Chapter 5

Taylor Series

An important tool in the study of numerical methods is the Taylor expansion of a function. Its basic use is to derive error estimates for numerical methods. Since numerical methods by in-large use discretize information, it is important to quantify the error in approximating a function by its value at a near by point; the Taylor series is the tool to get a handle on that error estimate. Here we derive the Taylor series expansion since it is rather simple.

The starting point for this derivation is the fundamental theorem of Calculus:

\[ u(x) = u(x_i) + \int_{x_i}^{x} u'(s) \, ds \]  

(5.1)

where \( x_i \) is a reference point, \( u' \) is the derivative of the function \( u(x) \) and \( s \) is a constant of integration. The only restriction is that \( u'(x) \) be continuous. This expression allows to compute the function \( u \) at a point \( x \) provided we know at a neighboring point \( x_i \) and we know how its derivative varies.

Since \( u(x) \) is arbitrary, the formula should hold with \( u(x) \) replaced by \( u'(x) \), i.e.,

\[ u'(s) = u'(x_i) + \int_{x_i}^{s} u''(t) \, dt \]  

(5.2)

provided \( u''(x) \) is itself continuous. Replacing this expression in the original formula and carrying out the integration (since \( u(x_i) \) is constant) we get:

\[ u(x) = u(x_i) + \int_{x_i}^{x} u'(x_i) \, ds + \int_{x_i}^{x} \int_{x_i}^{s} u''(t) \, dt \, ds \]  

(5.3)

Now notice that the term inside the first integral is constant, it does not vary with the integration variable \( s \), and hence it can be pulled out of the integral; the integrand can then be evaluated:

\[ \int_{x_i}^{x} u'(x_i) \, ds = \int_{x_i}^{x} ds u'(x_i) = [x]_{x_i}^{x} u'(x_i) = (x - x_i) u'(x_i) \]  

(5.4)
and substituted to get:

\[ u(x) = u(x_i) + (x - x_i)u'(x_i) + \int_{x_i}^{x} \int_{x_i}^{s} u''(t) \, dt \, ds \]  \tag{5.5}

The process can be repeated, provided \( u'''(x) \) with

\[ u''(t) = u''(x_i) + \int_{x_i}^{t} u'''(y) \, dy. \]  \tag{5.6}

The double integral of the above expression is:

\[
\int_{x_i}^{x} \int_{x_i}^{s} u''(t) \, dt \, ds = \int_{x_i}^{x} \int_{x_i}^{s} u''(x_i) \, dt \, ds + \int_{x_i}^{x} \int_{x_i}^{s} \int_{x_i}^{t} u'''(y) \, dy \, dt \, ds
\]

\[
= \int_{x_i}^{x} \int_{x_i}^{s} dt \, ds \, u''(x_i) + \int_{x_i}^{x} \int_{x_i}^{s} \int_{x_i}^{t} u'''(y) \, dy \, dt \, ds
\]

\[
= \int_{x_i}^{x} [(t - x_i)]^2 \int_{x_i}^{s} ds \, u''(x_i) + \int_{x_i}^{x} \int_{x_i}^{s} \int_{x_i}^{t} u'''(y) \, dy \, dt \, ds
\]

\[
= \left[ \frac{(s - x_i)^2}{2} \right]_{x_i}^{x} u''(x_i) + \int_{x_i}^{x} \int_{x_i}^{s} \int_{x_i}^{t} u'''(y) \, dy \, dt \, ds
\]

\[
= \frac{(x - x_i)^2}{2} u''(x_i) + \int_{x_i}^{x} \int_{x_i}^{s} \int_{x_i}^{t} u'''(y) \, dy \, dt \, ds \]  \tag{5.7}

Replacing the integral of \( u''(x) \) in 5.7 into equation 5.5 we get:

\[ u(x) = u(x_i) + (x - x_i)u'(x_i) + \frac{(x - x_i)^2}{2!} u''(x_i) + \int_{x_i}^{x} \int_{x_i}^{s} \int_{x_i}^{t} u'''(s) \, ds \, ds \, ds \]  \tag{5.8}

