

## **Instructions**

- You may rip off the last three pages as soon as you sit down.
- There are 53 marks available. It will be marked out of 50.
- No aides.
- Turn off all electronic media and store them under your desk.
- You may ask only one question during the examination: “May I go to the washroom?”
- Asking any other question will result in a deduction of 5 marks from the exam grade.
- If you think a question is ambiguous, write down your assumptions and continue.
- Do not leave during first hour or after there are only 15 minutes left.
- Do not stand up until all exams have been picked up.
- There are questions on both sides of the pages.
- If a question only asks for an answer, you do not have to show your work to get full marks; however, if your answer is wrong and no rough work is presented to show your steps, no part marks will be awarded.
- Answer the questions in the spaces provided. If you require additional space to answer a question, please use the provided blank page and refer to this page in your solutions.

1. [1] Multiply the following two numbers shown in the double-precision floating-point representation:

|                   |                               |
|-------------------|-------------------------------|
| c0100000000000000 | 1 100000000001 0000000000...0 |
| 3fe0000000000000  | 0 01111111110 0000000000...0  |

Each row is the same number, only the first is in the hexadecimal representation, and the second is in the binary representation. You may give your answer in either hexadecimal or in binary, as you wish.

**Solution:** The first number is  $-2^2 = -4$  and the second is  $2^{-1} = 0.5$ , so the answer is  $-2^1$ , which is c0000...0 or 1100000...0. Half a mark for the sign, and half a mark for the correct exponent. If the mantissa is anything other than all zeros, deduct half a mark.

2. [3] Show that the error of the approximation of the second derivative

$$y^{(2)}(t) \approx \frac{y(t) - 2y(t-h) + y(t-2h)}{h^2}$$

is equal to  $y^{(3)}(t)h + O(h^2)$  where you will use, for example,

$$y(t-h) = y(t) - y^{(1)}(t)h + \frac{1}{2}y^{(2)}(t)h^2 - \frac{1}{6}y^{(3)}(t)h^3 + O(h^4).$$

You should recall that  $O(16h^4) = O(h^4)$ ,  $O(h^4) \pm O(h^4) = O(h^4)$  and that, for example,  $\frac{O(h^4)}{5h} = O(h^3)$ . You must show and explain each step in your calculations. You will not be using the intermediate-value theorem.

**Solution:**

$$y(t-h) = y(t) - y^{(1)}(t)h + \frac{1}{2}y^{(2)}(t)h^2 - \frac{1}{6}y^{(3)}(t)h^3 + O(h^4)$$

$$y(t-2h) = y(t) - y^{(1)}(t)(2h) + \frac{1}{2}y^{(2)}(t)(2h)^2 - \frac{1}{6}y^{(3)}(t)(2h)^3 + O((2h)^4)$$

$$= y(t) - 2y^{(1)}(t)h + 2y^{(2)}(t)h^2 - \frac{4}{3}y^{(3)}(t)h^3 + O(h^4)$$

Adding  $-2$  times the first to the second yields

$$-2y(t-h) + y(t-2h) = -y(t) + y^{(2)}(t)h^2 - y^{(3)}(t)h^3 + O(h^4)$$

Bringing  $y(t)$  to the other side:

$$y(t) - 2y(t-h) + y(t-2h) + y^{(3)}(t)h^3 + O(h^4) = y^{(2)}(t)h^2$$

Rearranging yields

$$y^{(2)}(t)h^2 = y(t) - 2y(t-h) + y(t-2h) + y^{(3)}(t)h^3 + O(h^4)$$

$$y^{(2)}(t) = \frac{y(t) - 2y(t-h) + y(t-2h)}{h^2} + y^{(3)}(t)h + O(h^2)$$

(a) One mark for correctly writing out the expansion of  $y(t-2h)$ .

(b) One mark for adding the two equations together.

(c) One mark for isolating the second derivative, dividing by  $h^2$ , and getting the result.

Do not give marks out if they get the correct answer at the end without clearly showing that they got to the solution correctly. On the mid-term, some students wrote the correct result, but their calculations demonstrated that they did not actually arrive at that solution.

3. [4] Write down the system of linear equations as a numeric augmented matrix that must be solved to find  $\Delta \mathbf{u}_0$  when trying to find the minimum of the function

$$x^4 + y^4 + z^4 + xyz + xy - 2yz$$

where  $\mathbf{u} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$  and when using the gradient and Newton's method starting with the initial approximation  $\mathbf{u}_0 = \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}$ .

Assume the solution to the system of linear equations is  $\Delta \mathbf{u}_0 = \begin{pmatrix} 0.19 \\ -0.06 \\ -0.11 \end{pmatrix}$ . What is the next approximation of the minimum  $\mathbf{u}_1$ ?

**Solution:** The gradient is

$$\vec{\nabla}(\mathbf{f})(\mathbf{u}) = \begin{pmatrix} 4x^3 + yz + y \\ 4y^3 + xz + x - 2z \\ 4z^3 + xy - 2y \end{pmatrix}$$

The Jacobian of the gradient is

$$J(\vec{\nabla}(\mathbf{f}))(\mathbf{u}) = \begin{pmatrix} 12x^2 & z + 1 & y \\ z + 1 & 12y^2 & x - 2 \\ y & x - 2 & 12z^2 \end{pmatrix}$$

Evaluating these at  $\mathbf{u}_0$ , we have that we are solving

$$J(\vec{\nabla})(\mathbf{f})(\mathbf{u}) = \begin{pmatrix} 12 & 2 & 1 \\ 2 & 12 & -3 \\ 1 & -3 & 12 \end{pmatrix} \Delta \mathbf{u}_0 = \begin{pmatrix} 2 \\ 0 \\ -1 \end{pmatrix}$$

The given value of  $\Delta \mathbf{u}_0$  is very close to the solution, so a student could theoretically check their solution.

Thus,  $\mathbf{u}_1 = \begin{pmatrix} 0.81 \\ 0.94 \\ 0.89 \end{pmatrix}$ .

- (a) One mark for correctly or almost correctly calculating the gradient by taking the three partial derivatives. Ignore one or two very small errors, but for habitual mistakes, take off half a mark and if it is not even close to the correct answer, a full mark.
- (b) One mark for correctly or almost correctly calculating the Jacobian of the gradient.
- (c) One mark for correctly substituting the values (please try to take into account previous mistakes). It is important that the right-hand vector must be  $-\vec{\nabla}(\mathbf{f})(\mathbf{u}_0)$ , so half a mark off if the student forgets to negate the vector entries.
- (d) One mark for correctly calculating  $\mathbf{u}_1$ .

