Quadratic Gradient: Uniting Gradient Algorithm and Newton Method as One

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Abstract

It might be inadequate for the line search technique for Newton’s method to use only one floating point number. A column vector of the same size as the gradient might be better than a mere float number to accelerate each of the gradient elements with different rates. Moreover, a square matrix of the same order as the Hessian matrix might be helpful to correct the Hessian matrix. Chiang [4] applied something between a column vector and a square matrix, namely a diagonal matrix, to accelerate the gradient and further proposed a faster gradient variant called quadratic gradient. In this paper, we present a new way to build a new version of the quadratic gradient. This new quadratic gradient doesn’t satisfy the convergence conditions of the fixed Hessian Newton’s method. However, experimental results show that it sometimes has a better performance than the original one in convergence rate. Also, Chiang [4] speculates that there might be a relation between the Hessian matrix and the learning rate for the first-order gradient descent method. We prove that the floating number $\frac{1}{\varepsilon + \max_i |\lambda_i|}$ can be a good learning rate of the gradient methods, where $\varepsilon$ is a number to avoid division by zero and $\lambda_i$ the eigenvalues of the Hessian matrix.

1 Introduction

Chiang [4] introduced a novel gradient variant called quadratic gradient which could abstract the second-order information of the curve into the first-order information gradient. He also applied this gradient variant to the naive NAG method and obtained an enhanced NAG method for the binary logistic regression training. Experiments show that the enhanced NAG method converges faster than the raw NAG method.

Chiang [3] extended this work of binary LR training to multiclass LR training based on the fixed Hessian method of the multiclass LR model. Chiang [3] also presented the enhanced Adagrad method and applied it to multiclass LR training. From the construction of the quadratic gradient, Chiang [3] inferred that $\frac{1}{2}X^TXX$ can be a good fixed lower bound.

In this work, we first point out that there does exist a relation between the Hessian matrix and the learning rate of the first-order gradient (descent) method. That is, the eigenvalues of the Hessian matrix can provide reference information to the setting of the learning rate of the naive gradient descent methods. We then proposed the enhanced Adam method via quadratic gradient for general numerical optimization problems and test this enhanced method on several optimization functions. Finally, we provide a new way to construct a new quadratic gradient. We test this new quadratic-gradient version and the original one by using the enhanced Adam method on several optimization functions.
2 Preliminaries

For two symmetric matrices $A$ and $B$, $A \leq B$ is defined in the Loewner ordering iff their difference $B - A$ is positive semi-definite.

2.1 Chiang’s Quadratic Gradient

In the following work to [2] in which a simplified diagonal matrix satisfying the fixed Hessian method [1] is constructed, Chiang [4] proposed a faster gradient variant called quadratic gradient.

**Quadratic Gradient** Given a differentiable scalar-valued function $F(x)$ with its gradient $g$ and Hessian matrix $H$. For the maximization problem, we need to find a good lower bound matrix $\bar{H} \leq H$, where “$\leq$” denotes the Loewner ordering. For the minimization problem, we try to find a good upper bound $\bar{H}$ such that $H \leq \bar{H}$ in the Loewner ordering. Note that the Hessian matrix $H$ itself satisfies these two conditions and can substitute the good bound matrix $\bar{H}$. We attempt to find a fixed good bound matrix of the Hessian matrix for efficiency but could just directly use the Hessian matrix itself. To build the quadratic gradient, we first construct a diagonal matrix $\bar{B}$ from the good bound matrix $\bar{H}$ as follows:

$$
\bar{B} = \begin{bmatrix}
\frac{1}{\epsilon + \sum_{i=0}^{d} |h_{0i}|} & 0 & \cdots & 0 \\
0 & \frac{1}{\epsilon + \sum_{i=0}^{d} |h_{1i}|} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \frac{1}{\epsilon + \sum_{i=0}^{d} |h_{di}|}
\end{bmatrix},
$$

where $\epsilon$ is a small positive number to avoid dividing by zero and $\bar{h}_{ji}$ the elements of the matrix $\bar{H}$. We can then defined the quadratic gradient for the function $F(x)$ as $G = \bar{B} \cdot g$.

