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1 Taylor

Let $f \in C^n[a,b]$ and assume $f^{(n+1)}$ exists in (a,b). Then for any $c, x \in [a,b]$ there is some ζ between c and x s.t.

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(c)(x-c)^k}{k!} + E_n(x) \tag{1}$$

where

$$E_n(x) = \frac{f^{(n+1)}(\zeta)(x-c)^{n+1}}{(n+1)!}$$

Equation (1) is called the Taylor expansion of f around c.

Observation. The famous *mean value theorem* is simply the case $n = 0$ of Taylor's expansion: if $f \in C[a,b]$ and f' exists on (a,b), then for $x, c \in [a,b]$

$$f(x) = f(c) + f'(\zeta)(x-c)$$

where ζ is between c and x. Take $x = b, c = a$ and the theorem appears:

$$f(b) - f(a) = f'(\zeta)(b-a)$$

We typically extend the Taylor approximation of f around a point r, where $r = x + h$ is an approximation some value of interest x. This is useful because said approximation gives

$$f(r) = f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \ldots + \frac{f^{(n)}(x)}{n!}h^n + E_n(h)$$

In other words, this strategy allows us to extend $f(r)$ in terms of x and h, the approximation and its error. Usually, r, h are unknown but h can be bounded.

2 Alg. de Horner: Polynomial evaluation

Consider

$$p(x) = \sum_{i=0}^{n} a_i x^i$$

We wish to compute $p(k)$ for a given $k \in \mathbb{R}$ minimizing the number of operations. Directly computing $a_0 + a_1 k_1 + \ldots$ leads to n sums. The ith term requires computing k^i, which means i product operations, for a totall of $\sum_{i=1}^{n} i = \frac{n(n+1)}{2}$ products. The total number of operations is then

$$\Theta = n + n(n+1)/2$$

The associated complexity is $O(n^2)$.

Horner's method consists of re-writing $p(x)$ so that the number of products is reduced. One writes

$$p(x) = a_0 + x b_0$$

where $b_{n-1} = a_n$ and for $0 \leq i < n-1$:

$$b_{i-1} = a_i + x b_i$$

Let $p(x) = 3 + 5x - 4x^2 + 0x^3 + 6x^4$, giving $n = 4$. Then $b_3 = 6$ and

$$b_2 = a_3 + x b_3 = 6x, \qquad b_1 = a_2 + x b_2 = -4 + x(6x),$$
$$b_0 = a_1 + x b_1 = 5 + x(-4 + x(6x))$$

This finally gives

$$p(x) = 3 + x b_0 = 3 + x(5 + x(-4 + x(6x)))$$

Here, one must perform n sums again but only n products. Thus, there are $\Theta = n + n = 2n$ operations, giving a complexity of $O(n)$ (in the operation space). See the algorithm below:

$$
\begin{array}{l}
\textbf{input } n; a_i, i = 0, \ldots, n; x \\
b_{n-1} \leftarrow a_n \\
\textbf{for } i = n-2 \textbf{ to } i = 0 \\
\qquad b_i = a_{i+1} + x * b_{i+1} \\
\textbf{od} \\
y \leftarrow a_0 + x * b_0 \\
\textbf{return } y
\end{array}
$$

It is easy to see in this code that the **for** loop performs $n-1$ iterations, in each of which a single sum and a single product are computed. The nth sum and nth product are performed in the computation of y, the final result.

A more polished version includes the last computatoin (the one in the assignment of y) within the loop and makes no use of indexes:

$$
\begin{array}{l}
\textbf{input } n; a_i, i = 0, \ldots, n; x \\
b \leftarrow a_n \\
\textbf{for } i = n-2 \textbf{ to } i = -1 \\
\qquad b = a_{i+1} + x * b \\
\textbf{od} \\
\textbf{return } b
\end{array}
$$

In Python,

```
def horner(coefs, x):
  n = len(coefs)-1
  b = coefs[n]

  for i in reversed(range(-1, n-1)):
    b = coefs[i+1] + x*b

  return b
```

It is trivial to adapt the code so that it returns the coefficients $b_0, \ldots, b_{n-1}$ and not the final result, if needed.

3 Error

Let $r, \overline{r}$ be two real numbers s.t. the latter is an approximation of the first. We define the **error** of the approximation to be $r - \hat{r}$, and

$$\Delta r = |r - \overline{r}|, \qquad \delta r = \frac{\Delta r}{|r|}$$

With r unknown the strategy is to work with a known bound of r.

4 Non-linear equations

The general problem is to find members of the set $\mathcal{R}_f$ of roots of $f \in \mathbb{R} \to \mathbb{R}$. The numerical strategy is to iteratively approximate some $r \in \mathcal{R}_f$ until some pre-established threshold in the error of approximation is met.

More formally, the numerical strategy produces a sequence $\{x_k\}_{k \in \mathbb{N}}$ which satisfies

- $\lim_{k\to\infty} \{x_k\} = r$ for some $r \in \mathcal{R}_f$
- Either $e(x_k) < e(x_{k-1})$ or, more strongly, $\lim_{k\to\infty} e(x_k) = 0$, where $e(x_k)$ is some appropriate measure of the error of approximation.

4.1 Bisection

A very simple procedure: if a root exists in $[a, b]$, it iteratively shrinks $[a, b]$ in halves (keeping the halves which contain the root) until the interval is of sufficiently small length or the root is found.

Theorem 1 (Intermediate value)**.** If f is continuous in $[a, b]$ and $f(a)f(b) < 0$, then $\exists r \in \mathcal{R}_f$ s.t. $r \in [a, b]$.

Assume f is continuous. A root exists in $[a, b]$ if $f(a)f(b) < 0$ (**Theorem 1**). If that is the case, the midpoint $(a + b)/2$ is taken as the approximation x_0. It is also trivial to observe that x_0 is *at most* at a distance of $(b - a)/2$ from the real root, so $e_0 = |x_0 - r| \leq (b - a)/2$.

If $f(x_0) = 0$ the procedure must end because a root was found. Otherwise, sufficies to find which half of the interval contains a root computing $f(a)f(c)$ and, if needed, $f(c)f(b)$.

The iterations may stop after reaching a maximum number of steps, when $|f(c)|$ is sufficiently close to zero, or when the error bound $|e_k| \leq (b_k - a_k)/2$ (where $[a_k, b_k]$ is the interval of this iteration) is sufficiently small.

(!) The algorithm not always converges. Take $f(x) = 1/x$. Clearly, it has no root. Yet setting $a = -1, b = 1$ in the initial iteration falsely passes the test. (The problem obviously is that f is not continuous in $[-1, 1]$.) If one sets

```
Input : a, b, δ, M, f
Output : Tupla de la forma: (r, cota de error)
f_a ← f(a)
f_b ← f(b)

if f_a * f_b > 0
    return ?
fi

for i = 1 to i = M do
    c ← a + (b − a)/2
    f_c ← f(c)
    if f_c = 0 then
        return (c, 0)
    fi
    ϵ = (b − a)/2
    if ϵ < δ then
        break
    fi
    if f_a * f_c < 0 then
        b ← c
        f_b = f(b)
    else
        a ← c
        f_a = f(a)
    fi
od
return (c, ϵ)
```

```
def bisection(f : callable, a : float, b : float, delta : float, M : int):

  s, e = f(a), f(b) # function values at (s)tart, (e)nd of interval

  if s*e > 0:
    raise ValueError("Interval [a, b] contains no root.")

  for i in range(M):

    c = a + (b-a)/2
    m = f(c) # value of f at (m)idpoint

    if m == 0:
      return c, 0

    e = (b-a)/2
    if e < delta:
      return c, e

    if s*m < 0:
      b = c
      e = f(b)
    else:
      a = c
      s = f(a)

  return c, e
```

Theorem 2. If $\{[a_i, b_i]\}_{i=0}^{\infty}$ are the intervals generated by the bisection method on iterations $i = 0, 1, \ldots$, then:

1. $\lim_{n\to\infty} a_n = \lim_{n\to\infty} b_n$ is a member of $\mathcal{R}_f$.
2. If $c_n = \frac{1}{2}(a_n + b_n), r = \lim_{n\to\infty} c_n$, then $|r - c_n| \leq \frac{1}{2^{n+1}}(b_0 - a_0)$

Proof. **(1)** It is clear that $a_i \leq a_{i+1}$ and $b_i \geq b_{i+1}$, since the interval on each iteration shrinks in one direction.

$\therefore$ a_n, b_n are monotonous.

But clearly a_n is bounded by b_0 and b_n is bounded by a_0.

$\therefore$ a_n, b_n are monotonous and bounded.

$\therefore$ Their limits exist.

It is also clear that the interval shrinks to half its size on each iteration:

$$b_n - a_n = \frac{1}{2}(b_{n-1} - a_{n-1}), \qquad n \geq 1 \tag{1}$$

By recurrence on (1),

$$b_n - a_n = \frac{1}{2^n}(b_0 - a_0), \qquad n \geq 0 \tag{2}$$

Then

$$\lim_{n\to\infty} a_n - \lim_{n\to\infty} b_n = \lim_{n\to\infty}(a_n - b_n) = \lim_{n\to\infty}\frac{1}{2^n}(b_0 - a_0) = 0 \tag{3}$$

$\therefore$ $\lim_{n\to\infty} a_n = \lim_{n\to\infty} b_n$.

Since the limit of a_n, b_n exists and f is by assumption continuous, the composition limit theorem applies and:

$$\begin{aligned}
&\lim_{n\to\infty}(f(a_n)\cdot f(b_n)) \\
&= \lim_{n\to\infty} f(a_n)\cdot \lim_{n\to\infty} f(b_n) && \{\text{Product of limits}\} \\
&= f\left(\lim_{n\to\infty} a_n\right)\cdot f\left(\lim_{n\to\infty} b_n\right) && \{\text{Composition limit theorem}\} \\
&= [f(r)]^2 && \left\{r = \lim_{n\to\infty} a_n\right\}
\end{aligned} \tag{4}$$

The invariant of the algorithm is $f(a_n)f(b_n) < 0$. But due to the last result,

$$\lim_{n\to\infty} f(a_n)f(b_n) \leq 0 \iff [f(r)]^2 \leq 0 \iff f(r) = 0$$

$\therefore$ $r = \lim_{n\to\infty} a_n = \lim_{n\to\infty} b_n$ is a root.

(2) Follows directly from result (2)

$$
\begin{aligned}
|r - c_n| &= \left| r - \frac{1}{2}(b_n - a_n) \right| \\
&\le \left| \frac{1}{2}(b_n - a_n) \right| \\
&= \left| \frac{1}{2^{n+1}}(b_0 - a_0) \right| && \{\text{Result (2)}\}
\end{aligned}
$$

4.2 Newton's method

Assume $r \in \mathcal{R}_f$ and $r = x + h$, with x an approximation of r and h its error. Assume f'' exists and is continuous in some I around x s.t. $r \in I$. What we explained on Taylor expansions around a point gives:

$$0 = f(r) = f(x + h) = f(x) + f'(x)h + O(h^2)$$

If x is sufficiently close to r, h is small and h^2 even smaller, so that $O(h^2)$ is unconsiderable:

$$0 \approx f(x) + hf'(x)$$

Therefore,

$$h \approx -\frac{f(x)}{f'(x)} \tag{1}$$

From this follows that $r = x + h$ is approximated by

$$r \approx x - \frac{f(x)}{f'(x)}$$

Since the approximation in (5) truncated the terms of $O(h^2)$ complexity, this new approximation is closer to r than x originally was. In other words, $x - f(x)/f'(x)$ is a better approximation to r than x itself.

Thus, if x_0 is an original approximation, we can define

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \tag{2}$$

to produce a sequence of approximations. This is the fundamental idea of Newton's method.

Input: x_0, M, δ, ϵ;
$v \leftarrow f(x_0)$
if $|v| < \epsilon$ **then return** x_0 **fi**
for $k = 1$ **to** $k = M$ **do**
  $x_1 \leftarrow x_0 - \dfrac{v}{f'(x_0)}$
  $v \leftarrow f(x_1)$
  if $|x_1 - x_0| < \delta \vee v < \epsilon$ **then**
    return x_1
  fi
  $x_0 \leftarrow x_1$
od
return x_0

The predicate $|x_1 - x_0| < \delta$ checks whether our algorithm is adjusting x in a negligible degree. If that is the case, we should stop.

Theorem 3. If f'' continuous around $r \in \mathcal{R}_f$ and $f'(r) \neq 0$, then there is some $\delta > 0$ s.t. if $|r - x_0| \leq \delta$, then:

- $|r - x_n| \leq \delta$ for all $n \geq 1$.
- $\{x_n\}$ converges to r
- The convergence is quadratic, i.e. there is a constant $c(\delta)$ and a natural N s.t. $|r - x_{n+1}| \leq c\,|r - x_n|^2$ for all $n \geq N$.

Proof. Let $e_n = r - x_n$ be the error in the nth approximation. Assume f'' is continuous and $f(r) = 0$, $f'(r) \neq 0$. Then

$$\begin{aligned} e_{n+1} &= r - x_{n+1} \\ &= r - \left(x_n - \frac{f(x_n)}{f'(x_n)}\right) \\ &= r - x_n + \frac{f(x_n)}{f'(x_n)} \\ &= \frac{e_n f'(x_n) + f(x_n)}{f'(x_n)} \end{aligned} \tag{3}$$

Thus, the error at any given iteration is a function of the error at the previous iteration. Now consider the expansion of $f(r)$ as

$$f(r) = f(x_n - e_n) = f(x_n) + e_n f'(x_n) + \frac{e_n^2 f''(\zeta_n)}{2} \tag{4}$$

for ζ_n between x_n and r. This equation gives

$$e_n f'(x_n) + f(x_n) = -\frac{1}{2} f''(\zeta_n) e_n^2 \tag{5}$$

The expression in (5) is the numerator in (3), whereby we obtain via substitution:

$$e_{n+1} = -\frac{1}{2} \frac{f''(\zeta_n) e_n^2}{f'(x_n)} \tag{6}$$

Equation (6) ensures that the error scales quadratically. Now we wish to bound the error expression in (6). To bound e_{n+1}, we take $\delta > 0$ to define a neighbourhood of length δ around r. For any x in this neighbourhood, (6) reaches its maximum when the numerator is maximized and the denominator is minimized:

$$c(\delta) = \frac{1}{2} \frac{\max_{|x-r| \leq \delta} |f''(x)|}{\min_{|x-r| \leq \delta |f'(x)|}}$$

In other words, $c(\delta)$ is the maximum value which e_{n+1} can take if ζ_n, x_n are assumed to belong to the neighbourhood. Now we make two assumptions:

1. x_0 belongs to the neighbourhood, i.e. $|x_0 - r| \leq \delta$
2. δ is sufficiently small so that $\varrho := \delta c(\delta) < 1$.

Note that, since ζ_0 is between x_0 and r, assumption (1) ensures that ζ_0 is also in the neighbourhood, i.e. $|r - \zeta_0| \leq \delta$. Then we have:

$$|e_0| = \frac{1}{2} |f''(\zeta_0)/f'(x_0)| \leq c(\delta)$$

Then:

$$\begin{aligned}
|x_1 - r| &= |e_1| \\
&= \left| e_0^2 \cdot \frac{1}{2} f''(\zeta_0)/f'(x_0) \right| \\
&\leq |e_0^2| c(\delta) && \left\{ \frac{1}{2} f''(\zeta_0)/f'(x_0) \leq c(\delta) \right\} \\
&\leq |e_0| \delta c(\delta) && \{|e_0| \leq \delta\} \\
&= |e_0|\, \varrho && \{\varrho = \delta c(\delta)\} \\
&< |e_0| && \{\varrho < 1\} \\
&\leq \delta
\end{aligned}$$

$\therefore |e_1| < |e_0| \leq \delta$, which means the error decreases. This argument may be repeated inductively, giving:

$$
\begin{aligned}
|e_1| &\leq \varrho\, |e_0| \\
|e_2| &\leq \varrho\, |e_1| \leq \varrho^2\, |e_0| \\
|e_3| &\leq \varrho\, |e_2| \leq \varrho^3\, |e_0| \\
&\vdots
\end{aligned}
$$

In general, $|e_n| \leq \varrho^n\, |e_0|$. And since $0 \leq \varrho < 1$, we have $\varrho^n \to 0$ when $n \to \infty$, entailing that $|e_n| \to 0$ when $n \to \infty$.

Theorem 4. If f'' is continuous in $\mathbb{R}$, and if f is increasing, convex, and has a root, then said root is unique and Newton's method converges to it from any starting point.

Recall that f is convex if $f''(x) > 0$ for all x. Graphically, it is convex if the line connecting two arbitrary points of f lies above the curve of f between those two points.

4.3 Secant method

In Netwon's method,

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

The function of interest is f. We cannot escape computing $f(x_n)$, but it would be desirable to avoid the computation of $f'(x_n)$, which may potentially be expensive. Since

$$f'(x) = \lim_{h \to x} \frac{f(x) - f(h)}{x - h}$$

it is natural to suggest

$$f'(x_n) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}} \tag{1}$$

Graphically, this means we are not using the line tangent to the point $(x_n, f(x_n))$ but the line secant to the points $(x_n, f(x_n)$ and $(x_{n-1}, f(x_{n-1}))$. The point x_{n+1} is then the value of x where this secant line has a root.

4.4 Fixed point iteration

The key observation is this: if $r \in \mathcal{R}_f$, then $g(x) = x - kf(x)$ has r as fixed point, for any $k \in \mathbb{R}$. Inversely, if g has a fixed point in r, then $r \in \mathcal{R}_f$.

Theorem 5. (1) Let $g \in C[a, b]$ and assume $g(x) \in [a, b]$ for all $x \in [a, b]$. Then there is a fixed point of g in $[a, b]$.

(2) If, on top of previous conditions, g is differentiable in (a, b) and there is some $k < 1$ s.t. $|g'(x)| \leq k$ for all $x \in (a, b)$, then the fixed point referred in (1) is unique.

Theorem 6 (Mean value theorem)**.** Let $f : [a, b] \to \mathbb{R}$ continuous and differentiable on (a, b) with $a < b$. Then there is some $c \in (a, b)$ s.t.

$$f'(c) = \frac{f(b) - f(a)}{b - a}$$

The interpretation is simple: consider the line secant to f on a, b. The theorem ensures that there is some point c s.t. the line tangent to c is parallelt to said secant (equal slopes).

Proof. (1) If a or b are fixed points the proof is done so assume otherwise. Since $g(x) \in [a, b]$, we have $g(a) > a$ and $g(b) < b$.

Take $\varphi(x) = g(x) - x$, which is continuous and defined in $[a, b]$. Then

$$\varphi(a) = g(a) - a > 0, \qquad \varphi(b) = g(b) - b < 0$$

Then $\varphi(a)\varphi(b) < 0$. Then, by the intermediate value theorem, φ has a root in (a, b). In otherwords, there is at least one p s.t.

$$\varphi(p) = g(p) - p = 0$$

$\therefore g(p) = p$ is a fixed point of g.

(2) Assume two distinct fixed points p, q exist in $[a, b]$. The mean value theorem ensures the existence of some ζ between p, q (and thus in $[a, b]$) s.t.t

$$g'(\zeta) = \frac{g(a) - g(b)}{a - b} \iff g'(\zeta)(a - b) = g(a) - g(b) \tag{1}$$

By hypothesis, $|g'(x)| \leq k < 1$. Since p, q are assumed to be fixed points, equation (1) gives:

$$\begin{aligned} |p - q| &= |g(p) - g(q)| \\ &= |g'(\zeta)|\,|p - q| \\ &\leq k\,|p - q| < |p - q| \end{aligned}$$

But this is absurd. The contradiction arises from assuming p, q to be distinct. Therefore, the fixed point is unique.

The fixed point algorithm begins with an approximation p_0. Then,

$$p_n = g(p_{n-1})$$

If g continuous and the sequence converges, then it converges to a fixed point, since:

$$p := \lim_{n\to\infty} p_n = \lim_{n\to\infty} g(p_{n-1}) = g\left(\lim_{n\to\infty} p_{n-1}\right) = g(p)$$

Input: p, M, δ
$p_{\text{previous}} = p$
for $i = 1$ **to** $i = M$ **do**
  $p \leftarrow g(p)$
  if $\left|p - p_{\text{previous}}\right| < \delta$ **then**
    return p
  fi
  $p_{\text{previous}} = p$
od
return p

Theorem 7. Let $g \in C[a, b]$ be a self-map of $[a, b]$ differentiable in (a, b). Assume there is a constant $0 < k < 1$ s.t. $|g'(x)| \leq k$ for all $x \in (a, b)$.

For all $p_0 \in [a, b]$, the sequence $p_n = g(p_{n-1})$ converges to the unique f ixed point p in (a, b).

Proof. The mean value theorem ensures that

$$\begin{aligned} |p_n - p| &= |g(p_{n-1}) - g(p)| \\ &= |g'(\zeta_n)||(p_{n-1} - p)| \\ &\leq k\,|p_{n-1} - p| \end{aligned}$$

with $\zeta_n \in (a, b)$. More succintly, with $e_n := p_n - p$,

$$|e_n| \leq k\,|e_{n-1}| \leq k\,|e_{n-2}| \leq \ldots \leq k\,|e_0|$$

By recurrence,

$$|e_n| \leq k^n \, |e_0|$$

Since $0 < k < 1$, $k^n \to 0$ when $n \to \infty$, which entails $|e_n| \to 0$ when $n \to \infty$. It follows that $\{p_n\} \to p$ when $n \to \infty$.

Now let us consider the error of this method. Take $p_n = p + e_n$ and consider the Taylor expanssion of g around p evaluated at $p_n = p + e_n$:

$$g(p_n) = g(p + e_n) = \sum_{i=1}^{m-1} \frac{g^{(i)}(p)}{i!} e_n^i + \frac{f^{(m)}(\zeta_n)}{(n+1)!} e_n^m \tag{2}$$

See that in (2), n corresponds to the iteration we are dealing with, and thus ζ_n and e_n depend on it. On the contrary, m is the degree to which we expand the series of g around p evaluated at p_n. We also assume that ζ_n lies between p_n and p.

