# Overview

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special care must be taken if we are only looking for minima or maxima

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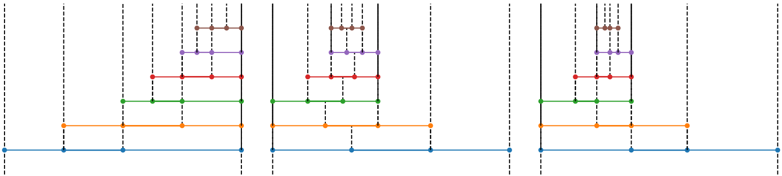
the conditions are satisfied when

$$x = \frac{\sqrt{5}+1}{2},$$

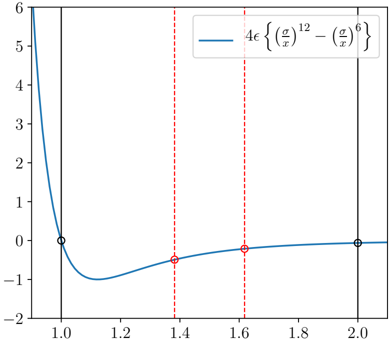
the golden ratio, hence the name, "golden section search."

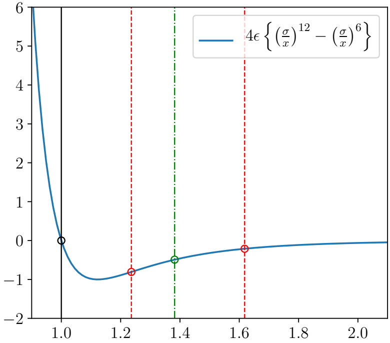
# Golden Section Search



- Uneven intervals (left), even, but suboptimal intervals (centre), and golden section search (right)

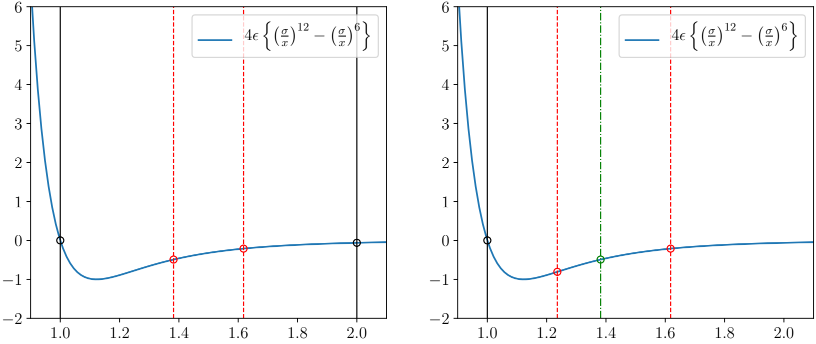
# Golden Section Search




- One iteration of the golden section search applied to the Lennard-Jones potential.

# Golden Section Search




- One iteration of the golden section search applied to the Lennard-Jones potential.
- The "c" point in the first bracket is reused as the "d" point in the second bracket.

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4. $(a, b, c) \leftarrow (b, c, d)$
5. continue until $|c - b| < \delta$
6. the order of convergence $q \approx 1.324$

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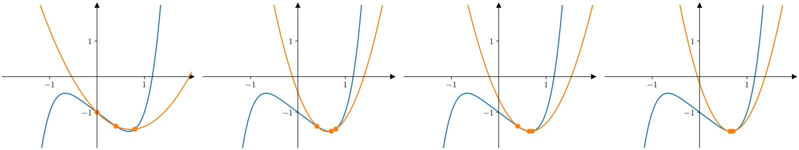
What if we only want to converge to minima?

1. find a bracket $(a, c, b)$;
2. find the new point $d$;
3. update with the new, narrower bracket,

$$(a, c, b) \leftarrow \begin{cases} (a, d, c) & d < c, \quad f(d) < f(c) \\ (d, c, b) & d < c, \quad f(d) > f(c) \\ (c, d, b) & d > c, \quad f(d) < f(c) \\ (a, c, d) & d > c, \quad f(d) > f(c) \,. \end{cases}$$

# Successive parabolic interpolation



- Successive parabolic interpolation applied to the quintic with $(a, b, c) = (0.0, 0.4, 0.8)$.

