I. INTRODUCTION

You are near the top of a long valley and are meeting your friend at the valley’s lowest point for a picnic. You could probably see the lowest point just by looking around and could walk right to it. To make things challenging you have decided to find the minimum in the same way that a computer would. First you blind-fold yourself, since the information that you get from your eyes, which includes the heights of a huge area around your location, would be far too costly for a computer to calculate. To find the lowest point in the valley while blindfolded you would probably walk down hill, continuously changing your orientation to always point in the direction of steepest descent, which you can determine with your feet alone. The path you would take is the same path that a ball would take if velocity was proportional to the force as in Aristotilian dynamics. Regardless, this method is also very costly for a computer, since it requires determination of the steepest descent direction at every point along one’s trajectory. So to make your path more closely match what a computer would do you have procured a magic scooter. You control the initial orientation of the scooter, hop on, and away you go. The scooter takes a straight line path and stops at the point where to go any farther would take you up hill. This is almost never the lowest point in the valley. When the scooter stops you can change its orientation and take another ride. This curious way of going downhill actually resembles the procedure many computer algorithms use to find the minimum of a function of many variables. Different methods vary only in their choice of which way to point the scooter at each step, and the method by which the scooter finds the local minimum along the ray determined by the scooter’s orientation. Finding a minimum along the length of the ray is the problem of finding the minimum of a function of one variable. Routines for doing this are described in several popular texts. In this paper we focus on the many variables aspect of the problem, the choice of which way to point the scooter, and in particular those choices that correspond to conjugate gradient and variable metric minimization.

Conjugate gradient and variable metric (sometimes called quasi-newton) optimization methods are very popular and successful algorithms for finding minima of functions of many variables. In this paper we motivate these optimization methods, and derive them in a unified manner in a way that emphasizes their essential similarity. The derivation in this paper encompasses the conjugate gradient method with and without conditioning, and the variable metric method. The common variants of these methods including Fletcher-Reeves, Polak-Ribiere, Davidon-Fletcher-Powell, and Broyden-Fletcher-Goldfarb-Shanno are described and motivated. In section II we describe what is wrong with the steepest descent method. In section III we derive a generalized optimization routine which is the starting point for all of the algorithms mentioned above. In section IV we take up some convergence proofs which are followed up in the Appendices. In section V we focus on conjugate gradient routines with and without conditioning and in section VI we turn to variable metric methods.

II. WHAT’S WRONG WITH STEEPEST DESCENT?

In this section we introduce numerical minimization of a function of many variables and show why the steepest descent minimization method is not an optimal choice. Consider a function $E(x)$ of $m$ unconstrained real variables collectively denoted by the $m$-component vector $x$. For concreteness you can consider the function to be the energy
of a configuration of ions. We seek the position of the ions for which the energy is minimized. As with finding the lowest point in a valley, we can think in terms of orienting and moving a single magic scooter but now the scooter moves in an m-dimensional space in which each point corresponds to a configuration of all of the ions. For example, if there are two ions labeled by coordinates \((x_1, y_1, z_1)\) and \((x_2, y_2, z_2)\) the scooter moves in the six dimensional space \(x = (x_1, y_1, z_1, x_2, y_2, z_2)\). In general the n+1 guess for the location of the scooter is determined by

\[
x_{n+1} = x_n + \lambda_n h_n
\]

where \(h_n\) is a vector, different for each minimization scheme, that points along the direction the scooter is headed and \(\lambda_n\) is a positive scaler that represents how far the scooter moves, in units of \(|h_n|\). Once \(h_n\) is chosen we find \(x_{n+1}\) by varying \(\lambda_n\) to minimize \(E(x_{n+1})\). The minimum is found where the derivative of the energy \(E\) with respect to \(\lambda_n\) is zero,

\[
\frac{\partial E}{\partial \lambda_n} = \nabla E(x_{n+1}) \cdot h_n = 0,
\]

or by multiplying by \(\lambda_n\)

\[
\nabla E(x_{n+1}) \cdot (x_{n+1} - x_n) = 0.
\]

This result tells us that the gradient, \(\nabla E(x_{n+1})\), at the new minimum \(x_{n+1}\) is perpendicular to the descent direction, \(x_{n+1} - x_n\), that took us to the minimum. This result is easy to visualize. The dot-product of the gradient of the energy with a particular vector represents the change in energy along that vector. The scooter stops when this is zero since that indicates that the energy is no longer decreasing in that direction.

Numerical minimization schemes differ in their choice for \(h_n\). A naive choice is the steepest decent direction at \(x_n\),

\[
h_n = -\nabla E(x_n).
\]

As well described in standard texts\(^3\), this choice turns out to be far from optimal since it forces each new decent direction to be orthogonal to the previous one. The path to the minimum using this method is a series of 90 degree jogs and it can take many steps of this sort to get close to the true minimum. Consider, for example, a valley with a long shallow axis and a short steep axis shaped like a canoe or a long wooden stirring spoon. Start the scooter somewhere away from the long axis. The steepest descent direction will point somewhere between the shortest path to the long axis, and the direct path to the minimum. Most people assume that the scooter will stop at the long axis and the next move will be along the long axis to the minimum. But the lowest point along the ray must overshoot the long axis by some amount for the next steepest descent direction to be 90 degrees from the path just taken. This is because the energy lost by going parallel to the long axis isn’t overtaken by the gain in going up the steep side until some distance beyond the long axis. For this reason, the steepest descent path constantly overshoots, taking many short 90 degree jogs along the long axis on the way to the minimum, when only two steps appear to be necessary. The way out of this dilemma, adopted by the conjugate gradient and variable metric methods, is to use some other direction than steepest descent for the descent direction. This is what we turn to in the next section.

