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# Chapter 3

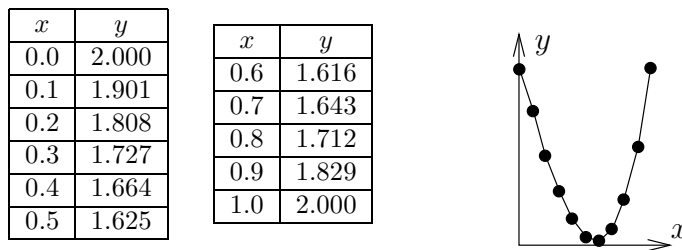
## First order numerical methods

### 3.1 Solving $y' = F(x)$ Numerically

Studied here is the creation of tables and graphs for the solution of the initial value problem

$$(1) \quad y' = F(x), \quad y(x_0) = y_0.$$

To illustrate the kinds of tables and graphs to be created, consider the initial value problem  $y' = 3x^2 - 1$ ,  $y(0) = 2$ . Quadrature gives  $y(x) = x^3 - x + 2$ . In Figure 1, evaluation of  $y(x)$  from  $x = 0$  to  $x = 1$  in increments of 0.1 gives the  $xy$ -table, whose entries represent the **dots** for the **connect-the-dots** graphic.



**Figure 1.** A table of  $xy$ -values for  $y = x^3 - x + 2$ . The graphic represents the table's rows as *dots*, which are joined to make the *connect-the-dots* graphic.

The interesting case is when quadrature in (1) encounters an integral  $\int_{x_0}^x F(t)dt$  that cannot be evaluated to provide an explicit equation for  $y(x)$ . Nevertheless,  $y(x)$  can be computed numerically.

Applied here are numerical integration rules from calculus: *rectangular*, *trapezoidal* and *Simpson*; see page 125 for a review of the three rules. The ideas lead to the numerical methods of Euler, Heun and Runge-Kutta, which appear later in this chapter.

**How to make an  $xy$ -table.** Given  $y' = F(x)$ ,  $y(x_0) = y_0$ , an equi-spaced table of  $xy$ -values is created as follows. The  $x$ -values are a distance  $h > 0$  apart. Each  $x, y$  pair in the table represents a *dot* in the *connect-the-dots* graphic of the explicit solution

$$y(x) = y_0 + \int_{x_0}^x F(t)dt.$$

**First table entry.** The *initial condition*  $y(x_0) = y_0$  identifies two constants  $x_0, y_0$  to be used for the first table entry. For example,  $y(0) = 2$  identifies  $X = 0, Y = 2$ .

**Second table entry.** The second table pair  $X, Y$  is computed from the first table pair  $x_0, y_0$  and a **recurrence**. The  $X$ -value is given by  $X = x_0 + h$ , while the  $Y$ -value is given by the numerical integration method being used, in accordance with Table 1 (the table is justified on page 128).

**Table 1. Three numerical integration methods.**

Rectangular Rule	$Y = y_0 + hF(x_0)$
Trapezoidal Rule	$Y = y_0 + \frac{h}{2}(F(x_0) + F(x_0 + h))$
Simpson's Rule	$Y = y_0 + \frac{h}{6}(F(x_0) + 4F(x_0 + h/2) + F(x_0 + h))$

**Third and higher table entries.** They are computed by letting  $x_0, y_0$  be the current table entry, then the next table entry  $X, Y$  is found exactly as outlined above for the second table entry.

It is expected, and normal, to compute the table entries using computer assist. In simple cases, a calculator will suffice. If  $F$  is complicated or Simpson's rule is used, then a computer algebra system or a numerical laboratory is recommended. See Example 2, page 122.

**How to make a connect-the-dots graphic.** To illustrate, consider the  $xy$ -pairs below, which are to represent the *dots* in the *connect-the-dots* graphic.

$$\begin{aligned} &(0.0, 2.000), (0.1, 1.901), (0.2, 1.808), (0.3, 1.727), (0.4, 1.664), \\ &(0.5, 1.625), (0.6, 1.616), (0.7, 1.643), (0.8, 1.712), (0.9, 1.829), \\ &(1.0, 2.000). \end{aligned}$$

**Hand drawing.** The method, unchanged from high school mathematics courses, is to plot the points as dots on an  $xy$ -coordinate system, then connect the dots with line segments. See Figure 2.

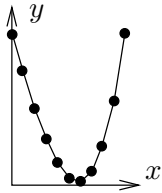


Figure 2. A computer-generated graphic made to simulate a hand-drawn connect-the-dots graphic.

**Computer algebra system graphic.** The computer algebra system maple has a primitive syntax especially made for connect-the-dots graphics. Below, L is a list of  $xy$ -pairs.

```
# Maple V.1
Dots:=[0.0, 2.000], [0.1, 1.901], [0.2, 1.808],
      [0.3, 1.727], [0.4, 1.664], [0.5, 1.625],
      [0.6, 1.616], [0.7, 1.643], [0.8, 1.712],
      [0.9, 1.829], [1.0, 2.000]:
plot([Dots]);
```

The plotting of *points only* can be accomplished by adding options into the plot command: `type=point` and `symbol=circle` will suffice.

**Numerical laboratory graphic.** The computer programs `matlab`, `octave` and `scilab` provide primitive plotting facilities, as follows.

```
X=[0, .1, .2, .3, .4, .5, .6, .7, .8, .9, 1]
Y=[2.000, 1.901, 1.808, 1.727, 1.664, 1.625,
  1.616, 1.643, 1.712, 1.829, 2.000]
plot(X,Y)
```

- 1 Example (Rectangular Rule)** Consider  $y' = 3x^2 - 2x$ ,  $y(0) = 0$ . Apply the rectangular rule to make an  $xy$ -table for  $y(x)$  from  $x = 0$  to  $x = 2$  in steps of  $h = 0.2$ . Graph the approximate solution and the exact solution  $y(x) = x^3 - x^2$  for  $0 \leq x \leq 2$ .

**Solution:** The exact solution  $y = x^3 - x^2$  is verified directly, by differentiation. It was obtained by quadrature applied to  $y' = 3x^2 - 2x$ ,  $y(0) = 0$ .