By definition, $g(p_n) = p_{n+1}$ so (2) is nothing but an expression for this value. Assume $g^{(k)}(p) = 0$ for $k = 1, 2, \ldots, m-1$, but $g^{(m)}(p) \neq 0$. Then

$$\begin{aligned} e_{n+1} &= p_{n+1} - p \\ &= g(p_n) - g(p) \\ &= \frac{g^{(m)}\,(\zeta_n)}{m!} e_n^m \end{aligned}$$

More succintly,

$$e_{n+1} = \frac{g^{(m)}\,(\zeta_n)}{m!} e_n^m$$

Then

$$\lim_{n \to \infty} \left| \frac{e_{n+1}}{e_n^m} \right| = \frac{|g^m(p)|}{m!}$$

which is a constant. In conclusion, if the derivatives of g are null in p up to the order $m-1$, the method as an order of convergence of at least m. Three results follow from this fact.

4.5 Exercises

(1) Let $f(x) = (x+2)(x+1)^2 x(x-1)^3(x-2)$. To which root does the biscection method converge on the following intervals?

$$[-1.5, 2.5], \qquad [-0.5, 2.4], \qquad [-0.5, 3], \qquad [-3, -0.5]$$

(a) The midpoint of $I_0 = [-1.5, 2.5]$ is $c_0 := (2.5 - 1.5)/2 = 1/2$. Since $f(a)f(c) < 0$, we have $I_1 = [-1.5, 0.5]$. The midpoint of I_1 is $c_1 = -0.5$, so I_2 will be $[-0.5, 0.5]$. The only root in this interval is $r = 0$, so the algorithm converges to it.

(b) The midpoint of $I_0 = [-0.5, 2.4]$ is $c := (2.4 - 0.5)/2 = 0.95$. Then $I_1 = [-1.5, 0.95]$. Same logic gives $c_1 = -0.725$ and then $I_2 = [-0.725, 0.95]$. The only root here is zero again.

(c, d) Same.

(2) We wish to find a root of f in $[a, b]$ using bisection method and ensuring that the error is not greater than $\epsilon \in \mathbb{R}^+$.

(a) Estimate the number of iterations sufficient to meet the criterion.

(b) What is the number of iterations for $a = 0, b = 1, \epsilon = 10^{-5}$?

Let $e_n = x_n - r$. It is trivial to note that $|e_n| \leq \frac{b_n - a_n}{2}$. Furthermore, the length of I_1 is half the length of I_0, that of I_2 is half that of I_1, etc. In other words,

$$|e_0| \leq \frac{b-a}{2}, \qquad |e_1| \leq \frac{b-a}{2^2}, \qquad |e_2| \leq \frac{b-a}{2^3}, \ldots$$

In general,

$$|e_n| \leq \frac{b-a}{2^{n+1}}$$

Imposing

$$|e_n| \leq \frac{b-a}{2^{n+1}} \leq \epsilon$$

we satisfy our criterion, but we wish to express this bound in terms of n. Now, clearly,

$$\begin{aligned}
&\frac{b-a}{2^{n+1}} \leq \epsilon \\
\iff &\frac{b-a}{\epsilon} \leq 2^{n+1} \\
\iff &\log_2\left(\frac{b-a}{\epsilon}\right) - 1 \leq n \\
\Longleftarrow &\log_2\left(\frac{b-a}{\epsilon}\right) \leq n \\
\iff &\frac{\ln\left(\frac{b-a}{\epsilon}\right)}{\ln 2} \leq n
\end{aligned}$$

which is our final answer.

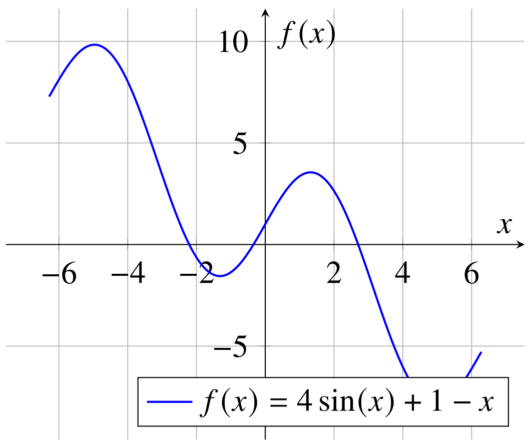
(b) For $a = 0, b = 1, \epsilon = 10^{-5}$, we need

$$n \geq \frac{\ln\left(\frac{1}{10^{-5}}\right)}{\ln 2} \approx 16.609$$

so $n = 17$ would suffice.

(3) Determine graphically some root of $f(x) = 4\sin x + 1 - x$ and perform three iterations of the bisection method to approximate. How many steps are needed to ensure an error less than 10^{-3}?

Let us unveil the full power of LaTex:



I'm too lazy to perform the steps of the algorithm. The number of steps needed again are given by

$$n \geq \frac{\ln\left(\frac{4-2}{10^{-3}}\right)}{\ln 2} \approx 10.96$$

so taking $n = 11$ suffices.

(4) Let $a > 0$. Computing $\sqrt{a}$ is equivalent to finding the root of $f(x) = x^2 - a$.

(a) Show that Newton's sequence for this case is

$$x_{n+1} = \frac{1}{2}\left(x_n + \frac{a}{x_n}\right)$$

(b) Prove that f or any $x_0 > 0$, the approximations $\{x_n\}$ satisfy $x_n \geq \sqrt{a}$ for $n \geq 1$.

(c) Prove $\{x_n\}$ is sdecreasing.

(d) Conclude that the sequence converges to $\sqrt{a}$

(a) In Newton's algorithm,

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

Clearly,

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

Therefore,

$$\begin{aligned} x_{n+1} &= x_n - \frac{x_n^2 - a}{2x_n} \\ &= x_n - \frac{1}{2}\left(x_n - \frac{a}{x_n}\right) \\ &= \frac{1}{2}x_n + \frac{1}{2}\frac{a}{x_n} \\ &= \frac{1}{2}\left(x_n + \frac{a}{x_n}\right) \qquad \blacksquare \end{aligned}$$

(b) Let $x_0 > 0$. Recall that, among all Pythagorean means, the arithmetic mean is the greatest, asuming positively-valued vectors. In particular, it is greater or equal to the geometric mean:

$$\frac{1}{N}\sum_{i=1}^{n} y_i \geq \sqrt[n]{\prod_{i=1}^{n} y_i}$$

for any set of points $y_1, \ldots, y_n$ all positive. In particular,

$$x_{n+1} = \frac{1}{2}\left(x_n + \frac{a}{x_n}\right) \geq \sqrt{x_n \frac{a}{x_n}} = \sqrt{a} \qquad \blacksquare$$

(c)

$$\begin{aligned}
& \frac{1}{2}\left(x_n + \frac{a}{x_n}\right) \leq x_n \\
\iff & x_n + \frac{a}{x_n} \leq 2x_n \\
\iff & \frac{a}{x_n} \leq x_n \\
\iff & a \leq x_n^2 \\
\iff & \sqrt{a} \leq x_n
\end{aligned}$$

which is true due to point (b).

(d) Let $e_n = x_n - \sqrt{a}$. We have shown $\{x_n\}$ to be decreasing and bounded below by $\sqrt{a}$. Therefore, it converges to a limit L (with L the infimum of $\{x_n\}$). Then

$$\lim_{n\to\infty} x_n = \frac{1}{2} \lim_{n\to\infty} \left(x_{n-1} + \frac{a}{x_{n-1}}\right) = \frac{1}{2}L + \frac{a}{2L}$$

This induces the equation

$$\begin{aligned}
L = \frac{L}{2} + \frac{a}{2L} \iff & \frac{L}{2} = \frac{a}{2L} \\
\iff & L^2 = a \\
\iff & L = \sqrt{a} \qquad \blacksquare
\end{aligned}$$

(5) Propose an iteration formula to approximate $\frac{1}{\sqrt{a}}$, with $a > 0$, using Newton's method. Decide the number of iterations needed so that the relative error in the approximation is less than 10^{-4} when starting from $x_0 = 1$ and taking $a = 5$.

Error: $e_n = r - x_n$, quadratitc, i.e. $|r - x_{n+1}| \leq c|r - x_n|^2$.

(a. Iteration formula) Let $a > 0$ and assume we wish to approximate $1/\sqrt{a}$. Let $\varphi = \frac{1}{a}$, so that $\frac{1}{\sqrt{a}} = \sqrt{\varphi}$. We see that we can express the problem of finding the reciprocal of a root in terms of a simple root.

We know from the previous exercise that the iteration formula for $\sqrt{\varphi}$ is

$$x_{n+1} = \frac{1}{2}\left(x_n + \frac{\varphi}{x_n}\right)$$

Now take $x_0 = 1$ and $a = 5$, so that $\varphi = \frac{1}{5}$. The relative error of approximation on iteration n is

$$e_n = \frac{\left|x_n - \frac{1}{\sqrt{5}}\right|}{\sqrt{5}}$$

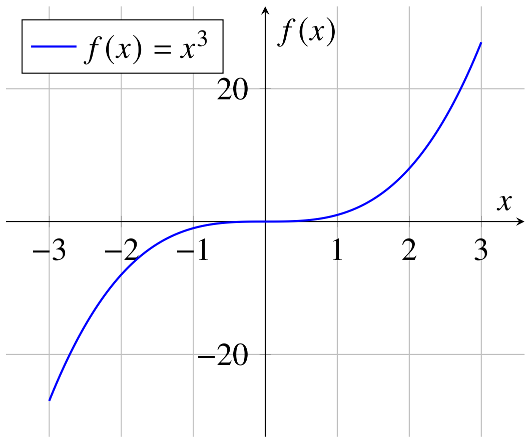
Brute-forcing allows us to see that x_0, x_1, x_2, x_3 do not meet the criterion, but

$$x_4 = 0.4472137791286728 \text{ (jaja)}$$

has $e_4 < 10^{-4}$.

(6) Propose an iteration formula for $\sqrt[3]{R}$ where $R > 0$. Plot the function to see where the procedure converges.

Observe that finding $\sqrt[3]{R}$ is equivalent to finding a root of $f(x) = x^3 - R$.



But $f(x)$ is simply a vertical displacement of x^3, so $\frac{d}{dx}x^3 = \frac{d}{dx}f(x)$ (which holds algebraically). In particular, the derivative of x^3 approaches 0 as $x \longrightarrow 0$, meaning that Newton's method will fail to converge for intervals of length L around 0 (with L unspecified). The graph suggests that an appropriate value for L is 1.

That said, since $\frac{d}{dx}f(x) = \frac{d}{dx}x^3$ (in other words, since the derivative of the function is independent of R), and $\frac{d}{dx}x^3 = 3x^2$, we propose

$$x_{n+1} = x_n - \frac{x_n^3}{3x_n^2} = x_n - \frac{x_n}{3} = \frac{2x_n}{3}$$

(7) (a) Utilizando el teorema del valor intermedio, demostrar que $g(x) = \arctan(x) - \frac{2x}{1+x^2}$ tiene raíz $\alpha \in [1, \sqrt{3}]$.

(b) Then show that if $\{x_n\}$ is the sequence generated by Newton's method for $f(x) = \arctan(x)$, with $x_0 = \alpha$, it is the case that $x_n = (-1)^n\alpha$.

(a) It is known that $\arctan x$ is continuous in $\mathbb{R}$. Since $1 + x^2 > 0$ for all x, $2x/(1 + x^2)$ is also continuous in $\mathbb{R}$. $\therefore$ g is continuous in $\mathbb{R}$. And it is easy to verify as well that $g(1)g(\sqrt{3}) < 0$.

$\therefore$ By virtue of the intermediate value theorem, there is a root α of g in $[1, \sqrt{3}]$.

(b) Let $g_1(x) = \arctan x$, $g_2(x) = \frac{2x}{1+x^2}$, so that $g = g_1 - g_2$. Since $\alpha > 0$, we have $g_1(\alpha) > 0$, $g_2(\alpha) > 0$. And since $g(\alpha) = 0$ if and only if $g_1(\alpha) - g_2(\alpha) = 0$, we conclude that $g_1(\alpha) = g_2(\alpha)$. In other words,

$$\arctan\alpha = \frac{2\alpha}{1+\alpha^2} \tag{1}$$

Since the derivative of $\arctan x$ is $1/(1 + x^2)$, equation (1) may be expressed as follows:

$$\arctan\alpha = 2\alpha\arctan'(\alpha) \tag{2}$$

This entails that

$$\arctan'\alpha = \frac{\arctan\alpha}{2\alpha} \tag{3}$$

Now take $x_0 = \alpha$ and consider Newton's sequence for $f(x) = \arctan x = g_1(x)$. Clearly,

$$\begin{aligned} x_1 &= \alpha - \frac{f(\alpha)}{f'(\alpha)} \\ &= \alpha - \arctan\alpha \times \frac{2\alpha}{\arctan\alpha} && \{\text{Eq. (3)}\} \\ &= \alpha - 2\alpha \\ &= -\alpha \end{aligned}$$

Same logic gives $x_2 = \alpha, x_3 = -\alpha, \ldots$ and the result should be easy to generalize.

(8) Consider for the fixed-point iteration the following functions, whose least positive root we wish to find:

$$\phi(x) = x^3 - x - 1, \qquad \psi(x) = 2x - \tan x, \qquad \varphi(x) = \exp(-x) - \cos x$$

Find an iteration function and an interval which guarantees the method's convergence.

(ϕ) Let us analyze ϕ in order to ascertain where its roots are.

Consider that $\phi'(x) = 3x^2 - 1$, which means ϕ' has roots wherever $3x^2 = 1$, which holds if and only if $x^2 = \frac{1}{3}$, or equivalently $x = \pm\frac{\sqrt{3}}{3}$. Furthermore, $\phi'(x) < 0$ in the region $(-\sqrt{3}/3, \sqrt{3}/3)$ and $\phi'(x) > 0$ elsewhere. In conclusion, ϕ is decreasing in $(-\sqrt{3}/3, \sqrt{3}/3)$ and increasing everywhere else.

Now, observe that $\phi\left(\sqrt{3}/3\right) < 0$. Combined with the fact that ϕ is increasing in $(\sqrt{3}/3, \infty)$, this means there is a root of ϕ in this interval. (Note that ϕ is a polynomial without asymptotic behavior.) Furthermore, $\phi\left(-\sqrt{3}/3\right) < 0$. Again, this means there is no root in $(\infty, \sqrt{3}/3)$.

$\therefore$ ϕ has one and only one root and it belongs to $(\sqrt{3}/3, \infty)$.

Now, suffices to note that $f(1.3)i < 0$, $f(1.4) > 0$, and the intermediate value theorem ensures that there is a root in $(1.3, 1.4)$. $\therefore$ The only root of ϕ lies within $(1.3, 1.4)$.

Now, we need only propose a function f s.t. r is a fixed-point of f and $f(x) \in (1.3, 1.4)$ for all $x \in (1.3, 1.4)$. Consider that

$$\phi(x) = 0 \iff x^3 = x + 1 \iff x = \sqrt[3]{x+1} \tag{4}$$

So letting $f(x) := \sqrt[3]{x+1}$ ensures that the fixed point of f is the root of ϕ. Furthermore, $f(1.3) \approx 1.32$, $f(1.4) \approx 1.33$. Now,

$$f'(x) = \frac{1}{\sqrt[3]{(x+1)^2}}$$

Since $f'(x) > 0$ (as is simple to note), we know f is increasing, which means all $f(x) \in (1.32, 1.33)$ for $x \in [1.3, 1.4]$. Furthermore, $f'(x) \in (0, 1)$ and $f'(x)$ is clearly decreasing. This means that in $[1.3, 1.4]$, f' has its maximum at $f'(1.4) \approx 0.573$. In other words, if we let $k = 0.573$, we know $|g'(x)| = g'(x) < k$ for all $x \in [1.3, 1.4]$.

$\therefore$ f is a self-map of $[1.3, 1.4]$, differentiable in $(1.3, 1.4)$, and there is a constant $k \in (0, 1)$ s.t. $|g'(x)| < k$ for all $x \in (1.3, 1.4)$—where incidentally this constant is $g'(1.3)$.]

$\therefore$ By virtue of **Theorem 7**, the fixed-point algorithm will converge to the unique root $r \in (1.3, 1.4)$ if using the iteration function $f(x) = \sqrt[3]{x+1}$ and the interval $[1.3, 1.4]$.

(ψ) Let $\psi(x) = 2x - \tan x$. A root exists for $\psi(x)$ whenever

$$x = \frac{\tan x}{2} = \frac{2 \sin x}{\cos x}$$

So we may define $g(x) := \tan x/2$ guarantying that any fixed point of g is a root of ψ. Now, $\tan 0 = 0$ entails that $g(0) = 0$. Furthermore, $g(\pi/4) = 1/2$. Since $g'(x) = \sec^2(x)/2$ is strictly positive, g is strictly increasing and this means for $x \in [0, \frac{\pi}{4}]$ we have $g(x) \in [0, 1/2] \subseteq [0, \frac{\pi}{4}]$.

$\therefore$ g is a self-map in $[0, \pi/4]$.

$\therefore$ There is a fixed-point of g in $[0, \pi/4]$.

Consider now $g'(x) = \frac{1}{2}\sec^2(x) = \frac{1}{2\cos^2 x}$. This is clearly bounded in $(0, 1]$. To be more precise, it is geometrically obvious that, for all $x \in [0, \pi/4]$, $\sqrt{2}/2 \leq \cos x \leq 1$, which means $1/2 \leq \cos^2 x \leq 1$. In particular, $g'(x)$ reaches its maximum when $\cos^2 x$ reaches its minimum, so $g'(x)$ reaches its maximum at $x = \frac{\pi}{4}$:

$$g'(\pi/4) = \frac{1}{2\cos^2 \frac{\pi}{4}} = \frac{1}{2 \cdot 1/2} = 1$$

It follows that there is some constant $k \in (0, 1)$ such that $|g'(x)| \leq k$ for all $x \in (0, \pi/4)$.

$\therefore$ There is a unique fixed point of g in $[0, \pi/4]$.

$\therefore$ There is a unique root of $\psi(x)$ in $[0, \pi/4]$ and the iteration method converges to it using this interval and the iteration function g.

(φ) Consider $\varphi(x) = \exp(-x) - \cos x$. This function is zero if and only if $e^{-x} = \cos x$, which may be expressed as $x = -\ln(\cos x)$. In other words, the roots of φ correspond to the fixed points of $f(x) = -\ln(\cos x)$.

Now, $-1 \le \cos x \le 1$ but ln is defined only in $\mathbb{R}^+$. From this follows that f is defined only when $\cos x > 0$, i.e. in the right-hand half of the unite circle. This corresponds to values of x in $[0, \pi/2)$ or $(3\pi/2, 2\pi]$ (extended by any factor $2\pi k$, $k \in \mathbb{Z}$).

Take $I := [0, \pi/4] \subseteq \mathrm{Dom}(f)$. See that $f(0) = -\ln(1) = 0$ and $f(\pi/4) = -\ln(\sqrt{2}/2) \approx 0.346 < \pi/4$. Furthermore, with $u = \cos x$,

$$\frac{df}{dx} = -\frac{d}{du}\ln(u) \times \frac{d}{dx}\cos x = \frac{\sin x}{\cos x} = \tan x$$

which is strictly positive in $[0, \pi/4]$. This suffices to prove that $f(x) \in [0, \pi/4]$ for all $x \in [0, \pi/4]$.

$\therefore$ f is a self-map of $[0, \pi/4]$.

$\therefore$ There is a fixed point of f in $[0, \pi/4]$.

Now, $\tan x$ is increasing in $[0, \pi/4]$ and, in particular, $\tan 0 = 0, \tan\frac{\pi}{4} = 1$. This suffices to show that $|g'(x)| < 1$ for all $x \in (0, \pi/4)$.

$\therefore$ There is a unique fixed point of f in $[0, \pi/4]$ and the fixed point iteration algorithm converges to it when starting from said interval with f as iteration function.

(10) Let $x_{n+1} = 2^{x_n - 1}$ the formula used to solve $2x = 2^x$. What interval should be chosen to ensure $\{x_n\}$ is convergent? Calculate its limit.

The fixed-point algorithm uses the formula $p_n = g(p_{n-1})$ where g is a function s.t. the fixed points of g are roots of some original function of interest f. In this case, clearly $g(x) = 2^{x-1}$. To ensure convergence, we must find an interval I s.t. g is a self-map of I and g' lies within a unit neighbourhood of 0.

Now, clearly the equation $2x = 2^x$ has solutions $x = 1, x = 2$, and no other. So whatever self-map I we build must contain either 1 or 2. So take $I = [0, 1]$.

Clearly, if $x \in I$, then $-1 \leq x - 1 \leq 0$. This means 2^{x-1} has exponent at least -1, when $g(0) = 2^{-1} = \frac{1}{2}$. Furthermore, 2^{x-1} has exponent at most 0, when $g(1) = 2^0 = 1$. This suffices to show that $g(x) \in I$ for all $x \in I$.

Now,

$$\frac{d}{dx}2^{x-1} = \frac{d}{du}2^u \times \frac{d}{dx}(x-1) = 2^u \ln u$$

In short, $g'(x) = 2^{x-1}\ln(2)$. For $x \in [0, 1]$, we have already established that $0 \leq 2^{x-1} \leq 1$. Therefore, $0 \leq g'(x) \leq \ln(2) < 0$ for all $x \in [0, 1]$. In other words, g' lies within a unit-distance of zero when its domain is restricted to I.

$\therefore$ The algorithm converges to the unique solution of $2x = 2^x$ in $[0, 1]$ (which is 1) when starting from said interval with iteration function g.

(11) Suppose $\{x_n\}$ converges to r and that $x_{n+1} = g(x_n)$ where $|g(y) - g(x)| \leq \lambda|y - x|$ for all x, y with $\lambda \in (0, 1)$. Determine the error bound on each iteration as a function of the difference between the last two iteration values. In other words, find C s.t.

$$|x_{n+1} - r| \leq C\,|x_{n+1} - x_n|$$

Recall that $x_{n+1} = g(x_n)$. This means

$$|x_{n+1} - r| = |g(x_n) - r|$$

But r is a fixed-point of g, i.e. $r = g(r)$. Then

$$|g(x_n) - r| = |g(x_n) - g(r)|$$

By assumption, then,

$$\begin{aligned} |x_{n+1} - r| &= |g(x_n) - g(r)| \\ &\leq \lambda\,|x_n - r| \end{aligned}$$

Recall that $|e_n| = |x_n - r| \leq k^n\,|e_{n-1}|$ for some $k \in (0, 1)$. Since the property above holds for any $\lambda \in (0, 1)$, it holds for said k.

