NEW STEP-SIZE CRITERION FOR THE STEEPEST DESCENT BASED ON GEOMETRIC NUMERICAL INTEGRATION

KENYA ONUMA AND SHUN SATO

ABSTRACT. This paper deals with unconstrained optimization problems based on numerical analysis of ordinary differential equations (ODEs). Although it has been known for a long time that there is a relation between optimization methods and discretization of ODEs, research in this direction has recently been gaining attention. In recent studies, the dissipation laws of ODEs have often played an important role. By contrast, in the context of numerical analysis, a technique called geometric numerical integration, which explores discretization to maintain geometrical properties such as the dissipation law, is actively studied. However, in research investigating the relationship between optimization and ODEs, techniques of geometric numerical integration have not been sufficiently investigated. In this paper, we show that a recent geometric numerical integration technique for gradient flow reads a new step-size criterion for the steepest descent method. Consequently, owing to the discrete dissipation law, convergence rates can be proved in a form similar to the discussion in ODEs. Although the proposed method is a variant of the existing steepest descent method, it is suggested that various analyses of the optimization methods via ODEs can be performed in the same way after discretization using geometric numerical integration.

1. INTRODUCTION

In this paper, we consider an unconstrained minimization problem

$$\min_{x \in \mathbb{R}^n} f(x),$$

where the function $f$ is assumed to be $L$-smooth and satisfies $\arg \min f \neq \emptyset$. Since problems of this form have appeared in various applications, optimization methods have been widely researched.

The steepest descent method, which is the simplest optimization method, can be regarded as a discretization of the gradient flow:

$$\dot{x} = -\nabla f(x), \quad x(0) = x_0,$$

where $x_0 \in \mathbb{R}^n$ is an initial condition. Investigations on the relationship between optimization methods and the discretization of ordinary differential equations (ODEs) have been reported in the 1980s (e.g., [1, 14, 18]). In addition, inspired by the pioneering work by Su, Boyd, and Candès [16] on Nesterov’s accelerated gradient method, research in this direction has been active again in recent years (see, e.g., [17] and references therein).

The gradient flow (2) itself is an important class of ODEs that describes various physical phenomena. Therefore, numerical methods for gradient flow (2) have also

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been intensively studied. In particular, specialized numerical schemes that replicate
the dissipation law \( \frac{d}{dt} f(x(t)) \leq 0 \) (Proposition 2.4) of the gradient flow have
been devised and investigated. Techniques devising and analyzing such a specialized
numerical scheme replicating a geometric property of ODEs are known as “geometric
numerical integration” (cf. [5]).

The discrete gradient method [4] (see also [10]) is the most popular specialized
numerical method for gradient flow (2). The schemes based on the discrete gradient
method are often superior to general-purpose methods, particularly for numerically
difficult differential equations.

Although these schemes allow us to employ a larger step size than general-
purpose methods, they are usually more expensive per step. Most of these schemes
require solving an \( n \)-dimensional nonlinear equation per step, and a scheme based
on the Itoh–Abe discrete gradient [8] requires solving a scalar nonlinear equation \( n \)
times per step.

If we return to the relation between ODEs and optimization problems, one may
think that geometric numerical integration techniques can be utilized immediately
as an optimization method. Indeed, because the discrete gradient method provides
a monotone non-increasing sequence \( \{ f(x_k) \}_{k=0}^{\infty} \), the discrete gradient method has
recently been applied to optimization problems [12, 13, 3].

However, as mentioned above, the discrete gradient method is usually computa-
tionally expensive. Although existing studies employ the Itoh–Abe discrete
gradient, a computationally cheaper one, it is still more expensive than practical
optimization methods.

Therefore, in this paper, we propose the use of the “Lagrange multiplier ap-
proach” recently devised by Cheng, Liu, and Shen [2]. Then, the resulting method

\[
\begin{align*}
\frac{x_{k+1} - x_k}{h} &= -\eta_k \nabla f(x_k) \\
f(x_{k+1}) - f(x_k) &= \eta_k \langle \nabla f(x_k), x_{k+1} - x_k \rangle
\end{align*}
\]

(3)

to obtain \( x_{k+1} \in \mathbb{R}^n \) (and \( \eta_k \in \mathbb{R} \)) from \( x_k \) can be regarded as the steepest descent
method with a new step-size criterion. Although (3) can be regarded as the steepest
descent method with a step size \( h \eta_k \), the parameter \( h \) is called “step size” in the
numerical analysis. It requires solving a scalar nonlinear equation with respect to
\( \eta_k \) per step. In other words, the computational cost is almost equivalent to that of
the steepest descent method with an exact line search.

Unfortunately, however, the existence and uniqueness of the scalar nonlinear
equation that appears in the Lagrange multiplier approach are not known in the
literature. Therefore, we establish the existence and uniqueness results for (3). We
also show the convergence rates for several cases: (i) general \( L \)-smooth functions, (ii)
convex functions, and (iii) functions that satisfy the Polyak–Lojasiewicz inequality.

Because the above method is still too expensive, we propose a relaxation tech-
nique to enhance computational efficiency. The resulting method

\[
\begin{align*}
\frac{x_{k+1} - x_k}{h} &= -\eta_k \nabla f(x_k) \\
f(x_{k+1}) - f(x_k) &\leq \eta_k \langle \nabla f(x_k), x_{k+1} - x_k \rangle
\end{align*}
\]

(4)

allows us to employ the backtracking technique, and satisfies the discrete dissipation
law (Theorem 5.1). Therefore, its computational cost is the same as that of the
standard steepest descent method with a backtracking line search. We also show similar convergence rates for the relaxed method (4).

The “step size” \( h \) can be any positive number, but it should be proportional to the reciprocal of the Lipschitz constant \( L \). However, when \( L \) is not known in advance, if \( h \) is too small, the convergence rate deteriorates, and if it is too large, the cost of backtracking increases. Therefore, we propose another method to adaptively change \( h \) at every step, and also show convergence rates for the adaptive method.

It may seem as though the methods proposed in this paper are merely variants of the basic existing method; moreover, as shown in numerical experiments later, the actual behavior is almost the same as that of the existing method.

However, the proposed methods in this paper have the advantage that the relationship between continuous and discrete systems is very clear in the proof of convergence rates (see, e.g., Theorems 2.7 and 4.1). To the best of the authors’ knowledge, in existing research considering the correspondence of continuous and discrete systems, although the discussion on continuous systems is simple, it is often very complicated to prove the corresponding property in discrete systems. A limitation of this paper is that we deal with the simplest gradient flows; however, it suggests that the above issues can be overcome by geometric numerical integration techniques even when we are dealing with more complicated ODEs that appear in optimization.

The remainder of this paper is organized as follows. Section 2 presents some basic concepts in optimization, discrete gradient methods, and the Lagrange multiplier approach. We show several existence results on a special case of the Lagrange multiplier approach in Section 3 and convergence rates of it in Section 4. In Section 5, we introduce the proposed methods, relaxation of the Lagrange multiplier approach, and show their convergence rates. These results are confirmed by numerical experiments in Section 6. Finally, Section 7 concludes the paper.

2. Preliminaries

2.1. Basic concepts in optimization. Throughout the paper, we assume the objective function \( f \) is \( L \)-smooth.

**Definition 2.1.** A function \( f : \mathbb{R}^n \to \mathbb{R} \) is \( L \)-smooth for \( L > 0 \) if its gradient \( \nabla f \) is \( L \)-Lipschitz continuous, that is, \( \| \nabla f(x) - \nabla f(y) \| \leq L \| x - y \| \) holds for all \( x, y \in \mathbb{R}^n \).

