1.00 Lecture 32

Integration

Reading for next time: Numerical Recipes 347-368

Packaging Functions in Objects

• Consider writing a method that evaluates, integrates or finds the roots of a function:
  – Evaluate: find f(x) when x=c
  – Root: find x such that f(x)= 0 on some interval [a, b]
• A general method that does this should have f(x) as an argument
  – Can’t pass functions in Java (unlike C++)
  – Include the function (method) in an object instead
    • Then pass the object reference to the evaluation, integration or root finding method as an argument
  – Define an interface that describes the object that will be passed to the numerical method
    • It must have a method, typically called f, that returns the value of the function f at a point defined by the arguments
Exercise: Passing Functions

- Write an interface MathFunction2
  ```java
  public interface MathFunction2 {
    public double f(double x1, double x2);  }
  ```
- Write a class Cubic that implements the interface for the function $5x_1^2 + 2x_2^3$
  ```java
  public class Cubic implements MathFunction2 { … }
  ```
- Write a class Evaluate that contains a method eval() that evaluates functions of two variables:
  ```java
  public class Evaluate {
    public static boolean eval(MathFunction2 func, double d1, double d2){…}
  }
  ```
- Write a main() method, in class Evaluate that:
  ```java
  – Invokes eval(), passing a Cubic object and two doubles $x_1=2$ and $x_2=-3$, and prints the boolean value returned
  ```
- No need for a constructor in Cubic (or Evaluate) classes
  ```java
  – Java will write a default (no argument) constructor automatically
  ```
- If you have time, create class Quadratic with $f(x)=x_1^2-x_2^2+2x_1x_2$

Elementary Integration Methods

- Rectangular rule
  $$A = f(x) \times h$$

- Trapezoidal rule
  $$A = \frac{(f(x_l)+f(x_r)) \times h}{2}$$

- Simpson’s method
  $$A = \frac{(f(x_l)+4f(x_m)+f(x_r)) \times h}{6}$$
Elementary Integration Methods

```java
class Quartic implements MathFunction {
    public double f(double x) { // f in MathFunction
        return x*x*x*x +2;  }
}

class Integration {
    public static double rect(MathFunction func, double a, double b, int n) {
        double h= (b-a)/n;
        double answer=0.0;
        for (int i=0; i < n; i++)
            answer += func.f(a+i*h);  // Left edge
        return h*answer;  }

    public static double trap(MathFunction func, double a, double b, int n) {
        double h= (b-a)/n;
        double answer= func.f(a)/2.0;
        for (int i=1; i <= n; i++)
            answer += func.f(a+i*h);  // Common edge
        answer -= func.f(b)/2.0;
        return h*answer;  }

    public static double simp(MathFunction func, double a, double b, int n) {
        // Each panel has area (h/6)*(f(x) + 4f(x+h/2) + f(x+h))
        double h= (b-a)/n;
        double answer= func.f(a);
        for (int i=1; i <= n; i++)
            answer += 4.0*func.f(a+i*h-h/2.0)+ 2.0*func.f(a+i*h);
        answer -= func.f(b);
        return h*answer/6.0;  }

    public static void main(String[] args) {
        double r= Integration.rect(new Quartic(), 0.0, 8.0, 200);
        System.out.println("Rectangle: "+ r);
        double t= Integration.trap(new Quartic(), 0.0, 8.0, 200);
        System.out.println("Trapezoid: "+ t);
        double s= Integration.simp(new Quartic(), 0.0, 8.0, 100);
        System.out.println("Simpson: "+ s);
    }
}
```

// Problems: no accuracy estimate, inefficient, only closed int
Quick Exercise

- Download and run Integration
  - The function is \( f(x) = x^4 + 2 \)
  - The integral is \( \int_0^8 (x^4 + 2) \, dx = (x^5 / 5 + 2x)^8_0 \)
  - What value do rectangular, trapezoidal and Simpson give for the function provided?
  - Compute the correct value via calculus
  - Which is the most accurate?