Since $|x_n - r| \leq k^n\,|e_{n-1}|$, and $k^n \in (0, 1)$ entails $k^n\,|e_{n-1}| < |e_{n-1}|$, we have $|x_n - r| < |x_{n-1} - r|$. In other words, successive approximations in the sequence become increasingly closer to r. This means

$$|x_{n+1} - r| \leq k\,|x_n - r|$$

Wtf now?

5 Polynomial interpolation

Teorema fundamental del álgebra. Every non-zero, single-variable, degree n polynomial with complex coefficients has, counted with multiplicity, exactly n complex roots.

Theorem 8. Given $x_0, \dots, x_n$, $y_0, \dots, y_n$, there is a unique polynomial p_n of degree $\mathrm{gr}(p_n) \leq n$ s.t. $p_n(x_i) = y_i$ for all i.

Proof. (Existence) If $n = 0$ simple $p_0(x) = y_0$ which is trivial. So take as inductive hypothesis the existence of p_{k-1}, of degree $\leq k-1$, s.t. $p_{k-1}(x_i) = y_i$ for $i = 0, \dots, k-1$. We will construct a polynomial p_k of degree $\leq k$ s.t. $p_k(x_i) = y_i$ for $0 \leq i \leq k$.

Consider

$$p_k(x) = p_{k-1}(x) + c(x - x_0)(x - x_1)\dots(x - x_{k-1})$$

with c yet to be determined. Its degree is $\leq k$ and it obviously interpolates the points $(x_0, y_0), \dots, (x_{k-1}, y_{k-1})$. Now consider the equation:

$$p_k(x_k) = y_k$$

or equivalently

$$p_{k-1}(x_k) + c(x_k - x_0)(x_k - x_1)\dots(x_k - x_{k-1})$$

Solving for c, we find

$$c = \frac{y_k - p_{k-1}(x_k)}{(x_k - x_0)\dots(x_k - x_{k-1})}$$

Notice that c is well defined because each $x_0, \dots, x_n$ is distinct and therefore the denominator is never zero. This proves the polynomial exists.

(Uniqueness) Assume two interpolating polynomoials p_n, q_n exist. Let $h = p_n - q_n$. Clearly, its degree is $\leq n$ and $h(x_i) = 0$ for each $0 \leq i \leq n$. But this means h has $n+1$ real roots. Then, for the fundamental theorem of algebra, $h(x) = 0$ for all x and then $p_n = q_n$.

5.1 Newton's form

Given $x_0, \dots, x_n$ we define Newton's basis polynomials:

$$\eta_i(x) = \prod_{j=0}^{i-1}(x - x_j), \qquad 0 \leq i \leq n$$

where $\eta_0(x) := 1$. Applying the construction seen in the last proof recurrently, we obtain:

$$p_k(x) = \sum_{i=0}^{k} c_i \eta_i(x) = \sum_{i=0}^{k} c_i \prod_{j=0}^{i-1} (x - x_j)$$

Here, each c_i is obtained as in the last proof.

Example. Consider the points $(1, 2), (2, 5), (3, 3)$. We begin with $p_0(x) = 2$, the first interpolation which interpolates $(1, 2)$.

Now,

$$\begin{aligned} p_1(x) &= p_0(x) + c_0(x - x_0) \\ &= 2 + c_0(x - 1) \end{aligned}$$

Now, we pose the equation:

$$\begin{aligned} p_1(x_1) &\iff y_1 \equiv p_1(2) = 5 \\ &\iff 2 + c_0(2 - 1) = 5 \\ &\iff c_0 = 3 \end{aligned}$$

Then $p_1(x) = 2 + 3(x - 1) = 3x - 1$. Now we repeat:

$$\begin{aligned} p_2(x) &= p_1(x) + c_1(x - x_0)(x - x_1) \\ &= (3x - 1) + c_1(x - 1)(x - 2) \end{aligned}$$

We pose the equation:

$$\begin{aligned} &(3 \cdot 3 - 1) + c_1(3 - 1)(3 - 2) = 3 \\ \iff &8 + 2c_1 = 3 \\ \iff &2c_1 = -5 \\ \iff &c_1 = -\frac{5}{2} \end{aligned}$$

from which we have

$$p_2(x) = (3x - 1) - \frac{5}{2}(x - 1)(x - 2)$$

In Newton's form,

$$\begin{aligned} p_2(x) &= 2 + 3(x - 1) - \frac{5}{2}(x - 1)(x - 2) \\ &= \sum_{i=0}^{2} c_i \eta_i(x) \end{aligned}$$

with $c_0 = 2, c_1 = 3, c_2 = -\frac{5}{2}$.

5.2 Lagrange's form

Given $(x_0, y_0), \ldots, (x_n, y_n)$, we define Lagrange's basic polynyomials:

$$\ell_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{(x - x_j)}{(x_i - x_j)}, \qquad i = 0, \ldots, n$$

Note that $\mathrm{gr}(\ell_i) = n$ for all i and $\ell_i(x_j) = \delta_{ij}$ for all i, j. In other words, $\ell_i(x)$ is nothing but a polynomial that becomes null at each x_j except at x_i, where it is one.

The Lagrange form of the interpolating polynomial es

$$p_n(x) = \sum_{i=0}^{n} y_i \ell_i(x)$$

Prove that $\sum_{i=0}^{n} \ell_i(x) = 1$.

Observe that the polynomial $\sum_{i=0}^{n} \ell_i(x)$ has roots x_0

Let $\gamma(x) = \sum_{i=0}^{n} \ell_i(x) - 1$. Any root of this polynomial is a value where the sum of each $\ell_i(x)$ is 1. Since $\ell_i(x_j) = \delta_{ij}$, it is the case that each x_j is a root of γ. Therefore, γ has at least $n + 1$ roots, but its degree is n. By the fundamental theorem of algebra, $\gamma(x) = 0$. But then $\sum_{i=0}^{n} \ell_i(x) = 1$ necessarily. ■

It should be clear from the fact that $\ell_i(x_j) = \delta_{ij}$ that Lagrange's form is a valid interpolation. We don't really care what its value is beyond the arguments $x_0, \ldots, x_n$.

5.3 Error of interpolation

Theorem 9 (Error of interpolation)**.** Let $f \in C^{n+1}[a, b]$ and p a polynomial of degree $\leq n$ which interpolates f on $n + 1$ distinct points within $[a, b]$. Then for each $x \in [a, b]$, there is a number $\zeta = \zeta_x \in (a, b)$ s.t.

$$f(x) - p(x) = \frac{f^{(n+1)}(\zeta)}{(n+1)!} \eta_{n+1}(x)$$

or equivalently

$$f(x) - p(x) = \frac{f^{(n+1)}(\zeta)}{(n+1)!} \prod_{j=0}^{n} (x - x_i)$$

5.4 Divided differences

In Newton's form, we use $f[x_0, \ldots, x_k]$ to denote c_k. In other words, we re-write

$$\begin{aligned} p_k(x) &= \sum_{i=0}^{k} f[x_0, \ldots, x_i] \eta_i(x) \\ &= f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_1)(x - x_2) + \ldots \end{aligned}$$

If $k = 0$, $f[x_0] = f(x_0)$; if $k = 1$,

$$f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

where f is the function being interpolated.

Theorem 10. Given $x_0, \dots, x_n$,

$$f[x_0, \dots, x_n] = \frac{f[x_1, \dots, x_n] - f[x_0, \dots, x_{n-1}]}{x_n - x_0}$$

This allows us to construct a table for the so called divided differences. For instance, with $n = 3$:

$$\begin{array}{c|c|c|c|c}
x_0 & f[x_0] & f[x_0, x_1] & f[x_0, x_1, x_2] & f[x_0, x_1, x_2, x_3] \\
x_1 & f[x_1] & f[x_1, x_2] & f[x_1, x_2, x_3] & \\
x_2 & f[x_2] & f[x_2, x_3] & & \\
x_3 & f[x_3] & & &
\end{array}$$

Example. Assume $f(3) = 1$, $f(1) = -3$, $f(5) = 2$, $f(6) = 4$ where these arguments are $x_0, \dots, x_3$. We begin the table thus:

$$\begin{array}{c|c|c|c|c}
3 & 1 & f[x_0, x_1] & f[x_0, x_1, x_2] & f[x_0, x_1, x_2, x_3] \\
1 & -3 & f[x_1, x_2] & f[x_1, x_2, x_3] & \\
5 & 2 & f[x_2, x_3] & & \\
6 & 4 & & &
\end{array}$$

This is information sufficient to compute $f[x_2, x_3]$, which is

$$f[x_2, x_3] = \frac{f(x_2) - f(x_3)}{x_2 - x_3} = \frac{2 - 4}{5 - 6} = 2$$

giving

$$\begin{array}{c|c|c|c|c}
3 & 1 & f[x_0, x_1] & f[x_0, x_1, x_2] & f[x_0, x_1, x_2, x_3] \\
1 & -3 & f[x_1, x_2] & f[x_1, x_2, x_3] & \\
5 & 2 & 2 & & \\
6 & 4 & & &
\end{array}$$

Same logic gives $f[x_1, x_2] = 5/4$ and $f[x_0, x_1] = 2$:

$$\begin{array}{c|c|c|c|c}
3 & 1 & 2 & f[x_0, x_1, x_2] & f[x_0, x_1, x_2, x_3] \\
1 & -3 & 5/4 & f[x_1, x_2, x_3] & \\
5 & 2 & 2 & & \\
6 & 4 & & &
\end{array}$$

Now, $f[x_0, x_1, x_2] = (f[x_1, x_2] - f[x_0, x_1])/(x_2 - x_0)$. Using the table, this gives $(5/4 - 2)/(2) = -3/8$. Similarly, $f[x_1, x_2, x_3] = (f[x_2, x_3] - f[x_1, x_2])/(x_3 - x_1) = (2 - 5/4)/(5) = 3/20$.

$$
\begin{array}{c|c|c|c|c}
3 & 1 & 2 & -3/8 & f[x_0, x_1, x_2, x_3] \\
1 & -3 & 5/4 & 3/20 & \\
5 & 2 & 2 & & \\
6 & 4 & & &
\end{array}
$$

The last value is computed in similar fashion.

Theorem 11 (Error of interpolation with divided differences)**.** Let p with degree $\leq n$ an interpolator of f on nodes $x_0, \ldots, x_n$. If $t \neq x_i$ for all i is a real number, then

$$
f(t) - p(t) = f[x_0, \ldots, x_n, t] \prod_{j=0}^{n} (t - x_j)
$$

($\star$) **Observation**. Assume $p(x)$ is of degree 1 (linear). Then $f(x) - p(x) = \frac{f^{(2)}(\zeta_x)}{2!}(x - x_0)(x - x_1)$ for some ζ_x in $[x_0, x_1]$, in accordance with the **Error of interpolation** theorem. See that $\varphi(x) = (x - x_0)(x - x_1)$ is a quadratic expression with roots x_0, x_1 and minimum at $x_m = (x_0 + x_1)/2$. And since $\varphi(x_m)$ is negative, $\varphi(x) \geq \varphi(x_m) \Rightarrow |\varphi(x)| \leq |\varphi(x_m)|$. In consequence,

$$
|\varphi(x)| \leq |(x - x_0)(x - x_1)| = \frac{|x_1 - x_0|^2}{4}
$$

In consequence,

$$
|f(x) - p(x)| \leq \frac{f^{(2)}(\zeta_x)}{8} |x_1 - x_0|^2
$$

If we choose M the maximum of $f^{(2)}(x)$ in $[x_0, x_1]$, then we have

$$
|f(x) - p(x)| \leq \frac{f^{(2)}(\zeta_x)}{8} |x_1 - x_0|^2 \leq \frac{M}{8} |x_1 - x_0|^2
$$

In consequence,

$$
|f(x) - p(x)| \leq \frac{\max_x f^{(2)}_{|[x_0, x_1]}(x)}{8} |x_1 - x_0|^2
$$

5.5 Hermite interpolation

Hermite interpolation consists of interpolating a function f *and its derivative* in certain nodes $x_0, \dots, x_n$. For instance, if two points are given, we wish

$$p(x_i) = f(x_i), \qquad p'(x_i) = f'(x_i), \qquad \text{for } i = 0, 1$$

See that this gives four conditions, which means it is reasonable to seek a solution in Π_3 the space of all polynomials of degree ≤ 3. (An element in Π_3 has four coefficients.) But instead of writing $p(x)$ in terms of the coefficients for $1, x, x^2, x^3$, we shall write

$$p(x) = a + b(x - x_0) + c(x - x_0)^2 + d(x - x_0)^2(x - x_1)$$

which gives

$$p'(x) = b + 2c(x - x_0) + 2d(x - x_0)(x - x_1) + d(x - x_0)^2$$

Writing the polynomial this way allows us to express the four conditions as follows:

$$\begin{aligned} a &= f(x_0) \\ b &= f'(x_0) \\ f(x_1) &= a + bh + ch^2 \\ f'(x_1) &= b + 2ch + dh^2 \end{aligned}$$

where $h = x_1 - x_0$. This approach readily gives a and b, c can be determined from the third equation, and d from the fourth equation.

Now, observe that from the third equation,

$$\begin{aligned} c = \frac{f(x_1) - a - bh}{h^2} &= \frac{f(x_1) - f(x_0)}{h^2} - \frac{f'(x_0)h}{h^2} \\ &= \frac{f(x_1) - f(x_0)}{(x_1 - x_0)^2} - \frac{f'(x_0)}{(x_1 - x_0)} \end{aligned}$$

5.6 Splines

A spline is an interval-based polynomial approximation. We say $S(x)$ defined on $[x_0, x_n]$ is a spline of degree k if

1. S is polynomial of degree $\leq k$ on each sub-interval $[x_i, x_{i+1})$ para $i = 0, \ldots, n-1$;
2. The derivaitves of $S^{(i)}$ are continuous $[x_0, x_n]$ for $i = 0, \ldots, k-1$.

A linear spline is a spline of the form:

$$S(x) = \begin{cases} S_2(x) = a_0 x + b_0 & x \in [x_0, x_1) \\ S_1(x) = a_1 x + b_1 & x \in [x_1, x_2) \\ \vdots & \\ S_{n-1}(x) = a_{n-1} x + b_{n-1} & x \in [x_{n-1}, x_n) \end{cases}$$

where each a_i, b_i is to be determined. This gives $2n$ conditions. Clearly, for a fixed i,

$$\begin{aligned} a_i x_i + b_i &= S_i(x_i) = f(x_i) \\ a_i x_{i+1} + b_i &= \lim_{x \to x_{i+1}} S_i(x) = S_{i+1}(x_{i+1}) = f(x_{i+1}) \end{aligned}$$

Subtracting the first equation in the second one,

$$a_i = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}, \qquad b_i = f(x_i) - a_i x_i$$

The error of approximation in a linear spline can be determined if we assume each $x_0, \ldots, x_n$ to be equidistant. In other words, assume f is two times continuously differentiable in $[a, b]$ and $x_k = a + kh$ for $h = (b-a)/n$ the length of each sub-interval. Then on each interval we have a degree 1 polynomial, which means the error of interpolation for each $x \in [a, b]$ satisfies

$$|e(x)| < \frac{M}{8} h^2$$

where $|f''(x)| \leq M$ for all $x \in [x_0, x_n]$. (See **Observation** marked with $\star$.)

5.6.1 Cubic splines

5.7 Exercises

(1) Construct the Lagrange and Newton interpolating polynomials for $f(x) = 1/x$ taking $x_0 = 2, x_1 = 2.5, x_2 = 4$. Compare them and give their degrees. Graph them. Analize the results (?).

(Newton) Newton's interpolating polynomial has the form

$$\varphi(x) = \sum_{i=0}^{n} a_i \eta_i(x)$$

where each a_i is to be determined and $\eta_i = \prod_{j=0}^{i-1}(x - x_j)$. We first do a brute construction, then a construction using divided differences.

(Newton, brute) Take $\varphi_0(x) = \frac{1}{2}$, a polynomial interpolating f at x_0. Now let $\varphi_1(x) = \varphi_0(x) + c(x - x_0)$ and solve $\varphi_1(x_1) = f(x_1)$:

$$\begin{aligned}
&\frac{1}{2} + c(2.5 - 2) = f(2.5) \\
\iff\ & c = 2 \times \left(\frac{2}{5} - \frac{1}{2}\right) \\
\iff\ & c = \frac{4}{5} - \frac{5}{5} \\
\iff\ & c = -\frac{1}{5}
\end{aligned}$$

$\therefore\ \varphi_1(x) = \frac{1}{2} - \frac{1}{5}(x - 2)$.

Now we let $\varphi_2(x) = \frac{1}{2} - \frac{1}{5}(x - 2) + c(x - 2)(x - 2.5)$ and solve for c in $\varphi_2(4) = f(4)$:

$$\begin{aligned}
&\frac{1}{2} - \frac{1}{5} \times 2 + 2 \times \frac{3}{2}c = \frac{1}{4} \\
\iff\ & \frac{1}{2} - \frac{2}{5} + 3c = \frac{1}{4} \\
\iff\ & c = \frac{1}{3}\left(\frac{10}{40} + \frac{16}{40} - \frac{20}{40}\right) \\
\iff\ & c = \frac{1}{3}\left(\frac{3}{20}\right) \\
\iff\ & c = \frac{1}{20}
\end{aligned}$$

So finally we have the following polynomial in Newton's form:

$$\varphi(x) = \frac{1}{2} - \frac{1}{5}(x-2) + \frac{1}{20}(x-2.5)(x-2)$$

which is of degree 2.

(Newton, divided diffs.) The table of divided differences to interpolate f on x_0, x_1, x_2 is

$$\begin{array}{c|c|c|c} x_0 & f[x_0] & f[x_0,x_1] & f[x_0,x_1,x_2] \\ x_1 & f[x_1] & f[x_1,x_2] & \\ x_2 & f[x_2] & & \end{array} \Rightarrow \begin{array}{c|c|c|c} 2 & 1/2 & f[x_0,x_1] & f[x_0,x_1,x_2] \\ 2.5 & 2/5 & f[x_1,x_2] & \\ 4 & 1/4 & & \end{array}$$

Now, $f[x_1,x_2] = (f[x_2] - f[x_1])/(x_2 - x_1) = (1/4 - 2/5)/(1.5) = -1/10$:

$$\begin{array}{c|c|c|c} 2 & 1/2 & f[x_0,x_1] & f[x_0,x_1,x_2] \\ 2.5 & 2/5 & -1/10 & \\ 4 & 1/4 & & \end{array}$$

Now, same rule gives $f[x_0,x_1] = -1/5$:

$$\begin{array}{c|c|c|c} 2 & 1/2 & -1/5 & f[x_0,x_1,x_2] \\ 2.5 & 2/5 & -1/10 & \\ 4 & 1/4 & & \end{array}$$

Lastly, $f[x_0,x_1,x_2] = (f[x_1,x_2] - f[x_0,x_1])/(x_2 - x_0) = 1/20$:

$$\begin{array}{c|c|c|c} 2 & 1/2 & -1/5 & 1/20 \\ 2.5 & 2/5 & -1/10 & \\ 4 & 1/4 & & \end{array}$$

Then,

$$\begin{aligned} \varphi(x) &= f[x_0] + f[x_0,x_1](x-x_0) + f[x_0,x_1,x_2](x-x_0)(x-x_1) \\ &= \frac{1}{2} - \frac{1}{5}(x-2) + \frac{1}{20}(x-2.5)(x-2) \end{aligned}$$

which is is what we had obtained before.

(Lagrange) Lagrange's polynomial has the form

$$\phi(x) = \sum_{i=0}^{n} y_i \ell_i(x)$$

where

$$\ell_i(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

Then,

$$\begin{aligned}
\ell_0(x) &= \left(\frac{x-2.5}{2-2.5}\right)\left(\frac{x-4}{2-4}\right) \\
&= \left(-\frac{1}{2}(x-2.5)\right)(-2(x-4)) \\
&= (x-2.5)(x-4)
\end{aligned}$$

$$\begin{aligned}
\ell_1(x) &= \left(\frac{x-2}{2.5-2}\right)\left(\frac{x-4}{2.5-4}\right) \\
&= -\frac{3}{4}(x-2.5)(x-4)
\end{aligned}$$

$$\begin{aligned}
\ell_2(x) &= \left(\frac{x-2}{4-2}\right)\left(\frac{x-2.5}{4-2.5}\right) \\
&= 3(x-2)(x-4)
\end{aligned}$$

Therefore,

$$\begin{aligned}
\phi(x) &= \frac{1}{2}\ell_0(x) + \frac{2}{5}\ell_1(x) + \frac{1}{4}\ell_2(x) \\
&= \frac{1}{2}(x-2.5)(x-4) - \frac{3}{10}(x-2.5)(x-4) + \frac{3}{4}(x-2)(x-4)
\end{aligned}$$

(2) Prove: If f polynomial of degree $\leq n$ then the polynomial of degree $\leq n$ that interpolates f at $x_0, \ldots, x_n$ is f itself.

It is a theorem that there exists a polynomial of degree $\leq n$ that interpolates f in the points $x_0, \ldots, x_n$, and that this polynomial is unique. f is a polynomial of degree $\leq n$ that interpolates f at $x_0, \ldots, x_n$. This concludes the proof.

Given $x_0, \ldots, x_n$, prove the following properties of Lagrange's basic polynomials $\ell_k(x)$:

1. Their sum is 1.
2. Their linear combination with coefficients $x_0, \ldots, x_n$ is x.
3. Their linear combinations with coefficients $x_0^m, \ldots, x_n^m$, with $m \leq n$, is x^m.

(1) This was already proven in a previous section.

(2) See that

$$\sum_{k=0}^{n} x_k \ell_k(x) = x \iff \sum_{k=0}^{n} x_k \ell_k(x) - x = 0 \tag{1}$$

Let $\phi(x) = \sum x_k \ell_k(x) - x$. Since $\ell_k(x_j) = \delta_{kj}$, $\varphi(x_j) = x_j - x_j = 0$, meaning that each x_j is root of ϕ. This means ϕ is a polynomial of degree $\leq n$ with $n+1$ roots. Then by virtue of the fundamental theorem of algebra, it is necessarily the case that $\phi(x) = 0$. Then the RHS of (1) holds, which concludes the proof.

