Newton’s Method for 1D Systems
Review:
Algorithm for Gradient Descent

The general procedure for numerical geometry optimization is as follows:

1. Calculate the force on all atoms for some configuration of an atomic system.
2. If the magnitude of the force is less than threshold, you have found a critical point! STOP.
3. If not, move the atoms such that they go towards a critical points

\[ r_{n+1} = r_n + \alpha F(r_n) \]

4. Repeat.
Example Gradient Descent

\[ V(r) = (r - 3)^2 \]

\[ r_{n+1} = r_n + \alpha F(r_n) \]

\[ r_4 = r_3 + \alpha F(r_3) = 2.5 + 0.25 \times 1 = 2.75 \]

4. Repeat until the magnitude of the force is less than 0.01

<table>
<thead>
<tr>
<th>Step #, n</th>
<th>( r_n )</th>
<th>( F(r_n) )</th>
<th>( r_{n+1} = r_n + \alpha F(r_n) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2.5</td>
</tr>
<tr>
<td>3</td>
<td>2.5</td>
<td>1</td>
<td>2.75</td>
</tr>
</tbody>
</table>
Newton’s Method

\[ V(r) = (r - 3)^2 \]

\[ \frac{dV}{dr} = V'(r) = 2(r - 3) \]

Since \( V \) is a parabola, the second derivative is a constant and the slope of the red line!

\[ V''(r_1) = \frac{V'(r_{opt}) - V'(r_1)}{r_{opt} - r_1} \]

Next, Solve for \( r_{opt} \) (Note: \( V'(r_{opt}) = 0 \))

\[ r_{opt} = r_1 - \frac{V'(r_1)}{V''(r_1)} \]
Newton’s Method

\[ V(r) = (r - 3)^2 \]

\[ \frac{dV}{dr} = V'(r) = 2(r - 3) \]

\[ V''(r) = 2 \]

Newton’s Method equation

\[ r_{opt} = r_1 - \frac{V'(r_1)}{V''(r_1)} \]

\[ r_{opt} = 1 - \frac{2(1 - 3)}{2} = 3 \]

We found the local minimum in one step!
Newton’s Method

- Newton’s Method for equations more complex than quadratic functions will not optimize in one step. Here is the equation for taking a step towards the minimum

\[ r_{n+1} = r_n - \frac{V'(r_n)}{V''(r_n)} \]
\[ V(r) = (r - 2.5)^4 \]
\[ V'(r) = 4(r - 2.5)^3 \]
\[ V''(r) = 12(r - 2.5)^2 \]

\[ r_0 = 1.5 \]

\[ r_1 = r_0 - \frac{V'(r_0)}{V''(r_0)} \]
\[ V(r) = (r - 2.5)^4 \]
\[ V'(r) = 4(r - 2.5)^3 \]
\[ V''(r) = 12(r - 2.5)^2 \]
\[ r_0 = 1.5 \]
\[ r_1 = r_0 - \frac{V'(r_0)}{V''(r_0)} \]
\[ r_1 = 1.833 \]
\[ V(r) = (r - 2.5)^4 \]
\[ V'(r) = 4(r - 2.5)^3 \]
\[ V''(r) = 12(r - 2.5)^2 \]

\[ r_0 = 1.5 \]

\[ r_1 = r_0 - \frac{V'(r_0)}{V''(r_0)} \]

\[ r_1 = 1.833 \]
\[ V(r) = (r - 2.5)^4 \]

\[ V'(r) = 4(r - 2.5)^3 \]

\[ V''(r) = 12(r - 2.5)^2 \]

\[ r_0 = 1.5 \]

\[ r_2 = r_1 - \frac{V'(r_1)}{V''(r_1)} \]

\[ r_1 = 1.833 \]

\[ r_2 = 2.05 \]
\[ V(r) = (r - 2.5)^4 \]
\[ V'(r) = 4(r - 2.5)^3 \]
\[ V''(r) = 12(r - 2.5)^2 \]

\[ r_0 = 1.5 \]
\[ r_{n+1} = r_n - \frac{V'(r_n)}{V''(r_n)} \]

\[ r_1 = 1.833 \]
\[ r_2 = 2.05 \]
\[ ... \]
\[ r_n \approx 2.5 \]