Trapezoid Rule

Individual trapezoid approximation:
\[
\int_{x_0}^{x_n} f(x) \, dx = h(0.5f_1 + 0.5f_2) + O(h^3 f''')
\]

Use this N-1 times for \((x_1, x_2), (x_2, x_3), ..., (x_{N-1}, x_N)\) and add the results:
\[
\int_{x_0}^{x_n} f(x) \, dx = h(0.5f_1 + f_2 + \cdots + f_{N-1} + 0.5f_N) + O(Nh^3 f''')
\]
Better Trapezoid Rule

N=1, requires two function evaluations

Better Trapezoid Rule

N=2, requires only one more function evaluation
Better Trapezoid Rule

N=4, requires only two more function evaluations

Better Trapezoid Rule

N=8, requires only 4 more function evaluations
Using Trapezoidal Rule

- Keep cutting intervals in half until desired accuracy met
  - Estimate accuracy by change from previous estimate
  - Each halving requires only half the work because past work is retained
- By using a quadratic interpolation (Simpson’s rule) to function values instead of linear (trapezoidal rule), we get better error behavior
  - By good fortune, errors cancel well with quadratic approximation used in Simpson’s rule
  - Computation same as trapezoid, but uses different weighting for function values in sum

Extended Trapezoid Method

```java
public class Trapezoid {
    public static double trapzd(MathFunction func, double a, double b, int n) {
        if (n == 1) {
            double s = 0.5*(b-a)*(func.f(a)+func.f(b));
            return s; }
        else {
            int it= 1; // Add1 interior points
            for (int j= 0; j < n-2; j++)
                it *= 2; // Subdivisions
            double tnm = it; // Double value of it
            double delta = (b-a)/tnm; // Spacing of points
            double x = a+0.5*delta; // Pt to evaluate f(x)
            double sum = 0.0; // Contrib of new pts x
            for (int j = 0; j < it; j++) {
                sum += func.f(x);
                x += delta;
            }
            s = 0.5*(s+(b-a)*sum/tnm); // Value of integral
            return s; }
        }
    private static double s; // Current value of integral
    }
```

Extended Simpson Method

Approximate function with quadratic, not linear form
(There is also a Simpson method using cubic form)

```java
public class Simpson {
    // NumRec p. 139
    public static double qsimp(MathFunction func, double a,
                               double b) {
        double ost= -1.0E30;
        double os= -1E30;
        for (int j=0; j < JMAX; j++) {
            double st= Trapezoid.trapzd(func, a, b, j+1);
            s= (4.0*st - ost)/3.0;      // See NumRec eq. 4.2.4
            if (j > 4)      // Avoid spurious early convergence
                if (Math.abs(s-os) < EPSILON*Math.abs(os) ||
                    (s==0.0 && os==0.0)) {
                    System.out.println("Simpson iter: " + j);
                    return s; }
            os= s;
            ost= st;
        }
        System.out.println("Too many steps in qsimp");
        return ERR_VAL;    }

    private static double s;   // Value of integral
    public static final double EPSILON= 1.0E-15;
    public static final int JMAX= 50;
    public static final double ERR_VAL= -1E10;  }
```

Using Extended Simpson

```java
public static void main(String[] args) {
    // Using extended Simpson method
    System.out.println("Simpson use");
    ans = qsimp(new Quartic(), 0.0, 8.0);
    System.out.println("Integral: " + ans);
}
}   // End Simpson class
```

```java
public class Quartic implements MathFunction {  // Same as before
    public double f(double x) {
        return x*x*x*x + 2;
    }
}
```

```java
public interface MathFunction {      // Same as before
    public double f(double x);
}
```

Quick Demo

- **Download Simpson and Trapezoid**
  - Run them with different values of m (trapezoid) and EPSILON (Simpson), which governs the size of the interval and number of iterations
  - **Trapezoid:**
    - Examine from m= 5 to m= 20 iterations
    - Number of intervals is $2^{m+1}$
    - $2^{20}$ is about a million
  - **Simpson:**
    - Experiment with EPSILON
  - Notice that Simpson is much more accurate with many times fewer iterations
Romberg Integration