(3) Assume $m \leq n$. See that:

$$\sum_{k=0}^{n} x_k^m \ell_k(x) = x^m \iff \sum_{k=0}^{n} x_k^m \ell_k(x) - x^m = 0 \tag{2}$$

Let $\phi(x) = \sum x_k^m \ell_k(x) - x^m$. The polynomial has degree $\leq n$ due to the fact that $m \leq n$. Once more, $\phi(x_j) = x_j^m - x_j^m = 0$. Etc.

(6) Let $f : [0,5] \to \mathbb{R}$, $f(x) = 2^x$. Let P_n a polynomial of degree at most n that interpolates f at $n+1$ distinct points in $[0,5]$. Prove that for any x in said interval,

$$|P(x) - f(x)| \leq \frac{32 \times 5^{n+1}}{(n+1)!}$$

Recall that for $x \in [0,5]$,

$$P(x) - f(x) = \frac{f^{(n+1)}(\zeta_x)}{(n+1)!}\eta_{n+1}(x)$$

for some $\zeta_x \in [0,5]$. Now, $\frac{d}{dx}2^x = \ln 2 \times 2^x$, whose derivative is $\ln^2 2 \times 2^x$, whose derivative is $\ln^3 2 \times 2^x$, etc. $\therefore\ f^{(n+1)}(x) = \ln^{n+1} 2 \times 2^x = (n+1)\ln 2 \times 2^x$.

$$\begin{aligned}\therefore\ P(x) - f(x) &= \frac{\ln^{n+1}(2) \times 2^{\zeta_x}}{(n+1)!}\prod_{j=0}^{n}(x - x_j)\\ &= \frac{\ln^{n+1}(2) \times 2^{\zeta_x}}{n!}\prod_{j=0}^{n}(x - x_j)\end{aligned}$$

Since $0 < \ln(2) < 1$, we know $0 < \ln^{n+1}(2) < 1$, and therefore

$$\frac{\ln^{n+1}(2) \times 2^{\zeta_x}}{(n+1)!}\prod_{j=0}^{n}(x - x_j) < \frac{2^{\zeta_x}}{(n+1)!}\prod_{j=0}^{n}(x - x_j)$$

Necessasrily, $2^{\zeta_x} \leq 5$ and

$$\prod_{j=0}^{n}(5 - x_j) \leq \prod_{j=0}^{n} 5 = 5^{n+1}$$

From this follows that

$$P(x) - f(x) \leq \frac{2^5 \times 5^{n+1}}{(n+1)!}$$

Since the RHS is positive, taking absolute value on both sides gives us the desired result.

(7) Prove that when interpolating $\cosh(x)$ with a polynomial $p(x)$ of degree ≤ 22 in $[-1, 1]$, the error is $\leq 5 \times 10^{-16}$.

A polynomial of degree $n = 22$ has 23 coefficients, corresponding to the need of determining 23 nodes $x_0, \ldots, x_{23}$. So we let $n = 23$. It is known that $\frac{d}{dx} \cosh x = \sinh x$, whose derivative is once more $\cosh x$. So, $\cosh^{(n+1)} = \cosh^{(24)} = \cosh$. In consequence,

$$p(x) - \cosh(x) = \frac{\cosh(\zeta_x)}{(n+1)!} \prod_{j=0}^{n} (x - x_j)$$

for some $\zeta_x \in (-1, 1)$. The graph of $\cos h$ is symmetric (the function is even). Therefore, it achieves its maximum (restricted to $[-1, 1]$) at $\cosh(1) = \cosh(-1) = (e^1 + e^{-1})/2 = (e^2 + 1)/2e$. So

$$\left|\frac{\cosh(\zeta_x)}{(n+1)!}\right| \left|\prod_{j=0}^{n} (x - x_j)\right| \leq \frac{e^2 + 1}{2e(n+1)!} \left|\prod_{j=0}^{n} (x - x_j)\right|$$

Now, since $x \in [-1, 1]$, it is obvious that the maximum value which the factorial (and its absolute value) can take is 1. So

$$\frac{e^2 + 1}{2e(n+1)!} \left|\prod_{j=0}^{n} (x - x_j)\right| \leq \frac{e^2 + 1}{2e(n+1)!}$$

Now, with a calculator one can see that $24! > 10^{16}$. Furthermore, $(e^2 + 1)/2e < 5$. So,

$$\frac{e^2 + 1}{2e(n+1)!} < \frac{5}{10^{16}} = 5 \times 10^{-16} \qquad \blacksquare$$

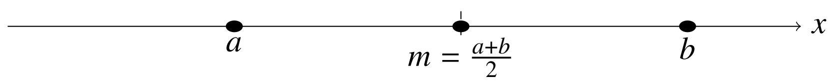
(8) (a) Let $a < b$, m the midpoint between them, $p = m - h$ and $q = m + h$ for $0 \leq h \leq (b-a)/2$. Prove that for all $x \in [a, b]$,

$$|(x-p)(x-q)| \leq \frac{(b-a)^2}{4}$$

(b) Let $x_i = a + i(\frac{b-a}{n})$ for $i = 0, \ldots, n$ equidistant points in $[a, b]$. Prove that for all $x \in [a, b]$,

$$|(x-x_0)\ldots(x-x_n)| \leq \frac{(b-a)^{n+1}}{2^{n+1}}$$

(a) See the graph below for reference.



Define $f(x)$ as the quadratic function with roots a, b and upward tails: $f(x) = (x-a)(x-b)$. We know that if $x_0 = p, x_1 = q$, then a linear interpolation of f at nodes x_0, x_1 on the interval $[a, b]$ satisfies:

$$|f(x) - p(x)| = \left|\frac{f''(\zeta_x)}{2!}\right| |(x-x_0)(x-x_1)| \leq \frac{M}{8}|x_1 - x_0|^2$$

with M the maximum of $|f''(x)|$ in $[a, b]$ and some $\zeta_x \in (a, b)$. Now,

$$|x_1 - x_0|^2 = |(m+h) - (m-h)|^2 = 4h^2$$

Therefore,

$$\begin{aligned}
&\left|\frac{f''(\zeta_x)}{2}\right| |(x-p)(x-q)| \leq \frac{4h^2 \times M}{8} \\
\Rightarrow &\left|\frac{f''(\zeta_x)}{2}\right| |(x-p)(x-q)| \leq \frac{M}{2}h^2 \\
\Rightarrow &|f''(\zeta_x)| \, |(x-p)(x-q)| \leq Mh^2
\end{aligned}$$

Here's the trick: since f is quadratic, f'' is constant and therefore $|f''(\zeta_x)| = |M|$. So dividing by $|M|$ on both sides we get

$$|(x-p)(x-q)| \leq h^2$$

Finally, we know $0 \leq h \leq (b-a)/2$, so

$$|(x-p)(x-q)| \leq h^2 \leq \left(\frac{b-a}{2}\right)^2 = \frac{(b-a)^2}{4}$$

which is what we wanted to show.

(b) Let $x_0, \ldots, x_n$ s.t. $x_i = a + i\frac{(b-a)}{n}$ for $0 \leq i \leq n$. We wish to show that for all $x \in [a,b]$,

$$|\eta_{n+1}(x)| \leq \frac{(b-a)^{n+1}}{2^{n+1}}$$

Take x_i, x_{i+1} and let f be the quadratic function with roots x_i, x_{i+1} and upward tails. Using the exact same reasoning of (a), we know

$$|(x-x_i)(x-x_{i+1})| \leq \frac{(x_{i+1}-x_i)^2}{2^2} \tag{3}$$

Since the points are equidistant, $x_{i+1} - x_i = \frac{b-a}{n}$, as is easy to prove algebraically, so equation (2) is equivalent to:

$$|(x-x_i)(x-x_{i+1})| \leq \left(\frac{b-a}{2n}\right)^2 \tag{4}$$

See that exercise (a) satisfied this formula, where had nodes x_0, x_1 and therefore $n = 1$. In other words, exercise (a) was the base case for an inductive proof and we can now assume that the statement holds for $n = k-1$ for some $k > 2$. Our inductive case consists of having points $x_0, \ldots, x_k$, where we wish to prove

$$|(x-x_0)\ldots(x-x_{k-1})| \leq \frac{(b-a)^k}{2^k} \Rightarrow |(x-x_0)\ldots(x-x_{k-1})(x-x_k)| \leq \frac{(b-a)^{k+1}}{2^{k+1}}$$

So assume

$$|\eta_k(x)| \leq \frac{(b-a)^k}{2^k}$$

Now take

$$|\eta_k(x)|\,|(x - x_{k+1})| \leq \frac{(b-a)^k}{2^k}\,|(x - x_{k+1})|$$

Since $x \in [a, b]$ and $x_{k+1} = b$ is the last node, $|x - x_{k+1}| \leq b - a$ (i.e. the maximum distance that x can take from b is when x is exactly a). So

$$|\eta_k(x)|\,|(x - x_{k+1})| \leq \frac{(b-a)^k}{2^k}\,|(x - x_{k+1})| \leq \frac{(b-a)^k}{2^k}(b-a)$$

Something's off. But should be along this lines.

(9) (a) Let $f(x) = \cos x\pi$. Find a polynomial of degree ≤ 3 that verifies:

$$p(-1) = f(-1), \qquad p(0) = f(0), \qquad p(1) = f(1), \qquad p'(1) = f'(1)$$

(b) Find a polynomial of degree ≤ 4 that verifies previous conditions and the added condition $p''(1) = f''(1)$.

(a) Let $x_0 = -1, x_2 = 0, x_3 = 1$. To keep track of which nodes have double (or more) conditions, let $z_0 = x_0, z_1 = x_1, z_2 = x_2, z_3 = x_2$ (since x_2 has two conditions, one for p and one for p'.) Then, our table of divided differences is

$$\begin{array}{c|c|c|c|c}
z_0 & f[z_0] & f[z_0, z_1] & f[z_0, z_1, z_2] & f[z_0, z_1, z_2, z_3] \\
z_1 & f[z_1] & f[z_1, z_2] & f[z_1, z_2, z_3] & \\
z_2 & f[z_2] & f[z_2, z_3] & & \\
z_3 & f[z_3] & & &
\end{array}$$

So now we simply compute the first column.

$$\begin{array}{c|c|c|c|c}
-1 & -1 & f[z_0, z_1] & f[z_0, z_1, z_2] & f[z_0, z_1, z_2, z_3] \\
0 & 1 & f[z_1, z_2] & f[z_1, z_2, z_3] & \\
1 & -1 & f[z_2, z_3] & & \\
1 & -1 & & &
\end{array}$$

Amazing. So now we compute $f[z_2, z_3] = f[x_2, x_2]$. Since this is a repeated node, by definition it corresponds to $f'(x_2) = f'(0)$. So, we see that $f'(0) = -\sin(0\pi)\pi = 0$. Similarly,

$$f[z_1, z_2] = \frac{f[z_2] - f[z_1]}{z_2 - z_1} = \frac{-2}{1} = -2$$

and

$$f[z_0, z_1] = \frac{f[z_1] - f[z_0]}{z_1 - z_0} = 2$$

So,

$$\begin{array}{c|c|c|c|c}
-1 & -1 & 2 & f[z_0, z_1, z_2] & f[z_0, z_1, z_2, z_3] \\
0 & 1 & -2 & f[z_1, z_2, z_3] & \\
1 & -1 & 0 & & \\
1 & -1 & & &
\end{array}$$

Now,

$$f[z_1, z_2, z_3] = \frac{f[z_2, z_3] - f[z_1, z_2]}{z_3 - z_1} = \frac{2}{1} = 2$$

$$f[z_0, z_1, z_2] = \frac{f[z_1, z_2] - f[z_0, z_1]}{z_2 - z_0} = -\frac{2}{2} = -2$$

$$\begin{array}{c|c|c|c|c}
-1 & -1 & 2 & -2 & f[z_0, z_1, z_2, z_3] \\
0 & 1 & -2 & 2 & \\
1 & -1 & 0 & & \\
1 & -1 & & &
\end{array}$$

At last,

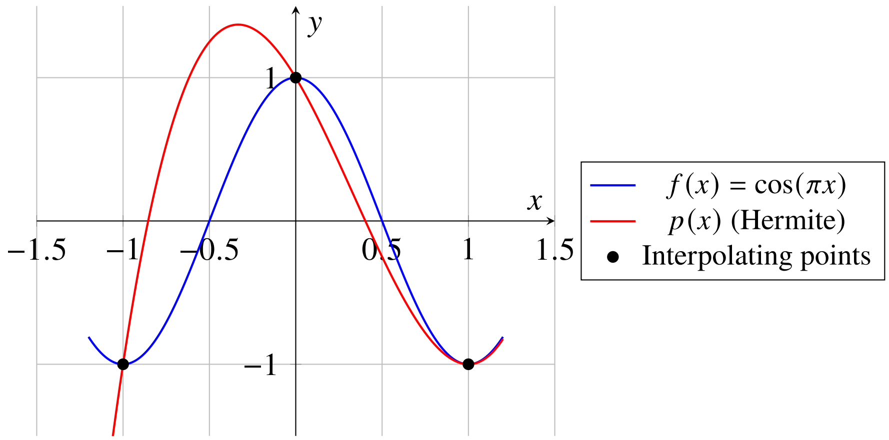
$$f[z_0, \ldots, z_3] = \frac{f[z_1, z_2, z_3] - f[z_0, z_1, z_2]}{z_3 - z_0} = 2$$

The interpolating polynomial is built using Newton's form—remember that $f[x_0], f[x_0, x_1], \ldots$ etc are the coefficients $c_0, c_1, \ldots$ in Newton's form $\sum_{i=0}^{n} c_i \eta_i(x)$. So,

$$p(x) = f[z_0] + f[z_0, z_1](x - z_0) + f[z_0, z_1, z_2](x - z_0)(x - z_1) + f[z_0, \ldots, z_3](x - z_0)(x - z_1)(x - z_2)$$

Simplifying,

$$p(x) = -1 + 2(x + 1) - 2(x + 1)x + 2(x + 1)x(x - 1)$$



y
x
1
−1
−1.5
−1
−0.5
0.5
1
1.5
f(x) = cos(πx)
p(x) (Hermite)
Interpolating points

(10) We wish to approximate $f(x) = \sqrt{x}$ with an error of at most 5×10^{-8} using a linear spline and quadratic interpolation every three nodes.

Determine the least number of nodes n of the form $x_i = 1 + \frac{i}{n}$, with $i = 0, \ldots, n$, and interval length h, so that the error bound is met.

(Linear spline) See that the desired approximation falls within $[1, 2]$. For a linear spline, the error of approximation obeys

$$|e(x)| < \frac{M}{8}h^2, \qquad x \in [1, 2] \text{ and } M = \max |f''|$$

where we can think of h as a function of n, i.e. $h(n) = \frac{1}{n}$ for $n \in \mathbb{N}$.

$$\begin{aligned} & \frac{M}{8}h(n)^2 \leq 5 \times 10^{-8} \\ \iff & \frac{M}{(n)^2} \leq 40 \times 10^{-8} \\ \iff & \frac{10^8 M}{40} \leq n^2 \\ \iff & \sqrt{\frac{10^8 M}{40}} \leq n \end{aligned}$$

Now, suffices to see that

$$f'(x) = \frac{1}{2\sqrt{x}}, \qquad f''(x) = -\frac{1}{4x^{3/2}}$$

Clearly then $|f''(x)|$ is decreasing and its maximum in $[1, 2]$ occurs at $x = 1$:

$$M = |f''(1))| = \frac{1}{4}$$

So, we require

$$
\begin{aligned}
&\sqrt{\frac{10^8}{40 \times 4}} \leq n \\
\iff &\frac{10^4}{\sqrt{160}} \leq n \\
\iff &\frac{10.000}{\sqrt{16 \times 10}} \leq n \\
\iff &\frac{10.000}{4\sqrt{10}} \leq n \\
\iff &\frac{2500}{\sqrt{10}} \leq n \\
\iff &790.569 \leq n
\end{aligned}
$$

So fixing $n = 791$ suffices.

(Quadratic interpolation) Assume we group $x_0, \ldots, x_n$ into x_0, x_1, x_2, then x_3, x_4, x_5, etc. Let $\overrightarrow{x}_i$ denote the ith grouping of three nodes. We are of course assuming that there are $n + 1 = 3k$ nodes with $k \in \mathbb{N}$. The function $h(n)$ which specifies the distance between nodes will be specified later.

Assume each $\overrightarrow{x}_i$ is used to fit a quadratic polynomial $q_i(x) = a_i x^2 + b_i x + c_i$. The error of interpolation will then be specific to each interval. In other words, for any x belonging to the interval specified by $\overrightarrow{x}_i$,

$$
|e(x)| = \left| \frac{f^{(3)}(\zeta_x)}{3!} \prod_{\widetilde{x} \in \overrightarrow{x}_i} (x - \widetilde{x}) \right|
$$

for some ζ_x in the interval of interest. Taking $M = \max \left| f^{(3)}(x) \right|$, with $f^{(3)}(x) = \frac{3}{8x^{\frac{5}{2}}}$, we obtain $M = 3/8$. Now the question becomes whether we can bound the factorial expression. See that

$$
\varphi(x) = (x - x_0)(x - x_1)(x - x_2)
$$

is a cubic function with distinct roots. (We could have chosen any successive values for x_0, x_1, x_2.) Consider φ as restricted to the interval $[x_0, x_2]$. We know that it will have three roots, a maximum x_M in $[x_0, x_1]$ and a minimum x_m at $[x_1, x_2]$. Since the roots are equidistant (root symmetry), φ is symmetric around the mid-root x_1 and $\varphi(x_m) = \varphi(x_M)$. But where is the critical point?

($\star$) Let us consider a centered cubic polynomial, without loss of generality. Let $\phi(x) = (x - a)x(x - b)$, with mid-root zero. Assuming root symmetry, $a = -b$. So letting $r = b$ we have

$$\phi(x) = (x-r)x(x+r) = x^3 - xr^2$$

Its derivative $\phi'(x) = 3x^2 - r^2$ is zero if and only if $x = \pm\frac{r}{\sqrt{3}}$. We have already established that these critical points are equal in their absolute values. Now it only suffices to see that

$$\phi\left(\frac{r}{\sqrt{3}}\right) = -\frac{2r^3}{3\sqrt{3}} = -\frac{(c-a)^3}{12\sqrt{3}}$$

(because $r = (c-a)/2$). Therefore,

$$\max|\phi(x)| = \frac{(c-a)^3}{12\sqrt{3}}$$

From ($\star$) readily follows that

$$\left|\prod_{\widetilde{x}\in\overrightarrow{x}_i}(x-\widetilde{x})\right| \leq \frac{h^3}{12\sqrt{3}}$$

where h is the distance between the last node in a grouping and the first (i.e. $x_2 - x_0 = x_5 - x_3 = \ldots$ etc.) In consequence,

$$|e(x)| = \left|\frac{f^{(3)}(\zeta_x)}{3!}\prod_{\widetilde{x}\in\overrightarrow{x}_i}(x-\widetilde{x})\right|$$
$$\Rightarrow |e(x)| \leq 3/8\frac{h^3}{12\sqrt{3}}$$

Here, h is a function of n. If $n = 2$ (three points), then $h = 2/3$. If $n = 5$ (six points), then each sub-interval is of length $1/6$ and $h = 2/6$. In general, if $n = 3k$, then $h = \frac{2}{n}$. So we have

$$|e(x)| \leq \frac{3}{8\times\sqrt{3}}\frac{2}{n} = \frac{3}{4\sqrt{3}n}$$

So now all that is needed is to bound the RHS expression to 5×10^{-8}:

$$\frac{3}{4\sqrt{3}n} \leq 5 \times 10^{-8} \iff \dots$$

bla bla. This is the simplest part of the problem so I skip it.

(10) Let $f(x) = \cos x$. Determine the step-length h and minimum number of nodes $n + 1$ needed to approximate $f(x)$ via linear spline in $[0, 2\pi]$ with an error less than or equal to 5×10^{-7}.

We know

$$|e(x)| \leq \frac{M}{8} h(n)^2$$

where $h(n) = \frac{2\pi}{n}$ anda $M = \max |f''(x)|$. Since $f''(x) = -\cos x$, its maximum in $[0, 2\pi]$ is 1. From this follows that

$$|e(x)| \leq \frac{4\pi^2}{8n^2} = \frac{1}{2}\left(\frac{\pi}{n}\right)^2$$

and all that is left is bounding said expression to be less than or equal to 5×10^{-7}. If one does the math, we obtain that said condition holds iff $n =\geq \pi \times 10^3 \approx 3141.59$, which means letting $n = 3142$ suffices. So the number of nodes needed is $n + 1 = 3143$. The step length h results $\frac{2\pi}{3142} \approx 0.001999 \approx 0.002$.

(12) (a) Determine α, β, γ such that

$$S(x) = \begin{cases} \alpha x^3 + \gamma x & 0 \le x \le 1 \\ -\alpha x^3 + \beta x^2 - 5\alpha x + 1 & 1 \le x \le 2 \end{cases}$$

is a cubic spline.

(b) With the determined values, decide if S interpolates $f(x) = 2^x + 1/2x^2 - 1/2x - 1$ in $[0,2]$ with nodes $\{0,1,2\}$.

(c) Graph f and S in $[0,2]$.

