Abstract

The goal of this paper is to debunk and dispel the magic behind the black-box optimizers and stochastic optimizers. It aims to build a solid foundation on how and why the techniques work. This manuscript crystallizes this knowledge by deriving from simple intuitions, the mathematics behind the strategies. This tutorial doesn’t shy away from addressing both the formal and informal aspects of gradient descent and stochastic optimization methods. By doing so, it hopes to provide readers with a deeper understanding of these techniques as well as the when, the how and the why of applying these algorithms.

Gradient descent is one of the most popular algorithms to perform optimization and by far the most common way to optimize machine learning tasks. Its stochastic version receives attention in recent years, and this is particularly true for optimizing deep neural networks. In deep neural networks, the gradient followed by a single sample or a batch of samples is employed to save computational resources and escape from saddle points. In 1951, Robbins and Monro published *A stochastic approximation method*, one of the first modern treatments on stochastic optimization that estimates local gradients with a new batch of samples. And now, stochastic optimization has become a core technology in machine learning, largely due to the development of the back propagation algorithm in fitting a neural network. The sole aim of this article is to give a self-contained introduction to concepts and mathematical tools in gradient descent and stochastic optimization. However, we clearly realize our inability to cover all the useful and interesting results concerning optimization methods and given the paucity of scope to present this discussion, e.g., the separated analysis of trust region methods, convex optimization, and so on. We refer the reader to literature in the field of numerical optimization for a more detailed introduction to the related fields.

The article is primarily a summary of purpose, significance of important concepts in optimization methods, e.g., vanilla gradient descent, gradient descent with momentum, conjugate descent, conjugate gradient, and the origin and rate of convergence of the methods which shed light on their applications. The mathematical prerequisite is a first course in linear algebra and calculus. Other than this modest background, the development is self-contained, with rigorous proof provided throughout.

**Keywords:** Gradient descent, Stochastic gradient descent, Steepest descent, Conjugate descent and conjugate gradient, Learning rate annealing, Adaptive learning rate, Second-order methods.
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1. Gradient Descent

Gradient descent (GD) is one of the most popular algorithms to perform optimization and by far the most common way to optimize machine learning tasks. And this is particularly true for optimizing neural networks. The neural networks or machine learning in general find the set of parameters $x \in \mathbb{R}^d$ in order to optimize an objective function $L(x)$. The gradient descent finds a sequence of parameters $x_1, x_2, \ldots, x_T$, (1.1) such that when $T \to \infty$, the objective function $L(x_T)$ achieves the optimal minimum value.

At each iteration $t$, a step $\Delta x_t$ is applied to change the parameters. Denoting the parameters at the $t$-th iteration as $x_t$. Then the update rule becomes

$$x_{t+1} = x_t + \Delta x_t.$$ (1.2)

The most naive method of gradient descents is the vanilla update: the parameter moves in the opposite direction of the gradient which finds the steepest descent direction since the gradients are orthogonal to level curves (a.k.a., level surface, see Lemma 16.4 in Lu (2022c)):

$$\Delta x_t = -\eta g_t = -\eta \frac{\partial L(x_t)}{\partial x_t} = -\eta \nabla L(x_t),$$ (1.3)

where the positive value $\eta$ is the learning rate and depends on specific problems, and $g_t = \frac{\partial L(x^t)}{\partial x_t} \in \mathbb{R}^d$ is the gradient of the parameters. The learning rate $\eta$ controls how large of a step to take in the direction of negative gradient so that we can reach a (local) minimum. While if we follow the negative gradient of a single sample or a batch of samples iteratively, the local estimate of the direction can be obtained and is known as the stochastic gradient descent (SGD) (Robbins and Monro, 1951). In the SGD framework, the objective function is stochastic that is composed of a sum of subfunctions evaluated at different subsamples of the data. However, the drawback of the vanilla update is that it is easy to get stuck in local minima (Rutishauser, 1959).

For a small step size, gradient descent makes a monotonic improvement at every iteration. Thus, it always converges, albeit to a local minimum. However, the speed of the vanilla GD method is usually slow, while it can take an exponential rate when the curvature condition is poor. While choosing higher than this rate may cause the procedure to diverge in terms of the objective function. Determining a good learning rate (either global or per-dimension) becomes more of an art than science for many problems. Previous work has been done to alleviate the need for selecting a global learning rate (Zeiler, 2012), while it is still sensitive to other hyper-parameters.

1.1 Gradient Descent by Calculus

An intuitive way to think of gradient descent is to imagine the path of a river originating from the top of a mountain. The goal of gradient descent is exactly what the river strives to achieve, namely, reach the bottom-most point (at the foothill) climbing down from the mountain.
To restate the problem, the objective function is $L(x)$, the input variable of $L$ is $x$ with $d$-dimension; our goal is to use algorithm to get the minimum of $L(x)$. To make this question more precise, let’s think about what happens when we move the ball a small amount $\Delta x_1$ in the $x_1$ direction, a small amount $\Delta x_2$ in the $x_2$ direction, \ldots, and a small amount $\Delta x_d$ in the $x_d$ direction. Calculus tells us that $L(x)$ changes as follows:

$$
\Delta L(x) \approx \frac{\partial L}{\partial x_1} \Delta x_1 + \frac{\partial L}{\partial x_2} \Delta x_2 + \ldots + \frac{\partial L}{\partial x_d} \Delta x_d.
$$

In this sense, we need to find a way of choosing $\Delta x_1, \ldots, \Delta x_d$ so as to make $\Delta L(x)$ negative, i.e., we’ll make the objective function decrease so as to minimize. Define $\Delta x = [\Delta x_1, \Delta x_2, \ldots, \Delta x_d]^\top$ to be the vector of changes in $x$ and gradients $\nabla L(x) = \frac{\partial L(x)}{\partial x} = [\frac{\partial L}{\partial x_1}, \frac{\partial L}{\partial x_2}, \ldots, \frac{\partial L}{\partial x_d}]^\top$ to be the gradient vector of $L(x)$ ¹. Then it follows that

$$
\Delta L(x) \approx \frac{\partial L}{\partial x_1} \Delta x_1 + \frac{\partial L}{\partial x_2} \Delta x_2 + \ldots + \frac{\partial L}{\partial x_d} \Delta x_d = \nabla L(x)^\top \Delta x.
$$

In a descent context, we want $\Delta L(x)$ to be negative so that a step $x_{t+1} = x_t + \Delta x_t$ will lead to a decrease in the loss function $L(x_{t+1}) = L(x_t) + \Delta L(x)$ since $\Delta L(x) \leq 0$. It can be shown that if the update step is given by $\Delta x = -\eta \nabla L(x)$ where $\eta$ is the learning rate, then it follows that

$$
\Delta L(x) \approx -\eta \nabla L(x)^\top \nabla L(x) = -\eta \|\nabla L\|_2^2 \leq 0.
$$

Strictly speaking, $\Delta L(x) < 0$ in the above equation, otherwise we find the optimal point with zero gradients. This shows the correctness of gradient descent. We can use the following update rule to update the next $x_{t+1}$:

$$
x_{t+1} = x_t - \eta \nabla L(x_t).
$$

This update rule will make the objective function drop to the minimum point steadily in a convex setting or local minima in a non-convex setting.

**Remark 1.1: Descent Condition**

In above construction, we let $\Delta x = -\eta \nabla L(x)$ where $-\nabla L(x)$ is the descent direction such that $\Delta L \approx -\eta \nabla L(x)^\top \nabla L(x) < 0$ (we assume $\nabla L(x) \neq 0$). More generally, any search direction $d_t \in \mathbb{R}^d \setminus \{0\}$ that satisfies the descent condition can be chosen as the descent direction:

$$
\frac{dL(x_t + \eta d_t)}{d\eta} \bigg|_{\eta=0} = \nabla L(x_t)^\top d_t < 0.
$$

In other words, by Taylor’s formula (Appendix A, p. 74)

$$
L(x_t + \eta d_t) \approx L(x_t) + \eta \nabla L(x_t)^\top d_t
$$

implies $L(x_t + \eta d_t) < L(x_t)$ when $\eta$ is sufficiently small. When $d_t = \nabla L(x_t)$, the descent direction is known as the steepest descent direction. When the learning rate

---

¹. Note the difference between $\Delta L(x)$ and $\nabla L(x)$.
\( \eta \) is not fixed and decided by exact line search, the method is called *steepest descent method* (see Section 2.4, p. 17).

**Gradient descent in a convex problems** We further consider the gradient descent in a convex problem. If the objective function is convex, then we have the fact that \( \nabla L(x_t)^\top (x_{t+1} - x_t) \geq 0 \) implies \( L(x_{t+1}) \geq L(x_t) \). This can be derived from the convex property of a convex function, i.e., \( L(x_{t+1}) \geq L(x_t)^\top (x_{t+1} - x_t) \).

In this sense, we need to make \( \nabla L(x_t)^\top (x_{t+1} - x_t) \leq 0 \) so as to make the objective function decrease. In gradient descent \( \Delta x_t = x_{t+1} - x_t \) is chosen to be negative gradient \(-\nabla L(x_t)\). However, there are many other descent methods, such as *steepest descent*, *normalized steepest descent*, *newton step*, and so on. The main idea of these methods is to make \( \nabla L(x_t)^\top \Delta x_t \leq 0 \) (Beck, 2017).

1.2 Gradient Descent by Greedy Search

We will be considering the greedy search such that \( x_{t+1} \leftarrow \arg \min_{x_t} L(x_t) \). Suppose we want to approximate \( x_{t+1} \) by a linear update on \( x_t \), i.e.,

\[
    x_{t+1} = x_t + \eta \nu.
\]

The problem now turns to the solution of \( \nu \) such that

\[
    \nu = \arg \min_{\nu} L(x_t + \eta \nu).
\]

By Taylor’s formula (Appendix A, p. 74), \( L(x_t + \eta \nu) \) can be approximated by

\[
    L(x_t + \eta \nu) \approx L(x_t) + \eta \nu^\top \nabla L(x_t),
\]

when \( \eta \) is small enough. Then a search under the condition \( ||\nu|| = 1 \) given positive \( \eta \) is as follows:

\[
    \nu = \arg \min_{||\nu|| = 1} L(x_t + \eta \nu) \approx \arg \min_{||\nu|| = 1} \left\{ L(x_t) + \eta \nu^\top \nabla L(x_t) \right\}.
\]

This is known as the *greedy search*. The optimal \( \nu \) can be obtained by

\[
    \nu = -\frac{\nabla L(x_t)}{||\nabla L(x_t)||},
\]

i.e., \( \nu \) is in the opposite direction of \( \nabla L(x_t) \). Therefore, the update of \( x_{t+1} \) is reasonable to be taken as

\[
    x_{t+1} = x_t + \eta \nu = x_t - \eta \frac{\nabla L(x_t)}{||\nabla L(x_t)||},
\]

which is usually called the *gradient descent* as aforementioned. If we further absorb the denominator into the step size \( \eta \), the gradient descent can be applied in the trivial way:

\[
    x_{t+1} = x_t - \eta \nabla L(x_t).
\]

1.3 Geometrical Interpretation of Gradient Descent
Lemma 1.2: (Direction of Gradients)
An important fact is that gradients are orthogonal to level curves (a.k.a., level surface).

Proof [of Lemma 1.2] This is equivalent to proving that the gradient is orthogonal to the tangent of the level curve. For simplicity, let’s first look at the 2-dimensional case. Suppose the level curve has the form \( f(x, y) = c \). This implicitly gives a relation between \( x \) and \( y \) such that \( y = y(x) \) where \( y \) can be thought of as a function of \( x \). Therefore, the level curve can be written as \( f(x, y(x)) = c \).

The chain rule indicates
\[
\frac{\partial f}{\partial x} \frac{dx}{dx} + \frac{\partial f}{\partial y} \frac{dy}{dx} = 0.
\]
Therefore, the gradient is perpendicular to the tangent:
\[
\left\langle \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y} \right \rangle \cdot \left\langle \frac{dx}{dx}, \frac{dy}{dx} \right \rangle = 0.
\]

Let us now treat the problem in full generality, suppose the level curve of a vector \( x \in \mathbb{R}^n \):
\( f(x) = f(x_1, x_2, \ldots, x_n) = c \). Each variable \( x_i \) can be regarded as a function of a variable \( t \) on the level curve \( f(x) = c \): \( f(x_1(t), x_2(t), \ldots, x_n(t)) = c \). Differentiate the equation with respect to \( t \) by chain rule:
\[
\frac{\partial f}{\partial x_1} \frac{dx_1}{dt} + \frac{\partial f}{\partial x_2} \frac{dx_2}{dt} + \ldots + \frac{\partial f}{\partial x_n} \frac{dx_n}{dt} = 0.
\]
Therefore, the gradients is perpendicular to the tangent in \( n \)-dimensional case:
\[
\left\langle \frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_n} \right \rangle \cdot \left\langle \frac{dx_1}{dt}, \frac{dx_2}{dt}, \ldots, \frac{dx_n}{dt} \right \rangle = 0.
\]
This completes the proof.

The lemma above reveals the geometrical interpretation of gradient descent. For finding a solution to minimize a convex function \( L(x) \), gradient descent goes to the negative gradient direction that can decrease the loss. Figure 1 depicts a 2-dimensional case, where \(-\nabla L(x)\) pushes the loss to decrease for the convex function \( L(x) \).

1.4 Regularization: A Geometrical Interpretation

The gradient descent can reveal the geometrical meaning of regularization. To avoid confusion, we denote the loss function without regularization by \( l(z) \) and the loss with regularization by \( L(x) = l(x) + \lambda \| x \|^2 \) where \( l(x) : \mathbb{R}^d \to \mathbb{R} \) (the notation is used only in this section). When minimizing \( l(x) \), the descent method will search in \( \mathbb{R}^d \) for a solution. However, in machine learning, searching in the whole space can cause overfitting. A partial solution is to search in a subset of the vector space, e.g., searching in \( x^\top x < C \) for some constant \( C \). That is
\[
\arg \min_x l(x), \quad \text{s.t.,} \quad x^\top x \leq C.
\]
Figure 1: Figure 1(a) shows a convex function surface plot and a contour plot (blue=low, yellow=high) where the upper graph is the surface plot, and the lower one is the projection of it (i.e., contour). Figure 1(b): $-\nabla L(x)$ pushes the loss to decrease for the convex function $L(x)$.

Figure 2: Constrained gradient descent with $x^T x \leq C$. The green vector $w$ is the projection of $v_1$ into $x^T x \leq C$ where $v_1$ is the component of $-\nabla l(x)$ perpendicular to $x_1$. The right picture is the next step after the update in the left picture. $x_*$ denotes the optimal solution of $\{ \min l(x) \}$.

As shown above, a trivial gradient descent method will go further in the direction of $-\nabla l(x)$, i.e., update $x$ by $x \leftarrow x - \eta \nabla l(x)$ for small step size $\eta$. When the level curve is $l(x) = c_1$ and the current position of $x = x_1$ where $x_1$ is the intersection of $x^T x = C$ and $l(x) = c_1$, the descent direction $-\nabla l(x_1)$ will be perpendicular to the level curve of $l(x_1) = c_1$ as shown in the left picture of Figure 2. However, if we further restrict that the optimal value can only be in $x^T x \leq C$, the trivial descent direction $-\nabla l(x_1)$ will lead $x_2 = x_1 - \eta \nabla l(x_1)$ outside of $x^T x \leq C$. A solution is to decompose the step $-\nabla l(x_1)$ into

$$-\nabla l(x_1) = a x_1 + v_1,$$
where \( ax_1 \) is the component perpendicular to the curve of \( x^\top x = C \), and \( v_1 \) is the component parallel to the curve of \( x^\top x = C \). Keep only the step \( v_1 \), then the update

\[
x_2 = \text{project}(x_1 + \eta v_1) = \text{project}\left(x_1 + \eta \left( -\nabla l(x_1) - ax_1 \right) \right)
\]

will lead to a smaller loss from \( l(x_1) \) to \( l(x_2) \) and it still matches the prerequisite of \( x^\top x \leq C \).

This is known as the projection gradient descent. It is not hard to see that the update \( x_2 = \text{project}(x_1 + \eta v_1) \) is equivalent to finding a vector \( w \) (shown by the green vector in the left picture of Figure 2) such that \( x_2 = x_1 + w \) is inside the curve of \( x^\top x \leq C \). Mathematically, the \( w \) can be obtained by \(-\nabla l(x_1) - 2\lambda x_1 \) for some \( \lambda \) as shown in the middle picture of Figure 2. This is exactly the negative gradient of \( L(x) = l(x) + \lambda \|x\|^2 \) such that

\[-\nabla L(x) = -\nabla l(x) - 2\lambda x,\]

and

\[w = -\nabla L(x) \quad \text{leads to} \quad x_2 = x_1 + w = x_1 - \nabla L(x).\]

And in practice, a small step size \( \eta \) can avoid going outside the curve of \( x^\top x \leq C \):

\[x_2 = x_1 - \eta \nabla L(x) .\]

### 1.5 Quadratic Form in Gradient Descent

We discuss further the (vanilla) gradient descent on the simplest model possible, the convex quadratic,

\[
L(x) = \frac{1}{2} x^\top Ax - b^\top x + c, \quad x \in \mathbb{R}^d ,
\]

where \( A \in \mathbb{R}^{d \times d}, b \in \mathbb{R}^d \), and \( c \) is a scalar constant. Though the quadratic form in Eq. (1.4) is an extremely simple model, it is rich enough to approximate many other functions, e.g., the Fisher information matrix (Amari, 1998) and capture key features of pathological curvature. The gradient of \( L(x) \) at point \( x \) is given by

\[
\nabla L(x) = \frac{1}{2} (A^\top + A)x - b \quad \text{(1.5)}
\]

The unique minimum of the function is the solution of the linear system \( \frac{1}{2}(A^\top + A)x = b \):

\[
x_* = 2(A^\top + A)^{-1}b \quad \text{(1.6)}
\]

If \( A \) is symmetric (for most of our discussions, we will restrict to symmetric \( A \) or even PD), the equation reduces to

\[
\nabla L(x) = Ax - b \quad \text{(1.7)}
\]

2. where the \text{project}(x) will project the vector \( x \) to the closest point inside \( x^\top x \leq C \). Notice here the direct update \( x_2 = x_1 + \eta v_1 \) can still make \( x_2 \) outside the curve of \( x^\top x \leq C \).
Then the unique minimum of the function is the solution of the linear system $Ax = b$ where $A, b$ are known matrix or vector, $x$ is an unknown vector; and the optimal point of $x$ is thus given by

$$x^* = A^{-1}b.$$ 

For different types of matrix $A$, the loss surface of $L(x)$ will be different as shown in Figure 3. When $A$ is positive definite, the surface is a convex bowl; when $A$ is negative definite, on the contrary, the surface is a concave bowl. $A$ also could be singular, in which case $Ax - b$ has more than one solution, and the set of solutions is a line (in the 2D case of Figure 3(c)) or a hyperplane (in the high-dimensional case). Moreover, $A$ could be none of the above, then there exists a saddle point where the gradient descent may fail. In this sense, other methods, e.g., perturbed GD (Jin et al., 2017; Du et al., 2017), can be applied to escape the saddle points.

Note here we don’t have to do any gradient descent, we can just jump directly to the minimum. However, we are concerned with the iterative updates of the convex quadratic...
function. Suppose we pick up a starting point \( x_1 \in \mathbb{R}^d \). The trivial way for the update at time step \( t \) is to set the learning rate \( \eta \) fixed; and the gradient descent update becomes:

\[
x_{t+1} = x_t + \eta d_t.
\]

This will create a monotonically decreasing sequence of \( \{L(x_t)\} \). When the descent direction is chosen to be the negative gradient, the update becomes

Vanilla GD: \( x_{t+1} = x_t - \eta (Ax_t - b) \). (1.8)

A concrete example is given in Figure 4 where \( A = \begin{bmatrix} 20 & 7 \\ 5 & 5 \end{bmatrix}, \ b = 0, \) and \( c = 0. \) Suppose at \( t \)-th iteration, \( x_t = [-3, 3.5]^{\top} \). Figure 4(a) shows the descent direction given by the negative gradient; Figure 4(b) and Figure 4(c) present 10 iterations afterwards with \( \eta = 0.02 \) and \( \eta = 0.08 \) respectively.

(a) Contour and the descent direction. The red dot is the optimal point.  
(b) Vanilla GD, \( \eta = 0.02. \)  
(c) Vanilla GD, \( \eta = 0.08. \)

**Figure 4:** Illustration for the linear search of quadratic form with \( A = \begin{bmatrix} 20 & 7 \\ 5 & 5 \end{bmatrix}, \ b = 0, \) and \( c = 0. \) The procedure is at \( x_t = [-3, 3.5]^{\top} \) for the \( t \)-th iteration.

