Queens College, CUNY, Department of Computer Science

Numerical Methods

CSCI 361 / 761

Fall 2017

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Final Exam Fall 2018

Monday Dec. 17, 2018 Solutions added

- **NOTE: It is the policy of the Computer Science Department to issue a failing grade to any student who either gives or receives help on any test.**
- This is an **open-book** test.
- Once you leave the classroom, you cannot come back to the test.
- **Any problem to which you give two or more (different) answers receives the grade of zero automatically.**
- Submit your solution in the envelope provided, with your name and student id on the cover.
  1. Write your answers in the blue book provided, with your name and student id on the cover of the blue book.
  2. If you require extra sheets of paper, write your name and student id at the top of each page and place the sheets in the envelope provided.
  3. **Answers must be written in legible handwriting: a failing grade will be awarded if the examiner is unable to decipher your handwriting.**
- Some questions require you to perform computations using a computer program.
  1. **Answers to questions which require a computer program will not be accepted if you do not submit your program code.**
  2. **Submit your program code on or before the date of the exam.**
  3. The code should implement the following:
     (a) Runge-Kutta RK4 algorithm.
     (b) Tridiagonal matrix algorithm.
  4. Programs may be written in C++ or Java.
  5. You are permitted to use the code in the online lectures (else write your own code).
  6. **You are NOT permitted to use online software (free or commercial software).**
  7. You ARE permitted to use Excel on your computer, and/or a pocket calculator.
- **Submit your program code via email, as a file attachment, to `Sateesh.Mane@qc.cuny.edu`.**

```
StudentId_first_last_CS361_final_Dec2018.zip
StudentId_first_last_CS761_final_Dec2018.zip
```

1 Question 1

- Solve the following linear equations for x_1, x_2 and x_3 using LU decomposition:

$$\begin{aligned} x_1 + 2x_2 + x_3 &= 3\,, \\ x_1 + 2x_2 + 4x_3 &= -6\,, \\ 2x_1 + 2x_2 + 3x_3 &= -1\,. \end{aligned} \tag{1.1}$$

- Write the matrix A associated with eq. (1.1).
- Write out the steps in the LU decomposition of A.
- Display the final matrix in LU form.
- Also write down the final value of the array of the swap indices.

$$(\text{swap array}) = \ldots$$

- Also write down the total number of swaps performed.
- Calculate the determinant of the matrix A.
- Solve eq. (1.1) for x_1, x_2 and x_3.

- **LU decomposition.**

1. Original matrix:

$$A = \begin{pmatrix} 1 & 2 & 1 \\ 1 & 2 & 4 \\ 2 & 2 & 3 \end{pmatrix} .$$

2. Scaled pivots, $\hat{a}_3$ is largest:

$$\hat{a}_1 = \frac{1}{2} = 0.5 \,, \qquad \hat{a}_2 = \frac{1}{4} = 0.25 \,, \qquad \hat{a}_3 = \frac{2}{3} = 0.666\ldots \quad (= \textbf{largest}) \,.$$

3. Swap rows 1 and 3. Swap array $= (3,2,1)$.

$$A_1 = \begin{pmatrix} 2 & 2 & 3 \\ 1 & 2 & 4 \\ 1 & 2 & 1 \end{pmatrix} .$$

4. Subtract (row 2)$-\frac{1}{2}\times$(row 1) and (row 3)$-\frac{1}{2}\times$(row 1), *fill in multipliers.*

$$A_2 = \begin{pmatrix} 2 & 2 & 3 \\ 0 & 1 & 2.5 \\ 0 & 1 & -0.5 \end{pmatrix} ,$$

$$A_3 = \begin{pmatrix} 2 & 2 & 3 \\ \frac{1}{2} & 1 & 2.5 \\ \frac{1}{2} & 1 & -0.5 \end{pmatrix} .$$