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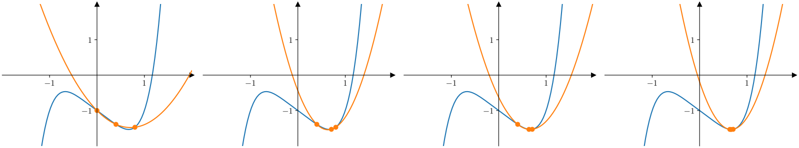


- Successive parabolic interpolation applied to the quintic with $(a, b, c) = (0.0, 0.4, 0.8)$.
- What happens if you set $(a, b, c) = (0.0, 0.5, 1.0)$?

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$$f\left(\xi\right) = f\left(x_0 + \epsilon_0\right) = f_0 + \epsilon_0 f_0' + \mathcal{O}\left(\epsilon_0^2\right)$$

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- to find only minima, take the absolute value of the second derivative in the update step,

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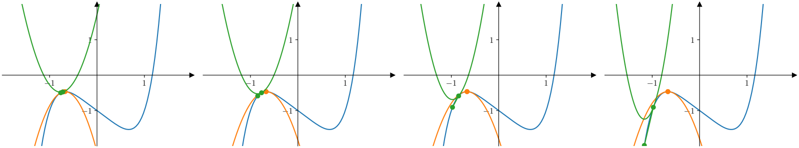


- Convergence to a minimum is not guaranteed...

# Secant Method (again)



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- You may have noticed that the secant method for zeros is equivalent to the NR method for zeros with the derivative approximated by first backward differences
- the secant method for stationary points works on a similar basis, with the second derivative term replaced by a first backward differences approximation of the first derivative...of the first derivative

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($\alpha$ is a small, positive, adjustable parameter, chosen to guarantee function decrease)

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- By construction, this method only finds minima
- to find maxima, a negative value of $\alpha$ should be employed

# Homework

## The gradient-descent (one dimensional)

Choosing the value of $\alpha$ is a critical consideration: if $\alpha$ is too small, convergence is slow; if $\alpha$ is too large, then we risk jumping back and forth over the minimum, which also results in slow convergence.

1. devise a simple algorithm to choose $\alpha$;
2. implement the gradient-descent method, using this algorithm.

# Backtracking line search



- consider the update

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where $\alpha$ is a positive, adjustable parameter, and $p = f'(x) / |f'(x)|$ is either 1 or $-1$

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- so we say the function value has decreased sufficiently if

$$f(x_0 - \alpha p) \leq f(x_0) - \alpha c m \tag{1}$$

where $m = p f'(x_0) = |f'(x_0)|$ and $c \in (0, 1)$ is a control parameter

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- if condition 1 is not satisfied, update $\alpha$ as $\alpha \leftarrow \tau\alpha$ where $\tau \in (0, 1)$ is another control parameter
- continue until condition 1 is satisfied
- typically, $c = 0.5$, $\tau = 0.5$

# Overview

# Solving linear equations

- Consider the system of equations,

$$\begin{aligned} 2x + y - z &= 8; \\ -3x - y + 2z &= -11; \\ -2x + y + 2z &= -3, \end{aligned}$$

- we can summarise these equations in an augmented matrix

$$\left[\begin{array}{ccc|c} 2 & 1 & -1 & 8 \\ -3 & -1 & 2 & -11 \\ -2 & 1 & 2 & -3 \end{array}\right]$$

# Solving linear equations



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2x + y - z &= 8; \\
-3x - y + 2z &= -11; \\
-2x + y + 2z &= -3,
\end{aligned}
$$

- $(R2) - \frac{3}{2}(R1)$, $(R3) + (R1)$

$$
\left[\begin{array}{ccc|c}
2 & 1 & -1 & 8 \\
0 & 0.5 & 0.5 & 1 \\
0 & 2 & 1 & 5
\end{array}\right]
$$