The \( L \)-smooth functions satisfy the following property:

**Lemma 2.2.** If \( f \) is \( L \)-smooth, the following inequalities hold for all \( x, y \in \mathbb{R}^n \):

\[
-\frac{L}{2} \| y - x \|^2 \leq f(y) - f(x) - \langle \nabla f(x), y - x \rangle \leq \frac{L}{2} \| y - x \|^2.
\]

We sometimes assume that the objective function \( f \) is convex or satisfies the Polyak–Lojasiewicz (PL) inequality.

**Definition 2.3** (cf. [9]). A function \( f : \mathbb{R}^n \to \mathbb{R} \) satisfies the Polyak–Lojasiewicz inequality with parameter \( \mu > 0 \) if

\[
\frac{1}{2} \| \nabla f(x) \|^2 \geq \mu (f(x) - f^*)
\]

holds for all \( x \in \mathbb{R}^n \).
Note that a $\mu$-strongly convex function satisfies the PL inequality with parameter $\mu$.

### 2.2. Discrete gradient method

The gradient flow (2) satisfies the dissipation law:

**Proposition 2.4** (Dissipation law). For any solution $x$ of the gradient flow (2) $\frac{d}{dt} f(x(t)) \leq 0$ holds.

**Proof.** A simple calculation
\[
\frac{d}{dt} f(x) = \langle \nabla f(x), \dot{x} \rangle = -\|\nabla f(x)\|^2 \leq 0
\]
implies the proposition. \qed

The explicit Euler method, the simplest one, for the gradient flow (2), is as follows:
\[
x_{k+1} - x_k = -\nabla f(x_k), \quad (6)
\]
where $x_k \approx x(kh)$ is a numerical solution. However, the explicit Euler method satisfies the discrete dissipation law
\[
f(x_{k+1}) \leq f(x_k) \quad (7)
\]
only when the step size $h$ is sufficiently small.

Because the dissipation law is an essential property of gradient flow (2), numerical methods that replicate the dissipation law have been studied in the literature. The discrete gradient method \([4, 10, 11]\) is one of the most popular numerical methods.

**Definition 2.5** (Discrete gradient). Let $f : \mathbb{R}^n \to \mathbb{R}$ be a differentiable function. A discrete gradient is a continuous mapping $\nabla f : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$ that satisfies the following two properties:

- (discrete chain rule) $f(x) - f(y) = \langle \nabla f(x, y), x - y \rangle$
- (consistency) $\nabla f(x, x) = \nabla f(x)$

for any $x, y \in \mathbb{R}^n$.

The first condition is essential and a discrete counterpart of the chain rule:
\[
\frac{d}{dt} f(x) = \langle \nabla f(x), \dot{x} \rangle
\]
which is used in the proof of Proposition 2.4. The second condition merely ensures that $\nabla f$ approximates the gradient $\nabla f$. Using the discrete gradient, we construct the scheme
\[
\frac{x_{k+1} - x_k}{h} = -\nabla f(x_{k+1}, x_k). \quad (8)
\]
For all $h > 0$, this method satisfies the discrete dissipation law (7):
\[
f(x_{k+1}) - f(x_k) = \langle \nabla f(x_{k+1}, x_k), x_{k+1} - x_k \rangle = -h\|\nabla f(x_{k+1}, x_k)\|^2 \leq 0.
\]

There are several constructions of the discrete gradient, e.g., the average vector field \([6]\), Gonzalez’s midpoint discrete gradient \([4]\), and Itoh–Abe’s discrete gradient \([8]\).
2.3. Discrete gradient method as an optimization method. In this section, we consider the unconstrained optimization problem (1). Because we assume that \( \text{arg min} f \neq \emptyset \), there is an optimal solution \( x^* \) and an optimal value \( f^* = f(x^*) \). In particular, we consider the relationship between the problem and gradient flow (2).

When \( f \) is strictly convex, the following proposition holds.

**Proposition 2.6** (cf. [7]). Let \( f \) be a strictly convex function. Then, \( f \) is a Lyapunov function of the gradient flow (2), and

\[
\lim_{t \to \infty} x(t) = x^*
\]

holds for any initial condition \( x_0 \in \mathbb{R}^n \).

Based on the fact above, some researchers have pointed out the idea of using a numerical method for gradient flow as an optimization method. For example, the explicit Euler method (6) coincides with the steepest descent method with a constant step size \( h \). However, we should carefully choose the step size \( h \) to ensure the convergence of this method.

Here, because the convergence in continuous time, such as in Proposition 2.6, are based on the dissipation law, the discrete gradient method can be regarded as an optimization method (see, e.g., [3]). Before stepping into the property in discrete systems, we review the property in continuous systems in this section. The gradient flow (2) satisfies the following three theorems.

**Theorem 2.7.** The solution \( x \) of the gradient flow (2) satisfies

\[
\min_{0 \leq \tau \leq t} \|\nabla f(x(\tau))\| \leq \sqrt{\frac{f(x_0) - f^*}{t}}.
\]

**Proof.** Since \( f^* \) is an optimal value,

\[
f(x_0) - f^* \geq f(x_0) - f(x(t)) \\
= \int_0^t \langle \nabla f(x(\tau)), \dot{x}(\tau) \rangle d\tau \\
= \int_0^t \|\nabla f(x(\tau))\|^2 d\tau \\
\geq t \min_{0 \leq \tau \leq t} \|\nabla f(x(\tau))\|^2
\]

holds. \( \square \)

**Theorem 2.8.** If \( f \) is convex, the solution \( x \) of the gradient flow (2) satisfies

\[
f(x) - f^* \leq \frac{\|x_0 - x^*\|^2}{2t}.
\]

**Proof.** Let \( \mathcal{E} \) be a function defined by

\[
\mathcal{E}(t) := t(f(x) - f^*) + \frac{1}{2}\|x - x^*\|^2.
\]

Then, \( \mathcal{E}(t) \) decreases along time:

\[
\dot{\mathcal{E}}(t) = f(x) - f^* + t(\nabla f(x), \dot{x}) + \langle x - x^*, \dot{x} \rangle \\
= f(x) - f^* + \langle x^* - x, \nabla f(x) \rangle - t\|\nabla f(x)\|^2 \\
\leq -t\|\nabla f(x)\|^2,
\]

\( \square \)
The last inequality is due to convexity. Therefore,

\[ t(f(x) - f^*) \leq \mathcal{E}(t) \leq \mathcal{E}(0) = \frac{1}{2} \|x_0 - x^*\|^2 \]

holds, which proves the theorem. \qed

**Theorem 2.9.** If \( f \) satisfies the Polyak–Lojasiewicz inequality (5) with parameter \( \mu > 0 \), the solution \( x \) of the gradient flow (2) satisfies

\[ f(x) - f^* \leq \exp(-2\mu)(f(x_0) - f^*). \]

**Proof.** Let \( \mathcal{L} \) be a function defined by \( \mathcal{L}(t) := f(x) - f^* \). Then,

\[ \dot{\mathcal{L}}(t) = \langle \nabla f(x), \dot{x} \rangle = -\|\nabla f(x)\|^2 \leq -2\mu(f(x) - f^*) = -2\mu\mathcal{L}(t); \]

therefore, \( \mathcal{L}(t) \leq \exp(-2\mu\mathcal{L}(0)) \)

holds, which proves the theorem. \( \square \)

As shown in Section 2.2, the discrete gradient method (8) satisfies the discrete dissipation law; however, whether the convergence rate such as Theorems 2.8 and 2.9 holds in discrete time is not trivial.

