Continuous Mathematics Memorandum

1 Derivatives and Taylor's theorem

- A function f is **continuous** at x if
$$\lim_{h\to 0} f(x+h) = f(x).$$
f is continuous if it is continuous at every point of its domain.

- A function $f : D \to \mathbb{R}$, where $D \subseteq \mathbb{R}$, is called **differentiable** at x if
$$\lim_{h\to 0} \frac{f(x+h) - f(x) - dh}{h} = 0$$
holds for some $d \in \mathbb{R}$. The value d is called the derivative at x. f is called differentiable if it is differentiable at every point of D.

- If f and g are continuous/differentiable*, then so are:

  $f + g$, *
  cf, for a constant $c \in \mathbb{R}$, *
  f^n, for a constant $n \in \mathbb{N}$, *
  fg, *
  $f \circ g$, *
  $\max(f, g)$,
  $|f|$,
  $\exp(f)$, *
  f^α, for a constant $\alpha \in \mathbb{R}$, **where f is strictly positive**, *
  $\frac{f}{g}$, **where g is nonzero**, *
  $\log(f)$, **where f is strictly positive**. *

- Rules for differentiation:

  $\frac{d}{dx}(f+g) = \frac{df}{dx} + \frac{dg}{dx}$,
  $\frac{d}{dx}(cf) = c\frac{df}{dx}$,
  $\frac{d}{dx}(fg) = f\frac{dg}{dx} + g\frac{df}{dx}$,
  $\frac{d}{dx}(\frac{f}{g}) = \frac{g\frac{df}{dx} - f\frac{dg}{dx}}{g^2}$,
  $\frac{d}{dx}(g \circ f) = (\frac{dg}{dx} \circ f)\frac{df}{dx}$.

- **Taylor's Theorem:** Let $f : D \to \mathbb{R}$ be a function, $k \geq 0$ an integer and $x_0, x_0 + h \in D$. Then, if f and its first $k+1$ derivatives exist and are continuous on an interval containing x_0 and $x_0 + h$, the following holds:
$$f(x_0+h) = f(x_0) + h\frac{df}{dx}(x_0) + \frac{h^2}{2!}\frac{d^2f}{dx^2}(x_0) + \cdots + \frac{h^k}{k!}\frac{d^kf}{dx^k}(x_0) + \frac{h^{k+1}}{(k+1)!}\frac{d^{k+1}f}{dx^{k+1}}(\xi),$$

for some $\xi \in (x0, x0 + h)$.
Equivalently, if we let $h = x - x_0$, we can write

$$f(x) = \hat{f}_k(x) + e_{k+1}(x, x_0),$$

where $\hat{f}_k(x)$ is the **Taylor polynomial of order** k,

$$\hat{f}_k(x) = \sum_{i=0}^{k} \frac{(x - x_0)^k}{k!} \frac{d^k f}{dx^k}(x_0),$$

and $e_{k+1}(x, x_0)$ is the **error term**,

$$e_{k+1}(x, x_0) = \frac{(x - x_0)^{k+1}}{(k+1)!} \frac{d^{k+1} f}{dx^{k+1}}(\xi).$$

We can Bound the approximation: if $\underline{C} \leq \frac{d^{k+1} f}{dx^{k+1}} \leq \overline{C}$, then

$$\hat{f}_k(x) + \underline{C} \leq f(x) \leq \hat{f}_k(x) + \overline{C}.$$

- A function $f : D \to \mathbb{R}$, for some $D \subseteq \mathbb{R}^n$, is called a **multivariate function** or a **scalar field**. Differentiating f with respect to a variable x, while holding all others constant, is called a **partial derivative** and written $\frac{\partial f}{\partial x}$.
- **Clairaut's theorem:** if f is continuous in x and y, then $\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x}$.
- We can collect all the partial derivatives in a vector and define the derivative of the function f:

$$\frac{df}{d\boldsymbol{x}} = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

- The **Hessian** of f, which is the equivalent of the second derivative, is a matrix that collects all the second partial derivatives:

$$\boldsymbol{H}(f) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{pmatrix}$$