4. [3] Show that one step of Newton's method for finding the root of a real-valued function of a real variable is  $O(h^2)$  where  $h = r - x_k$  if  $x_k$  is the current approximation of the root  $r$  using this method. You will show that  $r - x_{k+1}$  is a scalar multiple of  $(r - x_k)^2$  and finding that scalar multiple. Recall that

$$f(r) = f(x_k) + f^{(1)}(x_k)(r - x_k) + \frac{1}{2}f^{(2)}(\xi)(r - x_k)^2.$$

**Solution:**

$$\begin{aligned} f(r) &= f(x_k) + f^{(1)}(x_k)(r - x_k) + \frac{1}{2}f^{(2)}(\xi)(r - x_k)^2 \\ 0 &= f(x_k) + f^{(1)}(x_k)(r - x_k) + \frac{1}{2}f^{(2)}(\xi)(r - x_k)^2 \\ 0 &= \frac{f(x_k)}{f^{(1)}(x_k)} + r - x_k + \frac{1}{2}\frac{f^{(2)}(\xi)}{f^{(1)}(x_k)}(r - x_k)^2 \\ \frac{1}{2}\frac{f^{(2)}(\xi)}{f^{(1)}(x_k)}(r - x_k)^2 &= r - \left(x_k - \frac{f(x_k)}{f^{(1)}(x_k)}\right) \\ \frac{1}{2}\frac{f^{(2)}(\xi)}{f^{(1)}(x_k)}(r - x_k)^2 &= r - x_{k+1} \end{aligned}$$

The scalar multiple is  $\frac{1}{2}\frac{f^{(2)}(\xi)}{f^{(1)}(x_k)}$ .

- (a) One mark for having  $f(r) = 0$  and dividing by  $f^{(1)}(x_k)$ .
- (b) One mark for rewriting the expressions so that it is clear that we have one step of Newton's method through  $x_k - \frac{f(x_k)}{f^{(1)}(x_k)}$
- (c) One mark for clearly deducing the scalar multiple. The student doesn't have to explicitly point it out, but they should show that  $r - x_{k+1} = C(r - x_k)^2$ .

5. [1] If  $\mathbf{x}_5 = \begin{pmatrix} 1.5 \\ -1.2 \\ 1.8 \\ 2.4 \end{pmatrix}$  is one approximation of a solution to a system of linear equations, and

our next approximation is  $\mathbf{x}_6 = \begin{pmatrix} 1.2 \\ -1.4 \\ 1.7 \\ 2.5 \end{pmatrix}$  is our next approximation, suppose we want to use

successive over-relaxation by going an extra 10% in the direction of the better approximation. Find the updated vector  $\mathbf{x}_6$ .

6. [2] Use the 4<sup>th</sup>-order Runge Kutta method to approximate  $y(0.2)$  with  $h = 0.2$  for the initial-value problem

$$y^{(1)}(t) = 3t(t - 0.1)y(t)$$

with the initial condition  $y(0) = -2$ .

**Solution:**

$$s_0 \leftarrow f(0, -2) = 0$$

$$s_1 \leftarrow f(0.1, -2 + 0.1s_0) = f(0.1, -2) = 0$$

$$s_2 \leftarrow f(0.1, -2 + 0.1s_1) = f(0.1, -2) = 0$$

$$s_3 \leftarrow f(0.2, -2 + 0.1s_2) = f(0.2, -2) = 3 \cdot 0.2 \cdot 0.1 \cdot -2 = -0.12$$

$$y_1 \leftarrow -2 + 0.2 \frac{0 + 2 \cdot 0 + 2 \cdot 0 - 0.12}{6} = -2 - 0.004 = -2.004$$

- (a) One mark for correctly determining that the slopes are evaluated at  $(0, -2)$ ,  $(0.1, -2)$ ,  $(0.1, -2)$  and  $(0.2, -2)$ , getting the slopes to be the values shown. Ignore minor little errors in arithmetic, but don't ignore incorrect applications of the formulas.
- (b) One mark for correctly calculating  $y_1$ , but take into account any mistakes in the calculations above.

7. [4] Given the system of initial-value problems

$$\mathbf{y}^{(1)}(t) = \begin{pmatrix} y_1(t) + y_2(t) \\ y_1(t) - y_2(t) \end{pmatrix}$$

with the initial condition  $\mathbf{y}(0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ , perform one step of the Euler-Heun adaptive solving method with  $h = 0.1$  and determine the scaling factor  $a$  if the maximum error we are willing to accept per unit time is  $\epsilon_{\text{abs}} = 0.25$ , determine whether or not the approximation you found is sufficiently accurate, and in either case, determine what is the value of  $h$  you will use with the next iteration? Note: all calculations are straight-forward and can be easily done by hand.

**Solution:**

$$\mathbf{s}_0 = \mathbf{f}(0, \mathbf{y}_0) = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\mathbf{s}_1 = \mathbf{f}(0.1, \mathbf{y}_0 + 0.1\mathbf{s}_0) = \mathbf{f}\left(0.1, \begin{pmatrix} 0 \\ 1 \end{pmatrix} + 0.1 \begin{pmatrix} 1 \\ -1 \end{pmatrix}\right) = \mathbf{f}\left(0.1, \begin{pmatrix} 0.1 \\ 0.9 \end{pmatrix}\right) = \begin{pmatrix} 1 \\ -0.8 \end{pmatrix}$$

Thus, we have that

$$\mathbf{y} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} + 0.1 \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 0.1 \\ 0.9 \end{pmatrix}$$

and

$$\mathbf{z} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} + 0.1 \begin{pmatrix} 1 \\ -0.9 \end{pmatrix} = \begin{pmatrix} 0.1 \\ 0.91 \end{pmatrix}$$

Thus,  $\|\mathbf{y} - \mathbf{z}\|_2 = \left\| \begin{pmatrix} 0 \\ 0.01 \end{pmatrix} \right\| = 0.01$ , and the vector entry could be  $\pm 0.01$  depending on whether the student calculates  $\|\mathbf{y} - \mathbf{z}\|_2$  or  $\|\mathbf{z} - \mathbf{y}\|_2$ , but the 2-norm remains the same.

Thus  $a = \frac{0.1 \cdot 0.25}{0.02} = \frac{0.025}{0.02} = 1.25$ .

Therefore, the approximation is sufficiently accurate, and with the next iteration we will use the step size  $h \leftarrow 0.1 \cdot 0.9 \cdot 1.25 = 0.1125$ , but they don't have to multiply this out.

- (a) One mark for getting the two slope vectors correct.
- (b) One mark for getting the two approximations correct and correctly calculating  $\|\mathbf{y} - \mathbf{z}\|$ .
- (c) Correctly calculating  $a$  and making the appropriate deduction from its value, but do try to take into account previous errors.
- (d) One mark for writing out  $0.1 \cdot 0.9 \cdot a$ , where  $a$  is whatever value the student found previously.

8. [3] Suppose we are using Heun's method and the 4<sup>th</sup>-order Runge-Kutta method (RK4) to approximate a solution  $y(t_k + h)$  where our approximation of  $y(t_k)$  is  $y_k$ . These two techniques give us two approximations of  $y(t_k + h)$ , and let us label these as  $y$  and  $z$ , respectively. You know that Heun's method is  $O(h^3)$  for a single step and that the RK4 method for a single step is  $O(h^5)$ . Given  $y$  and  $z$ , we want to find that best scaling factor  $ah$  so that the error in approximating  $y(t + ah)$  is  $ah\epsilon_{\text{abs}}$ . Recall that for a method that is  $O(h^m)$ , this means the error  $2|y - z| \approx Ch^m$  for some  $C$ , and we want to ensure that  $C(ah)^m = ah\epsilon_{\text{abs}}$ . Find the scaling factor  $a$ . Explain why we are using  $2|y - z|$  and not just  $|y - z|$ .