# Solving linear equations



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- $(R3) - 4(R2)$

$$\left[\begin{array}{ccc|c} 2 & 1 & -1 & 8 \\ 0 & 0.5 & 0.5 & 1 \\ 0 & 0 & -1 & 1 \end{array}\right]$$

- at this point, we could solve by back-substitution
- we could also find the determinant of the original matrix as the product of the diagona elements
- additionally, if the matrix is symmetric, the signs of the eigenvalues of the matrix are the same as the signs of the diagonal elements

# Solving linear equations

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- reflect in the antidiagonal

$$\left[\begin{array}{ccc|c} -1 & 0 & 0 & 1 \\ 0.5 & 0.5 & 0 & 1 \\ -1 & 1 & 2 & 8 \end{array}\right]$$

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- $(R2) + \frac{1}{2}(R1)$, $(R3) - (R1)$

$$\left[\begin{array}{ccc|c} -1 & 0 & 0 & 1 \\ 0 & 0.5 & 0 & 1.5 \\ 0 & 1 & 2 & 7 \end{array}\right]$$

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- divide through by the diagonal

$$\left[\begin{array}{ccc|c} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & 3 \\ 0 & 0 & 1 & 2 \end{array}\right]$$

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- don't forget that we switched $x$ and $z$

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- the proof:

$$
\begin{aligned}
2(2) + (3) - (-1) &= 8 \\
-3(2) - (3) + 2(-1) &= -11 \\
-2(2) + (3) + 2(-1) &= -3
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- and finally solves to,

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- we can compute the inverse of the matrix of second derivatives, the Hessian matrix, using the matrix methods outlined above.

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- this condition is true iff all of the eigenvalues of the Hessian matrix are positive

- we can shift the eigenvalues of a symmetric matrix to positive values, while leaving the eigenvectors unchanged, by adding to it a multiple of the identity matrix,

$$\mathbf{B} = \mathbf{A} + \mu \mathbf{I}$$

where $\mu + \lambda_{min} > 0$, and $\lambda_{min}$ is the smallest (most negative) eigenvalue of $\mathbf{A}$

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- how do we choose the update?

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$$f''(x) \cdot h = f'(x) - f'(x-h) + \mathcal{O}\left(h^2\right)$$

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- re-writing in the above terms, we get

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- but... there is no unique solution to the secant equation!

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- this matrix is in general non-symmetric

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- so the update to $\mathbf{B}$ is,

$$\mathbf{B}_{k+1} = \mathbf{B}_k + \frac{\mathbf{y}_k\mathbf{y}_k^T}{\mathbf{y}_k^T\mathbf{s}_k} - \frac{\mathbf{B}_k\mathbf{s}_k\mathbf{s}_k^T\mathbf{B}_k^T}{\mathbf{s}_k^T\mathbf{B}_k\mathbf{s}_k}$$

(verify this for yourselves)

# Broyden–Fletcher–Goldfarb–Shanno (BFGS) method

- collecting these ideas together, recalling that $\mathbf{s}_k = \mathbf{x}_{k+1} - \mathbf{x}_k$, and $\mathbf{y}_k = \nabla f\left(\mathbf{x}_{k+1}\right) - \nabla f\left(\mathbf{x}_k\right)$,

$$\boxed{\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{x}_k - \mathbf{B}_k^{-1} \cdot \nabla f\left(\mathbf{x}_k\right) \qquad (3) \\ \mathbf{B}_{k+1} &= \mathbf{B}_k + \frac{\mathbf{y}_k \mathbf{y}_k^T}{\mathbf{y}_k^T \mathbf{s}_k} - \frac{\mathbf{B}_k \mathbf{s}_k \mathbf{s}_k^T \mathbf{B}_k^T}{\mathbf{s}_k^T \mathbf{B}_k \mathbf{s}_k}. \qquad (4) \end{aligned}}$$

BFGS UPDATES

- however, since we only need the inverse of **B**, we can rewrite the update using the Sherman–Morrison formula,

$$\mathbf{B}_{k+1}^{-1} = \left(\mathbf{I} - \frac{\mathbf{s}_k \mathbf{y}_k^T}{\mathbf{y}_k^T \mathbf{s}_k}\right) \mathbf{B}_k^{-1} \left(\mathbf{I} - \frac{\mathbf{y}_k \mathbf{s}_k^T}{\mathbf{y}_k^T \mathbf{s}_k}\right) + \frac{\mathbf{s}_k \mathbf{s}_k^T}{\mathbf{y}_k^T \mathbf{s}_k} \tag{5}$$

