Role of Lipschitz constant in Gradient Learning

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Abstract

Finding an optimal learning rate in gradient descent has typically been an empirical process. We attempt to mathematically compute an optimal value for the learning rate by exploiting functional properties of the loss function. By making only minimal assumptions about the functions, we argue that the inverse of the Lipschitz constant is this optimal value, and empirically show that this is indeed the case.

1 Introduction

Gradient descent is a popular optimization algorithm for finding optima for functions, and is used to find optima in loss functions in machine learning tasks. In an iterative process, it seeks to update randomly initialized weights to minimize the training error. These updates are typically small values proportional to the gradient of the loss function. The constant of proportionality is called the learning rate, and is usually manually chosen.

The gradient descent update rule is given by

$$\mathbf{w} := \mathbf{w} - \alpha \cdot \nabla_{\mathbf{w}} f$$

where f is the loss function. When the learning rate, α, is too small, then convergence takes a long time. However, when the learning rate is too large, the solution diverges.

For a function, the Lipschitz constant is the least positive constant L such that

$$\|f(\mathbf{w}_1) - f(\mathbf{w}_2)\| \leq L \|\mathbf{w}_1 - \mathbf{w}_2\|$$

for all $\mathbf{w}_1, \mathbf{w}_2$ in the domain of f. From the mean-value theorem for scalar fields, for any $\mathbf{w}_1, \mathbf{w}_2$, there exists $\mathbf{v}$ such that

$$
\begin{aligned}
\|f(\mathbf{w}_1) - f(\mathbf{w}_2)\| &= \|\nabla_{\mathbf{w}} f(\mathbf{v})\| \|\mathbf{w}_1 - \mathbf{w}_2\| \\
&\leq \sup_{\mathbf{v}} \|\nabla_{\mathbf{w}} f(\mathbf{v})\| \|\mathbf{w}_1 - \mathbf{w}_2\|
\end{aligned}
$$

Thus, $\sup_{\mathbf{v}} \|\nabla_{\mathbf{w}} f(\mathbf{v})\|$ is such an L. Since L is the least such constant,

$$L \leq \sup_{\mathbf{v}} \|\nabla_{\mathbf{w}} f(\mathbf{v})\|$$

In this paper, we use $\max |\nabla_{\mathbf{w}} f|$ to derive the Lipschitz constants. Our approach makes the minimal assumption that the functions are Lipschitz continuous and differentiable. Because the gradient of these loss functions is used in gradient descent, these conditions are guaranteed to be satisfied.

By setting $\alpha = \frac{1}{L}$, we have $\Delta\mathbf{w} \leq 1$, constraining the change in the weights. This makes it optimal to set the learning rate to the reciprocal of the Lipschitz constant. The following sections show the derivation for the Lipschitz constants for various loss functions. Note that the derived constants are in terms of the data, which is a constant with respect to the weight vector.

2 Least squares cost function

We have,

$$g(\mathbf{w}) = \frac{1}{2m} \sum_{i=1}^{m} \left(\mathbf{x}^{(i)}\mathbf{w} - y^{(i)} \right)^2$$

Thus,

$$
\begin{aligned}
g(\mathbf{w}) - g(\mathbf{v}) &= \frac{1}{2m} \sum_{i=1}^{m} \left(\mathbf{x}^{(i)}\mathbf{w} - y^{(i)} \right)^2 - \left(\mathbf{x}^{(i)}\mathbf{v} - y^{(i)} \right)^2 \\
&= \frac{1}{2m} \sum_{i=1}^{m} \left(\mathbf{x}^{(i)}(\mathbf{w}+\mathbf{v}) - 2y^{(i)} \right) \left(\mathbf{x}^{(i)}(\mathbf{w}-\mathbf{v}) \right) \\
&= \frac{1}{2m} \sum_{i=1}^{m} \left((\mathbf{w}+\mathbf{v})^T \mathbf{x}^{(i)T} - 2y^{(i)} \right) \left(\mathbf{x}^{(i)}(\mathbf{w}-\mathbf{v}) \right) \\
&= \frac{1}{2m} \sum_{i=1}^{m} \left((\mathbf{w}+\mathbf{v})^T \mathbf{x}^{(i)T}\mathbf{x}^{(i)} - 2y^{(i)}\mathbf{x}^{(i)} \right) (\mathbf{w}-\mathbf{v})
\end{aligned}
$$

The penultimate step is obtained by observing that $(\mathbf{w}+\mathbf{v})^T\mathbf{x}^{(i)T}$ is a real number, whose transpose is itself.