The first table entry 0, 0 is used to obtain the second table entry  $X = 0.2$ ,  $Y = 0$  as follows.

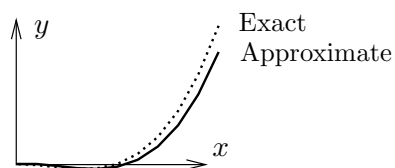
$x_0 = 0, y_0 = 0$	The current table entry, row 1.
$X = x_0 + h$	The next table entry, row 2.
$= 0.2,$	Use $x_0 = 0, h = 0.2$ .
$Y = y_0 + hF(x_0)$	Rectangular rule.
$= 0 + 0.2(0).$	Use $h = 0.2, F(x) = 3x^2 - 2x$ .

The remaining 9 rows of the table are completed by calculator, following the pattern above for the second table entry. The result:

**Table 2.** Rectangular rule solution and exact values for  $y' = 3x^2 - 2x$ ,  $y(0) = 0$  on  $0 \leq x \leq 2$ , step size  $h = 0.2$ .

$x$	$y$ -rect	$y$ -exact	$x$	$y$ -rect	$y$ -exact
0.0	0.000	0.000	1.2	0.120	0.288
0.2	0.000	-0.032	1.4	0.504	0.784
0.4	-0.056	-0.096	1.6	1.120	1.536
0.6	-0.120	-0.144	1.8	2.016	2.592
0.8	-0.144	-0.128	2.0	3.240	4.000
1.0	-0.080	0.000			

The  $xy$ -values from the table are used to obtain the comparison plot in Figure 3.



**Figure 3.** Comparison plot of the rectangular rule solution and the exact solution  $y = x^3 - x^2$  for  $y' = 3x^2 - 2x$ ,  $y(0) = 0$ .

**2 Example (Trapezoidal Rule)** Consider  $y' = \cos x + 2x$ ,  $y(0) = 0$ . Apply both the rectangular and trapezoidal rules to make an  $xy$ -table for  $y(x)$  from  $x = 0$  to  $x = \pi$  in steps of  $h = \pi/10$ . Compare the two approximations in a graphic for  $0 \leq x \leq \pi$ .

**Solution:** The exact solution  $y = \sin x + x^2$  is verified directly, by differentiation. It will be seen that the trapezoidal solution is nearly identical, graphically, to the exact solution.

The table will have 11 rows. The three columns are  $x$ ,  $y$ -rectangular and  $y$ -trapezoidal. The first table entry 0, 0, 0 is used to obtain the second table entry  $0.1\pi$ , 0.31415927, 0.40516728 as follows.

**Rectangular rule second entry.**

$$Y = y_0 + hF(x_0)$$

$$= 0 + h(\cos 0 + 2(0))$$

$$= 0.31415927.$$

Rectangular rule.

$$\text{Use } F(x) = \cos x + 2x, x_0 = y_0 = 0.$$

$$\text{Use } h = 0.1\pi = 0.31415927.$$

**Trapezoidal rule second entry.**

$$Y = y_0 + 0.5h(F(x_0) + F(x_0 + h))$$

$$= 0 + 0.05\pi(\cos 0 + \cos h + 2h)$$

$$= 0.40516728.$$

Trapezoidal rule.

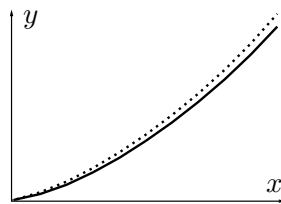
$$\text{Use } x_0 = y_0 = 0, F(x) = \cos x + 2x.$$

$$\text{Use } h = 0.1\pi.$$

The remaining 9 rows of the table are completed by calculator, following the pattern above for the second table entry. The result:

**Table 3.** Rectangular and trapezoidal solutions for  $y' = \cos x + 2x$ ,  $y(0) = 0$  on  $0 \leq x \leq \pi$ , step size  $h = 0.1\pi$ .

$x$	$y$ -rect	$y$ -trap	$x$	$y$ -rect	$y$ -trap
0.000000	0.000000	0.000000	1.884956	4.109723	4.496279
0.314159	0.314159	0.405167	2.199115	5.196995	5.638458
0.628319	0.810335	0.977727	2.513274	6.394081	6.899490
0.942478	1.459279	1.690617	2.827433	7.719058	8.300851
1.256637	2.236113	2.522358	3.141593	9.196803	9.869604
1.570796	3.122762	3.459163			



**Figure 4.** Comparison plot on  $0 \leq x \leq \pi$  of the rectangular (solid) and trapezoidal (dotted) solutions for  $y' = \cos x + 2x$ ,  $y(0) = 0$  for  $h = 0.1\pi$ .

**Computer algebra system.** The maple implementation for Example 2 appears below. Part of the interface is repetitive execution of a group, which is used here to avoid loop constructs. The code produces lists Dots1 and Dots2 which contain Rectangular (left panel) and Trapezoidal (right panel) approximations.

```
# Rectangular algorithm
# Group 1, initialize.
F:=x->evalf(cos(x) + 2*x):
x0:=0:y0:=0:h:=0.1*Pi:
Dots1:=[x0,y0]:

# Group 2, repeat 10 times
Y:=y0+h*F(x0):
x0:=x0+h:y0:=evalf(Y):
Dots1:=Dots1, [x0,y0]:

# Group 3, plot.
plot([Dots1]);

# Trapezoidal algorithm
# Group 1, initialize.
F:=x->evalf(cos(x) + 2*x):
x0:=0:y0:=0:h:=0.1*Pi:
Dots2:=[x0,y0]:

# Group 2, repeat 10 times
Y:=y0+h*(F(x0)+F(x0+h))/2:
x0:=x0+h:y0:=evalf(Y):
Dots2:=Dots2, [x0,y0]:

# Group 3, plot.
plot([Dots2]);
```

**3 Example (Simpson's Rule)** Consider  $y' = e^{-x^2}$ ,  $y(0) = 0$ . Apply both the rectangular and Simpson rules to make an  $xy$ -table for  $y(x)$  from  $x = 0$  to  $x = 1$  in steps of  $h = 0.1$ . In the table, include values for the exact solution  $y(x) = \frac{\sqrt{\pi}}{2} \operatorname{erf}(x)$ . Compare the two approximations in a graphic for  $0.8 \leq x \leq 1.0$ .