(a) $S(x)$ must satisfy the interpolation constraint and the continuity constraint. Note that $S(x)$ are polynomials with continuous first and second derivatives in $[0,2]$. Furthermore,

$$S'(x) = \begin{cases} 3\alpha x^2 + \gamma & 0 \le x \le 1 \\ -3\alpha x^2 + 2\beta x - 5\alpha & 1 \le x \le 2 \end{cases}, \qquad S''(x) = \begin{cases} 6\alpha x & 0 \le x \le 1 \\ -6\alpha x + 2\beta & 1 \le x \le 2 \end{cases}$$

For all f in $\{S, S', S''\}$ we wish that

$$\lim_{x \to 1(\leftarrow)} f(x) = \lim_{x \to 1(\rightarrow)} f(x)$$

$(a.a)$ Beginning with $S''(x)$, we impose

$$6\alpha = -6\alpha + 2\beta \Rightarrow 12\alpha = 2\beta \Rightarrow \beta = 6\alpha$$

$(a.b)$ Now taking $S'(x)$, we impose

$$3\alpha + \gamma = -3\alpha + 2\beta - 5\alpha$$

Substituting with $\beta = 6\alpha$, we find

$$\gamma = -6\alpha + 2(6\alpha) - 5\alpha \Rightarrow \gamma = \alpha$$

$(a.c)$ Now taking $S(x)$, we impose

$$\alpha + \gamma = -\alpha + \beta - 5\alpha + 1$$

Substituting with $\gamma = \alpha, \beta = 6\alpha$, we find

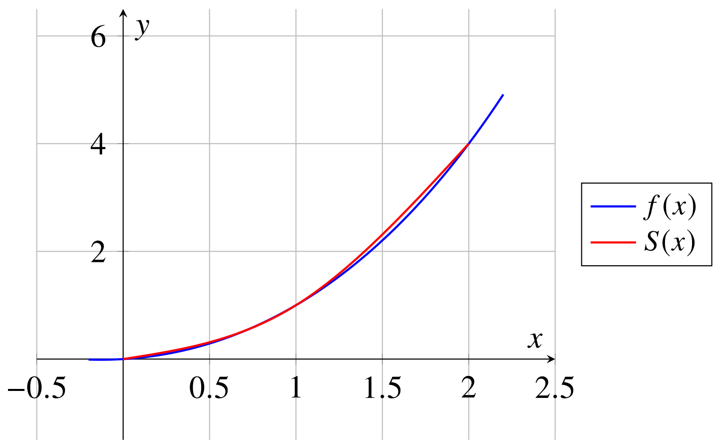
$$2\alpha = 1 \Rightarrow \alpha = \frac{1}{2}$$

So we finally obtain

$$\alpha = \frac{1}{2}, \beta = 3, \gamma = \frac{1}{2}$$

(b) It is simple to see that the spline does interpolate f simply by evaluating S and f on $0, 1, 2$.

(c)



6 Function approximation

6.1 Least squares method

Assume $(x_1, y_1), \ldots (x_m, y_m)$ are points from a function f we wish to approximate. A reasonable approach is to find a linear function with coefficients a_0, a_1 that minimize

$$E = \sum_{i=1}^{m} (y_i - (a_1 x_i + a_0))^2$$

Doing the standard things (take partial derivative, equate it to zero, etc.) we obtain the following normal equations to minimize E:

$$a_0 = \frac{\left(\sum x_i^2\right)\left(\sum y_i\right) - \left(\sum x_i y_i\right)\left(\sum x_i\right)}{m \sum x_i^2 - \sum x_i}, \qquad a_1 = \frac{m \sum x_i y_i - \left(\sum x_i\right)\left(\sum y_i\right)}{m \sum x_i^2 - \sum x_i}$$

where all sums range from $i = 1$ to m.

The general case is when f is approximated with a polynomial of degree $\leq n$, with $n < m - 1$. Now, we need to determine the coefficients $a_0, \ldots, a_n$ that minimize

$$\sum_{i=1}^{m} (y_i - p_n(x_i))^2$$

Again, doing the standard procedure, the following system of equation emerges for variables $a_0, \ldots, a_n$:

$$\begin{bmatrix} \sum x_i^0 & \sum x_i^1 & \sum x_i^2 & \ldots & \sum x_i^n \\ \sum x_i^1 & \sum x_i^2 & \sum x_i^3 & \ldots & \sum x_i^{n+1} \\ \vdots & \vdots & \vdots & \ldots & \vdots \\ \sum x_i^2 & \sum x_i^{n+1} & \sum x_i^{n+2} & \ldots & \sum x_i^{2n} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} \sum y_i x_i^0 \\ \sum y_i x_i^1 \\ \vdots \\ \sum y_i x_i^n \end{bmatrix}$$

6.2 Non-polynomial models

It is possible to propose a non-polynomial model for f, e.g. $\hat{f}(x) = be^{ax}$ or whatever. This produces a non-linear system of equations which cannot be solved simply. However, taking the logarithm of the proposed model allows for a linear approximation. For example, if $\hat{f}(x) = be^{ax}$ then

$$\ln \hat{f}(x) = \ln b + ax$$

which is a linear model that can be fitted using least squares. However, it is important to recall that the values $y_1, \ldots, y_m$ must be scaled with $\ln y_1, \ldots, \ln y_m$ to fit the logarithmic model.

6.3 Error of approximation

Assume $f \in C[a, b]$ and $P_n(x)$ of degree $\leq n$ an approximation via least squares. Then

$$E = E(a_0, \ldots, a_n) = \int_a^b (f(x) - P_n(x))^2 \; dx = \int_a^b \left[f(x) \; sum_{k=0}^n a_k x^k \right]^2 \; dx$$

In general, we wish to find $a_0, \ldots, a_n$ such that E is minimal. In general, the partial derivative of E with respect to a_j is zero if and only if

$$\sum_{k=0}^{n} \left(a_k \int_a^b x^{k+j} \; dx \right) = \int_a^b x^j f(x) \; dx, \qquad j = 0, \ldots, n$$

This readily provides a $(n+1) \times (n+1)$ system of equations which is to be solved to minimize the error:

$$\begin{bmatrix} \int_a^b \; dx & \int_a^b x \; dx & \ldots & \int_a^b x^n \\ \int_a^b x \; dx & \int_a^b x^2 \; dx & \ldots & \int_a^b x^{n+1} \\ \vdots & \vdots & \ldots & \vdots \\ \int_a^b x^n & \int_a^b x^{n+1} & \ldots & \int_a^b x^{2n} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} \int_a^b x^0 f(x) \; dx \\ \int_a^b x f(x) \; dx \\ \vdots \\ \int_a^b x^n f(x) \; dx \end{bmatrix}$$

Notice that, in LHS matrix, the coefficient c_{jk} is

$$\int_a^b x^{j+k} \; dx = \frac{b^{j+k+1} - a^{j+k+1}}{j+k+1}$$

which allows for a more direct computation of the system. The LHS matrix is called **Hilbert matrix** and it is famously ill-conditioned—i.e. small changes in the coefficients greatly affect the final result.

6.4 A few polynomial theorems

Recall that vectors $\phi_1, \ldots, \phi_n$ are linearly independent if $\sum_{i=0}^n c_i \phi_i = 0$ entails that $c_0 = \ldots = c_n = 0$. In particular, a function space $\mathcal{F}$ is a vector space such that $\Pi = \bigcup_{i=0}^{\infty} \Pi_i \subseteq \mathcal{F}$.

Theorem 12 (Polynomials of different degrees are linearly independent)**.** Let $\phi_0, \ldots, \phi_n$ such that $\phi_j \in \Pi_j$. Then $\{\phi_i\}_{i=0}^n$ is linearly independent in any interval $[a, b]$.

Proof. Assume $c_0, \ldots, c_n$ are such that $P(x) = c_0\phi_0(x) + \ldots + c_n\phi_n(x) = 0$ for any $x \in [a, b]$. Since $P(x)$ is null for all x in $[a, b]$, each exponentiation x^k must be zero. Since $c_n\phi_n(x)$ is the only term which includes x^n, we must have $c_n = 0$, which readily entails $P(x) = c_0\phi_0(x) + \ldots + c_{n-1}\phi_{n-1}(x)$. By recurrence, $c_0 = \ldots = c_n = 0$. ■

The previous theorem is highly general, since any polynomial of degree n is by definition a linear combination of $n+1$ polynomials of degree $0, 1, \ldots, n$. For instance, $1+3x+2x^2$ can be considered a linear combination of the polynomials $1, x, x^2$ with coefficients $1, 3, 2$, or of the polynomials $1, 3x, 4x^2$ with coefficients $1, 1, 1/2$, etc.

Theorem 13. Let $\{\phi_0, \ldots, \phi_n\}$ be a set of linearly independent polynomials for any interval $[a, b]$, each of degree $\leq n$. Then any polynomial of degree $\leq n$ can be expressed as a linear combination of $\{\phi_0, \ldots, \phi_n\}$.

6.5 Weighted function approximation: Diagonalizing Hilbert matrix

A weight function $\omega(x)$ on interval I is a function such that:

1. $\omega(x) > 0$ for all $x \in I$.
2. $\omega(x) \neq 0$ for all x in any arbitrary sub-interval of I.

Condition (2) means that ω cannot be constantly zero in any sub-interval, i.e. any zero mapping of ω must be a point. Weight function allow one to give more or less importance to approximations in different regions of an interval of interest.

Now assume we have a linearly independent set of functions $\{\phi_0, \ldots, \phi_n\}$ in $[a, b]$, a weight function ω defined on $[a, b]$, and f continuous in $[a, b]$ which we wish to approximate. Then there is a set of coefficients $a_0, \ldots, a_n$ of

$$P(x) = \sum_{k=0}^{n} a_k \phi_k(x)$$

that minimize the following error function:

$$E = E(a_0, \ldots, a_n) = \int_a^b \omega(x) \left[f(x) - P(x)\right]^2 \, dx$$

This is the same as we did before: we are approximating f via a polynomial by finding the coefficients that minimize the error of approximation. But now we are (a) including a weight function and (b) defining $P(x)$ as a linear combination of independent polynomials.

Once more, taking the derivative of E with respect to an arbitrary a_j, we find that said derivative is zero if and only if

$$\sum_{k=0}^{n} a_k \int_a^b \omega(x)\phi_k(x)\phi_j(x)\, dx = \int_a^b \omega(x) f(x) 0 \phi_j(x)\, dx, \qquad j = 0, \dots, n$$

which readily provides a system of equations. The system is complex, but it can be greatly simplified if we could choose $\{\phi_0, \dots, \phi_n\}$ such that

$$\int_a^b \omega(x)\phi_k(x)\phi_j(x)\, dx = \alpha_j \delta_{jk}$$

for some $\alpha_j > 0$. In that case, the equation would simplify to

$$a_j \int_a^b \omega(x)\phi_j^2(x)\, dx = \int_a^b \omega(x) f(x)\phi_j(x)\, dx, \qquad j = 0, \dots, n$$

By assumption, this would yield

$$a_j \alpha_j = \int_a^b \omega(x) f(x)\phi_j(x)\, dx, \qquad j = 0, \dots, n$$

or equivalently

$$a_j = \frac{1}{\alpha_j} \int_a^b \omega(x) f(x)\phi_j(x)\, dx, \qquad j = 0, \dots, n$$

In short, a relatively simple system of equations emerges if $\phi_0, \dots, \phi_n$ are intelligently chosen. But how to choose them intelligently?

[Ortogonal set] A set $\{\phi_0, \dots, \phi_n\}$ of functoins defined in $[a, b]$ is ortogonal with respect to a weight function ω iff

$$\int_a^b \omega(x)\phi_k(x)\phi_j(x)\, dx = \alpha_j \delta_{jk}, \qquad j = 0, \dots, n$$

for $\alpha_j > 0$. If $\alpha_j = 1$ for all $j = 0, \dots, n$ then we say the set is ortonormal.

We can formalize what was said so far as follows:

Theorem 14 (Ortogonal polynomial approximation theorem)**.** If $\{\phi_0, \dots, \phi_k\}$ defined in $[a, b]$ is ortogonal with respect to ω defined in $[a, b]$, then the least squared approximation of f weighted by ω is

$$P(x) = \sum_{k=0}^{n} a_k \phi_k(x)$$

with

$$a_k = \frac{1}{\alpha_k} \int_a^b \omega(x) f(x) \phi_k(x)\, dx$$

where $\alpha_k = \int_a^b \omega(x)\phi_k^2(x)\, dx$.

Theorem 15 (Ortogonal set generation)**.** The following is an ortogonal set of functions defined in $[a, b]$ with respect to a weight function ω:

$$\phi_0(x) = 1, \qquad \phi_1(x) = x - B_1, \qquad x \in [a, b]$$

where

$$B_1 = \frac{\int_a^b x\omega(x)\phi_0^2(x)\, dx}{\int_a^b \omega(x)\phi_0^2(x)\, dx}$$

For $k \geq 2$,

$$\phi_k(x) = (x - B_k)\phi_{k-1}(x) - C_k\phi_{k-2}(x), \qquad x \in [a, b]$$

with

$$B_k = \frac{\int_a^b x\omega(x)\phi_{k-1}^2(x)\, dx}{\int_a^b \omega(x)\phi_{k-1}^2(x)}, \qquad C_k = \frac{\int_a^b x\omega(x)\phi_{k-1}(x)\phi_{k-2}(x)\, dx}{\int_a^b \omega(x)\phi_{k-2}^2(x)\, dx}$$

In general, we will use a few ortogonal sets which are already known, built recurrently from the previous theorem:

1. **Legendre polynomials**:

$$\phi_0(x) = 1, \phi_1(x) = x, \phi_2(x) = x^2 - \frac{1}{3}, \phi_3(x) = x^3 - \frac{3}{5}x, \phi_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{25}, \ldots$$

2. More examples in the textbook.

6.6 Exercises

(1) Approximate $f(x)$ with a polynomial of degree 1 and $g(x)$ with a polynomial of degree two, where:

x	0	1	2	3	4	5	6	7	8	9
$\hat{f}(x)$	-0.1	1.1	1.9	3.2	3.8	5.0	6.0	7.3	8.1	8.9

and

x	-1	0	1	3	6
$\hat{g}(x)$	6.1	2.8	2.2	6	26.9

(f) We know $p(x) = a_0 + a_1 x + \ldots + a_n x^n$ is the least squared approximation of f if and only if $a_0, \ldots, a_n$ are solutions to the following system of equations:

$$\begin{bmatrix} \sum_{i=0}^m x_i^0 & \sum_{i=0}^m x_i^1 & \ldots & \sum_{i=0}^m x_i^m \mid \sum_{i=0}^m x_i^0 y_i \\ \sum_{i=0}^m x_i^1 & \sum_{i=0}^m x_i^2 & \ldots & \sum_{i=0}^{m+1} x_i^m \mid \sum_{i=0}^m x_i^1 y_i \\ \vdots & \vdots & \ldots & \vdots \\ \sum_{i=0}^m x_i^m & \sum_{i=0}^m x_i^{m+1} & \ldots & \sum_{i=0}^m x_i^{2m} \mid \sum_{i=0}^m x_i^m y_i \end{bmatrix}$$

where m is the number of points $(x_i, \hat{f}(x_i))$. Since we wish to approximate f with a polynomial of degree 1, this gives a 2×2 matrix with coefficients

$$c_{11} = \sum_{i=0}^{9} (1) = 10, \qquad c_{11} = \sum_{i=0}^{9} x = 45,$$

$$c_{21} = \sum_{i=0}^{9} x_i = 45, \qquad c_{22} = \sum_{i=0}^{n} x_i^2 = 285$$

The solution vector, on the other hand, is:

$$w_1 = \sum_{i=0}^{9} y_i = 45.2, \qquad w_2 = \sum_{i=0}^{9} x_i y_i = 286.7$$

So, suffices to solve the system

$$\begin{bmatrix} 10 & 45 & 45.2 \\ 45 & 285 & 286.7 \end{bmatrix} \to \begin{bmatrix} 1 & 4.5 & 4.52 \\ 1 & 6.33 & 6.371 \end{bmatrix} \to \begin{bmatrix} 1 & 4.5 & 4.52 \\ 0 & 1.83 & 1.85 \end{bmatrix}$$

So $a_1 = \frac{1.85}{1.83} a_2 = 1.01 a_2$, bla bla. Linear system, cursillo de ingreso.

(g) Not that different from (f): calculate the matrix, which will be 3×3 now (degree two polynomial), solve the resulting system. Calculating the matrix is computing sums (stupid), solving the system is solving a linear system (stupid).

(2) Prove that with $n + 1$ distinct points, the best polynomial approximation (in the sense of least squares) of degree n coincides with the interpolating polynomial.

Let $p_n(x)$ be the interpolating polynomial of f on points $x_0, \ldots, x_n$. Let $\ell_n(x)$ be the least squares approximation of degree n. Observe that

$$\sum_{i=0}^{n} (y_i - p_n(x_i))^2 = 0$$

Since $\ell_n(x)$ minimizes the error among all polynomials of degree n, and taking p_n we have an error of zero, we must have

$$\sum_{i=0}^{n} (y_i - \ell_n(x))^2 = 0$$

which holds if and only if $\ell_n(x)$ is an interpolating polynomial. But the interpolating polynomial is unique. $\therefore\ p_n(x) = \ell_n(x)$.

(3) Find the polynomial of degree 0 that best approximates $f : [a, b] \to \mathbb{R}$ on $x_1, \ldots, x_n$ in $[a, b]$.

We wish to find a constant polynomial $p_0(x) = c$ such that

$$S = \sum_{i=1}^{n} [y_i - p_0(x_i)]^2 = \sum_{i=1}^{n} [y_i - c]^2$$

is minimized. Taking

$$\begin{aligned}
\frac{\partial S}{\partial c} &= \sum_{i=1}^{n} \frac{\partial}{\partial c}(y_i - c)^2 \\
&= \sum_{i=1}^{n} \frac{\partial u^2}{\partial u} \frac{\partial}{\partial c}(y_i - c) \\
&= \sum_{i=1}^{n} 2(y_i - c)(-1) \\
&= 2\sum_{i=1}^{n}(c - y_i) \\
&= 2\left(cn - \sum_{i=1}^{n} y_i\right)
\end{aligned}$$

The expression above is zero if and only if

$$c = \frac{1}{n}\sum_{i=1}^{n} y_i$$

Therefore, the constant polynomial which best approximates f (in the sense of least squares) is the one whose value is the mean of $y_1, \ldots, y_n$.

(4) Approximate the following data with a model of the form $f(x) \sim ae^{bx}$.

x	-1	0	1	2
y	8.1	3	1.1	0.5

If $f(x) = ae^{bx}$ then $g(x) = \ln(f(x)) = \ln a + bx$. Now take the logarithm of the sampled image of f:

x	-1	0	1	2
y	2.09	1.09	0.09	-0.69

We can fit the linear model $g(x) = \ln a + bx$ to this data using the standard procedure. The 2×2 matrix associated to the system whose solutions are $\ln a, b$ is given by:

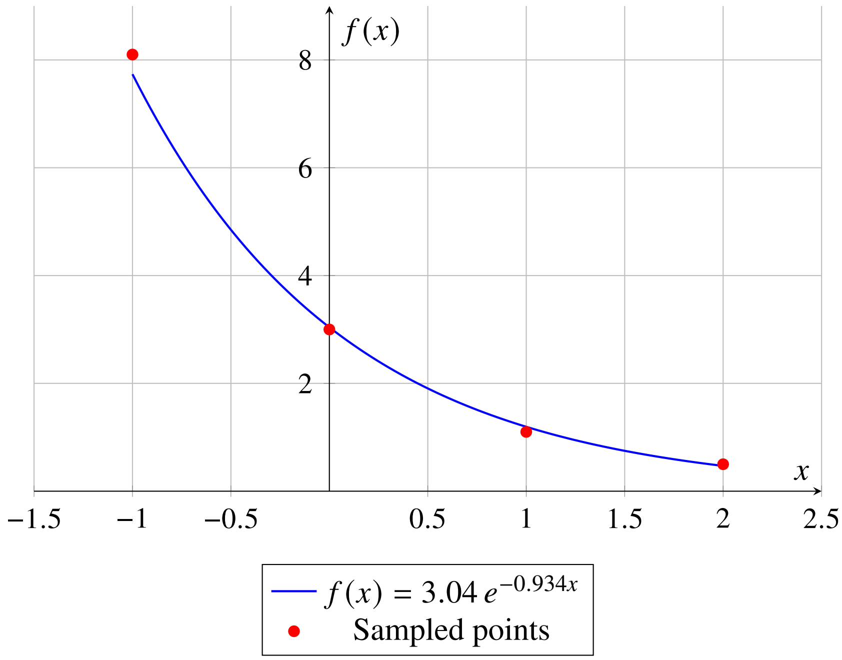
$$\sum_{i=0}^{3} x^0 = 4, \qquad \sum_{i=0}^{3} x_i 2, \qquad \sum_{i=0}^{3} x_i^2 = 6,$$
$$\sum_{i=0}^{3} x_i^0 y_i = 2.58, \qquad \sum_{i=0}^{3} x_i y_i = -3.38$$

In other words, the system is

$$\begin{bmatrix} 4 & 2 & 2.58 \\ 2 & 6 & -3.38 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 0 & 1.112 \\ 0 & 1 & -0.934 \end{bmatrix}$$

From this follows:

$$\ln a = 1.112 \text{ (or } a = e^{1.112} \approx 3.04), \qquad b = -0.934$$



$f(x)$
8
6
4
2
x
−1.5
−1
−0.5
0.5
1
1.5
2
2.5
$f(x) = 3.04\,e^{-0.934x}$
Sampled points

(5) Same, but with $f(x) \sim -e^{ax^2+bx+c}$ and values

x	-1	0	1	2
y	-1.1	-0.4	-0.9	-0.5

An obvious problem is that $\mathcal{D}(\ln) = \mathbb{R}^+$. So take

$$\phi(x) = \ln(-f(x)) = ax^2 + bx + c$$

so that the transformation we need to apply to the data is $\ln \circ \psi$ with ψ the negation function:

x	-1	0	1	2
y	0.09	-0.91	-0.1	-0.69

Since $n = 2$, we need to compute a 3×3 matrix with coefficients

$$\mathbf{A} = \begin{bmatrix} \sum x_i^0 & \sum x_i^1 & \sum x_i^2 \\ \sum x_i^1 & \sum x_i^2 & \sum x_i^3 \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 \end{bmatrix}$$

to create the system

$$\mathbf{A} \begin{bmatrix} a & b & c \end{bmatrix}^\top = \begin{bmatrix} \sum y_i & \sum x_i y_i & \sum x_i^2 y_i \end{bmatrix}^\top$$

Now,

$$\sum_{i=0}^{3} x^0 = 4, \qquad \sum_{i=0}^{3} x_i = 2, \qquad \sum_{i=0}^{3} x_i^2 = 6, \qquad \sum_{i=0}^{3} x_i^3 = 8, \qquad \sum_{i=0}^{3} x_i^4 = 18$$
$$\sum_{i=0}^{3} x_i^0 y_i = -1.61, \qquad \sum_{i=0}^{3} x_i y_i = -1.57, \qquad \sum_{i=0}^{3} x_i^2 y_i = -2.77$$

So the system can be expressed as:

$$\begin{bmatrix} 4 & 2 & 6 & -1.61 \\ 2 & 6 & 8 & -1.57 \\ 6 & 8 & 18 & -2.77 \end{bmatrix}$$

which solves to

$$a = -0.4285, \qquad b = -0.2555, \qquad c = 0.1025$$

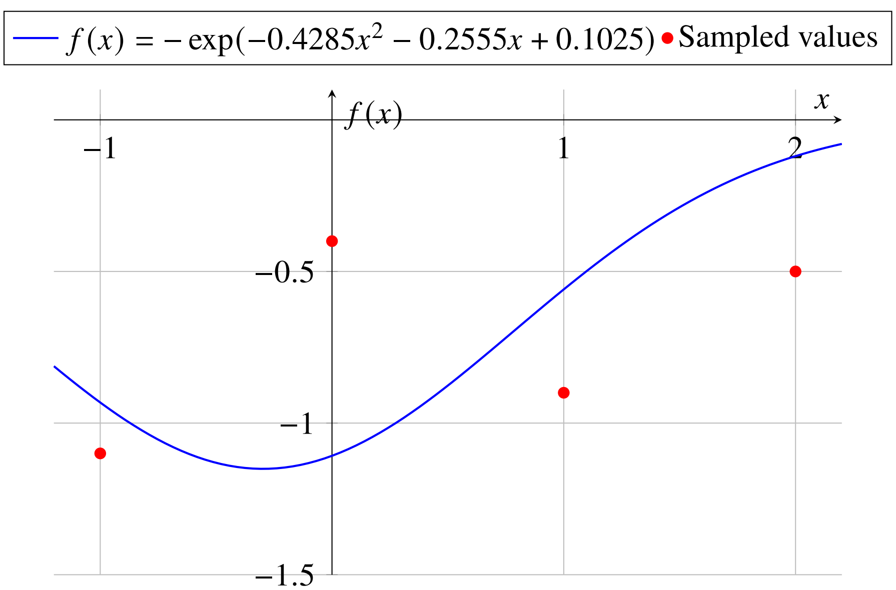
Now, since

$$\phi(x) = \ln(-f(x)) = ax^2 + bx + c$$

we find

$$f(x) = -\exp\left(ax^2 + bx + c\right) = -e^{-0.4285x^2 - 0.2555x + 0.1025}$$

to be the least square fit of our sampled values with model f.



