Numerical Methods

B.Tech all branches · GATE Engineering Mathematics

Uncodemy Handwritten Notes · free for students

1. Errors

- Numerical methods give **approximate** answers by repeated arithmetic. Used when exact answers are hard.
- **Absolute error** = abs(true − approx). **Relative error** = absolute error / abs(true). **Percentage error** = relative × 100.
- **Round-off error**: from keeping limited digits. **Truncation error**: from cutting an infinite process short (like a series).
- **Significant digits**: 0.004050 has 4 significant digits (4, 0, 5, 0).

EXAMPLE True value 2/3 = 0.666666..., approx 0.667. Absolute error ≈ 0.000333. Relative error ≈ 0.0005 = 0.05%.

2. Roots of Equations f(x) = 0

➤ Methods compared

Method	Needs	Order of convergence	Always converges?
Bisection	Interval [a, b] with sign change	1 (linear, halves each step)	Yes
Regula Falsi	Interval with sign change	1 (linear)	Yes
Secant	Two starting points	1.618	No
Newton–Raphson	One point, f'(x)	2 (quadratic)	No (fails if f' ≈ 0)
Fixed point x = g(x)	abs(g'(x)) < 1 near root	1	Only if abs(g') < 1

FORMULA Newton–Raphson: x(n+1) = x(n) − f(x(n)) / f'(x(n)).

FORMULA Regula Falsi: x = (a f(b) - b f(a)) / (f(b) - f(a)).

FORMULA Bisection steps for accuracy ε: n >= log2((b - a) / ε).

➤ Solved example (Newton–Raphson for sqrt(2))

- f(x) = x^2 - 2, f'(x) = 2x. Start x0 = 1.
- x1 = 1 - (1 - 2)/2 = 1.5.
- x2 = 1.5 - (2.25 - 2)/3 = 1.5 - 0.08333 = 1.41667.
- x3 = 1.41667 - (2.00694 - 2)/2.83333 = 1.41667 - 0.00245 = 1.41422. (True 1.41421.)

➤ Solved example (Bisection)

- f(x) = x^3 - x - 1 on [1, 2]. f(1) = -1, f(2) = 5.
- c = 1.5: f = 3.375 - 2.5 = 0.875 > 0 ⇒ root in [1, 1.5].
- c = 1.25: f = 1.953 - 2.25 = -0.297 < 0 ⇒ root in [1.25, 1.5].
- c = 1.375: f = 2.600 - 2.375 = 0.225 > 0 ⇒ root in [1.25, 1.375]. (True root ≈ 1.3247.)

TIP Newton's formula for sqrt(N): x(n+1) = (x(n) + N/x(n)) / 2. For 1/N: x(n+1) = x(n)(2 - N x(n)).

3. Linear Systems

➤ Direct methods

- **Gauss elimination**: forward elimination to upper triangular, then back substitution. Use **partial pivoting** (largest pivot) to reduce round-off.
- **Gauss–Jordan**: reduce to a diagonal / identity matrix. Also used to find A^-1.
- **LU (Doolittle / Crout)**: A = LU. Solve LY = B, then UX = Y.
- Operation count of Gauss elimination ≈ n^3 / 3 multiplications.

➤ Iterative methods

- **Jacobi**: every new value uses only old values.
- **Gauss–Seidel**: uses new values as soon as they are found. Usually about twice as fast as Jacobi.

- Both converge if the matrix is **diagonally dominant**: abs(a_ii) >= sum of abs of other entries in that row (strict in at least one row).

➤ Solved example (Gauss–Seidel)

- 4x + y = 6, x + 3y = 7. Start x = 0, y = 0.
- Iteration 1: x = (6 - 0)/4 = 1.5. y = (7 - 1.5)/3 = 1.8333.
- Iteration 2: x = (6 - 1.8333)/4 = 1.0417. y = (7 - 1.0417)/3 = 1.9861.
- Iteration 3: x = (6 - 1.9861)/4 = 1.0035. y = (7 - 1.0035)/3 = 1.9988.
- Converging to x = 1, y = 2 (check: 4 + 2 = 6, 1 + 6 = 7).