**Closed form for vanilla GD**  When \( A \) is symmetric, it admits spectral decomposition (Theorem 13.1 in Lu (2022c)):

\[
A = Q \Lambda Q^{\top} \in \mathbb{R}^{d \times d} \quad \text{leads to} \quad A^{-1} = Q \Lambda^{-1} Q^{\top},
\]

where the columns of \( Q = [q_1, q_2, \ldots, q_d] \) are eigenvectors of \( A \) and are mutually orthonormal, and the entries of \( \Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_d) \) are the corresponding eigenvalues of \( A \) which are real. If we further assume \( A \) is positive definite, then the eigenvalues are all positive. By convention, we order the eigenvalues such that \( \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d \). Define the following iterate vector at iteration \( t \)

\[
y_t = Q^{\top} (x_t - x_*),
\]

(1.9)

3. In some texts, the starting point is denoted as \( x_0 \), however, we will take it as \( x_1 \) in this article.
where $x_\star = A^{-1}b$ if we further assume $A$ is nonsingular as aforementioned. It then follows that
\[
y_{t+1} = Q^\top (x_{t+1} - x_\star) = Q^\top (x_t - \eta (Ax_t - b) - x_\star) = (x_{t+1} = x_t - \eta \nabla L(x_t))
\]
\[
= Q^\top (x_t - x_\star) - \eta Q^\top (Ax_t - b)
\]
\[
= y_t - \eta Q^\top (Q\Lambda Q^\top x_t - b)
\]
\[
= y_t - \eta (\Lambda Q^\top x_t - Q^\top b)
\]
\[
= y_t - \eta \Lambda Q^\top (x_t - x_\star) = y_t - \eta \Lambda y_t
\]
\[
= (I - \eta \Lambda)y_t = (I - \eta \Lambda)^t y_1
\]

where the second equality is from Eq (1.8). This reveals the error at each iteration:
\[
||x_{t+1} - x_\star||^2 = ||Q y_{t+1}||^2 = ||Q (I - \eta \Lambda)^t y_1||^2 = \left|\sum_{i=1}^d y_{1,i} \cdot (1 - \eta \lambda_i)^t q_i\right|^2.
\]  
(1.10)

where $y_1$ depends on the initial parameter $x_1$, and $y_{1,i}$ is the $i$-th element of $y_1$. An intuitive interpretation for $y_{t+1}$ is the error in the $Q$-basis at iteration $t+1$. By Eq (1.10), we realize that the learning rate should be chosen such that
\[
|1 - \eta \lambda_i| \leq 1, \quad \forall i \in \{1, 2, \ldots, d\}.
\]  
(1.11)

And the error is a sum of $d$ terms, each has its own dynamics and depends on the rate of $1 - \eta \lambda_i$; the closer the rate is to 1, the slower it converges in that dimension (Shewchuk et al., 1994; O’donoghue and Candes, 2015; Goh, 2017).

To converge, the learning rate should be satisfied that $|1 - \eta \lambda_i| \leq 1$. This implies $0 < \eta \lambda_i < 2$ for $i$ in $\{1, 2, \ldots, d\}$. And therefore, the overall rate of convergence is determined by the slowest component:
\[
rate(\eta) = \max\{|1 - \eta \lambda_1|, |1 - \eta \lambda_d|\},
\]
since $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d$. The optimal learning rate is obtained when the first and the last eigenvectors converge at the same rate, i.e., $\eta \lambda_1 - 1 = 1 - \eta \lambda_d$:
\[
\text{optimal } \eta = \arg \min_{\eta} \text{rate}(\eta) = \frac{2}{\lambda_1 + \lambda_d},
\]  
(1.12)

and
\[
\text{optimal rate} = \min_{\eta} \text{rate}(\eta) = \frac{\lambda_1/\lambda_d - 1}{\lambda_1/\lambda_d + 1} = \frac{\kappa - 1}{\kappa + 1}
\]  
(1.13)

where $\kappa = \frac{\lambda_1}{\lambda_d}$ is known as the condition number. When $\kappa = 1$, the convergence is fast with just one step; and when the condition number is larger, the gradient descent becomes slower. The rate of convergence (per iteration) is plotted in Figure 5. The more ill-conditioned the matrix, i.e., the larger its condition number, the slower the convergence of vanilla GD.
2. Line Search

In last section, we derive the gradient descent where the update step at step \( t \) is \(-\eta \nabla L(x_t) = -\eta g_t\) and the learning rate \( \eta \) controls how large of a step to take in the direction of negative gradient. Line search is a method that directly finds the optimal learning rate in order to provide the best improvement in the gradient movement. Formally, the line search solves the following problem at the \( t \)-th step of gradient descent:

\[
\eta_t = \arg\min_{\eta} L(x_t - \eta g_t).
\]

After performing the gradient update \( x_{t+1} = x_t - \eta_t g_t \), the gradient is computed at \( x_{t+1} \) for the next step \( t + 1 \). More generally, let \( d_t \) be the descent direction, then the gradient descent with line search (to differentiate, we call it steepest descent when \( d_t = -g_t \) in this article, and the fixed learning rate GD is known as the vanilla GD) can be described by:

\[
\eta_t = \arg\min_{\eta} L(x_t + \eta d_t).
\]

**Lemma 2.1: (Orthogonality in Line Search)**

The gradient of optimal point \( x_{t+1} = x_t + \eta d_t \) of a line search is orthogonal to the current update direction \( d_t \):

\[
\nabla L(x_{t+1})^\top d_t = 0.
\]

**Proof** [of Lemma 2.1] Suppose \( \nabla L(x_{t+1})^\top d_t \neq 0 \), then there exists a \( \delta \) and it follows by Taylor’s formula (Appendix A, p. 74) that

\[
L(x_t + \eta_t d_t + \delta d_t) \approx L(x_t + \eta_t d_t) \pm \delta d_t^\top \nabla L(x_t + \eta_t d_t).
\]

(2.1)

Since \( x_t + \eta_t d_t \) is the optimal move such that \( L(x_t + \eta_t d_t) \leq L(x_t + \eta_t d_t \pm \delta d_t) \) and \( \delta \neq 0 \). This leads to the claim

\[
d_t^\top \nabla L(x_t + \eta_t d_t) = 0.
\]
We complete the proof. □

In line search methods, the loss function is expressed in terms of $\eta$ at iteration $t$:

$$J(\eta) = L(x_t + \eta d_t).$$

And the problem then becomes

$$\eta_t = \arg \min_{\eta} L(x_t + \eta d_t) = \arg \min_{\eta} J(\eta).$$

This reveals that the (local) minimum of $\eta$ can be obtained by finding the solution of $J'(\eta) = 0$ if $J(\eta)$ is differentiable. The solution then follows that

$$J'(\eta) = d_t^\top \nabla L(x_t + \eta d_t) = 0,$$  \hspace{1cm} (2.2)

which again proves Lemma 2.1. When $\eta = 0$, we have (by Remark 1.1)

$$J'(0) = d_t^\top g_t \leq 0.$$  \hspace{1cm} (2.3)

One important property of typical line search settings is that the loss function $J(\eta)$ when expressed in terms of $\eta$ is often a unimodal function. And if we find a $\eta_{\text{max}}$ such that $J'(\eta_{\text{max}}) > 0$, the optimal learning rate is then in the range of $[0, \eta_{\text{max}}]$.

### 2.1 Bisection Line Search

In bisection line search, we start by setting the interval $[a, b]$ as $[\eta_{\text{min}}, \eta_{\text{max}}]$ where $\eta_{\text{min}}$ and $\eta_{\text{max}}$ are minimum and maximum boundaries for the learning rate $\eta$ ($\eta_{\text{min}}$ can be set to 0 by Eq (2.3)). The bisection line search evaluates the loss function $J(\eta)$ at the midpoint $a + \frac{b}{2}$. Since we know $J'(a) < 0$ and $J'(b) > 0$, the bisection line search follows that

$$\begin{cases} 
set a = \frac{a + b}{2}, & \text{if } J'\left(\frac{a + b}{2}\right) < 0; \\
set b = \frac{a + b}{2}, & \text{if } J'\left(\frac{a + b}{2}\right) > 0.
\end{cases}$$

The procedure is repeated until the range between $a$ and $b$ is small enough.

The bisection line search is also known as the binary line search. And in some cases, the derivative of $J(\eta)$ cannot be easily obtained; then the interval is narrowed by evaluating the objective function at two closely spaced points near $\frac{a+b}{2}$. To be more concrete, assume $J(\eta)$ is convex (since we are in the descent setting), we evaluate the loss function at $\frac{a+b}{2}$ and $\frac{a+b}{2} + \epsilon$ where $\epsilon$ is a numerically small value like $1e-8$. This allows us to evaluate whether the function is increasing or decreasing at $\frac{a+b}{2}$ by determining which of the two evaluations is larger. If the function is increasing at $\frac{a+b}{2}$, the interval is narrowed to $[a, \frac{a+b}{2} + \epsilon]$. Otherwise, it is narrowed to $[\frac{a+b}{2}, b]$.

$$\begin{cases} 
set b = \frac{a + b}{2} + \epsilon, & \text{if increasing at } \frac{a + b}{2}; \\
set a = \frac{a + b}{2}, & \text{otherwise}.
\end{cases}$$

And again, the procedure is repeated until the range is small enough or the interval is reached with the required level of accuracy.
2.2 Golden-Section Line Search

Similar to the bisection line search, the **golden-section line search** also finds the best learning rate \( \eta \) when \( J(\eta) \) is a unimodal function. Again, it starts with the interval \([a, b]\) as \([0, \eta_{\text{max}}]\).

However, instead of picking a midpoint, the golden-section search picks a pair of \(c_1, c_2\) such that \(a < c_1 < c_2 < b\). The procedure follows: when \( \eta = a \) yields the minimum value for \( J(\eta) \) (among the four values \( J(a), J(c_1), J(c_2) \) and, \( J(b) \)), we can exclude the interval \((c_1, b]\); when \( \eta = c_1 \) yields the minimum value, we can exclude the interval \((c_2, b]\); when \( \eta = c_2 \) yields the minimum value, we can exclude the interval \([a, c_1]\); and when \( \eta = b \) yields the minimum value, we can exclude the interval \([a, c_2]\). The four situations are shown in Figure 6. In other words, at least one of the intervals \([a, c_1]\) and \([c_2, b]\) can be dropped in the golden-section search method. To conclude, we have

- when \( J(a) \) is the minimum, exclude \((c_1, b]\);
- when \( J(c_1) \) is the minimum, exclude \((c_2, b]\);
- when \( J(c_2) \) is the minimum, exclude \([a, c_1]\);
- when \( J(b) \) is the minimum, exclude \([a, c_2]\).

As long as we exclude one of the above four intervals, the new bound \([a, b]\) can be set accordingly. The process is then repeated until the range is small enough.
2.3 Armijo Rule

Similar to Eq (2.1), by Taylor’s formula again, we have

\[ J(\eta) = L(x_t + \eta d_t) \approx L(x_t) + \eta d_t^T \nabla L(x_t). \]

Since \( d_t^T \nabla L(x_t) \leq 0 \) (by Remark 1.1), it follows that

\[ L(x_t + \eta d_t) \leq L(x_t) + \alpha \eta \cdot d_t^T \nabla L(x_t), \quad \alpha \in (0, 1). \] (2.4)

Let \( \tilde{J}(\eta) = J(0) + J'(0) \cdot \eta \) and \( \tilde{J}(\eta) = J(0) + \alpha J'(0) \cdot \eta \), the relationship of the two functions is shown in Figure 7 when \( J(\eta) \) is a convex function; and we note that \( \tilde{J}(\eta) > \tilde{J}(\eta) \) when \( \eta > 0 \).

The Armijo rule says that an acceptable \( \eta \) should satisfy \( J(\tilde{\eta}) \leq \tilde{J}(\tilde{\eta}) \) to ensure sufficient decrease and \( J(\tilde{\eta}/\beta) > \tilde{J}(\tilde{\eta}/\beta) \) to ensure the step size is not too small where \( \beta \in (0, 1) \) such that the (local) optimal learning rate is in the range of \( [\tilde{\eta}, \tilde{\eta}/\beta] \). By Eq (2.4), the two criteria above can also be described by:

\[
\begin{align*}
J(\tilde{\eta}) &\leq \tilde{J}(\tilde{\eta}); \\
J(\tilde{\eta}/\beta) &> \tilde{J}(\tilde{\eta}/\beta),
\end{align*}
\]

\[
\Rightarrow \quad \left\{ \begin{array}{l}
L(x_t + \tilde{\eta} d_t) - L(x_t) \leq \alpha \tilde{\eta} \cdot d_t^T \nabla L(x_t); \\
L(x_t + \tilde{\eta}/\beta d_t) - L(x_t) > \alpha \tilde{\eta}/\beta \cdot d_t^T \nabla L(x_t).
\end{array} \right.
\]

The full algorithm to calculate the learning rate at \( t \)-th iteration is formulated in Algorithm 1. In practice, the parameters are set to be \( \beta \in [0.2, 0.5] \) and \( \alpha \in [1e-5, 0.5] \). Moreover, the Armijo rule is inexact, and it works even when \( J(\eta) \) is not unimodal.

After developing the Armijo algorithm, the core idea behind the Armijo rule can be found that the descent direction \( J'(0) \) at that starting point \( \eta = 0 \) often deteriorates in terms of rate of improvement since it moves further along this direction. However, a fraction \( \alpha \in [1e-5, 0.5] \) of this improvement is acceptable. By Eq (2.4), the descent update at \((t+1)\)-th iteration \( L(x_t + \eta d_t) \) is at least \( \alpha \eta \cdot d_t^T \nabla L(x_t) \) smaller than that of \( t \)-th iteration.

**Algorithm 1 Armijo Rule at \( t \)-th Iteration**

**Require:** Start with \( \eta_t = s \), \( 0 < \beta < 1 \), and \( 0 < \alpha < 1 \);
1: isStop = False;
2: while isStop is False do
3: \quad if \( L(x_t + \eta_t d_t) - L(x_t) \leq \alpha \eta_t \cdot d_t^T \nabla L(x_t) \) then
4: \quad \quad isStop = True;
5: \quad else
6: \quad \quad \eta_t = \beta \eta_t;
7: \quad end if
8: end while
9: Output \( \eta_t \);

4. The tangent of \( J(\eta) \) at \( \eta = 0 \).
2.4 Quadratic Form in Steepest Descent

Following the discussion of the quadratic form in GD (Section 1.5, p. 9), we now discuss the quadratic form in GD with line search. By definition, we have

\[ J(\eta) = L(x_t + \eta d_t) = \frac{1}{2} (x_t + \eta d_t)^\top A (x_t + \eta d_t) - b^\top (x_t + \eta d_t) + c \]

\[ = L(x_t) + \eta d_t^\top \left( \frac{1}{2} (A + A^\top) x_t - b \right) + \frac{1}{2} \eta^2 d_t^\top A d_t, \]

which is a quadratic function with respect to \( \eta \) and there exists a closed form for the line search:

\[ \eta_t = -\frac{d_t^\top g_t}{d_t^\top A d_t}. \]  

(2.5)

We observe that \( d_t^\top A d_t > 0 \) when \( d_t \neq 0 \). As aforementioned, when the search direction is the negative gradient \( d_t = -g_t \), the method is known as the steepest descent. Then the descent update becomes

Steepest Descent:

\[ x_{t+1} = x_t + \eta_t d_t = x_t - \frac{d_t^\top g_t}{d_t^\top A d_t} d_t \]

\[ = x_t - \frac{g_t^\top g_t}{g_t^\top A g_t} g_t, \]  

(2.6)

where \( d_t = -g_t \) for the gradient descent case.

A concrete example is presented in Figure 8 where \( A = \begin{bmatrix} 20 & 7 \\ 5 & 5 \end{bmatrix} \), \( b = 0 \), and \( c = 0 \).

Suppose at \( t \)-th iteration, the parameter is at \( x_t = [-3, 3.5]^\top \). Figure 8(a) presents the descent direction via the negative gradient. The line search is to choose the learning rate \( \eta_t \) by minimizing \( J(\eta) = L(x_t + \eta d_t) \), and it is equivalent to choosing the point on the intersection of the vertical plane through the descent direction and the paraboloid defined by the loss function \( L(x) \) as shown in Figure 8(b). Figure 8(c) further shows the parabola defined by the intersection of the two surfaces. Figure 8(d) shows various gradients on the line through the descent direction where the gradient at the bottommost point is orthogonal to the gradient of the previous step \( \nabla L(x_{t+1})^\top d_t \) as proved in Lemma 2.1 (p. 13) where the black arrows are the gradients and the blue arrows are the projection of these gradients along \( d_t = -\nabla L(x_t) \). An intuitive reason for this orthogonality at the minimum is: the slope of the parabola (Figure 8(c)) at any point is equal to the magnitude of the projection of the gradients onto the search direction (Figure 8(d)) (Shewchuk et al., 1994). These projections represent the rate of increase of the loss function \( L(x) \) as the point traverses the search line; and \( L(x) \) is minimized where the projection is zero and where the gradient is orthogonal to the search line.

The example is run with 10 iterations in Figure 8(e), Figure 8(f), and Figure 8(g) by vanilla GD with \( \eta = 0.02 \), vanilla GD with \( \eta = 0.08 \), and steepest descent respectively. We notice the tedious choices in vanilla GD; and the zigzag path in the steepest GD with line search due to the orthogonality between each gradient and the previous gradient (Lemma 2.1, p. 13). While this drawback will be partly solved in conjugate descent (Section 5.4, p. 54).
(a) Contour and the descent direction. The red dot is the optimal point.

(b) Intersection of the loss surface and vertical plane through the descent direction.

(c) Intersection of the loss surface and vertical plane through the descent direction in 2-dimensional space.

(d) Various gradients on the line through the descent direction where the gradient at the bottommost point is orthogonal to the gradient of the previous step.

(e) Vanilla GD, $\eta = 0.02$.

(f) Vanilla GD, $\eta = 0.08$.

(g) Steepest descent.

**Figure 8:** Illustration for the line search of quadratic form with $A = \begin{bmatrix} 20 & 7 \\ 5 & 5 \end{bmatrix}$, $b = 0$, and $c = 0$. The procedure is at $x_t = [-3, 3.5]^\top$ for $t$-th iteration.
2.4.1 Special Case: Symmetric Quadratic Form

To further discuss the convergence results of steepest descent, we discuss some special cases. Following Shewchuk et al. (1994), we first introduce some definitions.

**Definition 2.2: Error and Residual Vector**

At iteration \( t \), the *error* is defined as \( e_t = x_t - x^* \), a vector indicates how far the iterate is from the solution, where \( x^* = A^{-1}b \) when \( A \) is symmetric and nonsingular. Substituting into Eq (2.6), the update for the error vector is

\[
e_{t+1} = e_t - \frac{g_t^T g_t}{g_t^T A g_t} g_t.
\]

(2.7)

Furthermore, the *residual* \( r_t = b - Ax_t \) indicates how far the iterate is from the correct value of \( b \). Note in this case, the residual is equal to the negative gradient and the descent direction, i.e., \( r_t = d_t = -g_t \) when \( A \) is symmetric (we may use \(-g_t\) and \( r_t \) interchangeably when \( A \) is symmetric).

We first consider the case where the error vector \( e_t \) at iteration \( t \) is an eigenvector with eigenvalue \( \lambda_t \), i.e., \( A e_t = \lambda_t e_t \). Then the gradient vector (for symmetric \( A \) by Eq. (1.7))

\[
g_t = A x_t - b = A \left( x_t - A^{-1}b \right) = A e_t = \lambda_t e_t
\]

is also an eigenvector of \( A \) with eigenvalue being \( \lambda_t \), i.e., \( A g_t = \lambda_t g_t \). By Eq (2.7), the update for \((t+1)\)-th iteration is

\[
e_{t+1} = e_t - \frac{g_t^T g_t}{\lambda_t g_t^T g_t} (\lambda_t e_t) = 0.
\]

Therefore, it takes only one step further to converge to the solution when \( e_t \) is an eigenvector of \( A \). A concrete example is shown in Figure 9(a) where \( A = \begin{bmatrix} 20 & 5 \\ 5 & 5 \end{bmatrix}, b = 0, c = 0 \).

2.4.2 Special Case: Symmetric with Orthogonal Eigenvectors

When \( A \) is symmetric, it admits spectral decomposition (Theorem 13.1 in Lu (2022c)):

\[
A = Q \Lambda Q^T \in \mathbb{R}^{d \times d} \quad \text{leads to} \quad A^{-1} = Q \Lambda^{-1} Q^T,
\]

where the columns of \( Q = [q_1, q_2, \ldots, q_d] \) are eigenvectors of \( A \) and are mutually orthonormal, and the entries of \( \Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_d) \) with \( \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d \) being the
corresponding eigenvalues of $A$, which are real. Since the eigenvectors are chosen to be mutually orthonormal:

$$q_i^\top q_j = \begin{cases} 1, & i = j; \\ 0, & i \neq j, \end{cases}$$

the eigenvectors also span the whole space $\mathbb{R}^d$ such that every error vector $e_t \in \mathbb{R}^d$ can be expressed as a combination of the eigenvectors:

$$e_t = \sum_{i=1}^d \alpha_i q_i,$$

(2.8)

where $\alpha_i$ indicates the component of $e_t$ in the direction of $q_i$. Then the gradient vector (for symmetric $A$ by Eq. (1.7))

$$g_t = A x_t - b = A e_t = A \sum_{i=1}^d \alpha_i q_i = \sum_{i=1}^d \alpha_i \lambda_i q_i,$$

(2.9)

i.e., a combination of eigenvectors with length at $i$-th dimension being $\alpha_i \lambda_i$. Again by Eq. (2.7), the update for $(t+1)$-th iteration is

$$e_{t+1} = e_t - \frac{g_t^\top g_t}{g_t^\top A g_t} g_t$$

$$= e_t - \sum_{i=1}^d \frac{\alpha_i^2 \lambda_i^2}{\sum_{i=1}^d \alpha_i^2 \lambda_i^3} \sum_{i=1}^d \alpha_i \lambda_i q_i = 0.$$
The above equation tells us that when only one component of \( \alpha_i \)'s is nonzero, the convergence is achieved in only one step as shown in Figure 9(a). More specially, when \( \lambda_1 = \lambda_2 = \ldots = \lambda_d = \lambda \), i.e., all the eigenvalues are the same, it then follows that

\[
e_{t+1} = e_t - \frac{g_t^\top g_t}{g_t^\top Ag_t} e_t \]

\[
= e_t - \frac{\sum_{i=1}^d \alpha_i^2}{\sum_{i=1}^d \alpha_i^2} e_t = 0.
\]

Therefore, it takes only one step further to converge to the solution for arbitrary \( e_t \). A concrete example is shown in Figure 9(b) where \( A = \begin{bmatrix} 20 & 0 \\ 0 & 20 \end{bmatrix} \), \( b = 0 \), \( c = 0 \).

