Queens College, CUNY, Department of Computer Science

Numerical Methods
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2 Lecture 2

2.1 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 $x \in [x_0, x_1]$,
  $$f(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}\, f''(a) + \cdots + \frac{(x-a)^n}{n!}\, f^{(n)}(a) + R_n\,. \tag{2.1.1}$$
  Here R_n is a remainder term whose value is finite and equal to
  $$R_n = \frac{(x-a)^{n+1}}{(n+1)!}\, f^{(n+1)}(b(x))\,. \tag{2.1.2}$$
  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
  $$\begin{aligned} f(x) &= f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}\, f''(a) + \frac{(x-a)^3}{3!}\, f'''(a) + \cdots \\ &= \sum_{n=0}^{\infty} \frac{(x-a)^n}{n!}\, f^{(n)}(a)\,. \end{aligned} \tag{2.1.3}$$

2.1.1 Example

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

$$f'(x) = \cos(x)\,, \quad f''(x) = -\sin(x)\,, \quad f'''(x) = -\cos(x)\,, \ \ldots \tag{2.1.4}$$

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

$$\sin(x) = \sin(a) + (x-a)\cos(a) - \frac{(x-a)^2}{2!}\sin(a) - \frac{(x-a)^3}{3!}\cos(a) + \cdots \tag{2.1.5}$$

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

$$\sin(31^\circ) = \frac{1}{2} + \left(\frac{\pi}{180}\right)\frac{\sqrt{3}}{2} - \frac{1}{2!}\left(\frac{\pi}{180}\right)^2\frac{1}{2} - \frac{1}{3!}\left(\frac{\pi}{180}\right)^3\frac{\sqrt{3}}{2} + \cdots \tag{2.1.6}$$

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

2.2 Multinomial coefficient

- Recall the **binomial coefficient** is

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}\,. \tag{2.2.1}$$

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

$$\begin{aligned}\binom{n}{k_1, k_2, \dots, k_m} &= \frac{n!}{k_!!k_2!\dots k_m!(n-k_1-k_2-\cdots-k_m)!} \\ &= \frac{n(n-1)\dots\bigl(n+1-\sum_i k_i\bigr)}{k_!!k_2!\dots k_m!}\quad.\end{aligned} \tag{2.2.2}$$

- We must have $k_1 + \cdots + k_m \le n$ else the value of the multinomial coefficient is zero.

- 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

$$\binom{x}{k_1, k_2, \dots, k_m} = \frac{x(x-1)\dots\bigl(x+1-\sum_i k_i\bigr)}{k_!!k_2!\dots k_m!}\quad. \tag{2.2.3}$$

2.3 Multinomial theorem (not for examination)

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

$$
\begin{aligned}
(1+x_1+x_2)^n &= 1 + \binom{n}{1,0}x_1 + \binom{n}{0,1}x_2 \\
&\quad + \binom{n}{2,0}x_1^2 + \binom{n}{1,1}x_1x_2 + \binom{n}{0,2}x_2^2 \\
&\quad + \binom{n}{3,0}x_1^3 + \binom{n}{2,1}x_1^2x_2 + \binom{n}{1,2}x_1x_2^2 + \binom{n}{0,3}x_2^3 \\
&\quad + \cdots \\
&= 1 + \Biggl[\sum_{k_1=0}^{n}\sum_{k_2=0}^{n}\binom{n}{k_1,k_2}x_1^{k_1}x_2^{k_2}\Biggr]_{k_1+k_2=1} \\
&\quad + \Biggl[\sum_{k_1=0}^{n}\sum_{k_2=0}^{n}\binom{n}{k_1,k_2,}x_1^{k_1}x_2^{k_2}\Biggr]_{k_1+k_2=2} \\
&\quad + \cdots \\
&= 1 + \sum_{j=1}^{\infty}\Biggl[\sum_{k_1=0}^{n}\sum_{k_2=0}^{n}\binom{n}{k_1,k_2}x_1^{k_1}x_2^{k_2}\Biggr]_{k_1+k_2=j} .
\end{aligned}
\tag{2.3.1}
$$

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

$$
\begin{aligned}
&(1+x_1+x_2+\cdots+x_m)^n \\
&\qquad = 1 + \sum_{j=1}^{\infty}\Biggl[\sum_{k_1=0}^{n}\cdots\sum_{k_m=0}^{n}\binom{n}{k_1,k_2,\dots,k_m}x_1^{k_1}x_2^{k_2}\dots x_m^{k_m}\Biggr]_{k_1+k_2+\cdots+k_m=j} .
\end{aligned}
\tag{2.3.2}
$$

- 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.

2.4 Multivariate Taylor series (not for examination)

- The multinomial coefficients appear in the formula for a Taylor series of a function of multiple variables $x_1, x_s, \dots, x_m$.
- 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{2.4.1}
$$

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

$$
\begin{aligned}
&f(x_1+\varepsilon_1, x_2+\varepsilon_2, \dots, x_m+\varepsilon_m) = f(x_1, x_2, \dots, x_m) \\
&\quad + \sum_{j=1}^{\infty}\Bigg[\sum_{k_1=0}^{n}\sum_{k_2=0}^{n}\cdots\sum_{k_m=0}^{n}\frac{1}{k_1!k_2!\cdots k_m!}\,\frac{\partial^j f}{\partial x_1^{k_1}\partial x_2^{k_2}\dots\partial x_m^{k_m}}\,\varepsilon_1^{k_1}\varepsilon_2^{k_2}\cdots\varepsilon_m^{k_m}\Bigg]_{k_1+k_2+\cdots+k_m=j}.
\end{aligned}
\tag{2.4.2}
$$