### III. A UNIVERSAL OPTIMIZATION PROCEDURE

In this section we improve upon the steepest descent method and develop a universal framework for optimization. The basic idea is to pick a descent direction that has some positive projection onto the steepest descent direction but also incorporates information about previous moves into our n+1 guess. A natural choice, as we will see below, for the n+1 guess constructs the direction vector from a linear combination of all previous displacements plus a new vector \(v_n\) that incorporates new information about \(E\) at \(x_n\),

\[
x_{n+1} = x_n + \lambda_n \left( v_n + \sum_{j=2}^{n} a_{j,n} (x_j - x_{j-1}) \right).
\]

For conjugate gradient minimization \(v_n = -\nabla E(x_n)\). For conjugate gradient with conditioning or variable metric minimization \(v_n = -H_n \nabla E(x_n)\) where \(H_n\) is an appropriately chosen symmetric matrix called the conditioner if it is independent of \(n\) or the variable metric if it depends on \(n\). The variables \(\lambda_n\) and \(a_{j,n}\) are varied either analytically or numerically to minimize the function in question. We will minimize \(E\) analytically with respect to the \(a_{j,n}\)’s. E
is then a function of the single variable $\lambda_n$ and can be minimized numerically using a routine to find the minimum of a function of one variable. Choosing $v_n$ and the $a_{j,n}$ beforehand determines $h_n$ and is like orienting the scooter. Determining $\lambda_n$ numerically is like taking a scooter ride.

When we take the derivative of the energy $E$ with respect to $\lambda_n$ at the point $x_{n+1}$ and set it to zero, we get Eq.(2.3), as before, but now $\nabla E(x_{n+1})$ is not the next descent direction so this condition does not constrain us to right angle turns as was the case for steepest descent minimization.

We get n-1 new conditions when we take the derivative of the energy $E$ with respect to $a_{j,n}$ at the point $x_{n+1}$ and set it to zero (In practice it is always clear that we are dealing with the n+1 guess so we have throughout the rest of this paper suppressed the second index in the $a_{j,n}$).

\[
\frac{\partial E}{\partial a_j} = \lambda_n \nabla E(x_{n+1}) \cdot (x_j - x_{j-1}) = 0 \quad 2 \leq j \leq n. \tag{3.2}
\]

Divided by $\lambda_n$ and combined with Eq.(2.3) we have

\[
\nabla E(x_{n+1}) \cdot (x_j - x_{j-1}) = 0 \quad 2 \leq j \leq n + 1. \tag{3.3}
\]

which tells us that the gradient at step $n + 1$ is orthogonal to all previous displacements. These relations will be a great aid in simplifying expressions.

We will get back to Eq.(3.2) shortly but first we need to express $\nabla E(x_{n+1})$ in terms of the $a_{j,n}$’s and known quantities. To do so we assume an explicit form for $E(x)$. We develop our optimization scheme assuming that our guess for the minimum is close enough to the true minimum $x_{\text{min}}$ that we can approximate $E(x)$ by its Taylor expansion to second order around its true minimum.

\[
E(x) = E(x_{\text{min}}) + \frac{1}{2}(x - x_{\text{min}}) \cdot A \cdot (x - x_{\text{min}}), \tag{3.4}
\]

where the first order term is zero since we are expanding $E(x)$ around its minimum. The $m \times m$ symmetric constant matrix $A$ is the diadic second derivative of $E(x)$ evaluated at $x_{\text{min}}$ with matrix elements $A_{i,j} = \partial^2 E(x_{\text{min}})/\partial x_i \partial x_j$. For a unique minimum, $A$ must have only positive eigenvalues.

The quadratic form for the energy Eq.(3.4) allows us to find an explicit expression for the gradient

\[
\nabla E(x) = A \cdot (x - x_{\text{min}}) = (x - x_{\text{min}}) \cdot A. \tag{3.5}
\]

However, for this to be useful we must express it in such a way that $x_{\text{min}}$ and $A$ do not explicitly appear since they are unknown. We can get rid of $x_{\text{min}}$ by subtracting the gradients at any two points in configuration space,

\[
\nabla E(x) - \nabla E(y) = A \cdot (x - y) = (x - y) \cdot A. \tag{3.6}
\]

This is an incredibly useful formula since it allows us to turn any expression with $A$, which we don’t know, into quantities we do know as long as we can arrange for $A$ to operate on a displacement. This is the reason why including previous displacements in our n+1 guess turns out to be the natural way to incorporate information from previous moves. We now have what we need to manipulate Eq.(3.2) to find the n-1 $a_{j,n}$’s.

First we use Eq.(3.6) to find an explicit expression for $\nabla E(x_{n+1})$ in Eq.(3.2) by setting $x = x_{n+1}$ and $y = x_n$,

\[
\nabla E(x_{n+1}) = \nabla E(x_n) + (x_{n+1} - x_n) \cdot A. \tag{3.7}
\]

We now use this expression for $\nabla E(x_{n+1})$ in Eq.(3.2) to get, after dividing by $\lambda_n$,

\[
\nabla E(x_n) \cdot (x_j - x_{j-1}) + (x_{n+1} - x_n) \cdot A \cdot (x_j - x_{j-1}) = 0 \quad 2 \leq j \leq n. \tag{3.8}
\]

The first term in Eq.(3.8) is zero via Eq.(3.3) with n+1 replaced with n. We are left with

\[
(x_{n+1} - x_n) \cdot A \cdot (x_j - x_{j-1}) = 0 \quad 2 \leq j \leq n. \tag{3.9}
\]

We can now, as promised, get rid of the unknown $A$ via Eq.(3.6) since it is operating on a displacement.

\[
(x_{n+1} - x_n) \cdot (\nabla E(x_j) - \nabla E(x_{j-1})) = 0 \quad 2 \leq j \leq n. \tag{3.10}
\]