For this issue, Ehrhardt, Riis, Ringholm, and Schönlieb [3] showed that the discrete gradient method (8) with several known constructions of the discrete gradient satisfies \( f(x_k) - f^* = O(1/k) \) for a convex function \( f \), and \( f(x_k) - f^* = O(\exp(-Ck)) \) for a function satisfying PL inequality (5) \((C > 0 \text{ is a constant})\).

### 2.4. Lagrange multiplier approach.

In this section, we review the numerical method proposed by Cheng, Liu, and Shen [2]. The method is based on splitting the function \( f \) in the form

\[ f(x) = \frac{1}{2}(x, Qx) + g(x), \quad (9) \]

where \( Q \in \mathbb{R}^{n \times n} \) is symmetric, and \( g : \mathbb{R}^n \to \mathbb{R} \) is a function. Note that the splitting is not unique \((g \text{ may contain a quadratic term})\); however, when we consider physical problems, the function \( f \) often includes a quadratic term so that we can naturally obtain a splitting \( (\text{see, e.g., [15]}). \)

By introducing an auxiliary variable \( \eta : \mathbb{R}_{\geq 0} \to \mathbb{R} \), we consider the following ODE:

\[ \begin{align*}
\dot{x} &= -(Qx + \eta \nabla g(x)), \\
\frac{d}{dt} \eta(t) &= \eta(\nabla g(x), \dot{x}).
\end{align*} \quad (10,11) \]

In view of the chain rule, the auxiliary variable \( \eta \) satisfies \( \eta(t) = 1 \) such that the ODE above is equivalent to the gradient flow (2).

Based on the reformulated ODE (10), (11), we consider the following scheme \((\eta_k \approx \eta(kh)):\)

\[ \begin{align*}
x_{k+1} - x_k &= -\left( Q \frac{x_{k+1} + x_k}{2} + \eta_k \nabla g \left( x^*_{k+1/2} \right) \right), \\
g(x_{k+1}) - g(x_k) &= \eta_k \left( \nabla g \left( x^*_{k+1/2} \right), x_{k+1} - x_k \right). \quad (12,13)
\end{align*} \]

Here, \( x^*_{k+1/2} \) is a numerical approximation of \( x((k + 1/2)h) \), which can be computed without the unknown variables \( x_{k+1} \) and \( \eta_k \). For example, Cheng, Liu, and Shen [2] employed \( x^*_{k+1/2} := (3x_k - x_{k-1})/2 \), and we employ \( x^*_{k+1/2} := x_k \) later.
Theorem 2.10 ([2]). A solution $x_{k+1}$ of the scheme (12), (13) satisfies the discrete dissipation law $f(x_{k+1}) \leq f(x_k)$.

Proof. By the splitting (9), we see

$$f(x_{k+1}) - f(x_k) = \left\langle Q\left(\frac{x_{k+1} + x_k}{2}\right), x_{k+1} - x_k \right\rangle + g(x_{k+1}) - g(x_k),$$

$$= \left\langle Q\left(\frac{x_{k+1} + x_k}{2}\right) + \eta_k \nabla g\left(x_{k+1/2}^*\right), x_{k+1} - x_k \right\rangle \quad (\because (13))$$

$$= -h\left\| Q\left(\frac{x_{k+1} + x_k}{2}\right) + \eta_k \nabla g\left(x_{k+1/2}^*\right) \right\|^2,$$

which proves the discrete dissipation law. □

Remark 2.11. The Lagrange multiplier approach is a special case of the discrete gradient method when $x_{k+1/2}^* = x_k$. In this case, $Q\left(\frac{x_{k+1} + x_k}{2}\right) + \eta_k \nabla g(x_k)$ satisfies the conditions of the discrete gradient (Definition 2.5).

By introducing $A_{\pm} := I_n \pm \frac{h}{2}Q$, we can rewrite (12) as follows:

$$x_{k+1} = A_{-1}^{-1}A_+ x_k - \eta_k h A_{-1}^{-1} \nabla g\left(x_{k+1/2}^*\right).$$

Then, $p_k := A_{-1}^{-1}A_+ x_k$ and $q_k := -h A_{-1}^{-1} \nabla g\left(x_{k+1/2}^*\right)$ can be computed by solving the linear equations with the same coefficient matrix $A_+$. Thus, we can compute $\eta_k$ by solving

$$F(\eta_k; x_k) := g(p_k + \eta_k q_k) - g(x_k) - \eta_k \left\langle \nabla g\left(x_{k+1/2}^*\right), p_k + \eta_k q_k - x_k \right\rangle = 0.$$

The scheme (12), (13) requires solving two linear equations with $n$ variables and a scalar nonlinear equation; moreover, because the coefficient matrix $A_+$ is constant, we can solve them quite efficiently. However, existence results for the nonlinear equation $F(\eta_k; x_k) = 0$ have not been established in the literature.

3. Existence results for Lagrange multiplier method

In this section, we establish some existence theorems for the Lagrange multiplier method (12), (13) under the assumption that $g = f$, $Q$ is the zero matrix, and $x_{k+1/2}^* = x_k$. In this case, the scheme can be written in the form

$$\frac{x_{k+1} - x_k}{h} = -\eta_k \nabla f(x_k), \quad (14)$$

$$f(x_{k+1}) - f(x_k) = \eta_k \left\langle \nabla f(x_k), x_{k+1} - x_k \right\rangle. \quad (15)$$

Then, $x_{k+1}$ can be computed by solving a scalar nonlinear equation

$$F(\eta_k; x_k) = f(x_k - \eta_k h \nabla f(x_k)) - f(x_k) + h(\eta_k)^2 \left\| \nabla f(x_k) \right\|^2 = 0.$$

This equation has a trivial solution $\eta_k = 0$, and we prove an existence theorem below for a nontrivial solution.

Theorem 3.1. For any $x_k \in \mathbb{R}^n$, there exists an $\eta_k$ that satisfies $F(\eta_k; x_k) = 0$ and

$$\eta_k \geq \eta_{LB} := \left(1 + \frac{Lh}{2}\right)^{-1} > 0.$$
In this proof, we use the notation $d_k := -\nabla f(x_k)$ for brevity. If $d_k = 0$, $F(\eta_k; x_k) = 0$ holds for any $\eta_k \in \mathbb{R}$ so that the theorem holds. Therefore, we focus on the case $d_k \neq 0$ hereafter. Then, because $\arg \min f \neq \emptyset$, $f$ is bounded from below so that $\lim_{\eta \to \infty} F(\eta; x_k) = \infty$ holds.

