Project list for Integration Workshop

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Objectives:

1. Make sure each student has a basic working knowledge of Matlab, Python, Julia, or some other high-level programming language for scientific computing.
2. Make sure each student has a basic working knowledge of LaTeX.
3. Make sure students can use computational approaches to solve math problems (turning mathematics into computer code).
4. Writing, reading, and discussing algorithms in a group setting.
5. Having fun!

1 The Fredholm Alternative & Least squares solutions

Sometimes we focus too much on solving the matrix equation $A\boldsymbol{x} = \boldsymbol{b}$ for situations where A is a square matrix, and we ignore situations where A is not square. In many practical applications, A is an $m \times n$ matrix with $m \neq n$. In this problem, we're going to explore what we mean by *solutions to the matrix equation for non-square matrices.*

The Fredholm Alternative

The Fredholm alternative states that for the matrix equation $Ax = b$, exactly one of the following statements is true:

- (Either) There exists an x that solves the matrix equation $Ax = b$.
- (Or) There exists a y that solves $A^\top y = 0$ such that $y^\top b \neq 0$.

Let A_m be the $3 \times m$ matrix (below), and let b' and b'' be the 3×1 vectors (below).

$$A_m = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 2 & 3 & \cdots & m \end{bmatrix}, \qquad b' = \begin{bmatrix} -1 \\ -1 \\ +1 \end{bmatrix}, \quad b'' = \begin{bmatrix} -1 \\ 0 \\ +1 \end{bmatrix}$$

(a) Plot the vectors that make the columns of A_m for $m = 5$, and use your figure to describe the column space of A_m.

(b) Use pencil-and-paper to verify the Fredholm Alternative for b' and for b''.

(c) Plot the vectors b' and b'' on the same figure from part (a), and use your figure to provide an intuitive explanation for the Fredholm Alternative.

Pseudo-inverses & Least Squares Solutions

When there is no solution to the matrix equation $Ax = b$, we may have to make and 'executive decision' and work with the 'next best thing'. Your co-worker suggests the following matrix-algebra to find the 'next best thing'.

$$Ax = b \quad \Rightarrow \quad A^\top Ax = A^\top b \quad \Rightarrow \quad x = (A^\top A)^{-1} A^\top b$$

(d) What are the dimensions of the matrix $(A^\top A)$? What are requirements on A for the matrix $(A^\top A)$ to be invertable?

(e) For $m = 2$, find the matrix $A^\dagger := (A_m^\top A_m) A_m^\top$ and compute the vectors $x' := A^\dagger b'$ and $x'' := A^\dagger b''$.

(f) Does $Ax' = b'$? What about $Ax'' = b''$? Can you describe what we mean when we say that $A^\dagger$ gives the 'next best thing'?

(g) (Bonus) Use some calculus to verify your answer in part (f).

2 Fitting functions using Lagrange interpolating polynomials. 'Discovery' of Lagrange interpolation points.

For a sequence of points in $\mathbb{R}^2$, $\{(x_k, y_k), k = 1, \ldots, N\}$ (with $x_k \neq x_j$ whenever $k \neq j$), the *Lagrange Interpolating polynomial* is defined as

$$L(x) = \sum_{k=1}^{N} \left(\prod_{j \neq k} \frac{x - x_j}{x_k - x_j} \right) y_k. \tag{2.1}$$

We wish to determine how well a Lagrange Interpolating polynomial can approximate the functions

$$f(x) = (x - .9)(x - .4)(x + .1)(x + .7)(x + .8) \tag{2.2}$$

and

$$g(x) = \frac{1}{1 + 10x^2} \qquad \text{for } -1 \leq x \leq 1 \tag{2.3}$$

(a) The Lagrange interpolating polynomial is linear combination of N terms in the form

$$T_k(x) := \left(\prod_{j \neq k} \frac{x - x_j}{x_k - x_j} \right) \tag{2.4}$$

Let $x_1 = -1$, $x_2 = 0$, and $x_3 = 1$. Plot the functions $T_k(x)$ for $k = 1, \ldots, 3$, and describe what you see.

(b) i. Sample $f(x)$ at the points $x_1 = -1$, $x_2 = 0$, and $x_3 = 1$. Compute and plot the Lagrange Interpolating polynomial given by these 3 equi-spaced points.

ii. Repeat part (b)(i) with 5 equi-spaced points, and again with 9 equi-spaced points. Plot your results and describe whether your approximation improves with more points.

(c) Repeat part (b) for the function $g(x)$.

(d) There is a well-known rule of thumb for improving numerical approximations: Sample your function with a higher density of sample points in regions where the error is biggest. Does this rule of thumb seem to work with the functions f and g?

3 Contour Integration of a Complex-valued Function

(This problem is probably out of reach for students who not yet taken a course in complex analysis. No worries, we will cover this topic during the first few weeks of Math 583A.)