When we put the formula for $x_{n+1}$, Eq.(3.1), into Eqs.(3.10) we get, after dividing by $\lambda_n$, what we have been after since the beginning of this section: n-1 equations for the n-1 $a_{j,n}$’s in terms of known quantities from previous steps,
By inverting these equations we can find a direction to orient our scooter that is closer to optimal the closer we are to the minimum and the closer the quadratic approximation is to $E$. This is already more than we had any right to expect but it gets even better! These $n-1$ equations are uncoupled since by combining Eq.(3.6) with Eq.(3.9) and using the fact that $A$ is symmetric, we have

$$
(x_k - x_{k-1}) \cdot A \cdot (x_j - x_{j-1}) = (x_k - x_{k-1}) \cdot (\nabla E(x_j) - \nabla E(x_{j-1}))
$$

$$
= (\nabla E(x_k) - \nabla E(x_{k-1})) \cdot (x_j - x_{j-1})
$$

$$
= \delta_{j,k} (\nabla E(x_j) - \nabla E(x_{j-1})) \cdot (x_j - x_{j-1})
$$

so that all terms in the $k$-sum of Eq.(3.11) drop out except the $k=j$ term. The resulting formula for $a_j$ is

$$
a_j = -\frac{v_n \cdot (\nabla E(x_j) - \nabla E(x_{j-1}))}{(\nabla E(x_j) - \nabla E(x_{j-1})) \cdot (x_j - x_{j-1})}.
$$

Plugging this into the update formula Eq.(3.1) we obtain the expression that all of the optimization schemes take as a starting point.

$$
x_{n+1} = x_n + \lambda_n \left( v_n - \sum_{j=1}^{n} (x_j - x_{j-1}) \frac{v_n \cdot (\nabla E(x_j) - \nabla E(x_{j-1}))}{(\nabla E(x_j) - \nabla E(x_{j-1})) \cdot (x_j - x_{j-1})} \right)
$$

This is the most important equation in this paper. Conjugate gradient and variable metric routines use this formula and only differ in their choice of $v_n$.

IV. CONVERGENCE

Of course, none of this is worth it unless Eq.(3.14) is demonstrably faster than steepest descent. And it is, at least for those cases where one is close enough to a minimum that the second order Taylor expansion for $E$ is a good approximation. For quadratic energies, this updating scheme will converge to the minimum of $E$ in no more steps than the number of components of $x$ (two for the canoe, not including the first guess), provided that the $v_n$’s are chosen to be linearly independent of each other. The proof is straightforward. Consider the $m+1$ step of Eq.(3.14).

As long as $v_m$ and the $m-1$ $(x_j - x_{j-1})$’s are linearly independent, which will be true if all the $v_n$’s are linearly independent, then by varying $\lambda_m$ and the $m-1$ $a_j$’s, $x_{n+1}$ spans the entire configuration space. Since $\lambda_m$ and all the $a_j$’s are minimized exactly (remember the $a_j$’s are exact only for quadratic functions) $x_{n+1}$ is guaranteed to be the minimum. So, our intuition that it should only take two steps to find the minimum of a canoe is correct, as long as we have a quadratic canoe.

We can achieve the minimum in fewer than $m$ steps with a clever choice of $v_n$, provided that $E$ is exactly given by Eq.(3.4). For example, the steepest descent method, $v_1 = -\nabla E(x_1)$, finds the minimum in one step regardless of the dimensionality of the configuration space for the maximally symmetric case of quadratic functions with $A$ proportional to the identity matrix (a circular parabolic bowl is an example). More generally one step minimization for quadratic functions is always possible with

$$
x_{\text{min}} = x_n - A^{-1} \cdot \nabla E(x_n),
$$

found by inverting Eq.(3.5). This motivates choosing $v_n = -H_n \cdot \nabla E(x_n)$ where the matrix $H_n$ is a possibly different symmetric positive definite matrix at each step and is ideally a good approximation for $A^{-1}$. Different choices for $H_n$ correspond to different conjugate gradient and variable metric routines.

In the appendix we show that optimization of quadratic functions with appropriate choices for $H_n$ converges to the minimum of $E$ in no more steps than the number of distinct eigenvalues of $H_1 A$, which can be much less than $m$ for highly symmetric systems (notice that this agrees with 1 step minimization when $H_1$ is proportional to $A^{-1}$). In the Appendix we also show that these schemes automatically construct a better approximation for $A^{-1}$ at each step so the optimal choice for $\lambda_n$ approaches 1 for large $n$, regardless of how poorly $H_1$ initially approximates $A^{-1}$.

Even if the energy is not well approximated by a quadratic function, positive definite $H_n$ still guarantees that the positive $\lambda_n$ direction points down hill. The proof is straightforward. Downhill is determined by
\[ \nabla E(x_n) \cdot (x_{n+1} - x_n) < 0. \]  
(4.2)

Replacing the displacement \( x_{n+1} - x_n \) with Eq.(3.14) and using Eq.(3.3) to remove all terms in the \( j \) sum we have

\[ -\lambda_n \nabla E(x_n) \cdot H_n \nabla E(x_n) < 0, \]
(4.3)

which guarantees that \( E \) decreases in the positive \( \lambda_n \) direction, at least initially, provided \( H_n \) is positive definite.

If the energy function is not quadratic, convergence to the minimum is not guaranteed for any finite number of steps since the \( a_j \)'s given by this procedure are no longer the true minima. Regardless, these methods are generally better than steepest descent, since smooth functions are generally closer to quadratic the closer one is to the minimum so the approximate \( a_j \)'s get progressively closer to their true values. Many implementations of these methods switch over to steepest descent minimization in the event that \( x_n \) is in a region that is sufficiently far from quadratic.