5. Scaled pivots, $\hat{a}'_3$ is largest:

$$\hat{a}'_2 = \frac{1}{2.5} = 0.4 \,, \qquad \hat{a}'_3 = \frac{1}{1} = 1 \quad (= \textbf{largest}) \,.$$

6. Swap rows 2 and 3. *Swap the multiplers also.* Swap array $= (3,1,2)$.

$$A_4 = \begin{pmatrix} 2 & 2 & 3 \\ \frac{1}{2} & 1 & -0.5 \\ \frac{1}{2} & 1 & 2.5 \end{pmatrix} .$$

7. Subtract (row 3)$-1\times$(row 2), *fill in multiplier.*

$$A_5 = \begin{pmatrix} 2 & 2 & 3 \\ \frac{1}{2} & 1 & -0.5 \\ \frac{1}{2} & 0 & 3 \end{pmatrix} ,$$

$$A_6 = \begin{pmatrix} 2 & 2 & 3 \\ \frac{1}{2} & 1 & -0.5 \\ \frac{1}{2} & 1 & 3 \end{pmatrix} .$$

- **Final matrix in LU form**

$$LU = \begin{pmatrix} 2 & 2 & 3 \\ 0.5 & 1 & -0.5 \\ 0.5 & 1 & 3 \end{pmatrix}, \qquad L = \begin{pmatrix} 1 & 0 & 0 \\ 0.5 & 1 & 0 \\ 0.5 & 1 & 1 \end{pmatrix}, \qquad U = \begin{pmatrix} 2 & 2 & 3 \\ 0 & 1 & -0.5 \\ 0 & 0 & 3 \end{pmatrix}.$$

- **Swap array** $(3,1,2)$ **or** $(2,0,1)$ **both are acceptable.**
- **Number of swaps = 2.**
- **Determinant** $\det(A) = (-1)^2 \det(U) = 2 \times 1 \times 3 = 6$**.**
- **Solution of equations.**
  1. **First backsubstitution** $L\boldsymbol{y} = \boldsymbol{b}_{\text{swap}}$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0.5 & 1 & 0 \\ 0.5 & 1 & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} b_3 \\ b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} -1 \\ 3 \\ -6 \end{pmatrix}.$$

  2. **Solution for** $\boldsymbol{y}$

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} -1 \\ 3.5 \\ -9 \end{pmatrix}.$$

  3. **Second backsubstitution** $U\boldsymbol{x} = \boldsymbol{y}$

$$U = \begin{pmatrix} 2 & 2 & 3 \\ 0 & 1 & -0.5 \\ 0 & 0 & 3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} -1 \\ 3.5 \\ -9 \end{pmatrix}.$$

  4. **Solution (verify by substituting into original equations)**

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 2 \\ 2 \\ -3 \end{pmatrix}.$$

- ***The solution is given by swapping the right-hand vector only.***

$$LU \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \underbrace{\begin{pmatrix} b_3 \\ b_1 \\ b_2 \end{pmatrix}}_{swap} = \begin{pmatrix} -1 \\ 3 \\ -6 \end{pmatrix} \longleftarrow \textit{swap right-hand vector only}.$$

- ***Some students swapped*** (x_1, x_2, x_3) ***as well. That is a mistake.***

$$LU \underbrace{\begin{pmatrix} x_3 \\ x_1 \\ x_2 \end{pmatrix}}_{\textit{WRONG}} \neq \begin{pmatrix} -1 \\ 3 \\ -6 \end{pmatrix}.$$

2 Question 2

- You are given the following ordinary differential equation:

$$\frac{dy}{dx} = \cos(\alpha x)\, y^{1/3}\,. \tag{2.1}$$

- The following is the exact solution of eq. (2.1) with the initial condition $y(0) = 1$.
  You do not have to prove that this is the answer.

$$y_{\text{exact}}(x) = \left[1 + \frac{2}{3\alpha}\,\sin(\alpha x)\right]^{3/2}. \tag{2.2}$$

