CPSC 340: Machine Learning and Data Mining

Feature Selection

Fall 2016

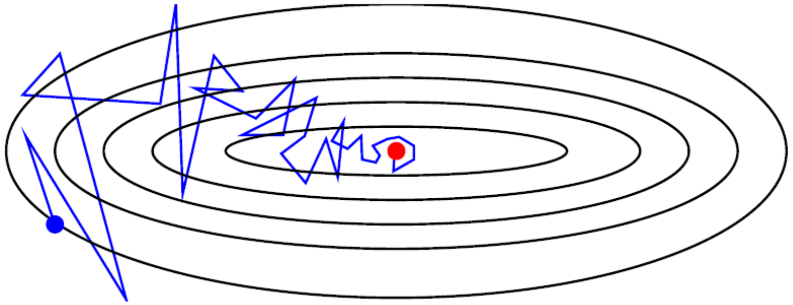
Admin

- Assignment 3:
  - Solutions will be posted after class Wednesday.
- Extra office hours Thursday:
  - 10:30-12 and 4:30-6 in X836.
- Midterm Friday:
  - Midterm from last year and list of topics posted (covers Assignments 1-3).
    - Tutorials this week will cover practice midterm (and non-1D version of Q5).
  - In class, 55 minutes, closed-book, cheat sheet: 2-pages each double-sided.

Last Time: Stochastic Gradient

- Stochastic gradient minimizes average of smooth functions:

$$f(w) = \frac{1}{n}\sum_{i=1}^{n} f_i(w)$$



  - Function $f_i(w)$ is error for example 'i'.

- Iterations perform gradient descent on one random example 'i':

$$w^{t+1} = w^t - \alpha^t \nabla f_i(w^t)$$

  - Very cheap iterations even when 'n' is large.
  - Doesn't always decrease 'f'.
  - But solves problem if α^t goes to 0 at an appropriate rate.

Last Time: Stochastic Gradient

- Practical tricks when using stochastic gradient:
  - Constant step-sizes, binary search for step, stop using validation error.

- Stochastic gradient converges very slowly:
  - But if your dataset is too big, there may not be much you can do.
  - Improved by “mini-batches” or “variance-reduced” methods (SAG, SVRG).

- It allows using infinite datasets:
  - Directly optimizes test error and cannot overfit.
  - But can underfit.

Motivation: Discovering Food Allergies

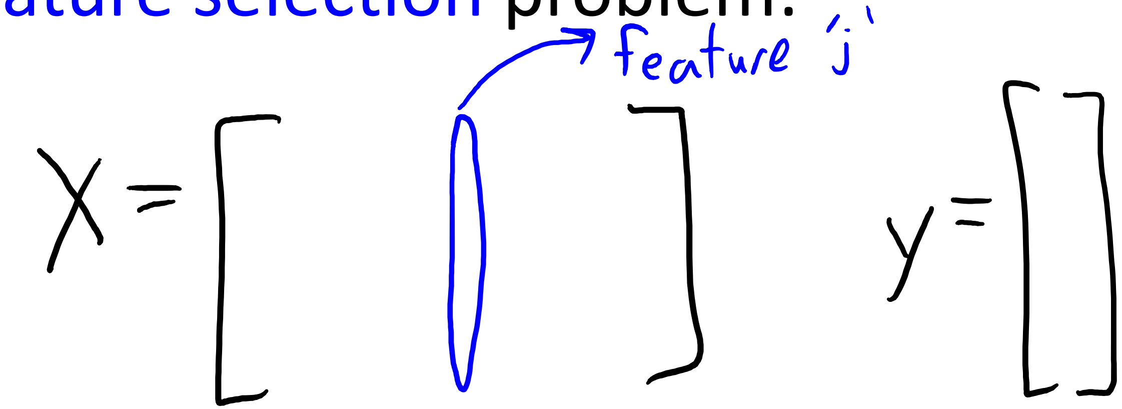
- Recall the food allergy example:

Egg	Milk	Fish	Wheat	Shellfish	Peanuts	…		Sick?
0	0.7	0	0.3	0	0		→	1
0.3	0.7	0	0.6	0	0.01		→	1
0	0	0	0.8	0	0		→	0
0.3	0.7	1.2	0	0.10	0.01		→	1

- Instead of predicting “sick”, we want to do feature selection:
  - Which foods are “relevant” for predicting “sick”.