**Solution:** The error function  $\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$  is a library function available in maple, mathematica, matlab and other computing platforms. It is known that the integral cannot be expressed in terms of elementary functions.

**The  $xy$ -table.** There will be 11 rows, for  $x = 0$  to  $x = 1$  in steps of  $h = 0.1$ . There are four columns:  $x$ ,  $y$ -rectangular,  $y$ -Simpson,  $y$ -exact.

The first row arises from  $y(0) = 0$ , giving the four entries 0, 0, 0, 0. It will be shown how to obtain the second row by calculator methods, for the two algorithms *rectangular* and *Simpson*.

**Rectangular rule second entry.**

$Y1 = y_0 + hF(x_0)$ $= 0 + h(e^0)$ $= 0.1.$	Rectangular rule. Use $F(x) = e^{-x^2}$ , $x_0 = y_0 = 0$ . Use $h = 0.1$ .
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**Simpson rule second entry.**

$Y2 = y_0 + \frac{h}{6}(F(x_0) + 4F(x_1) + F(x_2))$ $= 0 + \frac{h}{6}(e^0 + 4e^{.1/2} + e^1)$ $= 0.09966770540.$	Simpson rule, $x_1 = x_0 + h/2$ , $x_2 = x_0 + h$ . Use $F(x) = e^{-x^2}$ , $x_0 = y_0 = 0$ . Use $h = 0.1$ .
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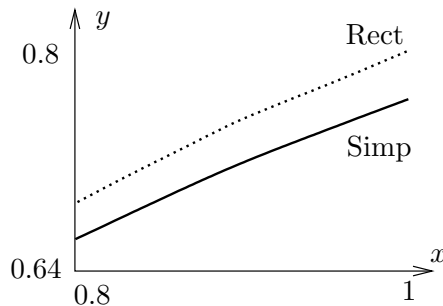
**Exact solution second entry.**

The numerical work requires the tabulated function  $\text{erf}(x)$ . The maple details:

<code>x0:=0:y0:=0:h:=0.1:</code>	Given.
<code>c:=sqrt(Pi)/2</code>	Conversion factor.
<code>Exact:=x-&gt;y0+c*erf(x):</code>	Exact solution $y = y_0 + \int_0^x e^{-t^2} dt$ .
<code>Y3:=Exact(x0+h);</code>	Calculate exact answer.
<code># Y3 := .09966766428</code>	

**Table 4. Rectangular and Simpson solutions for  $y' = e^{-x^2}$ ,  $y(0) = 0$  on  $0 \leq x \leq \pi$ , step size  $h = 0.1$ .**

$x$	$y$ -rect	$y$ -Simp	$y$ -exact
0.0	0.00000000	0.00000000	0.00000000
0.1	0.10000000	0.09966771	0.09966766
0.2	0.19900498	0.19736511	0.19736503
0.3	0.29508393	0.29123799	0.29123788
0.4	0.38647705	0.37965297	0.37965284
0.5	0.47169142	0.46128114	0.46128101
0.6	0.54957150	0.53515366	0.53515353
0.7	0.61933914	0.60068579	0.60068567
0.8	0.68060178	0.65766996	0.65766986
0.9	0.73333102	0.70624159	0.70624152
1.0	0.77781682	0.74682418	0.74682413



**Figure 5. Comparison plot on  $0.8 \leq x \leq 1.0$  of the rectangular (dotted) and Simpson (solid) solutions for  $y' = e^{-x^2}$ ,  $y(0) = 0$  for  $h = 0.1$ .**

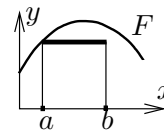
**Computer algebra system.** The maple implementation for Example 3 appears below. Part of the interface is repetitive execution of a group, which avoids loop constructs. The code produces two lists `Dots1` and `Dots2` which contain Rectangular (left panel) and Simpson (right panel) approximations.

<pre># Rectangular algorithm # Group 1, initialize. F:=x-&gt;evalf(exp(-x*x)): x0:=0:y0:=0:h:=0.1: Dots1:=[x0,y0]:  # Group 2, repeat 10 times Y:=evalf(y0+h*F(x0)): x0:=x0+h:y0:=Y: Dots1:=Dots1, [x0,y0];  # Group 3, plot. plot([Dots1]);</pre>	<pre># Simpson algorithm # Group 1, initialize. F:=x-&gt;evalf(exp(-x*x)): x0:=0:y0:=0:h:=0.1: Dots2:=[x0,y0]:  # Group 2, repeat 10 times Y:=evalf(y0+h*(F(x0)+ 4*F(x0+h/2)+F(x0+h))/6): x0:=x0+h:y0:=Y: Dots2:=Dots2, [x0,y0];  # Group 3, plot. plot([Dots2]);</pre>
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## Review of Numerical Integration

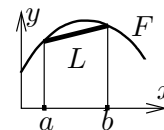
Reproduced here are calculus topics: the **rectangular rule**, the **trapezoidal rule** and **Simpson's rule** for the numerical approximation of an integral  $\int_a^b F(x)dx$ . The approximations are valid for  $b - a$  small. Larger intervals must be subdivided, then the rule applies to the small subdivisions.

**Rectangular Rule.** The approximation uses Euler's idea of replacing the integrand by a constant. The value of the integral is approximately the area of a rectangle of width  $b - a$  and height  $F(a)$ .



