Announcements:

- HW1 posted

Today:
- Review: bias variance
- Overfitting, overfitting overfitting
- Ridge regression
- Checking for overfitting: cross validation
Bias-Variance tradeoff – Intuition

- Model too “simple” ➔ does not fit the data well
  - A biased solution

- Model too complex ➔ small changes to the data, solution changes a lot
  - A high-variance solution
(Squared) Bias of learner

- Given dataset $D$ with $N$ samples, learn function $h_D(x)$
- If you sample a different dataset $D'$ with $N$ samples, you will learn different $h_D'(x)$
- **Expected hypothesis**: $E_D[h_D(x)]$

<table>
<thead>
<tr>
<th>Bias:</th>
<th>difference between what you expect to learn and truth</th>
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<td>Measures how well you expect to represent true solution</td>
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<td>Decreases with more complex model</td>
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<td>Bias$^2$ at one point $x$: $E_x \left( (h(x) - t(x))^2 \right)$</td>
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<td>Average Bias$^2$: $E_x \frac{1}{N} \sum_{i=1}^{N} (h(x) - t(x))^2$</td>
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Variance of learner

- Given dataset $D$ with $N$ samples, learn function $h_D(x)$
- If you sample a different dataset $D'$ with $N$ samples, you will learn different $h_D'(x)$
- **Variance**: difference between what you expect to learn and what you learn from a particular dataset

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<td>Measures how sensitive learner is to specific dataset</td>
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Training set error

\[ w^* = \arg \min_w \sum_j \left( t(x_j) - \sum_i w_i h_i(x_j) \right)^2 \]

- Given a dataset (Training data)
- Choose a loss function
  - e.g., squared error (L_2) for regression
- **Training set error:** For a particular set of parameters, loss function on training data:

\[
\text{error}_{train}(w) = \frac{1}{N_{train}} \sum_{j=1}^{N_{train}} \left( t(x_j) - \sum_i w_i h_i(x_j) \right)^2
\]
Training set error as a function of model complexity

\[
\text{error}_{\text{train}}(w) = \frac{1}{N_{\text{train}}} \sum_{i=1}^{N_{\text{train}}} (t(x_i) - \sum_j w_j h_j(x_i))^2
\]

Prediction error

- Training set error can be a poor measure of "quality" of solution
- **Prediction error**: We really care about error over all possible input points, not just training data:

\[
\text{error}_{\text{true}}(w) = \mathbb{E}_x \left[ \left( t(x) - \sum_i w_i h_i(x) \right)^2 \right] = \int_x \left( t(x) - \sum_i w_i h_i(x) \right)^2 p(x) dx
\]
Prediction error as a function of model complexity

\[ \text{error}_{\text{true}}(w) = \int_{x} \left( t(x) - \sum_{i} w_{i} h_{i}(x) \right)^{2} p(x) dx \]

Computing prediction error

- Computing prediction
  - Hard integral
  - May not know \( t(x) \) for every \( x \)

\[ \text{error}_{\text{true}}(w) = \int_{x} \left( t(x) - \sum_{i} w_{i} h_{i}(x) \right)^{2} p(x) dx \]

- Monte Carlo integration (sampling approximation)
  - Sample a set of i.i.d. points \( \{x_{1}, \ldots, x_{M}\} \) from \( p(x) \)
  - Approximate integral with sample average

\[ \text{error}_{\text{true}}(w) \approx \frac{1}{M} \sum_{j=1}^{M} \left( t(x_{j}) - \sum_{i} w_{i} h_{i}(x_{j}) \right)^{2} \]
Why training set error doesn’t approximate prediction error?

Sampling approximation of prediction error:

\[ error_{true}(w) \approx \frac{1}{M} \sum_{j=1}^{M} \left( t(x_j) - \sum_i w_i h_i(x_j) \right)^2 \]

Training error:

\[ error_{train}(w) = \frac{1}{N_{\text{train}}} \sum_{j=1}^{N_{\text{train}}} \left( t(x_j) - \sum_i w_i h_i(x_j) \right)^2 \]

Very similar equations!!!

- Why is training set a bad measure of prediction error???

Because you cheated!!!

Training error good estimate for a single \( w \),
But you optimized \( w \) with respect to the training error,
and found \( w \) that is good for this set of samples

Training error is a (optimistically) biased estimate of prediction error

Very similar equations!!!

