Newton's Method

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1 NEWTON'S METHOD

Newton's method is a technique used to find the root (based on an initial guess x_0) of a *differentiable*, univariate function f(x). The equation of the tangent line to the curve y = f(x) at $x = x_0$ is

$$y = f'(x_0)(x - x_0) + f(x_0)$$

where $f'(x_0)$ is the derivative of f(x) evaluated at x_0 . The x-intercept of this tangent line, $x = x_1$, can be solved by setting y = 0.

$$0 = f'(x_0)(x_1 - x_0) + f(x_0)$$

$$\therefore x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

 x_1 is an updated estimate of the root of f(x). To keep refining our estimate, we can keep iterating through this procedure using Eq. (1).

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$
 (1)

So how do we actually use Eq. (1)? Given an initial guess x_0 , we can keep coming up with new estimates of the root. But how do we know when to stop? To resolve this issue, we define the **error**² as

$$\boxed{\varepsilon = |x_{i+1} - x_i|} \tag{2}$$

Once ε is small enough, we say that the estimate of the root has **converged** to the true root, x^* , within some **tolerance** (which we denote as TOL). Therefore, if we predetermine that, at most, we can *tolerate* an error of TOL, then we will keep iterating Eq. (1) until ε < TOL. In some cases, the error may never decrease below TOL, or take too long to decrease to below TOL. Therefore, we also define the **maximum number of iterations** (i_{max}) so that the algorithm does not keep iterating forever, or for too long of a time [1, 2].

There are two basic algorithms for implementing Newton's method. The first implementation, shown in Algorithm 1 below, does *not* store the result of each iteration. On the other hand, the second implementation, shown in Algorithm 2, *does* store the result of each iteration. newtons method implements both of these algorithms.

Since Algorithm 2 first needs to preallocate a potentially huge array to store all of the intermediate solutions, Algorithm 1 is significantly faster. Even if $i_{\rm max}$ (determines size of the preallocated array) is set to be a small number (for example, 10), Algorithm 1 is still faster. The reason we still consider and implement Algorithm 2 is so that convergence studies may be performed.

Algorithm 1:

Newton's method ("fast" implementation).

Given:

- f(x) differentiable, univariate, scalar-valued function $(f : \mathbb{R} \to \mathbb{R})$
- f'(x) derivative of f(x)
- $x_0 \in \mathbb{R}$ initial guess for root
- $TOL \in \mathbb{R}$ tolerance
- $i_{\max} \in \mathbb{Z}$ maximum number of iterations

Often, a function f(x) will have multiple roots. Therefore, Newton's method typically finds the root closest to the initial guess x_0 . However, this is not always the case; the algorithm depends heavily on the derivative of f(x), which, depending on its form, may cause it to converge on a root further from x_0 .

Note that ε is an approximate error. The motivation behind using this definition of ε is that as i gets large (i.e. $i \to \infty$), $x_{i+1} - x_i$ approaches $x_{i+1} - x^*$ (assuming this sequence is convergent), where x^* is the true root (and therefore $x_{i+1} - x^*$ represents the exact error).

Procedure:

1. Initialize the error so that the loop will be entered.

$$\varepsilon = (2)(TOL)$$

2. Manually set the root estimate at the first iteration based on the initial guess.

$$x_{\text{old}} = x_0$$

3. Initialize x_{new} so its scope will not be limited to within the while loop.

$$x_{\text{new}} = 0$$

4. Find the root using Newton's method.

$$i = 1$$

while $(\varepsilon > \text{TOL})$ and $(i < i_{\text{max}})$

(a) Update root estimate.

$$x_{\text{new}} = x_{\text{old}} - \frac{f(x_{\text{old}})}{f'(x_{\text{old}})}$$

(b) Calculate error.

$$\varepsilon = |x_{\text{new}} - x_{\text{int}}|$$

(c) Store the current root estimate for the next iteration.

$$x_{\text{old}} = x_{\text{new}}$$

(d) Increment loop index.

$$i = i + 1$$

end

Return:

• $x^* = x_{\text{new}} \in \mathbb{R}$ - converged root

Algorithm 2:

Newton's method ("return all" implementation).

Given:

- f(x) differentiable, univariate, scalar-valued function $(f : \mathbb{R} \to \mathbb{R})$
- f'(x) derivative of f(x)
- $x_0 \in \mathbb{R}$ initial guess for root
- $TOL \in \mathbb{R}$ tolerance
- $i_{\max} \in \mathbb{R}$ maximum number of iterations

Procedure:

1. Initialize the error so that the loop will be entered.

$$\varepsilon = (2)(TOL)$$

- 2. Preallocate $\mathbf{x} \in \mathbb{R}^{i_{\max}}$ to store the estimates of the root at each iteration.
- 3. Manually set the root estimate at the first iteration based on the initial guess (note that x_1 is the first element of \mathbf{x} , while x_0 is the input initial guess).

$$x_1 = x_0$$

4. Find the root using Newton's method.

$$i = 1$$

while $(\varepsilon > \text{TOL})$ and $(i < i_{\text{max}})$

(a) Update root estimate.

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

(b) Calculate error.

$$\varepsilon = |x_{i+1} - x_i|$$

(c) Increment loop index.

$$i = i + 1$$

end

Return:

• $\mathbf{x} \in \mathbb{R}^n$ - vector where the first element is the initial guess for the root (x_0) , the subsequent elements are the intermediate root estimates, and the final element is the converged root (x^*)

REFERENCES 5

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[2] Newton's method. Wikipedia. Accessed: June 10, 2020. URL: https://en.wikipedia.org/wiki/Newton%27s_method.