**V. CONJUGATE GRADIENT OPTIMIZATION**

We are now ready to derive conjugate gradient optimization formulas. This section will be short since we have already done most of the work we need to do. Conjugate gradient optimization is just the general optimization procedure, Eq.(3.14) with \( v_n = -H \cdot \nabla E(x_n) \) where \( H \) called the conditioner, is an appropriately chosen symmetric positive definite matrix. This is motivated by the exact result in case of quadratic functions Eq.(4.1). If one has a good estimate for \( A^{-1} \) then one can use it for \( H \). Often no such information is known and the identity matrix is used for \( H \). The updating formula is

\[ x_{n+1} = x_n - \lambda_n \left( H \cdot \nabla E(x_n) - \sum_{j=2}^{n} (x_j - x_{j-1}) \frac{\nabla E(x_j) - \nabla E(x_{j-1})}{(x_j - x_{j-1}) \cdot (\nabla E(x_j) - \nabla E(x_{j-1}))} \right). \]
(5.1)

The conjugate gradient choice for \( v_n \) has the wonderful feature that it makes all terms in the \( j \) sum in Eq.(5.1) equal to zero except for the \( j=n \) term. To see this note that

\[ \nabla E(x_n) \cdot H \cdot \nabla E(x_j) = \nabla E(x_n) \cdot \left( H \cdot \nabla E(x_j) - \sum_{k=2}^{j} (x_k - x_{k-1}) \frac{\nabla E(x_k) - \nabla E(x_{k-1})}{(x_k - x_{k-1}) \cdot (\nabla E(x_k) - \nabla E(x_{k-1}))} \right), \]
(5.2)

for \( j \leq n \), where we have added terms that are zero via Eq.(3.3). Now using Eq.(5.1) we can replace the terms in parenthesis with the displacement so we get

\[ \nabla E(x_n) \cdot H \cdot \nabla E(x_j) = \nabla E(x_n) \cdot (x_{j+1} - x_j) / \lambda_j, \]
(5.3)

which by Eq.(3.3) is zero for \( j < n - 1 \), so that we have the result

\[ \nabla E(x_n) \cdot H \cdot \nabla E(x_j) = 0 \quad 2 \leq j \leq n - 1 \]
(5.4)

Eq.(5.4) makes all terms in the \( j \) sum zero in Eq.(5.1) except for \( j = n \). We are left with

\[ x_{n+1} = x_n - \lambda_n \left( H \cdot \nabla E(x_n) - (x_n - x_{n-1}) \frac{\nabla E(x_n) - \nabla E(x_{n-1})}{(x_n - x_{n-1}) \cdot (\nabla E(x_n) - \nabla E(x_{n-1}))} \right). \]
(5.5)

This expression for \( x_{n+1} \) is the Polak-Ribiere conjugate gradient updating formula (However, see Appendix A). One can come up with dozens of other formulas simply by adding or subtracting terms that are zero if the function is quadratic. Another popular choice is the Fletcher-Reeves updating formula which, using the fact that \( \nabla E(x_{n-1}) \cdot H \cdot \nabla E(x_n) = 0 \) from Eq.(5.4), simplifies Eq.(5.5) to

\[ x_{n+1} = x_n - \lambda_n \left( H \cdot \nabla E(x_n) - (x_n - x_{n-1}) \frac{\nabla E(x_n) \cdot H \cdot \nabla E(x_n)}{(x_n - x_{n-1}) \cdot (\nabla E(x_n) - \nabla E(x_{n-1}))} \right). \]
(5.6)

The Polak-Ribiere and the Fletcher-Reeves formulas are equal if the energy function is quadratic. If the energy function is not quadratic it is possible for the Polak-Ribiere numerator to be negative, while the Fletcher-Reeves numerator is always positive. Empirically the best form for the numerator appears to be
max(⟨∇E(x_n) − ∇E(x_{n-1}), H ∙ ∇E(x_n)⟩, 0) which uses the Polak-Ribiere numerator but restarts the conjugate gradient routine with a steepest descent step (assuming the conditioner is the identity) if the P-R numerator goes negative.

The conjugate gradient update formulas are swell but they don’t exactly look much like the one step formula Eq.(4.1) that we might have expected them to resemble. This can be remedied by taking advantage of the ability to create matrices by forming the outer product of two vectors. For the Polak-Ribiere formula we can write

\[ x_{n+1} = x_n - \lambda_n \left( H_n \cdot ∇E(x_n) - \sum_{j=2}^{n} (x_j - x_{j-1}) \cdot ∇E(x_{j-1}) \cdot H_n \cdot ∇E(x_n) \right) \cdot ∇E(x_n), \]  

(5.7)

in which \( \otimes \) commutes the outer product. A similar expression holds for the Fletcher-Reeves update formula. This change to the form of the descent direction is entirely cosmetic, and is given primarily to show the similarity with Eq.(4.1). However, Eq.(5.7) suggests the possibility that the expression in parenthesis, modified to exhibit symmetry, positive definiteness and other properties we expect of an approximation for \( A^{-1} \), would be an improvement over \( H \) that could profitably be used in the next update in its place. This is the motivation for variable metric minimization which is discussed in the next section.

### VI. VARIABLE METRIC OPTIMIZATION

For variable metric optimization we choose \( v_n = -H_n \cdot ∇E(x_n) \) where \( H_n \) is an appropriately chosen symmetric positive definite matrix that is updated at each step to more closely resemble \( A^{-1} \). The initial \( H_1 \) is often the identity matrix. \( A^{-1} \) has the useful property determined by the inverse of Eq.(3.6) that

\[ x - y = A^{-1} \cdot (∇E(x) - ∇E(y)) = (∇E(x) - ∇E(y)) \cdot A^{-1}, \]

(6.1)

which is good for any \( x \) and \( y \). Since \( H_n \) is supposed to be a good approximation for \( A^{-1} \) we will require that \( H_n \) is symmetric and satisfies Eq.(6.1) for \( x \) and \( y \) chosen from the set of \( x_j \) for \( j \leq n \). This will be so if we require

\[ H_n \cdot (∇E(x_j) - ∇E(x_{j-1})) = x_j - x_{j-1} \quad 2 \leq j \leq n. \]

(6.2)

For an \( H_n \) satisfying Eq.(6.2) the update formula

\[ x_{n+1} = x_n - \lambda \left( H_n \cdot ∇E(x_n) - \sum_{j=2}^{n} (x_j - x_{j-1}) \cdot (∇E(x_j) - ∇E(x_{j-1})) \cdot H_n \cdot ∇E(x_n) \right) \cdot ∇E(x_n) \]

(6.3)

simplifies to

\[ x_{n+1} = x_n - λ_n H_n \cdot ∇E(x_n), \]

(6.4)

via Eqn.’s (6.2) and (3.3). The resulting expression is naturally in the form resembling Eq.(4.1) so \( H_n \) is acting like an approximate \( A^{-1} \).