### 2.4.3 General Convergence Analysis for Symmetric PD Quadratic

To discuss the general convergence results, we further define the energy norm for error vector by \( ||e||_A = (e^\top A e)^{1/2} \). It can be shown that minimizing \( ||e_t||_A \) is equivalent to minimizing \( L(x_t) \) since

\[
||e||_A^2 = 2L(x_t) - 2b^\top x_t.
\]

By the definition of energy norm, Eq (2.7), and symmetric positive definiteness of \( A \), we have the update on the energy norm sequence:

\[
||e_{t+1}||_A^2 = e_{t+1}^\top Ae_{t+1}
\]

\[
= (e_t - \frac{g_t^\top g_t}{g_t^\top Ag_t} g_t)^\top A (e_t - \frac{g_t^\top g_t}{g_t^\top Ag_t} g_t)
\]

\[
= ||e_t||_A^2 + \left( \frac{g_t^\top g_t}{g_t^\top Ag_t} \right)^2 g_t^\top Ag_t - 2 \frac{g_t^\top g_t}{g_t^\top Ag_t} g_t^\top Ae_t
\]

\[
= ||e_t||_A^2 - \frac{(g_t^\top g_t)^2}{g_t^\top Ag_t} (Ae_t = g_t)
\]

\[
= ||e_t||_A^2 \cdot \left( 1 - \frac{(g_t^\top g_t)^2}{g_t^\top Ag_t} \cdot e_t^\top Ae_t \right)
\]

\[
= ||e_t||_A^2 \cdot \left( 1 - \frac{\sum_{i=1}^d \alpha_i^2 \lambda_i^2}{\left( \sum_{i=1}^d \alpha_i^2 \lambda_i \right)^2} \right)
\]

(by Eq (2.8), Eq (2.9))

\[
= ||e_t||_A^2 \cdot r^2,
\]

where

\[
r^2 = \left( 1 - \frac{\left( \sum_{i=1}^d \alpha_i^2 \lambda_i^2 \right)^2}{\left( \sum_{i=1}^d \alpha_i^2 \lambda_i \right)^2 \cdot \left( \sum_{i=1}^d \alpha_i^2 \lambda_i \right)^2} \right)
\]

determines the rate of convergence. As per convention, we assume \( \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d > 0 \), i.e., the eigenvalues are ordered in magnitude and positive as \( A \) is positive definite. Then the condition number is defined as \( \kappa = \frac{\lambda_1}{\lambda_d} \). Denote further \( \kappa_i = \lambda_i/\lambda_d \) and \( \sigma_i = \alpha_i/\alpha_1 \). It follows that

\[
r^2 = \left( 1 - \frac{(\kappa^2 + \sum_{i=2}^d \sigma_i^2 \kappa_i^2)^2}{(\kappa^3 + \sum_{i=2}^d \sigma_i^2 \kappa_i)(\kappa^3 + \sum_{i=2}^d \sigma_i^2 \kappa_i)} \right).
\]
Therefore, the rate of convergence is further controlled by $\kappa$, $\sigma_i$’s, and $\kappa_i$’s. We notice $|\kappa_i| \geq 1$ for $i \in \{2, 3, \ldots, d\}$.

**2-dimensional case** Specifically, when $d = 2$, we have

$$r^2 = 1 - \frac{(\kappa^2 + \sigma_2^2)^2}{(\kappa^3 + \sigma_2^2) \cdot (\kappa + \sigma_2^2)}. \quad (2.12)$$

Figure 10 depicts the value $r^2$ as a function of $\kappa$ and $\sigma_2$. When $d = 2$, from Eq (2.8), we have

$$e_t = \alpha_1 q_1 + \alpha_2 q_2. \quad (2.13)$$

This confirms the two special examples shown in Figure 9: when $e_t$ is an eigenvector of $A$, it follows that:

- **case 1**: $\alpha_2 = 0$ leads to $\sigma_2 = \alpha_2/\alpha_1 \to 0$;
- **case 2**: $\alpha_1 = 0$ leads to $\sigma_2 = \alpha_2/\alpha_1 \to \infty$,

i.e., the slope of $\sigma_2$ is either zero or infinite, the rate of convergence goes to zero and it converges instantly in just one step (example in Figure 9(a)). While if the eigenvalues are identical, $\kappa = 1$, once again, the rate of convergence is zero (example in Figure 9(b)).

**Worst case** We recall that $\sigma_2 = \alpha_2/\alpha_1$ decides the error vector $e_t$ (Eq (2.8) or Eq (2.13)) which in turn decides the point $x_t$ in the 2-dimensional case. It is then interesting to see the worst point to descent. Holding $\kappa$ fixed (i.e., $A$ and the loss function $L(x)$ are fixed), suppose further $t = 1$, we want to see the worst starting point $x_1$ to descent. It can be shown that the rate of convergence in Eq (2.12) is maximized when $\sigma_2 = \pm \kappa$:

$$r^2 \leq 1 - \frac{4\kappa^2}{\kappa^5 + 2\kappa^4 + \kappa^3} = \frac{(\kappa - 1)^2}{(\kappa + 1)^2}. \quad (2.12')$$
Substitute into Eq (2.11), we have

\[ ||e_{t+1}||_A^2 \leq ||e_t||_A^2 \cdot \frac{(\kappa - 1)^2}{(\kappa + 1)^2}, \]

leads to

\[ ||e_{t+1}||_A \leq ||e_1||_A \cdot \left(\frac{\kappa - 1}{\kappa + 1}\right)^t. \]

The upper bound of the rate of convergence (per iteration) is plotted in Figure 11. Again, the more *ill-conditioned* the matrix, the slower the convergence of steepest descent. We may notice that the (upper bound of the) rate of convergence is the same as that of the vanilla GD in Eq (1.13). However, the two are different in that the rate of the vanilla GD is described in terms of the \( y_t \) vector in Eq (1.9); while the rate of steepest descent is presented in terms of the energy norm. Moreover, the rate of vanilla GD in Eq (1.13) is obtained by selecting a specific learning rate as shown in Eq (1.12) which is not practical in vanilla GD since the learning rate is fixed at all iterations. This makes the rate of vanilla GD rather a tight bound. In practice, vanilla GD converges slower than steepest descent as the examples shown in Figure 8(e), Figure 8(f), and Figure 8(g).

3. Learning Rate Annealing and Warmup

We have discussed in Eq (1.3) that the learning rate \( \eta \) controls how large of a step to take in the direction of negative gradient so that we can reach a (local) minimum. In a wide range of applications, a fixed learning rate works well in practice. While there are other learning rate schedules that change the learning rate during learning and it is most often changed between epochs. We shall see in the sequel that per-dimension optimizers can change the learning rate in each dimension adaptively, e.g., AdaGrad, AdaDelta, RMSProp, and AdaSmooth (Duchi et al., 2011; Hinton et al., 2012b; Zeiler, 2012; Lu, 2022a); while in this section, we discuss how to decay or anneal the global learning rate, i.e., the \( \eta \) in Eq (1.3).
A constant learning rate often poses a dilemma to the analyst: a small learning rate used will cause the algorithm to take too long to reach anywhere close to an optimal solution. While a large initial learning rate will allow the algorithm to come reasonably close to a good (local) minimum in the cost surface at first; however, the algorithm will then oscillate back and forth around the point for a very long time. One method to prevent this challenge is to slow down the parameter updates by decreasing the learning rate. This can be done manually when the validation accuracy appears to plateau. On the other hand, decaying the learning rate over time based on how many epochs through the data have been done can naturally avoid these issues. The most common decay functions are step decay, inverse decay, and exponential decay. In the next section, we shall discuss the mathematical formulas for various learning rate annealing schemes.

3.1 Learning Rate Annealing

Step decay  Step decay scheduler drops the learning rate by a factor every epoch or every few epochs. Given the iteration $t$, number of iterations to drop $n$, initial learning rate $\eta_0$, and decay factor $d < 1$, the form of step decay is given by

$$\eta_t = \eta_0 \cdot d^\left\lfloor \frac{t}{n} \right\rfloor = \eta_0 \cdot d^s,$$

where $s = \left\lfloor \frac{t}{n} \right\rfloor$ is called the step stage to decay. Therefore, the step decay policy decays the learning rate every $n$ iterations.

Multi-step decay  Multi-step decay scheduler is a slightly different version of the step decay in that the step stage is the index where the iteration $t$ falls in the milestone vector $m = [m_1, m_2, \ldots, m_k]^T$ with $0 \leq m_1 \leq m_2 \leq \ldots \leq m_k \leq T$ and $T$ being the total number of iterations (or epochs)\(^5\). To be more concrete, the step stage $s$ at iteration $t$ is obtained by

$$s = \begin{cases} 0, & t < m_1; \\ 1, & m_1 \leq t < m_2; \\ \vdots & \\ k, & m_k \leq t \leq T. \end{cases}$$

As a result, given the iteration $t$, initial learning rate $\eta_0$, and decay factor $d < 1$, the learning rate at iteration $t$ is obtained by

$$\eta_t = \eta_0 \cdot d^s.$$

Exponential decay  Given the iteration $t$, the initial learning rate $\eta_0$, and the exponential decay factor $k$, the form of the exponential decay is given by

$$\eta_t = \eta_0 \cdot \exp(-k \cdot t),$$

where the parameter $k$ controls the rate of the decay.

---

\(^5\) When $T$ is the total number of iterations, it can be obtained by the number of epochs times the number of steps per epoch.
**Inverse decay** The inverse decay scheduler is a slightly different version of exponential decay in that the decaying effect is applied by the inverse function. Given the iteration number \( t \), the initial learning rate \( \eta_0 \), and the decay factor \( k \), the form of the inverse decay is obtained by

\[
\eta_t = \frac{\eta_0}{1 + k \cdot t},
\]

where, again, the parameter \( k \) controls the rate of the decay.

**Inverse square root** The inverse square root scheduler is a learning rate schedule

\[
\eta_t = \eta_0 \cdot \sqrt{w} \cdot \frac{1}{\sqrt{\max(t, w)}},
\]

where \( t \) is the current training iteration and \( w \) is the number of warm-up steps, and \( \eta_0 \) is the initial learning rate. This sets a constant learning rate for the first steps, then exponentially decays the learning rate until pre-training is over.

**Annealing polynomial decay** Given the iteration \( t \), max decay iteration \( M \), power factor \( p \), initial learning rate \( \eta_0 \), and final learning rate \( \eta_T \), the annealing polynomial decay at iteration \( t \) can be obtained by

\[
decay\_batch = \min(t, M);
\eta_t = (\eta_0 - \eta_T) \cdot \left(1 - \frac{t}{decay\_batch}\right)^p + \eta_T.
\]

In practice, the default values for the parameters are: initial rate \( \eta_0 = 0.001 \), end rate \( \eta_T = 1e - 10 \), the warm up steps \( M = T/2 \) where \( T \) is the maximal iteration number, and power rate \( p = 2 \).

Figure 12 compares step decay, multi-step decay, annealing polynomial decay, inverse decay, inverse square root, and exponential decay schedulers. One may find the exponential decay is the smoothest among the six, while multi-step decay is the least smooth one.

---

**Figure 12:** Demonstration of step decay, multi-step decay, annealing polynomial, inverse decay, inverse square root, and exponential decay schedulers. One may find the exponential decay is the smoothest among the six, while multi-step decay is the least smooth one.
- When $M$ is small, the decay gets closer to that of the exponential scheduler or step decay; however, the exponential decay has a longer tail. That is, the exponential scheduler decays slightly faster in the beginning iterations, while it decays slower in the last few iterations.
- When $M$ is large, the decay gets closer to that of multi-step decay; however, the multi-step scheduler behaves much more aggressively.

![Training Performance Graph](image)

**Figure 13:** Training and test performance with different learning rate schemes.

**Toy example** To see the effect of different schedulers, we employ a toy example with multi-layer perceptron (MLP) training on MNIST digit classification set (LeCun, 1998)\(^6\). Figure 13 shows the training and test performance in terms of negative log likelihood loss. The parameters for various schedulers are shown in Figure 12 (for 100 epochs). We observe that the stochastic gradient descent method with fixed learning rate may continue

\(^6\) It has a training set of 60,000 examples, and a test set of 10,000 examples.
to decrease the test loss. However, its test accuracy may get stuck at some point. The toy example shows learning rate annealing schemes in general can help optimization methods “find” better local minima with better performance.

### 3.2 Learning Rate Warmup

This warmup idea in training neural networks receive attention in recent years (He et al., 2016; Goyal et al., 2017; Smith and Topin, 2019). See also discussion in Popel and Bojar (2018) for a deep understanding of why the warmup scheduler works well in neural machine translation (NML). The learning rate annealing schedulers can be utilized in both epoch- and step-basis. However, the learning rate warmup schemes are usually applied in the step context where the total number of steps is the number of epochs times the number of steps per epoch as aforementioned (Vaswani et al., 2017; Howard and Ruder, 2018). Note that with this scheduler, early stopping should typically be avoided. In the rest of this section, we discuss two commonly used warmup policies, namely, the slanted triangular learning rates (STLR) and the Noam methods.

#### Slanted Triangular Learning Rates (STLR)

STLR is a learning rate schedule that first linearly increases the learning rate over some number of epochs and then linearly decays it over the remaining epochs. The rate at iteration $t$ is computed by

$$
cut = \left\lceil T \cdot \frac{1}{frac} \right\rceil;
$$

$$
p = \begin{cases} 
t / \cut, & \text{if } t < \cut; \\
1 - \frac{t - \cut}{\cut \cdot (1/frac - 1)}, & \text{otherwise}; 
\end{cases}
$$

$$
\eta_t = \eta_{\text{max}} \cdot \frac{1 + p \cdot (\text{ratio} - 1)}{\text{ratio}},
$$

where $T$ is the number of training iterations (the number of epochs times the number of updates per epoch), $frac$ is the fraction of iterations we want to increase the learning rate, $cut$ is the iteration when we switch from increasing to decreasing the learning rate, $p$ is the fraction of the number of iterations we have increased or decreased the learning rate respectively, $\text{ratio}$ specifies how much smaller the lowest learning rate is from the maximum learning rate $\eta_{\text{max}}$. In practice, the default values are $frac = 0.1$, $ratio = 32$ and $\eta_{\text{max}} = 0.01$ (Howard and Ruder, 2018).

#### Noam

The Noam scheduler is originally used in neural machine translation (NML) tasks and is proposed in Vaswani et al. (2017). This corresponds to increasing the learning rate linearly for the first “warmup steps” training steps and decreasing it thereafter proportionally to the inverse square root of the step number, scaled by the inverse square root of the dimensionality of the model (linear warmup for a given number of steps followed by exponential decay). Given the warmup steps $w$ and the model size $d_{\text{model}}$ (the hidden size parameter which dominates the number of parameters in the model), the learning rate $\eta_t$ at step $t$ can be calculated by

$$
\eta_t = \alpha \cdot \frac{1}{\sqrt{d_{\text{model}}}} \cdot \min \left( \frac{1}{\sqrt{t}}, \frac{t}{w^{3/2}} \right),
$$
where $\alpha$ is a smoothing factor. In the original paper, the warmup step $w$ is set to $w = 4000$. While in practice, $w = 25000$ can be a good choice.

Moreover, in rare cases, the model size is set to be the same as the warmup steps which is known as the warmup Noam scheduler:

$$\eta_t = \alpha \cdot \frac{1}{\sqrt{w}} \cdot \min \left( \frac{1}{\sqrt{t}}, \frac{t}{w^{3/2}} \right).$$

Figure 14 compares STLR and Noam schedulers with various parameters. We may observe that, in general, the Noam scheduler decays slower when the warmup finishes than the STLR.

### 3.3 Cyclical Learning Rate (CLR) Policy

The cyclical learning rate is a kind of generalization of warmup+decay (Noam scheme or STLR policy does just one cycle). The essence of this learning rate policy comes from the observation that increasing the learning rate might have a short term negative effect and yet achieves a long term beneficial effect. This observation leads to the idea of letting the learning rate vary within a range of values rather than adopting a stepwise fixed or exponentially decreasing value where minimum and maximum boundaries are set to make the learning rate vary between them. The simplest function to adopt this idea is the triangular window function that linearly increases and then linearly decreases (Smith, 2017).

Dauphin et al. (2014, 2015) argue that the difficulty in minimizing the loss arises from saddle points (toy example in Figure 3(d), p. 10) rather than poor local minima. Saddle points have small gradients that slow the pace of the learning process. However, increasing the learning rate allows more rapid traversal of saddle point plateaus. In this scenario, a cyclical learning rate policy with periodical increasing and decreasing of the learning rate between minimum and maximum boundaries is reasonable. The minimum and maximum boundaries are problem-specific. Usually one runs the model for several epochs for different learning rates between low and high learning rate values. This is known as the learning rate range test. In this case, plot the accuracy versus learning rate; when the accuracy starts to increase and when the accuracy slows, becomes ragged, or starts to fall, the two of which constitute good choices for the minimum and maximum boundaries.
The cyclical learning rate policies can be divided into two categories: the one based on iteration, and the one based on epoch. The former one does the annealing and warmup at each iteration and the latter one does this on an epoch-basis. However, there is no big difference between the two; any policy can be applied in either one of the two fashions. In the next paragraphs, we will discuss the update policies based on their original proposals.

**Triangular, Triangular2, and Exp Range**  
The *triangular* policy linearly increases the learning rate and then linearly decreases it. Given the initial learning rate $\eta_0$ (the lower boundary in the cycle), the max learning rate $\eta_{\text{max}}$, the step size $s$ (number of training iterations per half cycle), the learning rate $\eta_t$ at iteration $t$ can be obtained by:

\[
\text{triangular} : \begin{cases} 
\text{cycle} = \left\lfloor 1 + \frac{t}{2s} \right\rfloor; \\
x = \text{abs} \left( \frac{t}{s} - 2 \times \text{cycle} + 1 \right); \\
\eta_t = \eta_0 + (\eta_{\text{max}} - \eta_0) \cdot \max(0, 1 - x),
\end{cases}
\]

where the calculated $\text{cycle}$ records in which cycle the iteration $t$ is. The same as the *triangular* policy, the *triangular2* policy cuts in half at the end of each cycle:

\[
\text{triangular2} : \quad \eta_t = \eta_0 + (\eta_{\text{max}} - \eta_0) \cdot \max(0, 1 - x) \cdot \frac{1}{2^{\text{cycle} - 1}}.
\]

Less aggressive than the *triangular2* policy, the amplitude of a cycle in the *exp_range* policy is scaled exponentially based on $\gamma^t$ where $\gamma < 1$ is the scaling constant:

\[
\text{exp_range} : \quad \eta_t = \eta_0 + (\eta_{\text{max}} - \eta_0) \cdot \max(0, 1 - x) \cdot \gamma^t.
\]

A comparison of the three policies is shown in Figure 15. In practice, the step size $s$ usually is set to $2 \sim 10$ times the number of iterations in an epoch (Smith, 2017).

---

7. The total number of iterations equals the number of epochs times the number of updates per epoch.
Cyclical cosine  

*Cyclical cosine* is a type of learning rate schedule that has the effect of starting with a large learning rate that is relatively rapidly decreased to a minimum value before being increased rapidly again. The resetting of the learning rate acts as a simulated restart of the learning process and the re-use of good weights as the starting point of the restart is referred to as a “warm restart” in contrast to a “cold restart” where a new set of small random numbers may be used as a starting point (Loshchilov and Hutter, 2016; Huang et al., 2017). The learning rate $\eta_t$ at iteration $t$ is calculated as follows:

$$
\eta_t = \frac{\eta_0}{2} \left( \cos \left( \frac{\pi \text{mod}(t - 1, \lceil T/M \rceil)}{\lceil T/M \rceil} \right) + 1 \right),
$$

where $T$ is the total number of training iterations (note the original paper takes the iterations as epochs in this sense (Loshchilov and Hutter, 2016)), $M$ is the number of cycles, and $\eta_0$ is the initial learning rate. The scheduler anneals the learning rate from its initial value $\eta_0$ to a small learning rate approaching 0 over the course of a cycle. That is, we split the training process into $M$ cycles as shown in Figure 16(a), each of which starts with a large learning rate $\eta_0$ and then gets annealed to a small learning rate. The above equation can lower the learning rate at a very fast pace, encouraging the model to converge towards its first local minimum after a few epochs. The optimization then continues at a larger learning rate that can perturb the model and dislodge it from the minimum. The procedure is then repeated several times to obtain multiple convergences. In practice, the iteration $t$ usually refers to the $t$-th epoch. More generally, any learning rate with general function $f$ in the following form can have a similar effect:

$$
\eta_t = f(\text{mod}(t - 1, \lceil T/M \rceil)).
$$

Moreover, the learning rate can be set for each batch instead of prior to each epoch to give more nuance to the updates (Huang et al., 2017).

---

8. The goal of the procedure is similar to the perturbed SGD that can help escape from saddle points (Jin et al., 2017; Du et al., 2017).
Cyclical step  Similar to the cyclical cosine scheme, the cyclical step learning rate policy combines a linear learning rate decay with warm restarts (Mehta et al., 2019):

$$\eta_t = \eta_{\text{max}} - (t \mod M) \cdot \eta_{\text{min}}.$$

where in the original paper, $t$ refers to the epoch count, $\eta_{\text{min}}$ and $\eta_{\text{max}}$ are the ranges for the learning rate, and $M$ is the cycle length after which the learning rate will restart. The learning rate scheme can be seen as a variant of the cosine learning policy as discussed above and the comparison between the two policies is shown in Figure 16. In practice, $\eta_{\text{min}} = 0.1$, $\eta_{\text{max}} = 0.5$, and $M = 5$ are set as default values in the original paper.

Cyclical polynomial  The cyclical polynomial is a variant of the annealing polynomial decay (Eq (3.1)) scheme where the difference is that the cyclical polynomial scheme employs a cyclical warmup similar to the exp_range policy. Given the iteration number $t$, initial learning rate $\eta_0$, final learning rate, $\eta_T$, and maximal decay number $M < T$, the rate can be calculated by:

$$\text{decay\_batch} = M \cdot \left\lceil \frac{t}{M} \right\rceil$$

$$\eta_t = (\eta_0 - \eta_T) \cdot \left( 1 - \frac{t}{\text{decay\_batch} + \epsilon} \right)^p + \eta_T,$$

where $\epsilon = 1e - 10$ is applied for better condition when $t = 0$. Figure 17 presents cyclical polynomial scheme with various parameters.

