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Numerical Methods
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2 Lecture 2

2.1 Horner's rule

- In the material below, in general x can be a complex number, but we shall only consider x to be a real number.
- A polynomial is a finite sum of integer powers of x

$$p(x) = a_0 + a_1x + a_2x^2 + \cdots + a_nx^n \,. \tag{2.1.1}$$

- We say the above polynomial is of degree n. Obviously the value of a_n must be nonzero. The values of the other coefficients can be zero.
- An efficient way to compute the above polynomial numerically is known as *Horner's rule.*
- We nest the sum as follows.

$$p(x) = a_0 + x(a_1 + x(a_2 + \cdots + x(a_{n-1} + x(a_n)) \dots) \,. \tag{2.1.2}$$

- This can be coded in a loop as follows

```
sum = a[n];
for (i = n-1; i >= 0; --i) {
  sum = a[i] + x * sum;
}
```

- This loop requires n multiplications and n summations.
- Horner's rule has several nice features.
- If $|x|$ is small (and/or if the magnitudes of the coefficients $|a_i|$ decrease to small values for the high powers if x) then Horner's rule automatically takes care of underflow. As the nested sums are added in the loop, the contributions of the small terms disappear automatically.
- If the coefficients a_i alternate in sign (and/or if the value of x is negative), Horner's rule handles the cancellations better than a brute force summation of large terms of $+ - + - \dots$ opposing signs.

2.2 Horner's rule: additional ideas

- Many textbooks describe Horner's rule. It optimizes the summation of the powers of x.
- *But what about the coefficients* a_i*?*
- By and large, the coefficients are treated as a black box "input array" supplied by the user.
- However, depending on the situation, one can perform additional optimizations.
- Consider the exponential series

$$\exp(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots \tag{2.2.1}$$

  This is an infinite series. To evaluate it numerucally in practice, we truncate it after a finite number of terms, say N. Then we obtain a polynomial, say

$$p_{\exp}(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots + \frac{x^N}{N!}\,. \tag{2.2.2}$$

- If we apply Horner's rule to this, we obtain

$$p_{\exp}(x) = 1 + x\biggl(1 + x\biggl(\frac{1}{2!} + x\biggl(\frac{1}{3!} + \cdots + x\biggl(\frac{1}{N!}\biggr)\ldots\biggr)\,. \tag{2.2.3}$$

  The coefficients are $a_n = 1/n!$ for $n = 1, 2, \ldots, N$. Their values rapidly grow large as n increases.

- A better way to nest the summation is

$$p_{\exp}(x) = 1 + x\biggl(1 + \frac{x}{2}\biggl(1 + \frac{x}{3}\biggl(1 + \cdots + \frac{x}{N}\biggr)\ldots\biggr)\,. \tag{2.2.4}$$

- We not only nest the sums of the powers of x, but we also nest the computation of the coefficients.

***** Examine each problem on its merits *****

****** Use your imagination ******

2.3 Taylor series

- We know that $\sin(30^\circ) = \frac{1}{2}$. How do we compute the value of $\sin(31^\circ)$?
- We expect that it will be close to $\frac{1}{2}$, because $\sin(x)$ is continuous in x, but how do we compute an accurate answer?
- This is the sort of problem where Taylor series are useful.
- Basically, we know the value of a function at some point $x = a$, i.e. we know $f(a)$, and we wish to compute f for nearby values $x = a + \varepsilon$, where $|\varepsilon|$ is assumed small. Hence we seek to compute the value of $f(a + \varepsilon)$.
- If $a = 0$, the series is also called a Maclaurin series.
- (Taylor's theorem) If $f(x)$ and its first $(n+1)$ derivatives $f'(x), f''(x), \dots, f^{(n+1)}(x)$ all exist and are continuous and bounded in some interval $x_0 \le x \le x_1$, then if $a \in [x_0, x_1]$, then we can write, for $x \in [x_0, x_1]$,

$$f(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}\,f''(a) + \cdots + \frac{(x-a)^n}{n!}\,f^{(n)}(a) + R_n\,. \tag{2.3.1}$$

Here R_n is a remainder term whose value is finite and equal to

$$R_n = \frac{(x-a)^{n+1}}{(n+1)!}\,f^{(n+1)}(b(x))\,. \tag{2.3.2}$$

Here $b \in [x_0, x_1]$ but unfortunately the exact value of b is not known. At best we can place an upper bound on the value of $|R_n|$, i.e. an upper bound on the accuracy of the sum.