**Solution:** Because one step of Heun's method is  $O(h^3)$ , then the error is  $Ch^3 \approx 2|y - z|$ , and we want  $C(ah)^3 = ah\epsilon_{\text{abs}}$ . Thus,  $a^3Ch^3 = ah\epsilon_{\text{abs}}$ . Thus, substituting in the first equation, we have  $a^32|y - z| = ah\epsilon_{\text{abs}}$ . Thus, solving this for  $a$ , we have  $a^2 = \frac{h\epsilon_{\text{abs}}}{2|y - z|}$  or

$$a = \sqrt{\frac{h\epsilon_{\text{abs}}}{2|y - z|}}.$$

We use  $|y - z|$  because  $z$  is only approximately better an approximation than  $y$ , but it is not equal to  $y(t_k + h)$ . Thus,  $|y - z|$  may underestimate the error of  $y$ , and thus we will double this difference to ensure we are overestimating and not underestimating the error of  $y$ .

- (a) One mark for correctly having  $m = 3$  in the formula  $C(ha)^m$  and substituting to get  $a^32|y - z|$ .
- (b) One mark for the isolation of  $a$  to include the square root.
- (c) One mark for a reasonable description or argument as to why we use  $2|y - z|$ , hopefully referring to not under-estimating the error, but rather over-estimating it.

9. [2] Convert this third-order initial-value problem into a system of first-order initial-value problems:

$$x^{(3)}(t) = -x(t) + x^{(1)}(t) + 1$$

$$x(0) = 11$$

$$x^{(1)}(0) = 12$$

$$x^{(2)}(0) = 13$$

**Solution:** Define  $\mathbf{w}(t) = \begin{pmatrix} w_0(t) \\ w_1(t) \\ w_2(t) \end{pmatrix} = \begin{pmatrix} x(t) \\ x^{(1)}(t) \\ x^{(2)}(t) \end{pmatrix}$  and thus

$$\mathbf{w}^{(1)}(t) = \begin{pmatrix} w_1(t) \\ w_2(t) \\ -w_0(t) + w_1(t) + 1 \end{pmatrix}$$

where  $\mathbf{w}(0) = \begin{pmatrix} 11 \\ 12 \\ 13 \end{pmatrix}$ .

- (a) One mark for correctly writing down the vector-valued system of ordinary differential equations.
- (b) One mark for the correct initial condition.

10. [3] Suppose you are approximating a solution to a boundary-value problem using the shooting method. The right boundary value is given as  $u_b = 2$ . You calculated the initial slope to be  $s_0 = 0.6$  and with this initial slope, the approximation of  $u(b) = 2.4$ . You then calculate your next slope  $s_1 = 0.1$  and with this initial slope, the approximation of  $u(b) = 1.9$ . What method would you use to calculate the next initial slope  $s_2$ , and what value is the value of  $s_2$ .

What are the halting conditions if you are given  $\epsilon_{\text{step}}$  and  $\epsilon_{\text{abs}}$ ?

**Solution:**

- (a) One mark for saying that we use the secant method.
- (b) One mark for for determining that  $s_2 = 0.2$  (however the student finds it).
- (c) One mark for something approaching: We will stop once  $|s_{k+1} - s_k| < \epsilon_{\text{step}}$  and the approximation of  $u(b)$  with the initial slope  $s_{k+1}$  is closer than  $\epsilon_{\text{abs}}$  of 2, or to use the notation in class,  $|u_{s_{k+1}}(b) - 2| < \epsilon_{\text{abs}}$ .

11. [3] Show how we get from the heat equation in one spatial dimension  $\frac{\partial}{\partial t}u(x, t) = \alpha \nabla^2 u(x, t)$  to the equation

$$u_{k,\ell+1} \leftarrow u_{k,\ell} + \alpha \Delta t \frac{u_{k-1,\ell} - 2u_{k,\ell} + u_{k+1,\ell}}{h^2}$$

Describe each step, and be sure to indicate what it is that  $u_{k,\ell}$  is approximating. You may assume that  $x_k = a + kh$  and  $t_\ell = t_0 + \ell \Delta t$ .

**Solution:** First, we are approximating  $u(x_k, t_\ell)$  with  $u_{k,\ell}$ .

Next, we realize that the Laplacian is just the second partial with respect to the space variable  $x$ .

Next, we substitute the approximations of the partial derivatives into the equation:

$$\frac{u(x_k, t_\ell + \Delta t) - u(x_k, t_\ell)}{\Delta t} = \alpha \frac{u(x_k - h, t_\ell) - 2u(x_k, t_\ell) + u(x_k + h, t_\ell)}{h^2}$$

These are now replaced with

$$\frac{u_{k,\ell+1} - u_{k,\ell}}{\Delta t} = \alpha \frac{u_{k-1,\ell} - 2u_{k,\ell} + u_{k+1,\ell}}{h^2}$$

We now multiply both sides by  $\Delta t$  and bring the one term to the right side:

$$u_{k,\ell+1} = u_{k,\ell} + \alpha \Delta t \frac{u_{k-1,\ell} - 2u_{k,\ell} + u_{k+1,\ell}}{h^2}$$

- (a) One mark for noting that we are approximating  $u(x_k, t_\ell)$  with the unknown  $u_{k,\ell}$ .
- (b) One mark for substituting in the two approximations of the partial derivatives.
- (c) One mark for replacing the variables, multiplying by  $\Delta t$  and isolating  $u_{k,\ell+1}$ .

12. [3] Assume that the initial values for a system described by the heat equation (given in the previous question) are shown as given below in the table:

| $k$ | $u_{k,0}$       | $u_{k,1}$                   |
|-----|-----------------|-----------------------------|
| 0   | $u_{0,0} = 1.5$ | $u_{0,1} = 1.5$             |
| 1   | $u_{1,0} = 1.5$ | $u_{1,1}$                   |
| 2   | $u_{2,0} = 2.5$ | $u_{2,1}$                   |
| 3   | $u_{3,0} = 3.5$ | $u_{3,1}$                   |
| 4   | $u_{4,0} = 2.5$ | $u_{4,1}$                   |
| 5   | $u_{5,0} = 1.5$ | $u_{5,1}$                   |
| 6   | $u_{6,0} = 1.5$ | $u_{6,1}$                   |
| 7   | $u_{7,0} = 1.5$ | $u_{7,1}$                   |
| 8   | $u_{8,0} = 1.5$ | $u_{8,1}(\text{insulated})$ |

Assuming  $\alpha > 0$ ,

- (a) Which entries for  $\ell = 1$  will see the value go up from the previous value at that point? Just list the  $k$  values.
- (b) Which entries for  $\ell = 1$  will see the value go down from the previous value at that point? Just list the  $k$  values.
- (c) Which entry will see the largest change from the previous value (either up or down)? Just give the  $k$  value.
- (d) What will the value of  $u_{8,1}$  at the insulated boundary be?

This question does not require any explicit calculations. Note that the correct answers are independent of  $h > 0$  and  $\Delta t > 0$ .

**Solution:** The correct solutions:

- (a)  $k = 1, 5$
- (b)  $k = 3$
- (c)  $k = 3$
- (d) 1.5

Grading. The student does not have to show how the student got any of these answers.

- (a) For the first three, starting with 2,  $-0.5$  for any missing point or any value that should not be there, to a minimum of 0.
- (b) One mark for the correct value 1.5; no formula required. If the student writes down the correct formula, but does not calculate it correctly, subtract 0.5.