Consider the functions $f : \mathbb{C} \to \mathbb{C}$ and $g : \mathbb{C} \to \mathbb{C}$ defined as

$$f(z) = z^2 \qquad \text{and} \qquad g(z) = z^{-1}$$

(a) Plotting

(a) Make a surface plot showing $Re(f(z))$ and a surface plot showing $Im(f(z))$

(b) Make a surface plot showing $Re(g(z))$ and a surface plot showing $Im(g(z))$

Since g is undefined at $z = 0$ and since it is radially symmetric, the surface plots for g can look scary when done in cartesian co-ordinates. You may try switching to polar coordinates to make prettier plots

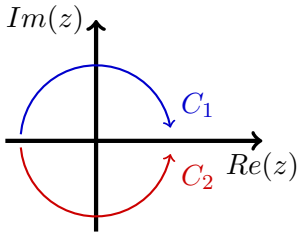
(b) We can approximate the line integral (or contour integral) of a function along a curve by discretizing the curve into $N + 1$ points $z(s) \to \{z_0, z_1, z_2, \ldots, z_N\}$ and then computing the sum:

$$\int_{z_o}^{z_t} f(z)dz \approx \sum_{k=1}^{N} f(z_k)\ (z_k - z_{k-1})$$

Define the two curves:

C_1 : The upper half circle of radius 1 centered at $z = 0$.

C_2 : The lower half circle of radius 1 centered at $z = 0$.



Approximate the line integrals of f and of g along the curves C_1 and C_2.

(c) (Bonus) Repeat (1) and (2) for the function $h(z) = z^{1/2}$.
Note: You may need to make some 'executive decisions' to make sure your problem is well-posed.

4 Forward-Euler Integrator

Consider the differential equation

$$\begin{cases} \dot{x}(t) = -y, & x(0) = 1 \\ \dot{y}(t) = \quad x, & y(0) = 0 \end{cases} \tag{4.1}$$

(Warm-up) Use pencil-and-paper to solve the ODE. Make a quiver plot. Sketch solutions.
(Project) We wish to build a numerical solver for differential equations like this one. We will test our solver on this ODE, and then use it to solve a more interesting ODE.

For this problem, we will discretize the time interval $0 \leq t \leq T$ into $n+1$ points, $t = \{t_0, t_1, \ldots, t_n\}$ with $t_k = k(\Delta t)$ so $t_0 = 0$ and $t_n = T$.

(a) For suitably small Δt (say $\Delta t = 0.1$), we can make what's called a *first-order forward difference* approximation of the derivatives $\dot{x}$ and $\dot{y}$ at each t as follows:

$$\dot{x}(t) \approx \frac{x(t+\Delta t) - x(t)}{\Delta t} \qquad \text{and} \qquad \dot{y}(t) \approx \frac{y(t+\Delta t) - y(t)}{\Delta t}. \tag{4.2}$$

Substitute equation (4.2) into equation (4.1) to show that we can approximate the differential equation by the discrete time-stepping process:

$$\begin{cases} x_{k+1} = x_k - (\Delta t) y_k, & x_0 = 1 \\ y_{k+1} = y_k + (\Delta t) x_k, & y_0 = 0 \end{cases} \tag{4.3}$$

Implement equation 4.3 for $0 \leq t \leq 1$ and plot the trajectory given by the solution. Is this approximation qualitatively correct? Will it remain qualitatively correct on $0 \leq t \leq T$ as T gets very large? Explain.

Hint: It may be useful to rewrite the system of difference equations in matrix form,

$$\boldsymbol{x}_{k+1} = \begin{bmatrix} 1 & -\Delta t \\ \Delta t & 1 \end{bmatrix} \boldsymbol{x}_k, \quad \boldsymbol{x}_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

and to analyze the eigenvalues of the matrix.

(b) We could have solved this problem by a different approach. We could also have used what's called a *first-order backward difference*:

$$\dot{x}(t) \approx \frac{x(t) - x(t-\Delta t)}{\Delta t} \qquad \text{and} \qquad \dot{y}(t) \approx \frac{y(t) - y(t\Delta t)}{\Delta t}. \tag{4.4}$$

Show that the backward difference gives the approximation

$$\begin{cases} x_k = x_{k-1} - (\Delta t) y_k, & x_0 = 1 \\ y_k = y_{k-1} + (\Delta t) x_k, & y_0 = 0 \end{cases} \tag{4.5}$$