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- as $\mathbf{B}_k^{-1}$ is symmetric, and both $\mathbf{y}_k^T \mathbf{B}_k^{-1} \mathbf{y}_k$ and $\mathbf{s}_k^T \mathbf{y}_k$ are scalars, we can write

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BFGS UPDATES (IMPROVED)

and we never need to invert a matrix ever again.

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BFGS UPDATES (IMPROVED)

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- we can use the real Hessian matrix as a starting guess, but it is often sufficient to start with the identity matrix...

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$$\mathbf{B}_{k+1}^{-1} = \left(\mathbf{I} - \frac{\mathbf{s}_k \mathbf{y}_k^T}{\mathbf{y}_k^T \mathbf{s}_k}\right) \mathbf{B}_k^{-1} \left(\mathbf{I} - \frac{\mathbf{y}_k \mathbf{s}_k^T}{\mathbf{y}_k^T \mathbf{s}_k}\right) + \frac{\mathbf{s}_k \mathbf{s}_k^T}{\mathbf{y}_k^T \mathbf{s}_k} \tag{5}$$

- as $\mathbf{B}_k^{-1}$ is symmetric, and both $\mathbf{y}_k^T \mathbf{B}_k^{-1} \mathbf{y}_k$ and $\mathbf{s}_k^T \mathbf{y}_k$ are scalars, we can write

$$\boxed{\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{x}_k - \mathbf{B}_k^{-1} \cdot \nabla f(\mathbf{x}_k) && (6) \\ \mathbf{B}_{k+1}^{-1} &= \mathbf{B}_k^{-1} + \frac{(\mathbf{s}_k^T \mathbf{y}_k + \mathbf{y}_k^T \mathbf{B}_k^{-1} \mathbf{y}_k)(\mathbf{s}_k \mathbf{s}_k^T)}{(\mathbf{s}_k^T \mathbf{y}_k)^2} - \frac{\mathbf{B}_k^{-1} \mathbf{y}_k \mathbf{s}_k^T + \mathbf{s}_k \mathbf{y}_k^T \mathbf{B}_k^{-1}}{\mathbf{s}_k^T \mathbf{y}_k} && (7) \end{aligned}}$$

BFGS UPDATES (IMPROVED)

and we never need to invert a matrix ever again.

- we can use the real Hessian matrix as a starting guess, but it is often sufficient to start with the identity matrix...
- ...at the first iteration, the update behaves like gradient descent, but in favourable circumstances, the approximate Hessian quickly approaches the values of the real Hessian

# Non-linear equations—Gradient Descent—again



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- we find that, if the function were linear, the function value would decrease by an amount,

$$\begin{aligned} f(\mathbf{x}_{k+1}) - f(\mathbf{x}_k) &= -\alpha \nabla f(\mathbf{x}_k)^T \mathbf{p} \\ &= -\alpha m \end{aligned}$$

where $m = f(\mathbf{x}_k)^T \mathbf{p}$

- as a condition for choosing $\alpha$, we say that the function value has decreased by a sufficient amount if it decreases by some amount,

$$\boxed{f(\mathbf{x}_{k+1}) - f(\mathbf{x}_k) < -\alpha c m} \tag{9}$$

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- in practice, the Newton and BFGS updates aren't always used directly—we use those equations to find a suitable search direction, then use a line search to find a suitable step size

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- then minimise in the direction obtained by projecting the eigenvector out of the gradient vector, using *e.g.*, BFGS,

$$\boxed{\nabla f_{\perp} = \nabla f - \left(\nabla f^{T} \cdot \mathbf{v}_{\text{min}}\right) \mathbf{v}_{\text{min}}} \tag{10}$$

EIGENVECTOR FOLLOWING PROJECTED GRADIENT

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- we can also use approximate Hessian matrices if exact ones are not available