Simple Variable Selection
LASSO: Sparse Regression

Machine Learning – CSE546
Sham Kakade
University of Washington

October 11, 2016

Announcements:

- HW1 due on Friday.
- Readings: please do them.
- Project Proposals: please start thinking about it!

- Today:
  - Review: cross validation
  - Feature selection
  - Lasso

Review: Cross-Validation

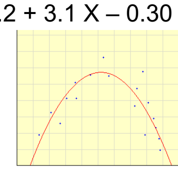
Machine Learning – CSE546
Sham Kakade
University of Washington

October 6, 2016

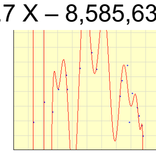
Regularization in Regression

- 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 + …



- ***Regularization:*** or "Shrinkage" procedure

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

- **How do we pick the regularization constant λ?? (and pick models?)**
  - We could use the test set? Or another hold out set?

(LOO) Leave-one-out cross validation

- Consider a **validation set with 1 example**:
  - D – training data
  - $D\backslash j$ – training data with j th data point moved to validation set
- **Learn classifier $h_{D\backslash j}$ with $D\backslash j$ dataset**
- **Estimate true error** as squared error on predicting $t(\mathbf{x}_j)$:
  - Unbiased estimate of $error_{true}(h_{D\backslash j})$!
  - 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 $h_{D\backslash j}$**
  - **Estimate error** as:

$$error_{LOO} = \frac{1}{N}\sum_{j=1}^{N}\left(t(\mathbf{x}_j) - h_{\mathcal{D}\backslash j}(\mathbf{x}_j)\right)^2$$

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**!
  - Asymptotically (for large N), under some conditions.
  - It is reasonable to use in practice.
  - **Great news: Use LOO error for model selection!! (e.g., picking λ)**
- **LOO is computationally costly**! (exception: see HW)
  - You have to run your algorithm N times.
  - Practice: "K-fold" cross validation

What you need to know…

- Never ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever train on the test data
- Use cross-validation to choose parameters
  - Leave-one-out is usually the best, but it is slow…
  - use k-fold cross-validation

Simple Variable Selection LASSO: Sparse Regression

Machine Learning – CSE546
Sham Kakade
University of Washington

October 11, 2016

Sparsity

- Vector **w** is sparse, if many entries are zero:
- Very useful for many tasks, e.g.,
  - **Efficiency**: If size(**w**) = 100B, each prediction is expensive:
    - If part of an online system, too slow
    - If **w** is sparse, prediction computation only depends on number of non-zeros
  - **Interpretability**: What are the relevant dimension to make a prediction?
    - E.g., what are the parts of the brain associated with particular words?
- But computationally intractable to perform "all subsets" regression

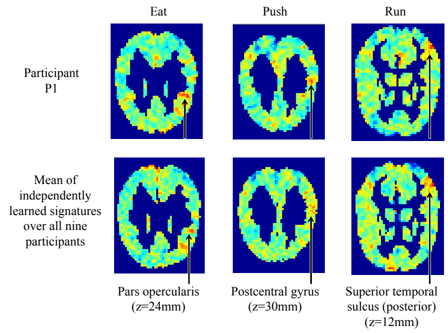


Figure from Tom Mitchell

Simple greedy model selection algorithm

- Pick a dictionary of features
  - e.g., polynomials for linear regression
- Greedy heuristic:
  - Start from empty (or simple) set of features $F_0 = \varnothing$
  - Run learning algorithm for current set of features F_t
    - Obtain weights for these features
  - Select **next best feature $h_i(x)^*$**
    - e.g., $h_j(x)$ that results in lowest training error learner when using $F_t + \{h_j(x)^*\}$
  - $F_{t+1} \leftarrow F_t + \{h_i(x)^*\}$
  - Recurse

Greedy model selection

- Applicable in many other settings:
  - Considered later in the course:
    - Logistic regression: Selecting features (basis functions)
    - Naïve Bayes: Selecting (independent) features $P(X_i|Y)$
    - Decision trees: Selecting leaves to expand
- Only a heuristic!
  - **Finding the best set of k features is computationally intractable!**
  - Sometimes you can prove something strong about it…
- There are many more elaborate methods out there

When do we stop???