4. Finite Differences and Interpolation

- Equal spacing h. **Forward difference** Δy0 = y1 - y0. **Backward** ∇y1 = y1 - y0.
- Shift operator E y(x) = y(x + h). Relations: Δ = E - 1, ∇ = 1 - E^(-1).
- For a polynomial of degree n, the nth differences are constant and (n+1)th differences are 0.

➤ Formulas

- **Newton forward** (near the start), u = (x - x0)/h:
  - y = y0 + u Δy0 + u(u-1)/2! Δ^2 y0 + u(u-1)(u-2)/3! Δ^3 y0 + ...
- **Newton backward** (near the end), u = (x - xn)/h:
  - y = yn + u ∇yn + u(u+1)/2! ∇^2 yn + ...
- **Lagrange** (unequal spacing): y = Σ yi Li(x), where Li(x) = Π (x - xj)/(xi - xj), j ≠ i.
- **Newton divided difference**: also for unequal spacing.

➤ Solved example (Lagrange)

- Points (1, 1), (2, 4), (3, 9). Find y at x = 2.5.
- L0 = (2.5-2)(2.5-3)/((1-2)(1-3)) = (0.5)(-0.5)/2 = -0.125.
- L1 = (2.5-1)(2.5-3)/((2-1)(2-3)) = (1.5)(-0.5)/(-1) = 0.75.
- L2 = (2.5-1)(2.5-2)/((3-1)(3-2)) = (1.5)(0.5)/2 = 0.375.
- y = 1(-0.125) + 4(0.75) + 9(0.375) = -0.125 + 3 + 3.375 = 6.25 (= 2.5^2, exact since data is from y = x^2).

5. Numerical Differentiation

- From Newton forward at x = x0: dy/dx = (1/h)[Δy0 - Δ^2 y0 / 2 + Δ^3 y0 / 3 - ...].
- Central difference: f'(x) ≈ (f(x + h) - f(x - h)) / 2h (error of order h^2).
- f''(x) ≈ (f(x + h) - 2f(x) + f(x - h)) / h^2.

6. Numerical Integration

Rule	Formula	Condition	Exact for
Trapezoidal	(h/2)[y0 + yn + 2(y1 + ... + y(n-1))]	Any n	Degree <= 1
Simpson 1/3	(h/3)[y0 + yn + 4(odd) + 2(even)]	n even	Degree <= 3
Simpson 3/8	(3h/8)[y0 + yn + 3(others) + 2(multiples of 3)]	n multiple of 3	Degree <= 3

- Error order: trapezoidal O(h^2), Simpson 1/3 O(h^4) (composite rules).

➤ Solved example

- ∫ (0 to 1) x^2 dx with h = 0.5. y0 = 0, y1 = 0.25, y2 = 1.
- Trapezoidal = (0.5/2)[0 + 1 + 2(0.25)] = 0.25 x 1.5 = 0.375.
- Simpson 1/3 = (0.5/3)[0 + 1 + 4(0.25)] = (1/6)(2) = 0.3333 (exact = 1/3).

REMEMBER Simpson 1/3 gives the exact answer for cubics too, because its error depends on the 4th derivative.

7. Numerical Solution of ODEs

- Problem: dy/dx = f(x, y), y(x0) = y0, step h.

Method	Formula	Order
Euler	y(n+1) = y(n) + h f(xn, yn)	1
Modified Euler (Heun)	average of slopes at start and predicted end	2
Runge-Kutta 4	y(n+1) = yn + (k1 + 2k2 + 2k3 + k4)/6	4

FORMULA RK4: $k1 = h\,f(x, y)$, $k2 = h\,f(x + h/2, y + k1/2)$, $k3 = h\,f(x + h/2, y + k2/2)$, $k4 = h\,f(x + h, y + k3)$.

- **Taylor series method** and **Picard's method** (successive integration) are also asked.
- **Milne's** and **Adams–Bashforth** are predictor–corrector (multi-step) methods.

