Overview

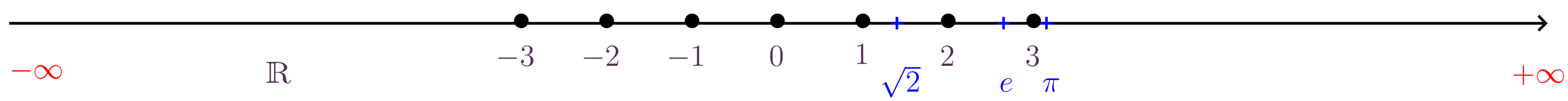
Motivation: A first application of function approximation is to devise procedures to find the roots or zeros of a real function of single variavle $f\colon [a,b] \to \mathbb{R}$. The procedures devised for scalar functions can be subsequently extended to multivariate and vector-valued functions

- Calculus of real functions of one variable
- The root-finding process
  - Root locations: qualitative plots
  - Interval reduction: bisection

- Calculus is the study of *continuous* change, based upon the fundamental concepts of:

Real numbers $\mathbb{R}$	Functions $f: D \to C$	Function limits $\lim_{x\to c} f(x)$

- Real numbers measure continuous quantities and are graphically represented by the *real axis*



- f associates input x from D (domain) to *a single* output y from C (codomain)

  $y = f(x)$ states that y is the single output of the function f for given input x

  f is *one-to-one* if output y is produced by *a single* input x, in which case $x = f^{-1}(y)$, f^{-1}: $C \to D$ is the inverse function of f.

- The limit $\lim_{x\to c} f(x)$ describes the function f *at an infinity of points* near to c.

  Formal definition: For any $\varepsilon > 0$ there exists a $\delta(\varepsilon)$ such that from $|x - c| < \delta(\varepsilon)$ it follows that $|f(x) - L| < \varepsilon$.

- Problem: $f\colon \mathbb{R} \to \mathbb{R}$, find $\mathcal{Z} = \{z_k\colon f(z_k) = 0, k \in \mathcal{K}\}$ *the null set* of f
- Assume $\mathcal{K} \subset \mathbb{N}$, $|\mathcal{K}| = m > 0$, $\mathcal{Z} = \{z_k\colon f(z_k) = 0, k = 1, 2, \ldots, m\}$
- Root-finding phases:
  - *Root localization*. Find intervals $[a_k, b_k]$, $a_k \leqslant z_k \leqslant b_k$, $z_j \notin [a_k, b_k]$ for $j \neq k$

$$f(a_k)\, f(b_k) \leqslant 0$$

  - *Interval reduction (optional)*. Find sequence of smaller intervals containing a root: $[a_k^{(n)}, b_k^{(n)}] \subset [a_k^{(n-1)}, b_k^{(n-1)}] \subset \ldots [a_k^{(1)}, b_k^{(1)}] \subset [a_k^{(0)}, b_k^{(0)}] = [a_k, b_k]$
  - *Root refinement*. Find approximation $z_k^{(n)}$ of z_k to within:
    - → *maximum residual* δ, $|f(z_k^{(n)})| \leqslant \delta$
    - → *maximum error* e, $|z_k^{(n)} - z_k| \leqslant e$ replaced usually by $|z_k^{(n+1)} - z_k^{(n)}| \leqslant e$
    - → *maximum relative error* ε

$$\frac{|z_k^{(n)} - z_k|}{|z_k|} \leqslant \varepsilon, \text{replaced by } \frac{|z_k^{(n+1)} - z_k^{(n)}|}{|z_k^{(n+1)}|} \leqslant \varepsilon$$

- How hard is the root-finding problem?
- Define root-finding *mathematical problem*, mapping $F: X \to Y$
  - Input set $X = \{f: \mathbb{R} \to \mathbb{R}\}$, the set of functions whose zero sets are sought
  - Output set $Y = \mathcal{Z} = \{z_k: f(z_k) = 0, k = 1, 2, \ldots, m\}$, the zero sets
- Note: the mathematical root-finding problem F is different from $f \in X$
- Example:
  - Find z solution of $f(x) = a\,x + b = 0$ for given $a, b \in \mathbb{R}$, $a \neq 0$.

$$X = \mathbb{R} \backslash \{0\} \times \mathbb{R}, Y = \mathbb{R}, z_1 = F(a, b) = -b/a.$$

    F is differentiable and has condition number

$$\kappa = \|\boldsymbol{J}\|, \boldsymbol{J} = \left[\begin{array}{cc} \frac{\partial F}{\partial a} & \frac{\partial F}{\partial b} \end{array}\right] = \left[\begin{array}{cc} -\frac{b}{a^2} & -\frac{1}{a} \end{array}\right]$$

    Intuitively, for $a \cong \epsilon$, the root finding problem is *hard*, $\kappa \gg 1$.
- In general $\kappa = \|\delta F / \delta f\|$ Gateaux derivative w.r.t. to function f.