Feature Selection

- General feature selection problem:



  - Find the features (columns) of ‘X’ that are important for predicting ‘y’.
    - “What are the relevant factors?”
    - “What is the right basis?”

- One of most important problems in ML/statistics:
  - But it’s very very messy…

Is “Relevance” Clearly Defined?

- Consider a supervised classification task:

gender	mom	dad
F	1	0
M	0	1
F	0	0
F	1	1

SNP
1
0
0
1

- Predict whether someone has a particular genetic variation (SNP).
  - Location of mutation is in “mitochondrial” DNA.
    - “You almost always have the same value as your mom”.

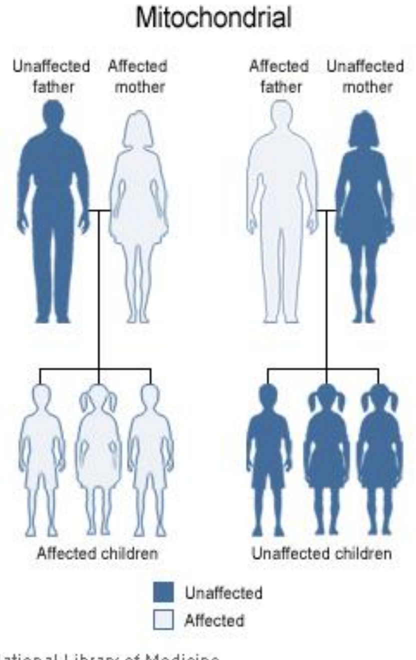
Is “Relevance” Clearly Defined?

- Consider a supervised classification task:

gender	mom	dad
F	1	0
M	0	1
F	0	0
F	1	1

SNP
1
0
0
1

- True model:
  - (SNP = mom) with very high probability.
  - (SNP != mom) with some very low probability.
- What are the “relevant” features for this problem?
  - Mom is relevant and {gender, dad} are not relevant.



U.S. National Library of Medicine

https://en.wikipedia.org/wiki/Human_mitochondrial_genetics

Is “Relevance” Clearly Defined?

- What if “mom” feature is repeated?

gender	mom	dad	mom2
F	1	0	1
M	0	1	0
F	0	0	0
F	1	1	1

SNP
1
0
0
1

- Are “mom” and “mom2” relevant?
  - Should we pick them both?
  - Should we pick one because it lets predict the other?

Neither of these is “correct”, but not picking either is incorrect.

- General problem (“dependence”, “collinearity” for linear models):
  - If features can be predicted from features, don’t know one(s) to pick.

Is “Relevance” Clearly Defined?

- What if we add “grandma”?

gender	mom	dad	grandma
F	1	0	1
M	0	1	0
F	0	0	0
F	1	1	1

SNP
1
0
0
1

- Is “grandma” relevant?
  - You can predict SNP very accurately from “grandma” alone.
  - But “grandma” is irrelevant if I know “mom”.
- General problem (conditional independence):
  - “Relevant” features may be irrelevant given other features.

Is “Relevance” Clearly Defined?

- What if we don’t know “mom”?

gender	grandma	dad
F	1	0
M	0	1
F	0	0
F	1	1

SNP
1
0
0
1

- Now is “grandma” is relevant?
  - Without “mom” variable, using “grandma” is the best you can do.
- General problem:
  - Features can be relevant due to missing information.

Is “Relevance” Clearly Defined?

- What if we don’t know “mom” or “grandma”?

gender	dad
F	0
M	1
F	0
F	1

SNP
1
0
0
1

- Now there are no relevant variables, right?
  – But “dad” and “mom” must have some common maternal ancestor.
  – “Mitochondrial Eve” estimated to be ~200,000 years ago.
- General problem (effect size):
  – “Relevant” features may have small effects.

Is “Relevance” Clearly Defined?

- What if we don’t know “mom” or “grandma”?

gender	dad
F	0
M	1
F	0
F	1

SNP
1
0
0
1

- Now there are no relevant variables, right?
  - What if “mom” likes “dad” because he has the same SNP as her?
- General problem (confounding):
  - Hidden effects can make “irrelevant” variables “relevant”.

Is “Relevance” Clearly Defined?

- What if we add “sibling”?

gender	dad	sibling
F	0	1
M	1	0
F	0	0
F	1	1

SNP
1
0
0
1

- Sibling is “relevant” for predicting SNP, but it’s not the cause.
- General problem (non-causality or reverse causality):
  – A “relevant” feature may not be causal, or may be an effect of label.