Because we assume that $f$ is $L$-smooth, the second inequality of Lemma 2.2 implies

$$F(\eta_k; x_k) \leq \langle \nabla f(x_k), \eta_k h d_k \rangle + \frac{L}{2} \eta_k^2 h^2 \|d_k\|^2 \geq \langle \nabla f(x_k), h d_k \rangle + \frac{L}{2} \|d_k\|^2 = \eta_k h \|d_k\|^2 \left( \eta_k \left( 1 + \frac{Lh}{2} \right) - 1 \right).$$

(16)

Therefore, $F(\eta_{LB}; x_k) \leq 0$ holds, which proves the theorem due to the intermediate value theorem.\hfill \Box

Theorem 3.2. Assume that $\nabla f(x_k) \neq 0$ and $h \leq 2/L$ hold. If $\eta_k > 0$ satisfies $F(\eta_k; x_k) = 0$, then

$$\eta_{LB} \leq \eta_k \leq \left( 1 - \frac{Lh}{2} \right)^{-1}$$

holds.

Proof. From (16), $F(\eta_k; x_k) < 0$ holds for any $\eta_k \in (0, \eta_{LB})$. Then, by using the first inequality in Lemma 2.2, we see

$$F(\eta_k; x_k) \geq \eta_k h \|d_k\|^2 \left( \eta_k \left( 1 - \frac{Lh}{2} \right) - 1 \right),$$

(the proof is similar to the proof of Theorem 3.1). Therefore, $F(\eta_k; x_k) > 0$ holds for any $\eta_k > (1 - \frac{Lh}{2})^{-1}$, which proves the theorem.\hfill \Box

Moreover, if $f$ is convex or satisfies the PL inequality (5), there is an upper bound that is valid for any step size $h$.

Theorem 3.3. If $f$ is convex and $\nabla f(x_k) \neq 0$ holds, then there exists a unique nontrivial solution $\eta_k$ of the nonlinear equation $F(\eta_k; x_k) = 0$ such that $\eta_{LB} \leq \eta_k \leq 1$ holds.

Proof. The convexity of $f$ implies that $F(\eta_k; x_k)$ is strictly convex with respect to $\eta_k$ such that the nontrivial solution is unique.

Since $f$ is convex, we see

$$F(1; x_k) = f(x_k + h d_k) - f(x_k) + h \|d_k\|^2 \geq \langle \nabla f(x_k), h d_k \rangle + h \|d_k\|^2 = 0,$$

which proves the theorem due to the intermediate value theorem.\hfill \Box

Theorem 3.4. If $f$ satisfies the PL inequality (5) with parameter $\mu > 0$ and $\nabla f(x_k) \neq 0$ holds, there exists a nontrivial solution $\eta_k$ of the nonlinear equation $F(\eta_k; x_k) = 0$ such that $\eta_{LB} \leq \eta_k \leq (2\mu h)^{-\frac{1}{2}}$ holds.
Proof. By introducing \( \eta = (2\mu h)^{-\frac{1}{2}} \), we obtain
\[
F(\eta; x_k) = f(x_k + \eta h) - f(x_k) + \frac{1}{2\mu} \| \nabla f(x_k) \|^2
\geq f(x_k + \eta h) - f(x_k) + (f(x_k) - f^*)
= f(x_k + \eta h) - f^*
\geq 0,
\]
which proves the theorem. \( \Box \)

4. Convergence rate of the Lagrange multiplier method

The Lagrange multiplier method described in the previous section can be interpreted as the steepest descent method with a new step-size criterion (15). In this section, we show the convergence rates corresponding to Theorems 2.7 to 2.9.

First, we establish the discrete counterpart of Theorem 2.7 as follows.

**Theorem 4.1.** Let \( \{x_k\}_{k=0}^{\infty} \) be a sequence satisfying (14), (15), and \( \eta_k \neq 0 \) for any non-negative integer \( k \). Then,
\[
\sum_{k=0}^{\infty} \| \nabla f(x_k) \|^2 \leq \left( \frac{Lh}{1} + 1 \right)^2 \frac{f(x_0) - f^*}{h}
\]
and
\[
\min_{0 \leq i \leq k} \| \nabla f(x_i) \| \leq \left( \frac{Lh}{2} + 1 \right) \sqrt{\frac{f(x_0) - f^*}{(k+1)h}}.
\]

**Proof.** Similar to the proof of Theorem 2.7, we see
\[
f(x_0) - f^* \geq f(x_0) - f(x_k)
= - \sum_{i=0}^{k-1} (f(x_{i+1}) - f(x_i))
= h \sum_{i=0}^{k-1} (\eta_k)^2 \| \nabla f(x_k) \|^2
\geq h(\eta_{LB})^2 \sum_{i=0}^{k-1} \| \nabla f(x_k) \|^2.
\]
By definition of \( \eta_{LB} \), the estimation above proves the theorem. \( \Box \)

From the theorem above, we obtain the global convergence result as follows when \( f \) is coercive.

**Theorem 4.2** (global convergence). Assume that \( f \) is coercive. Let \( \{x_k\}_{k=0}^{\infty} \) be a sequence satisfying (14), (15), and \( \eta_k \neq 0 \) for any non-negative integer \( k \). Then, the sequence \( \{x_k\}_{k=0}^{\infty} \) has an accumulation point, moreover, \( \nabla f(x^*) = 0 \) holds for any accumulation point \( x^* \).

**Proof.** The set \( \{ x \in \mathbb{R}^n \mid f(x) \leq f(x_0) \} \) is compact because \( f \) is coercive. Since the discrete dissipation law implies \( \{x_k\}_{k=0}^{\infty} \subset \{ x \in \mathbb{R}^n \mid f(x) \leq f(x_0) \}, \{x_k\}_{k=0}^{\infty} \) has an accumulation point.
For a fixed accumulation point $x^*$, there exists a convergent subsequence $\{x_{k(i)}\}_{i=0}^{\infty}$. The first equation of Theorem 4.1 implies that $\lim_{k \to \infty} \|\nabla f(x_k)\| = 0$. Due to the continuity of the norm and $\nabla f$, we see

$$\|\nabla f(x^*)\| = \|\nabla f\left(\lim_{i \to \infty} x_{k(i)}\right)\| = \lim_{i \to \infty} \|\nabla f(x_{k(i)})\| = 0,$$

which proves the theorem. \[\square\]

Moreover, if $f$ is convex or satisfies the PL inequality, we show the discrete counterparts of Theorems 2.8 and 2.9.

**Theorem 4.3.** Let $\{x_k\}_{k=0}^{\infty}$ be a sequence satisfying (14), (15), and $\eta_k \neq 0$ for any non-negative integer $k$. If $f$ is convex, the sequence $\{x_k\}_{k=0}^{\infty}$ satisfies

$$f(x_k) - f^* = O\left(\frac{1}{k}\right).$$

In particular, if $h \leq \frac{2}{L}$, then

$$f(x_k) - f^* \leq \left(\frac{Lh + 2}{4}\right) \frac{\|x_0 - x^*\|^2}{kh}$$

holds.