- If $|R_n| \to 0$ as $n \to \infty$, then we can extend the series to infinity and obtain a power series

$$f(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}\,f''(a) + \cdots = \sum_{n=0}^{\infty} \frac{(x-a)^n}{n!}\,f^{(n)}(a)\,. \tag{2.3.3}$$

- Example: compute $\sin(31^\circ)$. Hence $f(x) = \sin(x)$. We set $a = 30^\circ = \pi/6$. We know that

$$f'(x) = \cos(x)\,, \quad f''(x) = -\sin(x)\,, \quad f'''(x) = -\cos(x)\,, \ \dots$$

Also $\sin(\pi/6) = \frac{1}{2}$ and $\cos(\pi/6) = \frac{\sqrt{3}}{2}$. Hence

$$\sin(x) = \sin(a) + (x-a)\cos(a) - \frac{(x-a)^2}{2!}\,\sin(a) - \frac{(x-a)^3}{3!}\,\cos(a) + \cdots$$

Substitute $x - a = 1^\circ = \pi/180$ to obtain

$$\sin(31^\circ) = \frac{1}{2} + \Big(\frac{\pi}{180}\Big)\frac{\sqrt{3}}{2} - \frac{1}{2!}\Big(\frac{\pi}{180}\Big)^2\frac{1}{2} - \frac{1}{3!}\Big(\frac{\pi}{180}\Big)^3\frac{\sqrt{3}}{2} + \cdots$$

Sum the series until the answer converges to a desired tolerance.

2.4 Multinomial coefficient

- Recall the **binomial coefficient** is

$$\binom{n}{k} = \frac{n!}{k!(n-k)!} \,. \tag{2.4.1}$$

- The **multinomial coefficient** is the generalization for $m > 1$ variables $k_1, k_2, \dots, k_m$

$$\begin{aligned} \binom{n}{k_1, k_2, \dots, k_m} &= \frac{n!}{k_!!k_2! \dots k_m!(n-k_1-k_2-\cdots-k_m)!} \\ &= \frac{n(n-1)\dots\left(n+1-\sum_i k_i\right)}{k_!!k_2!\dots k_m!} \,. \end{aligned} \tag{2.4.2}$$

- The multinomial coefficient has the following combinatorial interpretation. Suppose we have a set of n objects and we wish to place them in m bins. The multinomial coefficient counts the number of ways to place k_1 objects in bin 1, k_2 objects in bin 2, etc. and finally k_m objects in bin m. The special case $m = 1$ is the binomial coefficient ("the number of ways to choose k objects from a set of n objects").

- The value of the multinomial coefficient is therefore a positive integer.

- It is obvious that the value of n can be generalized to a non-integer value.
  Let x be a real (or complex) number.
  The **generalized multinomial coefficient** is given by the finite product

$$\binom{x}{k_1, k_2, \dots, k_m} = \frac{x(x-1)\dots\left(x+1-\sum_i k_i\right)}{k_!!k_2!\dots k_m!} \,. \tag{2.4.3}$$

2.5 Multinomial theorem

- The multinomial coefficient is used to specify the coefficients in the **multinomial theorem**.
- Let us begin with $m = 2$ to illustrate.

$$\begin{aligned}
(1+x_1+x_2)^n &= 1 + \binom{n}{1,0}x_1 + \binom{n}{0,1}x_2 \\
&\qquad + \binom{n}{2,0}x_1^2 + \binom{n}{1,1}x_1x_2 + \binom{n}{0,2}x_2^2 \\
&\qquad + \binom{n}{3,0}x_1^3 + \binom{n}{2,1}x_1^2x_2 + \binom{n}{1,2}x_1x_2^2 + \binom{n}{0,3}x_2^3 + \cdots \\
&= 1 + \left[\sum_{k_1=0}^{n}\sum_{k_2=0}^{n}\binom{n}{k_1,k_2}x_1^{k_1}x_2^{k_2}\right]_{k_1+k_2=1} \\
&\qquad + \left[\sum_{k_1=0}^{n}\sum_{k_2=0}^{n}\binom{n}{k_1,k_2,}x_1^{k_1}x_2^{k_2}\right]_{k_1+k_2=2} + \cdots \\
&= 1 + \sum_{j=1}^{\infty}\left[\sum_{k_1=0}^{n}\sum_{k_2=0}^{n}\binom{n}{k_1,k_2}x_1^{k_1}x_2^{k_2}\right]_{k_1+k_2=j}.
\end{aligned} \tag{2.5.1}$$

- The last line tells us how to generalize to m terms

$$\begin{aligned}
&(1+x_1+x_2+\cdots+x_m)^n \\
&\qquad = 1 + \sum_{j=1}^{\infty}\left[\sum_{k_1=0}^{n}\cdots\sum_{k_m=0}^{n}\binom{n}{k_1,k_2,\dots,k_m}x_1^{k_1}x_2^{k_2}\dots x_m^{k_m}\right]_{k_1+k_2+\cdots+k_m=j}.
\end{aligned} \tag{2.5.2}$$

- Just as with the binomial theorem, the series terminates if the value of n is a nonnegative integer, and the series does not terminate otherwise.

