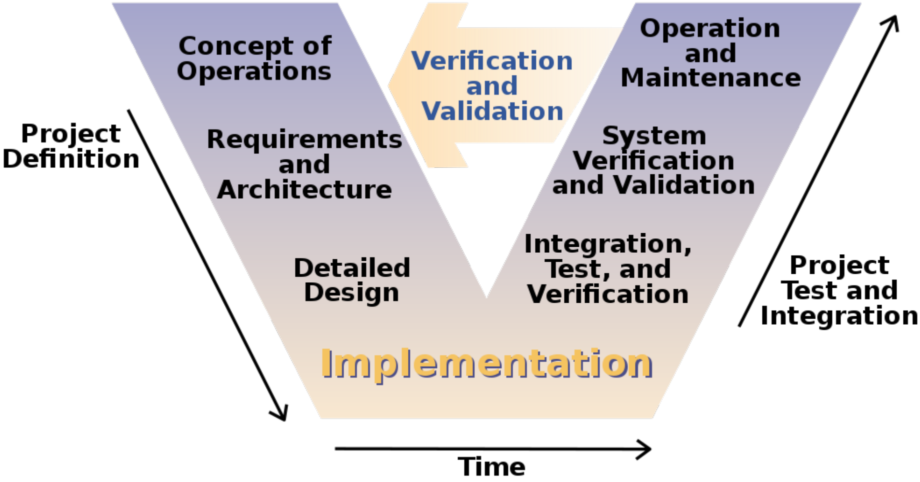
1. Computational methods and Taylor series

Design and building



Many team members
Many subproblems

Solving a quantitative problem as an engineer

Modeled in mathematical form (often, equations) using physics or empirical rules.

An *algorithm* gives step-by-step process (derived using *analytical* and *numerical* methods) to solve a math problem, which can be written as a program for a computer to solve.

The solution then needs to be interpreted in the original context.

Analytic and numeric methods

- Analytical methods: exact solutions derived for particular math problems, as in algebra and calculus (e.g. quadratic formula, simple harmonic oscillator)
- Numerical methods: solution process for more general math problems using arithmetic and logic operations as basic building blocks
  - Often approximate
  - Trade-off between accuracy and amount of computation
  - Need error analysis and error estimates

Computation

"Whenever someone speaks of using a computer to design an airplane, predict the weather, or otherwise solve a complex science or engineering problem, that person is talking about using numerical methods and analysis."

Simplification

- Given a complicated math problem, we can try to approximate it as something simpler that we know how to compute using arithmetic and logic
- Thus, many numerical methods are based on approximating arbitrary functions with simpler ones
  Some example of simple functions are
  - Constant: $f(x) = a$, for some number a
  - Linear: $f(x) = a_1 x + a_0$, for some a_0 and a_1
  - Quadratic: $f(x) = a_2 x^2 + a_1 x + a_0$
  - Polynomial: $f(x) = \sum_{i=0}^{n} a_i x^i$
- Taylor's theorem is important in numerical analysis because it gives us a way to approximate functions as polynomials, along with an expression for the error of the approximation

Taylor's theorem

If $f(x)$ has derivatives of order $0, 1, 2, \ldots, n+1$ on the closed interval $[b, c]$,
then for any x and a in this interval

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(a)\,(x-a)^k}{k!} + \frac{f^{(n+1)}(\xi)\,(x-a)^{n+1}}{(n+1)!},$$

where ξ is some number between x and a, and $f^{(k)}(x)$ is the kth derivative of f at x ($f^{(0)}$ is f)
The first $n+1$ terms form a polynomial of degree n
The rightmost term is the 'remainder', R_{n+1}.

Taylor series with different number of terms

- $n = 0$: $f(x) \approx f(a)$
- $n = 1$: $f(x) \approx f(a) + f'(a)(x - a)$
- $n = 2$: $f(x) \approx f(a) + f'(a)(x - a) + f''(a)(x - a)^2/2$
- In each case, how good the approximation is depends on the size of the left-out remainder term
- Full series: $\sum_{k=0}^{\infty} \frac{f^{(k)}(a)\,(x-a)^k}{k!}$ – should exactly equal $f(x)$ (if the remainder term goes to 0 as $n \to \infty$)

Alternative form of Taylor's theorem

If $f(x)$ has derivatives of order $0, 1, \ldots, n+1$ on the closed interval $[b, c]$,
then for any a in this interval and any h such that $a + h$ is in this interval,

$$f(a+h) = \sum_{k=0}^{n} \frac{f^{(k)}(a)\, h^k}{k!} + \frac{f^{(k+1)}(\xi)\, h^{n+1}}{(n+1)!},$$

where ξ is some number between a and $a + h$.