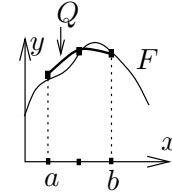
$$(2) \quad \int_a^b F(x)dx \approx (b - a)F(a).$$

**Trapezoidal Rule.** The rule replaces the integrand  $F(x)$  by a linear function  $L(x)$  which connects the planar points  $(a, F(a))$ ,  $(b, F(b))$ . The value of the integral is approximately the area under the curve  $L$ , which is the area of a trapezoid.



$$(3) \quad \int_a^b F(x)dx \approx \frac{b - a}{2} (F(a) + F(b)).$$

**Simpson's Rule.** The rule replaces the integrand  $F(x)$  by a quadratic polynomial  $Q(x)$  which connects the planar points  $(a, F(a))$ ,  $((a+b)/2, F((a+b)/2))$ ,  $(b, F(b))$ . The value of the integral is approximately the area under the quadratic curve  $Q$ .



$$(4) \quad \int_a^b F(x)dx \approx \frac{b-a}{6} \left( F(a) + 4F\left(\frac{a+b}{2}\right) + F(b) \right).$$

**Simpson's Polynomial Rule.** If  $Q(x)$  is a linear, quadratic or cubic polynomial, then (proof on page 126)

$$(5) \quad \int_a^b Q(x)dx = \frac{b-a}{6} \left( Q(a) + 4Q\left(\frac{a+b}{2}\right) + Q(b) \right).$$

Integrals of linear, quadratic and cubic polynomials can be evaluated *exactly* using Simpson's polynomial rule (5); see Example 4, page 126.

**Remarks on Simpson's Rule.** The right side of (4) is exactly the integral of  $Q(x)$ , which is evaluated by equation (5). The appearance of  $F$  instead of  $Q$  on the right in equation (4) is due to the relations  $Q(a) = F(a)$ ,  $Q((a+b)/2) = F((a+b)/2)$ ,  $Q(b) = F(b)$ , which arise from the requirement that  $Q$  connect three points along curve  $F$ .

The quadratic interpolation polynomial  $Q(x)$  is determined uniquely from the three data points; see *Quadratic Interpolant*, page 127, for a formula for  $Q$  and a derivation. It is interesting that Simpson's rule depends only upon the uniqueness and not upon the actual formula for  $Q$ !

**4 Example (Polynomial Quadrature)** Apply Simpson's polynomial rule (5) to verify  $\int_1^2 (x^3 - 16x^2 + 4)dx = -355/12$ .

**Solution:** The application proceeds as follows:

$$\begin{aligned} I &= \int_1^2 Q(x)dx && \text{Evaluate integral } I \text{ using } Q(x) = x^3 - 16x^2 + 4. \\ &= \frac{2-1}{6} (Q(1) + 4Q(3/2) + Q(2)) && \text{Apply Simpson's polynomial rule (5).} \\ &= \frac{1}{6} (-11 + 4(-229/8) - 52) && \text{Use } Q(x) = x^3 - 16x^2 + 4. \\ &= -\frac{355}{12}. && \text{Equality verified.} \end{aligned}$$

**Simpson's Polynomial Rule Proof.** Let  $Q(x)$  be a linear, quadratic or cubic polynomial. It will be verified that

$$(6) \quad \int_a^b Q(x)dx = \frac{b-a}{6} \left( Q(a) + 4Q\left(\frac{a+b}{2}\right) + Q(b) \right).$$



If the formula holds for polynomial  $Q$  and  $c$  is a constant, then the formula also holds for the polynomial  $cQ$ . Similarly, if the formula holds for polynomials  $Q_1$  and  $Q_2$ , then it also holds for  $Q_1 + Q_2$ . Consequently, it suffices to show that the formula is true for the special polynomials  $1, x, x^2$  and  $x^3$ , because then it holds for all combinations  $Q(x) = c_0 + c_1x + c_2x^2 + c_3x^3$ .

Only the special case  $Q(x) = x^3$  will be treated here. The other cases are left to the exercises. The details:

$\text{RHS} = \frac{b-a}{6} \left( Q(a) + 4Q\left(\frac{a+b}{2}\right) + Q(b) \right)$	Evaluate the right side of equation (6).
$= \frac{b-a}{6} \left( a^3 + \frac{1}{2}(a+b)^3 + b^3 \right)$	Substitute $Q(x) = x^3$ .
$= \frac{b-a}{6} \left( \frac{3}{2} \right) (a^3 + a^2b + ab^2 + b^3)$	Expand $(a+b)^3$ . Simplify.
$= \frac{1}{4} (b^4 - a^4),$	Multiply and simplify.
$\text{LHS} = \int_a^b Q(x) dx$	Evaluate the left hand side (LHS) of equation (6).
$= \int_a^b x^3 dx$	Substitute $Q(x) = x^3$ .
$= \frac{1}{4} (b^4 - a^4)$	Evaluate.
$= \text{RHS.}$	Compare with the RHS.

This completes the proof of Simpson's polynomial rule.

**Quadratic Interpolant  $Q$ .** Given  $a < b$  and the three data points  $(a, Y_0), ((a+b)/2, Y_1), (b, Y_2)$ , then there is a unique quadratic curve  $Q(X)$  which connects the points, given by

$$(7) \quad Q(X) = Y_0 + (4Y_1 - Y_2 - 3Y_0) \frac{X-a}{b-a} + (2Y_2 + 2Y_0 - 4Y_1) \frac{(X-a)^2}{(b-a)^2}.$$

**Proof:** The term *quadratic* is meant loosely: it can be a constant or linear function as well.

*Uniqueness* of the interpolant  $Q$  is established by subtracting two candidates to obtain a polynomial  $P$  of degree at most two which vanishes at three distinct points. By Rolle's theorem,  $P'$  vanishes at two distinct points and hence  $P''$  vanishes at one point. Writing  $P(X) = c_0 + c_1X + c_2X^2$  shows  $c_2 = 0$  and then  $c_1 = c_0 = 0$ , or briefly,  $P \equiv 0$ . Hence the two candidates are identical.

It remains to verify the given formula (7). The details are presented as two lemmas.<sup>1</sup> The first lemma contains the essential ideas. The second simply translates the variables.

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<sup>1</sup>What's a lemma? It's a helper theorem, used to dissect long proofs into short pieces.

**Lemma 1** Given  $y_1$  and  $y_2$ , define  $A = y_2 - y_1$ ,  $B = 2y_1 - y_2$ . Then the quadratic  $y = x(Ax + B)$  fits the data items  $(0, 0)$ ,  $(1, y_1)$ ,  $(2, 2y_2)$ .

