MS-C2105 - Introduction to Optimization
Lecture 8

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Outline of this lecture

Revision of calculus

General optimisation problems

Optimality conditions - unconstrained problems

Convexity of functions

One dimensional optimisation methods - line search

- Bisection method
- Newton's method

Reading: Taha: Chapter 20; Winston: Chapter 11

Tools from differential calculus

We focus on devising optimisation methods for general problems.

- No assumption of linearity.
- We consider first unconstrained problems.
- Later, we will include the consideration of constrains.

Let us first revise some important tools we will use.

Definition 1 (Limits and continuity)

Let $f : \mathbb{R} \to \mathbb{R}$ be a function. We say that $\lim_{x\to a} f(x) = c$ if, as x becomes closer to a, $f(x)$ becomes closer to c (asymptotically). Moreover, f is continuous at point a if $\lim_{x\to a} f(x) = f(a)$. If $\lim_{x\to a} f(x) = f(a)$ for all $a \in \mathbb{R}$, then function f is continuous.

Tools from differential calculus

Definition 2 (Differentiation)

The derivative of a function $f : \mathbb{R} \to \mathbb{R}$ at $x = a$ (denoted $f'(a)$) is defined as

$$\lim_{\Delta x \to 0} \frac{f(a + \Delta x) - f(a)}{\Delta x}.$$

If $f'(x)$ exists for every $x \in \mathbb{R}$, then f is differentiable.

Differentiability is used to infer local behaviour of f

- It is direction dependent: $\lim_{\Delta x \to 0^+}$ and $\lim_{\Delta x \to 0^-}$. If they are the same for all x, $f(x)$ is continuous.
- $f'(a)$ can be thought as the slope of f at a.
- $f'(x) > 0$ means that the function is increasing at x; i.e., for a arbitrarily small $\epsilon > 0$, $f(x + \epsilon) > f(x)$.
- Likewise, $f'(x) < 0$ means that the function is decreasing at x.

Tools from differential calculus

Function	Derivative
a	0
x	1
$af(x)$	$af'(x)$
$f(x)+g(x)$	$f'(x)+g'(x)$
x^n	nx^{n-1}
e^x	e^x
a^x	$a^x\ln(a)$
$\ln(x)$	$\frac{1}{x}$
$[f(x)]^n$	$nf(x)^{n-1}f'(x)$
$e^{f(x)}$	$e^{f(x)}f'(x)$
$a^{f(x)}$	$a^{f(x)}f'(x)\ln a$
$\ln f(x)$	$\frac{f'(x)}{f(x)}$
$f(x)g(x)$	$f(x)g'(x)+f'(x)g(x)$
$\frac{f(x)}{g(x)}$	$\frac{g(x)f'(x)-f(x)g'(x)}{g(x)^2}$

Tools from differential calculus

Definition 3 (n-order derivative)

The n^{th}-order derivative $f^{(n)}(a)$ of f at a is the derivative of $f^{(n-1)}(a)$ at a.

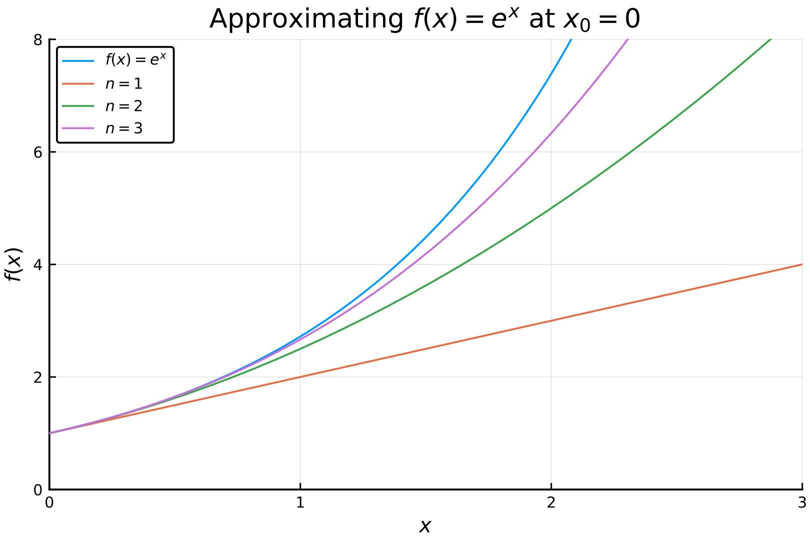
Higher derivatives are employed in Taylor series expansions, which are in turn used as general local approximations of function values.