Is “Relevance” Clearly Defined?

- What if we add “baby”?

gender	dad	baby
F	0	1
M	1	1
F	0	0
F	1	1

SNP
1
0
0
1

- “Baby” is relevant when (gender == F).
  - “Baby” is relevant (though causality is reversed).
  - Is “gender” relevant?
    - If we want to find relevant factors, “gender” is not relevant.
    - If we want to predict SNP, “gender” is relevant.
- General problems (context-specific relevance):
  - Adding a feature can make an “irrelevant” feature “relevant”.

Is “Relevance” Clearly Defined?

- Warnings about feature selection:
  - A feature is only “relevant” in the context of available features.
    - Adding/removing features can make features relevant/irrelevant.
  - Confounding factors can make “irrelevant” variables the most “relevant”.
  - If features can be predicted from features, you can’t know which to pick.
  - A “relevant” feature may have a tiny effect.
  - “Relevance” for prediction does not imply a causal relationship.

Is this hopeless?

- In the end, we often want to do feature selection we so have to try!

- We won't be able to resolve causality or confounding.
  - So "relevance" could mean "affect by confounding" or "affected by label".
  - This can sometimes be addressed by the way you collect data.

- Different methods will behave differently with respect to:
  - Tiny effects.
  - Context-specific relevance (is "gender" relevant if given "baby"?).
  - Variable dependence ("mom" and "mom2" have same information).
  - Conditional independence ("grandma" is irrelevant given "mom").

Application-Specific

You can do this wrong

“Association” Approach to Feature Selection

- A simple/common way to do feature selection:

```
for $j = 1:d$
    compute "similarity" between $X(:,j)$ and $y$
    Say 'j' is "relevant" if "similarity" is above a threshold.
```

  - “Similarity” could be correlation, mutual information, etc.
- Ignores tiny effects.
- Reasonable for variable dependence: it will take “mom” and “mom2”.
- Not reasonable for conditional independence:
  - It will take “grandma”, “great-grandma”, “great-great grandma”, etc.

  Systematically includes irrelevant variables.
- Not reasonable for context-specific relevance:
  - If two features aren’t relevant on their own, then both set as “irrelevant”. (This method will say “gender” is “irrelevant” given “baby”.)

"Regression Weight" Approach to Feature Selection

- A simple/common approach to feature selection:

  Fit 'w' using least squares

  Take all features 'j' where $|w_j|$ is greater than some threshold.

- Deals very badly with variable dependence:
  - If can take two irrelevant collinear variables:
    - Set one w_j hugely positive and the other hugely negative.

    } → Systematically adds irrelevant variables
  - Means it can allow tiny effects.
  - It could take any subset of {"mom","mom2","mom3"}, including none.

    → This is bad
- It should address conditional independence:
  - Should take "mom" but not "grandma" if you get enough data.
- It addresses context-specific relevance, if effect is linear.
  - This one says "gender" is "relevant".

“Regression Weight” Approach to Feature Selection

- A simple/common approach to feature selection:

  Fit 'w' using least squares with L_2-regularization.

  Take all features 'j' where $|w_j|$ is greater than some threshold.

- Same good properties with respect to independence/context.
- Deals less badly with collinearity:
  - If you two have irrelevant collinear variables, doesn’t take them.
  - No longer allows tiny affects.
  - But it could say “mom” and “mom2” are both irrelevant. → Bad!
    - Sum of their weights could be above threshold, with neither weight above threshold.

Common Approaches to Feature Selection

- 3 main “advanced” approaches to feature selection:
  1. Hypothesis testing.
  2. Search and score.
  3. L1-Regularization.

- None is ideal, but good to know advantages/disadvantages.

Feature Selection Approach 1: Hypothesis Testing

- Hypothesis testing ("constraint-based") approach:
  - Performs a sequence of conditional independence tests.

$$\underset{\text{feature 'j'}}{X_j} \perp \underset{\text{label}}{Y} \mid \underset{\text{other features 's'}}{X_s}$$

"If I know features in 's' does feature 'j' tell me anything about label?"

  - If they are independent, say that 'j' is "irrelevant".
- Common way to do the tests:
  - "Partial" correlation (numerical data).
  - "Conditional" mutual information (discrete data).

Hypothesis Testing

- Hypothesis testing ("constraint-based") approach:
  - Performs a sequence of conditional independence tests.

$$X_j \perp Y \mid X_s$$

feature 'j' label other features 's'

"If I know features in 's' does feature 'j' tell me anything about label?"

