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Paper: Mathematics – IV

UNIT-I

COMBINATORICS: Permutation and Combination, Repetition and Constrained Repetition, Binomial Coefficients, Binomial Theorem.

PROBABILITY: Definition of Probability, Conditional Probability, Baye's Theorem.

UNIT – II

PROBABILITY DISTRIBUTIONS: Review of Mean & Standard Deviation, Mathematical Expectation, Moments, Moment Generating Functions, Binomial, Poisson and Normal Distributions.

UNIT-III

INTERPOLATION: Operators: Shift; Forward Difference, Backward Difference Operators and their Inter-relation, Interpolation Formulae-Newton's Forward, Backward and Divided Difference Formulae: Lagrange's Formula.

SOLUTION OF NON LINEAR EQUATION: Bisection Method, False Position Method, Newton – Raphson Method for Solving Equation Involving One Variable only.

UNIT – IV

SOLUTION OF LINEAR SIMULTANEOUS EQUATIONS: Gaussian Elimination Method with and without Row Interchange: LU Decomposition: Gauss - Jacobi and Gauss-Seidel Method; Gauss – Jordan Method and to find Inverse of a Matrix by this Method.

NUMERICAL DIFFERENTIATION- First and Second Order Derivatives at Tabular and Non-Tabular Points, Numerical Integration, Trapezoidal Rule, Simpsons 1/3 Rule: Error in Each Formula (without proof).

UNIT -1

COMBINATORICS

Permutation and Combination

INTRODUCTION

Permutation and combination has lately emerged as an important topic for many entrance examinations. This is primary because questions from the topic require analytical skill and a logical bend of mind. Even students who do not have mathematics as a subject can handle them if they have a fairly good understanding of the concepts and their application. Hence anyone who is well-versed in different methods of counting and basic calculations will be able to solve these problems easily

IMPORTANT NOTATION

$n!$ (Read as n factorial)

Product of first n positive integers is called n factorial

$n! = 1 \times 2 \times 3 \times 4 \times 5 \times \ldots n$

$n! = (n - 1)!\ n \in N$

In special case $0! = 1$

MEANING OF PERMUTATION AND COMBINATION

Permutation

The arrangement made by taking some or all elements out of a number of things is called a permutation.

The number of permutations of n things taking r at a time is denoted by ${}^nP_r$ and it is defined as under:

$${}^n p_r = \lfloor n / \lfloor (n-r)$$

Combination

The group or selection made by taking some or all elements out of a number of things is called a combination.

The number of combinations of n things taking r at a time is denoted by ${}^nC_r$ or and it is defined as under:

$${}^nC_r = \lfloor n / \lfloor r \lfloor\ (n - r)$$

Here $n!$ = Multiple of n natural number

Some Important Results of Permutations

1. ${}^{n}P_{n-1} = {}^{n}P_{n}$
2. ${}^{n}P_{n} = n!$
3. ${}^{n}P_{r} = n\,({}^{n-1}P_{r-1})$
4. ${}^{n}P_{r} = (n - r + 1) \times {}^{n}P_{r-1}$
5. ${}^{n}P_{r} = {}^{n-1}P_{r} + r\,({}^{n-1}P_{r-1})$

Types of Permutations

When in a permutation of n things taken r at a time, a particular thing always occurs, then the required number of permutations = $r\,({}^{n-1}P_{r-1})$.

Q. If ${}^{n}C_{10} = {}^{n}C_{14}$ then find the value of n

Solution

${}^{n}C_{10} = {}^{n}C_{14} \Rightarrow n = (10 + 14) = 24 \quad (\because n = p + q)$

Permutations with Repetition

These are the easiest to calculate.

When you have ***n*** things to choose from ... you have ***n*** choices each time!

When choosing ***r*** of them, the permutations are:

n × n × ... *(r times)*

(In other words, there are **n** possibilities for the first choice, AND THEN there are **n** possibilities for the second choice, and so on, multiplying each time.)

Which is easier to write down using an exponent of **r**?

n × n × ... (r times) = n^r

Example: in the lock above, there are 10 numbers to choose from (0,1,..9) and you choose 3 of them:

10 × 10 × ... (3 times) = 10^3 = 1,000 permutations

Permutations without Repetition

In this case, you have to **reduce** the number of available choices each time.

For example, what order could 16 pool balls be in?

After choosing, say, number "14" you can't choose it again.

So, your first choice would have 16 possibilities, and your next choice would then have 15 possibilities, then 14, 13, etc. And the total permutations would be:

$$16 \times 15 \times 14 \times 13 \times \ldots = 20{,}922{,}789{,}888{,}000$$

But maybe you don't want to choose them all, just 3 of them, so that would be only:

$$16 \times 15 \times 14 = 3{,}360$$

In other words, there are 3,360 different ways that 3 pool balls could be selected out of 16 balls.

But how do we write that mathematically? Answer: we use the "factorial function"

The **factorial function** (symbol :!) just means to multiply a series of descending natural numbers. Examples:

- $4! = 4 \times 3 \times 2 \times 1 = 24$
- $7! = 7 \times 6 \times 5 \times 4 \times 3 \times 2 \times 1 = 5{,}040$
- $1! = 1$

There are also two types of combinations (remember the order does **not** matter now):

1. **Repetition is Allowed**: such as coins in your pocket (5,5,5,10,10)
2. **No Repetition**: such as lottery numbers (2,14,15,27,30,33)

1. Combinations with Repetition

Actually, these are the hardest to explain, so I will come back to this later.

2. Combinations without Repetition

This is how lotteries work. The numbers are drawn one at a time, and if you have the lucky numbers (no matter what order) you win!

The easiest way to explain it is to:

- assume that the order does matter (i.e. permutations),

- then alter it so the order does **not** matter.

Going back to our pool ball example, let us say that you just want to know which 3 pool balls were chosen, not the order.

We already know that 3 out of 16 gave us 3,360 permutations.

But many of those will be the same to us now, because we don't care what order!

For example, let us say balls 1, 2 and 3 were chosen. These are the possibilities:

Order does matter	Order doesn't matter
1 2 3	1 2 3
1 3 2	
2 1 3	
2 3 1	
3 1 2	
3 2 1	

So, the permutations will have 6 times as many possibilities.

In fact there is an easy way to work out how many ways "1 2 3" could be placed in order, and we have already talked about it. The answer is:

$$\mathbf{3! = 3 \times 2 \times 1 = 6}$$

(Another example: 4 things can be placed in $\mathbf{4! = 4 \times 3 \times 2 \times 1 = 24}$ different ways, try it for yourself!)

So, all we need to do is adjust our permutations formula to **reduce it** by how many ways the objects could be in order (because we aren't interested in the order any more):

$$\frac{n!}{(n-r)!} \times \frac{1}{r!} = \frac{n!}{r!(n-r)!}$$

That formula is so important it is often just written in big parentheses like this:

$$\frac{n!}{r!(n-r)!} = \binom{n}{r}$$

where ***n*** is the number of things to choose from, and you choose ***r*** of them

(No repetition, order doesn't matter)

It is often called "n choose r" (such as "16 choose 3")

And is also known as the "Binomial Coefficient"

Notation

As well as the "big parentheses", people also use these notations:

$$C(n,r) = {}^nC_r = {}_nC_r = \binom{n}{r} = \frac{n!}{r!(n-r)!}$$

Example

So, our pool ball example (now without order) is:

$$\frac{16!}{3!(16-3)!} = \frac{16!}{3!\times 13!} = \frac{20{,}922{,}789{,}888{,}000}{6\times 6{,}227{,}020{,}800} = 560$$

Or you could do it this way:

$$\frac{16\times 15\times 14}{3\times 2\times 1} = \frac{3360}{6} = 560$$

It is interesting to also note how this formula is nice and **symmetrical**:

$$\frac{n!}{r!(n-r)!} = \binom{n}{r} = \binom{n}{n-r}$$

In other words choosing 3 balls out of 16, or choosing 13 balls out of 16 have the same number of combinations.

$$\frac{16!}{3!\,(16-3)!} = \frac{16!}{13!\,(16-13)!} = \frac{16!}{3!\times 13!} = 560$$

Pascal's Triangle

You can also use Pascal's Triangle to find the values. Go down to row "n" (the top row is 0), and then along "r" places and the value there is your answer. Here is an extract showing row 16:

```
          1     14     91     364   ...
       1     15     105    455    1365   ...
  1     16    120    560    1820   4368   ...
```

1. Combinations with Repetition

OK, now we can tackle this one ...

