Overfitting

CMPUT 366: Intelligent Systems

P&M §7.4

Lecture Outline

1. Recap & Logistics
2. Causes of Overfitting
3. Avoiding Overfitting

Labs & Assignment #2

- **Assignment #2 was released on Friday**
  See the website under Assignments (or on the Schedule)
- Assignment #2 is due **Mar 4** before lecture
- Today's lab is from **5:00pm to 7:50pm** in **CAB 235**
  - Not mandatory
  - Opportunity to get help from the TAs

Recap: Linear Models

- Linear Regression and Classification
  - Fit a **linear function** to the input and target features
- Decision trees:
  - Split on a **condition** at each internal node
  - Prediction on the **leaves**
  - Simple, general; often a **building block** for other methods
  - **Stopping criteria**: too little data, too many nodes, etc. to avoid overfitting

Overfitting

- **Overfitting**: The learner makes predictions based on regularities that occur in the **training data** but **not** in the **underlying population**
    - Causes failure to **generalize**
- Combination of two factors:
    1. Learning **spurious correlations**: In any training data there may be coincidental associations that are not reflective of the process being learned
        - *Example:* More pictures of tanks taken on sunny days, more pictures without tanks taken on cloudy days. Learning agent learns that sunny pictures are predictive of tanks.
    2. **Overconfidence** in the learned model. The unseen data is assumed to be more **exactly like** the training data than is plausible.
        - *Example:* Just because my training data doesn't contain the word "squeegee" doesn't mean there is a literally **zero percent** chance of encountering it!

Example: Restaurant Ratings

- Suppose a website collects **ratings for restaurants** on a scale of 1 to 5 stars
- The website wants to display the **best** restaurants
  - Definition: Restaurants that future diners will like most
- **Question:** What rating **prediction** for a given restaurant optimizes the squared loss on the training data?
- **Question:** What would happen if the website just listed the restaurants with the highest rating predicted in this way?

Regression to the Mean

Regression to the mean: **Extreme** predictions perform worse

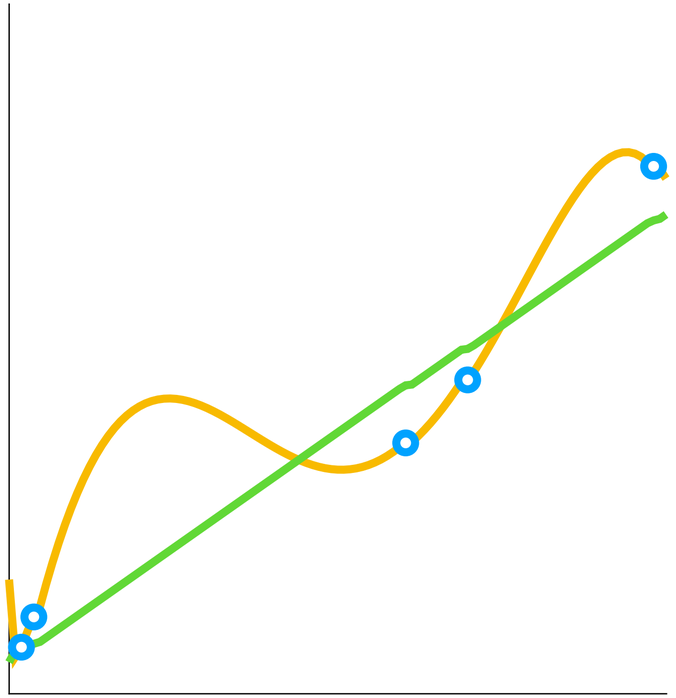
- Children of very tall parents are likely to be shorter than either parent
- The Sports Illustrated Cover curse: Players who have just appeared on the cover of Sports Illustrated often perform much worse subsequently
- There is no rating higher than five stars, so only possible noise in the data is too-low ratings

Model Complexity

- Adding **more parameters** to a model can almost always fit the training data better
    - Especially when the larger model is a **generalization** of the smaller model; it is then **mathematically inevitable**
- Intuition:
    - Simple models can't represent much, so they are forced to prioritize the largest/**most important** effects
    - Complex models can represent more effects, including small, **unimportant**, and or **spurious** effects

Example: Fitting Polynomials

- A linear fit **won't hit** every observation exactly
- A sufficiently high-degree polynomial **will**
- **Question:** Which model's predictions are more credible?