Theorem 4 (Taylor's theorem)

Let f be n-times differentiable on an open interval containing x and x_0. Then, the Taylor series expansion of f is

$$\begin{aligned} f(x) &= f(x_0) + \frac{1}{1} f'(x_0)(x - x_0) + \frac{1}{1 \times 2} f''(x_0)(x - x_0)^2 + \dots \\ &+ \frac{1}{n!} f^{(n)}(x_0)(x - x_0)^n + R_{n+1}(x) \\ &= \sum_{i=0}^{n} \frac{1}{i!} f^{(i)}(x_0)(x - x_0)^i + R_{n+1}(x) \end{aligned}$$

Tools from differential calculus



Tools from differential calculus

Remarks:

1. The term $R_n(x)$ is called the residual. For some $c \in (x_0, x)$,

$$R_{n+1}(x) = \frac{f^{(n+1)}(c)}{(n+1)!}(x - x_0)^{n+1}.$$

2. In particular, if $|f^{(n+1)}| \leq M$, then

$$R_{n+1}(x) \leq \frac{M|x - x_0|^{n+1}}{(n+1)!}.$$

3. Taylor's approximation is the Taylor's expansion without the residual term.
4. if $x_0 = 0$, Taylor's series reduce to the Maclaurin's series.

Nonlinear optimisation models

Nonlinear programming models are a more general class of optimisation problems.

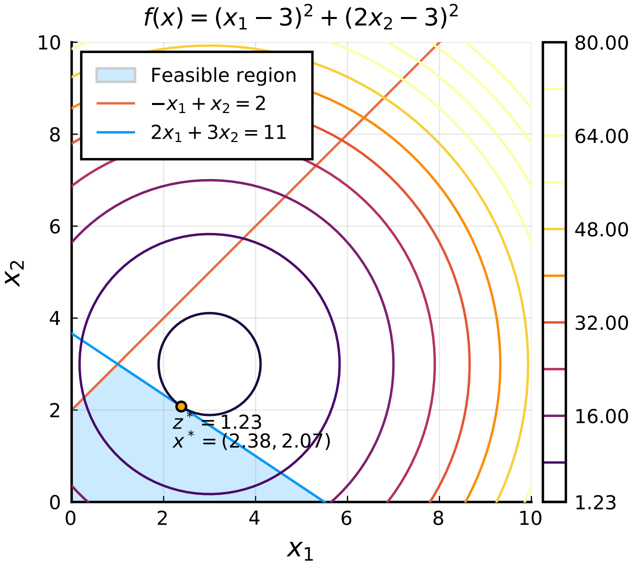
$$\begin{aligned} \text{min. } & f(x) \\ \text{s.t.: } & g_i(x) \leq 0, i = 1, \dots, m. \\ & x \in X \end{aligned}$$

Clearly, LP/ MIP models are a particular cases, to which dedicated efficient methods exist.

For more general problems

- optimal points might not be extreme points or be on the boundary of the feasible region.
- guarantees of global optimality might not exist.

Nonlinear optimisation models

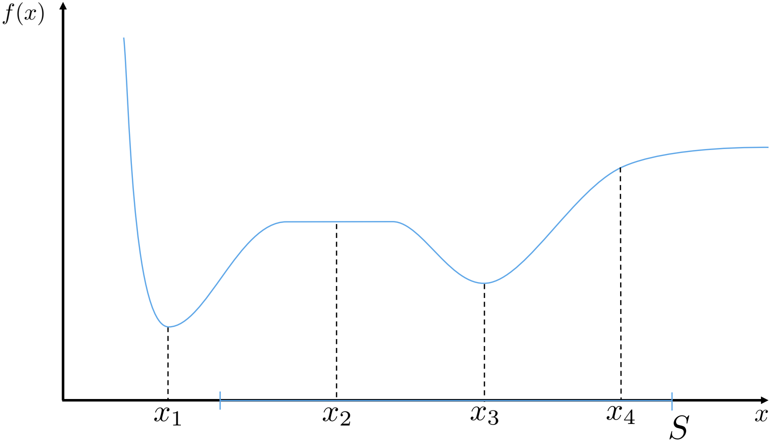


General optimality conditions

Let $f : \mathbb{R}^n \to \mathbb{R}$. Consider the problem (P) : min. $\{f(x) : x \in S\}$. Some important terminology:

- feasible solution: $x \in S$;
- local optimal solution: $\overline{x} \in S$ that has a neighbourhood $N_\epsilon(\overline{x}) = \{x : ||x - \overline{x}|| \leq \epsilon\}$ for some $\epsilon > 0$ such that $f(\overline{x}) \leq f(x)$ for each $x \in S \cap N_\epsilon(\overline{x})$.
- global optimal solution: $\overline{x} \in S$ with $f(\overline{x}) \leq f(x)$ for all $x \in S$.

General optimality conditions



Necessary optimality conditions

Candidates to local optima must be critical points.

Theorem 5 (First-order optimality condition)

Let $\overline{x}$ be a local optimum for f in $N_\epsilon(\overline{x})$ and assume that f is differentiable. Then $f'(\overline{x}) = 0$.

Proof.

Suppose $\overline{x}$ is a local minimum. Then, there exists $\delta > 0$ for which $f(\overline{x}) \leq f(x)$ for all $x \in (\overline{x} - \delta, \overline{x} + \delta) \subset N_\epsilon(\overline{x})$.

1. for any $h \in (0, \delta)$, it holds that $\frac{f(\overline{x}+h)-f(\overline{x})}{h} \geq 0$.
   Thus, $\lim_{h \to 0^+} \frac{f(\overline{x}+h)-f(\overline{x})}{h} = f'(\overline{x}) \geq 0$.
2. for any $h \in (-\delta, 0)$, it holds that $\frac{f(\overline{x}+h)-f(\overline{x})}{h} \leq 0$.
   Thus, $\lim_{h \to 0^-} \frac{f(\overline{x}+h)-f(\overline{x})}{h} = f'(\overline{x}) \leq 0$.

From the above, we conclude that $f'(\overline{x}) = 0$. $\square$

Sufficient optimality conditions

The condition $f'(x) = 0$ does not imply local optimality.

- Points satisfying $f'(x) = 0$ are called stationary.
- An additional certificate is necessary to state optimality.

Theorem 6 (n^{th}-order optimality condition)

Suppose f has a stationary point at x_0 and that $f'(x_0) = \cdots = f^{(n-1)}(x_0) = 0$, while $f^{(n)}(x_0) \neq 0$. If $f^{(n)}$ is continuous, then

1. *if n is even and $f^{(n)}(x_0) > 0$, then x_0 is a local minimum.*
2. *if n is even and $f^{(n)}(x_0) < 0$, then x_0 is a local maximum.*
3. *if n is odd, then x_0 is an inflection point.*

Sufficient optimality conditions

Proof.

With the first $n-1$ derivatives vanishing, using Taylor's expansion, we have that

$$f(x) - f(x_0) = R_n(x_0) = \frac{f^{(n)}(c)}{n!}(x - x_0)^n$$

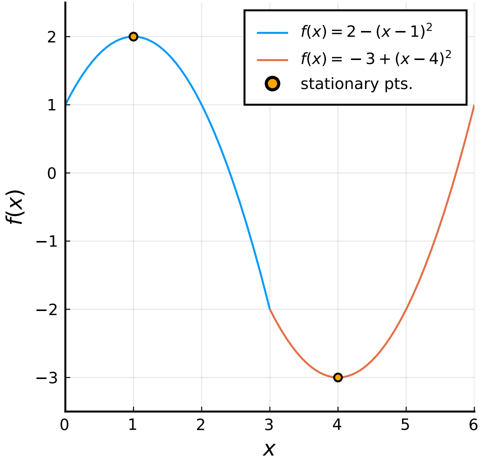
For n even, $(x - x_0)^n > 0$. $f^{(n)}(c)$ and $f^{(n)}(x^0)$ agree in sign, since they are arbitrarily close. Thus, $f(x) - f(x_0)$ will agree in sign of $f^{(n)}(x^0)$. If n is odd, $(x - x_0)^n$ and thus $f(x) - f(x_0)$ have opposite signs for $x < x_0$ and $x > x_0$. □

Sufficient conditions are posed considering $n = 2$, i.e.,

- if $f'(x_0) = 0$ and $f''(x_0) > 0$ then x_0 is a local minimum.
- if $f'(x_0) = 0$ and $f''(x_0) < 0$ then x_0 is a local maximum.
- if $f'(x_0) = 0$ and $f''(x_0) = 0$ then x_0 is a inflection point.

