COMS 4771 Machine Learning 2020
Problem Set #2

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Problem 1: A variant of Perceptron Algorithm

Given our Perceptron OR Variant with binary observations from a d-dimensional feature space, ($x \in \{0,1\}^d$) and output defined as an 'OR' of some of the features, we can show it makes at most $2 + 3r(1 + \log d)$ mistakes when the target concept is an OR of r variables.

(i) We can show that the Perceptron OR Variant makes $M_+ \leq r(1 + \log d)$ mistakes on positive examples: first consider the worst scenario in which positive mistakes are made. It can be observed that the algorithm will make the most mistakes when a vector with a single 1 element is given for the weights which has the weight of that element assigned to 1.

As a example for intuition, we can consider the case when $d = 4$, given an $x_i = [1, 0, 0, 0]$ predicted positively (x_0 is one of the terms in the target OR) we know that in order for the algorithm to predict positively for x_i, it must iterate the following weights:

start: $w = [1, 1, 1, 1]$

(1) $w = [2, 1, 1, 1]$

(2) $w = [4, 1, 1, 1]$

(3) $w = [8, 1, 1, 1]$

Notice that the algorithm will make $1 + \log d$ mistakes until the element w_i exceeds d (the requirement to successfully label x_i). Since this can occur for each of the terms in the target OR, there are r such instances above; meaning, there are at most $r(1+\log d)$ mistakes for any positive example.

(ii) Similar to the part above, we will consider the "boundary" case to provide a lower bound on the decrease in the total weight $\sum_i w_i$. In order for the algorithm to incorrectly classify a negative example, we have:

$$\hat{y} = 1, y = 0$$

Since $\hat{y} = \mathbb{1}[w \cdot x > d] = 1$, we have:

$$1 = \mathbb{1}[w \cdot x > d] \implies w \cdot x > d$$

Above, we have shown that each mistake made on a negative example is predicated on: $w \cdot x > d$. With this observation, we can prove a lower bound on the decrease in the total weight after the algorithm's update. First, consider we can rewrite:

$$w \cdot x > d$$

as

$$\sum_i w_i(\forall i : x_i = 1) > d.$$

After performing the update: $w_i \leftarrow w_i/2(for \forall i : x_i = 1)$, we can see that every term in the summation above is updated (divided by two) since they are predicated on the same expression. We have the following for the old w_i's:

$$\frac{1}{2}\sum_i w_i(\forall i : x_i = 1) > \frac{d}{2}.$$

And since the new w_i's are given by:

$$\frac{1}{2}\sum_i w_i(\forall i : x_i = 1)$$

, For the new w_i's we have:

$$\sum_i w_i(\forall i : x_i = 1) > \frac{d}{2}$$

We can effectively drop the predicate since $\sum_i w_i \geq \frac{1}{2}\sum_i w_i(\forall i : x_i = 1)$. This yields:

$$\sum_i w_i > \frac{d}{2}.$$

Thus, the updated weights at each negative mistake are decreased by at least $\frac{d}{2}$.

(iii) Let M_- denote the total number of mistakes on negative examples, and $TW(t)$ denote the total weight of w at iteration t. Observe that

$$0 < TW(t) \leq TW(0) + dM_+ - (d/2)M_-.$$

First, we can prove that

$$TW(t) \leq TW(0) - \frac{d}{2}M_-$$

since there are M_- total negative mistakes and each decreases the total weight by at least $\frac{d}{2}$, the total weight at iteration t must be at most the difference between the initial weight ($TW(0)$) and the accumulated changes to the weights since $t = 0$, $(d/2)M_-$.

Similarly, we can prove

$$TW(t) \leq TW(0) + dM_+.$$

First, consider the most that each mistake on a positive example can increase the total weight $\sum_i w_i$. Similar to (ii), we first predicate on $\hat{y} = 0, y = 1$. Since $\hat{y} = \mathbb{1}[w \cdot x > d] = 0$, we have:

$$0 = \mathbb{1}[w \cdot x > d] \implies w \cdot x \leq d$$

Then,

$$\sum_i w_i(\forall i : x_i = 1) \leq d.$$

In a similar vein as above, at each iteration in the algorithm, the update cannot exceed an addition of d to the total weight, since anytime element's corresponding weight is updated, it must be less than or equal to d (meaning the update from d to $2d$ is in fact the maximum - which is simply d).

Finally, we will rearrange the original observation and use $M_+ \leq r(1 + \log d)$:

$$0 < TW(t) \leq TW(0) + dM_+ - (d/2)M_-$$
$$\frac{d}{2}M_- < TW(t) + \frac{d}{2}M_- \leq TW(0) + dM_+$$

dropping the middle term:

$$\begin{aligned}
\frac{d}{2}M_- &\leq TW(0) + dM_+ \\
M_- &\leq \frac{2}{d}(TW(0) + dM_+) \\
M_- &\leq \frac{2}{d}(d + dM_+) \\
M_- &\leq 2 + 2M_+ \\
M_- &\leq 2 + 2(r(1 + \log d)) \\
M_- &\leq 2 + 2r + 2r\log d
\end{aligned}$$

Now that we have bounds on both M_- and M_+, we can establish a bound on the total number of mistakes:

$$\begin{aligned}
M_+ + M_- &\leq r(1 + \log d) + 2 + 2r + 2r\log d \\
M_+ + M_- &\leq r + r\log d + 2 + 2r + 2r\log d \\
M_+ + M_- &\leq 2 + 3r + 3r\log d \\
M_+ + M_- &\leq 2 + 3r(1 + \log d)
\end{aligned}$$

Thus, we can conclude that the total number of mistakes $(M_+ + M_-)$ is at most $2 + 3r(1 + \log d)$.

Problem 2: Inconsistency of the fairness definition

(i) Only trivial scenarios are able to satisfy all three fairness definitions simultaneously. Consider the problem of hiring ("hire" vs. "do not hire") where the sensitive attribute is gender ("male" vs. "female"). In this case, if there are an equal number of male and female candidates, and they are hired at exactly equal rates (and we have a perfect classifier), then all three fairness definitions can be satisfied. The number of men and number of women must be the same, as well as the number of men hired and the number of women hired.

(ii) Demographic Parity tells us that:

$$\mathbb{P}_0[\hat{Y} = \hat{y}] = \mathbb{P}_1[\hat{Y} = \hat{y}] \tag{1}$$

This implies that the predicted class is independent of the sensitive attribute:

$$\hat{Y} \perp A \tag{2}$$

and by the symmetry property of conditional independence:

$$A \perp \hat{Y} \tag{3}$$

On the other hand, Predictive parity is defined as:

$$\mathbb{P}_0[Y = y|\hat{Y} = \hat{y}] = \mathbb{P}_1[Y = y|\hat{Y} = \hat{y}] \tag{4}$$

Which tells us that the sensitive attribute is independent of the true class, given the predicted class:

$$A \perp Y|\hat{Y} \tag{5}$$

Thus, if $A \not\perp Y$,

$$A \not\perp \hat{Y} \tag{6}$$

which contradicts equation 3, showing that Demographic Parity and Predictive Parity cannot both hold if $A \not\perp Y$.

(iii) As in part (ii), demographic parity gives that:

$$\hat{Y} \perp A \tag{7}$$

The Equalized Odds fairness metric says that the predicted class is independent of the sensitive attribute, given the true class:

$$\hat{Y} \perp A|Y \tag{8}$$

By contraction:

$$\hat{Y} \perp A, Y \tag{9}$$

Then by decomposition:

$$\hat{Y} \perp A \tag{10}$$

AND

$$\hat{Y} \perp Y \tag{11}$$

For both equations to be true, either the sensitive attribute OR the predicted class must be independent of the actual class:

$$A \perp Y \tag{12}$$

OR

$$\hat{Y} \perp Y \tag{13}$$

Thus, if $A \not\perp Y$ and $\hat{Y} \not\perp Y$, both Demographic Parity (7) and Equalized Odds (8) cannot hold at the same time.

(iv) As shown in part (ii), when Equalized Odds holds:

$$\hat{Y} \perp A|Y \tag{14}$$

Which gives us that:

$$A \perp \hat{Y}|Y \tag{15}$$

And from part (i), the definition of Predictive Parity is:

$$Y \perp A|\hat{Y} \tag{16}$$

Which tells us:

$$A \perp Y|\hat{Y} \tag{17}$$

Combining equations 15 and 17 gives:

$$A \perp Y, \hat{Y} \tag{18}$$

By decomposition, $A \perp Y$, so if we are given $A \not\perp Y$, both Equalized Odds and Predictive Parity cannot hold.

Problem 3: Making data linearly separable by feature space mapping

(i) *Proof.* We are given that

$$\Phi_\alpha(x_i) = \begin{cases} \exp\left(-\dfrac{1}{1-(\frac{\alpha-x_i}{\sigma})^2}\right), & |\alpha - x_i| < \sigma \\ 0 \ , & \text{otherwise} \end{cases}$$

Because we are only concerned with a finite number of data points, $x_1 \ldots, x_n$, there exists some $\varepsilon > 0$ such that $|x_i - x_j| > \varepsilon$ for all $i, j \in \{1, \ldots, n\}$. Then, we have that $\varepsilon < \min_{i,j} |x_i - x_j|$. Using this fact, set $\sigma = \dfrac{\varepsilon}{2}$ so that for any x_i and x_j, where $x_i \neq x_j$, we have

$$\int_{-\infty}^{\infty} \Phi_\alpha(x_i)\Phi_\alpha(x_j)d\alpha = \int_{x_i-\sigma}^{x_i+\sigma} \Phi_\alpha(x_i)\Phi_\alpha(x_j)d\alpha = 0$$

Define our classifier to be such that $\text{sign}(w_i\Phi_\alpha(x_i)) = y_i, \ \forall i \in \{1, \ldots, n\}$.

Then set $\vec{\mathbf{w}} = \sum_{k=1}^{n} w_k y_k \Phi_\alpha(\vec{x_k})$. We then have the following:

$$\begin{aligned} \text{sign}\left(\vec{\mathbf{w}} \cdot \Phi_\alpha(\vec{x_i})\right) &= \text{sign}\left(\Phi_\alpha(\vec{x_i}) \cdot \sum_{k=1}^{n} w_k y_k \left(\Phi_\alpha(\vec{x_k})\right)\right) \\ &= \text{sign}\left(\int_{x_i-\sigma}^{x_i+\sigma} \sum_{k=1}^{n} w_k y_k \Phi_\alpha(\vec{x_k})\Phi_\alpha(\vec{x_i})d\alpha\right) \\ &= \text{sign}\left(w_i y_i \int_{x_i-\sigma}^{x_i+\sigma} \Phi_\alpha(\vec{x_i})\Phi_\alpha(\vec{x_i})d\alpha\right) \\ &= \text{sign}\left(w_i y_i \int_{x_i-\sigma}^{x_i+\sigma} \Phi_\alpha(\vec{x_i})^2 d\alpha\right) = y_i \end{aligned}$$

□

(ii) For arbitrary x and x', we want to express the dot product analytically. We have two cases: (1) $x \neq x'$, and (2) $x = x'$.