- Greedy heuristic:
  - …
  - Select **next best feature X_i^***
    - E.g. $h_j(x)$ that results in lowest training error learner when using $F_t + \{h_j(x)^*\}$
  - Recurse

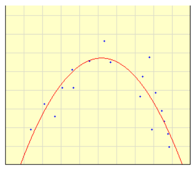
When do you stop???

- When training error is low enough?
- When test set error is low enough?
- Using cross validation?

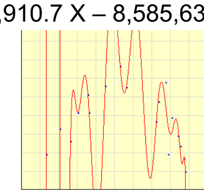
Regularization in Linear Regression

- 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

Variable Selection by Regularization

- Ridge regression: Penalizes large weights
- What if we want to perform "feature selection"?
  - E.g., Which regions of the brain are important for word prediction?
  - Can't simply choose features with largest coefficients in ridge solution
- Try new **(convex)** penalty: Penalize non-zero weights
  - Regularization penalty:
  - Leads to sparse solutions
  - Just like ridge regression, solution is indexed by a continuous param λ
  - Major impact in: statistics, machine learning & electrical engineering

LASSO Regression

- **LASSO:** least absolute shrinkage and selection operator

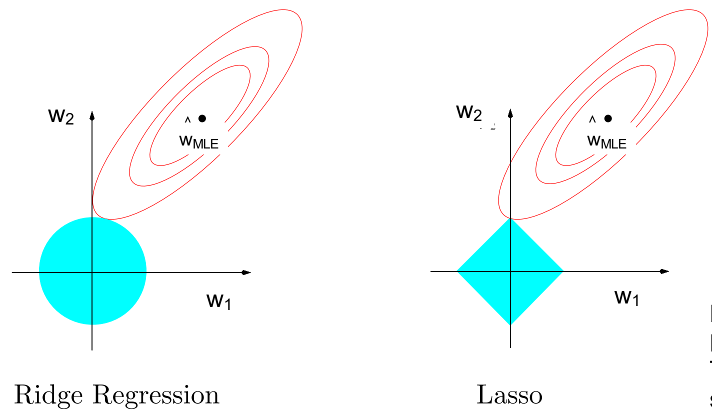
- New objective:

(Related) Constrained Optimization

- LASSO solution:

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

Geometric Intuition for Sparsity



From Rob Tibshirani slides

Optimizing the LASSO Objective

- LASSO solution:

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

Coordinate Descent

- Given a function F
  - Want to find minimum

- Often, hard to find minimum for all coordinates, but easy for one coordinate

- Coordinate descent:

- How do we pick next coordinate?

- Super useful approach for *many* problems
  - Converges to optimum in some cases, such as LASSO

Optimizing LASSO Objective One Coordinate at a Time

$$\sum_{j=1}^{N}\left(t(x_j)-(w_0+\sum_{i=1}^{k}w_ih_i(x_j))\right)^2+\lambda\sum_{i=1}^{k}|w_i|$$

- Taking the derivative:
  - Residual sum of squares (RSS):

$$\frac{\partial}{\partial w_\ell}RSS(\mathbf{w})=-2\sum_{j=1}^{N}h_\ell(x_j)\left(t(x_j)-(w_0+\sum_{i=1}^{k}w_ih_i(x_j))\right)$$

  - Penalty term:

Subgradients of Convex Functions

- Gradients lower bound convex functions:

- Gradients are unique at **w** iff function differentiable at **w**

- Subgradients: Generalize gradients to non-differentiable points:
  - Any plane that lower bounds function:

Taking the Subgradient

$$\sum_{j=1}^{N}\left(t(x_j) - (w_0 + \sum_{i=1}^{k} w_i h_i(x_j))\right)^2 + \lambda \sum_{i=1}^{k} |w_i|$$

- Gradient of RSS term:

$$\frac{\partial}{\partial w_\ell} RSS(\mathbf{w}) = a_\ell w_\ell - c_\ell$$

$$a_\ell = 2\sum_{j=1}^{N}(h_\ell(\mathbf{x}_j))^2$$

$$c_\ell = 2\sum_{j=1}^{N} h_\ell(\mathbf{x}_j)\left(t(\mathbf{x}_j) - (w_0 + \sum_{i\neq\ell} w_i h_i(\mathbf{x}_j))\right)$$