- A function $f : \mathbb{R}^n \to \mathbb{R}^m$ is sometimes called a **vector field**. We can break down f in the form of a vector, $\begin{pmatrix} f_1(\boldsymbol{x}) \\ f_2(\boldsymbol{x}) \\ \vdots \\ f_n(\boldsymbol{x}) \end{pmatrix}$. What acts as the derivative of f is called the **Jacobian**:

$$\boldsymbol{J}(\boldsymbol{f}) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n} \end{pmatrix}$$

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- For $f : \mathbb{R}^n \to \mathbb{R}$, $\boldsymbol{H}(f) = \boldsymbol{J}(\frac{df}{dx})^T$
- Rules for differentiation of multivariate functions:

$\frac{d}{d\boldsymbol{x}}(f+g) = \frac{df}{d\boldsymbol{x}} + \frac{dg}{d\boldsymbol{x}}$,
$\frac{d}{d\boldsymbol{x}}(cf) = c\frac{df}{d\boldsymbol{x}}$,
$\frac{d}{d\boldsymbol{x}}(fg) = f\frac{dg}{d\boldsymbol{x}} + g\frac{df}{d\boldsymbol{x}}$,
$\frac{d}{d\boldsymbol{x}}(\frac{f}{g}) = \frac{g\frac{df}{d\boldsymbol{x}} - f\frac{dg}{d\boldsymbol{x}}}{g^2}$,
If $f : \mathbb{R}^n \to \mathbb{R}$ and $g : \mathbb{R} \to \mathbb{R}$ then,
$\frac{d}{d\boldsymbol{x}}(g \circ f) = (\frac{dg}{d\boldsymbol{x}} \circ f)\frac{df}{d\boldsymbol{x}}$,
If $\boldsymbol{f} : \mathbb{R}^m \to \mathbb{R}^n$ and $g : \mathbb{R}^n \to \mathbb{R}$ then,
$\frac{d}{d\boldsymbol{x}}(g \circ \boldsymbol{f}) = \boldsymbol{J}(\boldsymbol{f})^T(\frac{dg}{d\boldsymbol{x}} \circ \boldsymbol{f})$,
$\boldsymbol{J}(\boldsymbol{f}+\boldsymbol{g}) = \boldsymbol{J}(\boldsymbol{f}) + \boldsymbol{J}(\boldsymbol{g})$,
$\boldsymbol{J}(c\boldsymbol{f}) = c\boldsymbol{J}(\boldsymbol{f})$,
$\boldsymbol{J}(\boldsymbol{A}\boldsymbol{f}) = \boldsymbol{A}\boldsymbol{J}(\boldsymbol{f})$,
$\boldsymbol{J}(\boldsymbol{f}^T\boldsymbol{g}) = \boldsymbol{g}^T\boldsymbol{J}(\boldsymbol{f}) + \boldsymbol{f}^T\boldsymbol{J}(\boldsymbol{g})$,
$\boldsymbol{J}(f\boldsymbol{g}) = \boldsymbol{g}\frac{df}{d\boldsymbol{x}}^T + f\boldsymbol{J}(\boldsymbol{g})$,
$\boldsymbol{J}(\boldsymbol{g} \circ \boldsymbol{f}) = (\boldsymbol{J}(\boldsymbol{g}) \circ \boldsymbol{f})\boldsymbol{J}(\boldsymbol{f})$.

- Standard derivatives:

$\frac{d}{d\boldsymbol{x}}\boldsymbol{a}^T\boldsymbol{x} = \frac{d}{d\boldsymbol{x}}\boldsymbol{x}^T\boldsymbol{a} = \boldsymbol{a}$,
$\frac{d}{d\boldsymbol{x}}\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} = (\boldsymbol{A} + \boldsymbol{A}^T)\boldsymbol{x}$,
$\boldsymbol{J}(\boldsymbol{x}) = \boldsymbol{I}$,
$\boldsymbol{J}(\boldsymbol{A}\boldsymbol{x}) = \boldsymbol{A}$.