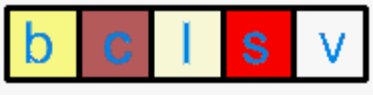
Let us say there are five flavors of ice-cream: **banana, chocolate, lemon, strawberry and vanilla**. You can have three scoops. How many variations will there be?

Let's use letters for the flavors: {b, c, l, s, v}. Example selections would be

- {c, c, c} (3 scoops of chocolate)
- {b, l, v} (one each of banana, lemon and vanilla)
- {b, v, v} (one of banana, two of vanilla)

(And just to be clear: There are **n=5** things to choose from and you choose **r=3** of them.
Order does not matter, and you **can** repeat!)

Now, I can't describe directly to you how to calculate this, but I can show you a **special technique** that lets you work it out.



Think about the ice cream being in boxes, you could say "move past the first box, then take 3 scoops, then move along 3 more boxes to the end" and you will have 3 scoops of chocolate!

So, it is like you are ordering a robot to get your ice cream, but it doesn't change anything, you still get what you want.

Now you could write this down as →○○○→→→(arrow means **move**, circle means **scoop**).

In fact the three examples above would be written like this:

{c, c, c} (3 scoops of chocolate): →○○○→→→

{b, l, v} (one each of banana, lemon and vanilla): ○→→○→→○

{b, v, v} (one of banana, two of vanilla): ○→→→→○○

OK, so instead of worrying about different flavors, we have a ***simpler*** problem to solve: "how many different ways can you arrange arrows and circles"

Notice that there are always 3 circles (3 scoops of ice cream) and 4 arrows (you need to move 4 times to go from the 1st to 5th container).

So (being general here) there are ***r*** + ***(n-1)*** positions, and we want to choose ***r*** of them to have circles.

This is like saying "we have ***r*** + ***(n-1)*** pool balls and want to choose ***r*** of them". In other words it is now like the pool balls problem, but with slightly changed numbers. And you would write it like this:

$$\binom{n+r-1}{r} = \frac{(n+r-1)!}{r!(n-1)!}$$

where ***n*** is the number of things to choose from, and you choose ***r*** of them
(Repetition allowed, order doesn't matter)

Interestingly, we could have looked at the arrows instead of the circles, and we would have then been saying "we have ***r*** + ***(n-1)*** positions and want to choose ***(n-1)*** of them to have arrows", and the answer would be the same...

$$\binom{n+r-1}{r} = \binom{n+r-1}{n-1} = \frac{(n+r-1)!}{r!(n-1)!}$$

So, what about our example, what is the answer?

$$\frac{(5+3-1)!}{3!\,(5-1)!} = \frac{7!}{3!\times 4!} = \frac{5040}{6\times 24} = 35$$

In Conclusion

Phew, that was a lot to absorb, so maybe you could read it again to be sure!

But knowing *how* these formulas work is only half the battle. Figuring out how to interpret a real world situation can be quite hard.

But at least now you know how to calculate all 4 variations of "Order does/does not matter" and "Repeats are/are not allowed".

BINOMIAL THEOREM

For any positive integral value

$(x + a) = nc_0x^n + nc_xx^{n-1}a + nc_2x^n - {}^2a^2 + \ldots + {}_na^n$

Proof

We can prove this theorem by using principle of mathematical Induction. First we shall verify the theorem for $n = 1$

$\therefore$ The result is true for some positive integral value of k or n.

$\therefore (x + a)^k = kc_0x^k + kc_1x^{k-1}a + kc_2x^{k-2}a^2 + \ldots + kc_ka^k$

Now multiplying both sides by x and a and adding the two results

$x\,(x + a)^k = kc_0x^{k+1} + kc_1xa + kc_2x^{k-1}a^2 + \ldots + kc_k\,xa^k$

and

$a(x + a)^k = kc_0x^ka + kc_1x^{k-1}a^2 + kc_2x^{k-2}a^3 + \ldots + kc_kxa^{k+1}$

$\therefore (x + a)^{k+1} = kc_0x^{k+1} + (kc_1 + kc_0)x^ka + (kc_2 + kc_1)x^{k-1}\,a^2 +$

$(kc_3 + kc_2)x^{k-2}a^3 + \ldots + kc_ka^{k+1}$

By using ${}^nc_r + {}^nc_{r-1} = {}^{n+1}c_r$ we can say that

$(x + a)^{k+1} = {}^kc_0x^{k+1} + {}^{(k+1)}c_1x^ka + {}^{(k+2)}c_2x^{k-1}a^2 + \ldots + {}^kc_ka^{k+1}$

GENERAL TERM OF BINOMIAL EXPANSION

We have derived binomial expansion as

$(x + a)^n = {}^nc_0x^n + {}^ac_1x^{n-1}a + {}^nc_2x^{n-2}a^2 + \ldots {}^nc_na^n$

Here $T_1 = {}^nc_0x^n$

$T_2 = {}^nc_2x^{n-1}a$

$T_3 = {}^nc_2x^{n-2}a^2$

∴ The $(r + 1)$ th term of the binomial expansion can be written as follows: $T_{r+1} = {}^nc_rx^{n-r}a^r$

The (r + 1) th term of binomial expansion is called the general term of expansion.

Probability:-

Probability is the likely percentage of times an event is *expected* to occur if the experiment is repeated for a large number of trials. The probability of rare event is close to zero percent and that of common event is close to 100%. Contrary to popular belief, it is not intended to accurately describe a single event, although people may often use it as such. For example, we all know that the probability of seeing the head side of a coin, if you were to randomly flip it, is 50%. However, many people misinterpret this as 1 in 2 times, 2 in 4 times, 5 in 10 times, etc

Conditional Probability

Conditional probability is the probability of one event occuring, given that another event occurs. The following expression describes the conditional probability of event A given that event B has occurred:

$$P(A|B)$$

If the events A and B are dependent events, then the following expression can be used to describe the conditional probability of the events:

$$P(A \mid B) = \frac{P(A, B)}{P(B)}.$$

$$P(B \mid A) = \frac{P(A, B)}{P(A)}.$$

This can be rearranged to give their joint probability relationship:

$$P(A, B) = P(B|A) * P(A) = P(A|B) * P(B)$$

This states that the probability of events A and B occurring is equal to the probability of B occurring given that A has occurred multiplied by the probability that A has occurred. A graphical representation of conditional probability is shown below:

Bayes' Theorem

Most probability problems are not presented with the probability of an event "A," it is most often helpful to condition on an event A"." At other times, if we are given a desired outcome of an event, and we have several paths to reach that desired outcome, Baye's Theorem will demonstrate the different probabilities of the pathes reaching the desired outcome. Knowing each probability to reach the desired outcome allows us to pick the best path to follow. Thus, Baye's Theorem is most useful in a scenario of which when given a desired outcome, we can condition on the outcome to give us the separate probabilities of each condition that lead to the desired outcome.

