



Slides adapted from Rob Schapire

Classification: Rademacher Complexity

Machine Learning: Jordan Boyd-Graber University of Colorado Boulder

LECTURE 6

Setup

Nothing new ...

- Samples $S = ((x_1, y_1), ..., (x_m, y_m))$
- Labels $y_i = \{-1, +1\}$
- Hypothesis $h: X \rightarrow \{-1, +1\}$
- Training error: $\hat{R}(h) = \frac{1}{m} \sum_{i=1}^{m} \mathbb{1}[h(x_i) \neq y_i]$

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$$= \frac{1}{m} \sum_{i}^{m} \begin{cases} 1 & \text{if } (h(x_i, y_i) == (1, -1) \text{ or } (-1, 1) \\ 0 & (h(x_i, y_i) == (1, 1) \text{ or } (-1, -1) \end{cases}$$
 (2)

(3)

(4)

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Correlation between predictions and labels

$$\hat{R}(h) = \frac{1}{m} \sum_{i}^{m} \mathbb{1} \left[h(x_i) \neq y_i \right]$$
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Minimizing training error is thus equivalent to maximizing correlation

$$\arg\max_{h} \frac{1}{m} \sum_{i}^{m} y_{i} h(x_{i}) \tag{5}$$

Playing with Correlation

Imagine where we replace true labels with Rademacher random variables

$$\sigma_i = \begin{cases} +1 & \text{with prob } .5\\ -1 & \text{with prob } .5 \end{cases}$$
 (6)

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This gives us Rademacher correlation—what's the best that a random classifier could do?

$$\hat{\mathcal{R}}_{\mathcal{S}}(H) \equiv \mathbb{E}_{\sigma} \left[\max_{h \in H} \frac{1}{m} \sum_{i}^{m} \sigma_{i} h(x_{i}) \right]$$
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Note: Empirical Rademacher complexity is with respect to a sample.

• What are the maximum values of Rademacher correlation?

Boulder

$$|H| = 1$$

$$|H|=2^m$$

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$$\frac{m}{m} = 1$$

- Rademacher correlation is larger for more complicated hypothesis space.
- What if you're right for stupid reasons?

We can generalize Rademacher complexity to consider all sets of a particular size.

$$\mathscr{R}_{m}(H) = \mathbb{E}_{S \sim D^{m}} \left[\hat{\mathscr{R}}_{S}(H) \right]$$
 (8)

Theorem

Convergence Bounds Let F be a family of functions mapping from Z to [0,1], and let sample $S=(z_1,\ldots,z_m)$ were $z_i\sim D$ for some distribution D over Z. Define $\mathbb{E}\left[f\right]\equiv \mathbb{E}_{z\sim D}\left[f(z)\right]$ and $\hat{\mathbb{E}}_S\left[f\right]\equiv \frac{1}{m}\sum_{i=1}^m f(z_i)$. With probability greater than $1-\delta$ for all $f\in F$:

$$\mathbb{E}\left[f\right] \leq \hat{\mathbb{E}}_{s}\left[f\right] + 2\mathcal{R}_{m}\left(F\right) + \mathcal{O}\left(\sqrt{\frac{\ln\frac{1}{\delta}}{m}}\right) \tag{9}$$

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Aside: McDiarmid's Inequality

If we have a function:

$$|f(x_1,...,x_i,...x_m)-f(x_1,...,x_i',...,x_m)| \le c_i$$
 (10)

then:

$$\Pr[f(x_1,\ldots,x_m) \ge \mathbb{E}\left[f(X_1,\ldots,X_m)\right] + \epsilon] \le \exp\left\{\frac{-2\epsilon^2}{\sum_{i}^{m} c_i^2}\right\}$$
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Proof in the back of the textbook.

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What function do we care about for Rademacher complexity? Let's define

$$\Phi(S) = \sup \left(\mathbb{E}[f] - \hat{\mathbb{E}}_{S}[f] \right) = \sup \left(\mathbb{E}[f] - \frac{1}{m} \sum_{i} f(z_{i}) \right)$$
 (12)

Step 1: Bounding divergence from true Expectation

Lemma

Moving to Expectation *With probability at least* $1 - \delta$,

$$\Phi(S) \leq \mathbb{E}_s[\Phi(S)] + \sqrt{\frac{\ln\frac{1}{\delta}}{2m}}$$

Since $f(z_1) \in [0,1]$, changing any z_i to z_i' in the training set will change $\frac{1}{m} \sum_i f(z_i)$ by at most $\frac{1}{m}$, so we can apply McDiarmid's inequality.