**Lemma 2** Given  $Y_0, Y_1$  and  $Y_2$ , define  $y_1 = Y_1 - Y_0$ ,  $y_2 = \frac{1}{2}(Y_2 - Y_0)$ ,  $A = y_2 - y_1$ ,  $B = 2y_1 - y_2$  and  $x = 2(X - a)/(b - a)$ . Then quadratic  $Y(X) = Y_0 + x(Ax + B)$  fits the data items  $(a, Y_0)$ ,  $((a + b)/2, Y_1)$ ,  $(b, Y_2)$ .

To verify the first lemma, the formula  $y = x(Ax + B)$  is tested to go through the given data points  $(0, 0)$ ,  $(1, y_1)$  and  $(2, 2y_2)$ . For example, the last pair is tested by the steps

$$\begin{aligned} y(2) &= 2(2A + B) && \text{Apply } y = x(Ax + B) \text{ with } x = 2. \\ &= 4y_2 - 4y_1 + 4y_1 - 2y_2 && \text{Use } A = y_2 - y_1 \text{ and } B = 2y_1 - y_2. \\ &= 2y_2. && \text{Therefore, the quadratic fits data item } (2, 2y_2). \end{aligned}$$

The other two data items are tested similarly, details omitted here.

To verify the second lemma, observe that it is just a change of variables in the first lemma,  $Y = Y_0 + y$ . The data fit is checked as follows:

$$\begin{aligned} Y(b) &= Y_0 + y(2) && \text{Apply formulas } Y(X) = Y_0 + y(x), y(x) = x(Ax + B) \text{ with } X = b \text{ and } x = 2. \\ &= Y_0 + 2y_2 && \text{Apply data fit } y(2) = 2y_2. \\ &= Y_2. && \text{The quadratic fits the data item } (b, Y_2). \end{aligned}$$

The other two items are checked similarly, details omitted here. This completes the proof of the two lemmas. The formula for  $Q$  is obtained from the second lemma as  $Q = Y_0 + Bx + Ax^2$  with substitutions for  $A$ ,  $B$  and  $x$  performed to obtain the given equation for  $Q$  in terms of  $Y_0, Y_1, Y_2, a, b$  and  $X$ .

**Justification of Table 1:** The method of quadrature applied to  $y' = F(x)$ ,  $y(x_0) = y_0$  gives an explicit solution  $y(x)$  involving the integral of  $F$ . Specialize this solution formula to  $x = x_0 + h$  where  $h > 0$ . Then

$$y(x_0 + h) = y_0 + \int_{x_0}^{x_0+h} F(t) dt.$$

All three methods in Table 1 are derived by replacement of the integral above by the corresponding approximation taken from the rectangular, trapezoidal or Simpson method on page 125. For example, the trapezoidal method gives

$$\int_{x_0}^{x_0+h} F(t) dt \approx \frac{h}{2} (F(x_0) + F(x_0 + h)),$$

whereupon replacement into the formula for  $y$  gives the entry in Table 1 as

$$Y \approx y(x_0 + h) \approx y_0 + \frac{h}{2} (F(x_0) + F(x_0 + h)).$$

This completes the justification of Table 1.

### Exercises 3.1

**Simpson's Rule.** The following exercises use formulas and techniques found in the proof on page 126 and in Example 4, page 126.

19. Verify with Simpson's rule (5) for cubic polynomials the equality  $\int_1^2 (x^3 + 16x^2 + 4)dx = 541/12$ .
20. Verify with Simpson's rule (5) for cubic polynomials the equality  $\int_1^2 (x^3 + x + 14)dx = 77/4$ .
21. Let  $f(x)$  satisfy  $f(0) = 1$ ,  $f(1/2) = 6/5$ ,  $f(1) = 3/4$ . Apply Simpson's rule with one division to verify that  $\int_0^1 f(x)dx \approx 131/120$ .
22. Let  $f(x)$  satisfy  $f(0) = -1$ ,  $f(1/2) = 1$ ,  $f(1) = 2$ . Apply Simpson's rule with one division to verify that  $\int_0^1 f(x)dx \approx 5/6$ .
23. Verify Simpson's equality (5), assuming  $Q(x) = 1$  and  $Q(x) = x$ .
24. Verify Simpson's equality (5), assuming  $Q(x) = x^2$ .

**Quadratic Interpolation.** The following exercises use formulas and techniques from the proof on page 127.

25. Verify directly that the quadratic polynomial  $y = x(7 - 4x)$  goes through the points  $(0, 0)$ ,  $(1, 3)$ ,  $(2, -2)$ .
26. Verify directly that the quadratic polynomial  $y = x(8 - 5x)$  goes through the points  $(0, 0)$ ,  $(1, 3)$ ,  $(2, -4)$ .
27. Compute the quadratic interpolation polynomial  $Q(x)$  which goes through the points  $(0, 1)$ ,  $(0.5, 1.2)$ ,  $(1, 0.75)$ .
28. Compute the quadratic interpolation polynomial  $Q(x)$  which goes through the points  $(0, -1)$ ,  $(0.5, 1)$ ,  $(1, 2)$ .
29. Verify the remaining cases in Lemma 1, page 128.
30. Verify the remaining cases in Lemma 2, page 128.

## 3.2 Solving $y' = f(x, y)$ Numerically

The numerical solution of the initial value problem

$$(1) \quad y'(x) = f(x, y(x)), \quad y(x_0) = y_0$$

is studied here by three basic methods. In each case, the current table entry  $x_0, y_0$  plus step size  $h$  is used to find the next table entry  $X, Y$ . Define  $X = x_0 + h$  and let  $Y$  be defined below, according to the algorithm selected (Euler, Heun, RK4)<sup>2</sup>. The *motivation* for the three methods appears on page 135.

**Euler's method.**

$$(2) \quad Y = y_0 + hf(x_0, y_0).$$

**Heun's method.**

$$(3) \quad \begin{aligned} y_1 &= y_0 + hf(x_0, y_0), \\ Y &= y_0 + \frac{h}{2} (f(x_0, y_0) + f(x_0 + h, y_1)). \end{aligned}$$

**Runge-Kutta RK4 method.**

$$(4) \quad \begin{aligned} k_1 &= hf(x_0, y_0), \\ k_2 &= hf(x_0 + h/2, y_0 + k_1/2), \\ k_3 &= hf(x_0 + h/2, y_0 + k_2/2), \\ k_4 &= hf(x_0 + h, y_0 + k_3), \\ Y &= y_0 + \frac{k_1 + 2k_2 + 2k_3 + k_4}{6}. \end{aligned}$$

The last quantity  $Y$  contains an average of six terms, where two appear in duplicate:  $(k_1 + k_2 + k_2 + k_3 + k_3 + k_4)/6$ . A similar average appears in Simpson's rule.