At this point, we take the norm on both sides, and then assume that $\mathbf{w}$ and $\mathbf{v}$ are bounded such that $\|\mathbf{w}\|, \|\mathbf{v}\| \leq K$. Taking norm on both sides,

$$\boxed{\frac{\|g(\mathbf{w}) - g(\mathbf{v})\|}{\|\mathbf{w}-\mathbf{v}\|} \leq \frac{K}{m} \left\| \mathbf{X}^T\mathbf{X} \right\| - \frac{1}{m} \left\| \mathbf{y}^T\mathbf{X} \right\|}$$

We are forced to use separate norms because the matrix subtraction $2K\mathbf{X}^T\mathbf{X} - 2\mathbf{y}^T\mathbf{X}$ cannot be performed. The RHS here is the Lipschitz constant. Note that the Lipschitz constant changes if the cost function is considered with a factor other than $\frac{1}{2m}$.

2.1 An alternate derivation

The least-squares system can also be formulated as

$$
\begin{aligned}
L(\mathbf{w}) &= \|\mathbf{X}\mathbf{w} - \mathbf{y}\| \\
&= (\mathbf{X}\mathbf{w} - \mathbf{y})^T (\mathbf{X}\mathbf{w} - \mathbf{y})
\end{aligned}
$$

Then, we have

$$L(\mathbf{b}) - L(\mathbf{a}) = (X\mathbf{b} - Y)^T(X\mathbf{b} - Y) - (X\mathbf{a} - Y)^T(X\mathbf{a} - Y)$$

$$= (\mathbf{b}^T X^T - Y^T)(X\mathbf{b} - Y) - (\mathbf{a}^T X^T - Y^T)(X\mathbf{a} - Y)$$

$$= \mathbf{b}^T X^T X\mathbf{b} - \mathbf{b}^T X^T Y - Y^T X\mathbf{b} + Y^T Y - \mathbf{a}^T X^T X\mathbf{a} + \mathbf{a}^T X^T Y + Y^T X\mathbf{a} - Y^T Y$$

$$= \mathbf{b}^T X^T X\mathbf{b} - \mathbf{b}^T X^T Y - Y^T X\mathbf{b} - \mathbf{a}^T X^T X\mathbf{a} + \mathbf{a}^T X^T Y + Y^T X\mathbf{a}$$

$$= \mathbf{b}^T X^T X\mathbf{b} - 2Y^T X\mathbf{b} - \mathbf{a}^T X^T X\mathbf{a} + 2Y^T X\mathbf{a}$$

$$= \mathbf{b}^T X^T X\mathbf{b} - \mathbf{a}^T X^T X\mathbf{a} - 2Y^T X(\mathbf{b} - \mathbf{a})$$

$$= (\mathbf{b} - \mathbf{a} + \mathbf{a})^T X^T X\mathbf{b} - \mathbf{a}^T X^T X\mathbf{a} - 2Y^T X(\mathbf{b} - \mathbf{a})$$

$$= (\mathbf{b} - \mathbf{a})^T X^T X\mathbf{b} + \mathbf{a}^T X^T X\mathbf{b} - \mathbf{a}^T X^T X\mathbf{a} - 2Y^T X(\mathbf{b} - \mathbf{a})$$

$$= (\mathbf{b} - \mathbf{a})^T X^T X\mathbf{b} + \mathbf{a}^T X^T X(\mathbf{b} - \mathbf{a}) - 2Y^T X(\mathbf{b} - \mathbf{a})$$