<u>Case 1 ($x \neq x'$):</u>

From part (i) we have the following for any two distinct points:

$$\Phi_\alpha(x) \cdot \Phi_\alpha(x) = \int_{-\infty}^{\infty} \Phi_\alpha(x)\Phi_\alpha(x')d\alpha \ = \ 0$$

Case 2 ($x = x'$):

$$\begin{aligned}
\Phi_\alpha(x) \cdot \Phi_\alpha(x) &= \int_{-\infty}^{\infty} \Phi_\alpha(x)\Phi_\alpha(x')d\alpha \\
&= \int_{-\infty}^{\infty} \Phi_\alpha(x)^2 d\alpha \\
&= \int_{x-\sigma}^{x+\sigma} \left(e^{-\frac{1}{1-(\frac{\alpha-x}{\sigma})^2}} \right)^2 d\alpha \\
&= \int_{x-\sigma}^{x+\sigma} e^{-\frac{2}{1-(\frac{\alpha-x}{\sigma})^2}} d\alpha
\end{aligned}$$

this integral can clearly be transformed into Gaussian form, which can subsequently be efficiently computed.

(iii) (a) The decision rule $h(x) = \begin{cases} +1 & \|\phi(x) - c_+\| \leq \|\phi(x) - c_-\| \\ -1 & otherwise \end{cases}$ is equivalent to the following:

$$\begin{aligned}
h(x) &= \operatorname{sign}\left(\|\phi(x) - c_-\| - \|\phi(x) - c_+\|\right) \\
&= \operatorname{sign}\left((\langle \phi(x), \phi(x)\rangle + \langle c_-, c_-\rangle - 2\langle \phi(x), c_-\rangle) - (\langle \phi(x), \phi(x)\rangle + \langle c_+, c_+\rangle - 2\langle \phi(x), c_+\rangle)\right) \\
&= \operatorname{sign}\left(\cancel{\langle \phi(x), \phi(x)\rangle} + \langle c_-, c_-\rangle - 2\langle \phi(x), c_-\rangle - \cancel{\langle \phi(x), \phi(x)\rangle} - \langle c_+, c_+\rangle + 2\langle \phi(x), c_+\rangle\right) \\
&= \operatorname{sign}\left(2\langle \phi(x), c_+\rangle - 2\langle \phi(x), c_-\rangle + \|c_-\|^2 - \|c_+\|^2\right) \\
&= \operatorname{sign}\left(2\left(\langle \phi(x), c_+\rangle - \langle \phi(x), c_-\rangle + \frac{1}{2}\|c_-\|^2 - \frac{1}{2}\|c_+\|^2\right)\right) \\
&= \operatorname{sign}\left(\langle \phi(x), c_+\rangle - \langle \phi(x), c_-\rangle + b\right) \\
&= \operatorname{sign}\left(\langle \phi(x), c_+ - c_-\rangle + b\right) \\
&= \operatorname{sign}\left(\langle \phi(x), w\rangle + b\right) \\
&= \operatorname{sign}\left(\langle w, \phi(x)\rangle + b\right)
\end{aligned}$$

(b) In part (a) we showed that $h(x) = \operatorname{sign}(\langle w, \phi(x)\rangle + b)$. We can expand $h(x)$ using $w = c_+ - c_-$ and $c_+ = \frac{1}{m_+}\sum_{i:y_i=+1} \phi(x_i)$ and $c_- = \frac{1}{m_-}\sum_{i:y_i=-1} \phi(x_i)$:

$$
\begin{aligned}
h(x) &= \operatorname{sign}\left(\langle w, \phi(x)\rangle + b\right) \\
&= \operatorname{sign}\left(\langle \phi(x), c_+ - c_-\rangle + b\right) \\
&= \operatorname{sign}\left(\langle \phi(x), c_+\rangle - \langle \phi(x), c_-\rangle + b\right) \\
&= \operatorname{sign}\left(\langle \phi(x), \frac{1}{m_+}\sum_{i:y_i=+1}\phi(x_i)\rangle - \langle \phi(x), \frac{1}{m_-}\sum_{i:y_j=-1}\phi(x_j)\rangle + b\right) \\
&= \operatorname{sign}\left(\frac{1}{m_+}\sum_{i:y_i=+1}\langle \phi(x), \phi(x_i)\rangle - \frac{1}{m_-}\sum_{i:y_j=-1}\langle \phi(x), \phi(x_j)\rangle + b\right) \\
&= \operatorname{sign}\left(\frac{1}{m_+}\sum_{i:y_i=+1}\underbrace{\langle \phi(x), \phi(x_i)\rangle}_{=K(x,x_i)} - \frac{1}{m_-}\sum_{i:y_i=-1}\underbrace{\langle \phi(x), \phi(x_i)\rangle}_{=K(x,x_i)} + b\right) \\
&= \operatorname{sign}\left(\frac{1}{m_+}\sum_{i:y_i=+1}K(x,x_i) - \frac{1}{m_-}\sum_{i:y_i=-1}K(x,x_i) \ + \ b\right)
\end{aligned}
$$

where

$$
\begin{aligned}
b = \frac{1}{2}\left(\|c_-\|^2 - \|c_+\|^2\right) &= \frac{1}{2}\left(\frac{1}{m_-^2}\sum_{y_i=y_j=-1}\langle \phi(x_i)\phi(x_j)\rangle - \frac{1}{m_+^2}\sum_{y_i=y_j=+1}\langle \phi(x_i)\phi(x_j)\rangle\right) \\
&= \frac{1}{2}\left(\frac{1}{m_-^2}\sum_{y_i=y_j=-1}K(x_i,x_j) - \frac{1}{m_+^2}\sum_{y_i=y_j=+1}K(x_i,x_j)\right)
\end{aligned}
$$

Therefore, $h(x)$ can be expressed as:

$$
\begin{aligned}
\operatorname{sign}\Bigg[&\frac{1}{m_+}\sum_{i:y_i=+1}K(x,x_i) - \frac{1}{m_-}\sum_{i:y_i=-1}K(x,x_i) \\
&+ \ \frac{1}{2}\left(\frac{1}{m_-^2}\sum_{y_i=y_j=-1}K(x_i,x_j) - \frac{1}{m_+^2}\sum_{y_i=y_j=+1}K(x_i,x_j)\right)\Bigg]
\end{aligned}
$$

Problem 4: Convexity

(i) We are given that f is twice differentiable and $\nabla^2 f \succeq 0$ (i.e., the Hessian of f is positive semidefinite). Then for $g(t) = f(tx + (1-t)y)$, where $t \in [0,1]$, we have the following:

$$g'(t) = \nabla f(tx + (1-t)y)^\top (x - y)$$
$$g''(t) = (x-y)^\top \nabla^2 f(tx + (1-t)y)(x-y)$$

Now, $\nabla^2 f \succeq 0$ implies that $v^\top \nabla^2 f(x) v \geq 0$ for any $v \in \mathbb{R}^d$.
Hence, $g''(t) = (x-y)^\top \nabla^2 f(tx + (1-t)y)(x-y) \geq 0 \implies g''(t) \geq 0$.

(ii) *Proof.* By the supposition, g is twice differentiable. Then by Taylor's theorem we have the following

$$\begin{aligned} g(0) &= g(t) + g'(t)(0-t) + \frac{g''(\alpha)}{2!}(0-t)^2 \\ &= g(t) + g'(t)(-t) + \frac{g''(\alpha)}{2}t^2 \end{aligned}$$

and

$$g(1) = g(t) + g'(t)(1-t) + \frac{g''(\beta)}{2}(1-t)^2$$

for some $\alpha \in (0,t)$ and $\beta \in (t,1)$. Note that $\frac{g''(\alpha)}{2}(-t)^2$ is the remainder term for the expansion of $g(0)$, and $\frac{g''(\beta)}{2}(1-t)^2$ is the remainder term for the expansion of $g(1)$. By part (i), $g''(t) \geq 0$, for any $t \in [0,1]$. Then, $g''(\alpha) \geq 0$ and $g''(\beta) \geq 0$. It follows that

$$g(0) = g(t) + g'(t)(-t) + \frac{g''(\alpha)}{2}(-t)^2 \ \geq \ g(t) + g'(t)(-t)$$

and

$$g(1) = g(t) + g'(t)(1-t) + \frac{g''(\beta)}{2}(1-t)^2 \ \geq \ g(t) + g'(t)(1-t)$$

□

(iii) In part (ii) we showed that

$$g(0) \geq \ g(t) + g'(t)(-t) \tag{19}$$
$$g(1) \geq \ g(t) + g'(t)(1-t) \tag{20}$$

Multiplying both sides of (19) by $(1-t)$ and both sides of (20) by t and adding the resulting inequalities together[1], we get

$$\begin{aligned} (1-t)g(0) + tg(1) &\geq (1-t)g(t) + (1-t)g'(t)(-t) + tg(t) + tg'(t)(1-t) \\ &= g(t) \end{aligned}$$

That is, $g(t) = g(t \times 1 + (1-t) \times 0) \leq tg(1) + (1-t)g(0)$.
Hence, g is convex.

[1]Stephen Boyd, *Convex Optimization* (New York: Cambridge University Press, 2004), 69-70

Problem 5: Empirical study of various gradient-based optimization procedures

(i) Overview of different optimization methods.[2]

(a) (Full) Gradient Descent (GD)
Gradient Descent is a popular computational optimization technique. It relies on the rather straightforward idea of finding minima via iteratively executing an algorithm to arrive at a local minima. This is done by calculating the gradient of a differentiable function and taking "steps" in the direction proportional to the negative of the gradient at the current step. In effect, this means starting at some location on a function and iteratively moving across the function, minimizing said function, until some max number of iterations, or until the steps become too small. It is worth noting that this method is essentially the root of all of the following methods. What follows simply tried to improve on many of GD's shortcomings. Chiefly, gradient descent incurs a large computational cost when applied to optimization problems in machine learning which often are large summations (requiring gradient descent to calculate the entire sum to find the gradient).

(b) Stochastic Gradient Descent (SGD)
The aforementioned problem with gradient descent is alleviated by stochastic gradient descent. The idea is as follows: when trying to optimize a function of the form:

$$L(w) = \frac{1}{n}\sum_{i=1}^{n} L_i(w)$$

This is often the case in machine learning since the optimization function - although a function of the parameters (weights) - is actually part of a larger function of the training data which effectively produces a large summation function of weights after the data is applied. Since many datasets are extremely large, calculating the entire summation at each iteration becomes computationally infeasible. This means

(c) SGD with Momentum (SGDM)
The addition of the momentum term is based on the intuition that if the algorithm is repeatedly moving in the same direction, it should more confidently move in that direction.[3] This momentum manifests in a means to track the history of updates and apply a simple scalar factor to add to the update term:

$$\Delta w := \alpha \Delta w - \eta \nabla Q_i(w)$$

This achieves one of the goals of our optimization: fast convergence. Theoretically, the momentum can provide faster convergence if the above intuition holds. We will see below that this additional momentum hyperparameter, α can lead to poor convergence if it is too large.