This process can be repeated under the assumption that \( u(x) \) is sufficiently differentiable, and we find:

\[ u(x) = u(x_i) + (x - x_i)u'(x_i) + \frac{(x - x_i)^2}{2!} u''(x_i) + \ldots + \frac{(x - x_i)^n}{n!} u^{(n)}(x_i) + R_{n+1} \]  \tag{5.9}

where the remainder is given by:

\[ R_{n+1} = \int_{x_i}^{x} \ldots \int_{x_i}^{x} u^{(n+1)}(s) \, (ds)^{n+1} \]  \tag{5.10}

Equation 5.9 is known as the Taylor series of the function \( u(x) \) about the point \( x_i \). Notice that the series is a polynomial in \( (x - x_i) \) (the signed distance of \( x \) to \( x_i \)), and the coefficients are the (scaled) derivatives of the function evaluated at \( x_i \). The series gives a mean to approximate the function \( u \) at \( x \) using information about \( u \) and its derivative at \( x_i \). Whether the series converges or not depends on
the existence and distance of singularities (discontinuities in the function or its
derivatives) to the point $x_i$.

Taylor’s formula is usually used to get information about the magnitude of the
error committed in deriving discrete approximations to continuous problem. Notice
that the coefficients of the polynomial depend solely on the derivative of the function
and are hence fixed, i.e. they do not depend on the numerical approximation
but are inherent to the function $u(x)$. The only \textit{numerical parameters} in this case
is the distance between the point $x$ and the reference point $x_i$. If the derivatives
are finite then the approximation can be improved by including additional terms
in the series, since for (scaled), $\Delta x < 1$, $\Delta x^n < \ldots < \Delta x^2 < \Delta x$.

We can further get a grip on the quality of the approximation by deriving
bounds on the remainder $R_{n+1}$. If the $(n+1)$-th derivative of the function $u$ has
minimum $m$ and maximum $M$ over the interval $[x; x]$ then we can write:

$$
\int_{x_i}^{x} \cdots \int_{x_i}^{x} m (ds)^{n+1} \leq R_{n+1} \leq \int_{x_i}^{x} \cdots \int_{x_i}^{x} M (ds)^{n+1} 
$$

(5.11)

$$
\frac{m (x - x_i)^{n+1}}{(n + 1)!} \leq R_{n+1} \leq \frac{M (x - x_i)^{n+1}}{(n + 1)!} 
$$

(5.12)

which shows that the remainder is bounded by the values of the derivative and the
distance of the point $x$ to the expansion point $x_i$ raised to the power $(n + 1)$. If
we further assume that $u^{(n+1)}$ is continuous then it must take all values between
$m$ and $M$ that is

$$
R_{n+1} = u^{(n+1)}(\xi) \frac{(x - x_i)^{n+1}}{(n+1)!} 
$$

(5.13)

for some $\xi$ in the interval $[x_i; x]$. 
Chapter 6

Trapezoidal integration

6.1 Error approximations for trapezoidal integration

Here we will illustrate how error estimates for the trapezoidal integration rule can be estimated. Let us concentrate on the interval \([x_{i-1}, x_i]\) and let us carry out a first manipulation of an integration by part:

\[
\delta A_i = \int_{x_{i-1}}^{x_i} f(x) \, dx \\
= \int_{x_{i-1}}^{x_i} f(x) \, d\left(x - x_{i-\frac{1}{2}}\right) \\
= \left[\left(x - x_{i-\frac{1}{2}}\right) f(x)\right]_{x_{i-1}}^{x_i} - \int_{x_{i-1}}^{x_i} \left(x - x_{i-\frac{1}{2}}\right) f'(x) \, dx \\
= \left[(x_i - x_{i-\frac{1}{2}}) f(x_i) - (x_{i-1} - x_{i-\frac{1}{2}}) f(x_{i-1})\right] - \int_{x_{i-1}}^{x_i} \left(x - x_{i-\frac{1}{2}}\right) f'(x) \, dx \\
= \left[\frac{\Delta x}{2} f_i - \frac{-\Delta x}{2} f_{i-1}\right] - \int_{x_{i-1}}^{x_i} \left(x - x_{i-\frac{1}{2}}\right) f'(x) \, dx \\
= \frac{\Delta x}{2} \left[\frac{f_{i-1} + f_i}{2}\right] - \int_{x_{i-1}}^{x_i} \left(x - x_{i-\frac{1}{2}}\right) f'(x) \, dx \\
\delta A_i = \frac{\Delta x}{2} \left[\frac{f_{i-1} + f_i}{2}\right] - \int_{x_{i-1}}^{x_i} \left(x - x_{i-\frac{1}{2}}\right) f'(x) \, dx \\
\delta E_i
\]