- **Taylor's theorem (multivariate functions):** Let $D \subseteq \mathbb{R}^n$. Fix a vector $\boldsymbol{x_0}$ and $\boldsymbol{h} = (h_1, h_2, \ldots, h_n)$ be another vector. Let $k \geq 0$ be an integer. If f and its first $k+1$ derivatives exist and are continuous on a region including $\boldsymbol{x_0}$ and $\boldsymbol{x_0} + \boldsymbol{h}$, then

$$\begin{aligned} f(\boldsymbol{x}+\boldsymbol{h}) = f(\boldsymbol{x}) & \\ &+ \left[\left(h_1\frac{\partial}{\partial x_1} + \cdots + h_n\frac{\partial}{\partial x_n}\right)f\right](\boldsymbol{x}) \\ &+ \frac{1}{2!}\left[\left(h_1\frac{\partial}{\partial x_1} + \cdots + h_n\frac{\partial}{\partial x_n}\right)^2 f\right](\boldsymbol{x}) \\ &+ \ldots \\ &+ \frac{1}{k!}\left[\left(h_1\frac{\partial}{\partial x_1} + \cdots + h_n\frac{\partial}{\partial x_n}\right)^k f\right](\boldsymbol{x}) \\ &+ \frac{1}{(k+1)!}\left[\left(h_1\frac{\partial}{\partial x_1} + \cdots + h_n\frac{\partial}{\partial x_n}\right)^{k+1} f\right](\boldsymbol{x} + \xi\boldsymbol{h}) \end{aligned}$$

2 Optimization

- The classic **optimization** problem is: find $\underset{\boldsymbol{x}\in F}{min} f(\boldsymbol{x})$ (or, more often, $\underset{\boldsymbol{x}\in F}{argmin} f(\boldsymbol{x})$). f is called the **objective function**, F is called the **feasible set**. If f takes values in $\mathbb{R}^n$ and F is the whole $\mathbb{R}^n$, the problem is called **unconstrained**. The **standard** form of a **constrained** F is:

$$F = \{x \in \mathbb{R}^n | g_1(\boldsymbol{x}) = 0, \ldots, g_l(\boldsymbol{x}) = 0, h_1(\boldsymbol{x}) \geq 0, \ldots, h_m(\boldsymbol{x}) \geq 0\},$$

where $g_i(\boldsymbol{x}) = 0$ are l **equality constraints** and $h_i(\boldsymbol{x}) \geq 0$ are m **inequality constrains**. If the constraints force $F = \emptyset$, the problem is called **infeasible** or **inconsistent**. If there is no minimum because the function can take arbitrarily low values, the problem is called **unbounded**.

- A **local minimum** for a function f is a point $\boldsymbol{x} \in F$ such that

$$f(\boldsymbol{x}) \leq f(\boldsymbol{x} + \boldsymbol{h})$$

for sufficiently small $\boldsymbol{h}$.

- $\boldsymbol{x_0}$ is a **stationary point** (or a **critical point**) if $\frac{df}{d\boldsymbol{x}}(\boldsymbol{x_0}) = 0$
- global minima $\subseteq$ local minima $\subseteq$ stationary points
- **Optimization in 1 dimension:**
  - Find all stationary points.
  - Classify them into local minima, local maxima and points of inflection (if the first nonzero derivative is of odd order, then we have a stationary point of inflection), otherwise we have a local minimum/maximum if that nonzero derivative is positive/negative.
  - Check only the local minimums disocovered.
- In multiple dimension, a stationary point can be a local minimum, local maximum, or a saddle point (the local behaviour of f near $\boldsymbol{x}$ depends on which coordinate you approach from).
- A symmetric matrix $\boldsymbol{A}$ is called **positive definite/positive semidefinite/negative definite/negative semidefinite** if $\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} > 0/\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} \geq 0/\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} < 0/\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} \leq 0$ for all nonzero $\boldsymbol{x}$. If it satisfies none of those, it is called **indefinite**.
- Positive definiteness properties:
  (i) $\boldsymbol{A}$ is positive definite/positive semidefinite if and only if all its eigenvalues (or pivots) are $> 0/\geq 0$.
  (ii) $\boldsymbol{A}$ is positive (semi)definite if and only if $-\boldsymbol{A}$ is negative (semi)definite.
  (iii) The sum of positive semidefinite matrices is positive semidefinite. The sum of a positive definite and a positive (semi)definite matrix is positive definite.
  (iv) For any symmetric matrix $\boldsymbol{C}$, $\boldsymbol{C} - \lambda\boldsymbol{I}$ is positive definite/positive semidefinite as long as $\lambda </\leq$ the smallest eigenvalue of $\boldsymbol{C}$.
  (v) if $\boldsymbol{A}$ and $\boldsymbol{B}$ are positive (semi)definite matrices of the same size, then so are:
    (a) $c\boldsymbol{A}$, for any constant $c > 0$,
    (b) $\boldsymbol{A}^{-1}$, which exists when $\boldsymbol{A}$ is positive definite,
    (c) any upper-left submatrix of $\boldsymbol{A}$,
    (d) $\boldsymbol{A}\boldsymbol{B}\boldsymbol{A}$,
    (e) $\boldsymbol{C}^T\boldsymbol{A}\boldsymbol{C}$, for any matrix $\boldsymbol{C}$ of full rank,
    (f) $\boldsymbol{A} - \boldsymbol{v}\boldsymbol{v}^T$, if $\boldsymbol{v}^T\boldsymbol{A}\boldsymbol{v} < 1$