With either form, we say that the Taylor expansion is *centered* at a or *about*/*around* a.
(The special case $a = 0$ is called the Maclaurin series.)

Taylor series example: exponential function

$f(x) = e^x$ or $\exp(x)$ has all its derivative equal to itself
Therefore, the Taylor series is

$$e^x = e^a(1 + (x-a) + \frac{(x-a)^2}{2} + \frac{(x-a)^3}{6} + \cdots),$$

For example, given e, we could approximate $e^{1.2}$ as

$$e^{1.2} \approx e(1 + 0.2 + \frac{0.04}{2} + \frac{0.008}{6}),$$

The remainder term would look like $\frac{f^{(n+1)}(\xi)\,(x-a)^{n+1}}{(n+1)!} = \frac{e^{\xi}(x-a)^{n+1}}{(n+1)!}$.
In this case, with $a = 1, x = 1.2, n = 3$, we can bound the error term as $\frac{(0.2)^4 e}{24} \leq R_{n+1} \leq \frac{(0.2)^4 e^{1.2}}{24}$, which is around 2×10^{-4}

Taylor series example: sine function

If $f(x) = \sin(x)$, $f'(x) = \cos(x)$ and so forth
Therefore, the Taylor series is

$$\sin(x) = \sin(a) + \cos(a)(x-a) - \sin(a)\frac{(x-a)^2}{2} - \cos(a)\frac{(x-a)^3}{6} + \cdots,$$

For example, given $a = 0$ we could approximate $\sin(0.5)$ as

$$\sin(0.5) \approx 0 + 0.5 - 0 - \frac{0.125}{6},$$

The remainder term with $a = 0, x = 0.5, n = 3$ would look like $\frac{f^{(n+1)}(\xi)\,(x-a)^{n+1}}{(n+1)!} = \frac{\sin(\xi)0.5^4}{4!}$. In this case, we can bound the error term as $0 \leq R_4 \leq \frac{\sin(0.5)}{24 \cdot 16}$, which is less than 1.25×10^{-3}

Cosine

If $f(x) = \cos(x)$, $f'(x) = -\sin(x)$ and so forth
Therefore, the Taylor series is

$$\cos(x) = \cos(a) - \sin(a)(x-a) - \cos(a)\frac{(x-a)^2}{2} + \sin(a)\frac{(x-a)^3}{6} + \cdots ,$$

For example, given $a = \pi/2$ we could approximate $\cos(2)$ as

$$\cos(2) \approx 0 - (2 - \pi/2) + \frac{(2-\pi/2)^3}{6},$$

The remainder term with $a = \pi/2, x = 2, n = 3$ would look like $\frac{f^{(n+1)}(\xi)\,(x-a)^{n+1}}{(n+1)!} = \frac{\cos(\xi)(2-\pi/2)^4}{4!}$. In this case, we can bound the error term as $\frac{\cos(2)(2-\pi/2)^4}{24} \leq R_4 \leq 0$, which is less than 6×10^{-4} in absolute value

Polynomial

If $f(x) = x^4$, we can use Taylor's theorem to approximate it as a degree-2 polynomial about $a = 1$ as

$$x^4 \approx 1 + 4(x-1) + 6(x-1)^2$$

For example, for $x = 1.1$, this approximation gives $f(x) \approx 1.46$, compared to the exact value $(1.1)^4 = 1.4641$

On the other hand, if x is not close to 1, this approximation is no longer close to x^4. In fact, we can see from the remainder term that the error of the approximation is proportional to $(x-1)^3$

Practice problem

Given $f(3) = 6, f'(3) = 8, f''(3) = 2$, and that all other higher order derivatives of $f(x)$ are zero at $x = 3$, and assuming the function and all its derivatives exist and are continuous between $x = 3$ and $x = 6$, what is the value of $f(6)$?