[2] https://en.wikipedia.org/wiki/Stochastic_gradient_descent
[3] https://towardsdatascience.com/learning-parameters-part-2-a190bef2d12

(d) Adaptive Gradient (AdaGrad)
AdaGrad is the first addressed which incorporates a per-parameter learning rate. The intuition is to increase/decrease the learning rate based on the relative sparsity of the parameters. In the case there are parameters which are sparse (zero most of the time) the gradient will likely be zero for that element in most inputs, thus the learned feature will get fewer updates than others. In the case that this feature happens to be sparse but is important, we would prefer to incorporate the information into the model more constructively. In adaptive optimization algorithms, they attempt to perform some sort of per-parameter tuning such that the information is included even in sparse features which would otherwise be discounted.

(e) RMSProp
Root Mean Square Propagation (RMSProp) is another "adaptive" algorithm.

The RMSprop optimizer is similar to the gradient descent algorithm with momentum. In particular, the RMSprop optimizer restricts the oscillations in the vertical direction, so one can increase the learning rate. As a result, the algorithm can take larger steps in the horizontal direction, resulting in faster convergence. The difference between RMSprop and gradient descent arises in the computation of the gradient. The following show the differences in computing the gradients for each algorithm. [4]

Gradient Descent with momentum:

$$v_{dw} = \beta v_{dw} + (1 - \beta) dw$$

$$v_{db} = \beta v_{dw} + (1 - \beta) db$$

$$W = W - \alpha v_{dw}$$

$$b = b - \alpha v_{db}$$

RMSProp:

$$v_{dw} = \beta v_{dw} + (1 - \beta) dw$$

$$v_{db} = \beta v_{dw} + (1 - \beta) db$$

$$W = W - \alpha v_{dw}$$

$$b = b - \alpha v_{db}$$

(f) AdaDelta
The method dynamically adapts over time using only first order information and has minimal computational overhead beyond vanilla stochastic gradient descent. The method requires no manual tuning of a learning rate and appears robust to noisy gradient information, different model architecture choices, various data modalities and selection of hyperparameters.

[4] https://int8.io/comparison-of-optimization-techniques-stochastic-gradient-descent-momentum-adagrad-and-adadelta/

(g) Adaptive Momentum (ADAM)
Adaptive Momentum (Adam) was published in 2015 and performed better than many of the aforementioned methods in terms of convergence speed and success. Adam provides more robust optimization via keeping running averages of the gradients and the second moments of the gradients. Our final non-convex test below assesses our success working with Adam compared to the other adaptive algorithms.

(h) Batch versions
In addition to the usual stochastic approach above, there is another which attempts to similarly alleviate computational cost by introducing random sampling (i.e. taking a single sample of the sum as in stochastic gradient descent) but reduce the randomness/errors by averaging across multiple samples instead of one.

(ii) Implementation and results. Our implementation was written in Python 3 and relied on Google's Jax autograd library. Instead of simply simulating specific datasets, our approach was a bit more traditional, as we generated functions which exhibited the properties we desired instead of jumping straight into optimization specifically for machine learning loss functions.

In the first part, a simple quadratic convex function was utilized to build intuition and observe the methods in an easy scenario which we new they would all succeed. Later a non-convex function is addressed. It is also worth noting that simple summations were used to add the sort of machine learning-like form which benefits so much from using stochastic methods.

(a) (Full) Gradient Descent (GD) vs Stochastic
Our experiment validated the hypothesis that stochastic gradient descent was faster than gradient descent (about 12x speedup per iteration); although the method suffered from its randomness and actually took about the same time to converge (quantitative analysis is omitted due to the arbitrary nature of the experiment). In Figure 2 the optimization paths are shown on a contour of the original function. The same learning rate is used, and it is easily seen that the stochastic nature actually harms the rate of convergence due to the lack of contribution of every term in the sum.

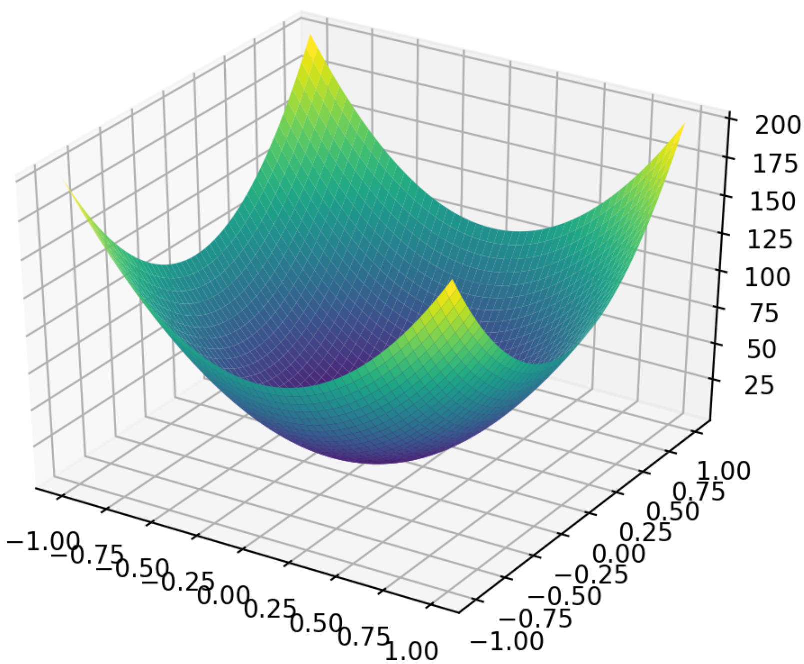


Figure 1: Easy test optimization function.

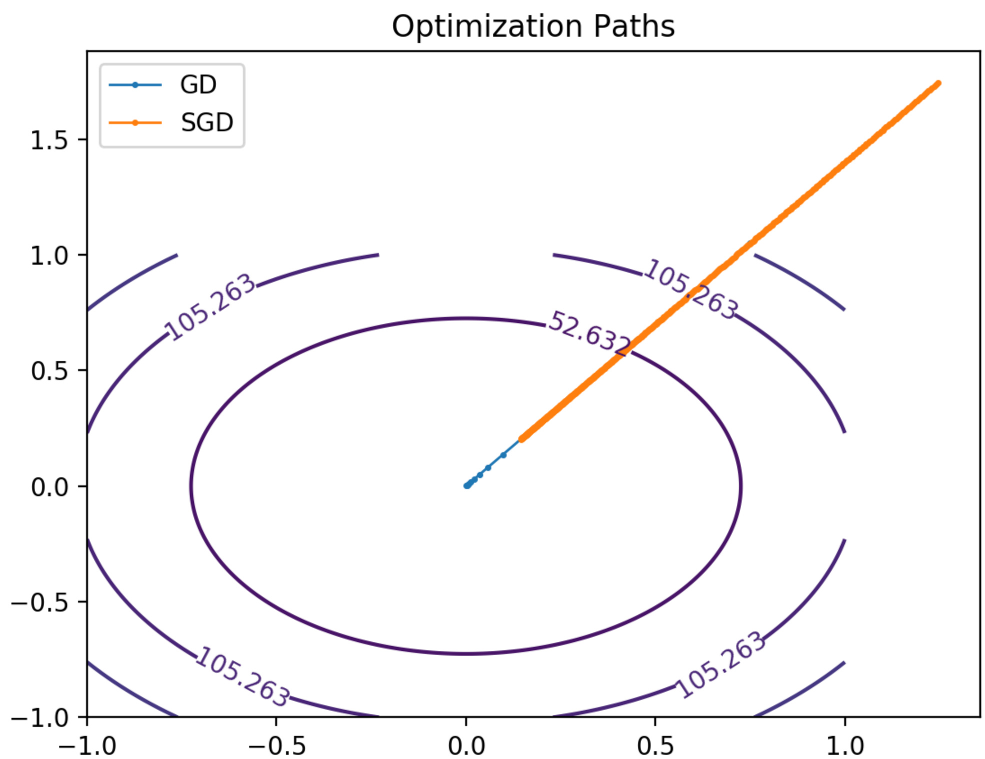


Figure 2: Gradient Descent and SGD optimization paths.

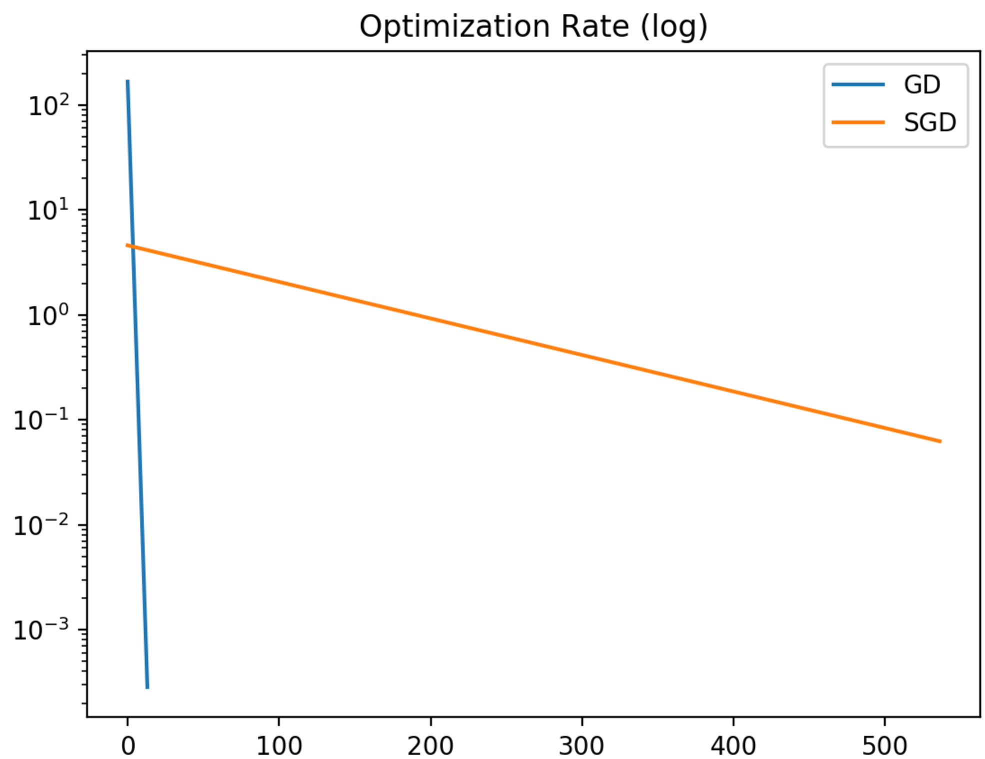


Figure 3: Gradient Descent and SGD optimization iterations.