2.6 Multivariate Taylor series

- The multinomial coefficients appear in the formula for a Taylor series of a function of multiple variables $x_1, x_s, \ldots, x_m$.
- Again, let us begin with $m = 2$ to illustrate.

$$
\begin{aligned}
f(x_1+\varepsilon_1, x_2+\varepsilon_2) &= f(x_1,x_2) + \binom{1}{1,0}\frac{\partial f}{\partial x_1}\,\varepsilon_1 + \binom{1}{0,1}\frac{\partial f}{\partial x_2}\,\varepsilon_2 \\
&\qquad + \frac{1}{2!}\binom{2}{2,0}\frac{\partial^2 f}{\partial x_1^2}\,\varepsilon_1^2 + \frac{1}{2!}\binom{2}{1,1}\frac{\partial^2 f}{\partial x_1 \partial x_2}\,\varepsilon_1\varepsilon_2 + \frac{1}{2!}\binom{2}{0,2}\frac{\partial^2 f}{\partial x_2^2}\,\varepsilon_2^2 \\
&\qquad + \frac{1}{3!}\binom{3}{3,0}\frac{\partial^3 f}{\partial x_1^3}\,\varepsilon_1^3 + \frac{1}{3!}\binom{3}{2,1}\frac{\partial^3 f}{\partial x_1^2 \partial x_2}\,\varepsilon_1^2\varepsilon_2 \\
&\qquad\qquad + \frac{1}{3!}\binom{3}{1,2}\frac{\partial^3 f}{\partial x_1 \partial x_2^2}\,\varepsilon_1\varepsilon_2^2 + \frac{1}{3!}\binom{3}{0,3}\frac{\partial^3 f}{\partial x_2^3}\,\varepsilon_2^3 + \cdots \\
&= f(x_1,x_2) + \frac{\partial f}{\partial x_1}\,\varepsilon_1 + \frac{\partial f}{\partial x_2}\,\varepsilon_2 \\
&\qquad + \frac{1}{2!}\frac{2!}{2!0!}\frac{\partial^2 f}{\partial x_1^2}\,\varepsilon_1^2 + \frac{1}{2!}\frac{2!}{1!1!}\frac{\partial^2 f}{\partial x_1 \partial x_2}\,\varepsilon_1\varepsilon_2 + \frac{1}{2!}\frac{2!}{0!2!}\frac{\partial^2 f}{\partial x_2^2}\,\varepsilon_2^2 \\
&\qquad + \frac{1}{3!}\frac{3!}{3!0!}\frac{\partial^3 f}{\partial x_1^3}\,\varepsilon_1^3 + \frac{1}{3!}\frac{3!}{2!1!}\frac{\partial^3 f}{\partial x_1^2 \partial x_2}\,\varepsilon_1^2\varepsilon_2 \\
&\qquad\qquad + \frac{1}{3!}\frac{3!}{1!2!}\frac{\partial^3 f}{\partial x_1 \partial x_2^2}\,\varepsilon_1\varepsilon_2^2 + \frac{1}{3!}\frac{3!}{0!3!}\frac{\partial^3 f}{\partial x_2^3}\,\varepsilon_2^3 + \cdots \\
&= f(x_1,x_2) + \frac{\partial f}{\partial x_1}\,\varepsilon_1 + \frac{\partial f}{\partial x_2}\,\varepsilon_2 \\
&\qquad + \frac{1}{2!0!}\frac{\partial^2 f}{\partial x_1^2}\,\varepsilon_1^2 + \frac{1}{1!1!}\frac{\partial^2 f}{\partial x_1 \partial x_2}\,\varepsilon_1\varepsilon_2 + \frac{1}{0!2!}\frac{\partial^2 f}{\partial x_2^2}\,\varepsilon_2^2 \\
&\qquad + \frac{1}{3!0!}\frac{\partial^3 f}{\partial x_1^3}\,\varepsilon_1^3 + \frac{1}{2!1!}\frac{\partial^3 f}{\partial x_1^2 \partial x_2}\,\varepsilon_1^2\varepsilon_2 \\
&\qquad\qquad + \frac{1}{1!2!}\frac{\partial^3 f}{\partial x_1 \partial x_2^2}\,\varepsilon_1\varepsilon_2^2 + \frac{1}{0!3!}\frac{\partial^3 f}{\partial x_2^3}\,\varepsilon_2^3 + \cdots \\
&= f(x_1,x_2) + \sum_{j=1}^{\infty}\Bigg[\sum_{k_1=0}^{n}\sum_{k_2=0}^{n}\frac{1}{k_1!k_2!}\frac{\partial^j f}{\partial x_1^{k_1}\partial x_2^{k_2}}\,\varepsilon_1^{k_1}\varepsilon_2^{k_2}\Bigg]_{k_1+k_2=j}.
\end{aligned}
\tag{2.6.1}
$$

- The last line tells us how to generalize to m terms

$$
\begin{aligned}
&f(x_1+\varepsilon_1, x_2+\varepsilon_2, \ldots, x_m+\varepsilon_m) = f(x_1, x_2, \ldots, x_m) \\
&\quad + \sum_{j=1}^{\infty}\Bigg[\sum_{k_1=0}^{n}\sum_{k_2=0}^{n}\cdots\sum_{k_m=0}^{n}\frac{1}{k_1!k_2!\cdots k_m!}\,\frac{\partial^j f}{\partial x_1^{k_1}\partial x_2^{k_2}\ldots\partial x_m^{k_m}}\,\varepsilon_1^{k_1}\varepsilon_2^{k_2}\cdots\varepsilon_m^{k_m}\Bigg]_{k_1+k_2+\cdots+k_m=j}.
\end{aligned}
\tag{2.6.2}
$$