**Relationship to calculus methods.** If the differential equation (1) is specialized to the equation  $y'(x) = F(x)$ ,  $y(x_0) = y_0$ , to agree with the previous section, then  $f(x, y) = F(x)$  is independent of  $y$  and the three methods of Euler, Heun and RK4 reduce to the rectangular, trapezoidal and Simpson rules.

To justify the reduction in the case of Heun's method, start with  $f(x, y) = F(x)$  and observe that by independence of  $y$ , variable  $Y_1$  is never used. Compute as follows:

$$Y = y_0 + \frac{h}{2} (f(x_0, y_0) + f(x_0 + h, Y_1)) \quad \text{Apply equation (3).}$$

<sup>2</sup>Euler is pronounced *oiler*. Heun rhymes with *coin*. Runge rhymes with *run key*.

$$= y_0 + \frac{h}{2} (F(x_0) + F(x_0 + h)). \quad \text{Use } f(x, y) = F(x).$$

The right side of the last equation is exactly the trapezoidal rule.

**5 Example (Euler's Method)** Solve  $y' = -y + 1 - x$ ,  $y(0) = 3$  by Euler's method for  $x = 0$  to  $x = 1$  in steps of  $h = 0.1$ . Produce a table of values which compares approximate and exact solutions. Graph both the exact solution  $y = 2 - x + e^{-x}$  and the approximate solution.

**Solution: Exact solution.** The homogeneous solution is  $y_h = ce^{-x}$ . A particular solution  $y_p = 2 - x$  is found by the extended equilibrium method. Initial condition  $y(0) = 3$  gives  $c = 1$  and then  $y = y_h + y_p = 2 - x + e^{-x}$ .

**Table of  $xy$ -values.** The table starts because of  $y(0) = 3$  with the two values  $X = 0, Y = 3$ . The  $X$ -values will be  $X = 0$  to  $X = 1$  in increments of  $h = 1/10$ , making 11 rows total. The  $Y$ -values are computed from

$$\begin{aligned} Y &= y_0 + hf(x_0, y_0) && \text{Euler's method.} \\ &= y_0 + h(-y_0 + 1 - x_0) && \text{Use } f(x, y) = -y + 1 - x. \\ &= 0.9y_0 + 0.1(1 - x_0) && \text{Use } h = 0.1. \end{aligned}$$

The pair  $x_0, y_0$  represents the two entries in the current row of the table. The next table pair  $X, Y$  is given by  $X = x_0 + h, Y = 0.9y_0 + 0.1(1 - x_0)$ . It is normal in a computation to do the *second pair* by hand, then use computing machinery to reproduce the hand result and finish the computation of the remaining table rows. Here's the second pair:

$$\begin{aligned} X &= x_0 + h && \text{Definition of } X\text{-values.} \\ &= 0.1, && \text{Substitute } x_0 = 0 \text{ and } h = 0.1. \\ Y &= 0.9y_0 + 0.1(1 - x_0), && \text{The simplified recurrence.} \\ &= 0.9(3) + 0.1(1 - 0) && \text{Substitute for row 1, } x_0 = 0, y_0 = 3. \\ &= 2.8. && \text{Second row found: } X = 0.1, Y = 2.8. \end{aligned}$$

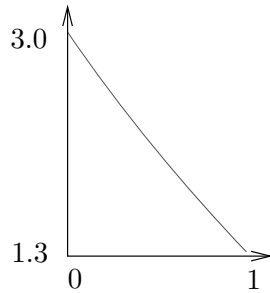
By the same process, the third row is  $X = 0.2, Y = 2.61$ . This gives the  $xy$ -table below, in which the exact values from  $y = 2 - x + e^{-x}$  are also tabulated.

**Table 5. Euler's method applied with  $h = 0.1$  on  $0 \leq x \leq 1$  to the problem  $y' = -y + 1 - x$ ,  $y(0) = 3$ .**

$x$	$y$	Exact	$x$	$y$	Exact
0.0	3.00000	3.0000000	0.6	1.93144	1.9488116
0.1	2.80000	2.8048374	0.7	1.77830	1.7965853
0.2	2.61000	2.6187308	0.8	1.63047	1.6493290
0.3	2.42900	2.4408182	0.9	1.48742	1.5065697
0.4	2.25610	2.2703200	1.0	1.34868	1.3678794
0.5	2.09049	2.1065307			

See page 133 for `maple` code which automates Euler's method. The approximate solution graphed in Figure 6 is nearly identical to the exact solution  $y = 2 - x + e^{-x}$ . The `maple` plot code for Figure 6:

```
L:= [0.0, 3.00000], [0.1, 2.80000], [0.2, 2.61000], [0.3, 2.42900],
     [0.4, 2.25610], [0.5, 2.09049], [0.6, 1.93144], [0.7, 1.77830],
     [0.8, 1.63047], [0.9, 1.48742], [1.0, 1.34868]:
plot({[L], 2-x+exp(-x)}, x=0..1);
```



**Figure 6.** Euler approximate solution for  $y' = -y + 1 - x$ ,  $y(0) = 3$  is nearly identical to the exact solution  $y = 2 - x + e^{-x}$ .

**6 Example (Euler and Heun Methods)** Solve  $y' = -y + 1 - x$ ,  $y(0) = 3$  by both Euler's method and Heun's method for  $x = 0$  to  $x = 1$  in steps of  $h = 0.1$ . Produce a table of values which compares approximate and exact solutions.

**Solution: Table of  $xy$ -values.** The Euler method was applied in Example 5. The first pair is 0, 3. The second pair  $X, Y$  will be computed by hand below.