Practice problem

Let $f(x) = x \cos x$.
Find a second-order polynomial that approximates $f(x)$ using Taylor's theorem about $a = 0$.
Use this polynomial to approximate $f(0.5)$.
Based on the remainder term, get an upper bound for the absolute error in the approximation.
How does the actual absolute error compare to this upper bound?

Practice problem

To what order in x should the Taylor series of $\sin(x)$ about 0 be taken so to make sure that it approximates $\sin(x)$ with absolute error less than 10^{-4} for all x between 0 and 0.2?

Some numerical methods derived from Taylor's theorem

- Newton's method
- Centered finite difference
- Euler's method

Newton's method for solving nonlinear equations

Suppose we have some known function f and want to find a value x such that $f(x) = 0$

Taylor theorem application

Writing the Taylor series about some guess x_i for x,

$$0 = f(x) = f(x_i) + f'(x_i)(x - x_i) + \frac{f''(\xi)(x - x_i)^2}{2},$$

so that

$$\begin{aligned} x &= x_i - \frac{f(x_i)}{f'(x_i)} + \frac{R_2}{f'(x_i)} \\ &\approx x_i - \frac{f(x_i)}{f'(x_i)} \end{aligned}$$

where the approximation should be good if x is close to x_i (and f'' not too large, and $f'(x_i)$ not too close to 0)

Newton's method as an iteration

- Given f, start with some initial guess x_0 for where it's equal to 0
- Derive a hopefully better estimate using

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

- Stop once $f(x_i)$ is close enough to 0

Example of using Newton's method

To find where $\cos(x)$ is equal to x,
Let $f(x) = \cos(x) - x$
If $x_0 = 0.5$, we get $x_1 = 0.75522, x_2 = 0.73914, x_3 = 0.73909$, and $f(x_3) = -1.2 \times 10^{-9}$ is quite close to 0

Practice problem

Do an iteration of Newton's method for finding the cube root of 6, starting from an initial guess of 2.

Centered finite difference for numerically approximating derivatives

Suppose we have some known function f and want to find a value $f'(x)$ at some given point x

Taylor theorem derivation

Centered finite difference uses the values of f at points $x+h$ and $x-h$, on either side of x

Writing the Taylor series up to order 2 about x for those two points,

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + R_{3,+}$$
$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - R_{3,-}$$

Combining those expressions, we can extract $f'(x)$ as

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{R_{3,+} + R_{3,-}}{2h} \approx \frac{f(x+h) - f(x-h)}{2h}$$

The remainder term can also be written as $\frac{1}{6}h^2 f'''(\xi)$ for some ξ between $x-h$ and $x+h$, so it normally gets smaller as h becomes closer to 0

Example of using centered finite difference

Find the derivative of $\cos(x)$ at $x = 0.5$.
With $h = 0.2$:
$\cos'(0.5) \approx \frac{\cos(0.7)-\cos(0.3)}{0.4} = -0.47624$
With $h = 0.1$:
$\cos'(0.5) \approx \frac{\cos(0.6)-\cos(0.4)}{0.2} = -0.47863$, which is more accurate compared to the actual derivative $-\sin(0.5) = -0.47943$

Euler's method for numerically solving a differential equation

Suppose we know that $y'(x) = f(x, y)$ and that $y(a) = y_1$, and we want to know $y(b)$
(an initial value problem)

Taylor theorem derivation

If F is the integral of f over x,

$$F(a+h) = F(a) + hF'(a) + \frac{h^2}{2}F''(\xi)$$

and hence

$$y(a+h) \approx y_1 + hf(a, y_1)$$

The remainder term normally gets smaller (making the approximation better) as h becomes closer to 0

Example of using Euler's method

Normally we would use the method with a small step size h for better accuracy, using the result from the last step as the initial value from the next step until we reach $x = b$

Find $y(2)$ if $y'(x) = -y$ and $y(1) = 3$.
With $h = 0.5$:
$y(1.5) \approx 3 + (0.5)(-3) = 1.5$
$y(2) \approx 1.5 + (0.5)(-1.5) = 0.75$

In this case, we can solve analytically to find that
$y(2) = 3/e = 1.1036$

Summary of Lecture 1

- Computation in engineering
- Characteristics of numerical methods
- Taylor's theorem
  - Finding unknown function values
  - Approximating functions as polynomials
  - Newton's method
  - Centered finite difference
  - Euler's method