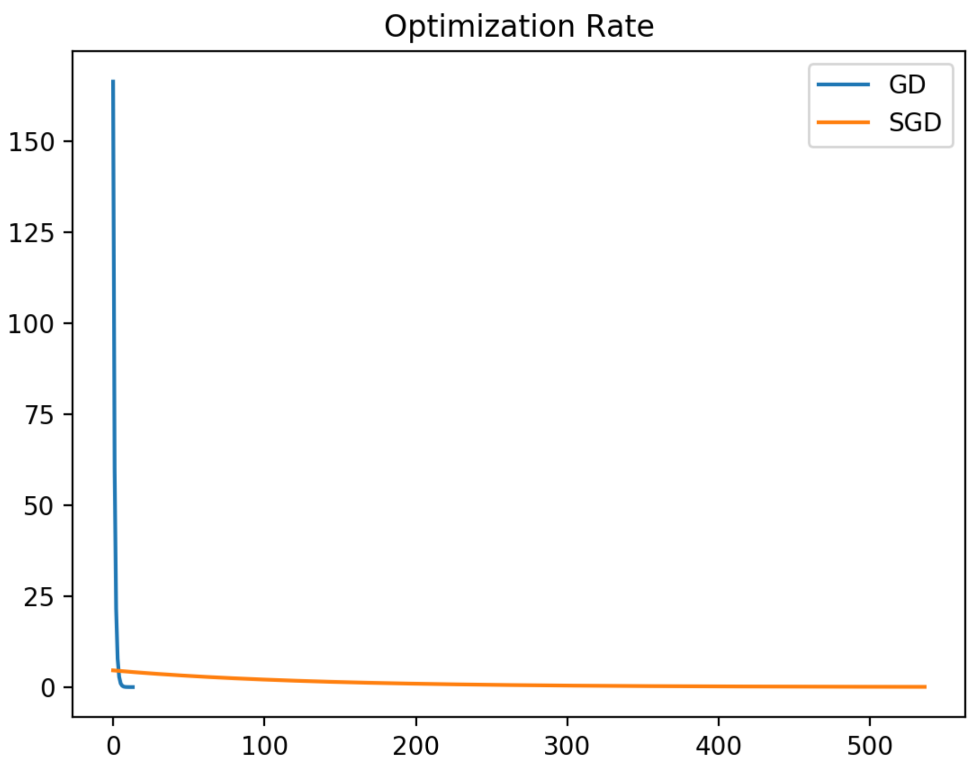


Figure 4: Gradient Descent and SGD optimization iterations.

(b) Stochastic Gradient Descent (SGD) vs Momentum
Whereas the above SGD proved to perform significantly worse than GD in order to achieve a speedup, adding a momentum term allowed for both faster iteration as in the case of SGD, but also better convergence.

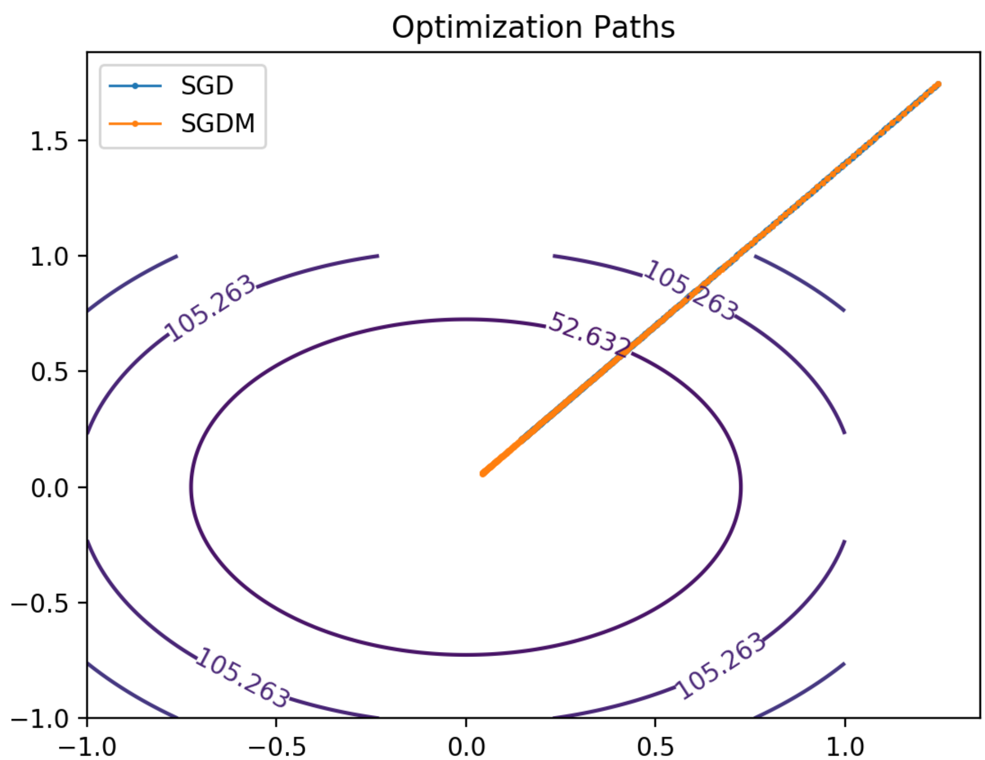


Figure 5: SGD and SGDM optimization paths.

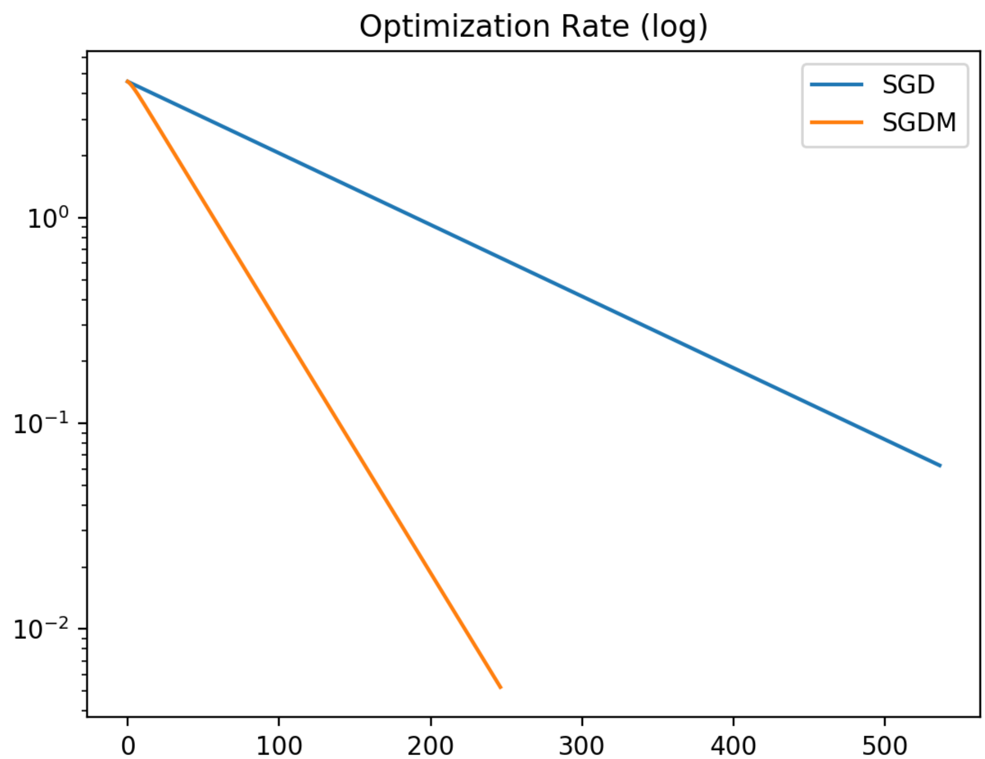


Figure 6: SGD and SGDM optimization iterations.

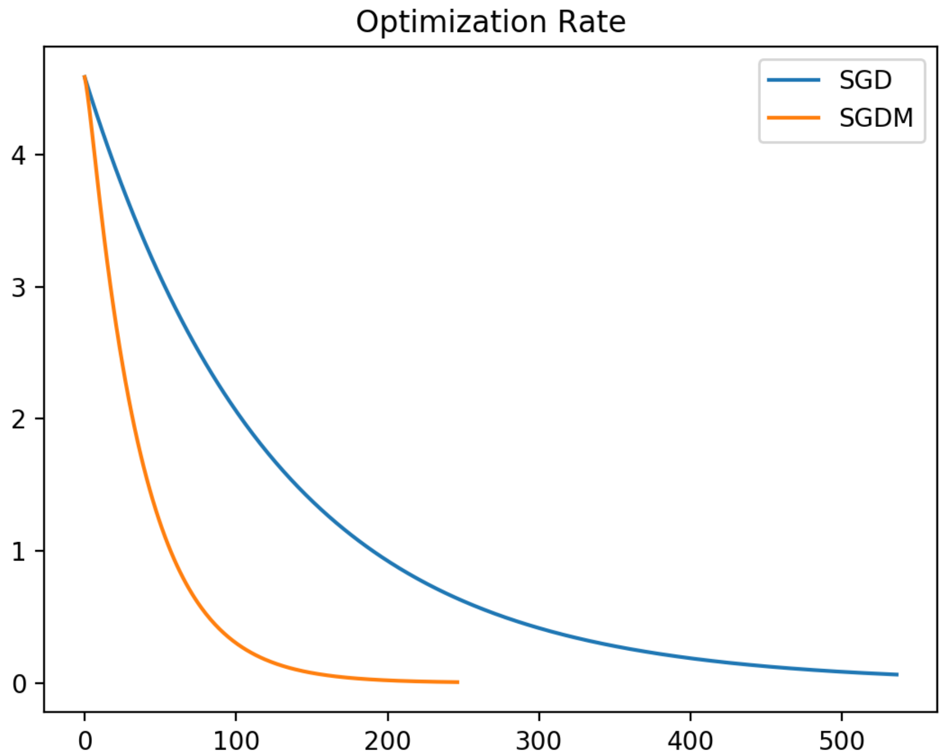


Figure 7: SGD and SGDM optimization iterations.

(c) Momentum anti-pattern
As momentum introduces a new hyperparameter, α, there are cases when it will perform significantly worse than SGD. Below illustrates such a case where the learning rate was set to .005 and the momentum was set too high at .9.