Define a ghost sample $S' = (z'_1, ..., z'_m) \sim D$. How much can two samples from the same distribution vary?

Lemma

Two Different Samples

$$\mathbb{E}_{\mathcal{S}}[\Phi(\mathcal{S})] = \mathbb{E}_{\mathcal{S}}\left[\sup_{f}(\mathbb{E}[f] - \hat{\mathbb{E}}_{\mathcal{S}}[f])\right]$$
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$$= \mathbb{E}_{\mathcal{S}} \left[\sup_{f \in F} (\mathbb{E}_{\mathcal{S}'} \left[\hat{\mathbb{E}}_{\mathcal{S}'} \left[f \right] \right] - \hat{\mathbb{E}}_{\mathcal{S}} [f]) \right]$$
(14)

(15)

The expectation is equal to the expectation of the empirical expectation of all sets S^\prime

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(15)
$$(16)$$

 ${\cal S}$ and ${\cal S}'$ are distinct random variables, so we can move inside the expectation

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$$\leq \mathbb{E}_{S,S'} \left[\sup_{f} (\hat{\mathbb{E}}_{S'}[f] - \hat{\mathbb{E}}_{S}[f]) \right]$$
 (15)

The expectation of a max over some function is at least the max of that expectation over that function

Step 3: Adding in Rademacher Variables

From S, S' we'll create T, T' by swapping elements between S and S' with probability .5. This is still iid from D. They have the same distribution:

$$\hat{\mathbb{E}}_{S'}[f] - \hat{\mathbb{E}}_{S}[f] \sim \hat{\mathbb{E}}_{T'}[f] - \hat{\mathbb{E}}_{T}[f]$$
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Let's introduce σ_i :

$$\hat{\mathbb{E}}_{T'}[f] - \hat{\mathbb{E}}_{T}[f] = \frac{1}{m} \begin{cases} f(z_i) - f(z_i') \text{ with prob .5} \\ f(z_i') - f(z_i) \text{ with prob .5} \end{cases}$$
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$$=\frac{1}{m}\sum_{i}\sigma_{i}(f(z_{i}^{\prime})-f(z_{i})) \tag{18}$$

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$$= \frac{1}{m} \sum_{i} \sigma_{i} (f(z'_{i}) - f(z_{i}))$$
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Thus:

$$\mathbb{E}_{\mathcal{S},\mathcal{S}'}\left[\sup\nolimits_{f\in\mathcal{F}}\left(\hat{\mathbb{E}}_{\mathcal{S}'}\left[f\right]-\hat{\mathbb{E}}_{\mathcal{S}}\left[f\right]\right)\right]=\mathbb{E}_{\mathcal{S},\mathcal{S}',\sigma}\left[\sup\nolimits_{f\in\mathcal{F}}\left(\sum\nolimits_{i}\sigma_{i}(f(z_{i}')-f(z_{i}))\right)\right].$$

Step 4: Making These Rademacher Complexities

Before, we had $\mathbb{E}_{\mathcal{S},\mathcal{S}',\sigma}\left[\sup_{f\in F}\sum_{i}\sigma_{i}(f(z_{i}')-f(z_{i}))\right]$

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$$\mathbb{E}_{S,S',\sigma}\left[\sup_{f\in F}\sum_{i}\sigma_{i}(f(z'_{i})-f(z_{i}))\right]$$

$$\leq \mathbb{E}_{S,S',\sigma} \left[\sup_{f \in F} \sum_{i} \sigma_{i} f(z'_{i}) + \sup_{f \in F} \sum_{i} (-\sigma_{i}) f(z_{i}) \right]$$
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Taking the sup jointly must be less than or equal the individual sup.