Derivation of Baye's Theorem: - The derivation of Baye's theorem is done using the third law of probability theory and the law of total probability.

Suppose there exists a series of events: $B_1, B_2, ..., B_n$ and they are mutually exclusive; that is,

This means that only one event, B_j, can occur. Taking an event "A" from the same sample space as the series of B_i, we have:

Using the fact that the events AB_i are mutually exclusive and using the third law of probability theory:

$$P(A) = \sum_j P(AB_j)$$

Conditioning on the above probability, the result below is also called "the law of total probability"

$$P(A) = \sum_j P(A \mid B_j)P(B_j)$$

UNIT-II

PROBABILITY DISTRIBUTIONS

In any probabilistic situation each strategy (course of action) may lead to a number of different possible outcomes. For example, a product whose sale is estimated around 100 units, may be equal to 100, less, or more. Here the sale (i.e., an outcome) of the product is measured in real numbers but the volume of the

sales is uncertain. The volume of sale which is an uncertain quantity and whose definite value is determined by chance is termed as *random (chance* or *stochastic) variable.* A listing of all the possible outcomes of a random variable with each outcome's associated probability of occurrence is called *probability distribution*. The numerical value of a random variable depends upon the outcome of an experiment and may be different for different trials of the same experiment. The set of all such values so obtained is called the *range space* of the random variable.

EXPECTED VALUE AND VARIANCE OF A RANDOM VARIABLE

Expected Value The mean (also referred as **expected value) of a random variable** is a typical value used to summarize a probability distribution. It is the weighted average, where the possible values of random variable are weighted by the corresponding probabilities of occurrence. If x is a random variable with possible values x_1, x_2,…, x_n occurring with probabilities P(x_1), P(x_2),…, $P(x_n)$, then the expected value of x denoted by E(x) or μ is the sum of the values of the random variable weighted by the probability that the random variable takes on that value.

Similarly, for the continuous random variable, the expected value is given by:

where $f(x)$ is the probability distribution function.

Binomial Probability Distribution

Binomial probability distribution is a widely used probability distribution for a discrete random variable. This distribution describes discrete data resulting from an experiment called a *Bernoulli process* (named after Jacob Bernoulli, 1654–1705, the first of the Bernoulli family of Swiss mathematicians). For each trial of an experiment, *there are only two possible complementary* (*mutually exclusive*) outcomes such as, defective or good, head or tail, zero or one, boy or girl. In such cases the outcome of interest is referred to as a '*success*' and the other as a '*failure*'. The term 'binomial' literally means two names.

> ***Bernoulli process:*** *It is a process wherein an experiment is performed repeatedly, yielding either a success or a failure in each trial and where there is absolutely no pattern in the occurrence of successes and failures. That is, the occurrence of a success or a failure in a particular trial does not affect, and is not affected by, the outcomes in any previous or subsequent trials. The trials are independent.*

Poisson Probability Distribution

Poisson distribution is named after the French mathematician S. Poisson (1781–1840), The Poisson process measures the number of occurrences of a particular outcome of a discrete random variable in a *predetermined time interval, space, or volume*, for which an *average number* of occurrences of the outcome is known or can be determined. In the Poisson process, the random variable values need counting. Such a count might be (i) number of telephone calls per hour coming into the switchboard, (ii) number of fatal traffic accidents per week in a city/state, (iii) number of patients arriving at a health centre every hour, (iv) number of organisms per unit volume of some fluid, (v) number of cars waiting for service in a workshop, (vi) number of flaws per unit length of some wire, and so on. The Poisson probability distribution provides a simple, easy-to compute and accurate approximation to a binomial distribution when the probability of success, p is very small and n is large, so that $\mu = np$ is small, preferably $np > 7$. It is often called the *'law of improbable'* events meaning that the probability, p, of a particular event's happening is very small. As mentioned above **Poisson distribution** occurs in business situations in which there are a few successes against a large number of failures or vice-versa (i.e. few successes in an interval) and has single independent events that are mutually exclusive. Because of this, the probability of success, p is very small in relation to the number of trials n, so we consider only the probability of success.

Variance and Standard Deviation

Another way to disregard the signs of negative deviations from mean is to square them. Instead of computing the absolute value of each deviation from mean, we square the deviations from mean. Then the sum of all such squared deviations is divided by the number of observations in the data set. This value is a measure called **population variance** and is denoted by $\boldsymbol{\sigma}^2$ (a lower-case Greek letter sigma). It is usually referred to as 'sigma squared'. Symbolically, it is written as:

Population variance,

where $d = x - A$ and A is any constant (also called assumed A.M.)

Since $\boldsymbol{\sigma}^2$ is the average or mean of squared deviations from arithmetic mean, it is also called the *mean square average.*

The population variance is basically used to measure variation among the values of observations in a population. Thus for a population of N observations (elements) and with μ, denoting the population mean, the formula for population variance . However, in almost all applications of statistics, the data being analyzed is a sample data. As a result, population variance is rarely determined. Instead, we compute a sample variance to estimate population variance, $\boldsymbol{\sigma}^2$.

Normal Probability Distribution Function

The formula that generates normal probability distribution is as follows:

where π = constant 3.1416

e = constant 2.7183

μ = mean of the normal distribution

σ = standard of normal distribution

The $f(x)$ values represent the relative frequencies (height of the curve) within which values of random variable x occur. The graph of a normal probability distribution with mean μ, and standard deviation σ is shown in Fig. 8.8. The distribution is symmetric about its mean μ, that locates at the centre.

Since the total area under the normal probability distribution is equal to 1, the symmetry implies that the area on either side of μ, is 50 per cent or 0.5. The *shape* of the distribution is determined by μ, and σ values.

UNIT-III

INTERPOLATION

Suppose that a function is defined by a table of values (x_r, y_r), $(r = 0, 1, 2, \ldots, n)$ or is tabulated for a number of equidistant values of the argument; for example, the tabulated values of logarithmic function or trigonometric function. We may have to estimate the value of the function at a point not coinciding with the given points. The process of estimating the value of y for an x belonging to the range $[x_0, x_n]$ is known as *interpolation*.

Here the points $x_0, x_1, \ldots, x_n$ are called the interpolation points .

The process of estimating the value of y for an x outside the range $[x_0, x_n]$ is known as *extrapolation.* Interpolation is to construct a new function $F(x)$ which coincides with the known function $f(x)$ at the tabulated $(n + 1)$ interpolation points.

INTERPOLATION FORMULAS FOR EQUAL INTERVALS

4.5.1 Newton[1]–Gregory[2] Forward Interpolation Formula

Let the values of $y_r = f(x_r)$ be given for equally spaced values of the independent variable

$$x_r = x_0 + rh,\ r = 0, 1, 2, \ldots, n$$

Suppose that the nth degree interpolating polynomial is

$$\phi(x) = a_0 + a_1 (x - x_0) + a_2 (x - x_0)(x - x_1) + \ldots + a_n (x - x_0) (x - x_1) (x - x_{n-1}) (
$$

Since the curve $y = \phi(x)$ passes through the points $[x_r, y_r]$, $r = 0 \ldots n$, we get the following equations for determining the constants $a_0, a_1, \ldots, a_n$.

Generally

Substituting these values of a_r in we get the Newton–Gregory forward interpolation formula

Putting $x = x_0 + ph$, $y(x_0) = y_0$ formula can be put in a simpler form as

INTERPOLATION WITH UNEQUAL INTERVALS

So far we have considered interpolation formulas for equally spaced values of x. We now develop two interpolation formulas for unequally spaced values of x.