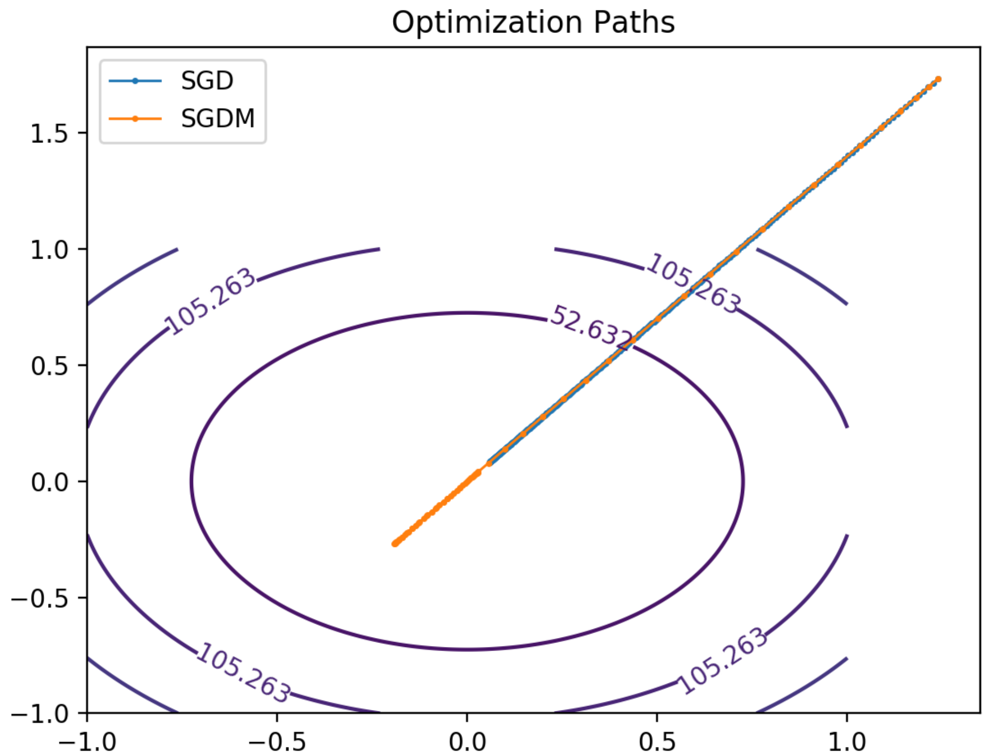


Figure 8: Poor momentum selection paths.

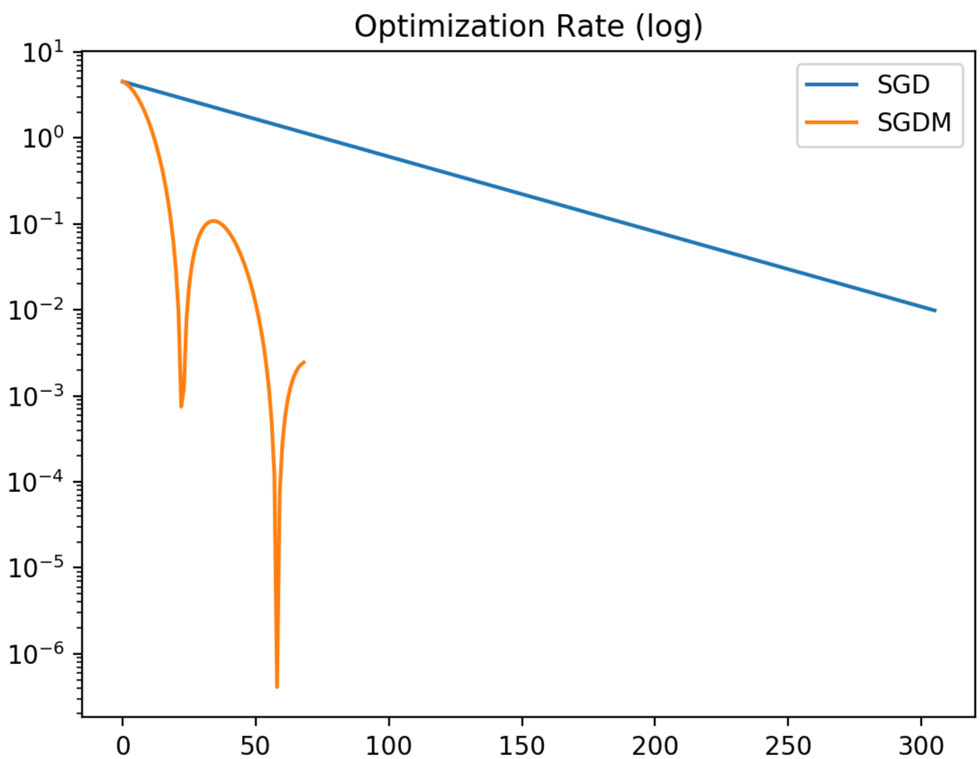


Figure 9: Poor momentum selection optimization iterations.

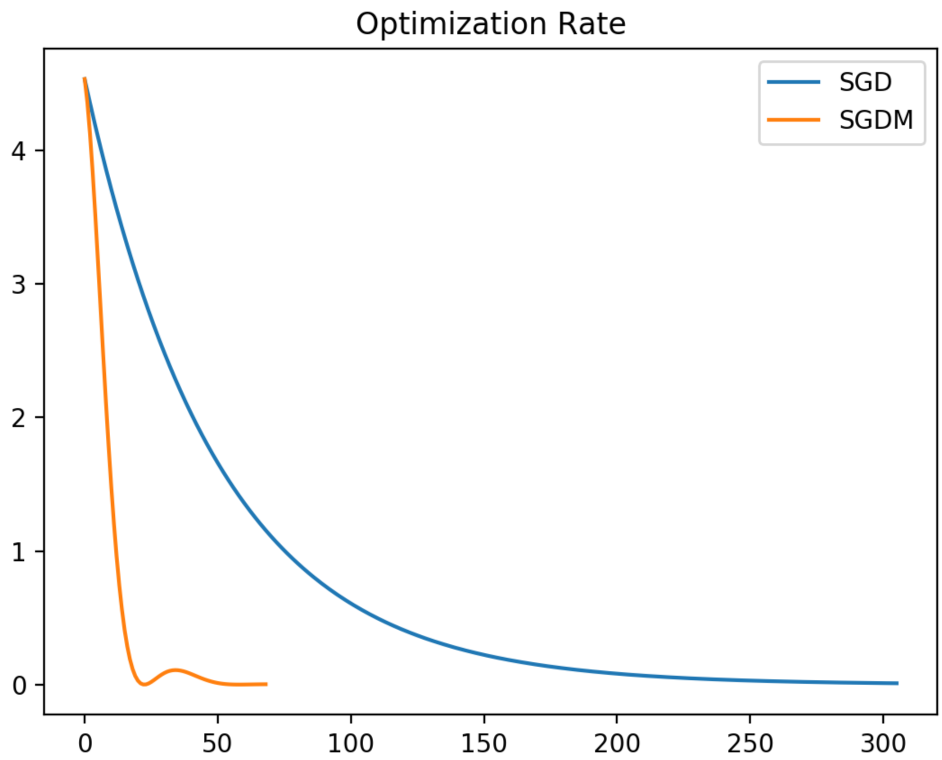


Figure 10: Poor momentum selection optimization iterations.

(d) Batching
Batching in each test provided expected results, greater convergence rate and slightly longer optimization times.