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(21)

Linearity

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(20)

$$= \mathcal{R}_m(F) + \mathcal{R}_m(F) \tag{21}$$

Definition

With probability $\geq 1 - \delta$:

$$\Phi(S) \le \mathbb{E}_{S}[\Phi(S)] + \sqrt{\frac{\ln \frac{q}{\delta}}{2m}}$$
 (22)

Step 1

With probability $\geq 1 - \delta$:

$$\sup_{f} \left(\mathbb{E}\left[f\right] - \hat{\mathbb{E}}_{S}\left[h\right] \right) \leq \mathbb{E}_{S}\left[\Phi(S)\right] + \sqrt{\frac{\ln\frac{q}{\delta}}{2m}}$$
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Definition of Φ

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Drop the sup, still true

With probability $\geq 1 - \delta$:

$$\mathbb{E}[f] - \hat{\mathbb{E}}_{S}[h] \leq \mathbb{E}_{S,S'} \left[\sup_{f} (\hat{\mathbb{E}}_{S'}[f] - \hat{\mathbb{E}}_{S}[f]) \right] + \sqrt{\frac{\ln \frac{q}{\delta}}{2m}}$$
(22)

Step 2

With probability $\geq 1 - \delta$:

$$\mathbb{E}\left[f\right] - \hat{\mathbb{E}}_{S}\left[h\right] \leq \mathbb{E}_{S,S',\sigma}\left[\sup_{f \in F} \left(\sum_{i} \sigma_{i}\left(f(z'_{i}) - f(z_{i})\right)\right)\right] + \sqrt{\frac{\ln \frac{q}{\delta}}{2m}}$$
(22)
Step 3

With probability $\geq 1 - \delta$:

$$\mathbb{E}[f] - \hat{\mathbb{E}}_{S}[h] \leq 2\mathscr{R}_{m}(F) + \sqrt{\frac{\ln\frac{q}{\delta}}{2m}}$$
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Recall that $\hat{\mathcal{R}}_{S}(F) \equiv \mathbb{E}_{\sigma}\left[\sup_{f} \frac{1}{m} \sum_{i} \sigma_{i} f(z_{i})\right]$, so we apply McDiarmid's inequality again (because $f \in [0,1]$:

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$$\widehat{\mathcal{R}}_{\mathcal{S}}(F) \le \mathcal{R}_{m}(F) + \sqrt{\frac{\ln \frac{1}{\delta}}{2m}}$$
 (23)

Putting the two together:

$$\mathbb{E}[f] \leq \hat{\mathbb{E}}_{s}[f] + 2\mathcal{R}_{m}(F) + \mathcal{O}\left(\sqrt{\frac{\ln\frac{1}{\delta}}{m}}\right)$$
 (24)

What about hypothesis classes?

Define:

$$Z \equiv X \times \{-1, +1\} \tag{25}$$

$$f_h(x,y) \equiv \mathbb{1} \left[h(x) \neq y \right] \tag{26}$$

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$$F_H \equiv \{ f_h : h \in H \} \tag{27}$$

We can use this to create expressions for generalization and empirical error:

$$R(h) = \mathbb{E}_{(x,y)\sim D}\left[\mathbb{1}\left[h(x) \neq y\right]\right] = \mathbb{E}\left[f_h\right]$$
(28)

$$\hat{R}(h) = \frac{1}{m} \sum_{i} \mathbb{1} [h(x_i) \neq y] = \hat{\mathbb{E}}_{S}[f_h]$$
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$$\hat{R}(h) = \frac{1}{m} \sum_{i} \mathbb{1} [h(x_i) \neq y] = \hat{\mathbb{E}}_{\mathcal{S}}[f_h]$$
 (29)

We can plug this into our theorem!

Generalization bounds

We started with expectations

$$\mathbb{E}[f] \leq \hat{\mathbb{E}}_{S}[f] + 2\hat{\mathcal{R}}_{S}(F) + \mathcal{O}\left(\sqrt{\frac{\ln\frac{1}{\delta}}{m}}\right)$$
(30)

• We also had our definition of the generalization and empirical error:

$$R(h) = \mathbb{E}_{(x,y)\sim D}\left[\mathbb{1}\left[h(x)\neq y\right]\right] = \mathbb{E}\left[f_h\right] \quad \hat{R}(h) = \frac{1}{m}\sum_{i}\mathbb{1}\left[h(x_i)\neq y\right] = \hat{\mathbb{E}}_{\mathcal{S}}\left[f_h\right]$$

Combined with the previous result:

$$\hat{\mathcal{R}}_{\mathcal{S}}(F_{H}) = \frac{1}{2}\hat{\mathcal{R}}_{\mathcal{S}}(H) \tag{31}$$

• All together:

$$R(h) \le \hat{R}(h) + \mathcal{R}_m(H) + \mathcal{O}\left(\sqrt{\frac{\log \frac{1}{\delta}}{m}}\right)$$
 (32)

Wrapup

- Interaction of data, complexity, and accuracy
- Still very theoretical
- Next time: How to evaluate generalizability of specific hypothesis classes