- **Set $\alpha = \frac{1}{2}\pi$ below for this question.**
- **Calculate the value of $y_{\text{exact}}(x)$ at $x = 2$. Call this value y_* below.**
- **If you use C++, you can obtain the value of π numerically via the following code:**

```
const double pi = 4.0*atan2(1.0,1.0);
```

- **Use Runge–Kutta fourth order `RK4` to integrate eq. (2.1) from $x = 0$ to $x = 2$ with the initial condition $y(0) = 1$.**

  1. Use n steps to calculate the value of y_n, i.e. the numerical solution for $y(x)$ at $x = 2$.
  2. Set $n = 500, 600, \ldots$ and fill the table below until you find a value of n such that $|y_n - y_*| < 10^{-4}$.

n	$\lvert y_n - y_*\rvert$
500	...
600	...
$\vdots$	...
...	stop when $\lvert y_n - y_*\rvert < 10^{-4}$

- **Not much to say here.**
- **Using Java, the tolerance can be satisfied using only $n = 10$.**
- **More serious is that some students used the following function (C++ or Java).**

```
return cos(0.5 * pi * x) * std::pow(y, 1/3);
return Math.cos(0.5 * Math.PI * x) * Math.pow(y, 1/3);
```

1. ***The use of*** $1/3$ ***is*** ***integer division*** ***so the above functions really compute*** `pow(y,0)`.
2. **You should not make such a mistake.**
3. **Several students made this mistake, and I was disappointed with them.**

- **One student wrote this, and submitted weird results.** ***Pay attention.***

```
const double pi = (4.0 * atan2(1.0, 1.0))/2;
double f(double x, double y)
{
    return cos(pi * x) * std::pow(y, 1/3);
}
```

- **Jumping ahead to Question 3 (the inhomogeneous equation), one student wrote this as the answer.**

$$y(x) = \left[1 + \frac{2}{3\alpha}\sin(\alpha x)\right]^{3/2} - \beta x\,.$$

1. ***This is wrong.***
2. **The differential equation eq. (3.2) is a** ***nonlinear differential equation.***
3. **The solution of eq. (3.2) is** ***not*** **given by adding (solution of homogeneous equation)+(particular solution).**

3 Question 3

- Set $\alpha = \frac{1}{2}\pi$ below for this question.
- Multiply your student id by 10^{-8} and define β as follows (hence $0 < \beta < 1$):

$$\beta = (\text{your student id}) \times 10^{-8} \,. \tag{3.1}$$

- You are given the following ordinary differential equation:

$$\frac{dy}{dx} = \cos(\alpha x)\, y^{1/3} - \beta \,. \tag{3.2}$$

- **Use Runge–Kutta fourth order `RK4` to integrate eq. (3.2) from $x = 0$ to $x = 2$ with the initial condition $y(0) = 1$.**

  1. **Use $n = 1000$ steps** to calculate the value of y_i for $i = 1, 2, \dots, n$.
  2. **Find the value of i and x_i where y_i attains its peak (maximum) value.**
  3. Write the values of i, x_i and y_i where y_i attains its peak (maximum) value.

$$\begin{aligned} i &= \dots \\ x_i &= \dots \\ y_i &= \dots \end{aligned}$$

- Sketch a graph of $y(x)$ for $0 \le x \le 2$.

  1. *The sketch is only approximate and does not have to be "to scale" etc.*
  2. Mark the peak (values of x and y).
  3. Write the value of y_n at $x = 2$.