    We can guarantee positive semidefiniteness in (e) if C is not of full rank and in (f) if the inequality is not strict.
- A set $D \subseteq \mathbb{R}^n$ is called convex if, for all $\boldsymbol{x_1}, \boldsymbol{x_2} \in D$ and $\alpha \in (0, 1)$,

$$(1 - \alpha)\boldsymbol{x_1} + \alpha\boldsymbol{x_2} \in D$$

- A function $f : D \in \mathbb{R}$, for some convex set $D \subseteq \mathbb{R}^n$, is convex/strictly convex/concave/strictly concave if for all $\boldsymbol{x_1}, \boldsymbol{x_2} \in D$ and $\alpha \in (0, 1)$,

$$f((1 - \alpha)\boldsymbol{x_1} + \alpha\boldsymbol{x_2}) \leq / < / \geq / > (1 - \alpha)f(\boldsymbol{x_1}) + (\boldsymbol{x - 2})$$

- For a convex function, global minima = local minima = stationary points.
- f is convex if and only if $\boldsymbol{H}(f)$ is positive semidefinite.// f is strictly convex if $\boldsymbol{H}(f)$ is positive definite.

- Convexity properties:

  (i) Only the linear function is both convex and concave.

  (ii) $f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}$ is convex/concave when $\boldsymbol{A}$ is is positive/negative semidefinite and strictly convex concave when $\boldsymbol{A}$ is positive/negative definite.

  (iii) If f and g are (strictly) convex functions, then so are:

    (a) $f + g$,

    (b) cf, for any constant $c > 0$,

    (c) $h(\boldsymbol{x}) = f(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b})$ (to preserve strict convexity, $\boldsymbol{A}$ must have full rank).

    (d) $max(f, g)$,

    (e) $exp(f)$.

  (iv) Let $f : \mathbb{R}^n \in \mathbb{R}, g_1, \ldots, g_n : \mathbb{R}^m \in \mathbb{R}$. If f is (strictly) convex, and for each $i = 1, \ldots, n$, either (a) f is (strictly) increasing in its i-th argument and g_i is (strictly) convex, or (b) f is (strictly) decreasing in its i-th argument and g_i is (strictly) concave, then $f \circ \boldsymbol{g}$ is (strictly) convex.

- **Jensen's inequality**: If f is convex and X any random variable taking values in its domain,

$$f(E[x]) \leq E[f(x)]$$

  .

- If g is a strictly increasing function, then

$$\underset{x \in F}{argmin} f(x) = \underset{x \in F}{argmin}\, g(f(x))$$

- If g is a $1-1$ function, then

$$g(\underset{x \in F}{argmin} f(x)) = \underset{x \in F}{argmin}\, f(g(x))$$

- **Optimization with equality constraints. Method of Lagrange multipliers.** We need to solve:

$$\text{minimize } f(\boldsymbol{x}) \text{ subject to } g_1(\boldsymbol{x}) = 0, \ldots, g_l(\boldsymbol{x}) = 0$$

  We form the **Lagrangian**

$$\Lambda(\lambda_1, \ldots, \lambda_l, \boldsymbol{x}) = f(\boldsymbol{x}) - \lambda_1 g_1(\boldsymbol{x}) - \cdots - \lambda_l g_l(\boldsymbol{x})$$

  and we use the fact that the stationary points of f are all stationary points of Λ, thus only needing to find and check the stationary points of Λ.