• Generalization of Simpson (NumRec p. 140)
  – Based on numerical analysis to remove more terms in error series associated with the numerical integral
    • Uses trapezoid as building block as does Simpson
  – Romberg is adequate for smooth (analytic) integrands, over intervals with no singularities, where endpoints are not singular
  – Romberg is much faster than Simpson or the elementary routines. For a sample integral:
    • Romberg: 32 iterations
    • Simpson: 256 iterations
    • Trapezoid: 8192 iterations
  – All are instances of Newton-Cotes methods

Improper Integrals

• Improper integral defined as having integrable singularity or approaching infinity at limit of integration
  – Use extended midpoint rule instead of trapezoid rule to avoid function evaluations at singularities or infinities
    • Must know where singularities or infinities are
  – Use change of variables: often replace $x$ with $1/t$ to convert an infinity to a zero
    • Done implicitly in many routines

• Last improvement: Gaussian quadrature
  – In Simpson, Romberg, etc. the $x$ values are evenly spaced. By relaxing this, we can get better efficiency and better accuracy
Midpoint Rule

See Numerical Recipes for discussion, code

Multidimensional integration

- Classical 1-D methods are of historic interest only
  - Rectangular, trapezoid, Simpson’s
  - Work well for integrals that are very smooth or can be computed analytically anyway
- Extended Simpson’s method is only elementary method of some utility for 1-D integration
- Multidimensional integration is tough
  - If region of integration and function values are smooth, use multidimensional Simpson’s (also called decomposition)
    - Numerical Recipes chapter 4 has multidimensional Simpson
  - If region of integration is complex but function values are smooth, use Monte Carlo integration (next exercise)
  - If region is simple but function is irregular, split integration into regions based on known sites of irregularity
  - If region is complex and function is irregular, or if sites of function irregularity are unknown, give up
Monte Carlo Integration

Cross section of jet engine thrust can look like this, for example

Integrate $f(x,y)$ over Circular Area

Randomly generate points in square $4r^2$. Odds that they’re in the circle are $\pi r^2 / 4r^2$, or $\pi / 4$.

This is Monte Carlo integration, with $f(x,y) = 1$

If $f(x,y)$ varies slowly, then evaluate $f(x,y)$ at each sample point in limits of integration, and sum them

This actually finds the volume of a cylinder
Integration over Circular Area

public class MonteCarloIntegration {
    public static double circularIntegral() {
        int nIter= 1000000;
        double sum= 0.0, radius= 0.5;
        for (int i=0; i < nIter; i++) {
            // Math.random() returns double d: 0 <= d < 1
            double x= Math.random() - radius;  // Ctr at 0,0
            double y= Math.random() - radius;
            double f= 1.0;  // f(x,y)—constant here
            if ((x*x + y*y) < radius*radius) // If in region
                sum += f;   // Increment integral sum
        }
        return sum/nIter;   // Integral value
    }
    public static void main(String[] args) {
        System.out.println("Result: " + circularIntegral() );
        System.out.println("Pi: " + 4.0*circularIntegral() );
    }
}   }  // Accuracy ~ sqrt(n) with random x,y.

Integration over Circular Area, 2

// To integrate f(x,y) = exp (x)/(y*y+1) over this area:
public class MonteCarloIntegration2 {
    public static double circularIntegral() {
        // for loop, random x, y same as previous slide
        // ...
        if ((x*x + y*y) < radius*radius){ // If in region
            double f= Math.exp(x)/(y*y+1);
            sum += f;   // Increment integral sum
        }
        return sum/nIter; // Integral value
    }
    public static void main(String[] args) {
        System.out.println("Result: " +circularIntegral() );
    }
} } // Numerical integration is used when functions and areas
// of integration are really complex and ugly
Exercise

- Find the shaded volume within circles below:
  - Use circularIntegral() as your starting point
  - Use f(x,y)= 1 to find the areas below using integration
  - Equation of circle is $(x-x_c)^2 + (y-y_c)^2 = r^2$

(Answer is $3\pi/16$, or .589)
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