Logistic Regression with L_2 Regularization

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1 INTRODUCTION

Machine Learning (ML) is a sub-discipline of Artificial Intelligence (AI) that focuses on the development and analysis of methods that produce models from data. An often referenced example application of ML is email spam filtering, but there is a wide variety of real-world problems where ML has been successful used, from object detection using a Microsoft Kinect sensor [1] to forecasting of power output from a photovoltaic solar farm [2].

ML algorithms are plentiful in number, but some are more suitable than others depending on the type of problem. Logistic regression is a ML algorithm well-suited to problems involving a set of real-valued inputs and a binary (Bernoulli) output. A real-world example of such a problem is whether a baseball player will hit a home run based on a collection of statistics (e.g. batting average, height, weight). The statistics are the real-valued inputs, whether he hits a home run is the binary output (1=yes, 0=no), and the probability of whether a player hits a home run is the determined using logistic regression.

In this paper we analyze logistic regressions capability for classification learning using a previously study as a baseline [3]. Aside from recreating the previous study's results, we also extend their work to comparing two gradient-based optimization methods for use in conjuction with the logistic regression: Stochastic Gradient Descent (SGD) and Limited-memory Broyden-Fletcher-Goldfarb-Shannon (L-BFGS).

2 DESIGN AND ANALYSIS OF ALGORITHMS

2.1 LOGISTIC REGRESSION

Given a set of real-valued features x with binary labels y (a training set), we can define logistic regression model as:

$$p(y|x;\alpha,\beta) = \frac{1}{1+\exp-[\sum_{j=0}^{d}\beta_j x_j]} \tag{1}$$

where d is the dimensionality of a training example, and β_j are parameters of the regression. To learn the logistic regression, we need deteremine β such that the Log Conditional Likelihood (LCL) is maximized. The LCL is defined as:

$$\text{LCL} = \sum_{i:y_i=1} logp_i + \sum_{i:y_i=0} log(1-p_i) \tag{2}$$

and is maximized when its derivative with respect to each parameter β_j is zero. For a single example the partial derivative of the LCL is:

$$\frac{\partial}{\partial\beta_j} logL(\beta;x,y) = (y-p)x_j \tag{3}$$

Stochastic gradient descent (SGD) and were each implemented in Matlab to maximize the total conditional log likelihood of each training data set. In brief, SGD incorporated a fixed learning rate λ to control the change in log likelihood, which was averaged over random mini-batches of size κ. To control over-fitting, logistic regression was used and change in the objective function was evaluated on a separate validation dataset containing 30% of all training examples selected at random. Convergence was reached when change in the objective function was less than ω or the total number of epochs was greater than ε (which ever came first). (Add brief overview of L-BFGS and cite MinFunc's implementation)

minFunc[4]

For each of these algorithms, the input training data is formatted as a set of n examples $x_i \ldots x_n$ where each x_j is a real-valued vector of d features. Each x_i is correlated to a binary (Bernoulli) outcome y_i by a global parameter vector β of length $d+1$. We assume this correlation follows the model below where $x_{i0} = 1$ for all i.

$$p_i = p(y_i|x_i;\beta) = \frac{1}{1+\exp-(\sum_{j=0}^{d}\beta_j\, x_{ij})} \tag{4}$$

2.2 L2 REGULARIZATION

In order to prevent overfitting of machine learning, a penalty was imposed to regulate the values of the parameters. A regularization constant μ was introduced into the LCL objective function:

$$\hat{B} = \text{argmax}_{\beta} LCL - \mu||\beta||_2^2 \tag{5}$$

where $||\beta||_2^2$ is the L_2 norm of the parameter vector. With this revision the derivative of the LCL becomes:

$$\frac{\partial}{\partial \beta_j}[logp(y|x;\beta) - \mu \sum_{j=0}^{d} \beta_j^2] = (y-p)x_j - 2\mu\beta_j \tag{6}$$

2.3 STOCHASTIC GRADIENT DESCENT

Our SGD implementation first randomized the order of input examples to avoid repeated computation of random numbers and partitioned the input data into $x_1 \ldots x_k$ *training* examples and $x_{k+1} \ldots x_n$ *validation* examples. Then sequential mini-batches of size $\kappa < k$ taken from the training set were used to update the parameter vector β (initialized to all zero values) by the following equation. The constant μ quantifies the trade-off between maximizing likelihood and minimizing parameter values for L_2 Regularization.

$$\beta := \beta + \frac{\lambda}{\kappa}\left[-2\mu\beta + \sum_{i=1}^{\kappa}(y_i - p_i)\, x_i\right] \tag{7}$$

After each update of β, absolute change in the objective $\widehat{\beta}$ was computed over all validation examples with the following function.

$$\widehat{\beta} = \mu\|\beta\|_2 + \sum_{i=k+1}^{n} -\log(p_i^{y_i}(1-p_i)^{1-y_i}) \tag{8}$$

Convergence was reached when change in the objective reached a value less than ω. Convergence was also reached if the total number of epochs was greater than ε. With this configuration, the time to run the SGD is O(nd).

2.3.1 Cross-Validation

SGD with cross-validation is represented by the following pseudo-code:

1. Initialize all parameter values β_j
2. Initialize all conditional probabilities p_i
3. Initialize the objective function and its difference value
4. Randomly divide the example set into two groups: testing set of m rows and validation set of (n-m) rows

5. while(objective function difference $\geq$ theshold AND number of epochs $<$ maximum epochs allowed
   (a) Randomly pick a sample of s rows out of the testing set
   (b) Update β_j for all features
   (c) Update the objective function

The algorithm was run ten times to generate 10 vectors of parameters. The ten vectors of parameters were averaged to calculate one vector with cross-validation. The result cross-validated vector was used to calculate the test error and its variance over all the instances. The test error was defined as the average value of the loss function:

$$\text{test error} = \sum_{i=1}^{n} -log(y_i|x_i;\beta) \tag{9}$$

2.4 LIMITED-MEMORY BFGS

Limited-memory Broyden-Fletcher-Goldfarb-Shannon (L-BFGS) is a quasi-Newton optimization method used to find local extrema.

3 DESIGN OF EXPERIMENTS

3.1 PRE-PROCESSING TRAINING DATA

normalization, concatation?

3.1.1 USPS-N

Digit 9 vs other digits

3.1.2 Web

anything special?

3.2 HYPERPARAMETERS

3.2.1 Learning Rate

How did we determine λ (the learning rate).

3.2.2 Regularization

How did we determine μ (the regularization constant).

4 RESULTS OF EXPERIMENTS

Results of experiments. Comparison of methods and data sets.

Table 1: Hyperparameters.

	λ	μ
SGD	1.0	1.0
SGD	0.1	1.0
SGD	0.01	1.0

4.1 USPS-N

How did SGD and L-BFGS perform on the USPS-N data sets.

4.2 WEB

How did SGD and L-BFGS perform on the Web data sets.

4.2.1 Figures

Figure 1: Comparison of SGD and L-BFGS for USPS-N (left) and Web (right) data sets.

5 FINDINGS AND LESSONS LEARNED

Findings and lessons learned.

References

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