- **Optimization with inequality constraints.** We need to solve:

$$\text{minimize } f(\boldsymbol{x}) \text{ subject to } h_1(\boldsymbol{x}) \geq 0, \ldots, h_m(\boldsymbol{x}) \geq 0$$

  . If, at the minimum, $h_i(\boldsymbol{x}) > 0$, constraint i will be called **slack**, otherwise it will be called **tight**. Not knowing from the beginning which constraints are slack and which are tight, we'll have to try all the 2^m cases in the worst case. After having fixed this, we solve the equality constrained problem that arises (with the tight constrains) using the previous method and we check if the slack constraints are satisfied. We eliminate those that don't and we check all the remaining possible solutions.

3 Algorithms for numerical integration

- If $f, F : \mathbb{R} \in \mathbb{R}$ and $\frac{dF}{dx} = f$, then
$$\int_a^b f(x)dx = F(a) - F(b)$$

- Single strip integration rules and their error bounds for approximating $\int_0^{2l} f(x)dx$:

Rule (X_1)	Approximation ($X_1[f,0,2l]$)	Error bounded by $err(X_1)[f,0,2l]$
Midpoint	$2lf(l)$	$-\frac{1}{3}l^3\frac{d^2f}{dx^2}$
Trapzeium	$l(f(0)+f(2l))$	$\frac{2}{3}l^3\frac{d^2f}{dx^2}$
Simpson's	$\frac{l}{3}(f(0)+4f(l)+f(2l))$	$\frac{1}{90}l^5\frac{d^4f}{dx^4}$
Boole's	$\frac{1}{45}(7f(0)+32f(\frac{l}{2})+16f(l)+32f(\frac{3l}{2})+7f(2l)$	$-\frac{1}{15120}l^7\frac{d^6f}{dx^6}$

- Composite strip integration rules and their error bounds for approximating $\int_a^b f(x)dx$, with $x_i = a + i\frac{b-a}{n}$:

Rule (X_n)	Approximation ($X_n[f,a,b]$)	Error bounded by $err(X_n)[f,a,b]$
Midpoint	$\frac{b-a}{n}(f(\frac{x_0+x_1}{2})+f(\frac{x_1+x_2}{2})+\cdots+f(\frac{x_{n-1}+x_n}{2}))$	$-\frac{(b-a)^3}{24n^2}\frac{d^2f}{dx^2}$
Trapzeium	$\frac{b-a}{2n}(f(x_0)+2f(x_1)+\cdots+2f(x_{n-1})+f(x_n))$	$\frac{(b-a)^3}{12n^2}\frac{d^2f}{dx^2}$
Simpson's	$\frac{b-a}{3n}(f(x_0)+4f(x_1)+2f(x_2)+\cdots+4f(x_{n-1})+f(x_n))$	$\frac{(b-a)^5}{180n^4}\frac{d^4f}{dx^4}$

- **Monte Carlo Integration:** For approximating $\int_R f(\boldsymbol{x})d\boldsymbol{x}$, pick a large number of continuous random variables $\boldsymbol{X_1}, \boldsymbol{X_2}, \ldots, \boldsymbol{X_N}$, all independently uniformly distributed over R, and the estimate is:
$$MC_N[f,r] = A(R)\frac{1}{N}\sum_i f(\boldsymbol{X_i}),$$
where $A(R)$ denotes the length/area/volume of region R.

- **Standard error** is equal to $\sqrt{\frac{\hat{V}}{N}}$

- Properties:

  (i) $E[MC_N[f,R]] = \int_R f(\boldsymbol{x})d\boldsymbol{x}$

  (ii) $Var[MC_N[f,R]] = \frac{V}{N}$, where V can be approximated by
$$\hat{V} = \frac{A(R)^2}{N}\sum_i f^2(\boldsymbol{x}) - \left(\frac{A(R)}{N}\sum_i f(\boldsymbol{x})\right)^2$$

  (iii) $P\left[|err(MC_N)[f,R]| \geq \epsilon\right] \to 0$ as $N \to \infty$, for any $\epsilon > 0$

  (iv) For large N, $err(MC_N)[f,R]$ approaces the normal distribution $N(0, \frac{V}{N})$. The same holds for $\hat{V}$.