**Proof.** Let us introduce the discrete counterpart

$$E_k := \left(\sum_{i=0}^{k-1} h\eta_i\right) (f(x_k) - f^*) + \frac{1}{2} \|x_k - x^*\|^2$$

of $E$ in the proof of Theorem 2.8. Then, we see

$$E_{k+1} - E_k = \left(\sum_{i=0}^{k} h\eta_i\right) (f(x_{k+1}) - f(x_k)) + h\eta_k (f(x_k) - f^*)$$

$$+ \frac{1}{2} \langle x_{k+1} - x_k, x_{k+1} + x_k - 2x^* \rangle.$$ 

Here, the last term on the right-hand side can be evaluated as follows:

$$\frac{1}{2} \langle x_{k+1} - x_k, x_{k+1} + x_k - 2x^* \rangle = \frac{1}{2} \langle x_{k+1} - x_k, x_{k+1} - x_k + 2(x_k - x^*) \rangle$$

$$= \frac{1}{2} \|h\eta_k \nabla f(x_k)\|^2 + \langle h\eta_k \nabla f(x_k), x^* - x_k \rangle$$

$$\leq \frac{1}{2} \|h\eta_k \nabla f(x_k)\|^2 + h\eta_k (f^* - f(x_k)).$$

Using this evaluation, we see

$$E_{k+1} - E_k \leq \left(\sum_{i=0}^{k} h\eta_i\right) (-h(\eta_k)^2\|\nabla f(x_k)\|^2) + \frac{1}{2} \|h\eta_k \nabla f(x_k)\|^2$$

$$= \left(\frac{1}{2} - \sum_{i=0}^{k} \eta_i\right) \|h\eta_k \nabla f(x_k)\|^2.$$
Because \( \eta_k \geq \left( \frac{Lh}{2} + 1 \right)^{-1} \), there exists \( k_0 \in \mathbb{N} \) such that \( \frac{1}{2} - \sum_{i=0}^{k} \eta_i \leq 0 \) holds for any \( k \geq k_0 \). Therefore, we see

\[
E_{k_0} \geq E_k \geq \left( \sum_{i=0}^{k} h \eta_i \right) (f(x_k) - f^*) \geq kh \left( \frac{Lh}{2} + 1 \right)^{-1} (f(x_k) - f^*) ,
\]

which implies \( f(x_k) - f^* = O \left( \frac{1}{k} \right) \). Moreover, if \( h \leq \frac{2}{L} \), then \( \eta_k \geq \left( \frac{Lh}{2} + 1 \right)^{-1} \geq \frac{1}{2} \) holds. Since \( E_{k+1} \leq E_k \) holds for any \( k \),

\[
\frac{1}{2} \| x_0 - x^* \|^2 = E_0 \geq E_k \geq kh \left( \frac{Lh}{2} + 1 \right)^{-1} (f(x_k) - f^*) \]

holds. \( \square \)

**Theorem 4.4.** Let \( \{x_k\}^{\infty}_{k=0} \) be a sequence satisfying (14), (15), and \( \eta_k \neq 0 \) for any non-negative integer \( k \). If \( f \) satisfies the Polyak–Łojasiewicz inequality (5) with parameter \( \mu > 0 \), the sequence \( \{x_k\}^{\infty}_{k=0} \) satisfies

\[
f(x_k) - f^* \leq \exp \left( -\frac{8\mu kh}{(Lh + 2)^2} \right) (f(x_0) - f^*). \]

**Proof.** We introduce the discrete counterpart \( L_k := f(x_k) - f^* \) of \( L \) in the proof of Theorem 2.9. Then, we see

\[
L_{k+1} - L_k = f(x_{k+1}) - f(x_k)
= -h(\eta_k)^2 \| \nabla f(x_k) \|^2
\leq -2\mu h (\eta_k)^2 (f(x_k) - f^*)
\leq -2\mu h \left( \frac{Lh}{2} + 1 \right)^{-2} L_k
\]

and

\[
L_{k+1} \leq \left( 1 - \frac{8\mu h}{(Lh + 2)^2} \right) L_k .
\]

Because \( 1 + r \leq e^r \) holds for any real number \( r \), we obtain

\[
L_k \leq \left( 1 - \frac{8\mu h}{(Lh + 2)^2} \right)^k L_0 \leq \exp \left( -\frac{8\mu kh}{(Lh + 2)^2} \right) (f(x_0) - f^*). \]

\( \square \)

### 5. Proposed methods: relaxation of Lagrange multiplier method

In view of the dissipation law (Theorem 2.10), condition (15) can be relaxed to \( F(\eta_k; x_k) \leq 0 \) as follows:

**Theorem 5.1.** A solution \( x_{k+1} \) of scheme (4) satisfies the discrete dissipation law \( f(x_{k+1}) \leq f(x_k) \)

**Proof.** We see

\[
f(x_{k+1}) - f(x_k) \leq \eta_k \langle \nabla f(x_k), x_{k+1} - x_k \rangle = -h(\eta_k)^2 \| \nabla f(x_k) \|^2 ,
\]

which proves the theorem. \( \square \)
This relaxation allows us to use the backtracking technique to find \( \eta_k \) satisfying the condition \( F(\eta_k; x_k) \leq 0 \). Because the discrete dissipation law is crucial in the discussion in the previous section, we can prove the convergence rates even after this relaxation (Section 5.1); moreover, we propose another method to adaptively change \( h \) at every step, and also show convergence rates for it in Section 5.2.

5.1. A relaxation of the Lagrange multiplier method. In this section, we consider Algorithm 1.

**Algorithm 1** Backtracking

**Input:** \( x_0 \in \mathbb{R}^n, h > 0, \epsilon > 0, \alpha \in (0, 1) \)

\[ k \leftarrow 0 \]

while \( \| \nabla f(x_k) \| \geq \epsilon \) do

\[ \eta_k \leftarrow 1 \]

while \( F(\eta_k; x_k) > 0 \) do

\[ \eta_k \leftarrow \alpha \eta_k \]

end while

\[ x_{k+1} \leftarrow x_k - h \eta_k \nabla f(x_k) \]

\[ k \leftarrow k + 1 \]

end while

\[ x \leftarrow x_k \]

**Output:** \( x \in \mathbb{R}^n \)

Because Theorems 2.7 to 2.9 rely on the lower bound of \( \eta_k \) as well as the discrete dissipation law, we establish the following lemma.

**Lemma 5.2.** The iteration of backtracking in Algorithm 1 stops at most \( \lceil \log_\alpha \eta_{\text{LB}} \rceil \) times so that \( \eta_k \geq \alpha \eta_{\text{LB}} \) holds.

**Proof.** As shown in the proof of Theorem 3.1, \( F(\eta; x_k) \leq 0 \) holds for any \( \eta \leq \eta_{\text{LB}} \). Because \( \alpha^{\lceil \log_\alpha \eta_{\text{LB}} \rceil} \leq \alpha^{\log_\alpha \eta_{\text{LB}}} = \eta_{\text{LB}} \), the iteration stops at most \( \lceil \log_\alpha \eta_{\text{LB}} \rceil \) times. Therefore, we see that \( \eta_k \geq \alpha^{\lceil \log_\alpha \eta_{\text{LB}} \rceil} \geq \alpha^{\log_\alpha \eta_{\text{LB}}} = \alpha \eta_{\text{LB}} \). \( \square \)

By using the lemma, we obtain the following convergence results. We omit the proof because it can be proved in a manner similar to that in Theorems 2.7 to 2.9.