- Consider $f \in C^2(a,b)$, construct plot of $f : \mathbb{R} \to \mathbb{R}$

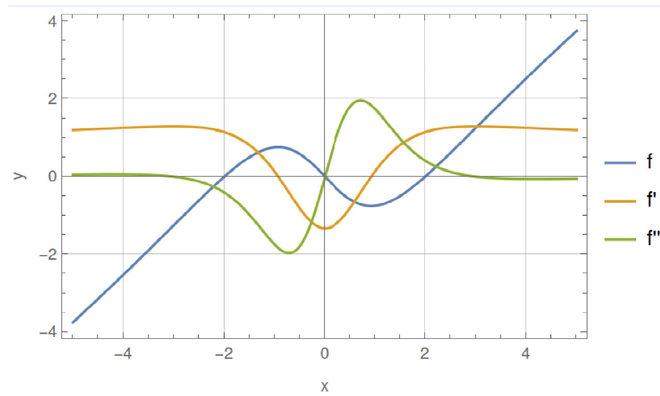


Figure 1. Qualitative function plot

x	$-\infty$	-2	-0.93	0	0.93	2	∞
f	$-\infty$	0		0		0	∞
f'	$+$	$+$	0	$-$	0	$+$	$+$
	$\nearrow$	$\nearrow$		$\searrow$		$\nearrow$	$\nearrow$
f''	0	$-$	$-$	0	$+$	$+$	0
		$\frown$	$\frown$		$\smile$	$\smile$	

Table 1. Root. Critical point. Inflection point. Increasing. Decreasing. Concave up, down.

- Qualitative function analysis furnishes root intervals $[a_k, b_k]$

- Idea:
  - Start from $[a,b]$ with $f(a)f(b) \leqslant 0$
  - Obtain smaller interval by computing $f(c)$, $c = (a+b)/2 = a + (b-a)/2$
    - $\rightarrow$ If $f(a)f(c) < 0$ then redefine $b = c$
    - $\rightarrow$ If $f(c)f(b) < 0$ then redefine $a = c$
- Obtain a sequence of intervals $[a_n, b_n]$ of decreasing length containing the root
  - $h_0 = (b-a)$
  - $h_n = h_0/2^n = b_n - a_n$
  - $z \in [a_n, b_n]$
- At iteration n, $z_n \cong c_n$

$$|z_n - z| \leqslant h_0/2^{n+1}$$

Linear order of convergence

$$\frac{|z_{n+1} - z|}{|z_n - z|} \cong \frac{1}{2} < 1.$$

- Computational complexity: *one* function evaluation ($f(c)$) per iteration

Algorithm - Bisection method

Input: f, a, b, ε
if $a > b$ then $\mathrm{swap}(a, b)$
$\mathrm{fa} \leftarrow f(a)$; $\mathrm{fb} \leftarrow f(b)$
$\delta \leftarrow b - a$
while $\delta > \varepsilon$ and $\mathrm{fa} \cdot \mathrm{fb} \leqslant 0$
  $\delta \leftarrow \delta/2$; $c \leftarrow a + \delta$; $\mathrm{fc} \leftarrow f(c)$
  if $\mathrm{fa} \cdot \mathrm{fc} \leqslant 0$
    $b \leftarrow c$; $\mathrm{fb} \leftarrow \mathrm{fc}$
  else
    $a \leftarrow c$; $\mathrm{fa} \leftarrow \mathrm{fc}$
return c

```
∴ function bisect(f,a,b,ε)
    if (a>b) a,b=b,a end
    fa=f(a); fb=f(b)
    δ=b-a; c=(a+b)/2
    while ((δ>ε) && (fa*fb<=0))
      δ=δ/2; c=a+δ; fc=f(c)
      if (fa*fc<=0)
        b,fb=c,fc
      else
        a,fa=c,fc
      end
    end
    return c
  end;
```

```
∴ f(x)=x^2-2; a=1; b=2; ε=0.01;
```

```
∴ [bisect(f,a,b,ε) sqrt(2.0)]
```

```
∴
```

- Computational complexity: *one* function evaluation ($f(c)$) per iteration

Algorithm - Bisection method

Input: f, a, b, ε
if $a > b$ then $\text{swap}(a, b)$
$\text{fa} \leftarrow f(a)$; $\text{fb} \leftarrow f(b)$
$\delta \leftarrow b - a$
while $\delta > \varepsilon$ and $\text{fa} \cdot \text{fb} \leqslant 0$
  $\delta \leftarrow \delta / 2$; $c \leftarrow a + \delta$; $\text{fc} \leftarrow f(c)$
  if $\text{fa} \cdot \text{fc} \leqslant 0$
    $b \leftarrow c$; $\text{fb} \leftarrow \text{fc}$
  else
    $a \leftarrow c$; $\text{fa} \leftarrow \text{fc}$
return c

```
∴ function bisect(f,a,b,ε)
    if (a>b) a,b=b,a end
    fa=f(a); fb=f(b)
    δ=b-a; c=(a+b)/2
    while ((δ>ε) && (fa*fb<=0))
      δ=δ/2; c=a+δ; fc=f(c)
      if (fa*fc<=0)
        b,fb=c,fc
      else
        a,fa=c,fc
      end
    end
    return c
  end;
```

```
∴ f(x)=x^2-2; a=1; b=2; ε=0.01;
```

```
∴ [bisect(f,a,b,ε) sqrt(2.0)]
```

$$\begin{bmatrix} 1.4140625 & 1.4142135623730951 \end{bmatrix} \tag{1}$$

```
∴
```