There are many ways to construct an \( H_n \) that satisfies Eq.(6.2). An interesting formula results if we choose \( v_n = -H_{n-1} \cdot ∇E(x_n) \) but insist that we still end up with Eq.(6.4) for \( x_{n+1} \). For this to be true we must have

\[ H_n \cdot ∇E(x_n) = H_{n-1} \cdot ∇E(x_n) - (x_n - x_{n-1}) \cdot (∇E(x_n) - ∇E(x_{n-1})) \cdot H_{n-1} \cdot ∇E(x_n) \]

(6.5)

An \( H_n \) that satisfies this is

\[ H_n = H_{n-1} - \frac{(x_n - x_{n-1}) \otimes H_{n-1} \cdot (∇E(x_n) - ∇E(x_{n-1}))}{(∇E(x_n) - ∇E(x_{n-1})) \cdot (x_n - x_{n-1})}, \]

(6.6)

which is an iterative form of Eq.(5.7). However, this \( H_n \) is a bad approximation for \( A^{-1} \) since it is neither symmetric nor does it satisfy Eq.(6.2). This can be remedied by amending \( H_n \) with terms that give zero for any \( E \), quadratic or not, when operating on \( ∇E(x_n) \):

\[ H_n = H_{n-1} - \frac{(x_n - x_{n-1}) \otimes H_{n-1} \cdot (∇E(x_n) - ∇E(x_{n-1}))}{(∇E(x_n) - ∇E(x_{n-1})) \cdot (x_n - x_{n-1})} - \frac{H_{n-1} \cdot (∇E(x_n) - ∇E(x_{n-1})) \otimes (x_n - x_{n-1})}{(∇E(x_n) - ∇E(x_{n-1})) \cdot (x_n - x_{n-1})} \]

\[ + a(x_n - x_{n-1}) \otimes (x_n - x_{n-1}). \]

(6.7)
The next to last term was added to make $H_n$ symmetric. The last term is allowed with any value of $a$. Remarkably, there is a special value:

$$a = \frac{1}{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot (x_n - x_{n-1})} \left(1 + \frac{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot H_{n-1} \cdot (\nabla E(x_n) - \nabla E(x_{n-1}))}{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot (x_n - x_{n-1})}\right)$$  \hspace{1cm} (6.8)

for which Eq.(6.2) is automatically satisfied, so that we are improving our approximation for $A^{-1}$ at every step. With this value for $a$, Eq.(6.7) is the Broyden-Fletcher-Goldfarb-Shanno variable metric updating formula. The proof that $H_n$ is positive definite, needed to guarantee that the positive $\lambda_n$ direction points downhill, is left for the Appendix.

Another popular variable metric update formula, the Davidon-Fletcher-Powell scheme, was developed with only Eq.(6.2) and symmetry in mind, with no regard for Eq.(6.5) (although it turns out to satisfy it as a proportionality rather than an equality as we show in the Appendix). It is

$$H_n = H_{n-1} - \frac{H_{n-1} \cdot (\nabla E(x_n) - \nabla E(x_{n-1})) \otimes H_{n-1} \cdot (\nabla E(x_n) - \nabla E(x_{n-1}))}{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot (x_n - x_{n-1})}$$

$$+ \frac{(x_n - x_{n-1}) \otimes (x_n - x_{n-1})}{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot (x_n - x_{n-1})}$$  \hspace{1cm} (6.9)

This is an arbitrary formula in that we can add the term $bu \otimes u$ to $H_n$ with

$$u = \frac{(x_n - x_{n-1})}{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot (x_n - x_{n-1})} - \frac{H_{n-1} \cdot (\nabla E(x_n) - \nabla E(x_{n-1}))}{\nabla E(x_n) - \nabla E(x_{n-1})}$$  \hspace{1cm} (6.10)

for any $b$ and still obey Eq.(6.2). The choice

$$b = \frac{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot H_{n-1} \cdot (\nabla E(x_n) - \nabla E(x_{n-1}))}{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot (x_n - x_{n-1})}$$  \hspace{1cm} (6.11)

corresponds to the BFGS scheme. It also is the only choice that makes $H_n$ linear in $H_{n-1}$. The Davidon-Fletcher-Powell scheme, for any $b$, is exactly equivalent to the Broyden-Fletcher-Goldfarb-Shanno scheme if the energy function is quadratic. Empirically, for more general nonquadratic energies, the Broyden-Fletcher-Goldfarb-Shanno scheme is usually better than the $b = 0$ Davidon-Fletcher-Powell scheme.

For quadratic energy functions variable metric and conjugate gradient methods are equivalent. The proof is in the appendix c. Variable metric minimization differs from conjugate gradient minimization for non-quadratic energy functions.

The variable metric method requires more memory than the conjugate gradient method since for variable metric optimization one is building up an $m \times m$ matrix. In practice, for large $m$, one can cut this way down by keeping information from only the last $q < m$ steps\(^8\). My experience has been that for nonquadratic functions the variable metric method with $q > 1$ converges faster than the conjugate gradient method (equivalent to variable metric with $q = 1$) but past performance is no guarantee of future returns.

**APPENDIX A: WILL THE REAL CONJUGATE GRADIENT FORMULA PLEASE STAND UP?**

Eq.(5.5) is the Polak-Ribiere conjugate gradient update formula and Eq.(5.6) is the Fletcher-Reeves formula. However, the conventions for conjugate gradient minimization and variable metric minimization are different. In this paper we have followed the variable metric convention throughout so our expressions for conjugate gradient updates are disguised. In what follows we make several changes in the appearance of Eq.(5.5) and Eq.(5.6) relying only on the orthogonality of a gradient with the most recent displacement, Eq.(2.3), which is always true regardless if the energy function is quadratic or not. The resulting formulas are the conventional expressions for the cg formulas that appear in most text books.