$$= (\mathbf{b} - \mathbf{a})^T X^T X(\mathbf{b} - \mathbf{a} + \mathbf{a}) + \mathbf{a}^T X^T X(\mathbf{b} - \mathbf{a}) - 2Y^T X(\mathbf{b} - \mathbf{a})$$

$$= (\mathbf{b} - \mathbf{a})^T X^T X\mathbf{a} + \mathbf{a}^T X^T X(\mathbf{b} - \mathbf{a}) + (\mathbf{b} - \mathbf{a})^T X^T X(\mathbf{b} - \mathbf{a}) - 2Y^T X(\mathbf{b} - \mathbf{a})$$

$$= \mathbf{a}^T X^T X(\mathbf{b} - \mathbf{a}) + \mathbf{a}^T X^T X(\mathbf{b} - \mathbf{a}) + (\mathbf{b} - \mathbf{a})^T X^T X(\mathbf{b} - \mathbf{a}) - 2Y^T X(\mathbf{b} - \mathbf{a})$$

$$= 2\mathbf{a}^T X^T X(\mathbf{b} - \mathbf{a}) + (\mathbf{b} - \mathbf{a})^T X^T X(\mathbf{b} - \mathbf{a}) - 2Y^T X(\mathbf{b} - \mathbf{a})$$

The triangle inequality now gives us,

$$L(\mathbf{b}) - L(\mathbf{a}) \le \left(2\|\mathbf{a}\| \|X^T X\| - 2\|Y^T X\| + \|\mathbf{b} - \mathbf{a}\| \|X^T X\|\right) \|\mathbf{b} - \mathbf{a}\|$$

Assuming $\|\mathbf{a}\|, \|\mathbf{b}\| \le K$,

$$L(\mathbf{b}) - L(\mathbf{a}) \le \left(2K\|X^T X\| - 2\|Y^T X\|\right) \|\mathbf{b} - \mathbf{a}\|$$

and so we can set the Lipschitz constant to

$$\boxed{L = 2K\|X^T X\| - 2\|Y^T X\|}$$

3   Binary cross-entropy function

We have,

$$g(\mathbf{w}) = \frac{1}{m}\sum_{i=1}^{m} -y^{(i)}\log\left(\frac{1}{1 + e^{-\mathbf{w}^T\mathbf{x}^{(i)}}}\right) - (1 - y^{(i)})\log\left(1 - \frac{1}{1 + e^{-\mathbf{w}^T\mathbf{x}^{(i)}}}\right)$$

The gradient is then,

$$\frac{\partial}{\partial \mathbf{w}_j} g(\mathbf{w}) = \frac{\partial}{\partial \mathbf{w}_j}\left(\frac{-1}{m}\sum_{i=1}^{m} y^{(i)}\log\left(h(\mathbf{x}^{(i)})\right) + (1 - y^{(i)})\log\left(1 - h(\mathbf{x}^{(i)})\right)\right)$$

$$= \frac{-1}{m}\sum_{i=1}^{m}\left(\frac{y^{(i)}}{h(\mathbf{x}^{(i)})}h'(\mathbf{x}^{(i)}) + \frac{1 - y^{(i)}}{1 - h(\mathbf{x}^{(i)})}(-h'(\mathbf{x}^{(i)}))\right)$$

$$= \frac{-1}{m}\sum_{i=1}^{m}\left(\frac{y^{(i)}}{h(\mathbf{x}^{(i)})}h(\mathbf{x}^{(i)})(1 - h(\mathbf{x}^{(i)}))(\mathbf{x}_j^{(i)}) - \frac{1 - y^{(i)}}{1 - h(\mathbf{x}^{(i)})}h(\mathbf{x}^{(i)})(1 - h(\mathbf{x}^{(i)}))(x_j^{(i)})\right)$$

$$= \frac{-1}{m}\sum_{i=1}^{m}\left(y^{(i)}(1 - h(\mathbf{x}^{(i)}))(\mathbf{x}_j^{(i)}) - (1 - y^{(i)})h(\mathbf{x}^{(i)})(x_j^{(i)})\right)$$