4. Stochastic Optimizer

Over the years, stochastic gradient-based optimization has become a core method in many fields of science and engineering such as computer vision and automatic speech recognition processing (Krizhevsky et al., 2012; Hinton et al., 2012a; Graves et al., 2013). Stochastic gradient descent (SGD) and deep neural network (DNN) play a core role in training stochastic objective functions. When a new deep neural network is developed for a given task, some hyper-parameters related to the training of the network must be chosen heuristically. For each possible combination of structural hyper-parameters, a new network is typically trained from scratch and evaluated over and over again. While much progress has been made on hardware (e.g., Graphical Processing Units) and software (e.g., cuDNN)
to speed up the training time of a single structure of a DNN, the exploration of a large set of possible structures remains very slow making the need of a stochastic optimizer that is insensitive to hyper-parameters. Efficient stochastic optimizers thus play a core role in training deep neural networks.

There are several variants of SGD to use heuristics for estimating a good learning rate at each iteration of the progress. These methods either attempt to accelerate learning when suitable or to slow down learning near a local minimum. In this section, we introduce a few stochastic optimizers that are in the two categories. Table 1 shows the number of papers that uses the optimizers to do the tasks and the date of publication. For alternative reviews, one can also check Zeiler (2012), Ruder (2016), Goodfellow et al. (2016), and many others.

| Method          | Year | Papers | Method          | Year | Papers |
|-----------------|------|--------|-----------------|------|--------|
| Adam            | 2014 | 7532   | AdamW           | 2017 | 45     |
| SGD             | 1951 | 1212   | Local SGD       | 2018 | 41     |
| RMSProp         | 2013 | 293    | Gravity         | 2021 | 37     |
| Adafactor       | 2018 | 177    | AMSGrad         | 2019 | 35     |
| Momentum        | 1999 | 130    | LARS            | 2017 | 31     |
| LAMB            | 2019 | 126    | MAS             | 2020 | 26     |
| AdaGrad         | 2011 | 103    | DFA             | 2016 | 23     |
| Deep Ensembles  | 2016 | 69     | Nesterov momentum| 1983 | 22     |
| FA              | 2014 | 46     | Gradient Sparsification | 2017 | 20     |

Table 1: Data retrieved on April 27th, 2022 via https://paperswithcode.com/.

4.1 Momentum

If the cost surface is not spherical, learning can be quite slow because the learning rate must be kept small to prevent divergence along the steep curvature directions (Polyak, 1964; Rumelhart et al., 1986; Qian, 1999; Sutskever et al., 2013). The SGD with momentum (that can be applied to full batch or mini-batch learning) attempts to use the previous step to speed up learning when suitable such that it enjoys better converge rates on deep networks. The main idea behind the momentum method is to speed up the learning along dimensions where the gradient consistently points in the same direction; and to slow the pace along dimensions in which the sign of the gradient continues to change. Figure 19(a) shows a set of updates for vanilla GD where we can find the update along dimension $x_1$ is consistent; and the move along dimension $x_2$ continues to change in a zigzag pattern. The GD with momentum keeps track of past parameter updates with an exponential decay, and the update method has the following step:

$$
\Delta x_t = \rho \Delta x_{t-1} - \eta \frac{\partial L(x_t)}{\partial x_t},
$$

where the algorithm remembers the latest update and adds it to the present update by multiplying a parameter $\rho$ called momentum parameter. That is, the amount we change the parameter is proportional to the negative gradient plus the previous weight change; the added momentum term acts as both a smoother and an accelerator. The momentum
parameter $\rho$ works as a decay constant where $\Delta x_1$ may have an effect on $\Delta x_{100}$; however, its effect is decayed by this decay constant. In practice, the momentum parameter $\rho$ is usually set to be 0.9 by default. Momentum simulates the concept of inertia in physics. It means that in each iteration, the update mechanism is not only related to the gradient descent, which refers to the dynamic term, but also maintains a component that is related to the direction of the last update iteration, which refers to the momentum.

![Surface and Contour Plot](image)

(a) A 2-dimensional surface plot for quadratic convex function. (b) The contour plot of $L(x)$. The red dot is the optimal point.

**Figure 18:** Figure 1(a) shows a function surface and a contour plot (blue=low, yellow=high) where the upper graph is the surface, and the lower one is the projection of it (i.e., contour). The quadratic function is with parameters $A = \begin{bmatrix} 4 & 0 \\ 0 & 40 \end{bmatrix}$, $b = [12, 80]^\top$, and $c = 103$. Or equivalently, $L(x) = 2(x_1 - 3)^2 + 20(x_2 - 2)^2 + 5$ and $\frac{\partial L(x)}{\partial x} = [4x_1 - 12, 8x_2 - 16]^\top$.

The momentum works extremely better in a ravine-shaped loss curve. Ravine is an area, where the surface curves are much steeper in one dimension than in another (see the surface and contour curve in Figure 18, i.e., a long narrow valley). Ravines are common near local minima in deep neural networks and vanilla GD or SGD has trouble navigating them. As shown by the toy example in Figure 19(a), GD tends to oscillate across the narrow ravine since the negative gradient will point down one of the steep sides rather than along the ravine towards the optimum. Momentum helps accelerate gradients in the correct direction and dampens oscillations as can be seen in the example of Figure 19(b).

As aforementioned, it does this by adding a fraction $\rho$ of the update vector of the past time step to the current update vector. When $\Delta x_t$ and $\Delta x_{t-1}$ are in the same direction, the momentum accelerates the update step (e.g., the blue arrow areas in Figure 19(b)); while they are in the opposite directions, the algorithm tends to update in the former direction if $x$ has been updated in this direction for many iterations. To be more concrete, look at the blue starting point, and then look at the cyan point we get to after one step in the step of the update without Momentum (Figure 19(a)), they have gradients that are pretty much equal and opposite. As a result, the gradient across the ravine has been canceled out. But the gradient along the ravine has not canceled out. Along the ravine, we’re going to keep building up speed, and so, after the momentum method has settled down, it’ll tend to go along the bottom of the ravine.
(a) Optimization without momentum. A higher learning rate may result in larger parameter updates in the dimension across the valley (direction of $x_2$) which could lead to oscillations back and forth across the valley.

(b) Optimization with momentum. Though the gradients along the valley (direction of $x_1$) are much smaller than the gradients across the valley (direction of $x_2$), they are typically in the same direction and thus the momentum term accumulates to speed up movement, dampen oscillations and cause us to barrel through narrow valleys, small humps and (local) minima.

Figure 19: The starting point is $[-2, 5]^T$. After 5 iterations, the squared loss from vanilla GD is 42.72, and the loss from GD with momentum is 35.41 in this simple case. The learning rates $\eta$ are set to be 0.04 in both cases.

From this figure, the problem with the vanilla GD is that the gradient is big in the direction in which we only want to travel a small distance; and the gradient is small in the direction in which we want to travel a large distance. However, one can easily find that the momentum term helps average out the oscillation along the short axis while at the same time adds up contributions along the long axis. In other words, although it starts off by following the gradient, however, when it has velocity, it no longer does steepest descent. We call this momentum, which makes it keep going in the previous direction.

4.1.1 Quadratic Form in Momentum

Following the discussion of quadratic form in GD (Section 1.5, p. 9) and steepest descent (Section 2.4, p. 17), we now discuss the quadratic form in GD with momentum. The update is:

$$\Delta x_t = \rho \Delta x_{t-1} - \eta \nabla L(x_t);$$
$$x_{t+1} = x_t + \Delta x_t,$$

where $\nabla L(x_t) = Ax_t - b$ if $A$ is symmetric for the quadratic form. The update becomes

$$\Delta x_t = \rho \Delta x_{t-1} - \eta (Ax_t - b);$$
$$x_{t+1} = x_t + \Delta x_t.$$

Again define the following iterate vectors

$$\begin{cases}
y_t = Q^T(x_t - x*) ; \\
z_t = Q^T \Delta x_t,
\end{cases}$$

34
where $x_* = A^{-1}b$ if we further assume $A$ is nonsingular and PD as aforementioned, $A = Q\Lambda Q^T$ is the spectral decomposition of matrix $A$. The construction yields the update rule:

$$z_t = \rho z_{t-1} - \eta \Lambda y_t;$$
$$y_{t+1} = y_t + z_t,$$

or after rearrangement:

$$\begin{bmatrix} z_t \\ y_{t+1} \end{bmatrix} = \begin{bmatrix} \rho I & -\eta \Lambda \\ \rho I & -\eta \Lambda + I \end{bmatrix} \begin{bmatrix} z_{t-1} \\ y_t \end{bmatrix}.$$

And this leads to the per-dimension update:

$$\begin{bmatrix} z_{t,i} \\ y_{t+1,i} \end{bmatrix} = \begin{bmatrix} \rho & -\eta \lambda_i \\ \rho & 1 - \eta \lambda_i \end{bmatrix}^t \begin{bmatrix} z_{0,i} \\ y_{1,i} \end{bmatrix} = B^t \begin{bmatrix} z_{0,i} \\ y_{1,i} \end{bmatrix},$$ (4.2)

where $z_{t,i}$ and $y_{t,i}$ are $i$-th element of $z_t$ and $y_t$ respectively, and $B = \begin{bmatrix} \rho & -\eta \lambda_i \\ \rho & 1 - \eta \lambda_i \end{bmatrix}$. Note here $z_0$ is initialized to be a zero vector, and $y_1$ is initialized to be $Q^T(x_1 - x_*)$ where $x_1$ is the initial parameter. Suppose the eigenvalue decomposition (Theorem 11.1 in Lu (2022c)) of $B$ admits

$$B = CDC^{-1},$$

where columns of $C$ contain eigenvectors of $B$ and $D$ is a diagonal matrix $\text{diag}(\alpha, \beta)$ containing the eigenvalues of $B$. Then $B^t = CDC^{-1}$. Alternatively, the eigenvalues of $B$ can be calculated by solving $\det(B - \alpha I) = 0$:

$$\alpha, \beta = \frac{(\rho + 1 - \eta \lambda_i) \pm \sqrt{(\rho + 1 - \eta \lambda_i)^2 - 4\rho}}{2}.$$

We then have by Williams (1992) that

$$B^t = \begin{cases} \alpha^t - \beta^t \frac{B - \beta I}{\alpha - \beta}, & \text{if } \alpha \neq \beta; \\ \alpha^t - \beta^t \frac{B - \alpha I}{\alpha - \beta}, & \text{if } \alpha = \beta. \end{cases}$$

And therefore it follows by substituting into Eq (4.2) that

$$\begin{bmatrix} z_{t,i} \\ y_{t+1,i} \end{bmatrix} = B^t \begin{bmatrix} z_{0,i} \\ y_{1,i} \end{bmatrix},$$

where the rate of convergence is controlled by the slower one, $\max\{|\alpha|, |\beta|\}$; when $\max\{|\alpha|, |\beta|\} < 1$, the GD with momentum is guaranteed to converge. When $\rho = 0$, the momentum reduces to vanilla GD, such that

$$\max\{|\alpha|, |\beta|\} = |1 - \eta \lambda_i| < 1, \quad \forall \quad i \in \{1, 2, \ldots, d\},$$

same as that in Eq (1.11).
Following the same example in Figure 18 and Figure 19 where \( A = \begin{bmatrix} 4 & 0 \\ 0 & 40 \end{bmatrix} \) with eigenvalues \( \lambda_1 = 4 \) and \( \lambda_2 = 40 \), and matrix \( B \) in Eq (4.2) being

\[
B_1 = \begin{bmatrix} \rho & -4\eta \\ \rho & 1 - 4\eta \end{bmatrix} \quad \text{and} \quad B_2 = \begin{bmatrix} \rho & -40\eta \\ \rho & 1 - 40\eta \end{bmatrix}
\]

respectively. Then it can be shown that when \( \eta = 0.04, \rho = 0.8 \), the rate of convergence is approximated to be 0.894; Figure 20(b) shows the updates for 20 iterations, though the motion is in a zigzag pattern, it can still converge. However, when \( \eta = 0.04, \rho = 1 \), the rate of convergence is equal to 1; Figure 20(c) shows the updates for 20 iterations, the movement diverges even it passes through the optimal point.

![Figure 20](image)

(a) Momentum \( \rho = 0.2 \), rate \( \approx 0.79 \). (b) Momentum \( \rho = 0.8 \), rate \( \approx 0.89 \). (c) Momentum \( \rho = 1 \), rate = 1.

**Figure 20:** Momentum creates its own oscillations. The learning rates \( \eta \) are set to be 0.04 for all scenarios.

### 4.2 Nesterov Momentum

Nesterov momentum (a.k.a., Nesterov accelerated gradient (NAG)) is a slightly different version of the momentum update and has recently been gaining popularity. The core idea behind Nesterov momentum is that when the current parameter vector is at some position \( x_t \), then looking at the momentum update above, we know that the momentum term alone (i.e., ignoring the second term with the gradient) is about to nudge the parameter vector by \( \rho \Delta x_{t-1} \). Therefore, if we are about to compute the gradient, we can treat the future approximate position \( x_t + \rho \Delta x_{t-1} \) as a lookahead - this is a point in the vicinity of where we are soon going to end up. Hence, it makes sense to compute the gradient at \( x_t + \rho \Delta x_{t-1} \) instead of at the old position \( x_t \). Finally, the step has this form:

\[
\Delta x_t = \rho \Delta x_{t-1} - \eta \frac{\partial L(x_t + \rho \Delta x_{t-1})}{\partial x}.
\]

Figure 21 shows the difference between momentum and Nesterov momentum. This important difference is thought to counterbalance too high velocities by “peeking ahead” actual objective values in the candidate search direction. In other words, one first makes a big jump in the direction of the previously accumulated gradient; then measures the gradient where you end up and make a correction. But in standard momentum, one first jumps by current gradient, then makes a big jump in the direction of the previously accumulated
Gradient Descent, Stochastic Optimization, and Other Tales

Gradient: $\eta \frac{\partial L(x_t)}{\partial x_t}$

Actual step: $\rho \Delta x_{t-1}$

(a) Momentum: evaluate gradient at the current position $x_t$, and momentum is about to carry us to the tip of the green arrow.

(b) Nesterov momentum: evaluate the gradient at this “looked-ahead” position $x_t + \rho \Delta x_{t-1}$.

---

**Figure 21:** Comparison of momentum and Nesterov momentum.

gradient. To make a metaphor, it turns out, if you’re going to gamble, it’s much better to gamble and then make a correction, than to make a correction and then gamble (Hinton et al., 2012c). Sutskever et al. (2013) show that Nesterov momentum has a provably better bound than gradient descent for convex, non-stochastic objectives settings.

4.3 AdaGrad

The learning rate annealing procedure modifies a single global learning rate that applies to all dimensions of the parameters (Section 3.1, p. 24). Duchi et al. (2011) proposed a method called AdaGrad where the learning rate is updated on a per-dimension basis. The learning rate for each parameter depends on the history of gradient updates of that parameter in a way such that parameters with a scarce history of updates are updated faster by using a larger learning rate. In other words, parameters that have not been updated much in the past are more likely to have higher learning rates now. Denoting the element-wise vector multiplication between $a$ and $b$ by $a \odot b$, formally, the AdaGrad has the following update step:

$$
\Delta x_t = -\frac{\eta}{\sqrt{\sum_{\tau=1}^{t} g_{\tau}^2 + \epsilon}} \odot g_t,
$$

(4.3)

where $\epsilon$ is a smoothing term to better condition the division, $\eta$ is a global learning rate shared by all dimensions, $g_{\tau}^2$ indicates the element-wise square $g_{\tau} \odot g_{\tau}$, and the denominator computes the $l2$ norm of a sum of all previous squared gradients in a per-dimension fashion. Though the global learning rate $\eta$ is shared by all dimensions, each dimension has its own dynamic learning rate controlled by the $l2$ norm of accumulated gradient magnitudes. Since this dynamic learning rate grows with the inverse of the accumulated gradient magnitudes, larger gradient magnitudes have smaller learning rates and smaller absolute values of gradients have larger learning rates. Therefore, the aggregated squared magnitude of the partial derivative with respect to each parameter over the course of the algorithm in the denominator has the same effects as the learning rate annealing.

One pro of AdaGrad is that it is very easy to implement, the code snippet in the following is the implementation of it by Python:
On the other hand, AdaGrad partly eliminates the need to tune the learning rate controlled by the accumulated gradient magnitude. However, AdaGrad’s main weakness is its unbounded accumulation of the squared gradients in the denominator. Since every added term is positive, the accumulated sum keeps growing or exploding during every training step. This in turn causes the per-dimension learning rate to shrink and eventually decrease throughout training and become infinitesimally small, eventually falling to zero and stopping training any more. Moreover, since the magnitudes of gradients are factored out in AdaGrad, this method can be sensitive to the initialization of the parameters and the corresponding gradients. If the initial magnitudes of the gradients are large or infinitesimally huge, the per-dimension learning rates will be low for the remainder of training. This can be partly combated by increasing the global learning rate, making the AdaGrad method sensitive to the choice of learning rate. Further, AdaGrad assumes the parameter with fewer updates should favor a larger learning rate; and one with more movement should employ a smaller learning rate. This makes it consider only the information from squared gradients or the absolute value of the gradients. And thus AdaGrad does not include information from the total move (i.e., the sum of updates; in contrast to the sum of absolute updates).

To be more succinct, AdaGrad has the following main drawbacks: 1) the continual decay of learning rates throughout training; 2) the need for a manually selected global learning rate; 3) considering only the absolute value of gradients.

### 4.4 RMSProp

RMSProp is an extension of AdaGrad that overcomes the main weakness of AdaGrad (Hinton et al., 2012b; Zeiler, 2012). The original idea of RMSProp is simple: it restricts the window of accumulated past gradients to some fixed size $w$ rather than $t$ (i.e., current time step). However, since storing $w$ previous squared gradients is inefficient, the RMSProp introduced in Hinton et al. (2012b); Zeiler (2012) implements this accumulation as an exponentially decaying average of the squared gradients. This is very similar to the idea of momentum term (or decay constant).

We first discuss the exact form of the RMSProp. Assume at time $t$ this running average is $E[g^2]_t$, then we compute:

$$E[g^2]_t = \rho E[g^2]_{t-1} + (1 - \rho)g^2_t,$$

where $\rho$ is a decay constant similar to that used in the momentum method and $g^2_t$ indicates the element-wise square $g_t \odot g_t$. In other words, the estimate is achieved by multiplying the current squared aggregate (i.e., the running estimate) by the decay constant $\rho$ and then adding $(1 - \rho)$ times the current squared partial derivative. This running estimate is initialized to $0$ which can cause some bias in early iterations; while the bias disappears over the long term. We notice that the old gradients decay exponentially over the course of the algorithm.

As Eq (4.4) is just the root mean squared (RMS) error criterion of the gradients, we can replace it with the criterion short-hand. Let $\text{RMS}[g]_t = \sqrt{E[g^2]_t} + \epsilon$, where again a
constant $\epsilon$ is added to better condition the denominator. Then the resulting step size can be obtained as follows:

$$\Delta x_t = -\frac{\eta}{\text{RMS}[g]^t} \odot g_t,$$

(4.5)

where again $\odot$ is the element-wise vector multiplication.

As aforementioned, the form in Eq (4.4) is originally from the exponential moving average (EMA). In the original form of EMA, $1 - \rho$ is also known as the smoothing constant (SC) where the SC can be written as $\frac{2}{N+1}$ and the period $N$ can be thought of as the number of past values to do the moving average calculation (Lu, 2022b):

$$\text{SC} = 1 - \rho \approx \frac{2}{N+1}. \quad (4.6)$$

The above Eq (4.6) links different variables: the decay constant $\rho$, the smoothing constant (SC), and the period $N$. If $\rho = 0.9$, then $N = 19$. That is, roughly speaking, $E[g^2]^t$ at iteration $t$ is approximately equal to the moving average of the past 19 squared gradients and the current one (i.e., the moving average of 20 squared gradients totally). The relationship in Eq (4.6) though is not discussed in Zeiler (2012), it is important to decide the lower bound of the decay constant $\rho$. Typically, a time period of $N = 3$ or 7 is thought to be a relatively small frame making the lower bound of decay constant $\rho = 0.5$ or 0.75; when $N \to \infty$, the decay constant $\rho$ approaches 1.

AdaGrad is designed to converge rapidly when applied to a convex function; while RMSProp performs better in nonconvex settings. When applied to a nonconvex function to train a neural network, the learning trajectory can pass through many different structures and eventually arrives at a region that is a locally convex bowl. AdaGrad shrinks the learning rate according to the entire history of the squared partial derivative leading to an infinitesimally small learning rate before arriving at such a convex structure. While RMSProp discards ancient squared gradients to avoid this problem. However, we can find that the RMSProp still only considers the absolute value of gradients and a fixed number of past squared gradients is not flexible which can cause a small learning rate near (local) minima as we will discuss in the sequel.

The RMSProp is developed independently by Geoff Hinton in Hinton et al. (2012b) and by Matthew Zeiler in Zeiler (2012) both of which are stemming from the need to resolve AdaGrad’s radically diminishing per-dimension learning rates. Hinton et al. (2012b) suggest $\rho$ to be set to 0.9 and the global learning rate $\eta$ to be 0.001 by default. The RMSProp further can be combined into the Nesterov momentum method (Goodfellow et al., 2016) where the comparison between the two is shown in Algorithm 2 and Algorithm 3.

4.5 AdaDelta

Zeiler (2012) further shows the units of the step size shown above in RMSProp do not match (so as the vanilla SGD, the momentum, and the AdaGrad). To overcome this weakness, from the correctness of the second-order method (more in Section 5, p. 51), the author considers rearranging Hessian to determine the quantities involved. It is well known that though the calculation of Hessian or approximation to the Hessian matrix is a tedious and computationally expensive task, its curvature information is useful for optimization, and the units in Newton’s method are well matched. Given the Hessian matrix $H$, the update
Algorithm 2 RMSProp

1: **Input:** Initial parameter $x_1$, constant $\epsilon$;
2: **Input:** Global learning rate $\eta$, by default $\eta = 0.001$;
3: **Input:** Decay constant $\rho$;
4: **Input:** Initial accumulated squared gradients $E[g^2]_0 = 0$;
5: **for** $t = 1 : T$ **do**

6: Compute gradient $g_t = \nabla L(x_t)$;
7: Compute running estimate $E[g^2]_t = \rho E[g^2]_{t-1} + (1 - \rho)g^2_t$;
8: Compute step $\Delta x_t = -\frac{\eta}{\sqrt{E[g^2]_{t-1} + \epsilon}} \odot g_t$;
9: Apply update $x_{t+1} = x_t + \Delta x_t$;
10: **end for**
11: **Return:** resulting parameters $x_t$, and the loss $L(x_t)$.