4 Accuracy

- If $u \in \mathbb{R}$ is the number we want to approximate and $\tilde{u} \in \mathbb{R}$ its approximation, there are three ways to measure the error:

  $\tilde{u} - u$ is the **error**,

  $|\tilde{u} - u|$ is the **absolute error**,

  $\frac{|u-u|}{|u|}$ is the **relative error**.

- Source of error:

  Truncation error is the error introduced when approximating an infinite procedure by a finite procedure. For example, when we use a finite Taylor polynomial to approximate a function, we have truncated a power series and the remainder term is the truncation error. Or when we perform numerical integration we have truncated a hypothetical infinite sum (perfectly accurate for continuous functions) by the finite sum over n strips.

  Roundoff error (also called numerical error) is error introduced by approximating a real number, for example in floating-point format. A common mistake is to think that roundoff error is called truncation error because it involves truncating the binary representation of a floating-point number. Roundoff error is not truncation error.

- If we have an **iterative numerical algorithm** A_n that attempts to approximate a true value x^* by starting with an initial guess x_0 and repeatedly refining the answer $x_{n+1} = f(x_n)$, let the error at the n-th step be $\epsilon_n = x_n - x^*$. The first goal of the algorithm is for the error to converge to zero: $|\epsilon_n| \to 0$. Moreover, if that happens, we can say that:

  (i) A_n **converges linearly** if, for some $0 < a < 1$, $\frac{|\epsilon_{n+1}|}{\epsilon_n} \to a$.

  (ii) A_n **converges sublinearly** if $\frac{|\epsilon_{n+1}|}{\epsilon_n} \to 1$,
  a special case, **logarithmic convergence**, if $\frac{\epsilon_{n+2}-\epsilon_{n+1}}{\epsilon_{n+1}-\epsilon n} \to 1$.

  (iii) A_n **converges superlinearly** if $\frac{|\epsilon_{n+1}|}{|\epsilon_n|} \to 0$,
  a special case, **order-q convergence**, if $\frac{|\epsilon_{n+1}|}{|\epsilon_n|^q} \to a$ for $a > 0, q > 1$.

- If A_n converges with order q, A_{2n} converges with order q^2.

5 Algorithms for root finding

- **Interval bisection (1 dimension).** Start with a **bracket** (a_0, b_0) where $f(a_0)$ and $f(b_0)$ have different signs, which implies that f has a root in this interval. Given a bracket (a_n, b_n), we can refine it to a bracket exactly half as big, by testing the sign of $f(x_n)$, where $x_n = \frac{a_n+b_n}{2}$. Either (a_n, x_n) or (x_n, b_n) becomes the new bracket (a_{n+1}, b_{n+1}). This algorithm has linear convergence.

- **Newton's method (1 dimension).** Start with an initial points x_0 and apply iteratively:

$$x_{n+1} = x_n - \frac{f(x_n)}{\frac{df}{dx}(x_n)}$$

  . Let f have two continuous derivatives and $f(x^*) = 0$, then:

  (i) If $x_n \in I = (x^* - c, x^* + c)$ and

$$A(c) = \frac{\max\limits_{\beta \in I} \left|\frac{d^2 f}{dx^2}(\beta)\right|}{\min\limits_{\alpha \in I} \left|\frac{d^2 f}{dx^2}(\alpha)\right|},$$

  then $|\epsilon_{n+1}| \leq \frac{A(c)}{2} {\epsilon_n}^2$

  (ii) If $x_0 \in I$, and further $\frac{cA(c)}{2} < 1$, then Newton's method converges at least quadratically to x^*.

  (iii) If $x^* \in (m - c, m + c)$ and $I = (m - 2c, m + 2c)$,

$$B(c) = \frac{\max\limits_{\beta \in I} \left|\frac{d^2 f}{dx^2}(\beta)\right|}{\min\limits_{\alpha \in I} \left|\frac{d^2 f}{dx^2}(\alpha)\right|},$$

  and further $\frac{cB(c)}{2} < 1$, then Newton's method starting with $x_0 = m$ converges at least quadratically.

(iv) Such an interval I exists if $\frac{df}{dx}(x^*) \neq 0$.