$$= \frac{-1}{m}\sum_{i=1}^{m}\left(y^{(i)}(1 - h(\mathbf{x}^{(i)})) - (1 - y^{(i)})h(\mathbf{x}^{(i)})\right)x_j^{(i)}$$

$$= \frac{1}{m}\sum_{i=1}^{m}\left(y^{(i)} - y^{(i)}h(\mathbf{x}^{(i)}) - h(\mathbf{x}^{(i)}) + y^{(i)}h(\mathbf{x}^{(i)})\right)x_j^{(i)}$$

$$= \frac{1}{m}\sum_{i=1}^{m}\left(h(\mathbf{x}^{(i)}) - y^{(i)}\right)x_j^{(i)}$$

where $h(\mathbf{x}^{(i)}) = \frac{1}{1+e^{-\mathbf{w}^T\mathbf{x}^{(i)}}}$. It is trivial to show that the maximum of this occurs when $h(\mathbf{x}^{(i)}) = \frac{1}{2}$.

Thus, the Lipschitz constant is

$$\boxed{L = \frac{1}{2m}\,\|\mathbf{X}\|}$$

4 Softmax loss function

The softmax loss is defined as

$$g(\mathbf{w}) = -\frac{1}{m}\sum_{i=1}^{m}\sum_{j=1}^{k}[y^{(i)} = j]\log\left(\frac{e^{\Theta_j^T\mathbf{x}^{(i)}}}{\sum_{l=1}^{k}e^{\Theta_l^T\mathbf{x}^{(i)}}}\right)$$

Here, we are using the Iverson notation: the expression $[y^{(i)} = j]$ is 1 if the condition is true, and 0 otherwise. To find the Lipschitz constant, we require the derivative of the softmax function, which is the fraction in the log term.

$$
\begin{aligned}
\frac{\partial}{\partial\Theta_p}\left(\frac{e^{\Theta_j^T\mathbf{x}^{(i)}}}{\sum_{l=1}^{k}e^{\Theta_l^T\mathbf{x}^{(i)}}}\right) &= \frac{\partial}{\partial\Theta_p^T\mathbf{x}^{(i)}}\left(\frac{e^{\Theta_j^T\mathbf{x}^{(i)}}}{\sum_{l=1}^{k}e^{\Theta_l^T\mathbf{x}^{(i)}}}\right)\cdot\frac{\partial}{\partial\Theta_p}\left(\Theta_p^T\mathbf{x}^{(i)}\right) \\
&= \frac{\frac{\partial}{\partial\Theta_p^T\mathbf{x}^{(i)}}\left(e^{\Theta_j^T\mathbf{x}^{(i)}}\right)\sum_{l=1}^{k}e^{\Theta_l^T\mathbf{x}^{(i)}} - e^{\Theta_j^T\mathbf{x}^{(i)}}\frac{\partial}{\partial\Theta_p^T\mathbf{x}^{(i)}}\left(\sum_{l=1}^{k}e^{\Theta_j^T\mathbf{x}^{(i)}}\right)}{\left(\sum_{l=1}^{k}e^{\Theta_l^T\mathbf{x}^{(i)}}\right)^2}\frac{\partial}{\partial\Theta_p^T}\left(\Theta_p^T\mathbf{x}^{(i)}\right) \\
&= \frac{[p=j]e^{\Theta_j^T\mathbf{x}^{(i)}}\sum_{l=1}^{k}e^{\Theta_l^T\mathbf{x}^{(i)}} - e^{\Theta_j^T\mathbf{x}^{(i)}}\cdot e^{\Theta_p^T\mathbf{x}^{(i)}}}{\left(\sum_{l=1}^{k}e^{\Theta_l^T\mathbf{x}^{(i)}}\right)^2}\cdot\mathbf{x}^{(i)} \\
&= \left(\frac{[p=j]e^{\Theta_j^T\mathbf{x}^{(i)}}}{\sum_{l=1}^{k}e^{\Theta_l^T\mathbf{x}^{(i)}}} - \frac{e^{\Theta_j^T\mathbf{x}^{(i)}}}{\sum_{l=1}^{k}e^{\Theta_l^T\mathbf{x}^{(i)}}}\cdot\frac{e^{\Theta_p^T\mathbf{x}^{(i)}}}{\sum_{l=1}^{k}e^{\Theta_l^T\mathbf{x}^{(i)}}}\right)\cdot\mathbf{x}^{(i)} \\
&= ([p=j]s_j - s_j s_p)\cdot\mathbf{x}^{(i)} \\
&= s_j([p=j] - s_p)\mathbf{x}^{(i)}
\end{aligned}
$$