The first term on the right hand side of 6.2, \(\delta \tilde{A}_i\), is clearly the trapezoidal formula for the interval \([x_{i-1}, x_i]\), and the second term is nothing but the error term, referred to as \(\delta E_i\) if the trapezoidal formula is used to approximate the error in that interval. What we need to do know is to find a way to bound this error term in terms of the numerical parameters and the features of the function to be integrated. We will illustrate that in two ways.
6.1.1 Integration by parts

The integration by parts stratagem can be used again to get:

\[
\delta E_i = -\int_{x_{i-1}}^{x_i} \left( x - x_{i-\frac{1}{2}} \right) f'(x) \, dx
\]

\[
= -\int_{x_{i-1}}^{x_i} f'(x) \left[ \frac{\left( x - x_{i-\frac{1}{2}} \right)^2}{2} + B \right] \, dx
\]

\[
= -\left[ \frac{\Delta x^2}{8} + B \right] \left[ f'(x_i) - f'(x_{i-1}) \right] + \int_{x_{i-1}}^{x_i} \left[ \frac{\left( x - x_{i-\frac{1}{2}} \right)^2}{2} + B \right] f''(x) \, dx
\]

where \( B \) is an integration constant and \( f''(x) \) is the second derivative of the function \( f \). Clearly these integration by parts can be done only if the derivatives of \( f \) up to second order exist. The optimal choice of \( B \) that would knock-off the first term if \( B = -\Delta x^2/8 \), that term would then vanish and would not contribute to the error estimate. And we are left with the following estimate for the magnitude of the error:

\[
|\delta E_i| = \left| \int_{x_{i-1}}^{x_i} \left[ \frac{\left( x - x_{i-\frac{1}{2}} \right)^2}{2} - \frac{\Delta x^2}{8} \right] f''(x) \, dx \right|
\]

\[
\leq \int_{x_{i-1}}^{x_i} \left[ \frac{\left( x - x_{i-\frac{1}{2}} \right)^2}{2} - \frac{\Delta x^2}{8} \right] |f''(x)| \, dx
\]

\[
\leq \int_{x_{i-1}}^{x_i} \left[ \frac{\left( x - x_{i-\frac{1}{2}} \right)^2}{2} - \frac{\Delta x^2}{8} \right] \max_{x_{i-1} \leq x \leq x_i} |f''(x)| \, dx
\]

\[
\leq \int_{x_{i-1}}^{x_i} \left[ \frac{\left( x - x_{i-\frac{1}{2}} \right)^2}{2} - \frac{\Delta x^2}{8} \right] \, dx \max_{x_{i-1} \leq x \leq x_i} |f''(x)|
\]

\[
(6.3)
\]

where \( \max_{x_{i-1} \leq x \leq x_i} |f''(x)| \) is the maximum magnitude of the second derivative over the interval \([x_{i-1}, x_i]\). What remains to be done is to estimate the quadratic term. It is easy to see that the quadratic polynomial vanishes at \( x_{i-1} \) and \( x_i \) and reaches a minimum of \(-\Delta x^2/8\) at \( x_{i-\frac{1}{2}}\); thus it is entirely negative in that region, and we have:

\[
\int_{x_{i-1}}^{x_i} \left[ \frac{\left( x - x_{i-\frac{1}{2}} \right)^2}{2} - \frac{\Delta x^2}{8} \right] \, dx = \frac{\Delta x^3}{12}
\]

\[
(6.4)
\]