Divided Differences

Suppose that the function y_x is given for values $x = a, b, c, d, \ldots$ where the intervals $b - a, c - b, d - c$ are not necessarily equal. We define the divided difference of y_a at b by

Linearity Property

The divided difference operator Δ' is linear (a) $\Delta'[f(x) + g(x)] = \Delta'f(x) + \Delta'g(x)$; (b) $\Delta'[cf(x)] = c\Delta'[f(x)]$.

Symmetrical Property

The divided differences are symmetrical in the symbols.

Vanishing of (n + 1) Divided Differences

If $y = y(x)$ is an nth degree polynomial then its nth order divided difference $\Delta'^n y_x$ is constant and higher order divided differences vanish.

Theorem If y_x is a polynomial of degree n then $\Delta'^n y_x$ is constant.

Proof

a polynomial of degree $(n - 1)$.

Now Δ' is a linear operator. Hence it follows that the first divided difference of $y_x = a_0 + a_1x + \ldots a_nx^n$ is a polynomial of degree $(n - 1)$; the second divided difference is a polynomial of degree $(n - 2)$; the nth divided difference is constant, and all higher divided differences are zero.

Newton's Divided Difference Formula

Consider the function y_x for the arguments $x, a, b, c, d \ldots j, k$. Then

We continue this process until nth differences are reached. Assuming that y_x is represented by an nth degree polynomial, all higher differences vanish and we have Newton's divided difference formula:
where there are $(n + 1)$ arguments $a, b, c, \ldots, k$ and $A = (x - a), B = (x - b), C = (x - c), \ldots, K = (x - k)$.

Corollary If the arguments $a, b, c, \ldots$ are taken as 0, 1, 2, … then and we obtain from equation

LAGRANGE'S INTERPOLATION FORMULA

In the inverse interpolation for a given value of y, the corresponding value of x is to be found. Interchanging the roles of x and $y = f(x)$ in Lagrange's interpolation formula we get Lagrange's inverse interpolation formula as

Newton's divided differences formula is

$$y = f(x) = f(x_0) + (x - x_0)\,[x_0, x_1] + (x - x_0)\,(x - x_1) \cdot [x_0, x_1, x_2] + (x - x_0)\,(x - x_1)\,(x - x_2) \cdot [x_0, x_1, x_2] + \cdots = 48 + 52\,(x - 4) + 15(x - 4)\,(x - 5) + 1(x - 4)\,(x - 5)\,(x - 7) = x^2(x - 1)$$

$$\therefore f(2) = 2^2\,(2 - 1) = 4$$

$$f(8) = 8^2\,(8 - 1) = 448$$

CONVERGENCE OF REGULA–FALSI METHOD

Let ξ be the actual root of the equation $f(x) = 0$. Thus, $f(\xi) = 0$. Let $x_n = \xi + \varepsilon_n$, where ε_n is the error involved at the nth step while determining the root.

NEWTON–RAPHSON METHOD

If the derivative of a function f can be easily found and is a simple expression, then the real roots of the equation $f(x) = 0$ can be computed rapidly by Newton–Raphson method.

Let x_0 denote the approximate value of the desired root and let h be the correction which must be applied to x_0 to give the exact value of the root x. Thus, $x = x_0 + h$ and so the equation $f(x) = 0$ reduces to $f(x = x_0 + h) = 0$. Expanding by Taylor's Theorem, we have

Hence,

If h is relatively small, we may neglect the term containing h^2 and have

$$f(x_0) + hf'(x_0) = 0.$$

SQUARE ROOT OF A NUMBER USING NEWTON–RAPHSON METHOD

Suppose that we want to find the square root of N. Let

We have

$$f(x) = x^2 - N = 0.$$

Then, Newton–Raphson method yields

For example, if $N = 10$, taking $x_0 = 3$ as an initial approximation, the successive approximations are

$$x_1 = 3.166666667, x_2 = 3.162280702,$$
$$x_3 = 3.162277660, x_4 = 3.162277660$$

correct up to nine decimal places.

However, if we take $f(x) = x^3 - Nx$ so that if $f(x) = 0$ then Now $f'(x) = 3x^2 - N$ and so the Newton–Raphson method gives

Taking $x_0 = 3$, the successive approximations to are

$$x_1 = 3.176, x_2 = 3.1623, x_3 = 3.16227, x_4 = 3.16227$$

correct up to five decimal places.

Suppose that we want to find the pth root of N. Then consider $f(x) = x^p - N$ The Newton–Raphson formula yields

UNIT -IV

Linear Systems of Equations. Gauss Elimination

We now come to one of the most important use of matrices, that is, using matrices to solve systems of linear equations. We showed informally of how to represent the information contained in a system of linear equations by a matrix, called the augmented matrix. This matrix will then be used in solving the linear system of equations. Our approach to solving linear systems is called the Gauss elimination method. Since this method is so fundamental to linear algebra, the student should be alert.

A shorter term for systems of linear equations is just **linear systems**. Linear systems model many applications in engineering, economics, statistics, and many other areas. Electrical networks, traffic flow, and commodity markets may serve as specific examples of applications.

Inverse of a Matrix. Gauss–Jordan Elimination

In this section we consider* square *matrices exclusively.

The **inverse** of an $n \times n$ matrix $\mathbf{A} = [a_{jk}]$ is denoted by $\mathbf{A}^{-1}$ and is an $n \times n$ matrix such that

where **I** is the $n \times n$ unit matrix

If **A** has an inverse, then **A** is called a **nonsingular matrix**. If **A** has no inverse, then **A** is called a **singular matrix**.

If **A** *has an inverse, the inverse is unique.*

Indeed, if both **B** and **C** are inverses of **A**, then $\mathbf{AB} = \mathbf{I}$ and $\mathbf{CA} = \mathbf{I}$, so that we obtain the uniqueness from

We prove next that **A** has an inverse (is nonsingular) if and only if it has maximum possible rank n. The proof will also show that $\mathbf{Ax} = \mathbf{b}$ implies $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$ provided $\mathbf{A}^{-1}$ exists, and will thus give a motivation for the inverse as well as a relation to linear systems. (But this will ***not*** give a good method of solving $\mathbf{Ax} = \mathbf{b}$ ***numerically*** because the Gauss elimination requires fewer computations.)

NUMERICAL DIFFERENTIATION

INTRODUCTION

Situations arise frequently when the conventional calculus methods of differentiation and integration cannot be applied to a function, for instance,

1. when we do not know the exact function but know only values of it at a set of discrete points; and
2. when the function is known but is too complicated to apply the conventional methods of calculus.

In such cases we apply numerical methods. The method of finding the derivative dy/dx / integral of a function $y = f(x)$ using numerical techniques is called numerical differentiation /numerical integration.

6.1.1 Numerical Differentiation

Numerical differentiation is a process of computing the derivative of a function at some assigned value of x from a given set of data

$(x_i\ f_i)\ f_i = f(x_i)\ (i = 0, 1, 2, \ldots, n)$

MAXIMUM AND MINIMUM VALUES OF A TABULATED FUNCTION

We know that maximum and minimum values of a function are found by equating the first derivative to zero and solving for the variable. We can apply this procedure to a tabulated function as well.

Differentiating Newton's Forward interpolation formula

we have neglecting higher-order terms.

For an extreme value of y, we must have $dy/dp = 0$. This yields the quadratic in p:

$$a_0 + a_1 p + a_2 p^2 = 0$$

with The values of x are found from $x = x_0 + ph$.