First we can simplify the denominator in the Polak-Ribiere routine.

$$x_{n+1} = x_n - \lambda_n \left( H \cdot \nabla E(x_n) + (x_n - x_{n-1}) \frac{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot H \cdot \nabla E(x_n)}{(x_n - x_{n-1}) \cdot \nabla E(x_{n-1})} \right)$$  \hspace{1cm} (A1)

One is also always free, from the definition Eq.(2.1), to express the update scheme in terms of $h_{n-1}$ instead of $x_n - x_{n-1}$.

$$x_{n+1} = x_n - \lambda_n \left( H \cdot \nabla E(x_n) + h_{n-1} \frac{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot H \cdot \nabla E(x_n)}{h_{n-1} \cdot \nabla E(x_{n-1})} \right)$$  \hspace{1cm} (A2)

---

\(^8\) In my experience, for nonquadratic functions the variable metric method with $q > 1$ converges faster than the conjugate gradient method (equivalent to variable metric with $q = 1$) but past performance is no guarantee of future returns.
Next we expand the denominator using the cg form for $h_{n-1}$.

$$h_{n-1} \cdot \nabla E(x_{n-1}) = - \left( H \cdot \nabla E(x_{n-1}) + h_{n-2} \frac{\nabla E(x_{n-1}) - \nabla E(x_{n-2}) \cdot H \cdot \nabla E(x_{n-1})}{h_{n-2} \cdot \nabla E(x_{n-1})} \right) \cdot \nabla E(x_{n-1})$$

$$= -\nabla E(x_{n-1}) \cdot H \cdot \nabla E(x_{n-1}), \quad (A3)$$

where the second term was zero by orthogonality, Eq.(2.3). The update formula now looks like

$$x_{n+1} = x_n - \lambda_n \left( H \cdot \nabla E(x_n) - h_{n-1} \frac{\nabla E(x_n) - \nabla E(x_{n-1}) \cdot H \cdot \nabla E(x_{n})}{\nabla E(x_{n-1}) \cdot H \cdot \nabla E(x_{n-1})} \right), \quad (A4)$$

This is the formula that is conventionally used in implementations of the Polak-Ribiere update formula.

Similarly, the conventional Fletcher-Reeves update is

$$x_{n+1} = x_n - \lambda_n \left( H \cdot \nabla E(x_n) - h_{n-1} \frac{\nabla E(x_n) \cdot H \cdot \nabla E(x_{n})}{\nabla E(x_{n-1}) \cdot H \cdot \nabla E(x_{n-1})} \right), \quad (A5)$$

which we remind the reader is only equivalent to the Polak-Ribiere update formula for quadratic energy functions.

**APPENDIX B: PROOF THAT $H_n$ IS POSITIVE DEFINITE PROVIDED $H_{n-1}$ IS POSITIVE DEFINITE**

When finding the minimum of a function it is important to know which way is down. As shown in section IV, for conjugate gradient and variable metric minimization, downhill is in the direction of positive $\lambda_n$ guaranteed by making $H_n$ positive definite. For conjugate gradient minimization $H_n$ does not change with $n$ so positive definiteness is trivially guaranteed by making $H$ positive definite initially. For variable metric minimization, on the other hand $H_n$ is updated at each step so it is not obvious that if $H_1$ is chosen to be positive definite that $H_n$ will be too.

We will simultaneously show that the Broyden-Fletcher-Goldfarb-Shanno and Davidon-Fletcher-Powell forms of $H_n$ are positive definite provided that $H_{n-1}$ is positive definite, regardless if the energy is quadratic or not. We start with the BFGS expression for $H_n$, Eq.(6.7), and the DFP expression for $H_n$, Eq.(6.9) written in the alternative form

$$H_n = (1 - S^\dagger) \cdot H_{n-1} \cdot (1 - S) + \frac{(x_n - x_{n-1}) \bigotimes (x_n - x_{n-1})}{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot (x_n - x_{n-1})}, \quad (B1)$$

where

$$S = \frac{(\nabla E(x_n) - \nabla E(x_{n-1})) \bigotimes (x_n - x_{n-1})}{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot (x_n - x_{n-1})} \quad \text{BFGS}$$

$$= \frac{(\nabla E(x_n) - \nabla E(x_{n-1})) \bigotimes (\nabla E(x_n) - \nabla E(x_{n-1})) H_{n-1}}{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot H_{n-1} \cdot (\nabla E(x_n) - \nabla E(x_{n-1}))} \quad \text{DFP}. \quad (B2)$$

To prove positive definiteness we show that $v \cdot H_n \cdot v > 0$ for arbitrary $v$.

$$v \cdot H_n \cdot v = r \cdot H_{n-1} \cdot r + \frac{(v \cdot (x_n - x_{n-1}))^2}{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot (x_n - x_{n-1})}, \quad (B3)$$

in which

$$r = (1 - S) \cdot v. \quad (B4)$$

The denominator of the last term is always greater than zero provided that $H_{n-1}$ is positive definite,

$$(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot (x_n - x_{n-1}) = \lambda_{n-1} \nabla E(x_{n-1}) \cdot H_{n-1} \cdot \nabla E(x_{n-1}) > 0. \quad (B5)$$