Algorithm 3 RMSProp with Nesterov Momentum

1: **Input:** Initial parameter $x_1$, constant $\epsilon$;
2: **Input:** Global learning rate $\eta$, by default $\eta = 0.001$;
3: **Input:** Decay constant $\rho$, momentum constant $\alpha$;
4: **Input:** Initial accumulated squared gradients $E[g^2]_0 = 0$, and update step $\Delta x_0 = 0$;
5: **for** $t = 1 : T$ **do**

6: Compute interim update $\tilde{x}_t = x_t + \alpha \Delta x_{t-1}$;
7: Compute interim gradient $g_t = \nabla L(\tilde{x}_t)$;
8: Compute running estimate $E[g^2]_t = \rho E[g^2]_{t-1} + (1 - \rho)g^2_t$;
9: Compute step $\Delta x_t = \alpha \Delta x_{t-1} - \frac{\eta}{\sqrt{E[g^2]_{t-1} + \epsilon}} \odot g_t$;
10: Apply update $x_{t+1} = x_t + \Delta x_t$;
11: **end for**
12: **Return:** resulting parameters $x_t$, and the loss $L(x_t)$.

The step in Newton’s method can be described as follows (Becker and Le Cun, 1988; Dauphin et al., 2014):

$$
\Delta x_t \propto -H^{-1} g_t \propto \frac{\partial L(x_t)}{\partial x_t}.
$$

This implies

$$
\frac{1}{\partial^2 L(x_t)} = \frac{\Delta x_t}{\partial L(x_t)}
$$

i.e., the units of the Hessian matrix can be approximated by the right-hand side term of the above equation. Since the RMSProp update in Eq (4.5) already involves RMS[$g^2_t$ in the denominator, i.e., the units of the gradients. Putting another unit of the order of $\Delta x_t$ in the numerator can match the same order as Newton’s method. To do this, define another exponentially decaying average of the update steps:

$$
\text{RMS}[$\Delta x^2$]_t = \sqrt{E[\Delta x^2]_t}
$$

$$
= \sqrt{\rho E[\Delta x^2]_{t-1} + (1 - \rho)\Delta x^2_t}.
$$
Since $\Delta x_t$ for the current iteration is not known and the curvature can be assumed to be locally smoothed making it suitable to approximate $\text{RMS}[\Delta x_t]$ by $\text{RMS}[\Delta x_{t-1}]$. So we can use an estimation of $\frac{1}{\frac{\partial^2 L(x_t)}{\partial x_t^2}}$ to replace the computationally expensive $H^{-1}$:

$$\frac{\Delta x_t}{\frac{\partial L(x_t)}{\partial x_t}} \sim \frac{\text{RMS}[\Delta x_{t-1}]}{\text{RMS}[g_t]}.$$  

(4.10)

This is an approximation to the diagonal Hessian using only RMS measures of $g$ and $\Delta x$, and results in the update step whose units are matched:

$$\Delta x_t = -\frac{\text{RMS}[\Delta x_{t-1}]}{\text{RMS}[g_t]} \odot g_t.$$  

(4.11)

The idea of AdaDelta from the second-order method overcomes the annoying choosing of learning rate. Meanwhile, a web demo developed by Andrej Karpathy can be explored to find the convergence rates among SGD, SGD with momentum, AdaGrad, and AdaDelta.

A last note on using the RMSProp or AdaDelta method is to carefully notice that though the accumulated squared gradients in the denominator to compensate for the per-dimension learning rates, if we save the checkpoint of the neural networks at the end of some epochs and want to re-tune the parameter by loading the weights from the checkpoint, the first few batches of the re-tuning can perform poorly since there are not enough squared gradients to smooth the denominator. While this is not a big issue for the whole training progress as the loss can still go down from that point, a better choice might be saving the $E[g^2_t]$ along with the weights of the neural networks. A particular example is shown in Figure 22 where we save the weights and load them after each epoch; loss deterioration is observed after each epoch.

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9. see https://cs.stanford.edu/people/karpathy/convnetjs/demo/trainers.html.
4.6 AdaSmooth

In this section we will discuss the effective ratio based on previous updates in the stochastic optimization process and how to apply it to accomplish adaptive learning rates per-dimension via the flexible smoothing constant, hence the name AdaSmooth. The idea presented in the section is derived from the RMSProp method in order to improve two main drawbacks of the method: 1) consider only the absolute value of the gradients rather than the total movement in each dimension; 2) the need for manually selected hyper-parameters.

Effective Ratio (ER)  
Kaufman (2013, 1995) suggested replacing the smoothing constant in the EMA formula with a constant based on the efficiency ratio (ER). And the ER is shown to provide promising results for financial forecasting via classic quantitative strategies where the ER of the closing price is calculated to decide the trend of the asset (Lu, 2022b). This indicator is designed to measure the strength of a trend, defined within a range from -1.0 to +1.0 where the larger magnitude indicates a larger upward or downward trend. Recently, Lu and Yi (2022) show the ER can be utilized to reduce overestimation and underestimation in time series forecasting. Given the window size $M$ and a series $\{h_1, h_2, \ldots, h_T\}$, it is calculated with a simple formula:

$$e_t = \frac{s_t}{n_t} = \frac{h_t - h_{t-M}}{\sum_{i=0}^{M-1} |h_{t-i} - h_{t-1-i}|} = \frac{\text{Total move for a period}}{\text{Sum of absolute move for each bar}}$$

(4.12)

where $e_t$ is the ER of the series at time $t$. At a strong trend (i.e., the input series is moving in a certain direction, either up or down) the ER will tend to 1 in absolute value; if there is no directed movement, it will be a little more than 0.

Instead of calculating the ER of the closing price of the underlying asset, we want to calculate the ER of the moving direction in the update methods for each parameter. And in the descent methods, we care more about how much each parameter moves apart from its initial point in each period, either moving positively or negatively. So here we only consider the absolute value of the ER. To be specific, the ER for the parameters in the proposed method is calculated as follows:

$$e_t = \frac{s_t}{n_t} = \frac{|x_t - x_{t-M}|}{\sum_{i=0}^{M-1} |x_{t-i} - x_{t-1-i}|} = \frac{\sum_{i=0}^{M-1} \Delta x_{t-1-i}}{\sum_{i=0}^{M-1} |\Delta x_{t-1-i}|}$$

(4.13)

where $e_t \in \mathbb{R}^d$ whose $i$-th element $e_{t,i}$ is in the range of $[0, 1]$ for all $i$ in $[1, 2, \ldots, d]$. A large value of $e_{t,i}$ indicates the descent method in the $i$-th dimension is moving in a certain direction; while a small value approaching 0 means the parameter in the $i$-th dimension is moving in a zigzag pattern, interleaved by positive and negative movement. In practice, and in all of our experiments, the $M$ is selected to be the batch index for each epoch. That is, $M = 1$ if the training is in the first batch of each epoch; and $M = M_{\text{max}}$ if the training is in the last batch of the epoch where $M_{\text{max}}$ is the maximal number of batches per epoch. In other words, $M$ ranges in $[1, M_{\text{max}}]$ for each epoch. Therefore, the value of $e_{t,i}$ indicates the movement of the $i$-th parameter in the most recent epoch. Or even more aggressively, the window can range from 0 to the total number of batches seen during the whole training progress. The adoption of the adaptive window size $M$ rather than a fixed one has the benefit that we do not need to keep the past $M+1$ steps $\{x_{t-M}, x_{t-M+1}, \ldots, x_t\}$.
to calculate the signal and noise vectors \( \{s_t, n_t\} \) in Eq (4.13) since they can be obtained in an accumulated fashion.

**AdaSmooth** If the ER in magnitude of each parameter is small (approaching 0), the movement in this dimension is zigzag, the proposed AdaSmooth method tends to use a long period average as the scaling constant to slow down the movement in that dimension. When the absolute ER per-dimension is large (tend to 1), the path in that dimension is moving in a certain direction (not zigzag), and the learning actually is happening and the descent is moving in a correct direction where the learning rate should be assigned to a relatively large value for that dimension. Thus the AdaSmooth tends to choose a small period which leads to a small compensation in the denominator; since the gradients in the closer periods are small in magnitude when it’s near the (local) minima. A particular example is shown in Figure 23, where the descent is moving in a certain direction, and the gradient in the near periods is small in magnitude; if we choose a larger period to compensate for the denominator, the descent will be slower due to the large factored denominator. In short, we want a smaller period to calculate the exponential average of the squared gradients in Eq (4.4) if the update is moving in a certain direction without a zigzag pattern; while when the parameter is updated in a zigzag fashion, the period for the exponential average should be larger (Lu, 2022a).

The obtained value of ER is used in the exponential smoothing formula. Now, what we want to go further is to set the time period \( N \) discussed in Eq (4.6) to be a smaller value when the ER tends to 1 in absolute value; or a larger value when the ER moves towards 0. When \( N \) is small, SC is known as a “fast SC”; otherwise, SC is known as a “slow SC”.

For example, let the small time period be \( N_1 = 3 \), and the large time period be \( N_2 = 199 \). The smoothing ratio for the fast movement must be as for EMA with period \( N_1 \) (“fast SC” = \( \frac{2}{N_1+1} = 0.5 \)), and for the period of no trend EMA period must be equal to \( N_2 \) (“slow SC” = \( \frac{2}{N_2+1} = 0.01 \)). Thus the new changing smoothing constant is introduced, called the “scaled smoothing constant” (SSC), denoted by a vector \( c_t \in \mathbb{R}^d \):

\[
c_t = (\text{fast SC} - \text{slow SC}) \times e_t + \text{slow SC}.
\]
By Eq (4.6), we can define the fast decay constant $\rho_1 = 1 - \frac{2}{N_1+1}$, and the slow decay constant $\rho_2 = 1 - \frac{2}{N_2+1}$. Then the scaled smoothing constant vector can be obtained by:

$$c_t = (\rho_2 - \rho_1) \times e_t + (1 - \rho_2),$$

where the smaller $e_t$, the smaller $c_t$. For a more efficient influence of the obtained smoothing constant on the averaging period, Kaufman recommended squaring it. The final calculation formula then follows:

$$E[g^2]_t = c_t^2 \odot g^2_t + (1 - c_t^2) \odot E[g^2]_{t-1}. \quad (4.14)$$

or after rearrangement:

$$E[g^2]_t = E[g^2]_{t-1} + c_t^2 \odot (g^2_t - E[g^2]_{t-1}).$$

We notice that $N_1 = 3$ is a small period to calculate the average (i.e., $\rho_1 = 1 - \frac{2}{N_1+1} = 0.5$) such that the EMA sequence will be noisy if $N_1$ is less than 3. Therefore, the minimal value of $\rho_1$ in practice is set to be larger than 0.5 by default. While $N_2 = 199$ is a large period to compute the average (i.e., $\rho_2 = 1 - \frac{2}{N_2+1} = 0.99$) such that the EMA sequence almost depends only on the previous value leading to the default value of $\rho_2$ no larger than 0.99. Experimental study will show that the AdaSmooth update will be insensitive to the hyper-parameters in the sequel. We also carefully notice that when $\rho_1 = \rho_2$, the AdaSmooth algorithm recovers to the RMSProp algorithm with decay constant $\rho = 1 - (1 - \rho_2)^2$ since we square it in Eq (4.14). After developing the AdaSmooth method, we realize the main idea behind it is similar to that of SGD with momentum: to speed up (compensate less in the denominator) the learning along dimensions where the gradient consistently points in the same direction; and to slow the pace (compensate more in the denominator) along dimensions in which the sign of the gradient continues to change.

As discussed in the cyclical learning rate section (Section 3.3, p. 28), Dauphin et al. (2014, 2015) argue that the difficulty in minimizing the loss arises from saddle points rather than poor local minima. Saddle points have small gradients that slow the learning process. However, an adaptive smoothing procedure for the learning rates per-dimension can naturally find these saddle points and compensate less in the denominator or “increase” the learning rates when the optimization is in these areas allowing more rapid traversal of saddle point plateaus. When applied to a nonconvex function to train a neural network, the learning trajectory may pass through many different structures and eventually arrive at a region that is a locally convex bowl. AdaGrad shrinks the learning rate according to the entire history of the squared partial derivative and may have made the learning rate too small before arriving at such a convex structure. RMSProp partly solves this drawback since it uses an exponentially decaying average to discard ancient squared gradients making it more robust in a nonconvex setting compared to the AdaGrad method. The AdaSmooth goes further in two points: 1) when it’s close to a saddle point, a small compensation in the denominator can help it escape the saddle point; 2) when it’s close to a locally convex bowl, the small compensation further makes it converge faster.

Empirical evidence shows the ER used in the simple moving average (SMA) with a fixed windows size $w$ can also reflect the trend of the series/movement in quantitative strategies (Lu, 2022b). However, this again needs to store $w$ previous squared gradients in the AdaSmooth case, making it inefficient and we shall not adopt this extension.
Algorithm 4 Computing AdaSmooth: the proposed AdaSmooth algorithm. All operations on vectors are element-wise. Good default settings for the tested tasks are $\rho_1 = 0.5$, $\rho_2 = 0.99$, $\epsilon = 1e-6$, $\eta = 0.001$; see Section 4.6 or Eq (4.6) for a detailed discussion on the explanation of the decay constants’ default values. The AdaSmoothDelta iteration can be calculated in a similar way.

1: **Input:** Initial parameter $x_1$, constant $\epsilon$;
2: **Input:** Global learning rate $\eta$, by default $\eta = 0.001$;
3: **Input:** Fast decay constant $\rho_1$, slow decay constant $\rho_2$;
4: **Input:** Assert $\rho_2 > \rho_1$, by default $\rho_1 = 0.5$, $\rho_2 = 0.99$;
5: **for** $t = 1 : T$ **do**
6: Compute gradient $g_t = \nabla L(x_t)$;
7: Compute ER $e_t = \frac{|x_t - x_{t-1}|}{\sum_{i=0}^{M-1} |\Delta x_{t-1-i}|}$;
8: Compute scaled smoothing vector $c_t = (\rho_2 - \rho_1) \times e_t + (1 - \rho_2)$;
9: Compute normalization term $E[g^2]_t = c_t^2 \odot g_t^2 + (1 - c_t^2) \odot E[g^2]_{t-1}$;
10: Compute step $\Delta x_t = -\frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} \odot g_t$;
11: Apply update $x_{t+1} = x_t + \Delta x_t$;
12: **end for**
13: **Return:** resulting parameters $x_t$, and the loss $L(x_t)$.

**AdaSmoothDelta** We observe that the ER can also be applied to the AdaDelta setting:

$$\Delta x_t = -\frac{\sqrt{E[\Delta x^2]_t}}{\sqrt{E[g^2]_t + \epsilon}} \odot g_t, \quad (4.15)$$

where

$$E[g^2]_t = c_t^2 \odot g_t^2 + (1 - c_t^2) \odot E[g^2]_{t-1}, \quad (4.16)$$

and

$$E[\Delta x^2]_t = (1 - c_t^2) \odot \Delta x_t^2 + c_t^2 \odot E[\Delta x^2]_{t-1}, \quad (4.17)$$

in which case the difference in $E[\Delta x^2]_t$ is to choose a larger period when the ER is small. This is reasonable in the sense that $E[\Delta x^2]_t$ appears in the numerator while $E[g^2]_t$ is in the denominator of Eq (4.15) making their compensation towards different directions. Or even, a fixed decay constant can be applied for $E[\Delta x^2]_t$:

$$E[\Delta x^2]_t = (1 - \rho_2)\Delta x_t^2 + \rho_2 E[\Delta x^2]_{t-1},$$

The AdaSmoothDelta optimizer introduced above further alleviates the need for a hand specified global learning rate which is set to $\eta = 1$ from the Hessian context. However, due to the adaptive smoothing constants in Eq (4.16) and (4.17), the $E[g^2]_t$ and $E[\Delta x^2]_t$ are less locally smooth making it less insensitive to the global learning rate than the AdaDelta method. Therefore, a smaller global learning rate, e.g., $\eta = 0.5$ is favored in AdaSmoothDelta. The full procedure for computing AdaSmooth is then formulated in Algorithm 4.

We have discussed the step-points problem when reloading weights from checkpoints in the RMSProp or AdaDelta methods. However, this issue is less severe in the AdaSmooth
Figure 24: Demonstration of tuning parameter after each epoch by loading the weights. We save the weights and load them after each epoch such that there are step-points while re-training after each epoch. This issue is less severe in the AdaSmooth case than in the RMSProp method. A smaller loss deterioration is observed in the AdaSmooth example than that of the RMSProp case.

setting as a typical example shown in Figure 24 where a smaller loss deterioration is observed in the AdaSmooth example than that of the RMSProp case.

Figure 25: MLP: Comparison of descent methods on MNIST digit and Census Income data sets for 60 and 200 epochs with MLP.

Example: Multi-Layer Perceptron To see the difference between the discussed algorithms by far, we conduct experiments with different machine learning models; and different data sets including real handwritten digit classification task, MNIST (LeCun, 1998) \(^{10}\), and Census Income \(^{11}\) data sets are used. In all scenarios, the same parameter initialization is

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\(^{10}\) It has a training set of 60,000 examples, and a test set of 10,000 examples.

\(^{11}\) Census income data has 48842 number of samples and 70% of them are used as the training set in our case: https://archive.ics.uci.edu/ml/datasets/Census+Income.
adopted when training with different stochastic optimization algorithms. We compare the results in terms of convergence speed and generalization.

Multi-layer perceptrons (MLP, a.k.a., multi-layer neural networks) are powerful tools for solving machine learning tasks finding internal linear and nonlinear features behind the model inputs and outputs. We adopt the simplest MLP structure: an input layer, a hidden layer, and an output layer. We notice that rectified linear unit (ReLU) outperforms Tanh, Sigmoid, and other nonlinear units in practice making it the default nonlinear function in our structures. Since dropout has become a core tool in training neural networks (Srivastava et al., 2014), we adopt 50% dropout noise to the network architecture during training to prevent overfitting. To be more concrete, the detailed architecture for each fully connected layer is described by $F(\langle \text{num outputs} \rangle : \langle \text{activation function} \rangle)$; and for a dropout layer is described by $DP(\langle \text{rate} \rangle)$. Then the network structure we use can be described as follows:

$$F(128: \text{Relu})DP(0.5)F(\text{num of classes: Softmax}).$$

(4.18)

All methods are trained on mini-batches of 64 images per batch for 60 or 200 epochs through the training set. Setting the hyper-parameter to $\epsilon = 1e^{-6}$. If not especially mentioned, the global learning rates are set to $\eta = 0.001$ in all scenarios. While a relatively large learning rate ($\eta = 0.01$) is used for AdaGrad method since its accumulated decaying effect; learning rate for the AdaDelta method is set to 1 as suggested by Zeiler (2012) and for the AdaSmoothDelta method is set to 0.5 as discussed in Section 4.6. In Figure 25(a) and 25(b) we compare SGD with momentum, AdaGrad, RMSProp, AdaDelta, AdaSmooth and AdaSmoothDelta in optimizing the training set losses for MNIST and Census Income data sets respectively. The SGD with momentum method does the worst in this case. AdaSmooth performs slightly better than AdaGrad and RMSProp in the MNIST case and much better than the latters in the Census Income case. AdaSmooth shows fast convergence from the initial epochs while continuing to reduce the training losses in both the two experiments. We here show two sets of slow decay constant for AdaSmooth, i.e., $\rho_2 = 0.9$ and $\rho_2 = 0.95$. Since we square the scaled smoothing constant in Eq (4.14), when $\rho_1 = \rho_2 = 0.9$, the AdaSmooth recovers to RMSProp with $\rho = 0.99$ (so as the AdaSmoothDelta and AdaDelta case). In all cases, the AdaSmooth results perform better while there is almost no difference between the results of AdaSmooth with various hyper-parameters in the MLP model. Table 2 shows the best training set accuracy for different algorithms. While we notice the best test set accuracies for various algorithms are very close; we only present the best ones for the first 5 epochs in Table 3. In all scenarios, the AdaSmooth method converges slightly faster than other optimization methods in terms of the test accuracy for this toy example.