13. [4] For finding an approximation of a boundary-value problem where the ordinary differential equation is linear, we converted the ordinary differential equation into a finite-difference equation that gave us a system of  $n - 1$  linear equations in the  $n - 1$  unknowns  $u_1$  through  $u_{n-1}$ . Suppose we had a non-linear second-order differential equation  $u^{(2)}(x)u(x) = \sin(x)$ . We can substitute our divided-difference approximation of the second derivative, but we then get  $u(x_k - h)u(x_k) - 2u(x_k)^2 + u(x_k + h)u(x_k) = h^2 \sin(x_k)$ , which is not a linear equation. We can still approximate  $u(x_k)$  by an unknown  $u_k$ , but how can we find approximations of  $u_k$  where  $x_k = a + kh$  and  $h = \frac{b-a}{n}$ ? Specifically, what do we do about the first and last equations

$$\begin{aligned} u(x_0)u(x_1) - 2u(x_1)^2 + u(x_2)u(x_1) &= h^2 \sin(x_1) \\ u(x_{n-2})u(x_{n-1}) - 2u(x_{n-1})^2 + u(x_n)u(x_{n-1}) &= h^2 \sin(x_{n-1}) \end{aligned}$$

the boundary conditions are Dirichlet with  $u(a) = u(x_0) = 13$  and  $u(b) = u(x_n) = 15$ ? Hint: the tools we would use were taught in this course. Please do not try to actually solve for any of the values  $u_1$  through  $u_{n-1}$ .

**Solution:** This is quite straight-forward: turn it into a root-finding problem and apply Newton's method in  $n - 1$  dimensions.

$$u_{k-1}u_k - 2u_k^2 + u_{k+1}u_k - h^2 \sin(x_k) = 0$$

with the first and last being

$$13u_1 - 2u_1^2 + u_2u_1 - h^2 \sin(x_1) = 0$$

$$u_{n-2}u_{n-1} - 2u_{n-1}^2 + 15u_{n-1} - h^2 \sin(x_{n-1}) = 0$$

We would begin with an initial approximation of the solution, so say for example,  $u_k = u_a + k \frac{u_b - u_a}{n}$ , and this would form an  $n - 1$  dimensional vector  $u_1$  through  $u_{n-1}$ . The entries of the Jacobian matrix would be, for example,

$$\begin{pmatrix} 13 - 4u_1 + u_2 & 13u_2 & 0 & \cdots & 0 & 0 \\ u_2 & u_1 - 4u_2 + u_3 & u_3u_2 & \ddots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & u_{n-1} & u_{n-2} - 4u_{n-1} + 15 \end{pmatrix}$$

- (a) One mark for saying Newton's method in  $n$  dimensions.
- (b) One mark for converting the equation into a finite difference equation depending on  $u_k$  and then specifically showing that we could substitute 13 and 15 into the appropriate positions.
- (c) Two more marks for any reasonable discussion on the matter, such as, for example, the initial guess of the solution, or the Jacobian matrix, or just one line of the Jacobian matrix. These should be two distinct ideas that demonstrate some insights into the problem.

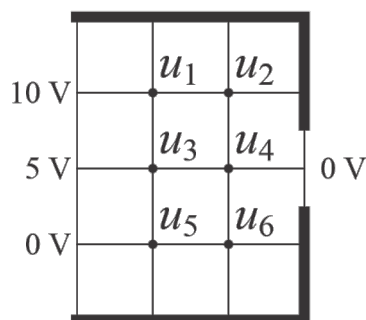


Figure 1: A rectangular region on a silicon wafer insulated along the boundary except where voltages are explicitly prescribed.

14. [2] Write down the system of linear equations as an augmented matrix that must be solved to approximate the steady-state potential in Figure 1; that is, the solution to Laplace's equation. Do not attempt to solve this system of linear equations.

**Solution:** Based on Project 4, the solution should be

$$\left( \begin{array}{cccccc|c} 3 & -1 & -1 & 0 & 0 & 0 & 10 \\ -1 & 2 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 4 & -1 & -1 & 0 & 5 \\ 0 & -1 & -1 & 4 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 3 & -1 & 0 \\ 0 & 0 & 0 & -1 & -1 & 2 & 0 \end{array} \right)$$

An alternative solution is

$$\left( \begin{array}{cccccc|c} 1 & -\frac{1}{3} & -\frac{1}{3} & 0 & 0 & 0 & \frac{10}{3} \\ -\frac{1}{2} & 1 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ -\frac{1}{4} & 0 & 1 & -\frac{1}{4} & -\frac{1}{4} & 0 & \frac{5}{4} \\ 0 & -\frac{1}{4} & -\frac{1}{4} & 1 & 0 & -\frac{1}{4} & 0 \\ 0 & 0 & -\frac{1}{3} & 0 & 1 & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & -\frac{1}{2} & 1 & 0 \end{array} \right)$$

or one could also negate all the entries.

- (a) One mark for correct diagonal entries, with only 0.5 if one or two entries are wrong, and 0 otherwise.
- (b) One mark for correct off-diagonal and vector entries, with only 0.5 if one or two entries are wrong, and 0 otherwise.

15. [4] The error of one step of Euler's method is  $\frac{1}{2}y^{(2)}(\tau)h^2$  where  $t \leq \tau \leq t+h$ . If we have the initial

condition  $y(t_0) = y_0$ , then show how we can determine that in approximating  $t_f$  with  $n$  steps has an error that is  $O(h)$ . Specifically, show how we go from summing the  $n$  errors  $\sum_{k=1}^n \frac{1}{2}y^{(2)}(\tau_k)h^2$  to  $\frac{1}{2}(t_f - t_0)hy^{(2)}(\tau)$  and explain what interval each of the  $\tau_k$  are found on, and why we know that  $t_0 \leq \tau \leq t_f$ . Recall  $h = \frac{t_f - t_0}{n}$ . Explain your reasoning and which tools you are using.

16. [1] Circle true or false. At least one of the techniques we have seen for finding minima is guaranteed to find a global minimum. True or False?

**Solution:** False.

17. [2] Apply two steps of the golden ratio to find the minimum of  $p(x) = x^2 - 13x + 16$  starting with interval  $[0, 10]$  and assuming that  $\frac{1}{\phi} = 0.6$ . Only calculate one new  $x$  value for the second step. For your information,

$$p(0) = 16, p(2) = -6, p(4) = -20, p(6) = -26, p(8) = -24, p(10) = -14$$

and

$$p(0.4) = 10.96, p(2.4) = -9.44, p(3.6) = -17.84, p(6.4) = -26.24, p(7.6) = -25.04, p(9.6) = -16.64$$

**Solution:** First,  $\ell = 4$  and  $r = 6$ , and  $p(4) = -20 > p(6) = -26$ , so discard the left boundary and continue with  $[4, 10]$ .

Second,  $\ell = 6$  while  $r = 7.6$ , and  $p(6) = -26 < p(7.6) = -25.04$ , so discard the right boundary and continue with  $[4, 7.6]$ .

- (a) One mark for calculating  $\ell$  and  $r$  correctly, and determining that we should continue with the right-hand interval  $[4, 10]$ . Half a mark off if either of these is wrong, but try to account for previous mistakes.
- (b) One mark for calculating  $\ell$  and  $r$  correctly, and determining that we should continue with the right-hand interval  $[4, 7.6]$ . Half a mark off if either of these is wrong, but try to account for previous mistakes.