The first step uses the chain rule for derivatives. The second step applies the quotient rule. The third step is obtained by noting that the partial derivative is taken with respect to $\Theta_p^T\mathbf{x}^{(i)}$. We then simplify, split the fraction into two, and cancel out terms. Finally, we use the notation s_j to denote the softmax function. In a more concise fashion, we write the above result as:

$$\frac{\partial}{\partial\Theta_p}s_j = s_j([p=j] - s_p)\mathbf{x}^{(i)} \tag{1}$$

4

We can now use (1) to find the gradient of g.

$$\nabla_{\boldsymbol{\Theta}_p} g = -\frac{1}{m} \sum_{i=1}^{m} \sum_{j=1}^{k} \nabla_{\boldsymbol{\Theta}_p} [y^{(i)} = j] \log s_j$$

$$= -\frac{1}{m} \sum_{i=1}^{m} \sum_{j=1}^{k} \frac{[y^{(i)} = j]}{s_j} \nabla_{\boldsymbol{\Theta}_p} s_j$$

$$= -\frac{1}{m} \sum_{i=1}^{m} \sum_{j=p} [y^{(i)} = j](1 - s_p)\mathbf{x}^{(i)} - \frac{1}{m} \sum_{i=1}^{m} \sum_{j\neq p} [y^{(i)} = j](-s_p)\mathbf{x}^{(i)}$$

$$= -\frac{1}{m} \sum_{i=1}^{m} \sum_{j=p} [y^{(i)} = j]\mathbf{x}^{(i)} + \frac{1}{m} \sum_{i=1}^{m} \sum_{j=p} [y^{(i)} = j]s_p\mathbf{x}^{(i)} + \frac{1}{m} \sum_{i=1}^{m} \sum_{j\neq p} [y^{(i)} = j]s_p\mathbf{x}^{(i)}$$

$$= -\frac{1}{m} \sum_{i=1}^{m} [y^{(i)} = p]\mathbf{x}^{(i)} + \frac{1}{m} \sum_{i=1}^{m} [y^{(i)} = p]s_p\mathbf{x}^{(i)} + \frac{1}{m} \sum_{i=1}^{m} [y^{(i)} \neq p]s_p\mathbf{x}^{(i)}$$

$$= -\frac{1}{m} \sum_{i=1}^{m} [y^{(i)} = p]\mathbf{x}^{(i)} + \frac{1}{m} \sum_{i=1}^{m} s_p\mathbf{x}^{(i)} \left([y^{(i)} = p] + [y^{(i)} \neq p] \right)$$

$$= -\frac{1}{m} \sum_{i=1}^{m} [y^{(i)} = p]\mathbf{x}^{(i)} + \frac{1}{m} \sum_{i=1}^{m} s_p\mathbf{x}^{(i)}$$

Thus,

$$\nabla_{\boldsymbol{\Theta}_p} g = \frac{1}{m} \sum_{i=1}^{m} \mathbf{x}^{(i)} \left(s_p - [y^{(i)} = p] \right) \tag{2}$$

In the limiting case, all the softmax values are equal, and $y^{(i)} = p$; for k classes, $s_p = \frac{1}{k}$, yielding $|s_p - 1| = \frac{k-1}{k}$ so we get the inequality

$$|[y^{(i)} = p](s_p - 1)| \leq \frac{k-1}{k} \tag{3}$$

Using (3) in (2), we get

$$|\nabla_{\boldsymbol{\Theta}_p} g| \leq \frac{k-1}{km} \sum_{i=1}^{m} \mathbf{x}^{(i)}$$

and thus we obtain the Lipschitz constant for the softmax loss function:

$$\boxed{L = \frac{k-1}{km} \|\mathbf{X}\|}$$

5   A note on regularization

It should be noted that this framework is extensible to the case where the loss function includes a regularization term.