4.7 Adam

Adaptive moment estimation (Adam) is yet another adaptive learning rate optimization algorithm (Kingma and Ba, 2014). The Adam algorithm uses a similar normalization by second-order information, the running estimates for squared gradient; however, it also incorporates first-order information into the update. In addition to storing the exponential moving average of past squared gradient (the second moment) like RMSProp, AdaDelta,
| Method                          | MNIST | Census |
|--------------------------------|-------|--------|
| SGD with Momentum ($\rho = 0.9$) | 98.64% | 85.65% |
| AdaGrad ($\eta=0.01$)          | 98.55% | 86.02% |
| RMSProp ($\rho = 0.99$)        | 99.15% | 85.90% |
| AdaDelta ($\rho = 0.99$)       | 99.15% | 86.89% |
| AdaSmooth ($\rho_1 = 0.5, \rho_2 = 0.9$) | **99.34%** | **86.94%** |
| AdaSmooth ($\rho_1 = 0.5, \rho_2 = 0.95$) | **99.45%** | **87.10%** |
| AdaSmoothDelta ($\rho_1 = 0.5, \rho_2 = 0.9$) | **99.60%** | **86.86%** |

Table 2: MLP: Best in-sample evaluation in training accuracy (%).

| Method                          | MNIST | Census |
|--------------------------------|-------|--------|
| SGD with Momentum ($\rho = 0.9$) | 94.38% | 83.13% |
| AdaGrad ($\eta=0.01$)          | 96.21% | 84.40% |
| RMSProp ($\rho = 0.99$)        | 97.14% | 84.43% |
| AdaDelta ($\rho = 0.99$)       | 97.06% | 84.41% |
| AdaSmooth ($\rho_1 = 0.5, \rho_2 = 0.9$) | 97.26% | 84.46% |
| AdaSmooth ($\rho_1 = 0.5, \rho_2 = 0.95$) | 97.34% | 84.48% |
| AdaSmoothDelta ($\rho_1 = 0.5, \rho_2 = 0.9$) | 97.24% | 84.51% |

Table 3: MLP: Best out-of-sample evaluation in test accuracy for the first 5 epochs.

and AdaSmooth, Adam also keeps an exponentially decaying average of the past gradients:

\[ m_t = \rho_1 m_{t-1} + (1 - \rho_1) g_t; \]
\[ v_t = \rho_2 v_{t-1} + (1 - \rho_2) g_t^2, \]  

(4.19)

where \( m_t \) and \( v_t \) are running estimates of the first moment (the mean) and the second moment (the uncentered variance) of the gradients respectively. The drawback of RMSProp is that the running estimate \( E[g^2] \) of the second-order moment is biased in the initial time steps since it is initialized to 0; especially when the decay constant is large (when \( \rho \) is close to 1 in RMSProp). Observing the biases towards zero in Eq (4.19) as well, Adam counteracts these biases by computing the bias-free moment estimates:

\[ \hat{m}_t = \frac{m_t}{1 - \rho_1^t}; \]
\[ \hat{v}_t = \frac{v_t}{1 - \rho_2^t}. \]

The first and second moment estimates are then incorporated into the update step:

\[ \Delta x_t = -\frac{\eta}{\sqrt{\hat{v}_t + \epsilon}} \odot \hat{m}_t. \]

And therefore the update becomes

\[ x_{t+1} = x_t - \frac{\eta}{\sqrt{\hat{v}_t + \epsilon}} \odot \hat{m}_t. \]

In practice, Kingma and Ba (2014) suggests to use \( \rho_1 = 0.9, \rho_2 = 0.999, \) and \( \epsilon = 1e - 8 \) for the parameters by default.
4.8 AdaMax

Going further from Adam, Kingma and Ba (2014) notices the high-order moment:

\[ v_t = \rho_p^2 v_{t-1} + (1 - \rho_p^2) |g_t|^p, \]

that is numerically unstable for large \( p \) values making \( l_1 \) and \( l_2 \) norms the common choices for updates. However, when \( p \to \infty \), the \( l_\infty \) also exhibits stable behavior. Therefore, the AdaMax admits the following moment update:

\[ u_t = \rho_2^\infty u_{t-1} + (1 - \rho_2^\infty) |g_t|^\infty = \max(\rho_2 u_{t-1}, |g_t|), \]

where we do not need to correct for initialization bias in this case, and this yields the update step

\[ \Delta x_t = -\eta \frac{u_t}{u_t} \odot \hat{m}_t. \]

In practice, Kingma and Ba (2014) suggests to use \( \eta = 0.002, \rho_1 = 0.9, \) and \( \rho_2 = 0.999 \) as the default parameters.

4.9 Nadam

Nadam (Nesterov-accelerated Adam) combines the ideas of Adam and Nesterov momentum (Dozat, 2016). We recall the momentum and NAG updates as follows:

**Momentum:**

\[
\begin{align*}
g_t &= \nabla L(x_t); \\
\Delta x_t &= \rho \Delta x_{t-1} - \eta g_t; \\
x_{t+1} &= x_t + \Delta x_t,
\end{align*}
\]

**NAG:**

\[
\begin{align*}
g_t &= \nabla L(x_t + \rho \Delta x_{t-1}); \\
\Delta x_t &= \rho \Delta x_{t-1} - \eta g_t; \\
x_{t+1} &= x_t + \Delta x_t,
\end{align*}
\]

Dozat (2016) first proposes a modification of NAG by using the current momentum vector to look ahead which we call \( \text{NAG}' \) here. That is, apply the momentum update twice for each update:

\[
\begin{align*}
\text{NAG}': \\
g_t &= \nabla L(x_t); \\
\Delta x_t &= \rho \Delta x_{t-1} - \eta g_t; \\
\Delta x' &= \rho \Delta x_t - \eta g_t; \\
x_{t+1} &= x_t + \Delta x',
\end{align*}
\]

By rewriting the Adam in the following form where a similar modification according to \( \text{NAG}' \) leads to the Nadam update:

**Adam:**

\[
\begin{align*}
m_t &= \rho_1 m_{t-1} + (1 - \rho_1) g_t; \\
\hat{m}_t &= \rho_1 \frac{m_{t-1}}{1 - \rho_1^2} + \frac{1 - \rho_1}{1 - \rho_1} g_t; \\
\Delta x_t &= -\frac{\eta}{\sqrt{v_t} + \epsilon} \odot \hat{m}_t; \\
x_{t+1} &= x_t + \Delta x_t,
\end{align*}
\]

leads to **Nadam:**

\[
\begin{align*}
m_t &= \rho_1 m_{t-1} + (1 - \rho_1) g_t; \\
\hat{m}_t &= \rho_1 \frac{m_{t-1}}{1 - \rho_1^{t+1}} + \frac{1 - \rho_1}{1 - \rho_1} g_t; \\
\Delta x_t &= -\frac{\eta}{\sqrt{v_t} + \epsilon} \odot \hat{m}_t; \\
x_{t+1} &= x_t + \Delta x_t.
\end{align*}
\]

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However, the $\rho_1 \frac{m_{t-1}}{1-\rho_1^t}$ in $\hat{m}_t$ of the Adam method can be replaced in a momentum fashion; by applying the same modification on NAG', the second version of Nadam has the following form (though it’s not originally presented in Dozat (2016)):

| Adam’ | Nadam’ |
|-------|--------|
| $m_t = \rho_1 m_{t-1} + (1-\rho_1) g_t$; | $\hat{m}_t = \rho_1 \hat{m}_{t-1} + \frac{1-\rho_1}{1-\rho_1^t} g_t$; |
| $\hat{m}_t = \rho_1 \hat{m}_{t-1} + \frac{1-\rho_1}{1-\rho_1^t} g_t$; | $\hat{m}_t' = \rho_1 \hat{m}_t + \frac{1-\rho_1}{1-\rho_1^t} g_t$; |
| $\Delta x_t = -\frac{\eta}{\sqrt{v_t} + \epsilon} \odot \hat{m}_t$; | $\Delta x_t = -\frac{\eta}{\sqrt{v_t} + \epsilon} \odot \hat{m}_t'$; |
| $x_{t+1} = x_t + \Delta x_t$; | $x_{t+1} = x_t + \Delta x_t'$; |

4.10 Problem in SGD

**Saddle points** When the Hessian of loss function is positive-definite, then the optimal point $x_*$ with vanishing gradient must be a local minimum. Similarly, when the Hessian is negative-definite, the point is a local maximum; when the Hessian has both positive and negative eigenvalues, the point is a saddle point (see later discussion in Eq (5.3), p. 53). The stochastic optimizers discussed above in practice are first order optimization algorithms: they only look at the gradient information, and never explicitly compute the Hessian. Such algorithms may get stuck at saddle points (toy example in Figure 3(d)). In the algorithms we show above, the vanilla update, AdaGrad, AdaDelta, RMSprop, and other algorithms will have such problem. AdaSmooth may have chance to go out of the saddle points as argued in Section 4.6. While, the mechanism of momentum and Nesterov momentum help point $x$ to go over the local minimum or saddle point because they have a term of previous step size (in general), but make the model more difficult to converge especially when momentum term $\rho$ is large.

**Low speed in SGD** However, although claimed in Rong Ge’s post 12, it is potential to converge to saddle points with high error rate. Dauphin et al. (2014) and Benjamin Recht’s post 13 point out that it is in fact super hard to converge to a saddle point if one picks a random initial point and run SGD. This is because the typical problem for both local minima and saddle points is that they are often surrounded by plateaus of small curvature in the error surface. In the SGD algorithms we discuss above, they are repelled away from a saddle point to a lower error by following the directions of negative curvature. In other words, there will be no so called saddle points problem in SGD algorithms. However, this repulsion can occur slowly due to the plateau with small curvature.

While, for the second-order methods, e.g., Newton’s method, it does not treat saddle points appropriately. This is partly because Newton’s method is designed to rapidly descend plateaus surrounding local minima by rescaling gradient steps by the inverse eigenvalues of the Hessian matrix (we will see shortly in the sequel).

---

12. http://www.offconvex.org/2016/03/22/saddlepoints/
13. http://www.offconvex.org/2016/03/24/saddles-again/
As argued in Dauphin et al. (2014), random Gaussian error functions over large $d$ dimensions are increasingly likely to have saddle points rather than local minima as $d$ increases. And the ratio of the number of saddle points to local minima increases exponentially with the dimensionality $d$. The author also argues that it is saddle points rather than local minima that provide a fundamental impediment to rapid high dimensional non-convex optimization. In this sense, local minima with high errors are exponentially rare in the dimensionality of the problem. So, the computation will be slow in SGD algorithms to escape from small curvature plateaus.

**First-order method to escape from saddle point** The post 14 by Rong Ge introduces a first-order method to escape from saddle point. He claims that saddle points are very unstable: if we put a ball on a saddle point, then slightly perturb it, the ball is likely to fall to a local minimum, especially when the second-order term $\frac{1}{2}\Delta x^\top H \Delta x$ (see later discussion in Eq (5.1), p. 52) is significantly smaller than 0 (i.e., there is a steep direction where the function value decreases, and assume we are looking for local minimum), which is called a strict saddle function in Rong Ge’s post. In this case, we can use noisy gradient descent:

$$x_{t+1} = x_t + \Delta x + \epsilon.$$

where $\epsilon$ is a noise vector that has zero mean 0. Actually, it is the basic idea of SGD, which uses the gradient of a mini batch rather than the true gradient. However, the drawback of the stochastic gradient descent is not the direction, but the size of the step along each eigenvector. The step, along any eigen-direction $q_i$, is given by $-\lambda_i \Delta v_i$ (see later discussion in Section 5.1, p. 52, feel free to skip this paragraph at first reading), when the steps taken in the direction with small absolute value of eigenvalues, the step is small. To be more concrete, as an example where the curvature of the error surface may not be the same in all directions. If there is a long and narrow valley in the error surface, the component of the gradient in the direction that points along the base of the valley is very small; while the component perpendicular to the valley walls is quite large even though we have to move a long distance along the base and a small distance perpendicular to the walls. This phenomenon can be seen in Figure 19(a) (though it’s partly solved by SGD with momentum).

We normally move by making a step that is some constant times the negative gradient rather than a step of constant length in the direction of the negative gradient. This means that in steep regions (where we have to be careful not to make our steps too large), we move quickly; and in shallow regions (where we need to move in big steps), we move slowly. This phenomenon again causes the SGD methods converging slower than second-order methods.

5. Second-Order Methods

We have discussed that the AdaDelta is from the correctness of the units in second-order methods (Section 4.5, p. 39). In this section, we shortly review Newton’s method and its common variants, namely, damped Newton’s method, Levenberg gradient descent. Furthermore, we also derive the conjugate gradient from scratch that utilizes second-order information to capture the curvature shape of the loss surface in order to favor a faster convergence.

14. http://www.offconvex.org/2016/03/22/saddlepoints/
5.1 Newton’s Method

Newton’s method is an optimization policy by applying Taylor’s expansion to approximate the loss function by a quadratic form and it guesses where the minimum is via the approximated quadratic equation. By Taylor’s formula (Appendix A, p. 74) and ignoring derivatives of higher order, the loss function $L(x + \Delta x)$ can be approximated by

$$L(x + \Delta x) \approx L(x) + \Delta x^\top \nabla L(x) + \frac{1}{2} \Delta x^\top H \Delta x,$$

(5.1)

where $H$ is the Hessian of the loss function $L(x)$ with respect to $x$. The optimal point (minimum point) of Eq (5.1) is then obtained at

$$x_* = x - H^{-1} \nabla L(x).$$

That is, the update step is rescaled by the inverse of Hessian. An intuitive interpretation of Newton’s update is the Hessian contains curvature information, when the curvature is steep, the inverse Hessian can scale more making the step smaller; while the curvature is flat, the inverse Hessian scales less resulting in a larger update. Here for nonlinear $L(x)$, we cannot just be able to hop to the minimum in one step. Similar to stochastic optimization methods we have introduced in previous sections, Newton’s method is updated iteratively as formulated in Algorithm 5 (Roweis, 1996; Goodfellow et al., 2016).

**Algorithm 5 Newton’s Method**

1: **Input:** Initial parameter $x_1$; 
2: for $t = 1 : T$ do 
3: Compute gradient $g_t = \nabla L(x_t)$; 
4: Compute Hessian $H_t = \nabla^2 L(x_t)$; 
5: Compute inverse Hessian $H_t^{-1}$; 
6: Compute update step $\Delta x_t = -H_t^{-1} g_t$; 
7: Apply update $x_{t+1} = x_t + \Delta x_t$; 
8: end for 
9: **Return:** resulting parameters $x_t$, and the loss $L(x_t)$.

The computational complexity of Newton’s method comes from the calculation of the inverse of Hessian at every training iteration. The number of entries in the Hessian matrix is squared in the number of parameters ($x \in \mathbb{R}^d, H \in \mathbb{R}^{d \times d}$) making the complexity of the inverse be of order $O(d^3)$ (Trefethen and Bau III, 1997; Boyd and Vandenberghe, 2018; Lu, 2021). As a consequence, only networks with a small number of parameters, e.g., shallow neural networks or multi-layer perceptrons, can be trained by Newton’s method in practice.

**Reparametrization of the space around critical point** A critical point is a point $x$ where the gradient of $L(x)$ vanishes. A useful reparametrization of the loss function $L$ around critical points is from Taylor’s expansion. Since the gradient vanishes, Eq (5.1) can be written as

$$L(x + \Delta x) \approx L(x) + \frac{1}{2} \Delta x^\top H \Delta x.$$  

(5.2)
Since Hessian $H$ is symmetric, it admits spectral decomposition (Theorem 13.1 in Lu (2022c)):

$$H = QQ^\top \in \mathbb{R}^{d \times d},$$

where the columns of $Q = [q_1, q_2, \ldots, q_d]$ are eigenvectors of $H$ and are mutually orthonormal and the entries of $\Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_d)$ are the corresponding eigenvalues of $A$, which are real. We define the following vector $\Delta v$:

$$\Delta v = \begin{bmatrix} q_1^\top \\ \vdots \\ q_d^\top \end{bmatrix}, \quad \Delta x = Q^\top \Delta x.$$

Then the reparametrization follows

$$L(x + \Delta x) \approx L(x) + \frac{1}{2} \Delta x^\top H \Delta x$$

$$= L(x) + \frac{1}{2} \Delta v^\top \Lambda \Delta v = L(x) + \frac{1}{2} \sum_{i=1}^{d} \lambda_i (\Delta v_i)^2,$$

where $\Delta v_i$ is the $i$-th element of $\Delta v$. A conclusion on the type of the critical point follows immediately from the reparametrization:

- If all eigenvalues are non-zero and positive, then the critical point is a local minimum;
- If all eigenvalues are non-zero and negative, then the critical point is a local maximum;
- If the eigenvalues are non-zero, and both positive and negative eigenvalues exist, then the critical point is a saddle point.

In vanilla GD, if an eigenvalue $\lambda_i$ is positive (negative), then the step moves towards (away) from $x$ along $\Delta v$ making the GD towards optimal $x_\star$. The step along any direction $q_i$ is given by $-\lambda_i \Delta v_i$. While in Newton’s method, the step is rescaled by the inverse Hessian, making the step along direction $q_i$ scaled into $-\Delta v_i$. This may cause problem when the eigenvalue is negative resulting in the opposite direction as that in vanilla GD (Dauphin et al., 2014).

The reparametrization shows that rescaling the gradient along the direction of each eigenvector can result in wrong direction when the eigenvalue $\lambda_i$ is negative. This suggests the rescale by its magnitude, i.e., scale by $1/|\lambda_i|$ rather than $1/\lambda_i$ preserving sign of the gradient and solving the slowness of GD at the same time. From Eq (5.3), when both positive and negative eigenvalues exist, both vanilla GD and Newton’s method have chance to be stuck in saddle points, achieving poor performance. However, scaling by $1/|\lambda_i|$ can partly solve this problem, since the movement around the saddle point can either increase the loss or decrease the loss from this rescaling rather than stay where it is (Nocedal and Wright, 1999; Dauphin et al., 2014).

### 5.2 Damped Newton’s Method

The Newton’s method solves the slowness problem by rescaling the gradients in each direction with the inverse of the corresponding eigenvalue, yielding the step $\Delta x_t = -H_t^{-1}g_t$ at iteration $t$. However, this approach can result in moving in the wrong direction when the
eigenvalue is negative. Newton’s step moves along the eigenvector in a direction opposite to the gradient descent step, thus increasing the error.

This problem can be solved by damping the Hessian, in which case we remove negative curvature by adding a constant $\alpha$ to its diagonal, yielding the step $\Delta x_t = -(\mathbf{H} + \alpha \mathbf{I})^{-1} \mathbf{g}_t$. We can view $\alpha$ as the tradeoff between Newton’s method and vanilla GD. When $\alpha$ is small, it is closer to Newton’s method; when $\alpha$ is large, it is closer to vanilla GD. In this case, we get the step $\frac{\lambda_i}{\lambda_i + \alpha} \Delta \mathbf{g}_t$. Therefore, obviously, the drawback of damping Newton’s method is that it potentially has a small step size in many eigen-directions incurred by the large damping factor $\alpha$.

5.3 Levenberg (-Marquardt) Gradient Descent

The quadratic rule is not universally better since it assumes a linear approximation of $L(\mathbf{x})$ which is only valid when it’s near a minimum. The Levenberg gradient descent goes further by blending the idea of damped Newton’s method and vanilla GD in which case we can use a steepest descent type method until we approach a minimum so that we switch to the quadratic rule. The distance from a minimum is described by evaluating the loss (Levenberg, 1944). If the loss is increasing, the quadratic approximation is not working well and we are not likely near a minimum, yielding a larger $\alpha$ in damped Newton’s method; while if the loss is decreasing, the quadratic approximation is working well and we are approaching a minimum, yielding a smaller $\alpha$ in damped Newton’s method.

Marquardt improved this method by incorporating the local curvature information, in which case one replaces the identity matrix in Levenberg’s method by the diagonal of the Hessian, resulting in the Levenberg-Marquardt gradient descent (Marquardt, 1963):

$$\Delta x_t = -\left(\mathbf{H} + \alpha \cdot \text{diag}(\mathbf{H})\right)^{-1} \mathbf{g}_t.$$

The Levenberg-Marquardt gradient descent method is nothing more than a heuristic method since it is not optimal for any well defined criterion of speed or error measurements and it is merely a well thought out optimization procedure. However, it is an optimization method that works extremely well in practice especially for medium sized nonlinear models.

5.4 Conjugate Gradient

We have shown that the vanilla GD (with the negative gradient as the descent direction) can move back and forth in a zigzag pattern when applied in a quadratic bowl (a ravine-shaped loss curve, see example in Figure 4(c), p. 11). The situation is severer if the learning rate is guaranteed by line search (Section 2, p. 13), since the gradient is orthogonal to the previous update step (Lemma 2.1, p. 2.1 and example in Figure 8(g), p. 18). The choice of orthogonal directions of descent do not preserve the minimum along the previous search directions and the line search will undo the progress we have already made in the direction of the previous line search. This results in the zigzag pattern in the movement.

Instead of favoring a descent direction that is orthogonal to previous search direction (i.e., $\mathbf{d}_{t+1}^\top \mathbf{d}_t = 0$), the conjugate descent chooses a search direction that is Hessian-orthogonal (i.e., $\mathbf{d}_{t+1}^\top \mathbf{Hd}_t = 0$, or conjugate with respect to $\mathbf{H}$) so that the movement is compensated by the curvature information of the loss function. In Figure 26, we show
examples of Hessian-orthogonal pairs when the eigenvalues of the Hessian matrix $H$ are different or identical. When the eigenvalues of the Hessian matrix are the same, the Hessian-orthogonality reduces to trivial orthogonal cases (this can be shown by the spectral decomposition of the Hessian matrix where the orthogonal transformation does not alter the orthogonality (Lu, 2021)).

![Surface plots for Hessian matrix](image)

(a) Surface plot: Hessian with different eigenvalues. (b) Surface plot: Hessian with same eigenvalues.

**Figure 26:** Illustration of $H$-orthogonal for different Hessian matrices in 2-dimensional case: $H = \begin{bmatrix} 40 & 5 \\ 7 & 10 \end{bmatrix}$ for Fig 26(a) and $H = \begin{bmatrix} 40 & 0 \\ 0 & 40 \end{bmatrix}$ for Fig 26(b). The $H$-orthogonal pairs are orthogonal when $H$ has identical eigenvalues.

We now give the formal definition of conjugacy as follows:

**Definition 5.1: Conjugacy**

Given a positive definite matrix $A \in \mathbb{R}^{d \times d}$, the vectors $u, v \in \mathbb{R}^{d}$ are *conjugate* with respect to $A$ if $u, v \neq 0$ and $u^\top A v = 0$.

In the method of *conjugate gradient* (CG), we find a descent direction that is conjugate to the previous search direction with respect to the Hessian matrix $H$ such that the new update step will not undo the progress made in the previous directions:

$$d_t = -\nabla L(x_t) + \beta_t d_{t-1},$$
where $\beta_t$ is a coefficient controlling how much the previous direction would add back to the current search direction. Three popular methods to compute the coefficient are

- **Fletcher-Reeves:**
  \[ \beta^F_t = \frac{\nabla L(x_t)^T \nabla L(x_t)}{\nabla L(x_{t-1})^T \nabla L(x_{t-1})}, \]

- **Polak-Ribi`ere:**
  \[ \beta^P_t = \frac{\left( \nabla L(x_t) - \nabla L(x_{t-1}) \right)^T \nabla L(x_t)}{\nabla L(x_{t-1})^T \nabla L(x_{t-1})}, \]

- **Hestenes–Stiefel:**
  \[ \beta^H_t = \frac{\left( \nabla L(x_t) - \nabla L(x_{t-1}) \right)^T \nabla L(x_t)}{\nabla L(x_{t-1})^T \nabla L(x_{t-1}) \cdot d_{t-1}}. \]

When the loss function is quadratic, the conjugate gradient ensures that the gradient along the previous direction does not increase in magnitude (Shewchuk et al., 1994; Nocedal and Wright, 1999; Iserles, 2009; Goodfellow et al., 2016). The full procedure of the conjugate gradient method is formulated in Algorithm 6 where we notice that the first step of CG is identical to a step of steepest descent when the learning rate is calculated by exact line search since $\beta_1 = 0$.