18. [4] The most trivial formula to approximate a double integral would be similar to a Riemann sum:

$$\int_a^b \int_c^d f(x, y) dx dy \approx f(a, c)(b - a)(d - c)$$

Propose a better formula that could be used to approximate this double integral  $\int_a^b \int_c^d f(x, y) dx dy$ , possibly considering a generalization of the trapezoidal rule. Next, suppose we wanted a better approximation of this integral. How could you use the techniques we saw in this class to find a better approximation? You don't have to write down the explicit formulas (which likely will use a double sum), but rather, you just have to explain your ideas.

**Solution:** This is an exploratory question. Basically, give one mark per useful or distinctive idea. For example, you could use the four corner values to find the interpolating polynomial  $ax + by + cxy + d$ . Alternatively, you could divide one of the intervals, say,  $[a, b]$  into steps, and then a composite integral rule along the other interval, and then add these up.

Alternatively, you could break both of the intervals  $[a, b]$  and  $[c, d]$  into smaller parts, and apply the Riemann sum formula on each smaller rectangle, but this is worth only one mark.

I can't think of any others, but the students may surprise you.

19. [2] Suppose you found an approximation to an initial-value problem  $y^{(1)}(t) = -y(t)$  using the 4<sup>th</sup>-order Runge Kutta method where you found that with the initial condition  $y(0) = 1$ , the approximation of  $y(1)$  with a single step is  $y(1) \approx 0.375$ . Write down the system of linear equations that must be solved to find the cubic spline connecting  $(0, 1)$ ,  $(1, 0.375)$  with the slopes at these two points being given by the ordinary differential equation.

**Solution:** The cubic polynomial is  $ax^3 + bx^2 + cx + d$ , and its derivative is  $3ax^2 + 2bx + c$ . The derivatives at the two points are  $-1$  and  $-0.375$ , respectively. Thus, we have one of the two forms:

$$d = 1$$

$$c = -1$$

$$a + b + c + d = 0.375$$

$$3a + 2b + c = -0.375$$

or they may write down the matrix

$$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 \\ 3 & 2 & 1 & 0 \end{pmatrix} \mathbf{a} = \begin{pmatrix} 1 \\ -1 \\ 0.375 \\ -0.375 \end{pmatrix}$$

(a) One mark for the matrix.

(b) One mark for the vector.

Give part marks as the get close to the correct solution.

20. [2] What is the direction from the point  $\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$  that has the steepest rate of descent of the polynomial  $x^2 + 3xy + 2y^2 - 4yz + 3z^2 - x + 2z + 125432$ .

**Solution:** The gradient is  $\begin{pmatrix} 2x + 3y - 1 \\ 3x + 4y - 4z \\ -4y + 6z + 2 \end{pmatrix}$ , and this evaluated at the given point is

$$\begin{pmatrix} 2 + 6 - 1 \\ 3 + 8 - 12 \\ -8 + 18 + 2 \end{pmatrix},$$

so the direction of maximum decrease is  $\begin{pmatrix} -7 \\ 1 \\ -12 \end{pmatrix}$ .

- (a) One mark for correctly calculating the gradient (−0.5 per error in the derivative or major calculation error).
- (b) One mark for negating the vector to get the direction of maximum decrease.

USE THIS PAGE IF ADDITIONAL SPACE IS REQUIRED

Clearly state the question number being answered and refer the marker to this page.

YOU MAY RIP THESE LAST THREE PAGES OFF

**Floating-point representations:**  $\pm\text{EENMMM}$  represents  $\pm\text{N.MMM} \times 10^{\text{EE}-49}$  and the 64 bits

seeeeeeeeeeebbbbbb...b

represents

$$(-1)^s 1.\text{bbbbbb} \dots \text{b} \times 2^{\text{eeeeeeeeee}-0111111111}$$

where  $0\text{b}0111111111 = 1023 = 0\text{x}3\text{ff}$ . Recall 1 is  $+491000$  or  $0\text{x}3\text{ff}00000000000000$ .

**Fixed-point theorem:** To approximate a solution to  $x = f(x)$ , choose  $x_0$  and let  $x_k \leftarrow f(x_{k-1})$ .

**Gaussian elimination with partial pivoting:** This is the Gaussian elimination algorithm but always swapping appropriate rows so that the largest entry is in the pivot position (the row that will be used to eliminate that term in all subsequent rows).

**$n^{\text{th}}$ -order Taylor series:** If  $h$  is small, expanding around  $x$  yields:

$$f(x+h) = \left( \sum_{k=0}^n \frac{1}{k!} f^{(k)}(x) h^k \right) + \frac{1}{(n+1)!} f^{(n+1)}(\xi) h^{n+1}$$

where  $x \leq \xi \leq x+h$ . Otherwise, if  $x$  is close to  $x_0$ , expanding around  $x_0$  yields:

$$f(x) = \left( \sum_{k=0}^n \frac{1}{k!} f^{(k)}(x_0) (x-x_0)^k \right) + \frac{1}{(n+1)!} f^{(n+1)}(\xi) (x-x_0)^{n+1}$$

where  $x_0 \leq \xi \leq x$ .

```
double horner( double a[], unsigned int const degree, double const x ) {
    // The coefficient of x^k is a[k]
    double result{ a[degree] };

    for ( std::size_t k{degree - 1}; k < degree; --k ) {
        result = result*x + a[k];
    }

    return result;
}
```

**Noise:** Averaging noisy values with zero bias mitigates the effect, while differentiating noisy values magnifies the effect. Use interpolating polynomials if the data is accurate and precise, but use least squares best-fitting polynomials if the data is accurate but not precise (that is, the data has significant noise). If the data is not accurate, we cannot recover the underlying signal.

**Evaluating interpolating polynomials:** For interpolating between  $t_k$  and  $t_{k-1}$  where  $t_k$  is the time of the most recent data point, shift and scale to  $\dots, -2.5, -1.5, -0.5$  and  $0.5$  to ensure that  $-0.5 < \delta < 0.5$  to evaluate the polynomial at the point  $\frac{t_{k-1}+t_k}{2} + \delta h$  where  $h$  is the time step between readings. Note, you do not have to know these formulas explicitly; rather, you must understand the idea behind deriving these. For example, why do we shift and scale so that our choice of  $\delta$  is such that  $|\delta| < 0.5$ .

**Derivatives:**

Centered three-point:

$$f^{(1)}(x) = f^{(1)}(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{1}{6} f^{(3)}(\xi) h^2$$

Backward two-point:

$$y^{(1)}(t) = \frac{y(t) - y(t-h)}{h} + \frac{1}{2} y^{(2)}(\tau) h$$

Backward three-point:

$$y^{(1)}(t) = \frac{3y(t) - 4y(t-h) + y(t-2h)}{2h} + \frac{1}{3} y^{(3)}(t) h^2 + O(h^3)$$

**Second derivatives:**

Centered three-point:

$$f^{(2)}(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{1}{12}f^{(4)}(\xi)h^2$$

Backward three-point:

$$y^{(2)}(t) = \frac{y(t) - 2y(t-h) + y(t-2h)}{h^2} + y^{(3)}(\tau)h$$

Backward four-point:

$$y^{(2)}(t) = \frac{2y(t) - 5y(t-h) + 4y(t-2h) - y(t-3h)}{h^2} + \frac{11}{12}y^{(4)}(t)h^2 + O(h^3)$$

**Integrals:**

Two-point (trapezoidal rule):

$$\int_{x_{k-1}}^{x_k} f(x) dx = \left( \frac{1}{2}f(x_{k-1}) + \frac{1}{2}f(x_k) \right) h - \frac{1}{12}f^{(2)}(\xi)h^3$$