**Theorem 5.3.** The sequence \( \{ x_k \}_{k=0}^\infty \) obtained by Algorithm 1 satisfies

\[
\min_{0 \leq i \leq k} \| \nabla f(x_i) \| \leq \frac{Lh + 2}{2\alpha} \sqrt{\frac{f(x_0) - f^*}{(k+1)h}}.
\]

Moreover, if \( f \) is convex,

\[ f(x_k) - f^* = O\left( \frac{1}{k} \right) \]

holds. If \( f \) satisfies the Polyak–Lojasiewicz inequality (5) with parameter \( \mu > 0 \),

\[ f(x_k) - f^* \leq \exp \left( -\frac{8\alpha^2 k \mu h}{(Lh + 2)^2} (f(x_0) - f^*) \right) \]

holds.
5.2. Adaptive step size. In this section, we consider adaptively changing the step size $h_k$ in every step. Here, instead of $F(\eta_k; x_k) \leq 0$, we use the condition $F_{h_k}(\eta_k; x_k) \leq 0$, where $F_{h_k}$ is defined as

$$F_{h_k}(\eta_k; x_k) = f(x_k - \eta_k h_k \nabla f(x_k)) - f(x_k) + h_k (\eta_k)^2 \|\nabla f(x_k)\|^2.$$ 

Then, $h_{k+1}$ is defined by $h_{k+1} = h_k \eta_k / \eta^*$, which is intended to maintain $\eta_{k+1}$ around a fixed constant $\eta^*$. As shown in the numerical experiments in the next section, this simple strategy reduces the number of backtracking iterations, and the numerical result does not depend significantly on the choice of $h_0$.

Algorithm 2 Adaptive step size

Input: $x_0 \in \mathbb{R}^n$, $h_0 > 0$, $\epsilon > 0$, $\alpha \in (0, 1)$, $\eta^* \in (0, \alpha)$

$k \leftarrow 0$

while $\|\nabla f(x_k)\| \geq \epsilon$ do

$\eta_k \leftarrow 1$

while $F_{h_k}(\eta_k; x_k) > 0$ do

$\eta_k \leftarrow \alpha \eta_k$

end while

$x_{k+1} \leftarrow x_k - h_k \eta_k \nabla f(x_k)$

$h_{k+1} \leftarrow \frac{h_k \eta_k}{\eta^*}$

$k \leftarrow k + 1$

end while

$x \leftarrow x_k$

Output: $x \in \mathbb{R}^n$

In view of Lemma 5.2, we see

$$\eta_k \geq \frac{2\alpha}{L h_k + 2}.$$ 

The assumption $\eta^* < \alpha$ ensures that $\{h_k\}_{k=0}^\infty$ is bounded from below, as shown in the lemma below. This lower bound of $\{h_k\}_{k=0}^\infty$ will be used in the proof of convergence rates.

Lemma 5.4. If $h_0 \geq h_{LB} := \frac{2(\alpha - \eta^*)}{\eta^* L}$, then $h_k \geq h_{LB}$ holds for any positive integer $k$.

Proof. We prove the lemma by induction. Suppose that $h_k \geq h_{LB}$ holds. Then we see

$$h_{k+1} = \frac{h_k \eta_k}{\eta^*} \geq \frac{2\alpha h_k}{\eta^*(L h_k + 2)} \geq \frac{2\alpha h_{LB}}{\eta^*(L h_{LB} + 2)} = h_{LB},$$

which proves the lemma. □

5.2.1. Convex functions. In this section, we deal with convex functions.

Theorem 5.5. We assume that $h_0 \geq h_{LB}$ and $\eta^* \geq \frac{1}{2}$ hold. If $f$ is convex, the sequence $\{x_k\}_{k=0}^\infty$ obtained by Algorithm 2 satisfies

$$f(x_k) - f^* \leq \left( \frac{L}{4(\alpha - \eta^*)} \right) \|x_0 - x^*\|^2 / k.$$
Proof. Let us introduce the discrete counterpart
\[ E_k := \left( \sum_{i=0}^{k-1} h_i \eta_i \right) (f(x_k) - f^*) + \frac{1}{2} \| x_k - x^* \|^2 \]
of \( E \) in the proof of Theorem 2.8. Then, we see
\[ E_{k+1} - E_k = \left( \sum_{i=0}^{k} h_i \eta_i \right) (f(x_{k+1}) - f(x_k)) + h_k \eta_k (f(x_k) - f^*) + \frac{1}{2} (x_{k+1} - x_k, x_{k+1} + x_k - 2x^*). \]

Similar to the proof of Theorem 4.3, the last term on the right-hand side can be evaluated as follows:
\[ \frac{1}{2} (x_{k+1} - x_k, x_{k+1} + x_k - 2x^*) \leq \frac{1}{2} \| h_k \eta_k \nabla f(x_k) \|^2 + h_k \eta_k (f^* - f(x_k)). \]
Using this evaluation, we see
\[ E_{k+1} - E_k \leq \left( \sum_{i=0}^{k} h_i \eta_i \right) (-h_k (\eta_k)^2 \| \nabla f(x_k) \|^2) + \frac{1}{2} \| h_k \eta_k \nabla f(x_k) \|^2 \]
\[ = \left( \frac{1}{2} h_k - \sum_{i=0}^{k} h_i \eta_i \right) h_k (\eta_k)^2 \| \nabla f(x_k) \|^2. \]

Since
\[ \frac{1}{2} h_k - \sum_{i=0}^{k} h_i \eta_i = \frac{1}{2} h_k - h_k \eta_k - \eta^* \sum_{i=0}^{k-1} h_{i+1} \]
\[ = \left( \frac{1}{2} - \eta_k - \eta^* \right) h_k - \eta^* \sum_{i=0}^{k-2} h_{i+1} \]
\[ \leq 0 \]
holds owing to the assumption \( \eta^* \geq \frac{1}{2} \), we see \( E_{k+1} - E_k \leq 0 \). Therefore, we see
\[ \frac{1}{2} \| x_0 - x^* \|^2 = E_0 \geq E_k \geq \sum_{i=0}^{k-1} h_i \eta_i (f(x_k) - f^*) \geq k \eta^* h_k \| f(x_k) - f^* \|, \]
which proves the theorem. \( \Box \)

5.2.2. Functions satisfying PL inequality. In this section, we deal with functions satisfying PL inequality. In this case, we need the upper bound of \( \{ h_k \}_{k=0}^{\infty} \) as well as the lower bound.

Lemma 5.6. Assume that \( f \) satisfies the Polyak–Lojasiewicz inequality (5) with parameter \( \mu > 0 \), and \( h_0 \leq h_{UB} := \frac{1}{2 \mu (\eta^*)^2} \) holds. Then, \( h_k \leq h_{UB} \) holds for any positive integer \( k \).

Proof. In a manner similar to the proof of Theorem 3.4, we see that \( \eta_k \leq \sqrt{\frac{1}{2 \mu h_k}} \). Then, we prove the lemma by induction. Suppose that \( h_k \leq h_{UB} \) holds. Then we see
\[ h_{k+1} = \frac{h_k \eta_k}{\eta^*} \leq \frac{1}{\eta^*} \sqrt{\frac{h_k}{2 \mu}} \leq \frac{1}{\eta^*} \sqrt{\frac{h_{UB}}{2 \mu}} = h_{UB}, \]
which proves the lemma. □

**Theorem 5.7.** Assume that \( h_0 \in [h_{LB}, h_{UB}] \) holds. If \( f \) satisfies the Polyak–Lojasiewicz inequality (5) with parameter \( \mu > 0 \), the sequence \( \{x_k\}_{k=0}^{\infty} \) obtained by Algorithm 2 satisfies

\[
f(x_k) - f^* \leq \exp\left( -\frac{16\alpha(\alpha - \eta^*)(\eta^*)^2}{\kappa (\kappa + 4(\eta^*)^2)} k \right) (f(x_0) - f^*),
\]

where \( \kappa := L/\mu \) is the condition number.