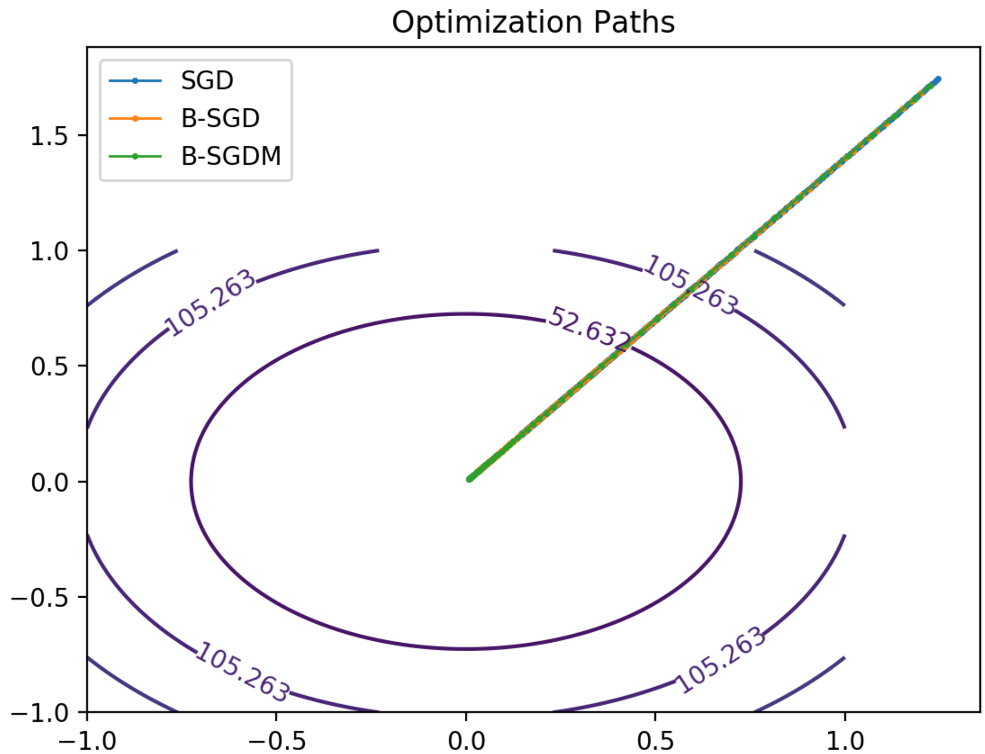


Figure 11: SGD vs Batching SGD and Batching SGDM

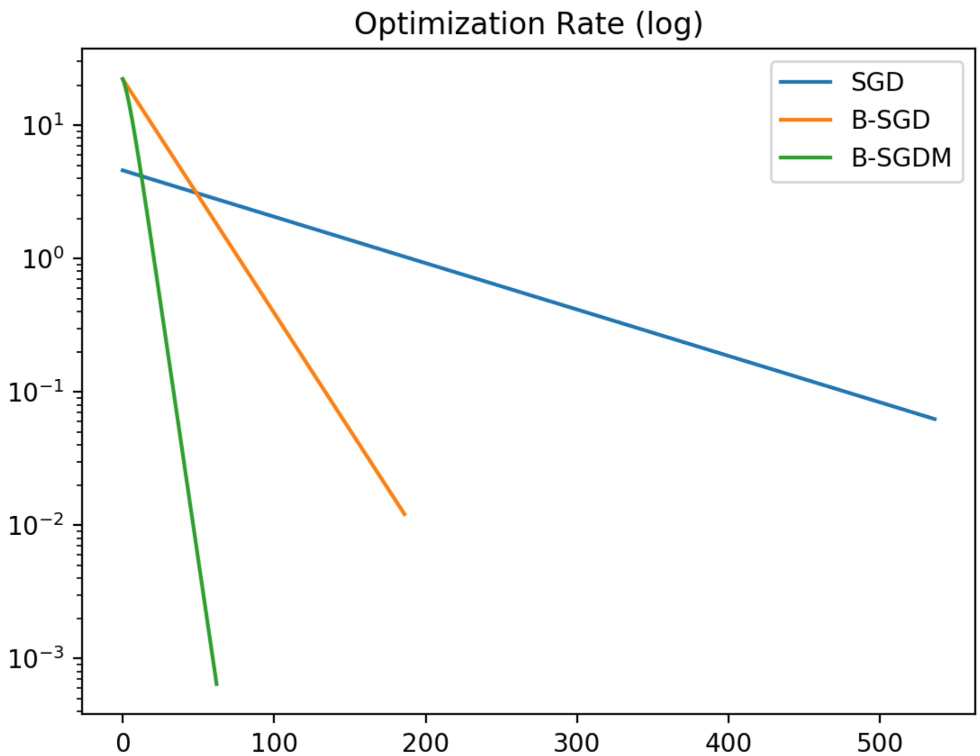


Figure 12: SGD vs Batching SGD and Batching SGDM

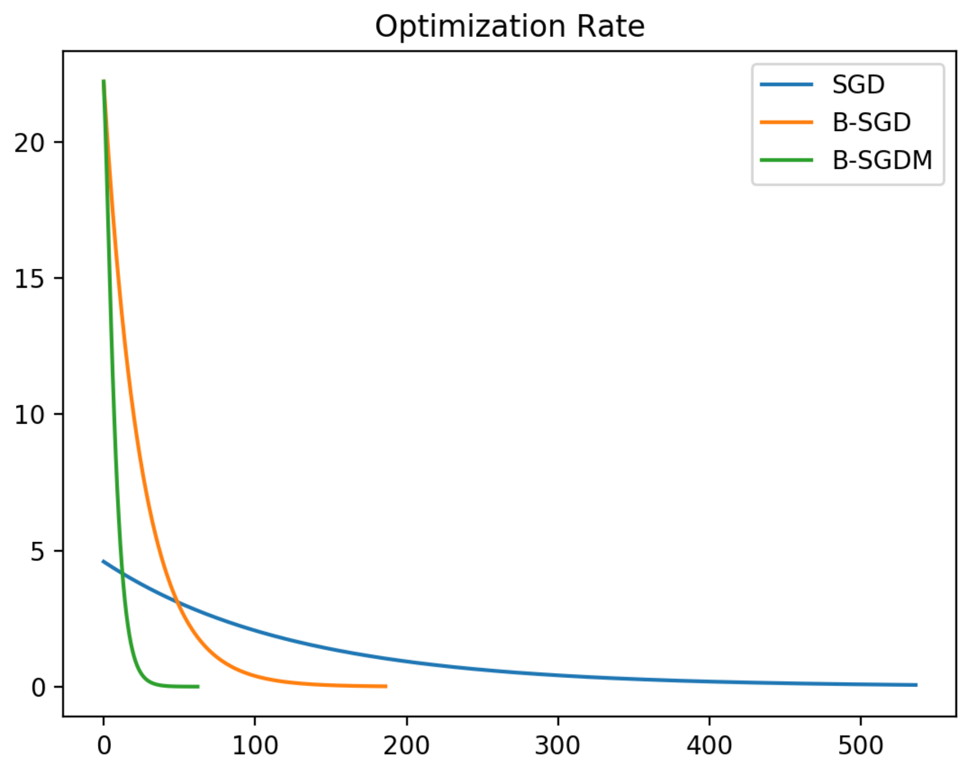


Figure 13: SGD vs Batching SGD and Batching SGDM

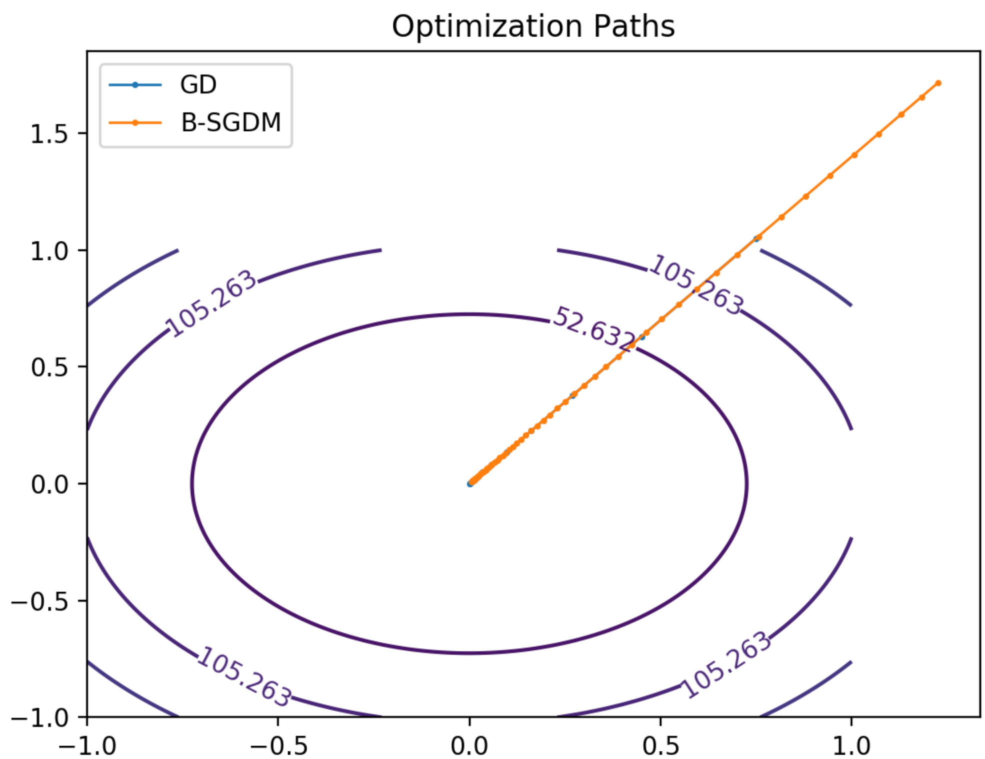


Figure 14: GD vs Batching SGDM

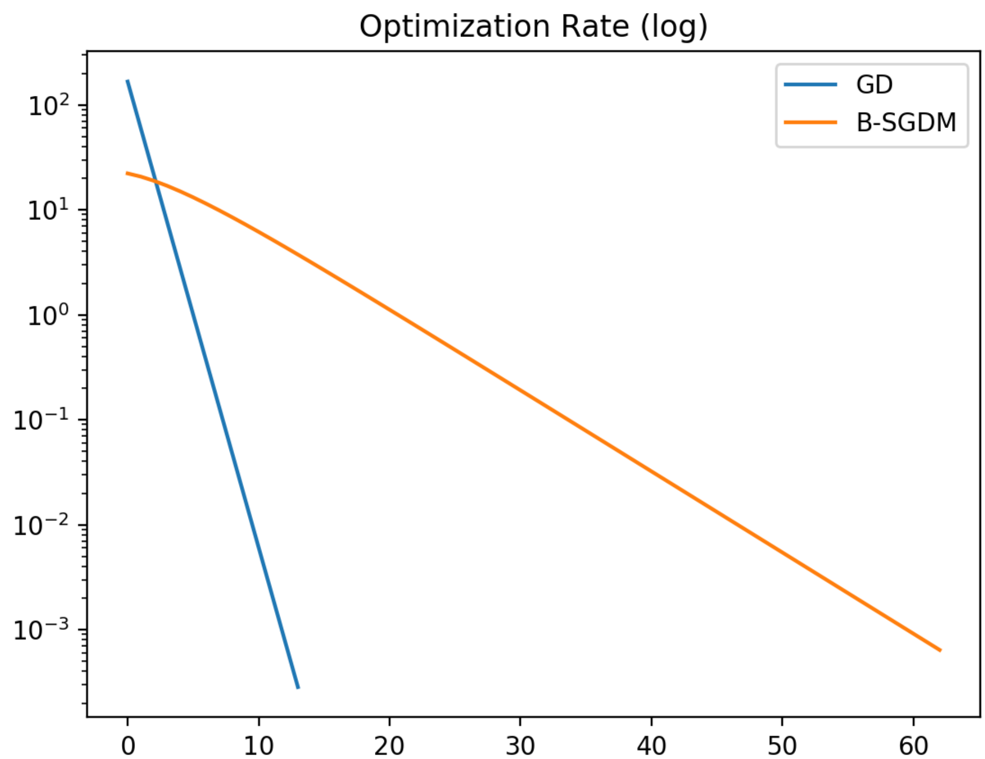


Figure 15: GD vs Batching SGDM

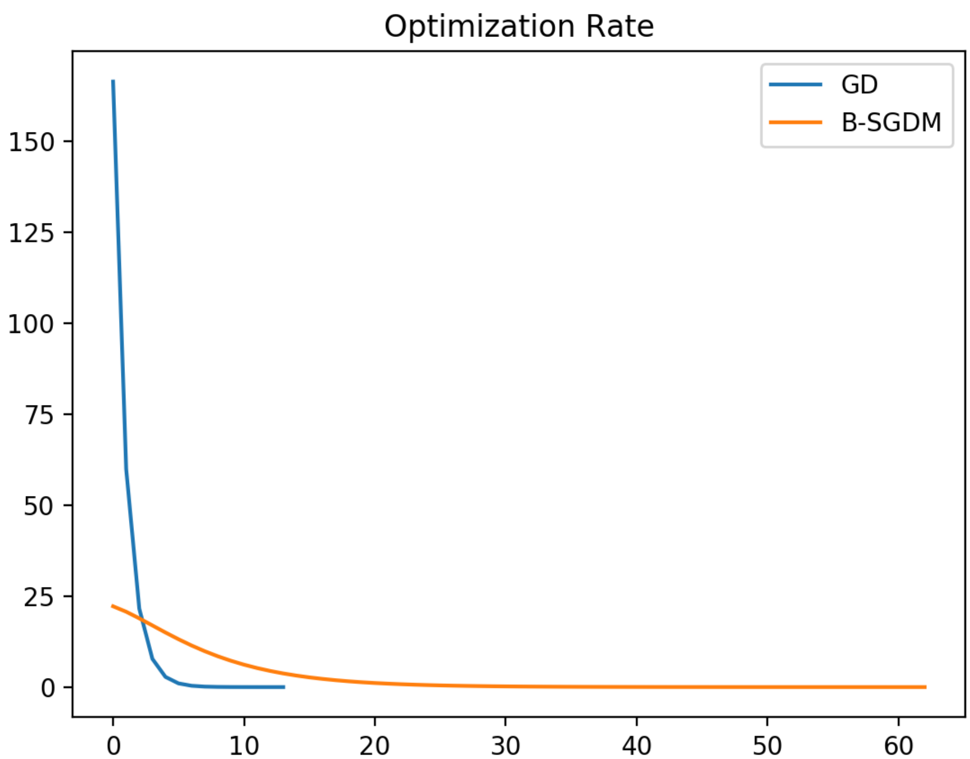


Figure 16: GD vs Batching SGDM

(e) Adaptive Methods
The adaptive methods provided more robust optimization although were not necessarily exhibited well in this simple convex function. See below for a better use-case.