  - If they are independent, say that 'j' is "irrelevant".
- Two many possible tests, "greedy" method is for each 'j' do:

First test if $X_j \perp Y$

If still dependent test $X_j \perp Y \mid X_s$ where 's' has one feature

If still dependent test $X_j \perp Y \mid X_s$ where 's' has one more feature

⋮

If still dependent when 's' includes all other features, declare 'j' relevant.

Often choose features to minimize dependence.

Hypothesis Testing Issues

- Advantages:
  - Deals with conditional independence.
  - Algorithm can explain why it thinks ‘j’ is irrelevant.
  - Doesn’t necessarily need linearity.
- Disadvantages:
  - Deals badly with variable dependence: doesn’t select “mom” or “mom2” if both present.
  - Usual warning about testing multiple hypotheses:
    - If you test $p < 0.05$ more than 20 times, you’re going to make errors.
  - Greedy approach may be sub-optimal.
- Neither good nor bad:
  - Allow tiny effects.
  - Says “gender” is irrelevant when you know “baby”.
  - This approach is better for finding relevant factors, not to select features for learning.

Feature Selection Approach 2: Search and Score

- Two components behind search and score methods:
  - Define a score function f(s) that says how "good" a set of variables 's' are:
  - Now search for the variables 's' with the best value of f(s).

- Under usual score functions, very hard to find the best 's'.
- Usual greedy approach is forward selection:
  - Start with 's' empty, add variable that increase score the most, repeat.

- Many variations like "backward" and "stagewise" selection.

Feature Selection Approach 2: Search and Score

- Two components behind search and score methods:
  - Define a score function f(s) that says how “good” a set of variables ‘s’ are:
  - Now search for the variables ‘s’ with the best value of f(s).

- Can’t use training error as the score: you’ll just add all features.
- Usual score functions:
  - Validation/cross-validation:
    - Good if your goal is prediction.
    - Tends to give false positives because you search over many subsets.
  - L0-”norm”:
    - Balance training error and number of non-zero variables.

L0-Norm

- In linear models, setting $w_j = 0$ is the same as removing feature ‘j’:

$$y_i = w_1 x_{i1} + \underbrace{w_2 x_{i2}}_{\downarrow \text{ set } w_2 = 0} + w_3 x_{i3} + \cdots + w_d x_{id}$$

$$y_i = w_1 x_{i1} + \underbrace{0}_{\text{ignore } x_{i2}} + w_3 x_{i3} + \cdots + w_d x_{id}$$

- The L0 “norm” is the number of non-zero values.

$$\text{If } w = \begin{bmatrix} 1 \\ 0 \\ 2 \\ 0 \\ 3 \end{bmatrix} \text{ then } \|w\|_0 = 3 \qquad \text{If } w = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \text{ then } \|w\|_0 = 0.$$

  - Not actually a true norm.
  - A vector with many elements set to 0 is called a sparse vector.

L0-Norm

- L0-norm regularization for feature selection:

$$f(w) = \frac{1}{2}\|Xw - y\|^2 + \lambda\|w\|_0$$

- Balances between training error and number of features.
- Different values of λ give common feature selection scores:
    - Akaike information criterion (AIC).
    - Bayesian information criterion (BIC).
- To we use f(w) to score features ‘s’:
    – Solve least squares problem using only features ‘s’.
    – Compute f(w) above with all other w_j set to zero.

Search and Score Issues

- Advantages:
  - Deals with conditional independence (if linear).
  - Sort of deals with collinearity:
    - Cross-validation picks at least one of “mom” and “mom2”.
    - L0-norm will pick only one of “mom” or “mom2”.
- Disadvantages:
  - Difficult to define ‘correct’ score:
    - Cross-validation often selects too many.
    - L0-norm selects too few/many depending on λ.
  - Under most scores, it’s hard to find optimal features.
- Neither good nor bad:
  - Does not take small effects.
  - Says “gender” is relevant if we know “baby”.
  - This approach is better for prediction than the previous approaches.

Summary

- Feature selection is task of choosing the relevant features.
  - Hard to define "relevant" and many problems that can have.
  - Obvious approaches have obvious problems.
- Hypothesis testing: find sets that make y_i and x_{ij} independent.
- Search and score: find features that optimize some score.

- Next time:
  - Midterm.