Centered four-point:

$$\int_{x_{k-1}}^{x_k} f(x) dx = \left( -\frac{1}{24}f(x_{k-2}) + \frac{13}{24}f(x_{k-1}) + \frac{13}{24}f(x_k) - \frac{1}{24}f(x_{k+1}) \right) h - \frac{11}{720}f^{(4)}(t_k)h^5 + O(h^6)$$

Simpson's rule:

$$\int_{x_{k-1}}^{x_{k+1}} f(x) dx = \left( \frac{1}{6}f(x_{k-1}) + \frac{4}{6}f(x_k) + \frac{1}{6}f(x_{k+1}) \right) (2h) - \frac{1}{90}f^{(4)}(\xi)h^5$$

Backward three-point (half Simpson's rule):

$$\int_{t_{k-1}}^{t_k} y(t) dx = \left( \frac{5}{12}y(t_k) + \frac{8}{12}y(t_{k-1}) - \frac{1}{12}y(t_{k-2}) \right) h - \frac{1}{24}y^{(3)}(t_k)h^4 + O(h^5)$$

Backward four-point:

$$\int_{t_{k-1}}^{t_k} y(t) dx = \left( \frac{9}{24}y(t_k) + \frac{19}{24}y(t_{k-1}) - \frac{5}{24}y(t_{k-2}) + \frac{1}{24}y(t_{k-3}) \right) h + \frac{19}{720}y^{(4)}(t_k)h^5 + O(h^6)$$

As Simpson's rule spans two time intervals, it is less useful, but it is interesting with its comparison with the trapezoidal rule applied twice versus one application of Simpson's rule.

Any integral formula can be applied repeatedly on the interval  $[a, b]$  by dividing the interval into  $n$  equally-spaced sub-intervals of width  $h = \frac{b-a}{n}$  and then setting  $x_k = a + kh$  or  $t_k = a + kh$ .

**Least squares:** In general, if we want to find the best approximation of an  $n$ -dimensional vector  $\mathbf{y}$  by a linear combination of  $m$  vectors  $\mathbf{v}_1, \dots, \mathbf{v}_m$  (where  $m < n$ ), we create the matrix  $V = (\mathbf{v}_1 \cdots \mathbf{v}_m)$  and solve  $V^T V \vec{\alpha} = V^T \mathbf{y}$ . More specific to this course, having shifted and scaled the  $n$  most recent  $t$ -values onto  $0, -1, -2, \dots, -n + 1$ , with  $y$  values  $\mathbf{y} = (y_k, y_{k-1}, y_{k-2}, \dots, y_{k-n+1})$ , we solve  $V^T V \vec{\alpha} = V^T \mathbf{y}$  for the coefficients of the least-squares best-fitting polynomial, generally of degree one (linear or  $\alpha_1 t + \alpha_0$ ) or two (quadratic or  $\alpha_2 t^2 + \alpha_1 t + \alpha_0$ ). We can find the  $2 \times n$  or  $3 \times n$  matrix to calculate  $\vec{\alpha} = (V^T V)^{-1} V^T \mathbf{y}$ .

| Value being estimated       | Linear estimation          |
|-----------------------------|----------------------------|
| $y(t_k)$                    | $\alpha_0$                 |
| $y(t_k + h)$                | $\alpha_0 + \alpha_1$      |
| $y^{(1)}(t_k)$              | $\alpha_1/h$               |
| $\int_{t_k-h}^{t_k} y(t)dt$ | $(\alpha_0 - \alpha_1/2)h$ |
| $\int_{t_k}^{t_k+h} y(t)dt$ | $(\alpha_0 + \alpha_1/2)h$ |

| Value being estimated       | Quadratic estimation                    |
|-----------------------------|-----------------------------------------|
| $y(t_k)$                    | $\alpha_0$                              |
| $y(t_k + h)$                | $\alpha_0 + \alpha_1 + \alpha_2$        |
| $y^{(1)}(t_k)$              | $\alpha_1/h$                            |
| $y^{(2)}(t_k)$              | $2\alpha_2/h^2$                         |
| $\int_{t_k-h}^{t_k} y(t)dt$ | $(\alpha_0 - \alpha_1/2 + \alpha_2/3)h$ |
| $\int_{t_k}^{t_k+h} y(t)dt$ | $(\alpha_0 + \alpha_1/2 + \alpha_2/3)h$ |

References to both binary search and interpolation search are not applicable to this course. Instead, they are introduced into the course to demonstrate parallels between the binary search and bisection method, and interpolation search and the bracketed secant method.

**Bisection:** Given an interval  $[a, b]$  with  $f(a)$  and  $f(b)$  having opposite signs, let  $m \leftarrow \frac{a+b}{2}$  and update whichever endpoint has the same sign as  $f(m)$ .  $O(h)$ .

**Bracketed secant:** Given an interval  $[a, b]$  with  $f(a)$  and  $f(b)$  having opposite signs, let  $c \leftarrow \frac{af(b)-bf(a)}{f(b)-f(a)}$  and update whichever endpoint has the same sign as  $f(c)$ .  $O(h)$ .

**Secant:** Given two initial approximations  $x_0$  and  $x_1$  with  $|f(x_0)| > |f(x_1)|$ , let  $x_2 \leftarrow \frac{x_0f(x_1)-x_1f(x_0)}{f(x_1)-f(x_0)}$ .  $O(h^{1.618})$ .

**Muller's:** Given three initial approximations, interpolate  $(x_0 - x_2, y_0)$ ,  $(x_1 - x_2, y_1)$  and  $(0, y_2)$  and find the smaller root of the interpolating quadratic, call this  $\delta$  and set  $x_3 = x_2 + \delta$ .  $O(h^{1.839})$ .

**Inverse quadratic interpolation:** Given three initial approximations, interpolate  $(y_0, x_0)$ ,  $(y_1, x_1)$  and  $(y_2, x_2)$  and find let  $x_3$  be the constant coefficient of this interpolating quadratic polynomial.  $O(h^{1.839})$ .

**Newton's:** Given an initial approximation  $x_0$ , let  $x_1 \leftarrow x_0 - \frac{f(x_0)}{f^{(1)}(x_0)}$ .  $O(h^2)$ .

**Fixed-point iteration for systems of linear equations:** Given a square  $n \times n$  matrix  $A$ , if  $D_A$  is the matrix corresponding to the diagonal entries of  $A$ , and  $A_{\text{off}}$  consists of all the off-diagonal entries of  $A$  (so  $A = D_A + A_{\text{off}}$ ), then we can rewrite  $A\mathbf{x} = \mathbf{b}$  as the equation  $\mathbf{x} = D_A^{-1}(\mathbf{b} - A_{\text{off}}\mathbf{x})$ . Let the entries of  $\mathbf{x}_k = (x_{k,1}, x_{k,2}, \dots, x_{k,n})$ .

**Jacobi:** Set  $x_k \leftarrow D_A^{-1}(\mathbf{b} - A_{\text{off}}\mathbf{x}_{k-1})$ .

**Successive over-relaxation:** Given the approximation  $x_{k-1}$  and having iterated an algorithm once more to get the approximation  $x_k$ , we can move an additional  $100\alpha\%$  in the direction of the newer approximation by updating  $x_k \leftarrow (1 + \alpha)x_k - \alpha x_{k-1}$ .