NUMERICAL INTEGRATION: INTRODUCTION

We can find the integral of a function $y = f(x)$ defined and continuous on an interval $[a, b]$if there exists a

function $F(x)$ such that $F'(x) = f(x)$. According to the Fundamental Theorem of Integral Calculus we

Geometrically, it represents the area under the curve $y = f(x)$ and between the ordinates $x = a$ and $x = b$.

In applications, evaluation of the integral may prove to be very complicated and not practical:

1. when we cannot find the anti derivative $F(x)$ of $f(x)$ and
2. when the integrand $f(x)$ is a tabulated function.

In such cases we have to resort to numerical evaluation which is also called mechanical quadrature. The basic idea is to replace $f(x)$ by an interpolating polynomial $\phi(x)$ using a suitable interpolation formula. We derive a general formula for numerical integration using Newton's Forward difference formula.

INTRODUCTION

Many engineering and scientific problems are modelled as differential equations. Forming differential equation, finding its solution and interpreting the results obtained are of utmost importance for engineers and scientists. Exact solutions of differential equations can be found only in a limited number of cases. Hence, there is need for numerical solution. Even in cases where closed-form solutions are possible to assess and analyse them we have to compute. Instead, we could solve the differential equation itself numerically and have a better understanding of the solution, especially now with the availability of high-speed digital computers.

Ordinary Differential Equation

An equation of the form

$F(x, y, y', y'', \ldots, y^{(n)}) = 0 \quad (7.1)$

Simpson's Method

In order to find $y(x_n)$ where $x_n = x_0 + nh$ by Milne's method we proceed in the following way.

Since the value $y_0 = y(x_0)$ is given to us, we compute $y_1 = y(x_1) = y(x_0 + h)$, $y_2 = y(x_2) = y(x_0 + 2h)$, $y_3 = y(x_3) = y(x_0 + 3h)$ by Picard's or Taylor's method. Next we calculate

To evaluate: $\int_{x_0}^{x_n} f(x)dx$

1. Divide $[x_o, x_n]$ into n segments ($n \geq 1$)

2. Within each segment approximate $f(x)$ by an m^{th} order polynomial,

$$p_m(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_m x^m$$

The polynomial order need not be the same for all segments. Then:

$$\int_{x_0}^{x_n} f(x)dx = \int_{x_0}^{x_1} p_{m_1}(x)dx + \int_{x_0}^{x_2} p_{m_2}(x)dx + \ldots + \int_{x_0}^{x_n} p_{m_n}(x)dx$$

the m_i's may be the same or different. Integrate each polynomial exactly.

Order m of polynomial $p_m(x)$ determines Newton-Cotes formulas:

m	Polynomial	Formula	Error
1	linear	Trapezoid	$O(h^2)$
2	quadratic	Simpson's 1/3	$O(h^4)$
3	cubic	Simpson's 3/8	$O(h^4)$
4	quartic	Boole's Rule	$O(h^6)$
5	quintic	Boole's Rule	$O(h^6)$

Trapezoid Rule

For each segment (or one segment), let $f(x) \approx p_1(x) = a_0 + a_1 x$

a. Determine $a_0 + a_1 x$ from Newton DD Polynomial:

$$p_1(x) = f(x_{i-1}) + \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}(x - x_{i-1})$$

b. Integrating [use trapezoid area formula, C&C 4th ed., Box 21.1]:

$$\int_{x_{i-1}}^{x_i} p_1(x)dx = (x_i - x_{i-1})\frac{f(x_i) + f(x_{i-1})}{2}$$

c. Truncation Error [C&C 4th ed., Box 21.2]:

$$\int_{x_{i-1}}^{x_i} f(x)dx = (x_i - x_{i-1})\frac{f(x_i) + f(x_{i-1})}{2} - \frac{1}{12}(x_i - x_{i-1})^3 f''(\xi)$$

Integrates a linear function correctly: $f''(\xi) = 0$.

Easily derived by considering Taylor Series.

Composite Trapezoid Rule

For multiple segments, sum segment areas to approximate integral:

$$I = \int_{x_0}^{x_n} f(x)dx = \sum_{i=1}^{n}\left[(x_i - x_{i-1})\frac{f(x_i)+f(x_{i-1})}{2} + E_{ti}\right]$$

where E_{ti} is truncation error in i^{th} interval.

If data are evenly spaced, i.e., $x_i - x_{i-1} = \frac{x_n - x_0}{n} = h$ for i=1,...,n

$$I \approx (x_n - x_0)\frac{f(x_0) + \left(2\sum_{i=1}^{n-1} f(x_i)\right) + f(x_n)}{2n}$$

or: $$I \approx h\left[\frac{1}{2}f(x_0) + \sum_{i=1}^{n-1} f(x_i) + \frac{1}{2}f(x_n)\right]$$

It can be shown that $\sum_{i=1}^{n} f''(\xi_i) \approx n\bar{f}''(\xi)$ so the error is

$$E_t = -\frac{nh^3}{12}\bar{f}'' = -\frac{(x_n - x_0)h^2}{12}\bar{f}''$$

Note: If n is doubled, h➔ h/2 and E_t ➔ $E_a/4$

NOTE: C&C notation is different

h = $(x_n-x_0)/n$ ==> (b-a)/n and $E_t = -\frac{nh^3}{12}\overline{f''} = -\frac{(b-a)^3}{12n^2}\overline{f''}$

Simpson 1/3 Rule

Improving the estimate of the integral

- fit Lagrange polynomials to **three** points (a pair of segments)
- integrate those polynomials to obtain a general formula for integrals.
- the resulting function must correctly integrate **quadratic** polynomials.

Evaluate $\int_{x_0}^{x_n} f(x)dx \approx \int_{x_0}^{x_n} p_2(x)dx$

For each pair of segments use Lagrange Interpolating Polynomial:

$$p_2(x) = \frac{(x-x_i)(x-x_{i+1})}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})} f(x_{i-1}) + \frac{(x-x_{i-1})(x-x_{i+1})}{(x_i-x_{i-1})(x_i-x_{i+1})} f(x_i) + \frac{(x-x_{i-1})(x-x_i)}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)} f(x_{i+1})$$

If points are *evenly spaced*, integrating yields:

$$\int_{x_{i-1}}^{x_{i+1}} f(x)dx = (x_{i+1}-x_{i-1})\frac{f(x_{i-1})+4f(x_i)+f(x_{i+1})}{6} = h\frac{f(x_{i-1})+4f(x_i)+f(x_{i+1})}{3}$$

Simpson's 1/3 Rule – Alternative derivation

Choose weights in $\omega_0 f(-1) + \omega_1 f(0) + \omega_2 f(1)$ so that over $[-1, +1]$:

a. $$\int_{-1}^{+1} 1\,dx = 2 = \omega_0(1) + \omega_1(1) + \omega_2(1)$$

$$\int_{-1}^{+1} x\,dx = 0 = \omega_0(-1) + \omega_1(0) + \omega_2(+1)$$

$$\int_{-1}^{+1} x^2\,dx = \frac{2}{3} = \omega_0(-1)^2 + \omega_1(0) + \omega_2(+1)^2$$

from 2nd equation: $\omega_0 = \omega_2$; from 3rd: $\omega_0 + \omega_2 = 2/3$;

hence $\omega_0 = \omega_2 = 1/3$ and from 1st equation $\omega_1 = 4/3$

b. General formula for evenly spaced points (note interval above had width of 2):

$$\int_{x_{i-1}}^{x_{i+1}} p_2(x)dx = (x_{i+1} - x_{i-1})\frac{f(x_{i-1}) + 4f(x_i) + f(x_{i+1})}{6}$$

c. Error: $\int_{x_{i-1}}^{x_{i+1}} f(x)\,dx = \int_{x_{i-1}}^{x_{i+1}} p_2(x)\,dx - \frac{1}{180}(x_2 - x_0)\ h^4\ f^{(4)}(\xi)$

➔ Integrates a cubic exactly: $f^{(4)}(\xi) = 0$.