$X = x_0 + h$	Definition of $X$ -values.
$= 0.1,$	Substitute $x_0 = 0$ and $h = 0.1$ .
$Y_1 = y_0 + hf(x_0, y_0)$	First Heun formula.
$= y_0 + 0.1(-y_0 + 1 - x_0)$	Use $f(x, y) = -y + 1 - x$ .
$= 2.8,$	Row 1 gives $x_0, y_0$ . Same as the Euler method value.
$Y = y_0 + h(f(x_0, y_0) + f(x_0 + h, Y_1))/2,$	Second Heun formula.
$= 3 + 0.05(-3 + 1 - 0 - 2.8 + 1 - 0.1)$	Use $x_0 = 0, y_0 = 3, Y_1 = 2.8$ .
$= 2.805.$	

Therefore, the second row is  $X = 0.1, Y = 2.805$ . By the same process, the third row is  $X = 0.2, Y = 2.619025$ . This gives the  $xy$ -table below, in which the exact values from  $y = 2 - x + e^{-x}$  are also tabulated.

**Table 6.** Euler and Heun methods applied with  $h = 0.1$  on  $0 \leq x \leq 1$  to the problem  $y' = -y + 1 - x$ ,  $y(0) = 3$ .

$x$	$y$ -Euler	$y$ -Heun	Exact
0.0	3.00000	3.00000	3.0000000
0.1	2.80000	2.80500	2.8048374
0.2	2.61000	2.61903	2.6187308
0.3	2.42900	2.44122	2.4408182
0.4	2.25610	2.27080	2.2703200
0.5	2.09049	2.10708	2.1065307
0.6	1.93144	1.94940	1.9488116
0.7	1.77830	1.79721	1.7965853
0.8	1.63047	1.64998	1.6493290
0.9	1.48742	1.50723	1.5065697
1.0	1.34868	1.36854	1.3678794

**Computer algebra system.** The implementation for maple appears below. Part of the interface is repetitive execution of a group, which is used here to avoid loop constructs. The code produces a list L which contains Euler (left panel) or Heun (right panel) approximations.

<pre># Euler algorithm # Group 1, initialize. f:=(x,y)-&gt;-y+1-x: x0:=0:y0:=3:h:=0.1:L:=[x0,y0]: # Group 2, repeat 10 times Y:=y0+h*f(x0,y0): x0:=x0+h:y0:=Y:L:=L,[x0,y0]: # Group 3, plot. plot([L]);</pre>	<pre># Heun algorithm # Group 1, initialize. f:=(x,y)-&gt;-y+1-x: x0:=0:y0:=3:h:=0.1:L:=[x0,y0]: # Group 2, repeat 10 times Y:=y0+h*f(x0,y0): Y:=y0+h*(f(x0,y0)+f(x0+h,Y))/2: x0:=x0+h:y0:=Y:L:=L,[x0,y0]: # Group 3, plot. plot([L]);</pre>
---	--

**Numerical laboratory.** The implementation of the Heun method for matlab, octave and scilab will be described. The code is written into files `f.m` and `heun.m`, which must reside in a default directory. Then `[X,Y]=heun(0,3,1,10)` produces the  $xy$ -table. The graphic is made with `plot(X,Y)`.

```
File f.m:      function yp = f(x,y)
                yp= -y+1-x;

File heun.m:   function [X,Y] = heun(x0,y0,x1,n)
                h=(x1-x0)/n;X=x0;Y=y0;
                for i=1:n;
                y1= y0+h*f(x0,y0);
                y0= y0+h*(f(x0,y0)+f(x0+h,y1))/2;
                x0=x0+h;
                X=[X;x0];Y=[Y;y0];
                end
```

**7 Example (Euler, Heun and RK4 Methods)** Solve  $y' = -y + 1 - x$ ,  $y(0) = 3$  by Euler's method, Heun's method and the RK4 method for  $x = 0$  to  $x = 1$  in steps of  $h = 0.1$ . Produce a table of values which compares approximate and exact solutions.

**Solution: Table of  $xy$ -values.** The Euler and Heun methods were applied in Example 6. The first pair is 0, 3. The second pair  $X, Y$  will be computed by hand calculator.

$X = x_0 + h$	Definition of $X$ -values.
$= 0.1,$	Substitute $x_0 = 0$ and $h = 0.1$ .
$k_1 = hf(x_0, y_0)$	First RK4 formula.
$= 0.1(-y_0 + 1 - x_0)$	Use $f(x, y) = -y + 1 - x$ .
$= -0.2,$	Row 1 supplies $x_0, y_0$ .
$k_2 = hf(x_0 + h/2, y_0 + k_1/2)$	Second RK4 formula.
$= 0.1f(0.05, 2.9)$	
$= -0.195,$	
$k_3 = hf(x_0 + h/2, y_0 + k_2/2)$	Third RK4 formula.
$= 0.1f(0.05, 2.9025)$	
$= -0.19525,$	
$k_4 = hf(x_0 + h, y_0 + k_3)$	Fourth RK4 formula.
$= 0.1f(0.1, 2.80475)$	
$= -0.190475,$	
$Y = y_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4),$	Last RK4 formula.
$= 3 + \frac{1}{6}(-1.170975)$	Use $x_0 = 0, y_0 = 3, Y_1 = 2.8$ .
$= 2.8048375.$	

Therefore, the second row is  $X = 0.1, Y = 2.8048375$ . Continuing, the third row is  $X = 0.2, Y = 2.6187309$ . This gives the  $xy$ -table below, in which the exact values from  $y = 2 - x + e^{-x}$  are also tabulated.

