DEN: Roots of functions numerically

Definition.
By a **root** of a function f we mean any number r such that $f(r) = 0$.

Fact.
Let f be a function on an interval $[a,b]$. If $f(a) \cdot f(b) < 0$ (i.e. $f(a)$ and $f(b)$ have opposite signs) and f is continuous on $[a,b]$, then f must have a root in the interval $[a,b]$.

Algorithm (bisection method for finding root of f)
Given: a function f continuous on interval $[a,b]$ and a tolerance ε.
Assumption: $f(a)$ and $f(b)$ have opposite signs.

0. Set $a_0 = a$, $b_0 = b$. Let $k = 0$.

1. Assumption: $f(a_k)$ and $f(b_k)$ have opposite signs.
Let $m_k = \frac{1}{2}(a_k + b_k) = a_k + \frac{1}{2}(b_k - a_k)$.

2. If $f(m_k) = 0$ or $|b_k - a_k| < \varepsilon$ then algorithm stops, output is m_k. Otherwise:
If $f(a_k)$ and $f(m_k)$ have opposite signs, set $a_{k+1} = a_k$, $b_{k+1} = m_k$, increase k by one and go back to step **1**.
If $f(m_k)$ and $f(b_k)$ have opposite signs, set $a_{k+1} = m_k$, $b_{k+1} = b_k$, increase k by one and go back to step **1**.

Algorithm (Newton method for finding root of a function f)
Given: a differentiable function f and a tolerance ε.

0. Choose x_0. Let $k = 0$.

1. Let $x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$.
If $|x_{k+1} - x_k| < \varepsilon$ or $|f(x_{k+1})| < \varepsilon$ then the algorithm stops, output is x_{k+1}.
Otherwise increase k by one and go back to step **1**.

Theorem.
Let f be a function on an interval $[a,b]$ such that $f(a) \cdot f(b) < 0$. Assume that f is twice continuously differentiable on (a,b) and $f' \neq 0$, $f'' \neq 0$ on (a,b).
If $x_0 \in (a,b)$ is chosen so that $f(x_0) \cdot f''(x_0) > 0$, then the sequence $\{x_n\}$ generated by the Newton methodou converges to a root $r \in [a,b]$ of f.

Stopping conditions:
- $|x_k - x_{k-1}| < \varepsilon$ absolute difference
- $\frac{|x_k - x_{k-1}|}{|x_k|} < \varepsilon$ relative difference
- $|f(x_k)| < \varepsilon$ value (residual)

Fact.
Let f be a function and $r \in \mathbb{R}$ its root. Assume that there is a neighborhood U of r and $m_1 > 0$ such that f is differentiable on U and $m_1 \leq |f'|$ on U.
Then for $\hat{r} \in U$ we have the estimate $|r - \hat{r}| \leq \frac{1}{m_1}|f(\hat{r})|$.

Definition.
Consider a sequence $\{x_k\}$ that converges to some x_∞.
We say that it converges with order (or rate) of convergence $q > 0$ if there is C such that
$|x_\infty - x_{k+1}| \leq C|x_\infty - x_k|^q$ for all k.
Sometimes this is called the Q-order.

We say that it converges with R-order (or R-rate) of convergence $q > 0$ if there is a sequence $\{e_k\}$ of upper estimates for $|x_\infty - x_k|$, that is, $|x_\infty - x_k| \leq e_k$ for all k, such that it Q-converges to zero.

Definition.
Consider a certain iterating method for finding roots of functions. We say that it is a **method of order** q, or that it has **error of order** q, where $q > 0$, if it satisfies the following condition:
Whenever this method produces a sequence $\{x_k\}$ converging to a certain root r of a function f, this root is simple and the function sufficiently smooth, then $\{x_k\}$ converges to r with rate q.

Theorem.
Assume that a function f continuous on $[a,b]$ satisfies $f(a)\cdot f(b) < 0$. Then the sequence $\{m_k\}$ generated by the bisection method with starting values $a_0 = a$, $b_0 = b$ converges to a root of f.
The bisection method is of linear order.

Theorem.
The Newton method is of order 2 for twice continuously differentiable functions.
For roots of higher multiplicity it is of order 1.

Algorithm (secant method for finding root of a function f)

Given: a continuous function f and a tolerance ε.

0. Choose x_0, x_1. Let $k = 1$.

1. Let $x_{k+1} = \frac{x_{k-1} f(x_k) - x_k f(x_{k-1})}{f(x_k) - f(x_{k-1})}$.
If $|x_{k+1} - x_k| < \varepsilon$ or $|f(x_{k+1})| < \varepsilon$ then algorithm stops, output is x_{k+1}.
Otherwise increase k by one and go back to step **1**.

Theorem.
The secant method is of order $\alpha = \frac{1+\sqrt{5}}{2} \approx 1.6$ for twice continuously differentiable functions.
For roots of higher multiplicity it is of order 1.

Definition.
Let φ be a function. By a **fixed point** of φ we mean any number x_f satisfying $\varphi(x_f) = x_f$.

Fact.
If a function φ is continuous on some closed bounded interval I and $\varphi[I] \subseteq I$, then φ has a fixed point $x_f \in I$.

Algorithm (fixed-point iteration)

Given: a continuous function φ and a tolerance ε.
0. Choose x_0. let $k = 0$.
1. Let $x_{k+1} = \varphi(x_k)$.
If $|x_{k+1} - x_k| < \varepsilon$ then algorithm stops, output is x_{k+1}.
Otherwise increase k by one and go back to step **1**.

Theorem.
Let φ be a function, $x_0 \in \mathbb{R}$ and $x_{k+1} = \varphi(x_k)$ for $k \in \mathbb{N}$. If $x_k \to x_f$ and φ is continuous at x_f, then x_f is a fixed point.

Definition.
Let φ be a function on an interval I. We say that it is **contractive** there, or that it is a **contraction**, if there exists $q < 1$ such that for all $x, y \in I$ we have

$$|\varphi(x) - \varphi(y)| \leq q \cdot |x - y|.$$

Theorem. (Banach's fixed-point theorem)
Let φ be a contractive function on $I = [a, b]$ with coefficient q such that $\varphi[I] \subseteq I$. Then there exists exactly one fixed point x_f of the function φ in I.
Moreover, for all choices of $x_0 \in I$ the sequence given by $x_{k+1} = \varphi(x_k)$ converges to x_f and satisfies

$$|x_f - x_{k+1}| \leq q|x_f - x_k| \quad \text{and} \quad |x_f - x_{k+1}| \leq \frac{q}{1-q}|x_{k+1} - x_k|.$$

Theorem.
Assume that function φ defined on an interval I has a continuous derivative on the interior I^O of I. If there is $q < 1$ such that $|\varphi'(t)| \leq q$ on I^O, then φ is a contraction on I with coefficient q.

Algorithm (relaxation for fixed-point iteration)

Given: a continuous function φ and a tolerance ε.

1. We choose some relaxation parameter λ and apply fixed-point iteration to $\varphi_\lambda(x) = \lambda\varphi(x) + (1-\lambda)x$.