Because $(x_2 - x_0) = 2h$, the error term becomes (C&C 4th ed., Table 21.2, p. 604):

$$-\frac{1}{90}h^5 f^{(4)}(\xi) = -\frac{(x_{i+1} - x_{i-1})^5}{2880} f^{(4)}(\xi)$$

Derivation of Simpson 1/3 Rule error term

Let: x = -h, 0, +h

$$I = \int_{-h}^{h} f(x)dx = \int (f_o + xf_o' + \frac{x^2}{2!} f_o'' + \ldots)\,dx$$

$$= 2hf_o + \frac{2h^3}{6} f_o'' + \frac{2h^5}{5!} f_o^{[4]} + \ldots \text{ (only odd powers of h survive)}$$

$$S = \frac{h}{3}\left[f(-h) + 4f(0) + f(+h)\right] = \frac{h}{3}\left[6f_o + 0 + \frac{2h^2}{2} f_o'' + 0 + \frac{2h^4}{4!} f_o^{[4]} + \ldots\right]$$

$$= 2hf_0 + \frac{2h^3}{6} f_0'' + \frac{2h^5}{3(4!)} f^{[4]} + \cdots$$

Both have only odd terms. I - S = Truncation Error:

$$= -\frac{(2h)h^4}{180} f^{[4]} + 2h\ 0(h^6) = -\frac{1}{90}h^5 f^{(4)}(\xi)$$

Composite Simpson 1/3 Rule

Sum pairs of segment areas to approximate the given integral:

$$I = \int_{x_0}^{x_n} f(x)dx = \sum_{i=1,3,5}^{n-1} \left((x_{i+1} - x_{i-1}) \frac{f(x_{i-1}) + 4f(x_i) + f(x_{i+1})}{6} + E_{ti} \right)$$

If all data are *evenly spaced*, i.e., $x_i - x_{i-1} = h$ for i=1,...,n:

$$I \approx \frac{h}{3}\left[f(x_0) + 4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n) \right]$$

It can also be shown that $\sum_{i=1}^{n} f^{(4)}(\xi_i) \approx n\overline{f^{(4)}}$ so:

$$E_t = -\frac{nh^5}{180}\overline{f^{(4)}} = -\frac{(x_n - x_0)h^4}{180}\overline{f^{(4)}} = -\frac{(x_n - x_0)^5}{180n^4}\overline{f^{(4)}}$$

Note: If n is doubled, h--> h/2 and E_t --> E_t/16

Simpson 3/8 Rule

For each triple of segments, let $f(x) \approx p_3(x) = a_0 + a_1x + a_2x^2 + a_3x^3$

a. Replace $a_0 + a_1x + a_2x^2 + a_3x^3$ w/ Lagrange Polynomials and integrate

b. For evenly spaced points:

$$\int_{x_0}^{x_3} p_3(x)dx = (x_3 - x_0)\frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8} = 3h\frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8}$$

c. Error: $\int_{x_0}^{x_3} f(x)dx = \int_{x_0}^{x_3} p_3(x)dx - \frac{1}{80}(x_3 - x_0)h^4 f^{(4)}(\xi)$

$$E_t = -\frac{1}{80}(x_3 - x_0)h^4 f^{(4)}(\xi) = -\frac{3}{80}h^5 f^{(4)}(\xi) = -\frac{(x_3 - x_0)^5}{6480} f^{(4)}(\xi)$$

Notes: 1. Composite Simpson 1/3 Rule and Simpson 3/8 Rule errors are

$$-\frac{(x_n - x_0)}{180} h^4 \overline{f^{(4)}} \quad \text{vs.} \quad -\frac{(x_n - x_0)}{80} h^4 \overline{f^{(4)}}$$

Simpson 1/3 rule is slightly more accurate over the interval $[x_0, x_n]$ when the two methods use the same value of h.

But both methods have the **same order** of accuracy.

2. Simpson 3/8 Rule requires multiples of **three** segments.

Simpson 1/3 Rule requires **even** number of segments.

3. Can use a combination of T, S 1/3, and/or S 3/8 when number of segments is neither even nor divisible by 3 or when data in unevenly spaced.

Higher order does not always yield higher accuracy.

Example: $I = \int_{0.2}^{1.5} c\, e^{-x^2} dx = 1.00000$

n	Trap.	Simp. 1/3	Simp. 3/8
1	1.05191		
2	1.00499*	0.98935	
3	1.00187*		0.99561
4	1.000990.99965		
6	1.000420.99994*	0.99985	
8	1.000230.99998*		
9	1.00019	0.99998*	
12	1.000111.00000*	1.00000*	
15	1.00008	1.00000*	
16	1.000061.00000*		

32 1.00001

64 1.00000Asterisk (*) denotes more accurate answer for each n.

Newton-Cotes Integration -- Other Cases:

1. NC formulas can be derived for any number of segments and spacing.

   Just integrate Lagrange Polynomial to get weight on each value of function:

   $f(x_i)$, i = 0,...,n;

   Formula can be open or closed.

2. Can always use multiple-application Trapezoidal Rule.

   Can use a Simpson Rule when adjacent segments have equal h's.

3. Integrate interpolating sp line.

Richardson Extrapolation

Given two numerical estimates obtained using different h's, compute a higher-order estimate.

Scheme:

Starting with a step size h_1, the exact value of some operation A is:

$$\mathbf{A} = A(h_1) + O(h_1^n)$$

Suppose we reduce step size to h_2

$$\mathbf{A} = A(h_2) + O(h_2^n)$$

Multiplying the second equation by $r = (h_1/h_2)^n$ and then subtracting the first equation yields [where the bracketed error terms tend to cancel]:

$$(r-1)\mathcal{A} = r\,A(h_2) - A(h_1) + [r\,O(h_2^n) - O(h_1^n)]$$

$$\mathbf{A} = \frac{\left(\frac{h_1}{h_2}\right)^n A(h_2) - A(h_1)}{\left(\frac{h_1}{h_2}\right)^n - 1} + O(h_1^m) \qquad m \geq n+1$$

Richardson Extrapolation Example -- Numerical Differentiation

$$D = \frac{\left(\frac{h_1}{h_2}\right)^n D(h_2) - D(h_1)}{\left(\frac{h_1}{h_2}\right)^n - 1}$$

Start with $O(h^2)$ centered first difference approx. from Table 23.3:

$$f'(x_i) \approx D(h) = \frac{f(x_i + h) - f(x_i - h)}{2h} = \frac{f_1 - f_{-1}}{2h}$$

Substituting $h_2 = h$ and $h_1 = 2h$, Richardson Extrapolation yields the next highest order centered first-difference formula in Table 23.3:

$$f'(x_i) = (1/3)\,[\,4\,D(h) - D(2h)\,] + O(h^4) =$$

$$= \frac{1}{3}\left[4\frac{1}{2h}(f_1 - f_{-1}) - \frac{1}{4h}(f_2 - f_{-2})\right] + O(h^4) =$$

$$= \frac{(-f_2 + 8f_1 - 8f_{-1} + f_{-2})}{12h} + O(h^4)$$

Richardson Extrapolation Example -- Numerical Integration

Suppose we use the Trapezoidal Rule to integrate. If we use step size h

$$I = T(2h) + O(4h^2).$$

To improve estimate, *reduce* step size:

$$I = T(h) + O(h^2).$$

Combining to eliminate error of order h^2 yields

$$I = \frac{2^2 T(h) - T(2h)}{2^2 - 1} + O(h^4) = \frac{1}{3}\,[\,4\,T(h) - T(2h)\,] + O(h^4)$$

1. Greater weight is placed on the more accurate estimate
2. Weighting coefficients sum to unity, i. e. $(4 - 1)/3 = 1$
3. Actually Simpson's 1/3 rule: $(h/3)[f(x_{i-1}) + 4f(x_i) + f(x_{i+1})]$

Romberg Integration

Systematic application of Richardson extrapolation with: $h_{i+1} = h_i/2$

Benefit: Get a high-order Newton-Cotes formula easily.