- Why is training set a bad measure of prediction error???
Test set error

Given a dataset, randomly split it into two parts:
- Training data – \{x_1, \ldots, x_{N_{\text{train}}}\}
- Test data – \{x_1, \ldots, x_{N_{\text{test}}}\}

Use training data to optimize parameters w

Test set error: For the final output \( \hat{\mathbf{w}} \), evaluate the error using:

\[
\text{error}_{\text{test}}(\mathbf{w}) = \frac{1}{N_{\text{test}}} \sum_{j=1}^{N_{\text{test}}} \left( t(x_j) - \sum_{i} w_i h_i(x_j) \right)^2
\]

Test set error as a function of model complexity
Overfitting

- **Overfitting**: a learning algorithm overfits the training data if it outputs a solution \( w \) when there exists another solution \( w' \) such that:

\[
[error_{train}(w) < error_{train}(w')] \land [error_{true}(w') < error_{true}(w)]
\]

How many points to I use for training/testing?

- Very hard question to answer!
  - Too few training points, learned \( w \) is bad
  - Too few test points, you never know if you reached a good solution
- Bounds, such as Hoeffding’s inequality can help:

\[
P(| \hat{\theta} - \theta^* | \geq \epsilon) \leq 2e^{-2N\epsilon^2}
\]

- More on this later this quarter, but still hard to answer
- Typically:
  - If you have a reasonable amount of data, pick test set “large enough” for a “reasonable” estimate of error, and use the rest for learning
  - If you have little data, then you need to pull out the big guns…
    - e.g., bootstrapping
Error estimators

\[ \text{error}_{\text{true}}(w) = \int_{\mathcal{X}} \left( t(x) - \sum_{i} w_i h_i(x) \right)^2 p(x)dx \]

\[ \text{error}_{\text{train}}(w) = \frac{1}{N_{\text{train}}} \sum_{j=1}^{N_{\text{train}}} \left( t(x_j) - \sum_{i} w_i h_i(x_j) \right)^2 \]

\[ \text{error}_{\text{test}}(w) = \frac{1}{N_{\text{test}}} \sum_{j=1}^{N_{\text{test}}} \left( t(x_j) - \sum_{i} w_i h_i(x_j) \right)^2 \]
Error estimators

Be careful!!!

Test set only unbiased if you never ever ever do any any any any any learning on the test data

For example, if you use the test set to select the degree of the polynomial... no longer unbiased!!! (We will address this problem later)

\[ \text{error}_{\text{test}}(w) = \frac{1}{N_{\text{test}}} \sum_{i=1}^{N_{\text{test}}} \left( f(x_i) - \sum_j w_j h_j(x_i) \right)^2 \]

What you need to know

- True error, training error, test error
  - Never learn on the test data
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- Overfitting
Regularization in Linear Regression

- Overfitting usually leads to very large parameter choices, e.g.:
  - $-2.2 + 3.1 X - 0.30 X^2$
  - $-1.1 + 4,700,910.7 X - 8,585,638.4 X^2 + \ldots$

- Regularized or penalized regression aims to impose a “complexity” penalty by penalizing large weights
  - “Shrinkage” method
Ridge Regression

- Aleviating issues with overfitting:
- New objective:

\[
\hat{w}_{ridge} = \arg \min_w \sum_{j=1}^{N} \left( t(x_j) - (w_0 + \sum_{i=1}^{k} w_i h_i(x_j)) \right)^2 + \lambda \sum_{i=1}^{k} w_i^2
\]

\[
= \arg \min_w (Hw - t)^T (Hw - t) + \lambda w^T I_{0+k} w
\]

residual error
Minimizing the Ridge Regression Objective

\[ \hat{w}_{ridge} = \arg \min_w \sum_{j=1}^{N} \left( t(x_j) - (w_0 + \sum_{i=1}^{k} w_i h_i(x_j)) \right)^2 + \lambda \sum_{i=1}^{k} w_i^2 \]

\[ = (Hw - t)^T (Hw - t) + \lambda \ w^T I_{0+k} w \]

Shrinkage Properties

\[ \hat{\hat{w}}_{ridge} = (H^T H + \lambda I_{0+k})^{-1} H^T t \]

- If orthonormal features/basis: \( H^T H = I \)
Ridge Regression: Effect of Regularization

\[ \hat{w}_{\text{ridge}} = \arg \min_w \sum_{j=1}^{N} \left( t(x_j) - (w_0 + \sum_{i=1}^{k} w_i h_i(x_j)) \right)^2 + \lambda \sum_{i=1}^{k} w_i^2 \]