Necessary and sufficient optimality conditions

Example: $f(x) = \begin{cases} 2 - (x-1)^2, & \text{if } x < 3 \\ -3 + (x-4)^2, & \text{if } x \geq 3. \end{cases}$



Convexity of functions

Convexity is a key feature in optimisation. In convex optimisation problems, local optimality always implies global optimality.

Definition 7 (Convexity of a function)

Let $f : \mathbb{R}^n \to \mathbb{R}$. The function f is said to be convex if

$$f(\lambda x_1 + (1-\lambda)x_2) \leq \lambda f(x_1) + (1-\lambda)f(x_2)$$

for each $x_1, x_2 \in \mathbb{R}^n$ and for each $\lambda \in (0, 1)$.

Remarks:

- f is concave if $-f$ is convex;
- if strict inequality holds, f is strictly convex.
- A nonconvex function can be convex within a specific set (e.g., $f(x) = x^3$ for $x \geq 0$)

Convexity of functions

Examples of convex functions:

1. $f(x) = a^\top x + b$;
2. $f(x) = e^x$;
3. $f(x) = x^p$ on $\mathbb{R}_+$ for $p \leq 0$ or $p \geq 1$; concave for $0 \leq p \leq 1$.
4. $f(x) = ||x||_p$ (p-norm);

Convexity of functions

Convexity preserving operations:

1. let $f_1, \dots, f_k : \mathbb{R}^n \to \mathbb{R}$ be convex. Then these are convex:
   - $f(x) = \sum_{j=1}^{k} \alpha_j f_j(x)$ where $\alpha_j > 0$ for $j = 1, \dots, k$;
   - $f(x) = \max\{f_1(x), \dots, f_k(x)\}$;
2. $f(x) = \frac{1}{g(x)}$ on S, where $g : \mathbb{R}^n \to \mathbb{R}$ is concave and $S = \{x : g(x) > 0\}$;
3. $f(x) = g(h(x))$, where $g : \mathbb{R} \to \mathbb{R}$ is a nondecreasing convex function and $h : \mathbb{R}^n \to \mathbb{R}$ is convex.
4. $f(x) = g(h(x))$, where $g : \mathbb{R}^m \to \mathbb{R}$ is convex and $h : \mathbb{R}^n \to \mathbb{R}^m$ is affine: $h(x) = Ax + b$ with $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$.

Example: $f(a) = (b - a^\top x)^2 + ||a||^2$. Is this function convex?

Convexity and optimality condition

The importance of convexity derives from this fundamental result:

Theorem 8 (Necessary and sufficient conditions)

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a convex differentiable function. Then any local optimum $\overline{x}$ of f is also a global optimum.

Proof.

By contradiction. **Assume that $\overline{x}$ is a local minimum in $N_\epsilon(\overline{x})$**, but not a global minimum. Then, for some x we will have $f(x) < f(\overline{x})$. As f is convex, we have for every $\lambda \in [0, 1]$ that

$$\begin{aligned} f(\lambda\overline{x} + (1-\lambda)x) &\leq \lambda f(\overline{x}) + (1-\lambda)f(x) \\ &< \lambda f(\overline{x}) + (1-\lambda)f(\overline{x}) = f(\overline{x}). \end{aligned}$$

Now, $1-\lambda$ can be made arbitrarily small such that $\lambda\overline{x} + (1-\lambda)x$ belongs to $N_\epsilon(\overline{x})$, contradicting the **initial assumption**. $\square$

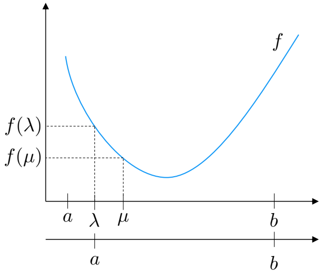
Line search methods

Most optimisation methods will iteratively search for points that satisfy first-order conditions.

One-dimensional (line) searches seek for $\overline{x}$ such that $f'(\overline{x}) = 0$.