The error estimate is thus:

\[
|\delta E_i| \leq \frac{\Delta x^3}{12} \max_{x_{i-1} \leq x \leq x_i} |f''(x)|
\]

\[
(6.5)
\]
6.1. ERROR APPROXIMATIONS FOR TRAPEZOIDAL INTEGRATION

Finally this error estimate need to be summed for all intervals used since \( A = \sum_{i=1}^{N} \delta A_i \), \( A_N = \sum_{i=1}^{N} \delta \bar{A}_i \), and \( E_n = \sum_{i=1}^{N} \delta E_i \). And thus we have

\[
E_N = \sum_{i=1}^{N} \delta E_i
\]

\[
|E_N| = \left| \sum_{i=1}^{N} \delta E_i \right|
\]

\[
|E_N| \leq \sum_{i=1}^{N} |\delta E_i| \leq \frac{\Delta x^3}{12} \sum_{i=1}^{N} \max_{x_{i-1} \leq x \leq x_i} |f''(x)| \leq \frac{\Delta x^3}{12} \sum_{i=1}^{N} \left( \max_{a \leq x \leq b} |f''(x)| \right)
\]

(6.6)

where \( \max_{a \leq x \leq b} |f''(x)| \) is the **global** maximum of \( f''(x) \) which must be greater than all the local maxima within each interval:

\[
\max_{x_{i-1} \leq x \leq x_i} |f''(x)| \leq \max_{a \leq x \leq b} |f''(x)|
\]

(6.7)

The bound in equation 6.6 can be simplified further by realizing that the global maximum is a constant that can be pulled out of the sum:

\[
|E_N| \leq \frac{\Delta x^3}{12} \max_{a \leq x \leq b} |f''(x)| \sum_{i=1}^{N} 1 = \frac{N \Delta x^3}{12} \max_{a \leq x \leq b} |f''(x)|
\]

(6.8)

Replacing \( \Delta x \) by \( (b - a)/N \) we get our final estimate:

\[
|E_N| \leq \frac{(b - a)}{12N^2} \max_{a \leq x \leq b} |f''(x)|
\]

(6.9)

The derivation of estimate 6.9 might appear involved, but the critical issue at this point is the interpretation of the error bound. First notice that the parameters appear on the right hand side of inequality 6.9 involve a mix of numerical and non-numerical parameters. The non-numerical parameters pertain to the width of the interval, \( b - a \), and to the maximum curvature of the integrand, \( \max_{a \leq x \leq b} |f''(x)| \). Both quantities are inherent to the problem formulation and are not at the disposal.
of the numerical user. Clearly the larger the interval and/or the curvature of the function, the larger the error grows. The only numerical parameter at our disposal is the number of interval, $N$. Several aspects of this parameter should be noted. First $N$ appears in the denominator, and hence the error bounds is guaranteed to decay to zero as the number of intervals is increased. Second, the error decays to zero as the second power of $N$, $N^{-2}$, that is we should expect a decrease of the error by a factor of 4 if the number of interval is doubled to $2N$; this is referred to as quadratic or second order convergence. Third, for this estimate to hold (for the analysis to be valid) the maximum curvature on the interval $[a \, b]$ must be finite.

6.1.2 Taylor Series

A few more facts about the errors behavior can be revealed by following a slightly different tack in estimating the error, namely that all error terms are dependent on negative even powers of $N$. This has implication with respect to improving on the basic of the trapezoidal rule using Richardson extrapolation.

The starting point here is to expand the derivative, $f'(x)$ in a Taylor series about $x_{i-\frac{1}{2}}$:

$$f'(x) = \frac{df}{dx}\bigg|_{x_{i-\frac{1}{2}}} + (x - x_{i-\frac{1}{2}}) \frac{d^2f}{dx^2}\bigg|_{x_{i-\frac{1}{2}}} + \frac{(x - x_{i-\frac{1}{2}})^2}{2!} \frac{d^3f}{dx^3}\bigg|_{x_{i-\frac{1}{2}}} + \cdots$$

$$+ \frac{(x - x_{i-\frac{1}{2}})^n}{n!} \frac{d^{n+1}f}{dx^{n+1}}\bigg|_{x_{i-\frac{1}{2}}} + \cdots + R_{M+1} \quad (6.10)$$