(8) Approximate the data with $f(x) \sim a\cos x + b\sin x$.

x	0	1	2	3	4	5	6	7	8	9	10
y	1.8	3.5	2.1	-1.0	-3.3	-2.7	0.9	3.3	2.8	-0.1	-3.0

There is no way to transform f into a polynomial model (that I kwow of). So let's brute-force this:

$$\begin{aligned} E = E(a,b) &= \sum_{i=0}^{n} (y_i - f(x_i))^2 \\ &= \sum_{i=0}^{n} (y_i - (a\cos x_i + b\sin x_i))^2 \\ &= \sum_{i=0}^{n} (y_i - a\cos x_i - b\sin x_i)^2 \end{aligned}$$

Now, it is easy to see that

$$\frac{\partial E}{\partial a} = 2\sum_{i=0}^{n}(a\cos x_i + b\sin x_i - y_i)\cos x_i, \qquad \frac{\partial E}{\partial b} = 2\sum_{i=0}^{n}(a\cos x_i + b\sin x_i - y_i)\sin x_i$$

Equating both expressions to zero, one obtains the system:

$$\begin{aligned} a\sum_{i=0}^{n}\cos^2 x_i + b\sum_{i=0}^{n}\sin x_i\cos x_i &= \sum_{i=0}^{n} y_i\cos x_i \\ a\sum_{i=0}^{n}\cos x_i\sin x_i + b\sum_{i=0}^{n}\sin^2 x_i &= \sum_{i=0}^{n} y_i\sin x_i \end{aligned}$$

In other words, we readily obtain the system

$$\begin{bmatrix} \sum_{i=0}^{n}\cos^2 x_i & \sum_{i=0}^{n}\sin x_i\cos x_i & \sum_{i=0}^{n} y_i\cos x_i \\ \sum_{i=0}^{n}\cos x_i\sin x_i & \sum_{i=0}^{n}\sin^2 x_i & \sum_{i=0}^{n} y_i\sin x_i \end{bmatrix}$$

Suffices to evaluate these sums using a calculator and solving the system to obtain the coefficients a, b which minimize the squared distances from the model to the set of data points.

(9) Consider Legendre's polynomials $\mathcal{P} := \{P_0, P_1, P_2\}$ on $[-1, 1]$ given by

$$P_0(x) = 1, \qquad P_1(x) = x, \qquad P_2(x) = x^2 - 1/3$$

Verify that the set $\mathcal{P}$ is ortogonal.

The set $\mathcal{P}$ is ortogonal (in $[a, b]$) if and only if there is a weight function ω such that

$$\int_a^b \omega(x) P_k(x) P_j(x)\ dx = \alpha_j \delta_{jk}, \qquad j = 0, 1, 2$$

for some $\{\alpha_0, \alpha_1, \alpha_2\}$ all positive. In particular, if $\alpha_0 = \alpha_1 = \alpha_2 = 1$, the set is ortonormal. Now, consider that $\Omega(x) = 1$ is a weight function. It is easy to verify that

$$\int_{-1}^1 \Omega(x) P_j^2(x)\ dx > 0$$

for $j = 0, 1, 2$. Now, $\int_{-1}^1 \Omega(x) P_0(x) P_1(x)\ dx = \int_{-1}^1 x\ dx = 0$. Similarly,

$$\int_{-1}^1 \Omega(x) P_0(x) P_2(x)\ dx \int_{-1}^0 x^2 - 1/3\ dx = \frac{2}{3} - \frac{2}{3} = 0$$

Etc. This excercise is silly as it amounts to solving integrals.

(10) Determine the linear and quadratic approximations of $f(x) = e^x$ in the least squares sense using Legendre's polynomials in $[-1, 1]$.

Let $\Phi = \left\{1, x, x^2 - 1/3\right\}$, and use ϕ_0, ϕ_1, ϕ_2 to refer to the elements in this set in the order I wrote them. We know Φ to be ortogonal.

(Linear approximation) There is a set of coefficients a_0, a_1 of

$$P(x) = \sum_{k=0}^{n} a_k \phi_k(x)$$

which minimizes

$$\int_{-1}^{1} [f(x) - P(x)]^2 \ dx$$

Since Φ is ortonormal, we have

$$a_j = \frac{1}{\alpha_j} \int_a^b f(x)\phi_j(x) \ dx, \qquad j = 0, 1$$

Recall that

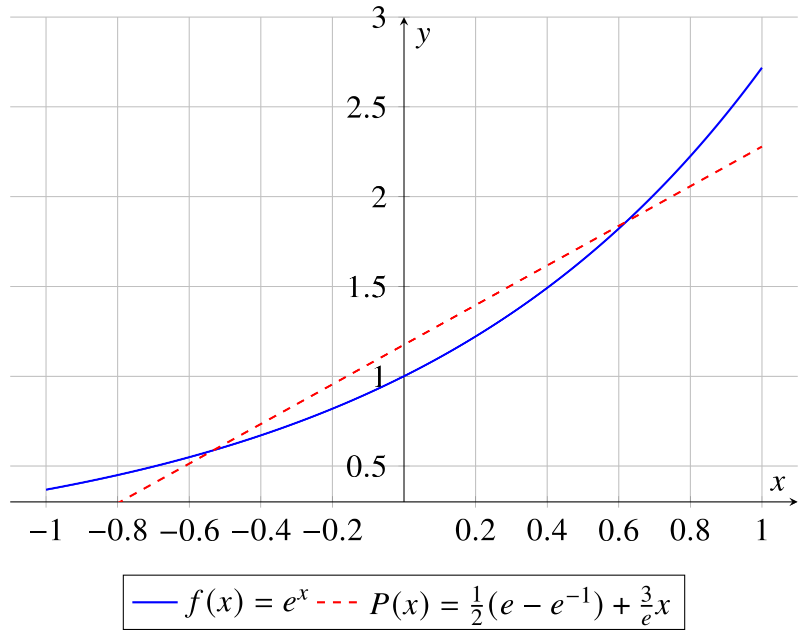
$$\alpha_0 = \int_{-1}^{1} \phi_0^2(x) = 2, \qquad \alpha_1 = \int_{-1}^{1} \phi_1^2(x) \ dx = \frac{2}{3}, \qquad \alpha_2 = \int_{-1}^{2} \phi_2^2(x) \ dx = \frac{8}{45}$$

This readily gives the system of equations:

$$\begin{aligned} a_0 &= \frac{1}{2} \int_{-1}^{1} e^x \ dx = \frac{1}{2}(e - e^{-1}) \\ a_1 &= \frac{3}{2} \int_{-1}^{1} x e^x \ dx = \frac{3}{2} \left[e^{-1} + e^{-1}\right] = \frac{3 \cdot 2}{2e} = \frac{3}{e} \end{aligned}$$

Hence, the desired polynomial approximation of $f(x) = e^x$ on $[-1, 1]$ is:

$$P(x) = \frac{1}{2}(e - e^{-1}) + \frac{3}{e} \cdot x$$

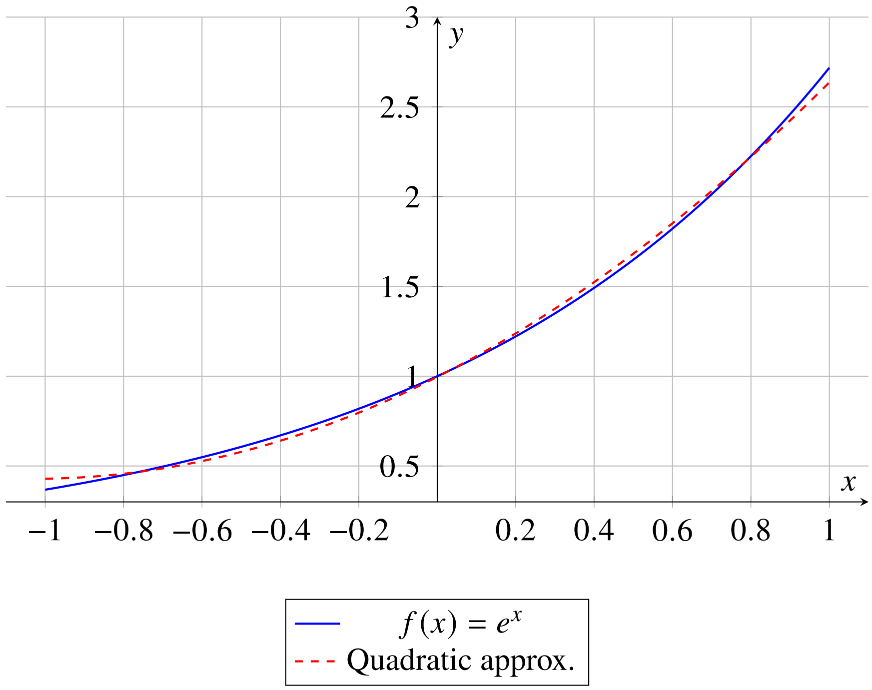


(Quadratic approximation) For a quadratic approximation, we now compute as well

$$a_2 = \frac{45}{8} \int_{-1}^{1} e^x (x^2 - 1/3)\, dx = \frac{15(2e^2 - 14)}{8e}$$

So, the approximation is

$$P(x) = \frac{1}{2}(e - e^{-1}) + \frac{3}{e} \cdot x + \frac{15(2e^2 - 14)}{8e} \left(x^2 - \frac{1}{3}\right)$$



3
2.5
2
1.5
1
0.5
y
x
−1
−0.8
−0.6
−0.4
−0.2
0.2
0.4
0.6
0.8
1
$f(x) = e^x$
Quadratic approx.

(10) Approximate $f(x) = e^{-3x}$ for $x \in (0, \infty)$ with a quadratic polynomial using least squares with weight function $\omega(x) = e^{-x}$, considering Laguerre polynomials defined as:

$$\phi_k(x) = \frac{e^x}{k!}\frac{d^k}{dx^k}(x^k e^{-x})$$

for all $x \in [0, \infty)$, $k = 0, 1, 2, \ldots$. Help: For each $n \in \mathbb{N}$, we know

$$\int_0^\infty x^n e^{-x}\, dx = n!$$

We will need ϕ_0, ϕ_1, ϕ_2 for a quadratic polynomial, so we might just as well begin by finding these polynomials. See the calculations below for their derivation.

Derivation of ϕ_1, ϕ_2, ϕ_3: See that

$$\begin{aligned}\phi_0(x) &= e^x(x^0 e^{-x}) \\ &= e^{x-x} \\ &= 1\end{aligned}$$

Furthermore,

$$\begin{aligned}\phi_1(x) &= e^x \frac{d}{dx}(xe^{-x}) \\ &= e^x\,(e^{-x} - xe^{-x}) \\ &= 1 - x\end{aligned}$$

Lastly, since

$$\frac{d}{dx}x^2e^{-x} = 2xe^{-x} - x^2e^{-x}$$

then the second derivative of x^2e^{-x} is:

$$2 \cdot \frac{d}{dx}(xe^{-x}) - \frac{d}{dx}x^2e^{-x} = 2\,(e^{-x} - xe^{-x}) - (2xe^{-x} - x^2e^{-x})$$

Por lo tanto,

$$
\begin{aligned}
\phi_2(x) &= \frac{e^x}{2!}\frac{d^2}{dx^2}\left(x^2 e^{-x}\right) \\
&= \frac{e^x}{2}\left[2e^{-x} - 2xe^{-x} - 2xe^{-x} + x^2 e^{-x}\right] \\
&= \frac{2 - 2x - 2x + x^2}{2} \\
&= (x^2 - 4x + 2)1/2
\end{aligned}
$$

In summary,

$$\phi_1(x) = 1, \qquad \phi_2(x) = -x + 1, \qquad \phi_2(x) = (x^2 - 4x + 2)1/2$$

We know these polynomials are orthogonal with respect to ω, which simply means that the Hilbert matrix with coefficients

$$a_{ij} = \int_0^\infty \omega(x)\phi_i(x)\phi_j(x)$$

satisfies

$$a_{ij} = \delta_{ij}\alpha_j, \qquad j = 0, 1, 2$$

for some values $\alpha_0, \alpha_1, \alpha_2$ which we must determine. Expressed differently, the coefficients a_0, a_1, a_2 of the polynomial which approximates f are given by

$$a_j = \frac{1}{\alpha_j}\int_0^\infty \omega(x) f(x)\phi_j^2(x)\, dx$$

So let us now compute $\alpha_0, \alpha_1, \alpha_2$.

Computation of the α coefficients. See that

$$
\begin{aligned}
\alpha_0 = \int_0^\infty \omega(x)\phi_0^2(x)\ dx &= \int_0^\infty x^0 e^{-x}\ dx \\
&= 1
\end{aligned}
$$

$$
\begin{aligned}
\alpha_1 = \int_0^\infty \omega(x)\phi_1^2(x)\ dx &= \int_0^\infty e^{-x}(1-x)^2\ dx \\
&= \int_0^\infty e^{-x}(1-2x+x^2)\ dx \\
&= \int_0^\infty e^{-x}\ dx - 2\int_0^\infty xe^{-x}\ dx + \int_0^\infty x^2 e^{-x}\ dx \\
&= 0! - 2\times 1! + 2! \\
&= 1 - 2 + 2 \\
&= 1
\end{aligned}
$$

For the last problem, see that the numerator of ϕ_2 squared is:

$$
\begin{aligned}
(x^2-4x+2)(x^2-4x+2) &= (x^4-4x^3+2x^2) + (-4x^3+16x^2-8x) + (2x^2-8x+4) \\
&= x^4 + (-4x^3-4x^3) + (2x^2+16x^2+2x^2) + (-8x-8x) + 4 \\
&= x^4 - 8x^3 + 20x^3 - 16x + 4
\end{aligned}
$$

Then

$$
\begin{aligned}
\alpha_2 &= \int_0^\infty \omega(x)\phi_2^2(x)\ dx \\
&= \int_0^\infty e^{-x}\left(x^2-4x+2\right)^2 (1/4)\ dx \\
&= \frac{1}{4}\int_0^\infty e^{-x}\left(x^4-8x^3+20x^2-16x+4\right)\ dx \\
&= \frac{1}{4}\left[4! - 8\times 3! + 20\times 2! - 16\times 1! + 4\times 0!\right] \\
&= \frac{1}{4}\left[24-48+40-16+4\right] \\
&= \frac{1}{4}\left[68-64\right] \\
&= 1
\end{aligned}
$$

So we have $\alpha_0 = \alpha_1 = \alpha_2 = 1$. This means

$$a_j = \int_0^\infty \omega(x)\phi_j(x)f(x)\ dx$$

I don't know how to do the following fast without using the Gamma function:

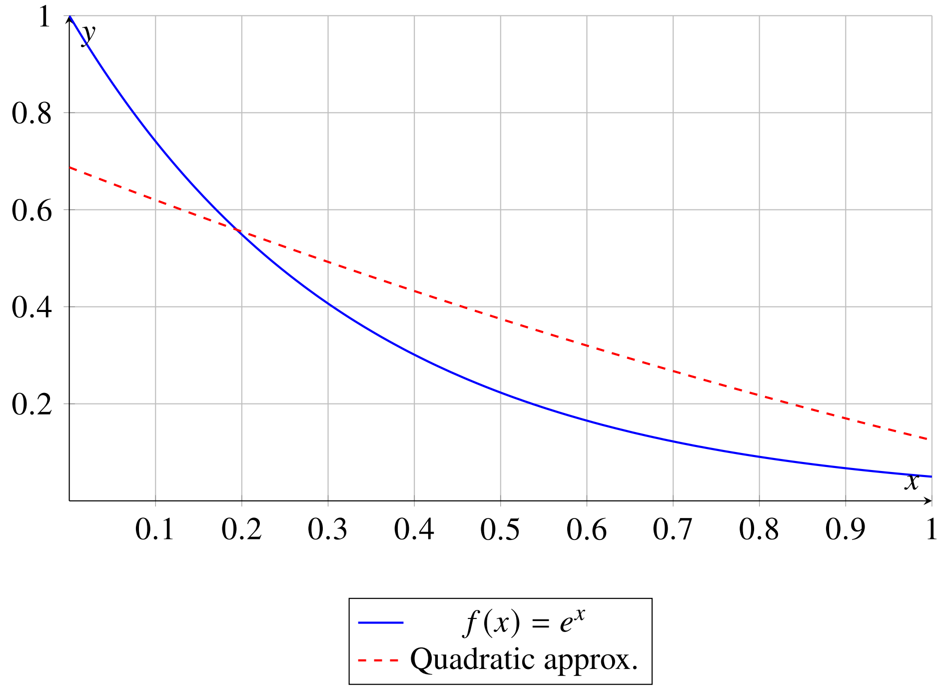
$$\int_0^\infty x^n e^{-kx}\ dx = \frac{n!}{k^{n+1}}$$

But we have:

$$\begin{aligned}
a_0 &= \int_0^\infty e^{-x}e^{-3x}\ dx = \int_0^\infty e^{-4x}\ dx = \frac{1}{4} \\
a_1 &= \int_0^\infty e^{-x}(1-x)e^{-3x}\ dx \\
&= \int_0^\infty e^{-4x}(1-x)\ dx \\
&= \int_0^\infty e^{-4x}\ dx - \int_0^\infty e^{-4x}x\ dx \\
&= \frac{1}{4} - \frac{1}{4^2} \\
a_2 &= \frac{1}{2}\int_0^\infty e^{-x}(x^2-4x+2)e^{-3x}\ dx \\
&= \frac{1}{2}\int_0^\infty e^{-4x}(x^2-4x+2)\ dx \\
&= \frac{1}{2}\left[\int_0^\infty x^2e^{-4x}\ dx - 4\int_0^\infty xe^{-4x}\ dx + 2\int_0^\infty e^{-4x}\ dx\right] \\
&= \frac{1}{2}\left[\frac{2!}{4^3} - 4\frac{1!}{4^2} + 2\frac{1}{4}\right] \\
&= \frac{1}{2}\left[1/4 - 1/4 + 1/2\right] \\
&= 1/4
\end{aligned}$$

So the approximating polynomial is

$$
\begin{aligned}
P(x) &= \sum_{i=0}^{2} a_i \phi_i(x) \\
&= \frac{1}{4} + \frac{3}{16}(-x+1) + \frac{1}{4}\frac{x^2-4x+2}{2} \\
&= \frac{1}{4} - \frac{3}{16}x + \frac{3}{16} + \frac{1}{8}x^2 - \frac{1}{2}x + \frac{1}{4} \\
&= \frac{1}{8}x^2 - \frac{11}{16}x + \frac{11}{16}
\end{aligned}
$$



7 Numerical integration

We'll estimate $\int_a^b f(x)\ dx$ via $\sum_{i=0}^n a_i f(x_i)$, where $(x_0, y_0), \ldots, (x_n, y_n)$ are known values of f (which itself might be unknown) in the interval $[a, b]$.

More generally, take $\{x_i\}_{i=0}^n$ in $[a, b]$ and P_n the interpolating polynomial of f in those nodes in Lagrange's form. Then we have

$$P_n(x) = \sum_{i=0}^n f(x_i)\ell_i(x), \qquad e_n(x) = \frac{f^{(n+1)(\zeta_x)}}{(n+1)!}\eta_{n+1}(x)$$

for $\zeta_x \in (x_0, x_n)$. Using the fact that $f(x) = P_n(x) + e_n(x)$,

$$\begin{aligned}
\int_a^b f(x)\ dx &= \int_a^b P_n(x)\ dx + \int_a^b e_n(x)\ dx \\
&= \int_a^b \sum_{i=0}^n f(x_i)\ell_i(x)\ dx + \int_a^b \frac{f^{(n+1)(\zeta_x)}}{(n+1)!}\eta_{n+1}(x)\ dx \\
&= \sum_{i=0}^n a_i f(x_i) + \frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\zeta_x) eta_{n+1}(x)\ dx
\end{aligned}$$

from $\zeta_x \in (x_0, x_n)$ and $a_i = \int_a^b \ell_i(x)\ dx$, $i = 0, \ldots, n$.

$$\therefore \int_a^b f(x)\ dx \approx \sum_{i=0}^n a_i f(x_i) \tag{1}$$

with an error

$$E_n(f) = \frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\zeta_x)\eta_{n+1}(x)\ dx \tag{2}$$

7.1 Trapeze rule

Summary.

$$\int_a^b f(x)\ dx \approx \frac{h}{2}\left[f(a) + f(b)\right], \qquad E(x) = -\frac{h^3}{12}f''(\zeta)$$

for some $\zeta \in (a, b)$ and $h = b - a$.

