

User Manual 3.4.1 Numerical differentiation and integration

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Introduction

Scope

This section details numerical differentiation and integration (not to be misunderstood with numerical integration of ODE). A focus is realised on:

- differentiation methods of real univariate functions: Ridders and finite difference.
- integration methods of real univariate functions : Trapezoidal and Simpson.

Javadoc

The numerical differentiator objects are available in the package `org.apache.commons.math3.analysis.differentiation` in the Commons Math Library. The numerical integrator objects are available in the package `org.apache.commons.math3.analysis.integration` in the Commons Math Library.

Library

Javadoc

Commons Math [Package org.apache.commons.math3.analysis.differentiation](#)

Commons Math [Package org.apache.commons.math3.analysis.integration](https://commons.wikimedia.org/wiki/Package_org.apache.commons.math3.analysis.integration)

Links

Links to the implemented integration methods :

<http://mathworld.wolfram.com/TrapezoidalRule.html>

<http://mathworld.wolfram.com/SimpsonsRule.html>

Useful Documents

None as of now.

Package Overview

The numerical differentiation conception is described hereafter :



Accuracy of integration method (all examples are based on sinus function):

Default setting	Value
Maximum absolute error	1.0e-15
Maximum relative error	1.0e-6
Maximum number of iterations	64
Minimum number of iterations	3

Note : the accuracy of the results and the computing time are directly dependent on the value of maximum relative error.

Features Description

Numerical differentiation

Finite difference

Finite difference is the discrete analog of the derivative. The user can choose the number of points to use and the step size (the gap between each point).

Ridders algorithm

The derivative of a function at a point x is computed using the Ridders method of polynomial extrapolation.

Numerical Integration

Trapezoidal method

The trapezoidal rule works by approximating the region under the graph of the function as a trapezoid and calculating its area.

```
UnivariateFunction f = new SinFunction();
UnivariateIntegrator integrator = new TrapezoidIntegrator();
double r = integrator.integrate(10000, f, 0, FastMath.PI);
```

Result : r = 1.9999996078171345 (exact result = 2)

And :

```
integrator = new TrapezoidIntegrator(1.e-12, 1.0e-15, 3, 64);
r = integrator.integrate(10000000, f, 0, FastMath.PI);
```

Result : r = 1.9999999999904077

But :

```
integrator = new TrapezoidIntegrator(1.e-13, 1.0e-15, 3, 64);
r = integrator.integrate(10000000, f, 0, FastMath.PI);
```

Result : r = no result (infinite time !)

Simpson method

Simpson's rule is a Newton-Cotes formula for approximating the integral of a function using quadratic polynomials (i.e., parabolic arcs instead of the straight line segments used in the trapezoidal rule). In general, this method has faster convergence than the trapezoidal rule for functions which are twice continuously differentiable, though not in all specific cases.

```
UnivariateFunction f = new SinFunction();
UnivariateIntegrator integrator = new SimpsonIntegrator();
double r = integrator.integrate(10000, f, 0, FastMath.PI);
```

Result : r = 2.000000064530001 (exact result = 2)

Getting Started

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Interfaces

Interface	Summary	Javadoc
UnivariateFunctionDifferentiator	This interface represents a generic numerical differentiator.	...
UnivariateIntegrator	Interface for univariate integration algorithms.	...

Classes

Class	Summary	Javadoc
FiniteDifferencesDifferentiator	Apply the finite difference method to differentiate a function.	...
RiddersDifferentiator	Apply the Ridders algorithm to differentiate a function.	...
TrapezoidIntegrator	The class implements the Trapezoidal rule	...
SimpsonIntegrator	The class implements the Simpson rule	...

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