**Newton's method in two dimensions:** Given functions  $f(x, y)$  and  $g(x, y)$  and an approximation to a simultaneous root  $(x_k, y_k)$ , we can solve

$$\begin{pmatrix} \frac{\partial}{\partial x} f(x_k, y_k) & \frac{\partial}{\partial y} f(x_k, y_k) \\ \frac{\partial}{\partial x} g(x_k, y_k) & \frac{\partial}{\partial y} g(x_k, y_k) \end{pmatrix} \begin{pmatrix} \Delta x_k \\ \Delta y_k \end{pmatrix} = \begin{pmatrix} -f(x_k, y_k) \\ -g(x_k, y_k) \end{pmatrix}$$

and then let  $x_{k+1} \leftarrow x_k + \Delta x_k$  and  $y_{k+1} \leftarrow y_k + \Delta y_k$ .

**Newton's method in  $n$  dimensions:** More generally, approximating  $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ , given an approximation  $\mathbf{x}_k$ , solve  $\mathbf{J}(\mathbf{f})(\mathbf{x}_k)\Delta\mathbf{x}_k = -\mathbf{f}(\mathbf{x}_k)$  and then let  $\mathbf{x}_{k+1} \leftarrow \mathbf{x}_k + \Delta\mathbf{x}_k$ .

**Initial-value problems (IVPs):** Given the ordinary-differential equation (ODE) and initial value

$$y^{(1)}(t) = f(t, y(t)) \text{ and } y(t_0) = y_0,$$

we will approximate  $y_{k+1} \approx y(t_{k+1})$ .

Given the system of ODEs and initial values

$$\mathbf{y}^{(1)}(t) = \mathbf{f}(t, \mathbf{y}(t)) \text{ and } \mathbf{y}(t_0) = \mathbf{y}_0$$

we will approximate  $\mathbf{y}_{k+1} \approx \mathbf{y}(t_{k+1})$ .

**Euler's method:**

$$y_{k+1} \leftarrow y_k + hf(t_k, y_k) \quad \mathbf{y}_{k+1} \leftarrow \mathbf{y}_k + h\mathbf{f}(t_k, \mathbf{y}_k)$$

**Heun's method:**

$$\begin{aligned} s_0 &\leftarrow f(t_k, y_k) & \mathbf{s}_0 &\leftarrow \mathbf{f}(t_k, \mathbf{y}_k) \\ s_1 &\leftarrow f(t_k + h, y_k + hs_0) & \mathbf{s}_1 &\leftarrow \mathbf{f}(t_k + h, \mathbf{y}_k + h\mathbf{s}_0) \\ y_{k+1} &\leftarrow y_k + h\frac{s_0 + s_1}{2} & \mathbf{y}_{k+1} &\leftarrow \mathbf{y}_k + h\frac{\mathbf{s}_0 + \mathbf{s}_1}{2} \end{aligned}$$

**The 4<sup>th</sup>-order Runge-Kutta method:**

$$\begin{aligned} s_0 &\leftarrow f(t_k, y_k) & \mathbf{s}_0 &\leftarrow \mathbf{f}(t_k, \mathbf{y}_k) \\ s_1 &\leftarrow f\left(t_k + \frac{1}{2}h, y_k + \frac{1}{2}hs_0\right) & \mathbf{s}_1 &\leftarrow \mathbf{f}\left(t_k + \frac{1}{2}h, \mathbf{y}_k + \frac{1}{2}h\mathbf{s}_0\right) \\ s_2 &\leftarrow f\left(t_k + \frac{1}{2}h, y_k + \frac{1}{2}hs_1\right) & \mathbf{s}_2 &\leftarrow \mathbf{f}\left(t_k + \frac{1}{2}h, \mathbf{y}_k + \frac{1}{2}h\mathbf{s}_1\right) \\ s_3 &\leftarrow f(t_k + h, y_k + hs_2) & \mathbf{s}_3 &\leftarrow \mathbf{f}(t_k + h, \mathbf{y}_k + h\mathbf{s}_2) \\ y_{k+1} &\leftarrow y_k + h\frac{s_0 + 2s_1 + 2s_2 + s_3}{6} & \mathbf{y}_{k+1} &\leftarrow \mathbf{y}_k + h\frac{\mathbf{s}_0 + 2\mathbf{s}_1 + 2\mathbf{s}_2 + \mathbf{s}_3}{6} \end{aligned}$$

A single step of these three methods are  $O(h^2)$ ,  $O(h^3)$  and  $O(h^5)$ , respectively; however, multiple steps are one order less:  $O(h)$ ,  $O(h^2)$  and  $O(h^4)$ , respectively.

For Euler's method, the error of one step may be found from Taylor series:

$$y(t+h) = y(t) + y^{(1)}(t)h + \frac{1}{2}y^{(2)}(\tau)h^2$$

where

$$y(t_{k+1}) = y_k + f(t_k, y_k)h + \frac{1}{2}y^{(2)}(\tau)h^2$$

assuming that  $y_k$  is exact.

**The adaptive Euler-Heun method** Given an ODE and an initial value together with a maximum absolute error per unit step  $\epsilon_{\text{abs}}$ , start with an initial step size  $h$  and determine both minimum and maximum step sizes  $h_{\text{min}}$  and  $h_{\text{max}}$ , respectively. Also, let  $k \leftarrow 0$ .

1. If  $h < h_{min}$ , set  $h \leftarrow h_{min}$ , and if  $h > h_{max}$ , set  $h \leftarrow h_{max}$ .
2. Given  $y_k$ , calculate  $s_0 \leftarrow f(t_k, y_k)$  and  $s_1 \leftarrow f(t_k + h, y_k + hs_0)$ .
3. Estimate  $y(t_k + h)$  with
  - $y \leftarrow y_k + hs_0$  (the worse approximation), and
  - $z \leftarrow y_k + h \frac{s_0 + s_1}{2}$  (the better approximation).
4. Let  $a \leftarrow \frac{h\epsilon_{abs}}{2|y-z|}$ , and
  - if  $a \geq 1$  or  $h = h_{min}$ , let  $t_{k+1} \leftarrow t_k + h$  and let  $y_{k+1} \leftarrow z$  and then set  $h \leftarrow 0.9ah$  and  $k \leftarrow k + 1$ , and we will continue with the next step;
  - otherwise  $a < 1$  and we will try again.
5. If  $0.9a \leq 0.5$ , set  $h \leftarrow 0.5h$  (don't shrink  $h$  by more than a factor of two), else if  $0.9a \geq 2$ , set  $h \leftarrow 2h$  (don't grow  $h$  by more than a factor of two), else set  $h \leftarrow 0.9ah$ .