The multiplication between the diagonal matrix $\bar{B}$ and the gradient $g$, the quadratic gradient $G$, is of the same size as the gradient $g$. To use the quadratic gradient $G$, we can just use it the same way as the gradient but need a learning rate larger than 1. The well-studied first-order gradient descent methods can also be applied to develop enhanced methods via quadratic gradient.

2.2 Enhanced Methods via Quadratic Gradient

Chiang [4] presented the enhanced NAG method via quadratic gradient for binary LR training:

$$
V_{t+1} = \beta_{t} + (1 + \alpha_{t}) \cdot G, \quad \beta_{t+1} = (1 - \gamma_{t}) \cdot V_{t+1} + \gamma_{t} \cdot V_{t},
$$

Chiang [3] proposed the enhanced Adagrad method via quadratic gradient for multiclass LR training:

$$
\beta_{[i]}^{(t+1)} = \beta_{[i]}^{(t)} - \frac{1 + \eta}{\epsilon + \sqrt{\sum_{k=1}^{t} G_{[i]}^{(k)} \cdot G_{[i]}^{(k)}}} \cdot G_{[i]}^{(t)},
$$

In this work, we propose the enhanced Adam method, which is to apply the quadratic gradient to the Adam method. The naive Adam method and the enhanced Adam method are described in detail in Algorithms [1] and [2], respectively. See the [5] for the detailed description of the parameters in these two Algorithms.
Algorithm 1 The Adam method

Input: $\alpha$: Stepsize; $\beta_1, \beta_2 \in [0, 1)$: Exponential decay rates; $f(\theta)$: Objective function with parameters $\theta \theta_0$: Initial parameter vector

Output: $\theta_t$: Resulting parameters
1: $m_0 \leftarrow 0$: Initialize 1st moment vector
2: $v_0 \leftarrow 0$: Initialize 2nd moment vector
3: $t \leftarrow 0$: Initialize timestep
4: while $\theta_t$ not converged do
5: $t \leftarrow t + 1$
6: $g_t \leftarrow \nabla_{\theta} f_t(\theta_{t-1})$
7: $\hat{m}_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot g_t$
8: $m_t \leftarrow \beta_2 \cdot m_{t-1} + (1 - \beta_2) \cdot g_t^2$
9: $\tilde{m}_t \leftarrow m_t / (1 - \beta_1^t)$
10: $\hat{v}_t \leftarrow \beta_1 \cdot v_{t-1} + (1 - \beta_1) \cdot g_t^2$
11: $v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 - \beta_2) \cdot G_t$
12: $\theta_t \leftarrow \theta_{t-1} - \alpha \cdot \tilde{m}_t / (\sqrt{v_t} + \varepsilon)$
13: end while
14: return $\theta_t$ ▷ Resulting parameters

Algorithm 2 Enhanced Adam method

Input: $\eta$: Stepsize; $\beta_1, \beta_2 \in [0, 1)$: Exponential decay rates; $f(\theta)$: Objective function with parameters $\theta \theta_0$: Initial parameter vector

Output: $\theta_t$: Resulting parameters
1: $m_0 \leftarrow 0$: Initialize 1st moment vector
2: $v_0 \leftarrow 0$: Initialize 2nd moment vector
3: $t \leftarrow 0$: Initialize timestep
4: while $\theta_t$ not converged do
5: $t \leftarrow t + 1$
6: $g_t \leftarrow \nabla_{\theta} f_t(\theta_{t-1})$
7: $G_t \leftarrow B \cdot g_t$
8: $m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot G_t$
9: $v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 - \beta_2) \cdot G_t^2$
10: $\hat{m}_t \leftarrow m_t / (1 - \beta_1)$
11: $\hat{v}_t \leftarrow v_{t-1} / (1 - \beta_2)$
12: $\theta_t \leftarrow \theta_{t-1} - \eta \cdot \hat{m}_t / (\sqrt{\hat{v}_t} + \varepsilon)$
13: end while
14: return $\theta_t$

3 Hessian Matrix and Learning Rate

We show the relation between the Hessian matrix and the learning-rate setting of the first-order gradient (descent) method. By constructing special quadratic gradients, we can draw the conclusion that the eigenvalues of the Hessian matrix can be used to the setting of the learning rate. Such learning-rate settings can actually be seen as a further simplified fixed Hessian method and thus ensure convergence.