- Solution is indexed by the regularization parameter \( \lambda \)
- Larger \( \lambda \)
- Smaller \( \lambda \)
- As \( \lambda \to 0 \)
- As \( \lambda \to \infty \)

Ridge Coefficient Path

Typical approach: select \( \lambda \) using cross validation, more on this later in the quarter
Error as a function of regularization parameter for a fixed model complexity

\[
\frac{1}{N_{\text{train}}} \sum_{i=1}^{N_{\text{train}}} \left( f(x_i) - \sum_{j=1}^{d} w_j h(x_i)_j \right)^2 + \lambda \left( \sum_{j=1}^{d} w_j^2 \right)
\]

\[
\lambda = \infty \quad \lambda = 0
\]

What you need to know…

■ Regularization
  - Penalizes for complex models

■ Ridge regression
  - L_2 penalized least-squares regression
  - Regularization parameter trades off model complexity with training error
Cross-Validation

Test set error as a function of model complexity

\[
\text{error}_{\text{test}}(w) = \frac{1}{N_{\text{test}}} \sum_{i=1}^{N_{\text{test}}} (f(x_i) - \sum_{j=1}^{p} w_j h_j(x_i))^2
\]
How... How... How????????

- How do we pick the regularization constant $\lambda$...
  - And all other constants in ML, 'cause one thing ML doesn't lack is constants to tune... 😊

- We could use the test data, but...

(LOO) Leave-one-out cross validation

- Consider a validation set with 1 example:
  - $D$ – training data
  - $D_j$ – training data with $j$th data point moved to validation set

- Learn classifier $h_j$ with $D_j$ dataset

- Estimate true error as squared error on predicting $t(x)$:
  - Unbiased estimate of $error_{true}(h_j)$!
  - Seems really bad estimator, but wait!

- LOO cross validation: Average over all data points $j$:
  - For each data point you leave out, learn a new classifier $h_j$
  - Estimate error as:
    
    $$error_{LOO} = \frac{1}{N} \sum_{j=1}^{N} (t(x_j) - h_{D \setminus j}(x_j))^2$$
LOO cross validation is (almost) unbiased estimate of true error of $h_D$!

- When computing LOOCV error, we only use $N-1$ data points
  - So it's not estimate of true error of learning with $N$ data points!
  - Usually pessimistic, though – learning with less data typically gives worse answer

- LOO is almost unbiased!

Great news!
- Use LOO error for model selection!!!
- E.g., picking $\lambda$

Using LOO to Pick $\lambda$

$$\lambda = \infty \quad \quad \lambda = 0$$
Using LOO error for model selection

\[ \text{error}_{\text{LOO}} = \frac{1}{N} \sum_{j=1}^{N} (y_j - \hat{h}(x_j))^2 \]

Computational cost of LOO

- Suppose you have 100,000 data points
- You implemented a great version of your learning algorithm
  - Learns in only 1 second
- Computing LOO will take about 1 day!!!
  - If you have to do for each choice of basis functions, it will take foooooorreeevvve'!!!
- Solution 1: Preferred, but not usually possible
  - Find a cool trick to compute LOO (e.g., see homework)
Solution 2 to complexity of computing LOO:

(More typical) Use \textit{k-fold cross validation}

- Randomly divide training data into \( k \) equal parts
  - \( D_1, \ldots, D_k \)
- For each \( i \)
  - Learn classifier \( h_{D_i} \) using data point not in \( D_i \)
  - Estimate error of \( h_{D_i} \) on validation set \( D_i \)
    \[
    \text{error}_{D_i} = \frac{k}{N} \sum_{x_j \in D_i} \left( t(x_j) - h_{D\setminus D_i}(x_j) \right)^2
    \]
- \textit{k-fold cross validation error is average} over data splits:
  \[
  \text{error}_{k-fold} = \frac{1}{k} \sum_{i=1}^{k} \text{error}_{D_i}
  \]
- \textit{k-fold cross validation properties:}
  - Much faster to compute than LOO
  - More (pessimistically) biased – using much less data, only \( m(k-1)/k \)
  - Usually, \( k = 10 \)

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What you need to know...

- Never train on the test data
- Use cross-validation to choose magic parameters such as \( \lambda \)
- Leave-one-out is the best you can do, but sometimes too slow
  - In that case, use k-fold cross-validation

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