$$R_{M+1} = \frac{(x - x_{i-\frac{1}{2}})^M}{(M + 1)!} \frac{d^{M+2}f}{dx^{M+2}}\bigg|_{\xi} \quad (6.11)$$

where the derivative in the remainder term $R_{M+1}$ is evaluated at an undetermined point $\xi$ in the interval $[x_{i-1} \, x_i]$. Notice that the remainder has the same form as the other term except that the derivative in it is evaluated at an unknown location $\xi$. The integral of the function $f$ can now be done via its Taylor approximation. Since the derivatives are evaluated at the fixed mid-point of the interval they can be pulled out of the integrand to get:

$$\delta E_i = \int_{x_{i-1}}^{x_i} (x - x_{\frac{i}{2}}) f'(x) \, dx$$

$$= \sum_{n=0}^{M} \left[ \frac{1}{n!} \int_{x_{i-1}}^{x_i} (x - x_{i-\frac{1}{2}})^{n+1} \, dx \frac{d^{n+1}f}{dx^{n+1}}\bigg|_{x_{i-\frac{1}{2}}} \right] + \int_{x_{i-1}}^{x_i} R_{M+1} \, dx \quad (6.12)$$

We are thus simply required to integrate powers of $(x - x_{i-\frac{1}{2}})$. It is easy to show
that

\[
\int_{x_{i-1}}^{x_i} (x - x_{i-\frac{1}{2}})^{n+1} \, dx = \left[ \frac{(x - x_{i-\frac{1}{2}})^{n+2}}{n+2} \right]_{x_{i-1}}^{x_i} = \frac{(x_i - x_{i-\frac{1}{2}})^{n+2}}{n+2} - \frac{(x_{i-1} - x_{i-\frac{1}{2}})^{n+2}}{n+2} = \frac{(\Delta x)^{n+2}}{n+2} - \frac{(-\Delta x)^{n+2}}{n+2} = \begin{cases} 0 & \text{if } n \text{ is even} \\ \frac{\Delta x^{n+2}}{2^{n+1}(n+2)} & \text{if } n \text{ is odd} \end{cases}
\]

Hence all the odd powers drop out of the summation and only the even powers remain.

\[
\delta E_i = \sum_{n=1,3,5,...}^{N} \left[ \frac{1}{n!} \frac{\Delta x^{n+2}}{2^{n+1}(n+2)} \left( \frac{d^{n+1}f}{dx^{n+1}} \right)_{i-\frac{1}{2}} \right] + \int_{x_{i-1}}^{x_i} R_{N+1} \, dx = \frac{\Delta x^3}{12} \left( \frac{d^2f}{dx^2} \right)_{i-\frac{1}{2}} + \frac{\Delta x^5}{480} \left( \frac{d^4f}{dx^4} \right)_{i-\frac{1}{2}} + \frac{\Delta x^7}{53760} \left( \frac{d^6f}{dx^6} \right)_{i-\frac{1}{2}} + \cdots
\]

\[
+ \frac{\Delta x^{2M+1}}{(2M-1)! \, 2^{2M}(2M+1)} \left( \frac{d^{2M}f}{dx^{2M}} \right)_{\xi}
\]

where we have changed notation slightly to indicate that only even derivatives of \(f\) survive. The leading term in the above series is nothing but the error bounds derived previously in equation 6.5. The estimate for the total error can now be obtained by summing over all intervals to get:

\[
E_N = \frac{\Delta x^3}{12} \sum_{i=1}^{N} \left( \frac{d^2f}{dx^2} \right)_{i-\frac{1}{2}} + \frac{\Delta x^5}{480} \sum_{i=1}^{N} \left( \frac{d^4f}{dx^4} \right)_{i-\frac{1}{2}} + \frac{\Delta x^7}{53760} \sum_{i=1}^{N} \left( \frac{d^6f}{dx^6} \right)_{i-\frac{1}{2}} + \cdots
\]