Lemma 1. Given the Hessian matrix $H$ with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$, it holds that $\lambda_1 I \leq H \leq \lambda_n I$ in the Loewner ordering. To build the quadratic gradients, we can use $\lambda_1 I$ for the maximization problems with the eigenvalues being negative and $\lambda_n I$ for the minimization problems with the eigenvalues being positive. The real absolute value function can be used to unify the two conditions and therefore the float number $\frac{1}{\max(|\lambda_i|)+\varepsilon}$ can be used as the learning rate of the first-order gradient (descent) method, which can be seen as the further simplified fixed Hessian method [2] and ensures the convergence of the method.

Proof. To prove $\lambda_1 I \leq H \leq \lambda_n I$ in the Loewner ordering, we have to prove that $x^T \lambda_1 I x \leq x^T H x \leq x^T \lambda_n I x$ for any nonzero vector $x$. The Rayleigh quotient $RQ(H, x)$ for the Hessian $H$ and the nonzero vector $x$ is: $RQ(H, x) = \frac{x^T H x}{x^T x}$. By the property of Rayleigh quotient, we get: $\lambda_1 \leq RQ(H, x) \leq \lambda_n$, which leads to: $x^T \lambda_1 I x \leq x^T H x \leq x^T \lambda_n I x$, and we conclude that $\lambda_1 I \leq H \leq \lambda_n I$.

By the construction of the quadratic gradient, we can use $\lambda_1 I$ or $\lambda_n I$ to build the quadratic gradient depending on whether the optimization question is to maximize the function or to minimize the function. These two cases both result in the quadratic gradient being $g = \frac{1}{\max(|\lambda_i|)+\varepsilon} \cdot g$. It is straightforward that the naive quadratic gradient methods have the iterations $x = x + \frac{1}{\max(|\lambda_i|)+\varepsilon} \cdot g$ and $x = x - \frac{1}{\max(|\lambda_i|)+\varepsilon} \cdot g$ for the maximization problems and minimization problems respectively. Thus, when we set $\frac{1}{\max(|\lambda_i|)+\varepsilon}$ as the learning rate of the first-order gradient method, we actually adopt the (simplified) fixed Hessian method even though it looks like we just use the first-order gradient method.

The diagonal matrix $\frac{1}{\max(|\lambda_i|)+\varepsilon} I$ might not be a good bound for the simplified fixed Hessian method. However, as a learning rate of the naive gradient method, it possesses the merit of the second-order fixed Hessian Newton’s method, which ensures that in this way the first-order gradient method would process toward the final optimization solution and would eventually converge.
Performance Evaluation We can apply the above learning-rate setting to adapt three methods:

1. Method 1: we directly use $\frac{1}{\max\{|\lambda_i|+\epsilon\}}$ as the learning rate in each iteration for the naive gradient descent method:
   
   $$x = x - \frac{1}{\max\{|\lambda_i|+\epsilon\}} \cdot g.$$

2. Method 2: we use the naive NAG method as a baseline method with the $\frac{1}{\max\{|\lambda_i|+\epsilon\}}$ being the learning rate:
   
   $$lr_t = \frac{1}{\max\{|\lambda_i|+\epsilon\}}$$
   
   $$V_{t+1} = \beta_t + lr_t \cdot \nabla J(\beta_t),$$
   
   $$\beta_{t+1} = (1 - \gamma_t) \cdot V_{t+1} + \gamma_t \cdot V_t.$$

3. Method 3: we use $\frac{1}{\max\{|\lambda_i|+\epsilon\}}$ as the learning rate in each iteration for the enhanced NAG method with the $B$ in quadratic gradient $B \cdot g$ built from the Hessian matrix itself:
   
   $$lr_t = \frac{1}{\max\{|\lambda_i|+\epsilon\}}$$
   
   $$V_{t+1} = \beta_t + (1 + lr_t) \cdot B \cdot \nabla J(\beta_t),$$
   
   $$\beta_{t+1} = (1 - \gamma_t) \cdot V_{t+1} + \gamma_t \cdot V_t.$$

We evaluate the three adapted methods on three functions: Rosenbrock Function, Beale Function, and Booth Function. See Figure 1 for the comparison results.