In particular, if an L_2 regularization term, $\frac{\lambda}{2} \|\mathbf{w}\|_2^2$ is added, it is trivial to show that the Lipschitz constant increases by λK, where K is the upper bound for $\|\mathbf{w}\|$. More generally, if a Tikhonov regularization term, $\|\boldsymbol{\Gamma}\mathbf{w}\|_2^2$ term is added, then the increase in the Lipschitz constant can be computed in the same way as shown in the alternate derivation for the least-squares loss above. For the sake of continuity, we show a succinct version of the derivation below:
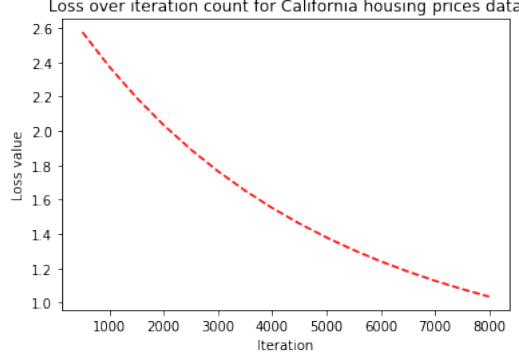
Figure 1: Loss function over iterations for California housing prices dataset

$$L(\mathbf{w}_1) - L(\mathbf{w}_2) = (\mathbf{\Gamma}\mathbf{w}_1)^T(\mathbf{\Gamma}\mathbf{w}_1) - (\mathbf{\Gamma}\mathbf{w}_2)^T(\mathbf{\Gamma}\mathbf{w}_2)$$
$$= \mathbf{w}_1^T\mathbf{\Gamma}^2\mathbf{w}_1 - \mathbf{w}_2^T\mathbf{\Gamma}^2\mathbf{w}_2$$
$$= 2\mathbf{w}_2^T\mathbf{\Gamma}^2(\mathbf{w}_1 - \mathbf{w}_2) + (\mathbf{w}_1 - \mathbf{w}_2)^T\Gamma^2(\mathbf{w}_1 - \mathbf{w}_2)$$
$$\frac{\|L(\mathbf{w}_1) - L(\mathbf{w}_2)\|}{\|\mathbf{w}_1 - \mathbf{w}_2\|} \leq 2\|\mathbf{w}_2\|\,\|\mathbf{\Gamma}^2\| + \|\mathbf{w}_1 - \mathbf{w}_2\|\,\|\mathbf{\Gamma}^2\|$$

Now by the assumption that $\mathbf{w}_1, \mathbf{w}_2$ are bounded by K,

$$\boxed{L = 2K\,\|\mathbf{\Gamma}^2\|}$$

This additional term may be added to the Lipschitz constants derived above when gradient descent is performed on a loss function including a Tikhonov regularization term. Clearly, for an L_2-regularizer, since $\mathbf{\Gamma} = \frac{\lambda}{2}\mathbf{I}$, $L = \lambda K$.

6 Experiments

This section discusses experiments demonstrating the faster convergence with our approach.

In each experiment, we randomly initialize weights, and use the same initial weight vector for gradient descent with both the learning rates. In all experiments, we scale each feature to [0, 1] before running gradient descent. This scale data is used to compute the Lipschitz constants, and consequently, the learning rates. Normalizing the data is particularly important because the Lipschitz constant may get arbitrarily large, thus making the learning rate too small. For the results obtained with a constant learning rate, the chosen value of α was 0.1.

6.1 Regression experiments

Rather than wait for absolute convergence, which may take many iterations, we instead choose to set a threshold for the value of the loss function. When the value of the cost function goes below this threshold, we stop the gradient descent procedure. A reasonable threshold value is chosen for each dataset separately.

For the least-squares cost function, an estimate of K is required. A good estimate of K would be obtained by running gradient descent with some fixed learning rate and then taking the norm of the final weight vectors. However, because this requires actually running the algorithm for which we want to find a parameter first, we need to estimate this value instead. In our experiments, we obtain a close approximation to the value obtained above through the formula below. For the experiments in this subsection, we use this formula to compute K.