Can watch convergence.

General formula

$$I_{j,k} = \frac{4^{k-1} I_{j+1,k-1} - I_{j,k-1}}{4^{k-1} - 1} = I_{j+1,k-1} + \frac{I_{j+1,k-1} - I_{j,k-1}}{4^{k-1} - 1}$$

where: j = level of subdivision

k = level of integration $O(h^{2k})$

Tabular Organization of Romberg Integration

$$I_{j,k} = I_{j+1,k-1} + \frac{I_{j+1,k-1} - I_{j,k-1}}{4^{k-1} - 1}$$

j	# Trap. segs. n	k = 1 $O(h^2)$ Trap	k = 2 $O(h^4)$ Simp 1/3	k = 3 $O(h^6)$ Boole 5	k = 4 $O(h^8)$	k = 5 $O(h^{10})$
1	1	$I_{1,1}$	$I_{1,2}$	**$I_{1,3}$**		
2	2	$I_{2,1}$	**$I_{2,2}$**			
3	4	**$I_{3,1}$**				
4	8					
5	16					
	$\frac{1}{4^{k-1}-1}$ =		1/3	1/15	1/63	1/255

Romberg Integration: Continuation of earlier integration example.

Example : $I = \int_{1.2}^{1.5} ce^{-x^2} dx = 1.0000000$

Trap n	Trap $O(h^2)$	Simpson $O(h^4)$	Boole $O(h^6)$	$O(h^8)$
1	1.0519096	0.9893489	1.0003403	0.9999970
2	1.0049891	0.9996533	1.0000024	1.0000000
4	1.0009873	0.9999806	1.0000000	1.0000000
8	1.0002322	0.9999988	1.0000000	1.0000000
16	1.0000572	0.9999999	1.0000000	
32	1.0000142	1.0000000		
64	1.0000036			

Example : $I = \int_0^1 (a+1)x^a \, dx$ **a = 6**

Trap	***Trapezoid***	**Simp 1/3**	**Boole 5-pt**		
n	**O(h²)**	**O(h⁴)**	**O(h⁶)**	**O(h⁸)**	**O(h¹⁰)**
1	3.500000	1.239583	1.002604	1.000000	1.000000
2	1.804688	1.017415	1.000041	1.000000	
4	1.214233	1.001127	1.000001		
8	1.054403	1.000071			
16	1.013654				

Example 3: $I = \int_0^1 (a+1)x^a \, dx$ **a = 1.5**

Trap	***Trapezoid***	**Simp 1/3**	**Boole 5-pt**		
n	**O(h²)**	**O(h⁴)**	**O(h⁶)**	**O(h⁸)**	**O(h¹⁰)**
1	1.250000	1.005922	1.000757	1.000124	1.000022
2	1.066942	1.001080	1.000134	1.000022	
4	1.017545	1.000193	1.000024		
8	1.004531	1.000034			
16	1.001159				

Gauss Quadrature

Requires: $f(x)$ to be explicitly known so we can pick any x_i

Approach: $$\int_{-1}^{+1} f(x)dx = \sum_{i=0}^{n-1} \omega_i f(x_i) + R_n$$

where: ω_i = weighting factors

x_i = sampling points selected optimally

R_n= truncation error

Pick points & weights cleverly to integrate a polynomial of order (2n - 1) exactly.

For **n = 2** Gauss Quadrature will be accurate for **cubics**.

Trapezoidal Rule is accurate for linear functions.

For **n=3** exact result for polynomials of order up to and including 5

With 3 points we want exact results for polynomials of order 5 over the interval [-1, +1].

$$\int_{-1}^{+1} 1dx = 2 = \omega_0 1 + \omega_1 1 + \omega_2 1$$

$$\int_{-1}^{+1} xdx = 0 = \omega_0 x_0 + \omega_1 x_1 + \omega_2 x_2$$

$$\int_{-1}^{+1} x^2 dx = \frac{2}{3} = \omega_0 x_0^2 + \omega_1 x_1^2 + \omega_2 x_2^2$$

$$\int_{-1}^{+1} x^3 dx = 0 = \omega_0 x_0^3 + \omega_1 x_1^3 + \omega_2 x_2^3$$

$$\int_{-1}^{+1} x^4 dx = \frac{2}{5} = \omega_0 x_0^4 + \omega_1 x_1^4 + \omega_2 x_2^4$$

$$\int_{-1}^{+1} x^5 dx = 0 = \omega_0 x_0^5 + \omega_1 x_1^5 + \omega_2 x_2^5$$

With *six* equations there are *six* unknowns,

i.e., 3 unknown weights (ω_0, ω_1, ω_2) and

3 unknown sampling points (x_0, x_1, x_2).

Solving these six equations for the six unknowns results in:

$\omega_0 = 0.555555556$ $\omega_1 = 0.888888889$ $\omega_2 = 0.555555556$

$x_0 = -0.774596669$ $x_1 = 0.000000000$ $x_2 = +0.774596669$

$$I \approx \omega_0 f(x_0) + \omega_1 f(x_1) + \omega_2 f(x_2)$$

See C&C Table 22.1, p. 626, for Gauss-Legendre formulas, n = 2, 3, 4, 5, and 6.

Gauss Quadrature Truncation Error

In general, n sampling points will provide an exact solution for a 2n–1 order polynomial. With n = # of sampling points

$$R_n = \frac{[2(b-a)]^{2n+1}(n!)^4}{(2n+1)[(2n)!]^3} f^{(2n)}(\xi)$$

(similar to C&C except their n = # pts.–1)

Because (b-a) = h, the error with the composite Gauss rule is $O(h^{2n})$ globally

with n = # of pts..

This shows a superiority of order over the Newton-Cotes formulas.

Higher order need not always mean higher accuracy.

Arbitrary intervals: Gauss Quadrature: When the limits of integration are [a,b] instead of [–1,+1] (C&C, p. 621)

We have a solution for the integral $\int_{-1}^{+1} f(x)dx$.