**Proof.** We introduce the discrete counterpart \( L_k := f(x_k) - f^* \) of \( L \) in the proof of Theorem 2.9. Then, we see

\[
L_{k+1} - L_k = f(x_{k+1}) - f(x_k) \\
\leq -h_k(\eta_k)^2 \|\nabla f(x_k)\|^2 \\
\leq -2\mu h_k(\eta_k)^2 (f(x_k) - f^*).
\]

By using \( h_k(\eta_k)^2 = \eta^* h_{k+1} \eta_k \geq \eta^* h_{LB} \frac{2\alpha}{L_k h_{LB + 2}} = \frac{8\mu(\alpha - \eta^*)(\eta^*)^2}{L(L + 4\mu(\eta^*)^2)} \), we obtain

\[
L_{k+1} \leq \left( 1 - \frac{16\alpha\mu^2 (\alpha - \eta^*)(\eta^*)^2}{L(L + 4\mu(\eta^*)^2)} \right) L_k,
\]

which proves the theorem. □

6. **Numerical experiments**

In this section, we compare Algorithms 1 and 2 with the steepest descent method with a fixed step size \( h = 1/L \) and the step size satisfying the standard Armijo rule

\[
f(x_k - h_k \nabla f(x_k)) - f(x_k) \leq -ch_k \|\nabla f(x_k)\|^2,
\]

where \( c \in (0, 1) \) is a parameter, where \( h_k \) is obtained by a standard backtracking line search with the parameter \( \alpha \in (0, 1) \).

Throughout the numerical experiment in this section, the parameter \( \alpha \) in the Armijo rule, Algorithms 1 and 2, is fixed at \( \alpha = 0.8 \). Because we investigate the difference in the results depending on the step size criteria in this experiment, we choose the parameter \( \alpha \) corresponding to a relatively precise line search. In addition, we fix the parameter \( \eta^* = 0.5 \) in view of Theorem 5.5.

6.1. **Quadratic function.** First, we consider the quadratic function

\[
f(x) = \frac{1}{2} \langle x, Ax \rangle + \langle b, x \rangle,
\]

where \( A \in \mathbb{R}^{n \times n} \) and \( b \in \mathbb{R}^n \). In this section, we fix \( n = 500 \) and \( b \in \mathbb{R}^n \), whose elements are independently sampled from the normal distribution \( \mathcal{N}(0, 5) \). We also fix the symmetric positive definite matrix \( A \in \mathbb{R}^{n \times n} \), defined as \( A = Q^T \Lambda Q \) by using a diagonal matrix \( \Lambda \), whose elements are sampled from a uniform distribution on \([0.001, 1]\), and an orthogonal matrix \( Q \) that was sampled from the Haar measure on the orthogonal group. The resulting matrix \( A \) has the maximum eigenvalue of \( L \approx 0.998 \) and minimum eigenvalue of \( \mu \approx 0.0022 \). We set the initial step size of the backtracking line search for the Armijo rule to 10.

Figure 1 summarizes the evolution of function values, and Table 1 summarizes the average step size and the number of backtracking iterations. In Figure 1, we omit the Armijo rule with \( c = 0.1 \), Algorithm 1 with \( h = 100 \), Algorithm 2
Figure 1. Evolution of function values for the quadratic function (17).

Table 1. Average step size and number of backtracking iterations for the quadratic function (17).

| Method | Armijo (c) | Algorithm 1 (h) | Algorithm 2 (h₀) |
|--------|------------|-----------------|------------------|
| Parameter | 10⁻¹⁴ | 0.1 | 0.5 | 1 | 10 | 100 | 1 | 10 | 100 |
| step size | 2.017 | 2.016 | 3.398 | 0.8 | 2.016 | 2.024 | 2.022 | 2.020 | 2.020 |
| # iterations | 7.19 | 7.19 | 6.16 | 1 | 7.19 | 17.51 | 3.10 | 3.11 | 3.12 |

with \( h₀ = 1, 100 \) because they are very similar to the Armijo rule with \( c = 10⁻¹⁴ \), Algorithm 1 with \( h = 10 \) and Algorithm 2 with \( h₀ = 10 \), respectively.

The results of Algorithm 1 with an appropriate \( h \) and Algorithm 2 are similar to those of the Armijo rule with a small \( c \). Because the Armijo rule with \( c = 0.5 \) is similar to the exact line search for quadratic functions, it overweights the other methods.

6.2. Log-Sum-Exp function. Second, we consider the Log-Sum-Exp function

\[
f(x) = \rho \log \left( \sum_{i=1}^{m} \exp \left( \frac{\langle a_i, x \rangle - b_i}{\rho} \right) \right) .
\]

(18)

where \( a_i \in \mathbb{R}^n \) (1 ≤ \( i \) ≤ \( m \)), \( b_i \in \mathbb{R} \) (1 ≤ \( i \) ≤ \( m \)) and \( \rho > 0 \). In this section, we fix \( n = 50, m = 200 \), and \( \rho = 20 \). We also fix \( a_i \) and \( b_i \), whose elements are independently sampled from the normal distribution \( \mathcal{N}(0, 1) \) and \( \mathcal{N}(0, \sqrt{2}) \), respectively. The resulting \( a_i \) satisfies \( \max_{1 \leq k \leq m} \|a_k\|^2 \approx 42.687 \), and the Lipschitz constant \( L \) satisfies \( L \leq \max_{1 \leq k \leq m} \|a_k\|^2 \). We set the initial step size of the backtracking line search for the Armijo rule to 100.

Table 2. Average step size and number of backtracking iterations for the Log-Sum-Exp function (18).

| Method | Armijo (c) | Algorithm 1 (h) | Algorithm 2 (h₀) |
|--------|------------|-----------------|------------------|
| Parameter | 10⁻¹⁴ | 0.1 | 0.5 | 1 | 10 | 100 | 1 | 10 | 100 |
| step size | 15.44 | 15.29 | 18.80 | 0.8 | 7.97 | 15.18 | 14.66 | 15.67 | 15.07 |
| # iterations | 8.42 | 8.46 | 8.14 | 1 | 1.02 | 8.48 | 2.80 | 3.02 | 3.22 |
6.3. A nonconvex function satisfying PL inequality. Finally, we consider the function

\[ f(x) = \|x\|^2 + 3\sin^2(\langle b, x \rangle) \]  

(19)

used in [3], where \( b \in \mathbb{R}^n \) is a vector that satisfies \( \|b\| = 1 \). This function is 8-smooth, nonconvex, and satisfies the Polyak–Lojasiewicz inequality (5) with parameter \( \mu = 1/32 \). In this section, we fix \( n = 50 \) and \( b = v/\|v\| \in \mathbb{R}^n \), where the elements of \( v \in \mathbb{R}^n \) are independently sampled from the normal distribution \( \mathcal{N}(0, 1) \). We set the initial step size of the backtracking line search for the Armijo rule to 10.
Table 3. Average step size and number of backtracking iterations for the nonconvex function (19).

| Method       | Armijo ($h$) | Algorithm 1 ($h$) | Algorithm 2 ($h_0$) |
|--------------|-------------|-------------------|---------------------|
| Parameter    | $10^{-4}$   | 0.1               | 0.5                 |
|              | 0.1         | 1                 | 10                  |
|              | 0.207       | 0.204             | 0.215               |
| step size    | 0.260       | 0.227             | 0.235               |
| # iterations | 16.6        | 17.2              | 17.2                |
|              | 1           | 7.1               | 16.8                |
|              | 3.04        | 3.15              | 3.26                |

7. Conclusion

In this paper, we show that the Lagrange multiplier approach, a recent geometric numerical integration technique, for the gradient system reads a new step-size criterion for the steepest descent method. Thanks to the discrete dissipation law, convergence rates of the proposed method for several cases can be proved in a form similar to the discussions in ODEs. In this paper we focused only on the simplest gradient flow, but the results suggest that geometric numerical integration techniques can be effective for other ODEs appear in optimization.