Observation. If $f'' \equiv 0$ then the rule is exact.

Trapeze's rule is the name for the case $n = 1$ (linear integration). By convention, $x_0 = a, x_1 = b, h = b - a$. The interpolating polynomial es

$$P_1(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)$$

with error

$$e_1(x) = \frac{f''(\zeta_x)}{2!}(x - x_0)(x - x_1)$$

Simplifying equation (1) for this case,

$$\begin{aligned}\int_a^b f(x)\, dx &\approx f(x_0) \int_a^b \frac{x - x_1}{x_0 - x_1}\, dx + f(x_1) \int_a^b \frac{x - x_0}{x_1 - x_0}\, dx \\ &= \frac{h}{2}\left(f(a) + f(b)\right)\end{aligned}$$

To simplify the expression of the error, the following theorem is used.

Theorem 16 (Pretty theorem)**.** Assume $f \in C[a, b]$ and g integrable and either always positive or always negative in $[a, b]$. Then there is some $c \in (a, b)$ such that

$$\int_a^b f(x)g(x)\, dx = f(c) \int_a^b g(x)\, dx$$

If $g(x) \equiv 1$ then $\int_a^b f(x)\, dx = f(c)(b - a)$, entailing that

$$f(c) = \frac{1}{b - a} \int_a^b f(x)\, dx$$

It is easy to see that $(x - x_0)(x - x_1)$ satisfies the conditions of the theorem, meaning that there is some ζ (independent of x) such that

$$
\begin{aligned}
\int_a^b (\zeta_x)(x-a)(x-b)\ dx &= f''(\zeta)\int_a^b (x-a)(x-b)\ dx \\
&= f''(\zeta)\left[\frac{x^3}{3} - \frac{a+b}{2}x^2 + abx\right]_a^b \\
&= f''(\zeta)\left(-\frac{h^3}{6}\right)
\end{aligned}
$$

In summary, the error is:

$$
E(x) = \frac{1}{2}f''(\zeta)\left(-\frac{h^3}{6}\right) = -\frac{h^3}{12}f''(\zeta)
$$

with $h = b - a$ and for some $\zeta \in (a, b)$ independent of x.

7.2 Simpson's rule

Simpson's rule is the name for the case $n = 2$ with three equidistant nodes $a = x_0, x_1 = \frac{a+b}{2}, x_2 = b$. We let

$$
h = \frac{b-a}{2},\ \text{which entails the nodes are } a, a+h, a+2h
$$

Three nodes allow us to construct an interpolating polynomoial of degree 2. The rule is:

$$
\int_a^b f(x)\ dx \approx \frac{h}{3}\left[f(a) + 4f\ (a+h) + f(a+2h)\right]
$$

with

$$
E = -\frac{h^5}{90}f^{(4)}(\zeta)
$$

for some $\zeta \in (a, b)$.

7.3 Rectangle's rule

Stupid:

$$\int_a^b f(x)\,dx \approx f(a)(b-a)$$

whicih is the area in the rectangle from a, b with height $f(a)$, giving

$$E = \frac{(b-a)^2}{2} f'(\zeta), \qquad \zeta \in (a, b)$$

One could take $x_0 = b$ and estimate via the rectangle from a, b with height $f(b)$.

7.4 Midpoint rule

Stupid: Exactly the same as the rectangle rule, but the rectangle has height $f(m)$, where $m = (a+b)/2$ is the midpoint of $[a, b]$:

$$\int_a^b f(x)\,dx = f\left(\frac{a+b}{2}\right)(b-a)$$

with error

$$E = \frac{(b-a)^3}{24} f''(\zeta), \qquad \zeta \in (a, b)$$

Since the error has a derivative of order 2, this method will integrate exactly all polynomials of degree 1.

7.5 Precision of estimation rules

The **precision** of a rule is the greatest non-negative integer n s.t. the formula is exact for x^k, for all $k = 0, \ldots, n$.

7.6 Composite rules

Simpson's composite rule. Let $f \in C^4[a, b]$, n a positive integer, $h = (b-a)/2n$ and $x_j = a + jH$ for $j = 0, \ldots, 2n$. There is some $\mu \in (a, b)$ such that the composite rule of Simpson for n sub-intervals is given by

Regla	Puntos	Fórmula	Error	Precisión
Rectángulo	1	$f(a)(b-a)$	$\frac{(b-a)^2}{2}f'(\xi)$	0
Punto medio	1	$f\left(\frac{a+b}{2}\right)(b-a)$	$\frac{(b-a)^3}{24}f''(\xi)$	1
Trapecio	2	$\frac{(b-a)}{2}[f(a)+f(b)]$	$-\frac{(b-a)^3}{12}f''(\xi)$	1
Simpson	3	$\frac{(b-a)/2}{3}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]$	$-\frac{((b-a)/2)^5}{90}f^{(4)}(\xi)$	3

Table 1: Fórmulas de integración numérica y sus errores

$$\int_a^b f(x) = \frac{h}{3}\left(f(x_0) + 2\sum_{j=1}^{n} f(x_{2j}) + 4\sum_{j=1}^{n} f(x_{2j-1}) + f(x_n)\right) - \frac{b-a}{180}h^4 f^{(4)}(\mu)$$

To estimate large intervals, the interval is segmented into k segments of equal length of relatively small size and the estimations within segment are summed.

In general, if $[a, b]$ is segmented in n sub-intervals of equal length, we obtain $(2n + 1)$ equally spaced points $x_j = a + jh$, with $j = 0, \ldots, 2n$ and $h = (b-a)/2n$. Then,

$$\int_a^b f(x)\,dx = \sum_{j=1}^{n} \int_{x_{2j-2}}^{x} {}_{2j} f(x)\,dx$$

For Simpson's rule, this gives

$$\int_a^b f(x)\,dx \approx \sum_{j=1}^{n} \left(\frac{h}{3}\left[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})\right] - \frac{h^5}{90} f^{(4)}(\zeta_j)\right)$$

with $\zeta_j \in (x_{2j-2}, x_{2j})$, $j = 1, \ldots, n$, $f \in C^4[a, b]$. For $j = 1, \ldots, n$, the term $f(x_{2j})$ appears both in $[x_{2j-2}, x_{2j}]$ and $[x_{2j}, x_{2j+2}]$, which allows us to simplify:

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left(f(x_0) + 2\sum_{j=1}^{n} f(x_{2j}) + 4\sum_{j=1}^{n} f(x_{2j-1}) + f(x_{2n})\right) - \frac{h^5}{90}\sum_{j=1}^{n} f^{(4)}(\zeta_j)$$

Since $f^{(4)}$ is assumed to be continuous in $[a, b]$, the extreme value theorem for continuous functions ensures:

- $f''(\zeta_j)$ is between the minimum and the maximum of $f^{(4)}$ in $[a, b]$.

- $\sum_{i=1}^{n} f^{(4)}(\zeta_j)$ is between n times the minimum and n times the maximum of $f^{(4)}$ in $[a, b]$.
- Dividing in (2) by n, we obtain

$$\min_{x\in[a,b]} f^{(4)}(x) \leq \frac{1}{n} f^{(4)}(\zeta_j) \leq \max_{x\in[a,b]} f^{(4)}(x)$$

The intermediate value theorem ensures then that there is some $\mu \in (a, b)$ such that

$$f^{(4)}(\mu) = \frac{1}{n} f^{(4)}(\zeta_j) \Rightarrow \sum_{j=1}^{n} f^{(4)}(\zeta_j) = n f^{f(4)}(\zeta_j)$$

Using this, the error can be expressed independently of ζ_j as:

$$E(f) = -\frac{h^5}{90} \sum_{j=1}^{n} f^{(4)}(\zeta_j) = -\frac{h^5}{90} n f^{(4)}(\mu)$$

7.7 Other composite rules

No time. Memorize the formulas from apunte.

7.8 Gaussian rules

Theorem 17. Let w a positive weight function in $[a, b]$ and $q \neq 0$ a polynomial of degree exactly $n + 1$ ortogonal to all polynomials of degree $\leq n$ (with respect to n). In other words, assume

$$\int_a^b q(x)p(x)w(x)\ dx = 0$$

Then if $x_0, x_1, \ldots, x_n$ are the $n + 1$ roots of q, then

$$\int_a^b f(x)w(x)\ dx \sum_{i=0}^{n} a_i f(x_i)$$

with $a_i = \int_a^b w(x)\ell_i(x)\ dx$ is exact for all polynomials f of degree $\leq 2n + 1$.

7.9 Excercises

(2) Define

$$f(x) = \begin{cases} x & 0 \leq x \leq 1/2 \\ 1 - x & 1/2 \leq x \leq 1 \end{cases}$$

in $[0,1]$. Estimate $\int_0^1 f(x)\ dx$ using (a) the trapeze rule in $[0,1]$, the trapez rule on a half-segmentation of $[0,1]$, (c) Simpson's rule on $[0,1]$. (d) What can you conclude?

Let us first observe that

$$\begin{aligned} \int_0^1 f(x)\ dx &= \int_0^{\frac{1}{2}} x\ dx + \int_{\frac{1}{2}}^1 1 - x\ dx \\ &= \frac{1}{8} + \frac{1}{2} - (\frac{1}{2} - \frac{1}{8}) \\ &= 1/4 \end{aligned}$$

(a) The trapeze rule was defined as

$$\int_a^b f(x)\ dx = \frac{h}{2}\left[f(a) + f(b)\right] - \frac{h^3}{12} f''(\zeta)$$

for some $\zeta \in (a,b)$. Here, $h = 1 - 0 = 1$, $f(0) = 0$, $f(1) = 0$. So its estimation gives $1/2(0) = 0$, with an error of 0.25.

(b) When using the rule on the two equal-split segments of the interval, we obtain

$$\begin{aligned} \int_0^1 f(x)\ dx &\approx \frac{1/2}{2}\left[f(0) + f(1/2)\right] + \frac{1/2}{2}\left[f(1/2) + f(1)\right] \\ &= \frac{1}{4} \times \frac{1}{2} + \frac{1}{4} \times \frac{1}{2} \\ &= 1/4 \end{aligned}$$

which is an exact approximation.

(c) Simpson's rule is defined for $n = 2$ (three points), so we select $1/2$ as midpoint having $h = 1/2$.

$$
\begin{aligned}
\int_0^1 f(x)\, dx &\approx \frac{h}{3}\,[f(0) + 4f(1/2) + f(1)] \\
&= \frac{1}{6}\,[0 + 4/2 + 0] \\
&= \frac{1}{3}
\end{aligned}
$$

(4) (a) Build a rule of the form

$$\int_{-1}^{1} f(x)\, dx \approx \alpha f\left(-\frac{1}{2}\right) + \beta f(0) + \gamma f\left(\frac{1}{2}\right)$$

that is exact for all polynomials f degree ≤ 2.

(b) Determine the precision of the formula for

$$\int_{-1}^{1} f(x)\, dx \approx \frac{4}{3} f\left(-\frac{1}{2}\right) - \frac{2}{3} f(0) + \frac{4}{3} f\left(\frac{1}{2}\right)$$

(a) Let $p_0(x) = 1, p_1(x) = x, p_2(x) = x^2$. For the formula to be exact for polynomials of degree ≤ 2, it must satisfy:

$$\begin{bmatrix} p_0\left(-\frac{1}{2}\right) & p_0\,(0)\; p_0\left(\frac{1}{2}\right) \\ p_1\left(-\frac{1}{2}\right) & p_1\,(0)\; p_1\left(\frac{1}{2}\right) \\ p_2\left(-\frac{1}{2}\right) & p_2\,(0)\; p_2\left(\frac{1}{2}\right) \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix} = \begin{bmatrix} \int_{-1}^{1} p_0(x)\, dx \\ \int_{-1}^{1} p_1(x)\, dx \\ \int_{-1}^{1} p_2(x)\, dx \end{bmatrix}$$

Let $\varphi_i = \int_{-1}^{1} p_i(x)\, dx$. Note that $\varphi_0 = 2, \varphi_1 = 0, \varphi_2 = \frac{2}{3}$. Then, we can express the problem more succintly. α, β, γ are solutions to the following system of equations:

$$\begin{bmatrix} 1 & 1 & 1 & \mid 2 \\ -\frac{1}{2} & 0 & \frac{1}{2} & \mid 0 \\ \frac{1}{4} & 0 & \frac{1}{4} & \mid \frac{2}{3} \end{bmatrix}$$

From the second row, we readily have $\alpha = \gamma$. Then, the third row expresses that

$$\frac{1}{2}\alpha = \frac{2}{3} \Rightarrow \alpha = \frac{4}{3}$$

Then, row one gives

$$\beta = 2 - \frac{8}{3} = -\frac{2}{3}$$

The formula then is

$$\int_{-1}^{1} f(x)\, dx \approx \frac{4}{3} f\left(-\frac{1}{2}\right) - \frac{2}{3} f(0) + \frac{4}{3} f\left(\frac{1}{2}\right)$$

(5) (a) Determine the number n of sub-intervals needed in the composite trapeze rule to approximate $\int_0^1 e^{-x^2}\ dx$ with an error $\leq \frac{1}{2}10^{-6}$, assuming e^{-x^2} can be computed precisely. (b) Repeat for Simpson's composite rule.

(a) If n sub-intervals are taken in $[0,1]$, then each sub-interval is of length $h(n) = \frac{1}{n}$. Note as well that if n sub-intervals are taken, then there are $n+1$ points forming intervals $[x_1, x_2], \ldots, [x_n, x_{n+1}]$. The composite approximation is

$$\int_0^1 f(x)\ dx \approx \sum_{i=1}^{n} \left(\frac{h(n)}{2} \left[f(x_i) + f(x_{i+1}) \right] - \frac{h^3}{12} f''(\zeta_i) \right)$$

where $\zeta_i \in (x_i, x_{i+1})$. We only care about the error here, which we can clear out, since

$$\begin{aligned} &\sum_{i=1}^{n} \left(\frac{h(n)}{2} \left[f(x_i) + f(x_{i+1}) \right] - \frac{h^3(n)}{12} f''(\zeta_i) \right) \\ &= \sum_{i=1}^{n} \left(\frac{1}{2n} \left[f(x_i) + f(x_{i+1}) \right] \right) - \frac{1}{12n^3} \sum_{i=1}^{n} f''(\zeta_i) \end{aligned}$$

Now, observe that

$$\frac{d}{dx} e^{-x^2} = \frac{d}{du} e^{u} \frac{d}{dx}(-x^2) = -2xe^{-x^2}$$

from which follows that the second derivative of f is

$$\frac{d}{dx} - 2xe^{-x^2} = -2\left(e^{-x^2} + x(-2xe^{-x^2})\right) = -2e^{-x^2} + 4x^2 e^{-x^2} = f''(x)$$

The derivative of this function is

$$-2(4e^{-x^2}x^3 - 6e^{-x^2}x)$$

which is always negative in $(0,1)$ (since e^{-x^2} is always positive in $(0,1)$). Therefore, f'' is a decreasing function and its maximum (in $(0,1)$) is bounded by $f''(0) = -2$. From this readily follows that the error term satisfies

$$-\frac{1}{12n^3}\sum_{i=1}^{n} f''(\zeta_i) \leq -\frac{1}{12n^3}\sum_{i=1}^{n}(-2) = \frac{2n}{12n^3} = \frac{1}{6n^2}$$

Using the fact that the error term is less than or equal to $1/6n^2$, we must simply bound

$$\frac{1}{6n^2} \leq \frac{1}{2}10^{-6}$$

(7) Estimate $\int_{-1}^{1} f(x)\, dx$ through a rule of the form

$$\int_{-1}^{1} f(x)\, dx = \alpha f(x_1) + \beta f(x_2) + \gamma f(x_3)$$

that is exact for polynomials of degree ≤ 5. Use it to approximate $f(x) = \cos x$.

We know from previous problems that $\varphi_0 = 2, \varphi_1 = 0, \varphi_2 = \frac{2}{3}$, where $\varphi_i = \int_{-1}^{1} x^i\, dx$.

$$\int_{-1}^{1} x^3\, dx = 0, \qquad \int_{-1}^{1} x^4\, dx = \frac{2}{5}, \qquad \int_{-1}^{1} x^5\, dx = 0$$

We will take $x_1 = -1, x_2 = 0, x_3 = 1$. Then, α, β, γ are the solutions of the following system of equations:

$$\begin{bmatrix} 1 & 1 & 1 & 2 \\ -1 & 0 & 1 & 0 \\ 1 & 0 & 1 & \frac{2}{3} \\ -1 & 0 & 1 & 0 \\ 1 & 0 & 1 & \frac{2}{5} \\ -1 & 0 & 1 & 0 \end{bmatrix} \tag{1}$$

8 Systems of equations

The problem is finding the solution to $Ax = b$ with $A \in \mathbb{R}^{n \times n}$ and $b \in \mathbb{R}^n$.

Diagonal case. Obviously, if A is diagonal and its determinant is non-zero (i.e. $a_{ii} \neq 0$ for all $i = 1, \ldots, n$) then $Ax = b$ (with $x, b \in \mathbb{R}^n$) has the single solution $x_i = \frac{b_i}{a_{ii}}$. So an algorithm is simply:

input n, A, b
for $i = 1, \ldots, n$ **do**
    $x_i \leftarrow b_i / a_{ii}$
od

with a computational complexity $O(n)$ (exactly n operations).

Triangular case. A matrix is upper-triangular iff $a_{ij} = 0$ for $i < j$ (lower-triangular if this holds for $i > j$). Assume $A \in \mathbb{R}^n$ is lower-triangular.

Assume A is lower-triangular and non-singular (i.e. invertible, i.e. non-zero determinant, ect.):

$$A = \begin{bmatrix} a_{11} & 0 & \ldots & 0 \\ a_{21} & a_{22} & \ldots & 0 \\ \vdots & \vdots & \ldots & 0 \\ a_{n1} & a_{n2} & \ldots & a_{nn} \end{bmatrix}$$

Then $Ax = b$ requires

$$\begin{cases} a_{11}x_1 & = b_1 \\ a_{21}x_1 + a_{22}x_2 & = b_2 \\ \vdots \\ a_{n1}x_1 + \ldots + a_{nn}x_n & = b_n \end{cases} \Rightarrow \begin{cases} x_1 & = b_1 / a_{11} \\ x_2 & = \frac{1}{a_{22}}(b_2 - a_{21}x_1) \\ \vdots \\ x_i & = \frac{1}{a_{ii}}\left(b_i \sum_{j=1}^{i-1} a_{ij}x_j\right) \\ \vdots \\ x_n & = \frac{1}{a_{nn}}\left(b_n - \sum_{j=1}^{n-1} a_{nj}x_j\right) \end{cases}$$

Therefore, an algorithm is simply setting for $i = 1, \ldots, n$ the value

$$x_i \leftarrow \left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j \right) / a_{ii}$$

Esto hace $O(n^2)$ operaciones.

8.1 Gaussian elimination

Gaussian elimination consists of solving $Ax = b$ by finding $(n-1)$ transformations of A and b,

$$A^{(1)}, \ldots, A^{(n-1)}, \qquad b^{(1)}, \ldots, b^{(n-1)}$$

satisfying that $U = A^{(n-1)}$ is upper-triangular and therefore contains the solution to the system. Let us show the transitions in part before generalizing.

(Transition $A \to A^{(1)}$) Take a_{11} as pivot. We want to convert all values under a_{11} (first column except a_{11}) into zeros. So for each row, we compute the multiplicative factor

$$m_i^{(1)} = \frac{a_{i1}}{a_{11}}$$

Observe that this factor is such that $a_{i1} - m_i^{(1)} a_{11} = 0$, in other words it is the number such that the row operation

$$i\text{th row} - \text{first row } \times m_i \tag{1}$$

ensures $a_{i1} = 0$. We then perform precisely the operation specified in (1), which gives $A^{(1)}$ with coefficients

$$a_{ij}^{(1)} = \begin{cases} a_{11} & i = j = 1 \\ 0 & 1 < i \leq n, j = 1 \\ a_{ij} - m_i^{(1)} a_{1j} & c.c. \end{cases}, \qquad b_i^{(1)} = \begin{cases} b_1 & i = 1 \\ b_i - m_i b_1 & 1 < i \leq n \end{cases}$$

How many operations are involved? Well, we can ignore the direct assignments and consider only the updating of non-zero values. In the matrix, there are $(n-1) \times (n-1) = (n-1)^2$ such computations to be made, each of which consists of substracting from an existing coefficient a product. Then $(n-1)$ such computations must be performed in vector b as well. So the passing $A \to A^{(1)}$ requires $(n-1)^2 + n - 1$ products, $(n-1)^2 + (n-1)$ sums.

However, before the passing, we must also compute $m_2, \ldots, m_n$, which involves $n-1$ quotients. So we have in total:

$$\textbf{\#Products} = (n-1)^2 + 2(n-1) = n^2 - 1, \qquad \textbf{\#Sums} = (n-1)^2 + (n-1) = n^2 - n \tag{2}$$

($A^{(1)} \to A^{(2)}$) We have all zeros in the first column (except for a_{11}), so now we want all zeros in the second column (except a_{12}, a_{22}). This involves in doing exactly the same as we did before, but in the $(n-1)^2$ sub-matrix that has a_{22} as pivot. So the same reasoning applies.

(General case: $A^{(k)} \to A^{(k+1)}$) The pivot is $a_{(k+1)(k+1)}$, the multiplicative factor is $m_i^{(k+1)} = \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}}$, and the operations are:

$$a_{ij}^{(k+1)} = \begin{cases} a_{ij}^{(k)} & 1 \le i \le k, 1 \le j \le n \\ 0 & k+1 \le i \le n, j = k \\ a_{ij}^{(k)} - m_i^{(k+1)} a_{kj}^{(k)} & k \le i \le n, k+1 \le j \le n \end{cases}$$

The number of operations are the same, but instead of dealing with matrix A of n^2 dimensions, we are dealing with matrix A^k of $(n-k)$ dimensions.

8.2 LU factorization

It is an excercise to show that the computational cost of Gaussian elimination is $\mathcal{O}\left(\frac{2}{3}n^3\right)$.

Assume several equations $Ax = b_1, Ax = b_2$, etc. wish to be solved. Same matrix, different b vectors. It'd be stupid to recompute the transformation of A.