Theorem 9 (Line search reduction)

Let $f : \mathbb{R} \to \mathbb{R}$ be convex over the interval $[a, b]$, and let $\lambda, \mu \in [a, b]$ such that $\lambda < \mu$. If $f(\lambda) > f(\mu)$, then $f(z) \geq f(\mu)$ for all $z \in [a, \lambda]$. If $f(\lambda) \leq f(\mu)$, then $f(z) \geq f(\lambda)$ for all $z \in [\mu, b]$.



Line search: bisection method

The bisection method uses gradient information to infer whether function is increasing or decreasing.

- Iteratively trim the search space (using Theorem 9).
- Relies on first-order conditions (presuming convexity/ sufficiency).

The main idea of the method is

1. if $f'(\lambda_k) = 0$, then λ_k is a minimiser.
2. if $f'(\lambda_k) > 0$, then, for $\lambda > \lambda_k$, we have $f(\lambda) \geq f(\lambda_k)$ since f is convex. Therefore, the new search interval becomes $[a_{k+1}, b_{k+1}] = [a_k, \lambda_k]$.
3. if $f'(\lambda_k) < 0$, the new search interval becomes $[a_{k+1}, b_{k+1}] = [\lambda_k, b_k]$.
4. To maximise interval reduction, we set $\lambda_k = \frac{1}{2}(b_k + a_k)$.

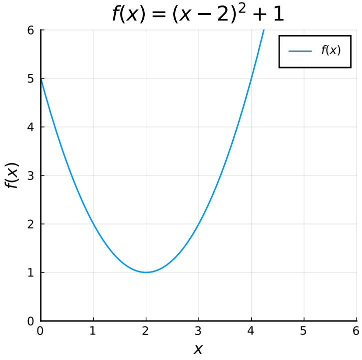
Line search: bisection method

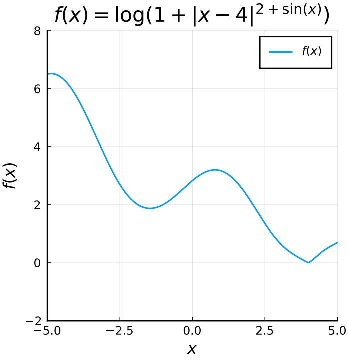
Algorithm Bisection method (minimisation)

```
1: initialise. tolerance l > 0, [a_0, b_0] = [a, b], k = 0.
2: while b_k − a_k > l do
3:     λ_k = (b_k + a_k)/2 and evaluate f′(λ_k).
4:     if f′(λ_k) = 0 then return λ_k.
5:     else if f′(λ_k) > 0 then
6:         a_{k+1} = a_k, b_{k+1} = λ_k.
7:     else
8:         a_{k+1} = λ_k, b_{k+1} = b_k.
9:     end if
10:    k = k + 1.
11: end while
12: return λ̄ = (a_k + b_k)/2.
```

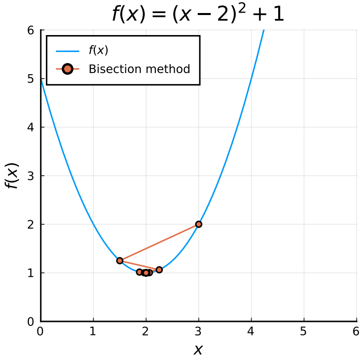
Remark: if maximising, the condition in Line 5 must be replaced with $f'(x) < 0$ and concavity is presumed.

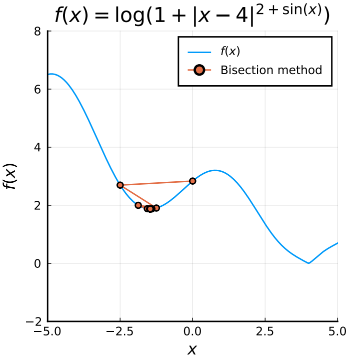
Bisection method: example



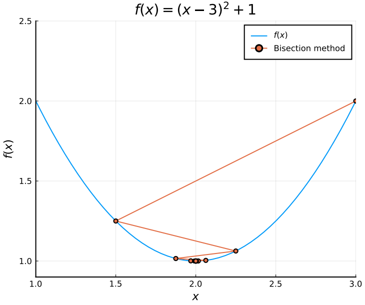


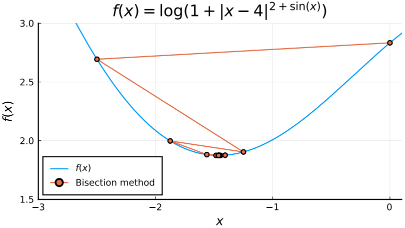
Bisection method: example





Bisection method: example (zoom in)





