
Secant Method

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1 SECANT METHOD

Newton's method is a root-finding technique that uses the derivative of a function to find its root¹. Newton's method is defined iteratively as [2, Eq. (1)]

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

But what if we don't know $f'(x)$? Then we need to approximate it using some numerical method. Specifically, for the secant method, we use the backward approximation of a derivative, given by Eq. (2) below.

$$f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \quad (2)$$

This approximation can be visualized using the finite difference stencil shown in Fig. 1.

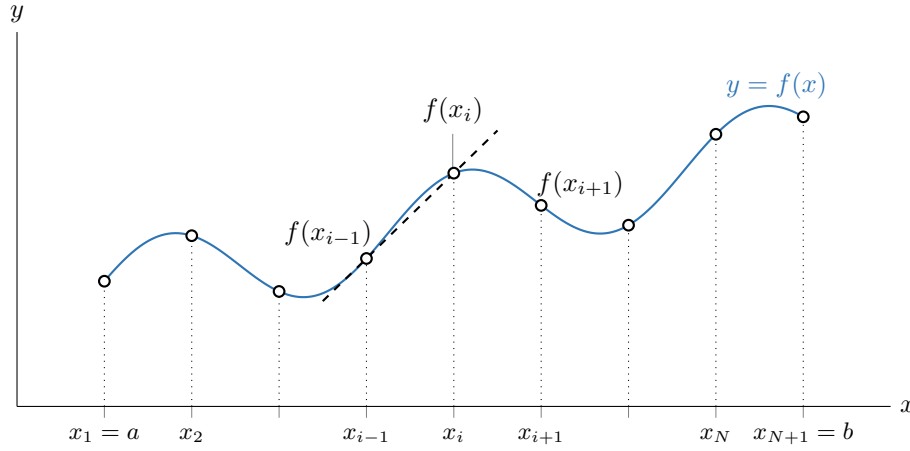


Figure 1: Backward approximation.

Substituting Eq. (2) into Eq. (1),

$$\begin{aligned} x_{i+1} &= x_i - \left[\frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})} \right] f(x_i) = \frac{[f(x_i) - f(x_{i-1})] x_i}{f(x_i) - f(x_{i-1})} - \frac{(x_i - x_{i-1}) f(x_i)}{f(x_i) - f(x_{i-1})} \\ &= \frac{x_i f(x_i) - x_i f(x_{i-1})}{f(x_i) - f(x_{i-1})} + \frac{x_{i-1} f(x_i) - x_i f(x_i)}{f(x_i) - f(x_{i-1})} = \frac{x_i f(x_i) - x_i f(x_i) + x_{i-1} f(x_i) - x_i f(x_{i-1})}{f(x_i) - f(x_{i-1})} \\ &\boxed{x_{i+1} = \frac{x_{i-1} f(x_i) - x_i f(x_{i-1})}{f(x_i) - f(x_{i-1})}} \end{aligned} \quad (3)$$

Equation (3) iteratively defines the **secant method**, which can be essentially thought of as a finite difference approximation of Newton's method for finding the root of a univariate function (based on an initial guess²). But how do we actually use Eq. (3)? 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**³ as

$$\varepsilon = |x_{i+1} - x_i| \quad (4)$$

¹ For a discussion/MATLAB implementation of Newton's method, see [2].

² Often, a function $f(x)$ will have multiple roots. Therefore, the secant 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 .

³ Note that ε is an *approximate* error. The motivation behind using this definition of ε is that as i gets large (i.e. $i \rightarrow \infty$), $x_{i+1} - x_i$ 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).

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. (3) until $\varepsilon < \text{TOL}$. 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.

In any implementation, we first have to make an initial guess x_0 for the root. Additionally, we need to set the root estimate at the first iteration (i.e. x_1) to a value slightly different than x_0 – otherwise, the denominator of the right hand side of Eq. (3) will be 0 (since $f(x_1) - f(x_0) = f(x_0) - f(x_0) = 0$ if $x_1 = x_0$) and x_2 will be undefined. We can think of this as “kick-starting” the algorithm [1, 3, 4].

There are two basic algorithms for implementing the secant 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. `secant_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_{\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:

Secant method [“fast” implementation].

Given:

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

Procedure:

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

$$\varepsilon = (2)(\text{TOL})$$

2. Manually set the root estimates at the first and second iterations based on the initial guess.

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

$$x_{\text{int}} = x_0 + 0.001$$

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 the secant method.

$$i = 2$$

```

while ( $\varepsilon > \text{TOL}$ ) and ( $i < i_{\max}$ )
    (a) Update root estimate.

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


    (b) Calculate error.

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


    (c) Store current and previous estimates for next iteration.

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

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


    (d) Increment loop index.

        
$$i = i + 1$$

end

```

Return:

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

Algorithm 2:

Secant method ["return all" implementation].

Given:

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

Procedure:

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

$$\varepsilon = (2)(\text{TOL})$$

2. Preallocate $\mathbf{x} \in \mathbb{R}^{i_{\max}}$ to store the estimates of the root at each iteration.
3. Manually set the root estimates at the first and second iterations based on the initial guess.

$$x_1 = x_0$$

$$x_2 = 1.01x_0$$

4. Find the root using the secant method.

$$i = 2$$

```
while ( $\varepsilon > \text{TOL}$ ) and ( $i < i_{\max}$ )  
    (a) Update root estimate.  
        
$$x_{i+1} = \frac{x_{i-1}f(x_i) - x_i f(x_{i-1})}{f(x_i) - f(x_{i-1})}$$
  
    (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^*)

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