Although the series involve odd powers of \(\Delta x\), one should not forget the influence of the individual sums which also increase as \(\Delta x\) decreases (or \(N\) increases). If one introduces the average of the derivative at the mid-points of the interval, namely

\[
\left( \frac{d^{2m}f}{dx^{2m}} \right) = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{d^{2m}f}{dx^{2m}} \right)_{i-\frac{1}{2}}
\]

The series in the error term can thus be written as:

\[
E_N = \frac{(b-a)^2}{12N^2} \left( \frac{d^2f}{dx^2} \right) + \frac{(b-a)^4}{480N^4} \left( \frac{d^4f}{dx^4} \right) + \frac{(b-a)^6}{53760N^6} \left( \frac{d^6f}{dx^6} \right) + \cdots
\]

If the calculations are repeated with different number of intervals, say \(2N\) and \(4N\) the series expansion of the integral takes the form:

\[
E_{2N} = \frac{(b-a)^2}{12(2N)^2} \left( \frac{d^2f}{dx^2} \right) + \frac{(b-a)^4}{480(2N)^4} \left( \frac{d^4f}{dx^4} \right) + \frac{(b-a)^6}{53760(2N)^6} \left( \frac{d^6f}{dx^6} \right) + \cdots
\]
E_{4N} = \frac{(b-a)^2}{12(4N)^2} \left\langle \frac{d^2 f}{dx^2} \right\rangle + \frac{(b-a)^4}{480(4N)^4} \left\langle \frac{d^4 f}{dx^4} \right\rangle + \frac{(b-a)^6}{53760(4N)^6} \left\langle \frac{d^6 f}{dx^6} \right\rangle + \cdots \quad (6.18)

The series suggest a mean to improve our estimates of the integral:

\begin{align*}
A & = A_N + E_N \quad (6.19) \\
A & = A_{2N} + E_{2N} \quad (6.20) \\
A & = A_{4N} + E_{4N} \quad (6.21)
\end{align*}

By forming linear combination of the different estimates, $A_N, A_{2N}, A_{4N}$ one can attempt to reduce the error further without major additional computations. If I set, for example, $A_{2N,N} = \alpha A_{2N} + \beta A_N$, what is the optimal choice of $\alpha$ and $\beta$ to guarantee a reduction in the error. The error estimate is clearly an asset here, and our goal should to knock off the leading error term. Now assuming for the time-being that the averages of the derivative terms do not change much as $N$ is increased, then the following combination: has

\begin{align*}
A_{2N,N} &= \frac{4A_{2N} - A_N}{3} + \frac{4E_{2N} - E_N}{3} \quad (6.22) \\
\frac{4E_{2N} - E_N}{3} &= \frac{1}{3} \left( \frac{4}{2^4} - 1 \right) \frac{(b-a)^4}{480N^4} \left\langle \frac{d^4 f}{dx^4} \right\rangle + \frac{1}{3} \left( \frac{4}{2^6} - 1 \right) \frac{(b-a)^6}{53760N^6} + \left\langle \frac{d^6 f}{dx^6} \right\rangle \quad (6.23)
\end{align*}

a leading error term that starts with $N^{-4}$, i.e. the error is fourth order in $N$. Similarly we have:

\begin{align*}
A_{4N,2N} &= \frac{4A_{4N} - A_{2N}}{3} + \frac{4E_{4N} - E_{2N}}{3} \quad (6.24) \\
\frac{4E_{4N} - E_{2N}}{3} &= \frac{1}{3} \left( \frac{4}{4^4} - \frac{1}{2^4} \right) \frac{(b-a)^4}{480N^4} \left\langle \frac{d^4 f}{dx^4} \right\rangle + \frac{1}{3} \left( \frac{4}{4^6} - \frac{1}{2^6} \right) \frac{(b-a)^6}{53760N^6} + \left\langle \frac{d^6 f}{dx^6} \right\rangle \quad (6.25)
\end{align*}

Notice that the process can be continued and a sixth-order estimate can be formed by combining the two fourth order estimates.

\begin{align*}
A_{4N,2N,N} &= \frac{16}{15} \left( A_{4N,2N} - \frac{1}{16} A_{2N,N} \right) + O(N^{-6}) \quad (6.26)
\end{align*}