Line search: Newton's method

Explores the quadratic approximation q of f at a given point x_k:

$$q(x) = f(x_k) + f'(x_k)(x - x_k) + \frac{1}{2}f''(x_k)(x - x_k)^2$$

Letting x_{k+1} be the point at which $q'(x) = 0$, we have

$$q'(x_{k+1}) = f'(x_k) + f''(x_k)(x_{k+1} - x_k) = 0,$$

which implies

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}.$$

Remarks:

1. The search terminates when $|x_{k+1} - x_k| < \epsilon$ or $|f'(x_k)| < \epsilon$.
2. The same as applying Newton-Raphson's method (for finding roots of functions) to first-order optimality condition.

Line search: Newton's method

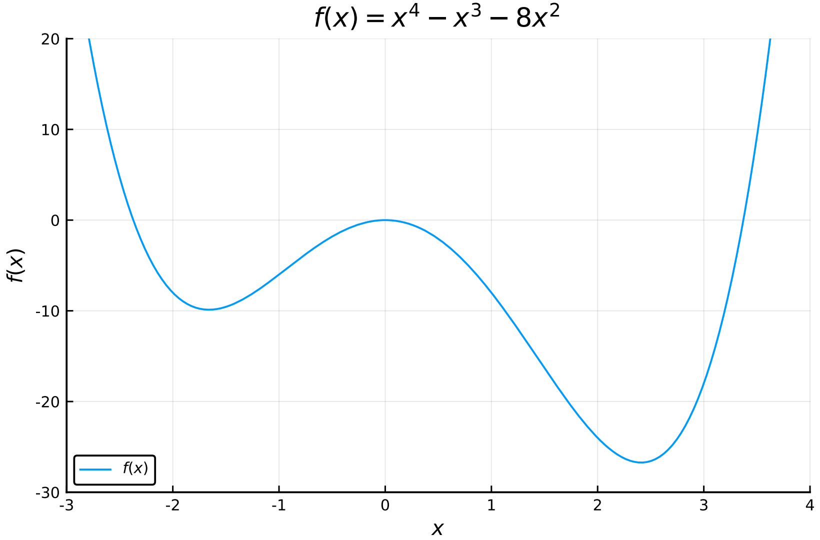
Algorithm Newton's method

1: **initialise.** tolerance $\epsilon > 0$, initial step size x_0, iteration count $k = 0$.
2: **while** $|f'(x_k)| > \epsilon$ **do**
3: $\quad x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}$.
4: $\quad k = k + 1$.
5: **end while**
6: **return** $\overline{x} = x_k$.

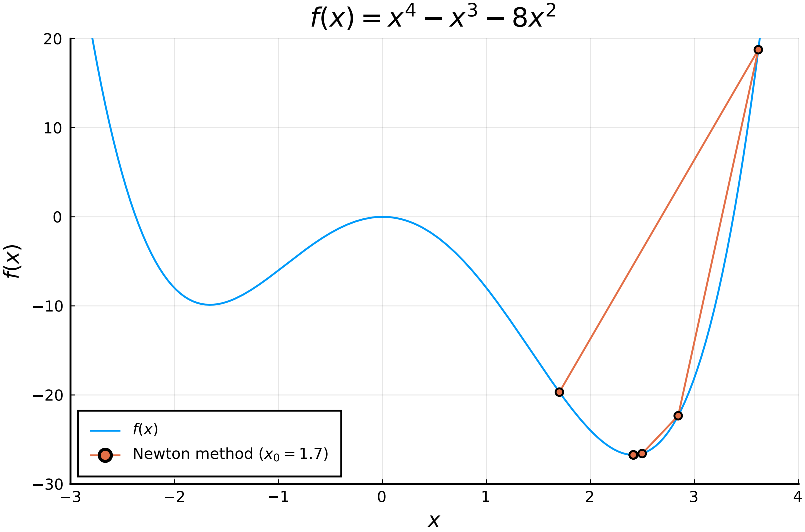
Remarks:

1. Newton's method is the backbone of several optimisation algorithms.
2. Has convergence issues if x_0 is too far away from optimal.
3. For quadratic problems, the approximation q is exact, meaning that only one iteration is needed.