- **The answer depends on your student id.**
- **Fig. 1 displays a graph of the solution of eq.** (3.2) **for** $\beta = 0.2$**.**
- **For the student ids in this class, the values of** β **lie in the interval** $0.1 < \beta < 0.3$**.**
- **In this interval of values, the coordinates of the peak** $(x_{\text{peak}}, y_{\text{peak}})$ **and the end value** y_n **at** $x = 2$ **are given by the following approximate quadratic formulas.**

$$
\begin{aligned}
x_{\text{peak}} &\simeq 1.0 - 0.5223\beta - 0.1686\beta^2 \,, \\
y_{\text{peak}} &\simeq 1.7002 - 1.0715\beta + 0.2989\beta^2 \,, \\
y_n &\simeq 1.0 - 1.7975\beta + 0.1768\beta^2 \,.
\end{aligned}
$$

- **You can compute the above values using your value for** β **and compare to your numerical results. The difference may be about** 10^{-3}**.**

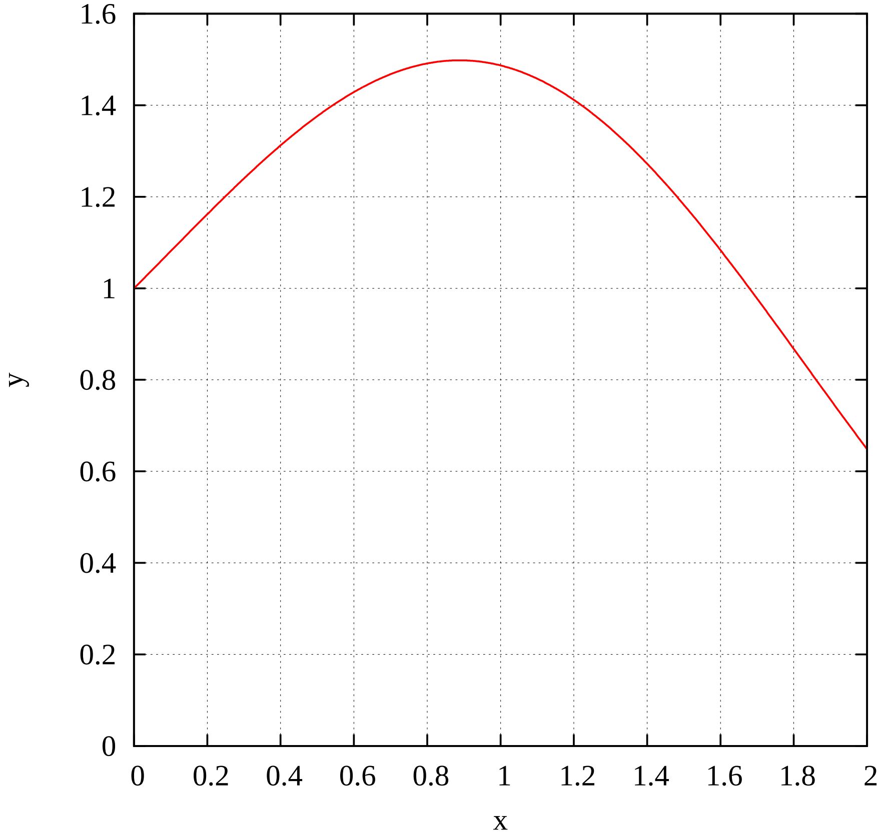

Figure 1: Graph of the solution of eq. (3.2) in Question 3 for $\beta = 0.2$.

4 Question 4

- Multiply your student id by 10^{-8} and define β as follows (hence $0 < \beta < 1$):

$$\beta = (\text{your student id}) \times 10^{-8}\,. \tag{4.1}$$

- You are given the following inhomogeneous linear second order differential equation:

$$\frac{d^2y}{dx^2} + \beta\,\frac{dy}{dx} + xy = 1\,. \tag{4.2}$$

- We shall employ the tridiagonal matrix algorithm to solve eq. (4.2) numerically.