Big Data

- More **examples** usually gives better **predictions** (**why**?)
- But this is not a cure-all
- Often when we have access to more **examples**, we also have access to more **features** of the examples
    - More features require more examples for efficient learning

Bias

What causes **test set error**? **Bias** + variance + noise

- **Bias** is error from systematically finding an **imperfect model**
  - **Representation bias:** Hypothesis class does not contain a model close enough to the **ground truth**
  - **Search bias:** Algorithm was not able to **find** a good enough hypothesis in the hypothesis space
- **Decision trees** can represent **any function** of categorical variables, so they have **low representational bias**
  - The space of decision trees is too large to search systematically, so they can have a **high search bias**
- **Linear regression** is a very simple class of models, so it has **high representation bias**
  - But the optimal linear model can be found analytically, so it has **zero search bias**

Variance

What causes **test set error**? Bias + **variance** + noise

- The smaller the training dataset, the more **different** we can expect our model estimates to be
    - *Restaurant Example:* how different would the estimates be from two training sets of **1 rating each**? How different would they be from two training sets of **100,000 ratings each**? (**why**?)
- **Variance** is the error from having **too little data** to train from
    - or, from having **too complex** a model for the amount of data that we have
    - More complex models require more data to fit
- **Bias-variance tradeoff** (for a given fixed amount of data):
    - Complicated models will contain better hypotheses, but be harder to estimate
    - Simple models will be easier to estimate, but representational bias means they cannot be as accurate

Noise

What causes **test set error**? Bias + variance + **noise**

- Sometimes the underlying process that generates our data is **inherently random**
  - In this case, we **cannot predict exactly** no matter how many we have
  - *Example:* Biased coin toss
- Sometimes the underlying process is not random, but we are **missing measurements** for important features
  - In this case, we also cannot predict exactly
  - The missing features make the process **appear** random
  - *Example:* Ice cream trucks only come out when it's sunny, but our dataset doesn't record the weather

Avoiding Overfitting

There are multiple approaches to avoiding overfitting

1. **Pseudocounts**: Explicitly account for **regression to the mean**

2. **Regularization**: Explicitly **trade off** between fitting the data and model complexity

3. **Cross-validation**: **Detect** overfitting using some of the training data

Pseudocounts

- When we have not observed all the **values** of a variable, those variables should not be assigned probability zero
- If we don't have very much **data**, we should not be making very extreme predictions
- Solution: artificially add some "pretend" observations for each value of a variable (**pseudocounts**)
    - When there is not much data, predictions will tend to be less extreme (**why**?)
    - When there is more data, the pseudocounts will have less effect on the predictions

Regularization

- We shouldn't choose a complicated model unless there is clear evidence for it

- Instead of optimizing directly for training error, optimize training error plus a penalty for complexity:

$$\arg\min_{h \in \mathcal{H}} \sum_{e} error(e, h) + \lambda \times regularizer(h)$$

- *regularizer* measures the **complexity** of the hypothesis

- λ is the regularization parameter: indicates how important hypothesis complexity is compared to fit

    - Larger λ means complexity is more important

Types of Regularizer

- Number of **parameters**
- **Degree** of polynomial
- **L2** regularizer ("ridge regularizer"): sum of squares of weights
  - Prefers models with **smaller** weights
- **L1** regularizer ("lasso regularizer"): sum of absolute values of weights
  - Prefers models with **fewer nonzero** weights
  - Often used for **feature selection**: only features with nonzero weights are used

Cross-Validation

- Previous methods require us to already know how simple a model "should" be:
    - How many **pseudocounts** to add?
    - What should **regularization parameter** be?
- Ideally we would like to be able to answer these questions **from the data**
- **Question:** Can we use the **test data** to see which of these work best?
    - Idea: Use some of the **training data** as an **estimate** of the test data

Cross-Validation Procedure

Cross-validation can be used to estimate most bias-control parameters (**hyperparameters**)

1. **Randomly remove** some datapoints from the training set; these examples are the **validation set**

2. Train the model on the training set using some values of hyperparameters (pseudocounts, polynomial degree, regression parameter, etc.)

3. Evaluate the results on the validation set

4. Update values of **hyperparameters**

5. Repeat

k-Fold Cross-Validation

- We want our training set to be as large as possible, so we get better models
- We want our validation set to be as large as possible, so that it is an accurate estimation of test performance
- ***k*-fold cross-validation** lets us use every one of our examples for both validation and training

k-Fold Cross-Validation Procedure

1. **Randomly partition** training data into *k* approximately equal-sized sets (**folds**)

2. Train *k* times, each time using all the folds but one; **remaining fold** is used for **validation**

3. Optimize hyperparameters based on **validation errors**

- Each example is used exactly **once** for **validation** and ***k*-1 times** for **training**

- **Extreme case**: *k=n* is called **leave-one-out** cross-validation

Summary

- **Overfitting** is when a learned model fails to **generalize** due to **overconfidence** and/or learning **spurious regularities**
- **Bias-variance tradeoff**: More **complex** models can be more **accurate**, but also require more **data** to train
- Techniques for avoiding overfitting:
  - **Pseudocounts**: Add **imaginary** observations
  - **Regularization**: **Penalize** model complexity
  - **Cross-validation**: Reserve **validation data** to estimate test error