Assume that there is a variable x which is linearly related to x_d such that:

$y = a_0 + a_1 x$

If y = a, corresponds to x = –1 and y = b, corresponds to x = 1, then

$a = a_0 + a_1(-1)$ and $b = a_0 + a_1(+1)$

Solving these two equations yields:

$a_0 = (b+a)/2$ and $a_1 = (b-a)/2$

which gives the change of variables:

$$y = \frac{b+a}{2} + \frac{b-a}{2} x \quad \text{and} \quad dy = \frac{b-a}{2} dx$$

Thus, $$\int_a^b f(y)dy = \int_{-1}^{+1} f\left(\frac{(b+a)+(b-a)x}{2}\right)\frac{b-a}{2}dx \approx \frac{b-a}{2}\sum_{i=0}^{n-1}\omega_i f(y[x_i])$$

(*The x_i are the tabulated Gauss points (Table 22.1) in C&C)*

Example : Evaluate $\int_{0.2}^{1.5} e^{y^2} dy$ using 3-pt Gauss Quad:

1. Change of variables: $y = \frac{(1.5+0.2)+(15-0.2)x}{2} = 0.65\,x + 0.85$

$$dy = \frac{1.5-0.2}{2} dx = 0.65\,dx$$

2. With $\int_{0.2}^{1.5} e^{-y^2}\,dy = 0.65 \int_{-1}^{+1} e^{[0.65x+0.85]^2}\,dx$

$$I \approx 0.65\left\{\omega_0\, e^{-[0.65x_0+0.85]^2} + \omega_1\, e^{-[0.65x_1+0.85]^2} + \omega_2\, e^{-[0.65x_2+0.85]^2}\right\}$$

where: $\omega_0 = 0.555555556$ $\quad x_0 = -0.774596669$

$\omega_1 = 0.888888889$ $\quad x_1 = 0.000000000$

$\omega_2 = 0.555555556$ $\quad x_2 = +0.774596669$

$I_{true} = 0.65882$

$I_{gauss} = 0.65860,\ e_t = 0.03\%$

Note: with 3 points, i.e., 2 segments: $I_{trap} = 0.66211,\ e_t = 0.50\%$

$I_{Simp.1/3} = 0.65181,\ e_t = 1.06\%$

Example : $\int_0^1 \frac{c\,dy}{2+\cos(\pi\, y/2)}$

n	pts	Romberg	Gauss Quad
1	2	1.08253170	0.99955157
2	3	1.00066008	1.00000812
4	5	0.99999114	1.00000000
8	9	0.99999987	1.00000000

n	pts	Romberg	Gauss Quad
1	2	$O(h^2)$	$O(h^4)$
2	3	$O(h^4)$	$O(h^6)$
4	5	$O(h^6)$	$O(h^{10})$
8	9	$O(h^8)$	$O(h^{18})$

n = number of panels; pts = number of points

Gauss Quadrature Formulas for Special Integrals

In each of these schemes, f(x) is a "well behaved" function, that is, continuously differentiable. Also each of these schemes has its own tabulated sampling points and weighting factors (not in C&C).

Gauss-Legendre

$$\int_{-1}^{+1} f(x)\,dx$$

Gauss-Hermite

$$\int_{-\infty}^{+\infty} e^{-x^2} f(x)\,dx$$

Gauss-Laguerre

$$\int_{0}^{+\infty} e^{-x} f(x)\,dx$$

log-weighted

$$\int_{0}^{1} \ln(x) f(x)\,dx$$

Gauss-Chebyshev

$$\int_{-1}^{+1} \frac{f(x)}{\sqrt{1-x^2}}\,dx$$

Advantages (A) and Disadvantages (D) of Gauss Quadrature

A1) With n points obtain a formula that integrates polynomials 1, x, x^2, ..., x^{2n-1} because of 2n free parameters: very high order.

Excellent for well-behaved functions!

A2) Special formulas are available and can be derived for special weighting functions, and infinite and semi-infinite intervals.

D1) Errors can depend upon $f^{(2n)}(\xi)$ so the method is only dependable if high order derivatives are well behaved.

D2) When composite Gauss formulas are applied (Gauss Quadrature applied to separate panels), endpoints cannot be reused as they are with Trapezoid, Simpson and Romberg.

D3) With an adaptive strategy that selectively subdivides intervals where truncation error may be large, cannot reuse points as one can with Trapezoid and Simpson. Gauss also fails to provide an estimate of local error as do Trapezoid, Simpson, and Romberg by clever use of the same function values with different weights.

D4) Inconvenient to remember special Gauss points and Gauss weights.

Improper Integrals

1. Use Gauss Quadrature for that special interval.

2. Transform variables on the outer portion of the interval. (Beware of singularities at what was infinity.) For any function that approaches zero at least as fast as $1/x^2$ as x approaches infinity, perform change of variables:

$$x = \frac{1}{t} \quad \text{and} \quad dx = -dt/t^2$$

$$\int_{x=a}^{b} f(x)dx = \int_{t=1/b}^{t=1/a} \frac{1}{t^2} f\left(\frac{1}{t}\right) dt \qquad (22.27)$$

which is valid for ab > 0. For integration limits that pass through zero, implement the integration in two (or three) steps:

$$\int_{-\infty}^{b} f(x)\,dx = \int_{-\infty}^{-a} f(x)\,dx + \int_{-a}^{b} f(x)\,dx$$

where a > 0. The first integral may be evaluated using equation (22.27) and the second may be evaluated using a Newton-Cotes formula or Gauss Quadrature.

For a detailed example (on the **cumulative normal distribution**), see C&C Example 22.6, page 629-630.

Integration when the Integrand contains a singularity

In the following, the function f(x) is "well behaved," i.e., it is continuously differentiable in the neighborhood of the singularity of the integrand or its derivative. Here is an integral with a singularity at the lower limit:

$$I = \int_0^1 \frac{f(x)}{\sqrt{x}} dx \quad \Rightarrow \quad \text{problem at the singular point } x = 0$$

In addition, if the derivative of the integrand goes to infinity, it is possible that the error goes to infinity as well. An example of this situation is:

$$I = \int_0^u \sqrt{x}\, f(x) dx$$

To integrate, we need to control error near the singularity.

Divide the integration region to isolate singularity, ***then-------***

Approach 1a: Try to subtract out singularity and numerically integrate only the remainder.

Consider the case $\int_0^u \sqrt{x}\, f(x) dx$

where f(x) is continuously differentiable at x = 0.

a) Subtract out the singularity at x = 0, and integrate numerically:

$$\int_0^u [f(x) - f(0)]\, \sqrt{x}\, dx$$

Here the bracketed term in the integrand vanishes at the singularity

b) Integrate the singularity separately: $f(0)\int_0^u \sqrt{x}\,dx = f(0)\frac{u^{1.5}}{1.5}$

c) Add the singularity back in: $I = \int_0^u [f(x) - f(0)]\sqrt{x}\,dx + f(0)\frac{u^{1.5}}{1.5}$

Approach 1b: Even better, include the first derivative when isolating the singularity, i.e.,:

a) Subtract out the singularity at x = 0, and integrate numerically:

$$\int_0^u [f(x) - f(0) - xf'(0)]\sqrt{x}\,dx$$

b) Integrate the singularity separately:

$$\int_0^u [f(0) + xf'(0)]\sqrt{x}\,dx = f(0)\frac{u^{1.5}}{1.5} + f'(0)\frac{u^{2.5}}{2.5}$$

c) Add the singularity back in:

$$I = \int_0^u [f(x) - f(0) - xf'(0)]\sqrt{x}\,dx + f(0)\frac{u^{1.5}}{1.5} + f'(0)\frac{u^{2.5}}{2.5}$$

Approach 2: Try a change of variables for part of interval near singularity

$$\int_0^u x^a \; f(x)\,dx$$

- Let $x = y^2$, then $dx = 2ydy \Rightarrow x^a\, f(x)\,dx = 2\,y^{2a+1}\, f(y^2)\,dy$

  For $0 < a < 1$, $1 < 2a+1$ so the singularity is eliminated.

- Does not entirely solve the problem, but makes it less severe.
- Use Trapezoid or Simpson rule near the problem. For a = ½:

$$\int_0^u f(x)\sqrt{x}\,dx = \int_0^u f(y^2)\,y(2y)dy = 2\int_0^u f(y^2)\,y^2dy$$

Approach 3: Integrate by parts: $\int x^a f(x)dx = x^{a+1}f(x) - \int x^{a+1}f'(x)dx$

Approach 4: Use the appropriate Gauss Quadrature approaches specialized for the particular singular function

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