  1. Use centered finite differences (with a stepsize h) and derive equations of the form

  $$b_i y_{i-1} + a_i y_i + c_i y_{i+1} = d_i \qquad (i = 1, \dots, n-1)\,. \tag{4.3}$$

  2. **Write the expressions for a_i, b_i, c_i and d_i below, for $1 \le i \le n-1$:**

  $$\begin{aligned} a_i &= \text{function of } (x_i, \beta, h)\,, \\ b_i &= \text{function of } (x_i, \beta, h)\,, \\ c_i &= \text{function of } (x_i, \beta, h)\,, \\ d_i &= \text{function of } (x_i, \beta, h)\,. \end{aligned}$$

  3. **For sufficiently small $|h| \ll 1$ and $x_i > 0$, show that:**

  $$|a_i| < |b_i| + |c_i|\,. \tag{4.4}$$

  4. *Hence the coefficients in eq. (4.3) are NOT diagonally dominant. Do not worry.*

- Set $n = 10000 = 10^4$ in this question.

  1. Define a set of $n+1$ equally spaced points x_i with **$x_0 = 0$ and $x_n = 10$.**
  2. Hence the interval size we shall employ in this question is $h = 10/n = 0.001$.
  3. **The boundary conditions are $y = -1$ at $x = 0$ and $y = 1$ at $x = 10$.**

- **Solve for y_i numerically using the tridiagonal matrix algorithm with eq. (4.3) and the given boundary conditions.**

- The solution for $y(x)$ crosses zero multiple times in the interval $0 \le x \le 10$.

  1. Find the values of i such that y_i and y_{i+1} have opposite signs.
  2. Then because $y(x)$ is a continuous function, it crosses zero between x_i and x_{i+1}.
  3. Fill the following table with the relevant values of i and x_i.

i	x_i
...	...
...	...
etc.	

- Sketch a graph of $y(x)$ for $0 \le x \le 10$. *An approximate sketch is sufficient.*

- **The answer depends on your student id.**
- **From the left-hand boundary condition $y(0) = -1$, the values at $i = 0$ are**

$$a_0 = 1\,, \qquad b_0 = 0\,, \qquad c_0 = 0\,, \qquad d_0 = -1\,.$$

- **The finite differences yield the following expressions for eq. (4.3), for $1 \le i < n$:**

$$\begin{aligned}
a_i &= -2 + h^2 x_i\,, \\
b_i &= 1 - \frac{h\beta}{2}\,, \\
c_i &= 1 + \frac{h\beta}{2}\,, \\
d_i &= h^2\,.
\end{aligned}$$

- **From the right-hand boundary condition $y(10) = 1$, the values at $i = n$ are**

$$a_n = 1\,, \qquad b_n = 0\,, \qquad c_n = 0\,, \qquad d_n = 1\,.$$

- **Note that the arrays have length $n + 1$, from a_0 through a_n, etc.**
- **For $1 \le i < n$ and $|h| \ll 1$ and $x > 0$, we obtain the following:**

$$\begin{aligned}
|b_i| + |c_i| &= 1 - \frac{h\beta}{2} + 1 + \frac{h\beta}{2} &&= 2\,, \\
|a_i| &= |-2 + h^2 x_i| &&= 2 - h^2 x_i &&< 2\,, \\
|a_i| &< |b_i| + |c_i|\,.
\end{aligned}$$

- **The value of $y(x)$ oscillates and crosses zero seven times in the interval $0 \le x \le 10$.**
- **Fig. 2 displays a graph of the solution of eq. (4.2) for $\beta = 0.2$.**
- **For $\beta = 0.2$, the curve crosses zero between x_i and x_{i+1}, where**

$$x_i = \{0.269,\ 2.973,\ 4.487,\ 5.950,\ 7.106,\ 8.306,\ 9.301\}\,.$$

- **Some students made the mistake of using the wrong array length.**
  1. **Remember that for n intervals, there are $n + 1$ points.**
  2. **I explained this in class.**
- **Some students did not implement the boundary conditions correctly in the first and last rows. This produced some strange graphs.**