**Table 7. Euler, Heun and RK4 methods applied with  $h = 0.1$  on  $0 \leq x \leq 1$  to the problem  $y' = -y + 1 - x, y(0) = 3$ .**

$x$	$y$ -Euler	$y$ -Heun	$y$ -RK4	Exact
0.0	3.00000	3.00000	3.0000000	3.0000000
0.1	2.80000	2.80500	2.8048375	2.8048374
0.2	2.61000	2.61903	2.6187309	2.6187308
0.3	2.42900	2.44122	2.4408184	2.4408182
0.4	2.25610	2.27080	2.2703203	2.2703200
0.5	2.09049	2.10708	2.1065309	2.1065307
0.6	1.93144	1.94940	1.9488119	1.9488116
0.7	1.77830	1.79721	1.7965856	1.7965853
0.8	1.63047	1.64998	1.6493293	1.6493290
0.9	1.48742	1.50723	1.5065700	1.5065697
1.0	1.34868	1.36854	1.3678798	1.3678794

**Computer algebra system.** The implementation of RK4 for `maple` appears below, as a modification of the code for Example 6.



```
# Group 2, repeat 10 times.
k1:=h*f(x0,y0):
k2:=h*f(x0+h/2,y0+k1/2):
k3:=h*f(x0+h/2,y0+k2/2):
k4:=h*f(x0+h,y0+k3):
Y:=y0+(k1+2*k2+2*k3+k4)/6:
x0:=x0+h:y0:=Y:L:=L,[x0,y0];
```

**Numerical laboratory.** The implementation of RK4 for `matlab`, `octave` and `scilab` appears below, to be added to the code for Example 6. The code is written into file `rk4.m`, which must reside in a default directory. Then `[X,Y]=rk4(0,3,1,10)` produces the  $xy$ -table.

```
function [X,Y] = rk4(x0,y0,x1,n)
h=(x1-x0)/n;X=x0;Y=y0;
for i=1:n;
    k1=h*f(x0,y0);
    k2=h*f(x0+h/2,y0+k1/2);
    k3=h*f(x0+h/2,y0+k2/2);
    k4=h*f(x0+h,y0+k3);
    y0=y0+(k1+2*k2+2*k3+k4)/6;
    x0=x0+h;
    X=[X;x0];Y=[Y;y0];
end
```

**Motivation for the three methods.** The entry point to the study is the equivalent integral equation

$$(5) \quad y(x) = y_0 + \int_{x_0}^x f(t, y(t)) dt.$$

The ideas can be explained by replacement of the integral in (5) by the rectangular, trapezoidal or Simpson rule. Unknown values of  $y$  that appear are subsequently replaced by suitable approximations. These approximations, known as **predictors** and **correctors**, are defined as follows from the integral formula  $y(b) = y(a) + \int_a^b f(x, y(x)) dx$ , by assuming the integrand is a constant  $C$  (the idea is due to Euler).

**Predictor**  $Y = y(a) + (b - a)f(a, Y^*)$ . Given an estimate or exact value  $Y^*$  for  $y(a)$ , then variable  $Y$  predicts  $y(b)$ . The approximation assumes the integrand in (5) constantly  $C = f(a, Y^*)$ .

**Corrector**  $Y = y(a) + (b - a)f(b, Y^{**})$ . Given an estimate or exact value  $Y^{**}$  for  $y(b)$ , then variable  $Y$  corrects  $y(b)$ . The approximation assumes the integrand in (5) constantly  $C = f(b, Y^{**})$ .

**Euler's method.** Replace in (5)  $x = x_0 + h$  and apply the rectangular rule to the integral. The resulting approximation is known as **Euler's method**:

$$(6) \quad y(x_0 + h) \approx Y = y_0 + hf(x_0, y_0).$$

**Heun's method.** Replace in (5)  $x = x_0 + h$  and apply the trapezoidal rule to the integral, to get

$$y(x_0 + h) \approx y_0 + \frac{h}{2} (f(x_0, y(x_0)) + f(x_0 + h, y(x_0 + h))).$$

The troublesome expressions are  $y(x_0)$  and  $y(x_0 + h)$ . The first is  $y_0$ . The second can be estimated by the **predictor**  $y_0 + hf(x_0, y_0)$ . The resulting approximation is known as **Heun's method** or the **modified Euler method**:

$$(7) \quad \begin{aligned} Y_1 &= y_0 + hf(x_0, y_0), \\ y(x_0 + h) &\approx Y = y_0 + \frac{h}{2} (f(x_0, y_0) + f(x_0 + h, Y_1)). \end{aligned}$$

**RK4 method.** Replace in (5)  $x = x_0 + h$  and apply Simpson's rule to the integral. This gives  $y(x_0 + h) \approx y_0 + S$  where the Simpson estimate  $S$  is given by

$$(8) \quad S = \frac{h}{6} (f(x_0, y(x_0)) + 4f(M, y(M)) + f(x_0 + h, y(x_0 + h)))$$

and  $M = x_0 + h/2$  is the midpoint of  $[x_0, x_0 + h]$ . The troublesome expressions in  $S$  are  $y(x_0)$ ,  $y(M)$  and  $y(x_0 + h)$ . The work of Runge and Kutta shows that

- Expression  $y(x_0)$  is replaced by  $y_0$ .
- Expression  $y(M)$  can be replaced by either  $Y_1$  or  $Y_2$ , where  $Y_1 = y_0 + 0.5hf(x_0, y_0)$  is a **predictor** and  $Y_2 = y_0 + 0.5hf(M, Y_1)$  is a **corrector**.
- Expression  $y(x_0 + h)$  can be replaced by  $Y_3 = y_0 + hf(M, Y_2)$ . This replacement arises from the **predictor**  $y(x_0 + h) \approx y(M) + 0.5hf(M, y(M))$  by using **corrector**  $y(M) \approx y_0 + 0.5hf(M, y(M))$  and then replacing  $y(M)$  by  $Y_2$ .

The formulas of Runge-Kutta result by using the above replacements for  $y(x_0)$ ,  $y(M)$  and  $y(x_0 + h)$ , with the caveat that  $f(M, y(M))$  gets replaced by the **average** of  $f(M, Y_1)$  and  $f(M, Y_2)$ . In detail,

$$\begin{aligned} 6S &= hf(x_0, y(x_0)) + 4hf(M, y(M)) + hf(x_0 + h, y(x_0 + h)) \\ &\approx hf(x_0, y_0) + 4h \frac{f(M, Y_1) + f(M, Y_2)}{2} + hf(x_0 + h, Y_3) \\ &= k_1 + 2k_2 + 2k_3 + k_4 \end{aligned}$$

where the RK4 quantities  $k_1, k_2, k_3, k_4$  are defined by (4), page 130. The resulting approximation is known as the **RK4 method**.