- **Secant method (1 dimension).** Start with two initial points, x_0 and x_1, and apply iteratively:

$$x_{n+1} = x_n - \frac{f(x_n)(x_n - x_{n-1})}{f(x_n) - f(x_{n-1})}$$

. This method has order-ϕ convergence.

- If $f : \mathbb{R} \to \mathbb{R}$ has at least two continuous derivatives and $f(x) = 0$, then, for any $a, b \neq 0$,

$$\frac{f(x+a)}{a} - \frac{f(x+b)}{b} = \frac{a-b}{2}\frac{d^2f}{dx^2}(\xi)$$

- **Newton's method (d dimensions).** Start with an initial point $\boldsymbol{x_0}$ and apply iteratively:

$$\boldsymbol{x_{n+1}} = \boldsymbol{x_n} - (\boldsymbol{J}(\boldsymbol{f})(\boldsymbol{x_n}))^{-1}\boldsymbol{f}(\boldsymbol{x_n})$$

However, in practice, we should find a solution to $(\boldsymbol{J}(\boldsymbol{f})(\boldsymbol{x_n}))\boldsymbol{\Delta x} = -\boldsymbol{f}(\boldsymbol{x_n})$ and set $\boldsymbol{x_{n+1}} = \boldsymbol{x_n} + \boldsymbol{\Delta x}$.

- **Broyden's method (d dimensions).** In the Newton's method for d dimension, instead of using $\boldsymbol{J}(\boldsymbol{f})$, we will use its approximation at every step, $\hat{\boldsymbol{J}}_{\boldsymbol{n}}$. If we let $\boldsymbol{y_{n-1}} = \boldsymbol{f}(\boldsymbol{x_{n-1}})$, $\boldsymbol{y_n} = \boldsymbol{f}(\boldsymbol{x_n})$, $\boldsymbol{\Delta y} = \boldsymbol{y_n} - \boldsymbol{y_{n-1}}$ and $\boldsymbol{\Delta x} = \boldsymbol{x_n} - \boldsymbol{x_{n-1}}$, $\hat{\boldsymbol{J}}_{\boldsymbol{n}}$ will have to satisfy the secant equation:

$$\boldsymbol{y_n} = \boldsymbol{y_{n-1}} + \hat{\boldsymbol{J}}_{\boldsymbol{n}}(\boldsymbol{x_n} - \boldsymbol{x_{n-1}})$$

. This, along with other conditions, will lead to

$$\hat{\boldsymbol{J}}_{\boldsymbol{n}} = \hat{\boldsymbol{J}}_{\boldsymbol{n-1}} + \frac{\boldsymbol{\Delta y} - \hat{\boldsymbol{J}}_{\boldsymbol{n-1}}\boldsymbol{\Delta x}}{\boldsymbol{\Delta x}^2}\boldsymbol{\Delta x}^T,$$

$$\boldsymbol{x_{n+1}} = \boldsymbol{x_n} + \boldsymbol{\Delta x}, \text{ where } \hat{\boldsymbol{J}}_{\boldsymbol{n}}\boldsymbol{\Delta x} = \boldsymbol{f}(\boldsymbol{x_n})$$

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6 Algorithms for optimization

- **Golden section search (1 dimension).** Start with an initial bracket $(a0, b0, c0)$ satisfying $a0 < b0 < c0, f(b0) < f(a0), f(b0) < f(c0)$, which guarantees that a local minimum will lie there. This will ideally also be close to the ratio: $b0 - a0 : c0 - b0 \simeq \phi : 1 - \phi$. Afterwards, for refining a bracket (a_n, b_n, c_n), pick a point z in the larger interval between (a_n, b_n) and (b_n, c_n) that also splits that part in the same $\phi : 1 - \phi$ ratio. If $b_n - a_n > c_n - b_n / c_n - b_n > b_n - a_n$, pick $z = a_n + \phi(b_n - a_n)/z = c_n - \phi(c_n - b_n)$. If $f(z) < f(b)$, set $(a_{n+1}, b_{n+1}, c_{n+1})$ equal to $(a_n, z, b_n)/(b_n, z, c_n)$, otherwise, to $(z, b_n, c_n)/(a_n, b_n, z)$. This method has linear convergence.