It is also the case that $r$ and $v \cdot (x_n - x_{n-1})$ can not both be zero at the same time if $v \neq 0$. This is because $r = 0$ only when $v$ is proportional to $\nabla E(x_n) - \nabla E(x_{n-1})$ which makes $v \cdot (x_n - x_{n-1})$ unequal to zero via Eq.(B5). Therefore, assuming $H_{n-1}$ is positive definite, Eq.(B3) is the sum of two nonnegative numbers, of which at least one must be greater than zero. Hence $H_n$ is positive definite provided that $H_{n-1}$ is positive definite. Consequently the positive $\lambda_n$ direction points downhill for the variable metric routines just as it does for the conjugate gradient routines.
In this section we show that all of the variable metric and conjugate gradient schemes are equivalent for quadratic functions. We have already shown that the Polak-Ribiere and the Fletcher Reeves conjugate gradient routines are equivalent for quadratic functions. We will now show that the variable metric routines are equivalent to conjugate gradient routines, and that therefore they are also equivalent to each other. The proof is inductive and relies on the following proportionality relations for descent directions

\[ H_n \cdot \nabla E(x_n) \propto H_k \cdot \nabla E(x_n) - (x_n - x_{n-1}) \frac{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot H_k \cdot \nabla E(x_n)}{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot (x_n - x_{n-1})} \quad k < n. \tag{C1} \]

The weaker requirement of proportionality rather than equality is sufficient to guarantee that the descent directions are the same for different \( k \); the equality of the displacements and therefore the \( x_n \)'s is recovered when \( \lambda_n \) is varied numerically. This is trivially satisfied for \( k = n - 1 \) in the Broyden-Fletcher-Goldfarb-Shanno updating formula where the proportionality is the equality in Eq.(6.5), and was the motivation for the BFGS update scheme. The proportionality is also true for \( k = n - 1 \) for the Davidon-Fletcher-Powell updating formula as we will prove below. Putting off the \( k = n - 1 \) proof for the DFP formula for now, we will show that for either scheme if Eq.(C1) is satisfied for \( H_k \) then it is also true for \( H_{k-1} \). Once this is proven the equivalence between variable metric and conjugate gradient optimization is achieved by setting \( k = 1 \). Plugging either the BFGS expression for \( H_k \), Eq.(6.7), or the DFP expression for \( H_k \), Eq.(6.9), into Eq.(C1) gets us back Eq.(C1) with \( H_{k-1} \) provided that \( E \) is quadratic (so that we may make liberal use of Eq.(3.3)) and that

\[ (\nabla E(x_k) - \nabla E(x_{k-1})) \cdot H_{k-1} \cdot \nabla E(x_n) = 0. \quad k < n. \tag{C2} \]

The second part of this expression is zero via Eq.(3.3) since \( E(x_{k-1}) \cdot H_{k-1} \) is proportional to the displacement \( x_k - x_{k-1} \). To show that \( E(x_k) \cdot H_{k-1} \) is also proportional to a linear combinations of displacements depends on Eq.(C1) being true for \( k = n - 1 \). If it is then

\[ H_{k-1} \cdot E(x_k) = (x_k - x_{k-1}) \frac{(\nabla E(x_k) - \nabla E(x_{k-1})) \cdot H_{k-1} \cdot \nabla E(x_k)}{(\nabla E(x_k) - \nabla E(x_{k-1})) \cdot (x_k - x_{k-1})} + \gamma(x_{k+1} - k), \tag{C3} \]

where \( \gamma \) is a proportionality constant. This is zero when dotted into \( \nabla E(x_n) \) so the theorem is proved. Setting \( k = 1 \) in the displacement formula Eq.(C1) completes the proof of equivalence of the BFGS variable metric and conjugate gradient optimization for quadratic functions. To show that DFP variable metric optimization is also equivalent to conjugate gradient optimization for quadratic functions we must show that Eq.(C1) is satisfied for \( k = n - 1 \) using the DFP \( H_n \). To do so we operate with, Eq.(6.9), the DFP formula for \( H_n \) in terms of \( H_{n-1} \), on the gradient \( \nabla E(x_n) \). The result is

\[ H_n \cdot \nabla E(x_n) = H_{n-1} \cdot \nabla E(x_n) - H_{n-1} \cdot (\nabla E(x_n) - \nabla E(x_{n-1})) \frac{(\nabla E(x_n) - \nabla E(x_{n-1}))H_{n-1} \cdot \nabla E(x_n)}{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot H_{n-1} \cdot (\nabla E(x_n) - \nabla E(x_{n-1}))} \tag{C4} \]

Combining terms we get

\[ H_n \cdot \nabla E(x_n) = \frac{\nabla E(x_n) \cdot H_{n-1} \cdot \nabla E(x_{n-1})}{\nabla E(x_n) \cdot H_{n-1} \cdot \nabla E(x_n)} \left( H_{n-1} \cdot \nabla E(x_n) - (x_n - x_{n-1}) \frac{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot H_{n-1} \cdot \nabla E(x_n)}{(\nabla E(x_n) - \nabla E(x_{n-1})) \cdot (x_n - x_{n-1})} \right), \tag{C5} \]

where we have used the fact that \( H_{n-1} \cdot \nabla E(x_{n-1}) \) is proportional to \( x_n - x_{n-1} \), and we have used Eq.(3.3) to simplify the proportionality prefactor.

This completes the proof that all of the standard conjugate gradient and variable metric optimization routines produce exactly the same sequence of \( x_n \)'s for quadratic functions. We can use this fact to prove fast convergence of all of these routines for the case of quadratic functions merely by showing that it is true for one. This is what we do in the next section of the appendix.
APPENDIX D: PROOF OF FAST CONVERGENCE FOR QUADRATIC FUNCTIONS

In this section we show that optimization with \( v_j = -H \cdot \nabla E(x_j) \) converges to the minimum of quadratic functions in the number of steps equal to the number of distinct eigenvalues of \( H \cdot A \), regardless of the dimension of the configuration space. Since conjugate gradient and variable metric minimization is the same for quadratic functions, it is sufficient to show this for the conjugate gradient minimization. The proof is based on the one step minimization formula

\[
x_{\text{min}} = x - A^{-1} \nabla E(x), 
\]

and the little known fact, which we prove below, that if a matrix \( M \) has \( p \) distinct eigenvalues then \( M^{-1} \) is a polynomial in \( M \) with highest power \( p - 1 \),

\[
M^{-1} = \sum_{j=0}^{p-1} c_j(M)^j. 
\]

With \( M = HA \) we have

\[
A^{-1} = \sum_{j=0}^{p-1} c_j(HA)^jH. 
\]

Plugging this into Eq.(D1) we have

\[
x_{\text{min}} = x - \sum_{j=0}^{p-1} c_j(HA)^jH \cdot \nabla E(x). 
\]

In this appendix we prove that for quadratic functions, and for \( HA \) with \( p \) distinct eigenvalues, Eq.(D4) is equal to the conjugate gradient expression after \( p \) steps, not including the first guess.