Idea: Factor $A = LU$ were L is lower-triangular with $l_{ii} = 1$ and U is upper-triangular. Thus,

$$Ax = b \iff (LU)x = b \iff Ux = y \text{ and } Ly = b$$

Thus, once we know LU which factorizes A, instead of solving $Ax = b$ we solve the two triangular systems $Ux = y, Ly = b$. L, U are obtained via construction by posing:

$$\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ \ell_{21} & 1 & 0 & \cdots & 0 \\ \ell_{31} & \ell_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \ell_{n1} & \ell_{n2} & \ell_{n3} & \cdots & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} & \cdots & u_{1n} \\ 0 & u_{22} & u_{23} & \cdots & u_{2n} \\ 0 & 0 & u_{33} & \cdots & u_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & u_{nn} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix}.$$

8.3 Iterative methods

[Vector norm] A vector norm in $\mathbb{R}^n$ is a function $\|\cdot\| : \mathbb{R}^n \to \mathbb{R}^{>0}$ satisfying:

1. $\|\mathbf{x}\| > 0$ if $\mathbf{x} \neq \overrightarrow{0}$, and $\|\overrightarrow{0}\| = 0$.
2. $\|\alpha\mathbf{x}\| = |\alpha|\|\mathbf{x}\|$
3. $\|\mathbf{x}+\mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$

[Distance] The distance between two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ is $d(x, y) = \|\mathbf{x} - \mathbf{y}\|$.

[Matrix norm] A matrix norm in $\mathbb{R}^{n\times n}$ is a function mapping each matrix in the sapce to a non-negative real denoted $\|A\|$, such that for all $A, B \in \mathbb{R}^{n\times n}$ and all $\alpha \in \mathbb{R}$:

1. Same 3 points as in vector norm.
2. $\|AB\| \leq \|A\|\|B\|$.

If we have a vector norm $\|\cdot\|$ in $\mathbb{R}^n$, then we say

$$\|A\| = \sup_{x=0} \frac{\|Ax\|}{\|x\|}$$

is the matrix norm induced by $\|\cdot\|$. In general, if a matrix norm is induced by a vector norm,

- $\|Ax\| \leq \|A\|\|x\|$ for all $x \in \mathbb{R}^n$
- There is some $\widetilde{x}$ with $\|\widetilde{x}\| = 1$ such that $\|A\widetilde{x}\| = \|A\|$.

The point is to generate a sequence of vectors $\left\{\mathbf{x}^{(k)}\right\}$ that converge to a solution of $A\mathbf{x} = \mathbf{b}$ under certain hypothesis.

Assume we expressed A as $M - N$. Then

$$\begin{aligned} A\mathbf{x} = \mathbf{b} &\iff (M - N)\mathbf{x} = \mathbf{b} \\ &\iff M\mathbf{x} = N\mathbf{x} + b \\ &\iff \mathbf{x} = M^{-1}(N\mathbf{x} + b) \\ &\iff \mathbf{x} = \left(M^{-1}N\right)\mathbf{x} + M^{-1}\mathbf{b} \end{aligned}$$

which is recursive because $\mathbf{x}$ is defined in terms of $\mathbf{x}$. Given $\mathbf{x}^{(0)}$ an approximation, we can construct

$$\mathbf{x}^{(k+1)} = \left(M^{-1}N\right)x^{(k)} + M^{(-1)}b, \qquad k \geq \tag{1}$$

Theorem 18 (Convergence of iterative methods)**.** Let $\mathbf{b} \in \mathbb{R}^n, A = M - N \in \mathbb{R}^{n\times n}$, with A, M non-singular. If $\|M^{-1}N\| < 1$ for some induced matrix norm, then the sequence generated in equation (1) converges to the solution of $A\mathbf{x} = b$ for any initial vector $\mathbf{x}^{(0)}$.

Proof. Take

$$\mathbf{x}^{(k+1)} = (M^{-1}N)x^{(k)} + M^{(-1)}b, \qquad k \geq 0 \tag{2}$$

Substracting this from $x_* = (M^{-1}N)x + M^{-1}b$, we obtain

$$x^{(k+1)} - x_* = (M^{-1}N)(x^{(k)} - x_*), \qquad k \geq 0 \tag{3}$$

Now, given an induced matricial norm, we obtain

$$\|x^{(k+1)} - x_*\| = \|M^{-1}N\|\|x^{(k)} - x_*\|, \qquad k \geq 0 \tag{4}$$

Repeating the last step,

$$\|x^{(k+1)} - x_*\| = \|M^{-1}N\|^{k+1}\|x^{(0)} - x_*\|, \qquad k \geq 0 \tag{5}$$

Using the fact that $\|(M^{-1}N)\| < 1$, we t hen have

$$\lim_{k\to\infty} \|x^{(k)} - x_*\| = 0 \tag{6}$$

8.4 Jacobi

In Jacobi we use $M = D$ and therefore

$$N = M - A = D - (L + D + U) = -(L + U)$$

which means M is the diagonal matrix with the diagonal of A, and is a copy of A but has zeros in the diagonal.

A matrix A is diagonally dominant if

$$|a_{ii}| > \sum_{j=1, j\neq i}^{n} \left|a_{ij}\right|$$

Theorem 19 (Jacobi's convergence)**.** If A is diagonally dominant, the sequence generated by Jacobi's method converges to the solution of $Ax = b$ for any initial vector $x^{(0)} \in \mathbb{R}^n$.

Proof. In Jacobi's method, the matrix M is the diagonal of A and it must be invertible for the method to be well-defined, meaning that $a_{ii} \neq 0$ for all $i = 1, \ldots, n$. Then the iteration matrix is give nby

$$
\begin{aligned}
M^{-1}N &= -\begin{bmatrix} 1/a_{11} & 0 & \ldots & 0 \\ 0 & 1/a_{22} & \ldots & 0 \\ \vdots & \vdots & \ldots & \vdots \\ 0 & 0 & \ldots & a_{nn} \end{bmatrix} \begin{bmatrix} 0 & a_{12} & \ldots & a_{1n} \\ a_{21} & 0 & \ldots & a_{2n} \\ \vdots & \vdots & \ldots & \vdots \\ a_{n1} & a_{n2} & \ldots & 0 \end{bmatrix} \\
&= -\begin{bmatrix} 0 & a_{12}/a_{11} & \ldots & a_{1n}/a_{11} \\ a_{21}/a_{22} & 0 & \ldots & a_{2n}/a_{22} \\ \vdots & \vdots & \ldots & \vdots \\ a_{n1}/a_{nn} & a_{n2}/a_{nn} & \ldots & 0 \end{bmatrix}
\end{aligned}
$$

It follows that

$$
\|M^{-1}N\|_\infty = \max_{1 \leq i \leq n} \sum_{j=1}^{n} \frac{|a_{ij}|}{|a_{ii}|} < 1
$$

since A is diagonally dominant. Then the method converges by virtue of **Theorem 1**.

8.5 Gauss-Seidel method

Here, we take $N = M - a = L + D - (L + D + U) = -U$. In other words, we obtain M to be the lower-triangular conversion of A, including the diagonal, and N to be the upper-triangular version of A, with zeros on the diagonal. It can be shown that

$$
x_i^{(k+1)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k+1)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k)} \right), \qquad i = 1, \ldots, n
$$

Theorem 20. If A is diagonally dominant, then the sequence generated by the Gauss-Seidel method converges to the solution of $Ax = b$, for any initial vector $x^{(0)} \in \mathbb{R}^n$.

Define with $\rho(A)$ the spectral radius of A, defined as

$$
\max \{|\lambda| : \lambda \text{ is eigenvalue of } A\}
$$

Theorem 21. For any matrix $A \in \mathbb{R}^{n\times n}$, it holds that $\rho(A) = \inf\{\|A\|\}$ on all induced matrix norms,

Theorem 22. A necessary and sufficient condition for the convergence of an iterative method

$$x^{(k+1)} = (M^{-1}N)x^{(k)} + M^{-1}b, \qquad k \geq 0$$

for any initial vector $x^{(0)}$ is that $\rho\left(M^{-1}N\right) < 1$.

8.6 Eigenvalues, eigenvectors

In the iteration

$$\vec{x}^{(k+1)} = M^{-1}N\vec{x}^{(k)} + M^{-1}\vec{b},$$

we define the iteration matrix $T = M^{-1}N$. To analyze convergence of the method, we consider the behavior of powers of T applied to the initial vector. If $\rho(T) < 1$, convergence is guaranteed by Theorem 22. When $\rho(T) \geq 1$, however, a more refined analysis is needed.

Assume $\overrightarrow{b} = 0$. Assume T is diagonalizable, so there exists a basis of eigenvectors $\mathcal{E} = \{\vec{v}_1, \ldots, \vec{v}_n\}$ with corresponding eigenvalues $\lambda_1, \ldots, \lambda_n$. Then any vector $\vec{x}^{(k)} \in \mathbb{R}^n$ can be expressed as a linear combination:

$$\vec{x}^{(k)} = \sum_{i=1}^{n} a_i^{(k)}\vec{v}_i.$$

Applying the iteration:

$$\vec{x}^{(k+1)} = T\vec{x}^{(k)} = \sum_{i=1}^{n} \lambda_i a_i^{(k)}\vec{v}_i,$$

which implies:

$$a_i^{(k+1)} = \lambda_i a_i^{(k)} \quad \Rightarrow \quad a_i^{(k)} = \lambda_i^k a_i^{(0)}$$

Thus,

$$\vec{x}^{(k)} = \sum_{i=1}^{n} \lambda_i^k a_i^{(0)}\vec{v}_i. = (\lambda_1^k a_1^{(0)}, \ldots, \lambda_n^k a_n^{(0)})_{\mathcal{E}} \tag{1}$$

This means that finding the expression of $\overrightarrow{x}^{(0)}$ in the basis $\mathcal{E}$, with coefficients $a_1^{(0)}, \ldots, a_n^{(0)}$, is sufficient to compute $\overrightarrow{x}^{(k)}$ just in terms of these coefficients and powers of the eigenvalues.

Incidentally, this is the reason why we need all eigenvalues to be < 1 in absolute value to ensure convergence. Otherwise, the values $x^{(1)}, x^{(2)}, \ldots$ diverge as seen from equation (1).

8.7 Excercises

(3) Show that the operational cost of Gaussian elimination for solving $Ax = b$, $A \in \mathbb{R}^{n \times n}$, is $O\left(\frac{2}{3}n^3\right)$ flops.

Hint. Recall that

$$\sum_{k=1}^{n} k = \frac{n(n+1)}{2}, \qquad \sum_{k=1}^{n} k^2 = \frac{n(n+1)(2n+1)}{6}$$

The Gaussian elimination method performs the transitions

$$A \to A^{(1)} \to A^{(2)} \to \ldots \to A^{(n-1)} = U$$

for a total of n transitions. We know

$$P(k) = (n-k)^2 - 1, \qquad S(k) = (n-k)^2 - (n-k)$$

are the number of products (P) and sums (S) on the kth to $k+1$ transition. Obviously, as k increases across $0, \ldots, n-1$, the coefficient $(n-k)$ ranges from $n, n-1, \ldots, 1$. So ultimately,

$$\begin{aligned}
\sum_{k=0}^{n-1} P(k) + S(k) &= \sum_{k=0}^{n-1} (n-k)^2 - 1 + (n-k)^2 - (n-k) \\
&= \sum_{k=1}^{n} k^2 - 1 + k^2 - k \\
&= 2 \times \frac{n(n+1)(2n+1)}{6} - n - \frac{n(n+1)}{2} \\
&= \frac{n(n+1)(2n+1)}{3} - n - \frac{n^2+n}{2} \\
&= \frac{2n^3 + 3n^2 + n}{3} - n - \frac{n^2}{2} + \frac{n}{2} \\
&= \frac{2}{3}n^3 + n^2 + \frac{1}{3}n - \frac{1}{2}n^2 - \frac{1}{2}n \\
&= \frac{2}{3}n^3 + \frac{1}{2}n^2 + \frac{1}{3}n - \frac{1}{2}n
\end{aligned}$$

Clearly, the dominant term in the number of flops is $\frac{2}{3}n^3$, which means the number of operations satisfies the complexity bound $\frac{2}{3}n^3 + O(n^2)$. This suffices to show the number of flops is in the order $O\left(\frac{2}{3}n^3\right)$.

(4) Solve $Ax = b$ with

$$A = \begin{bmatrix} 2 & -2 & 1 \\ 1 & 1 & 3 \\ 0 & 4 & 1 \end{bmatrix}, \qquad b = \begin{bmatrix} -1 \\ 6 \\ 9 \end{bmatrix}$$

(a) First, solve via Gaussian elimination. (b) Then via LU decomposition.

(a) Observe that

$$\begin{aligned} A = \begin{bmatrix} 2 & -2 & 1 & -1 \\ 1 & 1 & 3 & 6 \\ 0 & 4 & 1 & 9 \end{bmatrix} &\to \begin{bmatrix} 2 & -2 & 1 & -1 \\ 0 & 2 & 2.5 & 6.5 \\ 0 & 4 & 1 & 9 \end{bmatrix} && (m = 1/2) \\ &\to \begin{bmatrix} 2 & -2 & 1 & -1 \\ 0 & 2 & 2.5 & 6.5 \\ 0 & 4 & 1 & 9 \end{bmatrix} && (m = 0) \\ &\to \begin{bmatrix} 2 & -2 & 1 & -1 \\ 0 & 2 & 2.5 & 6.5 \\ 0 & 0 & -4 & -4 \end{bmatrix} && (m = 4/2 = 2) \end{aligned}$$

This concludes Gaussian elimination, and it readily provides the U and L matrix for LU method:

$$U = \begin{bmatrix} 2 & -2 & 1 \\ 0 & 2 & 2.5 \\ 0 & 0 & -4 \end{bmatrix}, \qquad L = \begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ 0 & 2 & 1 \end{bmatrix}$$

Solving via Gaussian elimination entails applying the upper-triangular algorithm to the system obtained via Gaussian elimination, which gives:

$$x_3 = 1, \qquad x_2 = (6.5 - 2.5)/2 = 2, \qquad x_3 = (-1 + 2 \times 2 - 1 \times 1)/2 = 1$$

(b) To solve using LU decomposition, we note that $Ax = b$ if and only if $Ux = y$ and $Ly = b$. So, we begin solving $Ly = b$, which gives (according to matrix L)

$$\begin{bmatrix} 1 & 0 & 0 & -1 \\ \frac{1}{2} & 1 & 0 & 6 \\ 0 & 2 & 1 & 9 \end{bmatrix}$$

$$y_1 = -1, \qquad y_2 = 6.5, \qquad y_3 = -4$$

Then we solve $Ux = y$, i.e. the system

$$\begin{bmatrix} 2 & -2 & 1 & -1 \\ 0 & 2 & 2.5 & 6.5 \\ 0 & 0 & -4 & -4 \end{bmatrix}$$

which is exactly the same system solved in (a) and gives the same solutions.

(8) Consider the system

$$\begin{cases} x - y = 0 \\ x + y = 0 \end{cases}$$

Obtain the eigenvalues and eigenvectors of the associated iteration matrix (Gauss-Seidel) to decide if the method converges independently of the initial vector $\overrightarrow{x}_0$. Predict the behavior of the sequence with $\overrightarrow{x}_0 \in \{(2,0), (-0.03, 0.03), (0,1)\}$. Decide if Jacobi's method converges for these vectors.

The matrix associated to the system is simply

$$\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$

Recall that Gauss-Seidel's method writes $A = (M - N)\overrightarrow{x} = \overrightarrow{b}$ with M the lower-triangular of A (including diagonal), and N the (negative) upper-triangularo of A (with zeros in the diagonal). So we take

$$M = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}, \qquad N = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

Recall that the iteration is given by $\overrightarrow{x}^{(k+1)} = (M^{-1}N)\overrightarrow{x}^{(k)} + M^{-1}\overrightarrow{b}$, but since $\overrightarrow{b} = \overrightarrow{0}$ the second term disappears. Thus, all that is needed is to compute the iteration matrix $T = M^{-1}N$. It is straigthforward to see that the inverse of M is

$$M^{-1} = \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix}$$

which entails

$$T = M^{-1}N = \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & -1 \end{bmatrix}$$

The eigenvalues are the solutions to the characteristic equation $\det(T - \lambda I) = 0$. Clearly,

$$\det(T - \lambda I) = \det \begin{pmatrix} -\lambda & 1 \\ 0 & -1-\lambda \end{pmatrix} = -\lambda(-1-\lambda)$$

with roots $\lambda = 0, \lambda = -1$. We know a necessary and sufficient condition for an iterative method to converge independently of the initial vector is $\rho(T) = \rho(M^{-1}T) < 1$, where ρ is the spectral radius. However,

$$\rho(T) = \max\{|\lambda| : \lambda \text{ is eigenvalue of } T\} = 1 \nless 1$$

$\therefore$ The matrix does not converge independently of the initial vector.

(b) To determine of the matrix converges with the given initial vectors, we need to compute the eigenvectors of T. To do this, we solve $(T - \lambda I)\overrightarrow{v} = 0$ for each eigenvalue λ. Now, clearly

$$\begin{aligned}
&(T - 0 \times I)\overrightarrow{v} = 0 \\
\iff &T\overrightarrow{v} = 0 \\
\iff &v_1(0,0) + v_2(1,-1) = 0 \\
\iff &(v_2, -v_2) = 0 \\
\iff &v_2 = 0
\end{aligned}$$

Then any multiple of the eigenvector $\overrightarrow{e}_1 = (1,0)$ is an eigenvector. Similarly,

$$\begin{aligned}
&(T + I)\overrightarrow{v} = 0 \\
\iff &\begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}\overrightarrow{v} = 0 \\
\iff &\overrightarrow{v} = (1,-1)^\top
\end{aligned}$$

So the eigenvectors are $e_1 = (1,0), e_2 = (1,-1)$. Then these vectors are a base and any $\overrightarrow{x}^{(0)}$ is a linear combination of them. In other words,

$$\overrightarrow{x}^{(0)} = (x_1, x_2) = (a, 0) + (b, -b) = (a + b, -b)$$

for some $a, b \in \mathbb{R}$. We can then infer that $b = -x_2$ and $a = x_1 - b = x_1 + x_2$. In other words, given any vector (x_1, x_2), we can write it in terms of the eigen-basis using coefficients $x_1 + x_2$ and $-x_2$. Then

$$
\begin{aligned}
T\begin{bmatrix}x_1\\x_2\end{bmatrix} &= T\left((x_1+x_2)\begin{bmatrix}1\\0\end{bmatrix} - x_2\begin{bmatrix}1\\-1\end{bmatrix}\right)\\
&= (x_1+x_2)T\begin{bmatrix}1\\0\end{bmatrix} - x_2T\begin{bmatrix}1\\-1\end{bmatrix}\\
&= (x_1+x_2)\cdot 0\begin{bmatrix}1\\0\end{bmatrix} - x_2\cdot(-1)\begin{bmatrix}1\\-1\end{bmatrix}\\
&= (x_2, -x_2)
\end{aligned}
$$

Therefore, if $\overrightarrow{x}^{(k)} = (x, 0)$ for some $x \in \mathbb{R}$, immediately $\overrightarrow{x}^{(k+1)} = T\overrightarrow{x}^{(k)} = (0, 0)$, which means the method converges in one step. If $\overrightarrow{x}^{(0)} = (x, y)$ with $y \neq 0$, then

$$
\overrightarrow{x}^{(1)} = (y, -y), \qquad \overrightarrow{x}^{(2)} = (-y, y), \qquad \overrightarrow{x}^{(3)} = (y, -y), \ldots
$$

and the method does not converge.

9 Linear programming

A problem suited for linear programming consists in finding the solution to a system of equations

$$A\mathbf{x} = \mathbf{b}$$

which minimizes a cost function $f(\mathbf{x})$ and which operates under certain constraints, among which we must impose $\mathbf{x} > \overrightarrow{0}$. The cost can itself be written as a system in function of $\mathbf{x}$:

$$\mathbf{c}^\top \mathbf{x}$$

where c_i is the cost associated to each x_i. In general, it is very simple to translate a problem that does not fit the previous form into a problem that does. For instanace, if one of the constraitns is $2x_1 + 7x_2 - 3x_3 \leq 10$, we could write $2x_1 + 7x_2 - 3x_3 + s_1 = 10$ with $s_1 \geq 0$.

A few definitions.

[Hyperplane, semi-space] A hyperplane of $\mathbb{R}^n$ is a the set of solutions to an arbitrary n-dimensional system:

$$\{\mathbf{x} \in \mathbb{R} \mid a_1x_1 + \ldots + a_nx_n = b\}$$

A semi-space of $\mathbb{R}^n$ is

$$\{\mathbf{x} \in \mathbb{R}^n \mid a_1x_1 + \ldots + a_nx_n \leq b\}$$

[Convex set] A set S of $\mathbb{R}^n$ is convex if for any $\mathbf{x}, \mathbf{y} \in S$, the segment joingin these points is also within S. Formally, if

$$\alpha\mathbf{x} + (1 - \alpha)\mathbf{y} \in S$$

for $\alpha \in [0, 1]$.

Two facts: a finite intersection of convex sets is convex, and every semi-space is convex. A finite intersection of closed semi-spaces in $\mathbb{R}^n$ is called a **closed polyhedral region** of $\mathbb{R}^n$.

It follows that every closed polyhedral region is a convex set. Furthermore, the set of restrictions in a linear problem given by

$$\Omega = \{x \in \mathbb{R}^n \mid Ax = b \wedge Rx \leq s\}$$

is a closed polyhedral region. To characterize the polyhedral regions such as Ω, we find the vertices, i.e. the intersection among the semi-spaces. Take the following linear problem:

$$\begin{cases} 3x + 2y & \geq 3 \\ x + 3y & \geq 1.5 \\ 8x + 2y & \geq 4 \\ x & \geq 0 \\ y \geq 0 \end{cases}$$

The vertices among the lines are $P_1 = (0, 2), P_2 = \left(\frac{1}{5}, \frac{5}{6}\right), P_3 = \left(\frac{6}{7}, \frac{3}{14}\right), P_4 = \left\{\frac{3}{2}, 0\right\}$. For instance, P_2 is obtained from solving

$$3x + 2y = 3, \qquad 8x + 2y = 4$$

which are the hyperplanes (lines) in the first and third restrictions. Note that $\left(0, \frac{3}{2}\right)$ is a solution to $3x + 2y = 3, x = 0$ but it is not a vertix of om.