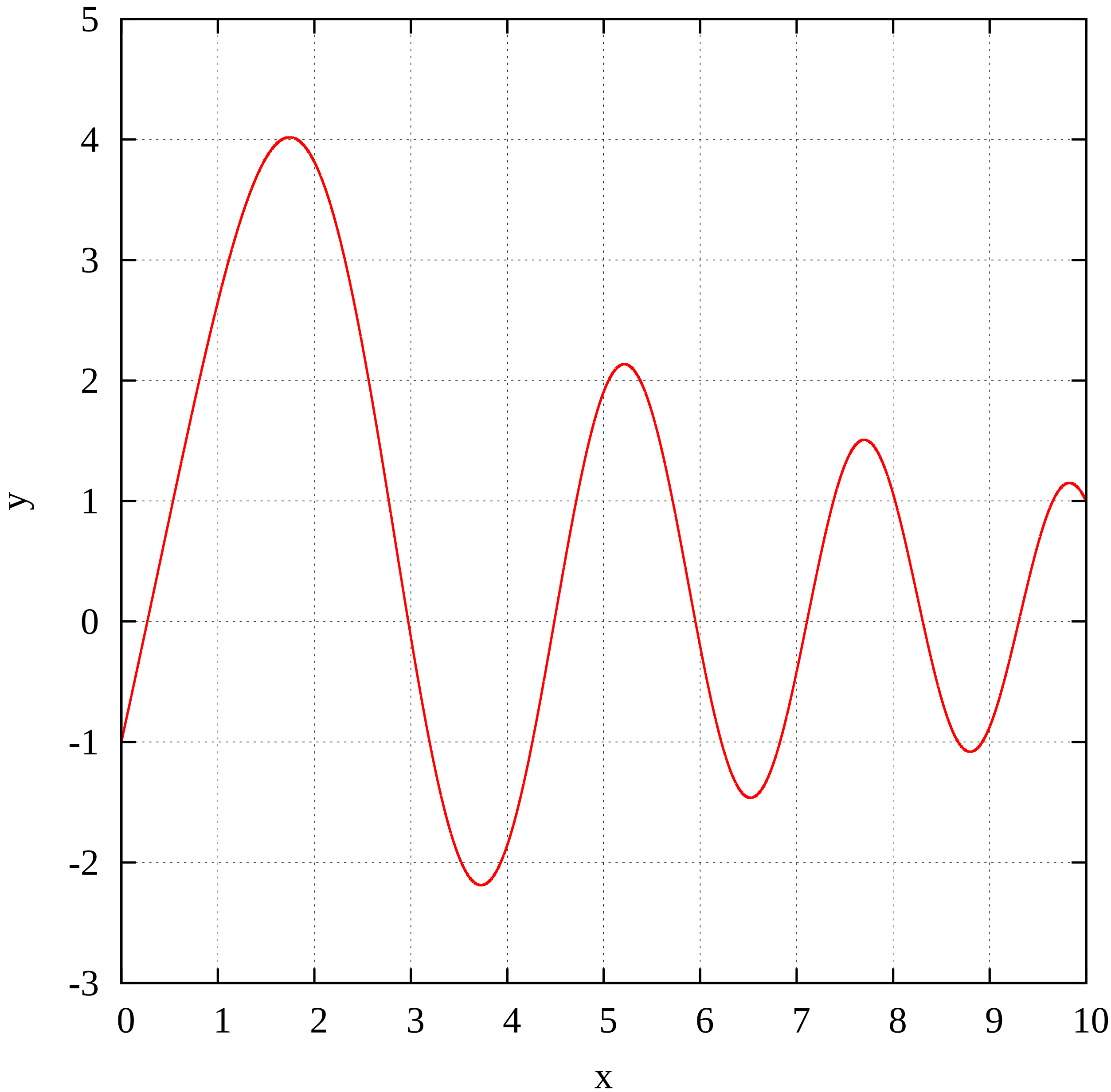

Figure 2: Graph of the solution of eq. (4.2) in Question 4 for $\beta = 0.2$.