4 A New Quadratic Gradient

In this section, we propose a new way to construct the quadratic gradient that includes the gradient information.

**Definition 4.1 (A New Quadratic Gradient).** Suppose that the Hessian matrix $H$ is invertible and both the gradient $g$ and the column vector $H^{-1} g$ contain no zero elements, we first construct a diagonal matrix $R$ such that $H^{-1} \cdot g = R^{-1} \cdot g$. We could then build a new quadratic gradient $G = R \cdot g$ where $R$ is constructed from $R$ in the same way as $B$ being constructed from the Hessian $H$ itself. Namely, $R = diag\{1/r_1, 1/r_2, \ldots, 1/r_n\}$, where $r_i$ is the element of $R$.

This new quadratic gradient doesn’t satisfy the convergence condition of the fixed Hessian method. For example, supposing that the optimization problem is to maximize the function $F(x_1, x_2) = -2x_1^2 + 2x_1x_2 - x_2^2$ with its Hessian matrix $H_F$ and gradient $g_F$ as follows:

$$H_F = \begin{bmatrix} -4 & 2 \\ 2 & -2 \end{bmatrix}$$

and $g_F = [-4x_1 + 2x_2, 2x_1 - 2x_2]^T$. At the point $(-1, -1.5)$, we can obtain the gradient $g_F(-1, -1.5) = [1, 1]^T$ and the $R = diag\{-1, -1.5\}$ such that $H_F^{-1} \cdot g_F = R^{-1} \cdot g_F$. From the construction of the quadratic gradient, we get the $B = diag\{-1 - \varepsilon, -1.5 - \varepsilon\}$ where $\varepsilon$ is a small positive float number. We can see that the $B$ doesn’t meet the convergence condition of the fixed Hessian method because it fails the inequality $R \leq H_F$ in the Laewner ordering.

Another problem about this new quadratic gradient is that, in the real-world applications, the Hessian matrix sometimes is singular and it is normal for the gradient to have zero elements. In these cases, we could use the Moore–Penrose inverse $(H \cdot D)^+ \cdot g$ to approximate the matrix $R$ where $D$ is the diagonal matrix whose diagonal elements are the elements of the gradient in the corresponding order: $D = diag\{g_0, g_1, \ldots, g_n\}$.

Performance Evaluation We compare the enhanced Adam method via the original quadratic gradient and that by the new quadratic gradient, through the Rosenbrock function with various variables. Figure 2 shows the comparison results.

There are some hidden bugs in the new version of the quadratic gradient (See Figure 3). What causes these would be studied in the near future. A lucky guess would be partly due to the error introduced by the Moore-Penrose inverse.
5 Conclusion

In this work, we proposed an enhanced Adam method via quadratic gradient and applied the quadratic gradient to the general numerical optimization problems. The quadratic gradient can indeed be used to build enhanced gradient methods for general optimization problems. There is a good chance that quadratic gradient can also be applied to quasi-Newton methods, such as the famous BFGS method.

All the python source code to implement the experiments in the paper is openly available at: https://github.com/petitioner/ML.QuadraticGradient.

Acknowledgments

自由與榮耀（Freedom with/and Honour）
- at 09:54 a.m. Saturday Sep 3 2022
- in 大綱, 大連
- by 西星 者
(a) The Rosenbrock Function with 2 variables
(b) The Rosenbrock Function with 5 variables
(c) The Rosenbrock Function with 10 variables
(d) The Rosenbrock Function with 20 variables

Figure 2: The Rosenbrock Functions with various variables

References

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(a) The Rosenbrock Function with 2 variables

(b) The Rosenbrock Function with 5 variables

(c) The Rosenbrock Function with 10 variables

(d) The Rosenbrock Function with 20 variables

Figure 3: The Rosenbrock Functions with various variables