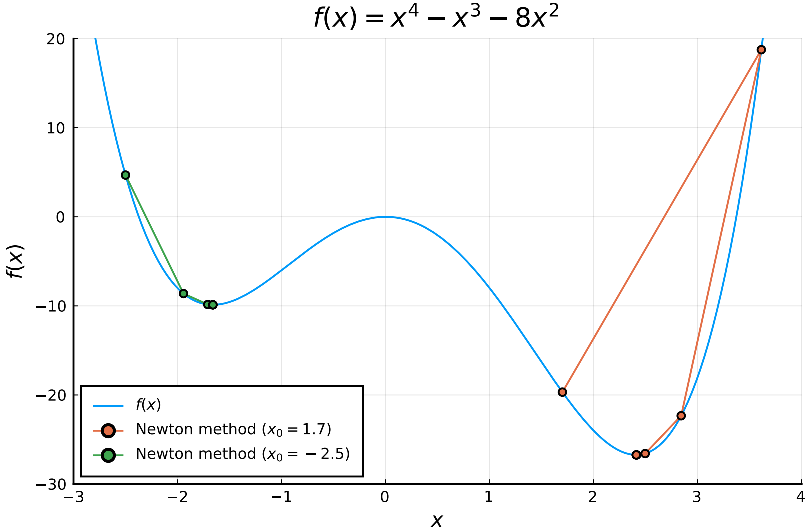
Newton's method: example



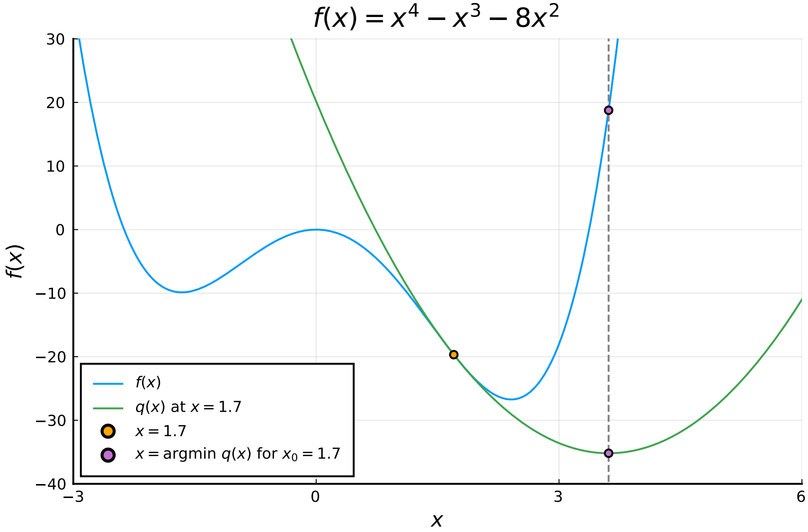
Newton's method: example



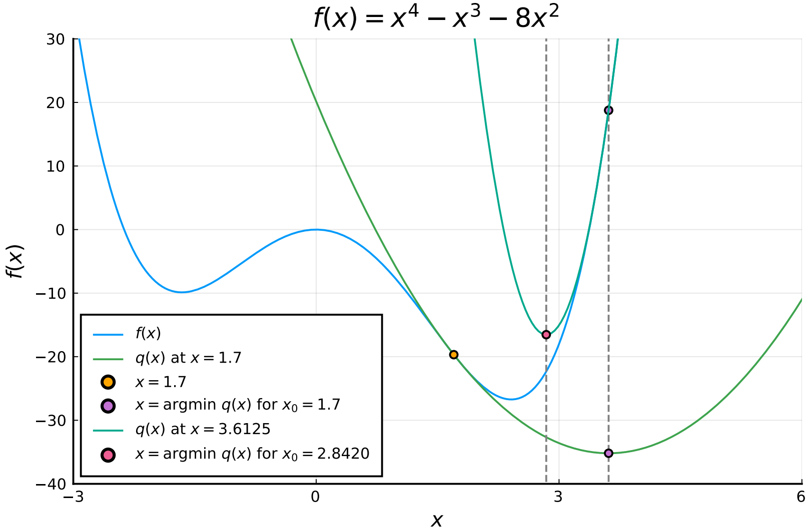
Newton's method: example



Newton's method: example



Newton's method: example



Newton's method: example