Computational methods-Lecture 1

1 Preliminaries

In solving the practical problems, we often do the following

(i) Modelling – This will introduce the modelling error, because "all models are wrong while some are useful"

(ii) Design numerical methods or algorithms to solve the models. This step introduces the so-called truncation error or method error. This is the main part that numerical analysis focuses on.

(iii) Using computers to compute will yield the roundoff errors. This is because the numbers are stored as float numbers in computer. See Section 1.2 of the book by Burden for details.

Let p be the true value while p^* be the approximation. The **absolute error** is defined by $|p - p^*|$; and the **relative error** is given by $|p - p^*|/|p|$. Note that the absolute value has units (or dimension). Hence, sometimes it is not easy to understand how large the error is by simplying staring at the absolute error. The relative error, however, is better for describing the bigness of the errors.

The approximation p^* is said to have m **significance digits** for approximating p, if

$$\frac{|p - p^*|}{|p|} < 5 \times 10^{-m}.$$

Intuitively, this means that the first m nonzero idigits in p^* have meanings while the subsequent digits in p^* make no sense because they are polluted by the errors. Hence, one should only keep m nonzero digits in the approximation.

For example: let $p = 0.012723$ and $p^* = 0.012815$. With the computation, $|p - p^*|/|p| = 0.0072 \cdots < 5 \times 10^{-2}$, one finds that $m = 2$. This means there are two significant digits in p^*, and we should keep it as $p^* = 0.013$. With this new approximation, the error is $0.0002 \cdots$ less one half of the mth nonzero digit. This then says the first m nonzero digits are good, while the error starts play the role from $(m + 1)$th digits.

The definition in Qingyang Li's book is as that:

There are n significant digits in p^* if

$$p^* = \pm 10^m (a_1 + a_2 10^{-1} + \cdots + a_n 10^{-(n-1)}),$$

and

$$|p - p^*| \leq 5 \times 10^{m-n}$$

Using this, the number of significant digits in our case is still 2.

Some comments

- For arithmetic computations, try to avoid divisions by small numbers, subtractions with comparable (big) numbers, additions between a very large and a very small number. These will reduce the significance digits.

- For numerical methods or algorithms, there are several aspects. Regarding complexity, try to avoid repeated computation and improve the complexity; regarding stability and convergence, we need the method to be well-posed. The concept of stability is very important. It roughly says that your local errors will not be amplified significantly in the eventual result. The so-called "condition number " can often indicate the stability of the system we are considering. This will be clear later.

2 Interpolation

The Weierstrass approximation theorem says that one an use polynomials to approximate any continuous function on a compact set. Particularly, in the 1D case, for $f \in C([a,b],\mathbb{R})$, and any $\epsilon > 0$, there exists a polynomial $P(x)$ such that

$$|f(x) - P(x)| < \epsilon, \ \forall x \in [a,b].$$

The above theorem does not tell us how to construct the approximating polynomials. The Taylor polynomials can charaterize the local behaviors of functions. However, in some problems, we know the function values at several points. Then, how can we approximate such functions?

We focus on problems where $x \in \mathbb{R}$ only.

Problem. *Given the function values of f at $n+1$ points: $(x_i, f(x_i))_{i=0}^n$, where $x_i \in \mathbb{R}$, find a polynomial such that $P(x_i) = f(x_i)$.*

2.1 Two point case

Given (x_0, y_0) and (x_1, y_1), we know there is a line going through them. The slope is

$$k = \frac{y_1 - y_0}{x_1 - x_0}.$$

Hence, the line is

$$y = y_0 + k(x - x_0) = y_0 + \frac{y_1 - y_0}{x_1 - x_0}(x - x_0). \tag{1}$$

Therefore, (1) satisfies the requirement. However, this cannot be generalized to cases with more points easily.

To solve the general cases, we rearrange the interpolation and combine the coefficients for y_0 and y_1:

$$y = y_0(1 - \frac{x - x_0}{x_1 - x_0}) + y_1 \frac{x - x_0}{x_1 - x_0} = y_0 \frac{x_1 - x}{x_1 - x_0} + y_1 \frac{x - x_0}{x_1 - x_0} = y_0 \ell_0(x) + y_1 \ell_1(x).$$

Observation:

$$\ell_0(x_0) = 1,\ \ell_0(x_1) = 0,$$

and

$$\ell_1(x_0) = 0,\ \ell_1(x_1) = 1.$$

Hence, ℓ_0 only picks out the value at x_0 and ℓ_1 only picks out the value at x_1. Clearly, ℓ_0 and ℓ_1 will span a linear vector space consisting of all polynomials of degree 1 that can interpolate functions with values known at x_0 and x_1.