First we prove Eq.(D2). For \( M \) with \( p \) distinct eigenvalues we have

\[
\prod_{j=1}^{p} (\epsilon_j - M) = 0 \tag{D5}
\]

where \( \epsilon_j \) are the distinct eigenvalue of \( M \). Therefore the identity can be written

\[
I = I - \beta \prod_{j=1}^{p} (\epsilon_j - M) \tag{D6}
\]

for any \( \beta \). Consequently

\[
M^{-1} = (I - \beta \prod_{j=1}^{p} (\epsilon_j - M))M^{-1} \tag{D7}
\]

for any \( \beta \). In general this is an implicit equation for \( M^{-1} \) but with \( \beta = 1/\prod_{k=1}^{p} \epsilon_k \) each term in parenthesis contains at least one power of \( M \), cancelling out \( M^{-1} \) on the right hand side. The final result expresses \( M^{-1} \) explicitly as a polynomial in \( M \) alone with highest power \( p - 1 \), as alleged in Eq.(D2). The results for \( p \) from one to four are

\[
M_1^{-1} = \frac{1}{\epsilon_1} I 
\]

\[
M_2^{-1} = \left( \frac{1}{\epsilon_1} + \frac{1}{\epsilon_2} \right) I - \frac{1}{\epsilon_1 \epsilon_2} M_2 \tag{D9}
\]

\[
M_3^{-1} = \left( \frac{1}{\epsilon_1} + \frac{1}{\epsilon_2} + \frac{1}{\epsilon_3} \right) I - \left( \frac{1}{\epsilon_1 \epsilon_2} + \frac{1}{\epsilon_1 \epsilon_3} + \frac{1}{\epsilon_2 \epsilon_3} \right) M_3 + \frac{1}{\epsilon_1 \epsilon_2 \epsilon_3} M_3^2 \tag{D10}
\]

\[
M_4^{-1} = \left( \frac{1}{\epsilon_1} + \frac{1}{\epsilon_2} + \frac{1}{\epsilon_3} + \frac{1}{\epsilon_4} \right) I - \left( \frac{1}{\epsilon_1 \epsilon_2} + \frac{1}{\epsilon_1 \epsilon_3} + \frac{1}{\epsilon_1 \epsilon_4} + \frac{1}{\epsilon_2 \epsilon_3} + \frac{1}{\epsilon_2 \epsilon_4} + \frac{1}{\epsilon_3 \epsilon_4} \right) M_4
+ \left( \frac{1}{\epsilon_1 \epsilon_2 \epsilon_3} + \frac{1}{\epsilon_1 \epsilon_2 \epsilon_4} + \frac{1}{\epsilon_1 \epsilon_3 \epsilon_4} + \frac{1}{\epsilon_2 \epsilon_3 \epsilon_4} \right) M_4^2 - \frac{1}{\epsilon_1 \epsilon_2 \epsilon_3 \epsilon_4} M_4^3 \tag{D11}
\]
Next we show that conjugate gradient minimization is equal to Eq. (D4) after \( p \) steps. The proof is inductive. We will prove that for conjugate gradient minimization

\[
x_n = x_1 + P_{n-2}(HA)H \nabla E(x_1)
\]

(D12)

where \( P_{n-2}(HA) \) is a polynomial of order \( n - 2 \). First, it is trivially true for \( n = 2 \) since \( x_2 = x_1 - H \nabla E(x_1) \). We will now prove that if it is true for the \( p \)th step then it is also true for the \( p+1 \)th step where

\[
x_{p+1} = x_p - \lambda_p H \cdot \nabla E(x_n) + \lambda_p \sum_{j=2}^{p} a_j (x_j - x_{j-1}),
\]

(D13)

in which the \( a_j \)’s are the coefficients of your favorite conjugate gradient routine. Using Eq.(3.6) we can put things in terms of \( x_1 \).

\[
x_{p+1} = x_1 + (x_p - x_1) - \lambda_p H \cdot (\nabla(E(x_1) + A(x_p - x_1))) + \lambda_p \sum_{j=2}^{p} a_j ((x_j - x_1) - (x_{j-1} - x_1))
\]

(D14)

Therefore using Eq.(D12) we have

\[
x_{p+1} = x_1 + \left( -\lambda_p HAP_{p-2}(HA) + P_{p-2}(HA) + \lambda_p \sum_{j=2}^{p} a_j (P_{j-2}(HA) - P_{j-3}(HA)) - \lambda_p \right) \cdot H \cdot (\nabla E(x_1)), \quad \text{(D15)}
\]

where \( P_{-1} = 0 \). The expression in parenthesis, because of its first term, is a polynomial of order \( p - 1 \). Indeed it can be any polynomial of order \( p - 1 \) since \( \lambda_p \) and the \( p-1 \) \( a_j \)’s in principle can be varied arbitrarily. In particular it can be the polynomial in Eq.(D4). The conjugate gradient formula picks out the polynomial of order \( p - 1 \) that minimizes \( E(x_{p+1}) \). Since \( E \) is minimized for \( x_{p+1} = x_{\text{min}} \), Eq.(D15) must equal Eq.(D4) and the theorem is proved.

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1 The scooter represents a routine that minimizes the function along a particular ray. A real line minimization routine moves quite unlike the motion of any real scooter, more like several pogo sticks bouncing along the ray until the minimum is found. If there is more than one minima, such routines can not guarantee that the minima found is the closest one to your starting point. References for line minimization routines can be found in the next citation.

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