Table 1: Regression experiments on various datasets with $\alpha = 0.1$ and $\alpha = \frac{1}{L}$

Dataset	Loss threshold	Inverse Lipschitz constant	#it with $\alpha = 0.1$	#it with $\alpha = \frac{1}{L}$
Boston housing prices	200	9.316	46,041	555
California housing prices	2.8051	5163.5	24,582	2
Energy efficiency [2]	100	12.78	489,592	3,833
Online news popularity [1]	73,355,000	1.462	10,985	753

Table 2: Binary classification experiments on various datasets with $\alpha = 0.1$ and $\alpha = \frac{1}{L}$

Dataset	Inverse Lipschitz constant	Accuracy with $\alpha = 0.1$	Accuracy with $\alpha = \frac{1}{L}$
Iris	830.22	50%	100%
Covertype	189.35M	43.05%	57.21%
Breast cancer	4280.22	43.23%	90.5%

$$a = \frac{1}{m} \sum_{j=1}^{n} \sum_{i=1}^{m} x_j^{(i)}$$

$$b = \frac{1}{n} \sum_{j=1}^{n} \max_i x_j^{(i)}$$

$$K = \frac{a+b}{2}$$

In the above formulas, the notation $x_j^{(i)}$ refers to the jth column of the ith training example. Note that a is the sum of the means of each column, and b is the mean of the maximum of each column.

Table 1 shows the results of our experiments on some datasets. Clearly, our choice of α outperforms a random guess in all the datasets. Our proposed method yields a learning rate that adapts to each dataset to converge significantly faster than with a guess. In some datasets, our choice of learning rate gives over a 100x improvement in training time.

While the high learning rates may raise concerns of oscillations rather than convergence, we have checked for this in our experiments. To do this, we continued running gradient descent, monitoring the value of the loss function every 500 iterations. Figure 1 shows this plot, demonstrating that the high learning rates do lead to convergence.

6.2 Binary classification experiments

For classification, our experiments were conducted by running gradient descent for 1000 iterations, and then comparing accuracy scores over the two learning rates. Table 2 summarizes the results of these experiments. Note that even with high learning rates, the algorithm outperforms a small choice of learning rate.

For the iris dataset, we removed one class to make the problem a binary classification one. For the covertype data, we considered only the first two out of seven classes. This resulted in 495,141 rows. We also considered only ten features to speed up computation time.

6.3 Multi-class classification experiments

For multi-class classification, the experiments were conducted in the same manner as for binary classification. However, we did not scale the data in this case. Further, the target variable was one-

Table 3: Softmax classification experiments on various datasets with $\alpha = 0.1$ and $\alpha = \frac{1}{L}$

Dataset	Inverse Lipschitz constant	Accuracy with $\alpha = 0.1$	Accuracy with $\alpha = \frac{1}{L}$
Iris	1.936	93.33%	97.78%
Digits	0.635	91.3%	94.63%
MNIST*	0.036	67.02%	67.02%

hot encoded before running gradient descent. Finally, we ran gradient descent for 200 iterations, rather than 1000. Table 3 summarizes the results of these experiments.

For MNIST, we handled the data differently. Because running gradient descent caused overflows even for learning rates of 10^{-4}, we standardized the data first. However, we observed a major difference between train and test accuracies, indicating overfitting. Thus, we added a regularization term, with $\lambda = 10$. To compute the Lipschitz constant, we proceeded as in section 5, but adding $\lambda \cdot \log c$ instead of $\lambda \cdot c$, since the log loss is used.

- format wants line after the table heading
- try MNIST with different scalers.
- for classification, also perform experiments like regression
- SVM analogy
- replace line search in BFGS with our approach

References

[1] Kelwin Fernandes, Pedro Vinagre, and Paulo Cortez. A proactive intelligent decision support system for predicting the popularity of online news. In *Portuguese Conference on Artificial Intelligence*, pages 535–546. Springer, 2015.

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