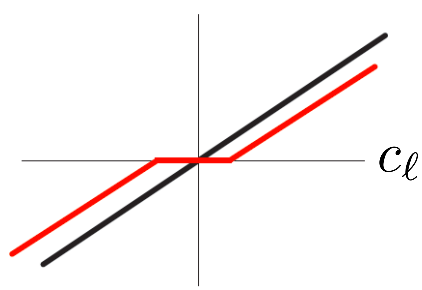
  - If no penalty:
- Subgradient of full objective:

Setting Subgradient to 0

$$\partial_{w_\ell} F(\mathbf{w}) = \begin{cases} a_\ell w_\ell - c_\ell - \lambda & w_\ell < 0 \\ [-c_\ell - \lambda, -c_\ell + \lambda] & w_\ell = 0 \\ a_\ell w_\ell - c_\ell + \lambda & w_\ell > 0 \end{cases}$$

Soft Thresholding

$$\hat{w}_\ell = \begin{cases} (c_\ell + \lambda)/a_\ell & c_\ell < -\lambda \\ 0 & c_\ell \in [-\lambda, \lambda] \\ (c_\ell - \lambda)/a_\ell & c_\ell > \lambda \end{cases}$$



From
Kevin Murphy
textbook

Coordinate Descent for LASSO (aka Shooting Algorithm)

- Repeat until convergence
  - Pick a coordinate *l* at (random or sequentially)
    - Set:

$$\hat{w}_\ell = \begin{cases} (c_\ell + \lambda)/a_\ell & c_\ell < -\lambda \\ 0 & c_\ell \in [-\lambda, \lambda] \\ (c_\ell - \lambda)/a_\ell & c_\ell > \lambda \end{cases}$$

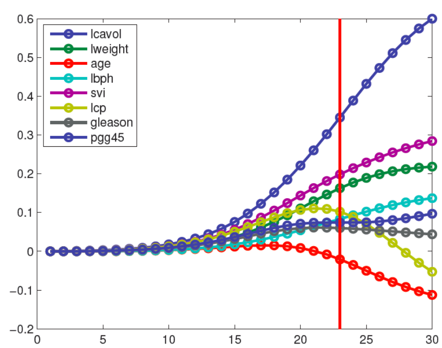
    - Where:

$$a_\ell = 2\sum_{j=1}^{N}(h_\ell(\mathbf{x}_j))^2$$

$$c_\ell = 2\sum_{j=1}^{N} h_\ell(\mathbf{x}_j)\left(t(\mathbf{x}_j) - (w_0 + \sum_{i\neq\ell} w_i h_i(\mathbf{x}_j))\right)$$

  - For convergence rates, see Shalev-Shwartz and Tewari 2009
- Other common technique = LARS
  - Least angle regression and shrinkage, Efron et al. 2004

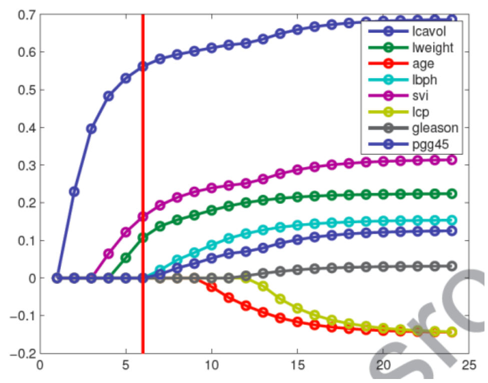
Recall: *Ridge Coefficient Path*



From Kevin Murphy textbook

- Typical approach: select λ using cross validation

Now: *LASSO Coefficient Path*



From
Kevin Murphy
textbook

What you need to know

- Variable Selection: find a sparse solution to learning problem
- L_1 regularization is one way to do variable selection
  - Applies beyond regression
  - Hundreds of other approaches out there
- LASSO objective non-differentiable, **but convex** ➔ Use subgradient
- No closed-form solution for minimization ➔ Use coordinate descent
- Shooting algorithm is simple approach for solving LASSO