Several issues still remain to be investigated. First, it is interesting to investigate the application of geometric numerical integration techniques to other ODEs that appear during optimization. Second, the existence results in this paper are only for a special case of the Lagrange multiplier approach. Though it is enough for the application to gradient flow (2), it is important to generalize the results for future development, as described in the previous section.

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Appendix A. Existence results for generalized gradient flow

The results in Section 3 for the gradient flow (2) can be extended to that of the generalized gradient flow

$$\dot{x} = -A\nabla f(x), \quad x(0) = x_0,$$

where $A \in \mathbb{R}^{n \times n}$ is positive definite but is not necessarily symmetric. In this case, the scheme can be written in the form

$$\frac{x_{k+1} - x_k}{h} = -\eta_k A\nabla f(x_k),$$

$$f(x_{k+1}) - f(x_k) = \eta_k \langle \nabla f(x_k), x_{k+1} - x_k \rangle.$$

Then, $x_{k+1}$ can be computed by solving a scalar nonlinear equation

$$G(\eta_k; x_k) = f(x_k - \eta_k h A\nabla f(x_k)) - f(x_k) + h(\eta_k)^2 \langle \nabla f(x_k), A\nabla f(x_k) \rangle = 0.$$

In this section, $\lambda_{\text{min}}$ denotes the smallest eigenvalue of the matrix

$$M = \frac{1}{2} \left( A^{-1} + (A^{-1})^T \right).$$
Theorem A.1. For any $x_k \in \mathbb{R}^n$, there exists an $\eta_k$ that satisfies $G(\eta_k; x_k) = 0$ and

$$\eta_k \geq \left(1 + \frac{Lh}{2\lambda_{\min}}\right)^{-1} > 0.$$

Proof. In this proof, we use the notation $d_k := -\nabla f(x_k)$ for brevity. If $d_k = 0$, $G(\eta_k; x_k) = 0$ holds for any $\eta_k \in \mathbb{R}$ such that the theorem holds. Therefore, we focus on the case $d_k \neq 0$ hereafter. Because $\arg \min f \neq \emptyset$, $f$ is bounded from below, such that $\lim_{\eta \to \infty} G(\eta; x_k) = \infty$ holds.

Because we assume that $f$ is $L$-smooth, the second inequality of Lemma 2.2 implies

$$G(\eta_k; x_k) \leq \langle \nabla f(x_k), \eta_k h A d_k \rangle + \frac{L}{2} \|\eta_k h A d_k\|^2 + h(\eta_k)^2 \langle d_k, A d_k \rangle$$

$$= \eta_k h \langle d_k, A d_k \rangle \left(\eta_k \left(1 + \frac{Lh}{2} \frac{\|A d_k\|^2}{\langle d_k, A d_k \rangle}\right) - 1\right)$$

$$\leq \eta_k h \langle d_k, A d_k \rangle \left(\eta_k \left(1 + \frac{Lh}{2\lambda_{\min}}\right) - 1\right),$$

where the last inequality comes from

$$\langle d_k, A d_k \rangle = \langle A d_k, A^{-1} A d_k \rangle = \langle A d_k, M A d_k \rangle \geq \lambda_{\min} \|A d_k\|^2.$$

Therefore, $G\left(\eta_k; x_k\right) < 0$ holds for any $\eta_k > 0$ satisfies $G(\eta_k; x_k) = 0$, which proves the theorem due to the intermediate value theorem.

Theorem A.2. Assume that $\nabla f(x_k) \neq 0$ and $h \leq 2\lambda_{\min}/L$ hold. If $\eta_k > 0$ satisfies $G(\eta_k; x_k) = 0$, then

$$\left(1 + \frac{Lh}{2\lambda_{\min}}\right)^{-1} \leq \eta_k \leq \left(1 - \frac{Lh}{2\lambda_{\min}}\right)^{-1}.$$

Proof. From (20), $G(\eta_k; x_k) < 0$ holds for any $\eta_k \in \left(0, \left(1 + \frac{Lh}{2\lambda_{\min}}\right)^{-1}\right)$.

Then, by using the first inequality in Lemma 2.2, we see

$$G(\eta_k; x_k) \geq \langle d_k, A d_k \rangle \left(\eta_k \left(1 - \frac{Lh}{2\lambda_{\min}}\right) - 1\right)$$

(the proof is similar to the proof of Theorem A.1). Therefore, $G(\eta_k; x_k) > 0$ holds for any $\eta_k > \left(1 - \frac{Lh}{2\lambda_{\min}}\right)^{-1}$, which proves the theorem.

Theorem A.3. If $f$ is a convex function and $\nabla f(x_k) \neq 0$ holds, there exists a unique nontrivial solution $\eta_k$ of the nonlinear equation $G(\eta_k; x_k) = 0$ such that

$$\left(1 + \frac{Lh}{2\lambda_{\min}}\right)^{-1} \leq \eta_k \leq 1$$

holds.
Proof. The convexity of $f$ implies that $G(\eta_k; x_k)$ is strictly convex with respect to $\eta_k$ such that the nontrivial solution is unique.

Since $f$ is convex, we see
\[
G(1; x_k) = f(x_k + hAd_k) - f(x_k) + h\langle d_k, Ad_k \rangle \\
\geq (\nabla f(x_k), hAd_k) + h\langle d_k, Ad_k \rangle \\
= 0,
\]
which proves the theorem due to the intermediate value theorem. □

Theorem A.4. If $f$ satisfies the PL inequality (5) with parameter $\mu > 0$ and $\nabla f(x_k) \neq 0$ holds, there exists a nontrivial solution $\eta_k$ of the nonlinear equation $G(\eta_k; x_k) = 0$ such that
\[
\left(1 + \frac{Lh}{2\lambda_{\min}}\right)^{-1} \leq \eta_k \leq (2\mu h\lambda_{\min})^{-\frac{1}{2}}
\]
holds.

Proof. By introducing $\overline{\eta} = (2\mu h\lambda_{\min})^{-\frac{1}{2}}$, we obtain
\[
G(\overline{\eta}; x_k) = f(x_k + \overline{\eta}hAd_k) - f(x_k) + \frac{1}{2\mu \lambda_{\min}} (\nabla f(x_k), A\nabla f(x_k)) \\
\geq f(x_k + \overline{\eta}hAd_k) - f(x_k) + \frac{1}{2\mu} \|\nabla f(x_k)\|^2 \\
\geq f(x_k + \overline{\eta}hAd_k) - f(x_k) + (f(x_k) - f^*) \\
= f(x_k + \overline{\eta}hAd_k) - f^* \\
\geq 0,
\]
which proves the theorem. □

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Department of Mathematical Informatics, Graduate School of Information Science and Technology, The University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo, 113-0033, Japan

Department of Mathematical Informatics, Graduate School of Information Science and Technology, The University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo, 113-0033, Japan

Email address: shun@mist.i.u-tokyo.ac.jp