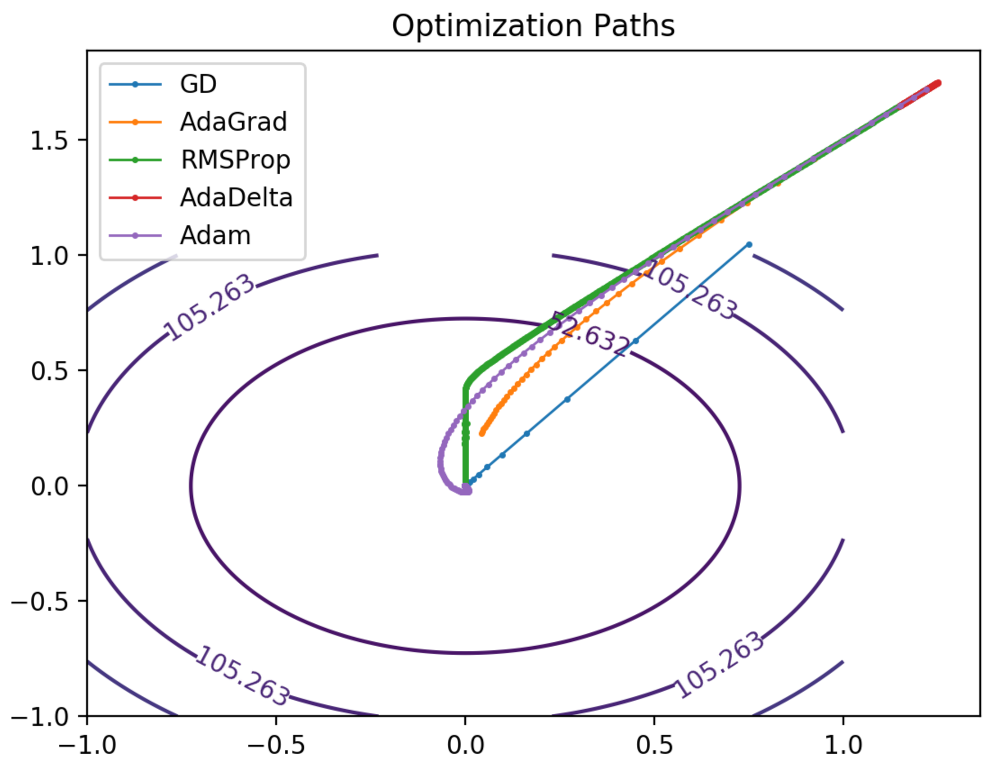


Figure 17: Adaptive methods optimization paths.

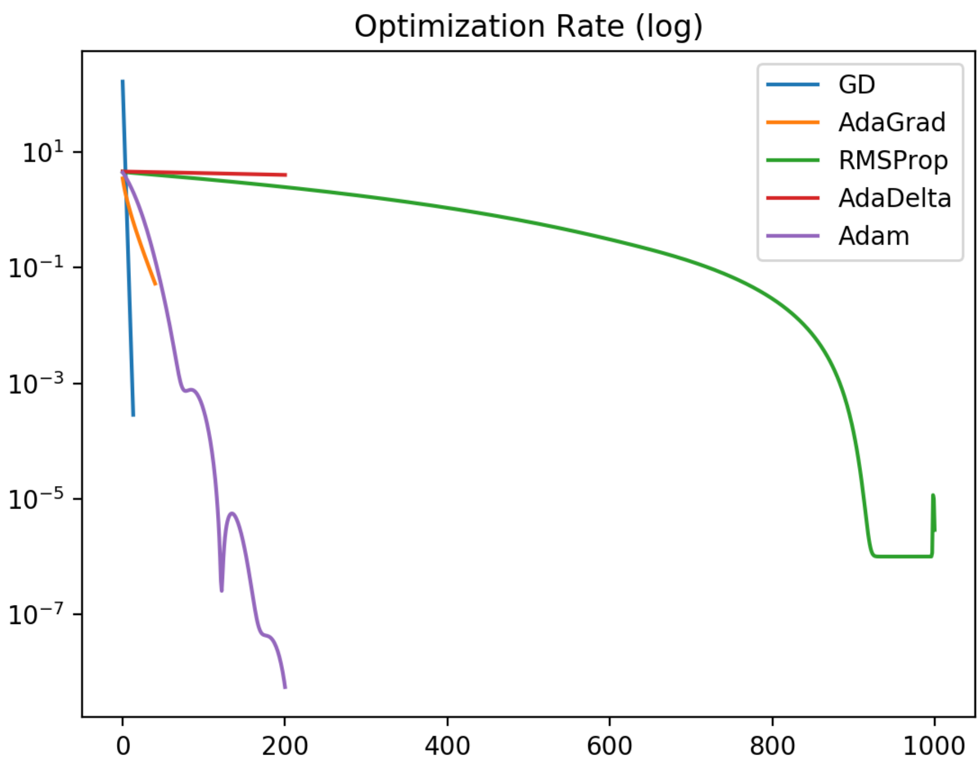


Figure 18: Adaptive methods optimization iterations.

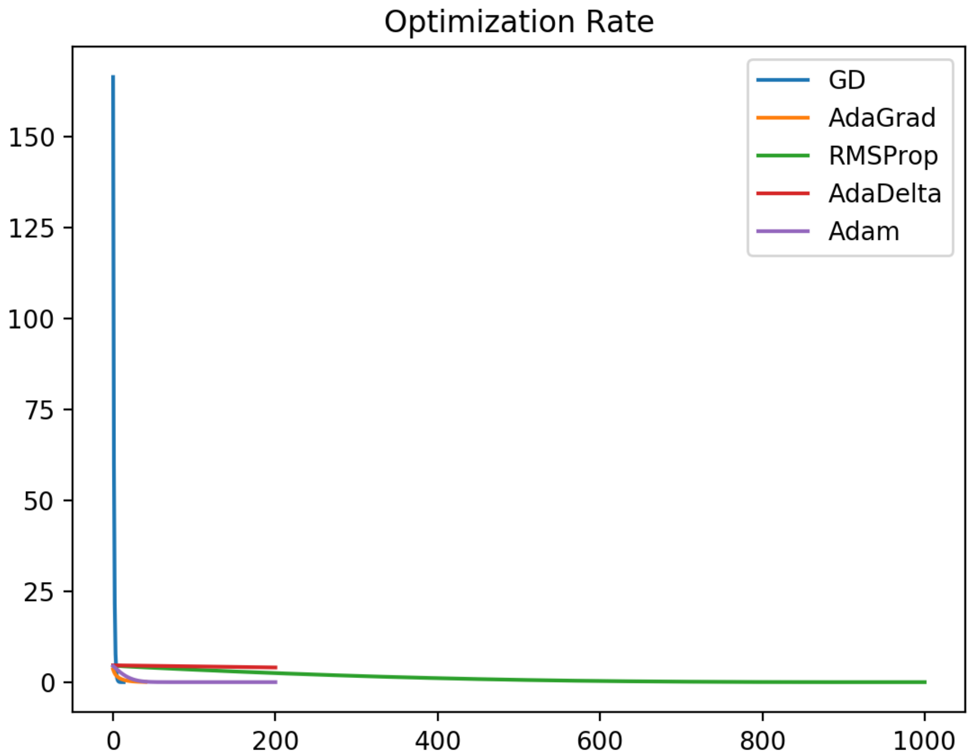


Figure 19: Adaptive methods optimization iterations.

(f) Non-convex Function

To test how many of these methods react to a more difficult optimization function (akin to what would be encountered in real-world data), we simulated the following non-convex function:

$$f(x, y) = 1 - e^{-(10x^2+y^2)}$$

In general, our results were what we expected: Adam performed the best and was capable of optimization while nearly all the others couldn't.

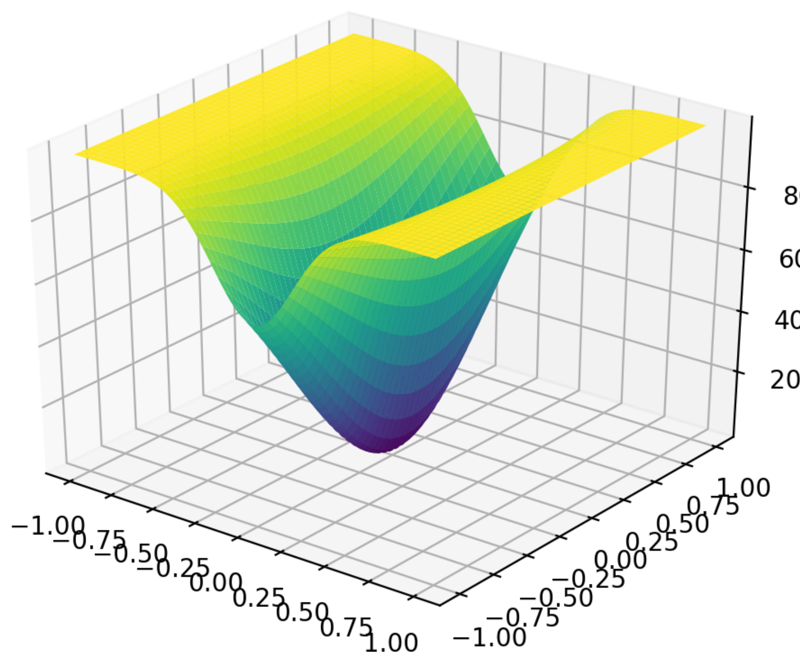


Figure 20: Non-convex optimization function.

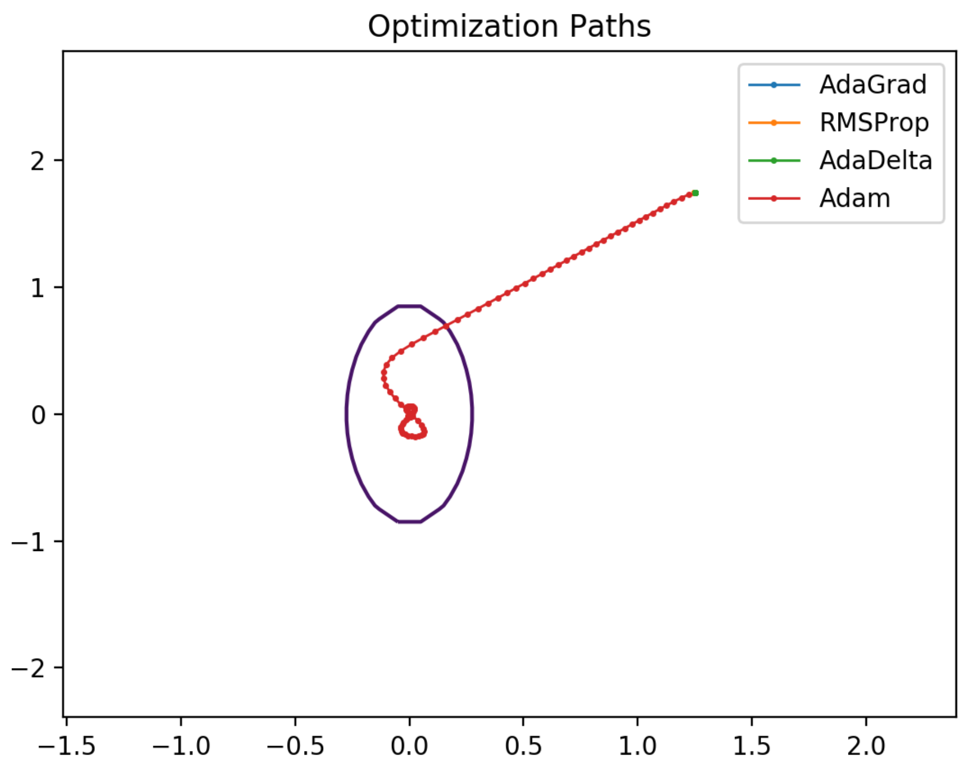


Figure 21: Non-convex optimization function paths.