2.2 General cases

Consider the $n + 1$ points: $(x_i, f(x_i))_{i=0}^n$. The idea is again the same. We aim to construct the interpolation basis functions $\ell_{n,k}(x)$ such that:

$$\ell_{n,k}(x_j) = \delta_{kj} = \begin{cases} 1 & \text{if } k = j, \\ 0 & \text{otherwise.} \end{cases}$$

Then,

$$L(x) = \sum_{k=0}^{n} f(x_k)\ell_{n,k}(x)$$

will be a desired polynomial.

Considering that the polynomial is zero at other points and thus it must contain factor $(x - x_j)$ for $j \neq k$. Hence, it is not hard to construct:

$$\ell_{n,k} = \frac{(x - x_0)\cdots(x - x_{k-1})(x - x_{k+1})\cdots(x - x_n)}{(x_k - x_0)\cdots(x_k - x_{k-1})(x_k - x_{k+1})\cdots(x_k - x_n)} = \prod_{i=0,\ i\neq k}^{n} \frac{(x - x_i)}{(x_k - x_i)}.$$

Letting

$$\omega_{n+1}(x) = \prod_{j=0}^{n} (x - x_j).$$

Then, it is not hard to see

$$\ell_{n,k} = \frac{\omega_{n+1}(x)}{(x - x_k)\omega'_{n+1}(x_k)}.$$

The polynomial $L(\cdot)$ is called the nth **Lagrange interpolation polynomial**.

2.3 Some theoretical results

The first question is: how many polynomials that will satisfy the condition?

Theorem 1. *Let $\{x_k\}_{k=0}^n$ be $n+1$ points, and $f(\cdot)$ is a given function. Then, there is a unique polynomial $P(x)$ with degree at most n such that*

$$P(x_k) = f(x_k),$$

and this polynomial is exactly the Lagrange interpolation polynomial.

Proof. The existence has been shown by the construction above. Now, let us consider uniqueness. In fact, if there is another polynomial $Q(x)$ satisfying the same conditions. Then, $Q(x) - L(x)$ is a polynomial with degree at most n, but has $n+1$ zeros. As well-known, a polynomial with degree m, $m \geq 1$ has m zeros only (repeated roots will count). Hence, the degree of $Q - L$ must be 0 and it must be zero. $\square$

Of course, if you consider polynomials with higher degree, they will not be unique.

Another question: what is the error for the polynomial approximation?

Theorem 2. *Suppose that $\{x_k\}_{k=0}^n$ are $n+1$ distinct points on the interval $[a, b]$. $f \in C^{(n+1)}([a, b]; \mathbb{R})$. Let $L(\cdot)$ be the Lagrange interpolation polynomial at these $n+1$ points. Then, for any $x \in [a, b]$, there exists $\xi \in (a, b)$ (depending on x) such that*

$$f(x) - L(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\omega_{n+1}(x).$$

Consider
$$K(x) = \frac{f(x) - L(x)}{\omega_{n+1}(x)}$$
Intuitively, this is indeed like the $(n+1)$th order derivative because the denominator is $(\Delta x)^{n+1}$ small. Proving such claims is just like how you prove the Lagrange mean value theorem. This gives
$$f(x) - L(x) - K(x)\omega_{n+1}(x) = 0.$$

Proof. Consider
$$K(x) = \frac{f(x) - L(x)}{\omega_{n+1}(x)},$$
which is continuous and bounded.

Define
$$\varphi(t) = f(t) - L(t) - K(x)\omega_{n+1}(t)$$
This function has zeros at $x_0, x_1, \ldots, x_n$ and x. If x equals x_j for some j, we have repeated roots. For such a function, there is ξ such that
$$\varphi^{(n+1)}(\xi) = 0.$$
It is easily seen that $L^{(n+1)}(x) \equiv 0$, and $\omega_{n+1}^{(n+1)} = (n+1)!$. Hence,
$$f^{(n+1)}(\xi) - K(x)(n+1)! = 0.$$
The result then follows. $\square$

Example Let $h = 1/N$ and $x_j = jh$ for $0 \leq j \leq N$. Suppose that we use piecewise linear interpolation for the function $f(x) = e^x$ between these grid points. Find an error bound for these piecewise linear interpolation.

Example Consider $f(x) = \ln(1+x)$. Let $x_0 = 0, x_1 = 0.5, x_2 = 1$. If we use the quadratic polynomial to interpolate this function, estimate the error for $x = 0.6$.