies$ finite hypothesis space $\mathcal{H}$
- Hypotheses $h \in \mathcal{H}$ are independent of test set $\mathcal{D}'$
- Let $g_{\mathcal{D}'}$ be the hypothesis $h \in H$ with lowest error on test set $\mathcal{D}'$
- Hoeffding with union bound applies!

$$\mathbb{P}[|E_{\mathcal{D}'}(g_{\mathcal{D}'}) - E_{\text{out}}(g_{\mathcal{D}'})| > \varepsilon] \leq 2m \exp \left(-2\varepsilon^2|\mathcal{D}'|\right).$$
References

- Concentration bounds for infinite model classes: see introduction to VC dimension in “Learning from Data” by Abu-Mostafa et al.
- Concentration bounds for time series: see papers by Cosma Shalizi