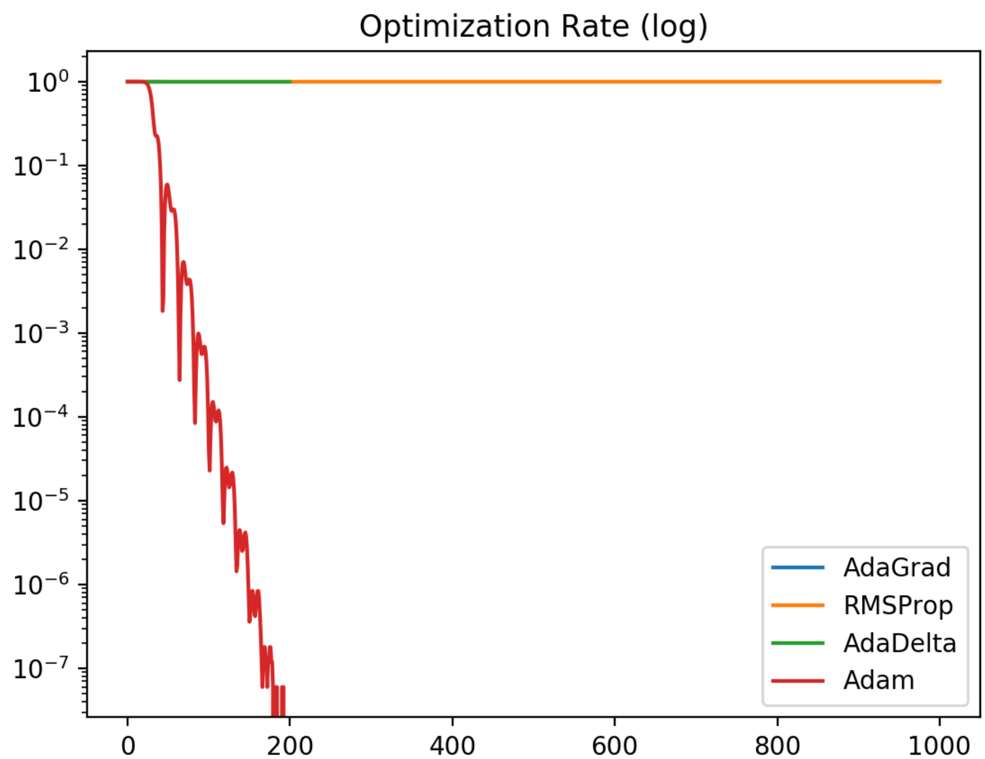


Figure 22: Non-convex optimization function iterations.

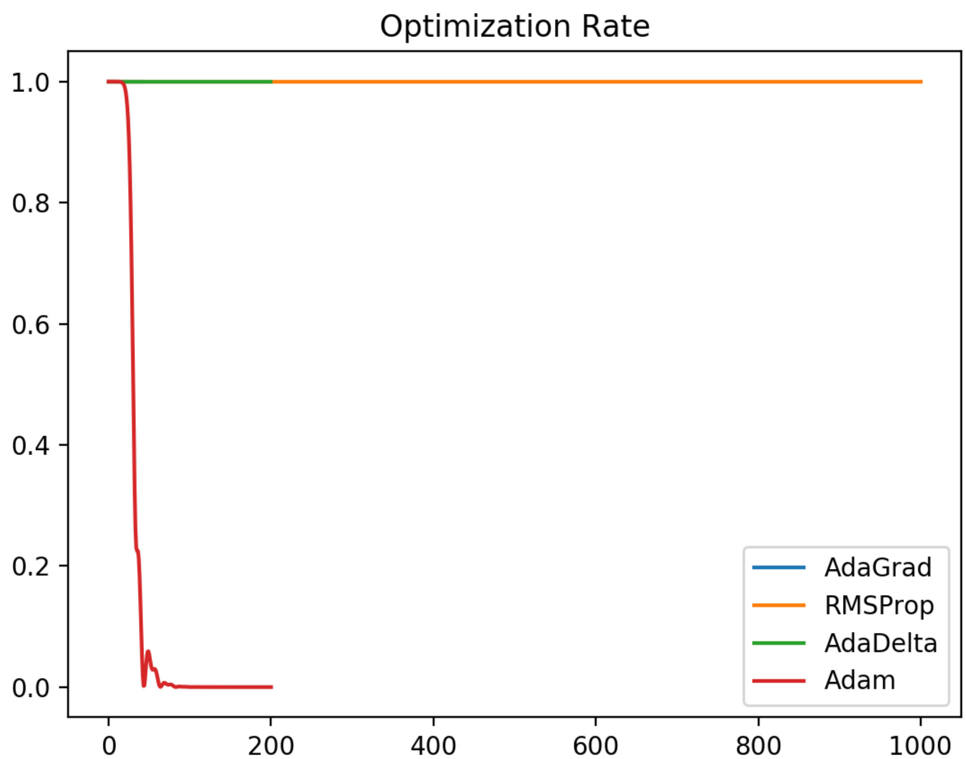
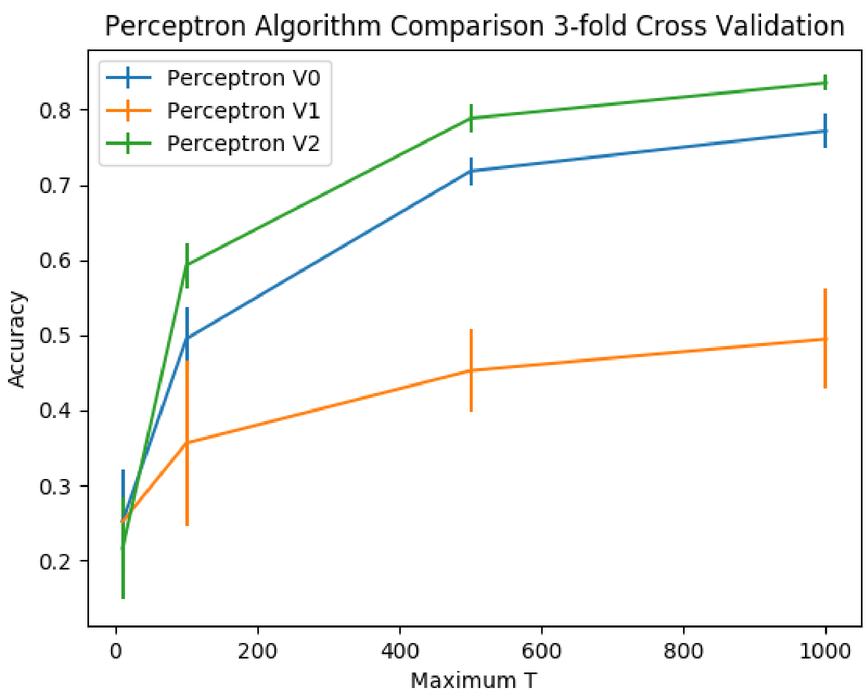


Figure 23: Non-convex optimization function iterations.

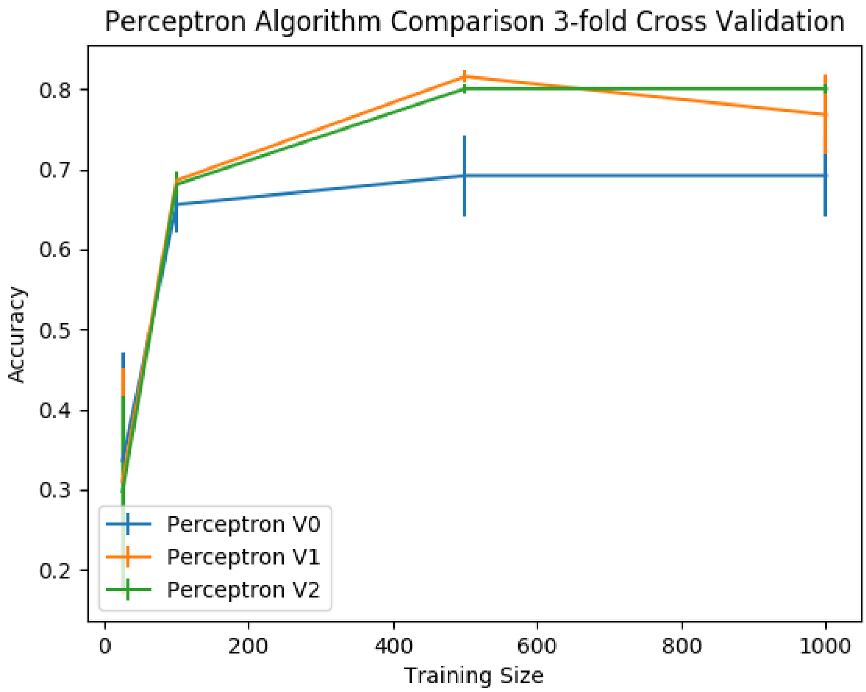
Problem 6: Perceptron case study

(i) We implemented the 3 versions of Perceptron first as binary classifiers, and then extended to a multiclass case using one-versus-all comparison. To double check our work, we ran synthetic, 2-class data through both the binary and extended multiclass versions, and for each version of Perceptron, we got exactly matching results between the binary and multiclass implementations. We then applied these algorithms to the MNIST dataset.

(ii) A three-fold cross-validation analysis was done of the three Perceptron versions at various maximum iterations (values of T). At very low values of T, all three versions of Perceptron are comparably bad (though still better than random guessing, which would have an accuracy of approximately 0.1). As the value of T increases, Perceptron V2 emerges as the most effective classifier for this MNIST task, followed by V0, and finally by V1.



A similar 3-fold cross-validation experiment was done with different sized training sets. In this experiment, Perceptron V1 and Perceptron V2 performed comparably, and both outperformed V0.



(iii) For the Kernel Perceptron, we once again turned to a synthetic binary dataset to ensure that our binary and multi-class implementations were working as expected. On our synthetic set, the performance was:

Perceptron	Binary Accuracy	"Multiclass" Accuracy
V0	0.724	0.724
V1	0.632	0.632
V2	0.736	0.736
Kernel	0.748	0.748

The fact that our implementations have matching performace on a two-class problem for both the base and multi-class implementations show that the multi-class extension is implemented correctly. As expected, the Kernel Perceptron is the best performer. When we generated the synthetic data, we intentionally set it to NOT be linearly separable. Thus, the Kernel version probably improves performance because the data is separable in a transformed space. For completeness, we also tested true multi-class (5 class) data through the implementations:

Perceptron	Multiclass Accuracy
V0	0.376
V1	0.192
V2	0.384
Kernel	0.456

We, once again, see that the Kernel version is the top performer.