**Algorithm 6** Fletcher-Reeves Conjugate Gradient

1. **Input:** Initial parameter $x_1$;
2. **Input:** Initialize $d_0 = 0$ and $g_0 = d_0 + \epsilon$;
3. for $t = 1 : T$ do
   4. Compute gradient $g_t = \nabla L(x_t)$;
   5. Compute coefficient $\beta_t = \frac{g_t^T g_t}{g_{t-1}^T g_{t-1}}$ (Fletcher-Reeves);
   6. Compute descent direction $d_t = -g_t + \beta_t d_{t-1}$;
   7. Fixed learning rate $\eta_t = \eta$ or find it by line search: $\eta_t = \arg \min L(x_t + \eta d_t)$;
   8. Compute update step $\Delta x_t = \eta_t d_t$;
   9. Apply update $x_{t+1} = x_t + \Delta x_t$;
4. end for
5. **Return:** resulting parameters $x_t$, and the loss $L(x_t)$.

While our derivation of the conjugate gradient in the next sections is based on the assumption of symmetric positive definite $A$, it can be easily adapted to asymmetric ones. A comparison among vanilla GD, steepest descent, and conjugate gradient is shown in Figure 27 where we observe that the updates in CG have less zigzag pattern than vanilla GD and steepest descent.

### 5.4.1 Quadratic Form in Conjugate Direction (CD) Method

Following the discussion of quadratic form in GD (Section 1.5, p. 9), quadratic form in steepest descent (Section 2.4, p. 17), and quadratic form in momentum (Section 4.1.1, p. 34), we now discuss the quadratic form in CG.
Gradient Descent, Stochastic Optimization, and Other Tales

(a) Vanilla GD, fixed $\eta = 0.08$. 
(b) Steepest descent. 
(c) Conjugate descent, fixed $\eta = 0.06$. 
(d) Conjugate descent, exact line search.

Figure 27: Illustration for the vanilla GD, steepest descent, and CG of quadratic form with $A = \begin{bmatrix} 20 & 7 \\ 5 & 5 \end{bmatrix}$, $b = 0$, and $c = 0$. Starting point to descent is $x_1 = [-3, 3.5]^T$. 

To introduce the conjugate gradient (CG) method, we first discuss the conjugate direction (CD) method where the distinction between them will be clear in the sequel. By the definition of conjugacy (Definition 5.1), it is easy to show that any set of vectors $\{d_1, d_2, \ldots, d_d\} \in \mathbb{R}^d$ satisfying this property with respect to the symmetric positive definite Hessian matrix $H = \frac{1}{2}(A^T + A)$:

$$d_i^T H d_j, \quad \forall i \neq j, \quad (5.4)$$

is also linearly independent. That is, the set span the whole $\mathbb{R}^d$ space:

$$\text{span}\{d_1, d_2, \ldots, d_d\} = \mathbb{R}^d.$$ 

Given the initial parameter $x_1$ and a set of conjugate directions $\{d_1, d_2, \ldots, d_d\}$ (defined in Eq (5.4)), the update at time $t$ is given by

$$x_{t+1} = x_t + \eta_t d_t, \quad (5.5)$$

where $\eta_t$ is the learning rate at time $t$ and is obtained by minimizing the one-dimensional quadratic function $J(\eta) = L(x_t + \eta d_t)$ as that in Eq (2.5) (p. 17):

$$\eta_t = -\frac{d_t^T g_t}{d_t^T A d_t} \quad \text{with} \quad g_t = \nabla L(x_t). \quad (5.6)$$

Then, we have the following theorem that the updates following from the conjugate directions will converge in $d$ steps (the dimension of the parameter) when $A$ is symmetric positive definite.

**Theorem 5.2: (Converge in $d$ Steps)**

For any initial parameter $x_1$, the sequence $\{x_t\}$ generated by the conjugate direction algorithm Eq (5.5) converges to the solution $x_*$ in at most $d$ steps when $A$ is symmetric positive definite.

**Proof** [of Theorem 5.2] Since conjugate directions $\{d_1, d_2, \ldots, d_d\}$ span the whole $\mathbb{R}^d$ space, the initial error vector $e_1 = x_1 - x_*$ (Definition 2.2, p. 19) then can be expressed as a linear combination of the conjugate directions:

$$e_1 = x_1 - x_* = \gamma_1 d_1 + \gamma_2 d_2 + \ldots + \gamma_d d_d. \quad (5.7)$$
The \( \gamma_i \)'s can be obtained by the following equation:

\[
d_i^\top H e_1 = \sum_{i=1}^{d} \gamma_i d_i^\top H d_i = \gamma_t d_t^\top H d_t \quad \text{(by conjugacy, Eq (5.4))}
\]

leads to

\[
\gamma_t \rightarrow \frac{d_t^\top H e_1}{d_t^\top A d_t} = \frac{d_t^\top H (e_1 + \sum_{i=1}^{t-1} \eta_i d_i)}{d_t^\top H d_t} \quad \text{(by conjugacy, Eq (5.4))}
\]

\[
= \frac{d_t^\top H e_t}{d_t^\top H d_t}.
\]

When \( A \) is further symmetric and nonsingular, we have \( e_t = x_t - x^* = x_t - A^{-1} b \) and \( H = A \). It can be shown \( \gamma_t \) is equal to \( \frac{d_t^\top g_t}{d_t^\top A d_t} \). This is exactly the same form (in magnitude) as the learning rate at time \( t \) in steepest descent: \( \gamma_t = -\eta_t \) (see Eq (2.5), p. 17). Substitute into Eq (5.7), it follows that

\[
x^* = x_1 + \eta_1 d_1 + \eta_2 d_2 + \ldots + \eta_d d_d.
\]

Moreover, we have updates by Eq (5.5) that

\[
x_{d+1} = x_d + \eta_d d_d
\]

\[
= x_{d-1} + \eta_{d-1} d_{d-1} + \eta_d d_d
\]

\[
= \ldots
\]

\[
= x_1 + \eta_1 d_1 + \eta_2 d_2 + \ldots + \eta_d d_d = x^*.
\]

which completes the proof.

The above theorem states the conjugate direction by Eq (5.5) converges in \( d \) steps, i.e., \( x_{d+1} \) minimizes quadratic function \( L(x) = \frac{1}{2} x^\top A x - b^\top x + c \) over the whole space \( \mathbb{R}^d \). Furthermore, we can prove that at each iteration \( t \leq d \), the update \( x_{t+1} \) minimizes the quadratic function over a subspace of \( \mathbb{R}^d \).

**Theorem 5.3: (Expanding Subspace Minimization)**

For any initial parameter \( x_1 \), the sequence \( \{x_t\} \) generated by the conjugate direction algorithm Eq (5.5). Then it follows that

\[
g_{t+1}^\top d_i = 0, \quad \forall i = 1, 2, \ldots, t, \text{ and } t \in \{1, 2, \ldots, d\}, \tag{5.8}
\]

where \( g_t = Ax_t - b \) (i.e., the gradient when \( A \) is symmetric), and \( x_{t+1} \) is the minimizer of \( L(x) = \frac{1}{2} x^\top A x - b^\top x + c \) with symmetric positive definite \( A \) over the subspace

\[
\mathbb{D}_t = \{x \mid x = x_1 + \text{span}\{d_1, d_2, \ldots, d_t\}\} . \tag{5.9}
\]

**Proof** [of Theorem 5.3] We first prove \( g_{t+1}^\top d_i \) by induction. When \( t = 1 \), since \( \eta_1 \) is obtained to minimize \( J(\eta) = L(x_1 + \eta_1 d_1) \), by Lemma 2.1 (p. 13), we have \( g_2 = \nabla L(x_2) \) that is orthogonal to \( d_1 \). Suppose now for general \( t - 1 \), the induction hypothesis is satisfied with \( g_t^\top d_i = 0 \) for \( i = 0, 1, \ldots, t - 1 \). The \( g_t \) has the following update

\[
g_{t+1} = Ax_{t+1} - b = A(x_t + \eta_t d_t) - b
\]

\[
= g_t + \eta_t A d_t . \tag{5.10}
\]
By conjugacy and the induction hypothesis, we have $\mathbf{g}_{t+1}^\top \mathbf{d}_i = 0$ for $i = \{0, 1, \ldots, t-1\}$. If we further prove $\mathbf{g}_{t+1}^\top \mathbf{d}_t$, we complete the proof. The again follows from Lemma 2.1 (p. 13), the current gradient is orthogonal to the previous search direction $\mathbf{d}_t$.

For the second part, we define $f(\eta) = L(x_1 + \eta_1 \mathbf{d}_1 + \eta_2 \mathbf{d}_2 + \ldots + \eta_t \mathbf{d}_t)$ which is a strictly convex quadratic function over $\eta = [\eta_1, \eta_2, \ldots, \eta_t]^\top$ such that

$$\frac{\partial f(\eta)}{\partial \eta_i} = 0, \quad \forall i = 1, 2, \ldots, t.$$ 

This yields

$$\nabla L(x_1 + \eta_1 \mathbf{d}_1 + \eta_2 \mathbf{d}_2 + \ldots + \eta_t \mathbf{d}_t)^\top \mathbf{d}_i = 0, \quad \forall i = 1, 2, \ldots, t.$$ 

That is, $x_{t+1} \in \{x | x = x_1 + \text{span}\{\mathbf{d}_1, \mathbf{d}_2, \ldots, \mathbf{d}_t\}\}$ is the minimizer of $L(x)$.

### 5.4.2 Quadratic Form in Conjugate Gradient (CG) Method

We have stated that the conjugate gradient (CG) method is different from the conjugate descent (CD) method. The distinction is in that the CG method computes a new vector $\mathbf{d}_{t+1}$ using only the previous vector $\mathbf{d}_t$ rather than all of the sequence $\{\mathbf{d}_1, \mathbf{d}_2, \ldots, \mathbf{d}_t\}$. And $\mathbf{d}_{t+1}$ will automatically be conjugate to the sequence in this sense. In the CG method, each search direction $\mathbf{d}_t$ is chosen to be a linear combination of negative gradient $-\mathbf{g}_t$ (search direction in steepest descent) and the previous direction $\mathbf{d}_{t-1}$:

$$\mathbf{d}_t = -\mathbf{g}_t + \beta_t \mathbf{d}_{t-1}. \quad (5.11)$$

This yields

$$\beta_t = \frac{\mathbf{g}_t^\top A \mathbf{d}_{t-1}}{\mathbf{d}_{t-1}^\top A \mathbf{d}_{t-1}}.$$ 

This choice of $\beta_t$ and $\mathbf{d}_t$ actually results in the conjugate sequence $\{\mathbf{d}_1, \mathbf{d}_2, \ldots, \mathbf{d}_t\}$. To see this, we first give the definition of the *Krylov subspace of degree $t$ for vector $\mathbf{v}$ with respect to matrix $A$*:

$$\mathcal{K}(\mathbf{v}; t) = \text{span}\{\mathbf{v}, A\mathbf{v}, \ldots, A^{t-1}\mathbf{v}\}.$$ 

**Theorem 5.4: (Converge in $d$ Steps)**

For any initial parameter $x_1$, the sequence $\{x_t\}$ generated by the conjugate descent algorithm with search direction generated by Eq (5.11) converges to the solution $x_*$ in at most $d$ steps when $A$ is symmetric positive definite. The result follows from the following claims:

$$\mathbf{g}_i^\top \mathbf{g}_i = 0, \quad \text{for } i = \{1, 2, \ldots, t-1\}; \quad (5.12)$$

$$\text{span}\{\mathbf{g}_1, \mathbf{g}_2, \ldots, \mathbf{g}_t\} = \text{span}\{\mathbf{g}_1, A\mathbf{g}_1, \ldots, A^{t-1}\mathbf{g}_1\} = \mathcal{K}(\mathbf{g}_1; t); \quad (5.13)$$

$$\text{span}\{\mathbf{d}_1, \mathbf{d}_2, \ldots, \mathbf{d}_t\} = \text{span}\{\mathbf{g}_1, A\mathbf{g}_1, \ldots, A^{t-1}\mathbf{g}_1\} = \mathcal{K}(\mathbf{g}_1; t); \quad (5.14)$$

$$\mathbf{d}_i^\top A \mathbf{d}_i = 0, \quad \text{for } i = \{1, 2, \ldots, t-1\}, \quad (5.15)$$
where Eq (5.15) says the sequence \(\{d_t\}\) is conjugate.

**Proof** [of Theorem 5.4] The proof follows from induction. Eq (5.13) and Eq (5.14) is trivial when \(t = 1\). Suppose for \(t\), Eq (5.13), Eq (5.14), and Eq (5.15) hold as well; if we can show the two equations still hold for \(t + 1\), then we complete the proof. By the induction hypothesis, we have

\[
g_t \in \text{span}\{g_1, Ag_1, \ldots, A^{t-1}g_1\}, \quad d_t \in \text{span}\{g_1, Ag_1, \ldots, A^{t-1}g_1\}.
\]

Left multiply by \(A\), it follows that

\[
Ad_t \in \text{span}\{Ag_1, A^2g_1, \ldots, A^tg_1\}. \tag{5.16}
\]

Since

\[
g_{t+1} = Ax_{t+1} - b = A(x_t + \Delta x_t) - b = A(x_t + \eta_t d_t) - b = g_t + \eta_t Ad_t. \tag{5.17}
\]

Then, we have

\[
g_{t+1} \in \text{span}\{g_1, Ag_1, A^2g_1, \ldots, A^tg_1\}. \tag{5.18}
\]

Combine Eq (5.18) and Eq (5.13), we have

\[
\text{span}\{g_1, g_2, \ldots, g_t, g_{t+1}\} \subseteq \text{span}\{g_1, Ag_1, \ldots, A^{t-1}g_1, A^tg_1\}.
\]

To see the reverse inclusion, by Eq (5.14), it follows that

\[
A^tg_1 = A(A^{t-1}g_1) \in \text{span}\{Ad_1, Ad_2, \ldots, Ad_t\}.
\]

Again, by Eq (5.17), we have \(Ad_t = (g_{t+1} - g_t)/\eta_t\). Therefore

\[
A^tg_1 \in \text{span}\{g_1, g_2, \ldots, g_t, g_{t+1}\}.
\]

Combine with Eq (5.13), we have

\[
\text{span}\{g_1, Ag_1, \ldots, A^{t-1}g_1, A^tg_1\} \subseteq \text{span}\{g_1, g_2, \ldots, g_t, g_{t+1}\}.
\]

Therefore, Eq (5.13) holds for \(t + 1\). Eq (5.14) follows similarly and also holds for \(t + 1\).

To see Eq (5.15) holds for \(t + 1\), we have

\[
d_{t+1}^\top Ad_t = (-g_{t+1} + \beta_{t+1}d_t)^\top Ad_t.
\]

By Theorem 5.3, we have

\[
g_{t+1}^\top d_i = 0 \quad \text{for} \quad i \in \{1, 2, \ldots, t\}. \tag{5.19}
\]

Further by Eq (5.16) and Eq (5.14), we have

\[
Ad_t \in \text{span}\{Ag_1, A^2g_1, \ldots, A^tg_1\} \subseteq \text{span}\{d_1, d_2, \ldots, d_t, d_{t+1}\}. \tag{5.20}
\]

Combine Eq (5.19) and Eq (5.20), it then follows that

\[
d_{t+1}^\top Ad_i = 0, \quad \text{for} \quad i \in \{1, 2, \ldots, t-1\}.
\]
We need to further prove $d_{t+1}^\top A d_t = 0$ (which is trivial since we invent the algorithm to be like this).

To see Eq (5.12) holds, we have $d_i = -g_i + \beta_i d_{i-1}$. Therefore, $g_i \in \text{span}\{d_i, d_{i-1}\}$.

Again by Eq (5.19), we prove $g_i^\top g_i = 0$ for $i \in \{1, 2, \ldots, t\}$. By Theorem 5.2, the CG method thus converges in at most $d$ steps (when $A$ is symmetric PD). The full procedure is then formulated in Algorithm 7.

**Algorithm 7** Vanilla Conjugate Gradient Method for Quadratic Function

1: **Require:** Symmetric positive definite $A \in \mathbb{R}^{d \times d}$;
2: **Input:** Initial parameter $x_1$;
3: **Input:** Initialize $d_0 = 0$ and $g_0 = d_0 + \epsilon$;
4: for $t = 1 : d$ do
5: Compute gradient $g_t = \nabla L(x_t)$;
6: Compute coefficient $\beta_t = \frac{d_t^\top Ad_{t-1}}{d_{t-1}^\top Ad_{t-1}}$;
7: Compute descent direction $d_t = -g_t + \beta_t d_{t-1}$;
8: Learning rate $\eta_t = -\frac{d_t^\top g_t}{d_t^\top Ad_t}$;
9: Compute update step $\Delta x_t = \eta_t d_t$;
10: Apply update $x_{t+1} = x_t + \Delta x_t$;
11: end for
12: **Return:** resulting parameters $x_t$, and the loss $L(x_t)$.

To further reduce the complexity of the CG algorithm, we first introduce the notion of floating operation (flop) counts. We follow the classical route and count the number of floating-point operations (flops) that the algorithm requires. Each addition, subtraction, multiplication, division, and square root counts as one flop. Note that we have the convention that an assignment operation does not count as one flop. The calculation of the complexity extensively relies on the complexity of the multiplication of two matrices so that we formulate the finding in the following lemma.

**Lemma 5.5: (Vector Inner Product Complexity)**

Given two vectors $v, w \in \mathbb{R}^n$. The inner product of the two vectors $v^\top w$ is given by $v^\top w = v_1 w_1 + v_2 w_2 + \ldots + v_n w_n$ which involves $n$ scalar multiplications and $n - 1$ scalar additions. Therefore the complexity for the inner product is $2n - 1$ flops.

The matrix multiplication thus relies on the complexity of the inner product.

**Lemma 5.6: (Matrix Multiplication Complexity)**

For matrix $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times k}$, the complexity of the multiplication $C = AB$ is $mk(2n - 1)$ flops.
By Theorem 5.4, we can replace the formula for calculating learning rate into:

$$\eta_t = -\frac{d_t^\top g_t}{d_t^\top Ad_t} \quad \text{leads to} \quad \eta_t = -\frac{g_t^\top g_t}{d_t^\top Ad_t}. $$

By Eq (5.10), it follows that $\eta_t Ad_t = g_{t+1} - g_t$. Combine with Eq (5.8) and Eq (5.12), $\beta_t$ can also be written as

$$\beta_t = -\frac{g_t^\top g_t}{d_{t-1}^\top g_{t-1}} = \frac{g_t^\top g_t}{g_{t-1}^\top g_{t-1}}. $$

This reduces the complexity from $O(4d^2)$ to $O(4d)$. This practical CG method is then formulated in Algorithm 8.

**Algorithm 8** Practical Conjugate Gradient Method for Quadratic Function

1: **Require:** Symmetric positive definite $A \in \mathbb{R}^{d \times d}$;  
2: **Input:** Initial parameter $x_1$;  
3: **Input:** Initialize $d_0 = 0$ and $g_0 = d_0 + \epsilon$;  
4: for $t = 1 : d$ do  
5: \hspace{1em} Compute gradient $g_t = \nabla L(x_t)$;  
6: \hspace{1em} Compute coefficient $\beta_t = -\frac{g_t^\top g_t}{d_{t-1}^\top g_{t-1}}$; $\triangleright$ set $\beta_1 = 0$ by convention  
7: \hspace{1em} Compute descent direction $d_t = -g_t + \beta_t d_{t-1}$;  
8: \hspace{1em} Learning rate $\eta_t = -\frac{g_t^\top g_t}{d_t^\top Ad_t}$;  
9: \hspace{1em} Compute update step $\Delta x_t = \eta_t d_t$;  
10: \hspace{1em} Apply update $x_{t+1} = x_t + \Delta x_t$;  
11: end for  
12: **Return:** resulting parameters $x_t$, and the loss $L(x_t)$.