➤ Solved example (Euler)

- $dy/dx = x + y$, $y(0) = 1$, $h = 0.1$. Find $y(0.2)$.
- $y1 = 1 + 0.1(0 + 1) = 1.1$.
- $y2 = 1.1 + 0.1(0.1 + 1.1) = 1.1 + 0.12 = 1.22$.
- (Exact $y = 2e^x - x - 1$ gives $y(0.2) = 1.2428$. Euler error is about 0.02.)

TIP In RK4 numericals, write k1, k2, k3, k4 in a small table with 4 decimal places. Most marks are lost by rounding too early.

➤ Solved example (RK4, one step)

- $dy/dx = x + y$, $y(0) = 1$, $h = 0.1$.
- $k1 = 0.1(0 + 1) = 0.1$.
- $k2 = 0.1(0.05 + 1.05) = 0.11$.
- $k3 = 0.1(0.05 + 1.055) = 0.1105$.
- $k4 = 0.1(0.1 + 1.1105) = 0.12105$.
- $y(0.1) = 1 + (0.1 + 0.22 + 0.221 + 0.12105)/6 = 1 + 0.110342 = 1.110342$.
- Exact $2e^{0.1} - 1.1 = 1.110342$. RK4 is correct to 6 decimals here.

8. Curve Fitting and Eigenvalues

➤ Least squares straight line $y = a + bx$

- Choose a and b so that the sum of squared errors $\Sigma (y - a - bx)^2$ is minimum.

FORMULA Normal equations: $\Sigma y = na + b\Sigma x$ and $\Sigma xy = a\Sigma x + b\Sigma x^2$.

Solved example

x	y	xy	x^2
1	2	2	1
2	3	6	4
3	5	15	9
4	6	24	16

- Sums: Σx = 10, Σy = 16, Σxy = 47, Σx^2 = 30, n = 4.
- 16 = 4a + 10b and 47 = 10a + 30b.
- Multiply the first by 2.5: 40 = 10a + 25b. Subtract: 7 = 5b ⇒ b = 1.4. Then 4a = 16 − 14 ⇒ a = 0.5.
- y = 0.5 + 1.4x.
- Parabola y = a + bx + cx^2 needs three normal equations (Σy, Σxy, Σx^2 y).
- Curves like y = a e^(bx) are fitted by taking log: ln y = ln a + bx (a straight line).

Power method (largest eigenvalue)

- Start with a vector X0 (like (1, 1)). Repeat: Y = A Xk, take out the largest entry as λ, Xk+1 = Y / λ.
- λ converges to the eigenvalue of largest absolute value; Xk to its eigenvector.

EXAMPLE A = [2 1; 1 2], X0 = (1, 0). AX0 = (2, 1) = 2(1, 0.5). A(1, 0.5) = (2.5, 2) = 2.5(1, 0.8). A(1, 0.8) = (2.8, 2.6). The values move towards λ = 3 with X = (1, 1).

9. Most Asked Questions (practice)

1. Find a root of x^3 − 2x − 5 = 0 by bisection (4 steps).
2. Find a root of x e^x = 1 by Newton–Raphson correct to 3 decimals.
3. Derive the Newton–Raphson formula and show it has quadratic convergence.
4. Solve a 3 x 3 system by Gauss–Seidel (diagonally dominant).
5. Using Newton forward formula, find y(1.5) from a given table.
6. Fit a polynomial through 4 unequally spaced points by Lagrange's formula.
7. Evaluate ∫ (0 to 1) 1/(1 + x^2) dx by trapezoidal and Simpson 1/3 (h = 0.25). Estimate π.

8. Solve $dy/dx = y - x$, $y(0) = 2$ by RK4 for $x = 0.1$.

9. Compare Euler and modified Euler for $dy/dx = x + y$.

10. Explain truncation and round-off errors with examples.

TIP GATE asks Newton–Raphson iterations, trapezoidal/Simpson values and Euler/RK steps. These are calculator-based, so practise speed and order of convergence facts.