Given a system of ODEs and initial values with a similar set-up:

1. If  $h < h_{min}$ , set  $h \leftarrow h_{min}$ , and if  $h > h_{max}$ , set  $h \leftarrow h_{max}$ .
2. Given  $y_k$ , calculate  $\mathbf{s}_0 \leftarrow \mathbf{f}(t_k, \mathbf{y}_k)$  and  $\mathbf{s}_1 \leftarrow \mathbf{f}(t_k + h, \mathbf{y}_k + h\mathbf{s}_0)$ .
3. Estimate  $\mathbf{y}(t_k + h)$  with
  - $\mathbf{y} \leftarrow \mathbf{y}_k + h\mathbf{s}_0$  (the worse approximation), and
  - $\mathbf{z} \leftarrow \mathbf{y}_k + h \frac{\mathbf{s}_0 + \mathbf{s}_1}{2}$  (the better approximation).
4. Let  $a \rightarrow \frac{h\epsilon_{abs}}{2\|\mathbf{y}-\mathbf{z}\|_2}$  where  $\|\cdot\|_2$  is the 2-norm (or Euclidean norm), and
  - if  $a \geq 1$  or  $h = h_{min}$ , let  $t_{k+1} \leftarrow t_k + h$  and let  $\mathbf{y}_{k+1} \leftarrow \mathbf{z}$  and then set  $h \leftarrow 0.9ah$  and  $k \leftarrow k + 1$ , and we will continue with the next step;
  - otherwise  $a < 1$  and we will try again.
5. If  $0.9a \leq 0.5$ , set  $h \leftarrow 0.5h$  (don't shrink  $h$  by more than a factor of two), else if  $0.9a \geq 2$ , set  $h \leftarrow 2h$  (don't grow  $h$  by more than a factor of two), else set  $h \leftarrow 0.9ah$ .

**Boundary-value problems (BVPs)** Given a 2<sup>nd</sup>-order ODE  $u^{(1)}(x) = f(x, u(x), u^{(1)}(x))$  with two boundary conditions  $u(a) = u_a$  and  $u(b) = u_b$ , we can approximate a solution to this BVP as follows. First, create the IVP  $u^{(1)}(x) = f(x, u(x), u^{(1)}(x))$  with the two initial conditions  $u(a) = u_a$  and  $u^{(1)}(a) = s$  where  $s$  is an initial slope we can choose. Let us use any technique you wish (preferably Dormand Prince), and let  $u_s(x)$  be an approximation to the solution of this IVP with the initial slope  $s$ . Then the approximation of  $u(b)$  using this technique and initial slope is  $u_s(b)$ . Proceed as follows:

1. Let  $s_0 = \frac{u_b - u_a}{b - a}$  and find  $u_{s_0}(b)$ . If  $u_{s_0}(b) = u_b$ , we are done, otherwise, continue.
2. Let  $s_1 = \frac{2u_b - u_{s_0}(b) - u_a}{b - a}$  and find  $u_{s_1}(b)$ . If  $u_{s_1}(b) = u_b$ , we are done, otherwise, continue.
3. Define the function  $f(s) = u_b - u_s(b)$ , which is a function of a single variable  $s$ , and use  $s_0$  and  $s_1$  as the first two approximations for the secant method.

**Linear boundary-value problems (BVPs)** Given a 2<sup>nd</sup>-order linear ODE (LODE)  $c_2(x)u^{(2)}(x) + c_1(x)u^{(1)}(x) + c_0(x)u(x) = g(x)$  with two boundary conditions  $u(a) = u_a$  and  $u(b) = u_b$ , we convert the LODE into a linear finite-difference equation and let  $x_k = a + hk$  for  $h = \frac{b-a}{n}$ , so if we define

for each  $k = 1, \dots, n-1$  the three values  $p_k = 2c_2(x_k) - hc_1(x_k)$ ,  $q_k = -4c_2(x_k) + 2h^2c_0(x_k)$  and  $r_k = 2c_2(x_k) + hc_1(x_k)$ , we have

$$p_k u_{k-1} + q_k u_k + r_k u_{k+1} = 2h^2 g(x_k)$$

For Dirichlet boundary conditions, the corresponding linear equations are:

$$q_1 u_1 + r_1 u_2 = 2h^2 g(x_1) - p_1 u_a$$

$$p_{n-1} u_{n-2} + q_{n-1} u_{n-1} = 2h^2 g(x_{n-1}) - r_{n-1} u_b$$

For Neumann boundary conditions, the corresponding linear equations are:

$$\begin{aligned} \left(q_1 + \frac{4}{3}p_1\right) u_1 + \left(r_1 - \frac{1}{3}p_1\right) u_2 &= 2h^2 g(x_1) + \frac{2}{3}hp_1 u_a^{(1)} \\ \left(p_{n-1} - \frac{1}{3}r_{n-1}\right) u_{n-2} + \left(q_{n-1} + \frac{4}{3}r_{n-1}\right) u_{n-1} &= 2h^2 g(x_{n-1}) - \frac{2}{3}hr_{n-1} u_b^{(1)} \end{aligned}$$

after which

$$\begin{aligned} u_0 &\leftarrow -\frac{2}{3}hu_a^{(1)} + \frac{4}{3}u_1 - \frac{1}{3}u_2 \\ u_n &\leftarrow \frac{2}{3}hu_b^{(1)} + \frac{4}{3}u_{n-1} - \frac{1}{3}u_{n-2} \end{aligned}$$

and this simplifies for insulated boundary conditions where  $u_a^{(1)} = 0$  or  $u_b^{(1)} = 0$ .

**Heat equation:** For the heat equation  $\frac{\partial u}{\partial t} = \alpha \nabla^2 u$ , we have  $u_{init}(x)$ ,  $u_a(t)$  and  $u_b(t)$ , and we convert the partial-differential equation (PDE) into a finite-difference equation with  $x_k \leftarrow a + kh$  and  $t_\ell \leftarrow t_0 + \ell \Delta t$  so that  $u_{k,0} \leftarrow u_{init}(x_k)$ ,

$$u_{k,\ell+1} \leftarrow u_{k,\ell} + \frac{\alpha \Delta t}{h^2} (u_{k-1,\ell} - 2u_{k,\ell} + u_{k+1,\ell})$$

where  $u_{0,\ell} \leftarrow u_a(t_\ell)$  and  $u_{n,\ell} \leftarrow u_b(t_\ell)$ .

**Laplace's equation:** On a grid  $x_j = a_x + jh$  and  $y_k \leftarrow a_y + kh$ , we convert the PDE into the linear finite difference equation:

$$4u_{j,k} - u_{j-1,k} - u_{j+1,k} - u_{j,k-1} - u_{j,k+1} = 0$$

replacing any points on the boundary with their boundary value. Note that each value is the average of the surrounding points. If there are insulated boundaries, each entry must be the average of all the points around it that are not insulated boundary points.

**Newton's:** Use Newton's method on  $f^{(1)}(x)$ .

**Golden ratio search:** To minimize, given an interval  $[a, b]$  with a minimum on that interval, let  $m_1 \leftarrow b - (b-a)/\phi$  and  $m_2 \leftarrow a + (b-a)/\phi$  and update  $a \leftarrow m_1$  if  $f(m_2) < f(m_1)$  and update  $b \leftarrow m_2$  otherwise.

**Successive parabolic interpolation:** Formula not necessary: given three points, find the interpolating polynomial  $ax^2 + bx + c$  and let the next point be  $-\frac{b}{2a}$ .

**Newton's:** Use Newton's method on  $\vec{\nabla} f$ .

**Gradient descent:** Calculate or approximate  $\vec{\nabla} f(\mathbf{x}_k)$ , and then use a one-dimensional algorithm to find a minimum of  $f(\mathbf{x}_k - s\vec{\nabla} f(\mathbf{x}_k))$  and when we find the value  $s_k$  that gives us the minimum, set  $\mathbf{x}_{k+1} \leftarrow \mathbf{x}_k - s_k \vec{\nabla} f(\mathbf{x}_k)$ .