5.4.3 Convergence Analysis for Symmetric Positive Definite Quadratic

We further discuss the convergence results of CG method. By Eq (5.14), there exists a set of $\{\sigma_1, \sigma_2, \ldots, \sigma_t\}$ coefficients such that

$$x_{t+1} = x_t + \eta_1 d_1 + \eta_2 d_2 + \ldots + \eta_t d_t = x_t + \sigma_1 g_1 + \sigma_2 Ag_1 + \ldots + \sigma_t A^{t-1} g_1$$  \hspace{1em} (5.21)

$$= x_t + P_{t-1}(A) g_1,$$

where $P_{t-1}(A) = \sigma_1 I + \sigma_2 A + \ldots + \sigma_t A^{t-1}$ is a polynomial of degree $t - 1$ with coefficients $\{\sigma_1, \sigma_2, \ldots, \sigma_t\}$ that is a special case of the polynomial of degree $t - 1$ with random coefficients $\{\omega_1, \omega_2, \ldots, \omega_t\}$, namely $P_{t-1}(A) = \omega_1 I + \omega_2 A + \ldots + \omega_t A^{t-1}$. (Note here, $P_{t-1}$ can take either a scalar or a matrix as its argument). Suppose symmetric positive definite $A$ admits spectral decomposition (Theorem 13.1 in Lu (2022c)):

$$A = Q\Lambda Q^\top \in \mathbb{R}^{d \times d} \quad \text{leads to} \quad A^{-1} = Q\Lambda^{-1}Q^\top,$$
where the columns of $Q = [q_1, q_2, \ldots, q_d]$ are eigenvectors of $A$ and are mutually orthonormal, and the entries of $\Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_d)$ with $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d > 0$ are the corresponding eigenvalues of $A$, which are real and ordered by magnitude (the eigenvalues are positive since $A$ is assumed to be positive-definite). It then follows that any eigenvector of $A$ is also an eigenvector of $P_{t-1}(A)$:

$$P_{t-1}(A)q_i = P_{t-1}(\lambda_i)q_i, \quad \forall i \in \{1, 2, \ldots, d\}.$$ 

Moreover, since the eigenvectors span the whole space $\mathbb{R}^d$, there exists a set of $\{\nu_1, \nu_2, \ldots, \nu_d\}$ coefficients such that the initial error vector $e_1$ can be expressed as

$$e_1 = x_1 - x_* = \sum_{i=1}^{d} \nu_i q_i,$$  \hspace{1cm} (5.22)

where $x_1$ is the initial parameter. Combining Eq (5.21) and Eq (5.22), this yields the update of the error vector:

$$e_{t+1} = x_{t+1} - x_* = x_1 + P_{t-1}^*(A)g_1 - x_* = x_1 + P_{t-1}^*(A)(Ax_1 - A^{-1}b) - x_* = x_1 + P_{t-1}^*(A)x_1 - x_* = (I + P_{t-1}^*(A))A(x_1 - x_*) = \left(I + P_{t-1}^*(A)A\right)(x_1 - x_*) = \left(I + P_{t-1}^*(A)A\right)\sum_{i=1}^{d} \nu_i q_i = \sum_{i=1}^{d} \left(1 + \lambda_i P_{t-1}^*(A)\right) \nu_i q_i$$ \hspace{1cm} (5.23)

To further discuss the convergence results, we still need to use the notion of energy norm for error vector $||e||_A = (e^\top A e)^{1/2}$ as defined in Section 2.4.3 (p. 21) where it can be shown that minimizing $||e||_A$ is equivalent to minimizing $L(x_t)$ by Eq (2.10) (p. 21).

**Remark 5.7: Polynomial Minimization**

Since we proved in Theorem 5.3 that $x_{t+1}$ minimizes $L(x)$ over the subspace $\mathbb{D}_t$ defined in Eq (5.9), it also minimizes the energy norm $||e||_A$ over the subspace $\mathbb{D}_t$ at iteration $t$. It then follows that $P_{t-1}^*(A)$ minimizes over the space of all possible polynomials of degree $t - 1$:

$$P_{t-1}^*(A) = \arg\min_{P_{t-1}(A)} ||x_1 + P_{t-1}(A)g_1 - x_*||_A.$$
Then the update of the squared energy norm can be obtained by

\[ \|e_{t+1}\|^2_A = e_{t+1}^\top A e_{t+1} = e_{t+1}^\top \left( \sum_{i=1}^{d} \lambda_i q_i q_i^\top \right) e_{t+1} \]

\[ = \sum_{i=1}^{d} \lambda_i (e_{t+1}^\top q_i)^2 \]

\[ = \sum_{i=1}^{d} \lambda_i \left( q_i^\top \left( \sum_{j=1}^{d} \left( 1 + \lambda_j P_{t-1}(A) \right) v_j q_j \right) \right)^2 \quad \text{(by Eq (5.23))} \]

\[ = \sum_{i=1}^{d} \left( 1 + \lambda_i P_{t-1}(\lambda_i) \right)^2 \lambda_i \nu_i^2 \]

\[ = \min_{P_{t-1}} \sum_{i=1}^{d} \left( 1 + \lambda_i P_{t-1}(\lambda_i) \right)^2 \lambda_i \nu_i^2 \]

\[ \leq m_t \sum_{i=1}^{d} \lambda_i \nu_i^2 \]

\[ \leq m_t \cdot \|e_1\|^2_A. \]

Therefore, the rate of convergence for the CG method is controlled by

\[ m_t = \min_{P_{t-1}} \max_{1 \leq j \leq d} \left( 1 + \lambda_j P_{t-1}(\lambda_j) \right)^2. \quad (5.24) \]

**Special Case: A Has Only r Distinct Eigenvalues**

We then consider some special cases. Firstly, we want to show the CG method terminates in exactly r iterations if symmetric positive definite \( A \) has only r distinct eigenvalues. To see this, suppose \( A \) has distinct eigenvalues \( \mu_1 < \mu_2 < \ldots < \mu_r \). And we define a polynomial \( Q_r(\lambda) \) by

\[ Q_r(\lambda) = \frac{(-1)^r}{\mu_1 \mu_2 \ldots \mu_r} (\lambda - \mu_1)(\lambda - \mu_2) \ldots (\lambda - \mu_r), \]

where \( Q_r(\lambda_i) = 0 \) for \( i = \{1, 2, \ldots, d\} \) and \( Q_r(0) = 1 \). Therefore, it follows that the polynomial

\[ R_{r-1}(\lambda) = \frac{Q_r(\lambda) - 1}{\lambda} \]

is a polynomial of degree \( r - 1 \) with root at \( \lambda = 0 \). Set \( t - 1 = r - 1 \) in Eq (5.24), we have

\[ 0 \leq m_r = \min_{P_{r-1}} \max_{1 \leq j \leq d} \left( 1 + \lambda_j P_{r-1}(\lambda_j) \right)^2 \]

\[ = \max_{1 \leq j \leq d} \left( 1 + \lambda_j R_{r-1}(\lambda_j) \right)^2 = \max_{1 \leq j \leq d} Q_r^2(\lambda_j) = 0. \]

Therefore \( m_r = 0 \), and \( \|e_{r+1}\|_A = 0 \) such that \( x_{r+1} = x_\star \) and the algorithm terminates at iteration r. A specific example is shown in Figure 28 where Figure 28(a) terminates in 2 steps since it has two distinct eigenvalues and Figure 28(b) terminates in just 1 step as it has 1 distinct eigenvalue.
Gradient Descent, Stochastic Optimization, and Other Tales

Figure 28: Illustration of special cases for CG with exact line search of quadratic forms.

Closed Form by Chebyshev Polynomials

It can be shown that Eq (5.24) is minimized by a Chebyshev polynomial such that

\[ 1 + \lambda_j P_{t-1}(\lambda_j) = \frac{T_t \left( \frac{\lambda_{\text{max}} + \lambda_{\text{min}} - 2\lambda}{\lambda_{\text{max}} - \lambda_{\text{min}}} \right)}{T_t \left( \frac{\lambda_{\text{max}} + \lambda_{\text{min}}}{\lambda_{\text{max}} - \lambda_{\text{min}}} \right)}, \]

where \( T_t(w) = \frac{1}{2} \left[ (w + \sqrt{w^2 + 1})^t + (w - \sqrt{w^2 - 1})^t \right] \) is the Chebyshev polynomial of degree \( t \).

**Proof** To see this, we can rewrite the \( m_t \) in Eq (5.24) by

\[ m_t = \min_{P_{t-1}} \max_{1 \leq j \leq d} \left( 1 + \lambda_j P_{t-1}(\lambda_j) \right)^2 = \min_{P_{t-1}} \max_{1 \leq j \leq d} \left( \tilde{P}_t(\lambda_j) \right)^2, \]

where \( \tilde{P}_t(\lambda) = 1 + \lambda P_{t-1}(\lambda) = 1 + w_1 \lambda + \ldots + w_t \lambda^t \) is a special polynomial of degree \( t \) with \( \tilde{P}_t(0) = 1 \). We note that the Chebyshev polynomial can be expressed on the region \( w \in [-1, 1] \) as

\[ T_t(w) = \cos(t \cos^{-1} w), \quad w \in [-1, 1] \quad \text{leads to} \quad |T_t(w)| \leq 1, \quad \text{if} \ w \in [-1, 1]. \]

We may then notice \( \tilde{P}_t(\lambda) \) oscillates in the range \( \pm T_t \left( \frac{\lambda_{\text{max}} + \lambda_{\text{min}} - 2\lambda}{\lambda_{\text{max}} - \lambda_{\text{min}}} \right)^{-1} \) on the domain \( [\lambda_{\text{min}}, \lambda_{\text{max}}] \).

Suppose there exists a polynomial \( S_t(\lambda) \) of degree \( t \) such that \( S_t(0) = 1 \) and \( S_t \) is better than \( \tilde{P}_t \) on the domain \( [\lambda_{\text{min}}, \lambda_{\text{max}}] \). It then follows that the \( S_t - \tilde{P}_t \) has a zero at \( \lambda = 0 \) and other \( t \) zeros on the range \( [\lambda_{\text{min}}, \lambda_{\text{max}}] \), making it has \( t + 1 \) zeros which leads to a contradiction. Therefore \( \tilde{P}_t \) is the best polynomial of degree \( t \). This completes the proof. \( \blacksquare \)
Therefore, it follows that

\[ ||e_{t+1}||_A \leq T_t \left( \frac{\lambda_{\max} + \lambda_{\min}}{\lambda_{\max} - \lambda_{\min}} \right)^{-1} \cdot ||e_1||_A \]

\[ = T_t \left( \frac{\kappa + 1}{\kappa - 1} \right)^{-1} \cdot ||e_1||_A \]

\[ = 2 \left[ \left( \sqrt{\kappa + 1} \right)^t + \left( \sqrt{\kappa - 1} \right)^t \right]^{-1} \cdot ||e_1||_A, \]

where \( \kappa = \frac{\lambda_{\max}}{\lambda_{\min}} \) is the condition number, and \( \left( \sqrt{\kappa - 1} \right)^t \to 0 \) as iteration \( t \) grows. A weaker inequality is then obtained by

\[ ||e_{t+1}||_A \leq 2 \left( \frac{\sqrt{\kappa}}{\sqrt{\kappa} + 1} \right)^t \cdot ||e_1||_A. \]

Figure 29 then compares the rate of convergence in steepest descent and CG per iteration. The convergence of CG is much faster than that of steepest descent.

**Figure 29:** Illustration of the rate of convergence for CG and steepest descent.

**(a)** Rate of convergence in steepest descent per iteration (same as Figure 11). The y-axis is \( \frac{\kappa - 1}{\kappa + 1} \).

**(b)** Rate of convergence in CG per iteration. The y-axis is \( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \).

---

**Preconditioning**

Since the smaller the condition number \( \kappa \), the faster the convergence (Figure 29(b)). We can accelerate the convergence of CG by transforming the linear system to improve the eigenvalue distribution of \( A \); the procedure is known as *preconditioning*. The variable \( x \) is transformed to \( \hat{x} \) via a nonsingular matrix \( P \) such that

\[ \hat{x} = Px; \]

\[ \hat{L}(\hat{x}) = \frac{1}{2} \hat{x}^\top (P^{-\top} A P^{-1}) \hat{x} - (P^{-\top} b)^\top \hat{x} + c. \]
When \( A \) is symmetric, the solution of \( \hat{L}(\hat{x}) \) is equivalent to the solution of the linear equation

\[
(P^{-\top}AP^{-1})\hat{x} = P^{-\top}b
\]

leads to \( P^{-\top}Ax = P^{-\top}b \)

leads to \( Ax = b \).

That is, we can solve \( Ax = b \) indirectly by solving \( P^{-\top}Ax = P^{-\top}b \). Therefore, the rate of convergence of the quadratic form \( \hat{L}(\hat{x}) \) depends on the condition number of \( P^{-\top}AP^{-1} \) that can be controlled by the nonsingular matrix \( P \). Intuitively, the preconditioning is a procedure to stretch the quadratic form to make it more spherical so that the eigenvalues are clustered in a smaller range. A specific example is given in Figure 28 that we want to transform the elliptical contour in Figure 28(a) into the spherical contour in Figure 28(b). Based on Algorithm 8, the preconditioned CG method is formulated in Algorithm 9.

### Algorithm 9 Transformed-Preconditioned CG for Quadratic Function

1. **Require:** Symmetric positive definite \( A \in \mathbb{R}^{d\times d} \);
2. **Input:** Initial parameter \( \hat{x}_1 \);
3. **Input:** Initialize \( d_0 = 0 \) and \( \hat{g}_0 = \hat{d}_0 + \epsilon \);
4. **for** \( t = 1 : d \) **do**
   5. Compute gradient \( \hat{g}_t = \nabla \hat{L}(\hat{x}_t) = (P^{-\top}AP^{-1})\hat{x} - P^{-\top}b \);
   6. Compute coefficient \( \hat{\beta}_t = \frac{\hat{g}_t^\top \hat{g}_t}{\hat{g}_{t-1}^\top \hat{g}_{t-1}} \);
   7. Compute descent direction \( \hat{d}_t = -\hat{g}_t + \hat{\beta}_t \hat{d}_{t-1} \);
   8. Learning rate \( \hat{\eta}_t = -\frac{\hat{g}_t^\top \hat{g}_t}{d_t^\top (P^{-\top}AP^{-1})d_t} \);
   9. Compute update step \( \Delta \hat{x}_t = \hat{\eta}_t \hat{d}_t \);
   10. Apply update \( \hat{x}_{t+1} = \hat{x}_t + \Delta \hat{x}_t \);
5. **end for**
6. **Return:** resulting parameters \( x_t = P^{-1}\hat{x}_t \), and the loss \( L(x_t) \).

However, the procedure in Algorithm 9 is not desirable since we need to transform \( x \) into \( \hat{x} = Px \) and untransformed back by \( x = P^{-1}\hat{x} \) as highlighted in blue texts of Algorithm 9. This may cause extra computation. Let \( M = P^\top P \), Algorithm 10 then formulates the untransformed-preconditioned CG that is more efficient than Algorithm 9.

**Second perspective of preconditioning** The matrices \( M^{-1}A \) and \( P^{-\top}AP^{-1} \) have the same eigenvalues. To see this, suppose the eigenpair of \( M^{-1}A \) is \( (M^{-1}A)v = \lambda v \), it follows that

\[
(P^{-\top}AP^{-1})(Pv) = P^{-\top}Av = PP^{-\top}P^{-\top}Av = PM^{-1}Av = \lambda(Pv).
\]

Therefore, the preconditioning can be understood from two perspectives. While the second perspective is to solve \( M^{-1}Ax = M^{-1}b \) where the condition number is decided by matrix \( M^{-1}A \). The simplest preconditioner \( M^{-1} \) is thus a diagonal matrix whose diagonal entries are identical to those of \( A \), known as diagonal preconditioning, in which case we scale the quadratic form along the coordinate axes. In contrast, the perfect preconditioner is \( M = A \)
Algorithm 10 Untransformed-Preconditioned CG for Quadratic Function

1: Require: Symmetric positive definite $A \in \mathbb{R}^{d \times d}$;
2: Input: Initial parameter $x_1$;
3: Input: Initialize $d_0 = 0$ and $g_0 = d_0 + \epsilon$;
4: for $t = 1 : d$ do
5:   Compute gradient $g_t = \nabla L(x_t)$; \hspace{1cm} $\triangleright$ Same as that of Algorithm 8
6:   Compute coefficient $\hat{\beta}_t = \frac{g_t^T M^{-1} g_t}{g_{t-1}^T M^{-1} g_{t-1}}$; \hspace{1cm} $\triangleright$ Same as that of Algorithm 9
7:   Compute descent direction $\tilde{d}_t = -M^{-1} g_t + \hat{\beta}_t \tilde{d}_{t-1}$; \hspace{1cm} $\triangleright$ $-P^{-1} \tilde{d}_t$ in Algorithm 9
8:   Learning rate $\hat{\eta}_t = -\frac{(g_t^T M^{-1} g_t)}{(\tilde{d}_t)^T A \tilde{d}_t)}$; \hspace{1cm} $\triangleright$ Same as that of Algorithm 9
9:   Compute update step $\Delta x_t = \hat{\eta}_t \tilde{d}_t$; \hspace{1cm} $\triangleright$ $-P^{-1} \Delta \tilde{x}_t$ in Algorithm 9
10: Apply update $x_{t+1} = x_t + \Delta x_t$;
11: end for
12: Return: resulting parameters $x_t$, and the loss $L(x_t)$.

Figure 30: Illustration of preconditioning for $A = \begin{bmatrix} 20 & 5 \\ 5 & 5 \end{bmatrix}$. $P$ is obtained by the Cholesky decomposition such that $M = A = P^\top P$.

Figure 30 shows the perfect preconditioning on $M = A = \begin{bmatrix} 20 & 5 \\ 5 & 5 \end{bmatrix}$ such that the eigenvalues of $P^{-\top} A P^{-1}$ are identical and the condition number is thus equal to 1.

5.4.4 General Conjugate Gradient Method

Now we come back to the general CG method as introduced in Fletcher and Reeves (1964). The method is already formulated in Algorithm 6; we may notice the Fletcher-Reeves Conjugate Gradient method (Algorithm 6) is just the same as the Practical Conjugate Gradient
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method (Algorithm 8) when the loss function is strongly convex quadratic and the learning rate $\eta_t$ is selected to be exact line search.

To see why the Fletcher-Reeves Conjugate Gradient algorithm (Algorithm 6) works, the search direction $d_t$ must satisfy the descent condition (Remark 1.1, p. 5) such that $g_t^\top d_t < 0$. The descent condition is satisfied when the learning rate is calculated by exact line search in which case the gradient $\nabla L(x_t) = g_t$ is orthogonal to search direction $d_{t-1}$ (Lemma 2.1, p. 13): $g_t^\top d_{t-1} = 0$. Therefore,

$$g_t^\top d_t = g_t^\top (-g_t + \beta_t d_{t-1}) = -||g_t||^2 + \beta_t g_t^\top d_{t-1} < 0$$

when $\eta_t$ is calculated by exact line search. However, when $\eta_t$ is fixed or calculated by inexact line search, the descent condition $g_t^\top d_t$ may not be satisfied. This problem, however, can be attacked by strong Wolfe conditions (Nocedal and Wright, 1999); and we will not give the details.

**Polak-Ribière conjugate gradient** We have mentioned previously that the $\beta_t$ can also be computed by the Polak-Ribière coefficient:

$$\text{Polak-Ribière: } \beta_t^P = \frac{\left( \nabla L(x_t) - \nabla L(x_{t-1}) \right)^\top \nabla L(x_t)}{\nabla L(x_{t-1})^\top \nabla L(x_{t-1})} = \frac{(g_t - g_{t-1})^\top g_t}{g_{t-1}^\top g_{t-1}}.$$  

When the loss function is strongly convex quadratic and the learning rate is chosen by exact line search, the Polak-Ribière coefficient $\beta_t^P$ is identical to the Fletcher-Reeves coefficient $\beta_t^F$ since $g_{t-1}^\top g_t = 0$ by Theorem 5.4.

**Hestenes–Stiefel conjugate gradient** Hestenes–Stiefel coefficient is yet another variant of the Polak-Ribière coefficient:

$$\text{Hestenes–Stiefel: } \beta_t^H = \frac{\left( \nabla L(x_t) - \nabla L(x_{t-1}) \right)^\top \nabla L(x_t)}{\left( \nabla L(x_t) - \nabla L(x_{t-1}) \right)^\top d_{t-1}} = \frac{(g_t - g_{t-1})^\top g_t}{(g_t - g_{t-1})^\top d_{t-1}}.$$  

When the loss function is strongly convex quadratic and the learning rate is chosen by exact line search, the Hestenes–Stiefel coefficient $\beta_t^H$ is identical to the Fletcher-Reeves coefficient $\beta_t^F$ since $g_{t-1}^\top g_t = 0$ by Theorem 5.4 and $g_t^\top d_{t-2} = g_{t-1}^\top d_{t-2} = 0$ by Theorem 5.3.

Moreover, numerical experiments show that the Polak-Ribière coefficient and Hestenes–Stiefel coefficient are more robust than Fletcher-Reeves coefficient in nonconvex settings (Nocedal and Wright, 1999).
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Appendix A. Taylor’s Expansion

Theorem A.1: (Taylor’s Expansion with Lagrange Remainder)

Let \( f(x) : \mathbb{R} \to \mathbb{R} \) be \( k \)-times continuously differentiable on the closed interval \( I \) with endpoints \( x \) and \( y \), for some \( k \geq 0 \). If \( f^{(k+1)} \) exists on the interval \( I \), then there exists a \( x^* \in (x,y) \) such that

\[
f(x) = f(y) + f'(y)(x - y) + \frac{f''(y)}{2!}(x - y)^2 + \ldots + \frac{f^{(k)}(y)}{k!}(x - y)^k + \frac{f^{(k+1)}(x^*)}{(k+1)!}(x - y)^{k+1}
\]

The Taylor’s expansion can be extended to a function of vector \( f(x) : \mathbb{R}^n \to \mathbb{R} \) or a function of matrix \( f(X) : \mathbb{R}^{m \times n} \to \mathbb{R} \).

The Taylor’s expansion, or also known as the Taylor’s series, approximates the function \( f(x) \) around the value of \( y \) by a polynomial in a single indeterminate \( x \). To see where does this series come from, we recall from the elementary calculus course that the approximated function around \( \theta = 0 \) for \( \cos(\theta) \) is given by

\[
\cos(\theta) \approx 1 - \frac{\theta^2}{2}.
\]

That is, the \( \cos \theta \) is approximated by a polynomial with degree of 2. Suppose we want to approximate \( \cos \theta \) by the more general polynomial with degree of 2 by \( f(\theta) = c_1 + c_2\theta + c_3\theta^2 \).

A intuitive idea is to match the gradients around the 0 point. That is,

\[
\begin{align*}
\cos(0) &= f(0); \\
\cos'(0) &= f'(0); & \text{leads to} & \begin{cases} 
1 = c_1; \\
-\sin(0) = 0 = c_2; \\
-\cos(0) = -1 = 2c_3.
\end{cases} \\
\cos''(0) &= f''(0);
\end{align*}
\]

This makes \( f(\theta) = c_1 + c_2\theta + c_3\theta^2 = 1 - \frac{\theta^2}{2} \) and agrees with our claim that \( \cos(\theta) \approx 1 - \frac{\theta^2}{2} \) around the 0 point. We shall not give the details of the proof.