5 Question 5

- You are given the following linear equations in the variables x_1, x_2 and x_3:

$$\begin{aligned} x_1 + 2x_2 + x_3 &= 1\,, \\ \boldsymbol{a_{21}}x_1 + 2x_2 + 7x_3 &= \boldsymbol{r_2}\,, \\ 2x_1 + 2x_2 + 3x_3 &= 3\,. \end{aligned} \tag{5.1}$$

- Here a_{21} and r_2 are constants.
- **Find the value of a_{21} such that the LU decomposition encounters a zero pivot.**
- Denote that value of a_{21} by α_{21}.
- *Hint: Process the equations "as is" and do not attempt to swap rows.*
- **Set $a_{21} = \alpha_{21}$ and then find the value of r_2 such that the equations are consistent.**
- *Note: Do NOT attempt to solve the resulting equations.*
  The equations are consistent but not linearly independent, hence there is no unique solution.

- **There are different ways to solve this. We do not have to begin with column 1.**
  1. **No swaps. Subtract (row 2)$-$(row 1) and (row 3)$-$(row 1):**

$$A_1 = \begin{pmatrix} 1 & 2 & 2 \\ a_{21}-1 & 0 & 6 \\ 1 & 0 & 2 \end{pmatrix} .$$

  2. **Subtract (row 2)$-3\times$(row 3):**

$$A_2 = \begin{pmatrix} 1 & 2 & 2 \\ a_{21}-4 & 0 & 0 \\ 1 & 0 & 2 \end{pmatrix} .$$

  3. **If all three elements in row 2 are zero, then we cannot avoid a zero pivot.**
  4. **Therefore we want $a_{21}-4=0$. The answer is**

$$a_{21} = 4 .$$

  5. **Then $\det(A)=0$, which is necessary if we cannot avoid a zero pivot.**

- ***You don't like it?* I didn't begin with column 1? Let us do it this way:**
  1. **No swaps. Subtract (row 2) $-a_{21}\times$(row 1) and (row 3) $-2\times$(row 1):**

$$A_3 = \begin{pmatrix} 1 & 2 & 2 \\ 0 & 2-2a_{21} & 7-a_{21} \\ 0 & -2 & 1 \end{pmatrix} .$$

  2. **Add (row 3) $+2/(2-2a_{21})\times$(row 2):**

$$A_4 = \begin{pmatrix} 1 & 2 & 2 \\ 0 & 2-2a_{21} & 7-a_{21} \\ 0 & 0 & 1+\frac{7-a_{21}}{1-a_{21}} \end{pmatrix} .$$

  3. **We require the last element in row 3 must equal zero. This yields the solution:**

$$\begin{aligned} 1+\frac{7-a_{21}}{1-a_{21}} &= 0 , \\ \frac{8-2a_{21}}{1-a_{21}} &= 0 , \\ 8-2a_{21} &= 0 , \\ a_{21} &= 4 . \end{aligned}$$

  4. **It is the same answer, as it must be.**

- **Some students derived $a_{21}=1$, but if you swap rows the LU decomposition does not encounter a zero pivot and $\det(A)\neq 0$ and the equations have a well-defined solution.**

- **Using $\alpha_{21} = 4$ we obtain the following.**

$$\begin{aligned}
\textbf{(row 3)} - \textbf{(row 1)} &= x_1 + 2x_3 && = 2\,, \\
\textbf{(row 2)} - \textbf{(row 3)} &= 2x_1 + 4x_3 && = r_2 - 3\,, \\
\textbf{(row 2)} + 2\textbf{(row 1)} - 3\textbf{(row 3)} &= 0 && = r_2 + 2 - 9 \qquad = r_2 - 7\,.
\end{aligned}$$

- **Therefore to obtain consistent equations we must have $r_2 = 7$.**