- **Gradient Descent Methods (d dimensions)** The general concept works as follows: given $\boldsymbol{x_n}$, and perhaps some information about the gradient (denoted by $\boldsymbol{g_n}$ here) and hessian of f at or near $\boldsymbol{x_n}$, choose a direction $\boldsymbol{d_n}$ and a step size α_n, the next iteration being

$$\boldsymbol{x_{n+1}} = \boldsymbol{x_n} + \alpha_n \boldsymbol{d_n}$$

. Desirable properties for $\boldsymbol{d_n}$ and α_n:

(i) d_n should be a descent direction: $\frac{df(\boldsymbol{x_n} + \alpha \boldsymbol{d_n})}{d\alpha} < 0 \iff \boldsymbol{g_n}^T \boldsymbol{d_n} < 0$,

(ii) the directions $\boldsymbol{d_n}, \boldsymbol{d_{n-1}}, \ldots$ should not veer widely, with each some previous work

(iii) α_n should loosely minimise $f(\boldsymbol{x_n} + \alpha_n \boldsymbol{d_n})$

(iv) the method must not reach a stop:

$$\sum_{n=1}^{\infty} \alpha_n = \infty$$

Methods of choosing $\boldsymbol{d_n}$:

- **co-ordinate gradient descent:** $\boldsymbol{d_n}$ repeatedly cycles through unit vectors $\boldsymbol{e_i}$ in some order, minimizing each direction on its own,
- **steepest decent:** $\boldsymbol{d_n} = -\boldsymbol{g_n}$,
- **conjugate gradient descent**(approximate): $\boldsymbol{d_n} = -\boldsymbol{g_n} + \boldsymbol{d_{n-1}} \frac{\boldsymbol{g_n - g_{n-1} g_n}}{\boldsymbol{gn-1}^T \boldsymbol{g_{n-1}}}$.

Methods of choosing α_n:

- use a one-dimensional minimization algorithm (like the golden ratio search or a one-dimensional Newton method),
- **backtracking** method: choose an initial step $\alpha_n = \alpha^{'}$ and repeatedly multiply it by a factor $0 < \rho < 1$ until we satisfy either:

  $f(\boldsymbol{x_n} + \alpha_n \boldsymbol{d_n}) < f(\boldsymbol{x_n})$
  $f(\boldsymbol{x_n} + \alpha_n \boldsymbol{d_n}) < f(\boldsymbol{x_n}) + \sigma \alpha_n \boldsymbol{g_n}^T \boldsymbol{d_n}$ (**Armijo rule**)

  $\alpha^{'}$ can be chosen as:

  $$\alpha^{'} = \alpha_{n-1} \frac{\boldsymbol{g_{n-1}}^T \boldsymbol{d_{n-1}}}{\boldsymbol{g_n}^T \boldsymbol{d_n}}$$

- **Newton method (d dimensions):** apply Newton's method for root finding to the gradient, and the iterationa becomes:

  $$\boldsymbol{x_{n+1}} = \boldsymbol{x_n} - (\boldsymbol{H}(f)(\boldsymbol{x_n}))^{-1} \boldsymbol{g_n}$$

- **Quasi-Newton Methods (d dimensions)** very similar to those for root finding, but have to give a slighly different formula for $\hat{\boldsymbol{H}}_{\boldsymbol{n}}$, since it has to remain symmetric:

$$\hat{\boldsymbol{H}}_{\boldsymbol{n}} = \hat{\boldsymbol{H}}_{\boldsymbol{n-1}} + \frac{\boldsymbol{\Delta g \Delta g}^T}{\boldsymbol{\Delta g}^T \boldsymbol{\Delta x}} - \frac{\hat{\boldsymbol{H}}_{\boldsymbol{n-1}} \boldsymbol{\Delta x \Delta x}^T \hat{\boldsymbol{H}}_{\boldsymbol{n-1}}}{\boldsymbol{\Delta x}^T \hat{\boldsymbol{H}}_{\boldsymbol{n-1}} \boldsymbol{\Delta x}}$$

and, similarly, $\boldsymbol{x_n} = \boldsymbol{x_{n-1}} - \hat{\boldsymbol{H}}_{\boldsymbol{n}} \boldsymbol{g_n}$.