which can be rewritten as

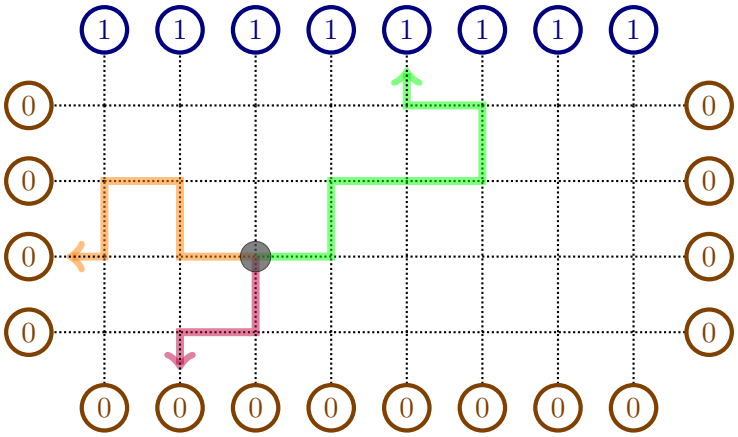
$$\boldsymbol{x}_k = \left(\begin{bmatrix} 1 & \Delta t \\ -\Delta t & 1 \end{bmatrix} \right)^{-1} \boldsymbol{x}_{k-1}, \quad \boldsymbol{x}_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Implement equation (4.5) for $0 \leq t \leq 1$ and plot the trajectory given by the solution. Is this approximation qualitatively correct? Will it remain qualitatively correct on $0 \leq t \leq T$ as T gets very large? Explain.

(c) (The really fun stuff) Perhaps solve $\dot{x} = -y$, $\dot{y} = \sin x$. Maybe this is too hard.

5 Use a random walk to solve Laplace's equation on a grid

A 'particle' takes a random walk on a 4×8 grid. At each step of the walk, the particle may move up, down, left, or right with equal probability. The particle continues this process until it exits the grid. If the particle exits the top of the grid, the particle scores 1 point for the walk. If the particle exits the left, bottom or right sides of the grid, the particle scores 0 points for the walk.



The figure shows three sample paths of the random walk that all begin at the initial point (3,2). For the red path, the particle (randomly) takes the steps $(\downarrow, \leftarrow, \downarrow)$, and exits the grid at the bottom scoring zero points for the walk. The other paths are the results of the steps listed below

Steps: $(\downarrow \leftarrow \downarrow)$	(See red path)	Exit: Bottom	Score: 0
Steps: $(\leftarrow \uparrow \leftarrow \downarrow \leftarrow)$	(See orange path)	Exit: Left	Score: 0
Steps: $(\rightarrow \uparrow \rightarrow \rightarrow \uparrow \leftarrow \uparrow)$	(See green path)	Exit: Top	Score: 1

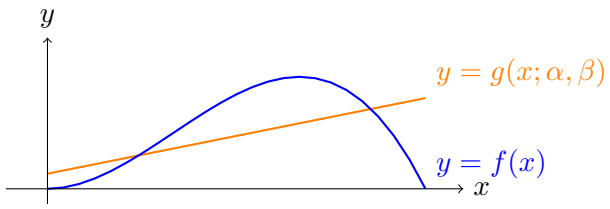
Compute the expected score of the particle as a function of the starting coordinates.

Hint: For each starting point, you may estimate the expected score of the particle by simulating many, many random paths and taking their average score.

Bonus: In this project, we have computed the solution to a problem by simulating many random events. This 'indirect' approach is always computationally inefficient, so it is often worth looking for a 'direct' approach. For this problem, there *is* a method of computing the solution directly. Can you find it?

6 Bias and Variance of fitting a function in 1-D

Let $f(x) = x^2(1-x)$ where $0 \leq x \leq 1$. We wish to find the 'best' linear model (or approximation) for f. That is, for functions in the form $g(x;\alpha,\beta) = \alpha + \beta x$, we wish to find the parameters α and β that minimize the error we would expect to incur if we used the function g to model (or approximate) the function f.



For this problem, we will define the error as

$$\text{Error}(f,g) = \int_0^1 \Big(f(x) - g(x;\alpha,\beta)\Big)^2 dx.$$

Use pencil-and-paper (or Mathematica, WolframAlpha, etc) to find a simplified expression for the error between f and g as a function of the parameters α and β. Find the values of α and β that minimize this error.

Terminology: The error we expect to incur when we use our best possible candidate is called the *bias* of the model.

In many practical applications, we only have imperfect knowledge of f, and therefore it is impossible to know the parameters of the *best possible* candidate $g(x,\alpha,\beta)$. Often, we must commit to a choice of sub-optimal parameters that are chosen after only a small glimpse of f. In this project, we will estimate how much more error we expect to incur by using an imperfect choice of parameters.

Repeat the following recipe to estimate how well a linear function parameterized by two random data points can be used to approximate f.

`Loop until you are confident you have reasonably accurate answers.`

1. `Generate two random data points on` $x_1, x_2 \in [0,1]$`.`
2. `Using only` x_1 `and` x_2`, compute a 'best guess' for parameters` α `and` β`.`
3. `Test the performance of your (sub-optimal) parameters by generating new data points and computing the mean square error on the new points. Record the mean square error.`

`Analyze the expected error by taking averages and plotting histograms.`

Terminology: The 'extra error' that we expect to typically incur by using 'best guess' parameters is called the variance of the model.

You will need to write:

1. a function that randomly generates two values in $[0, 1]$
2. a function called `train_g`.
   - Arguments (Input): Two values x_1, and x_2.
   - Functionality: Evaluate $y_1 := f(x_1)$ and $y_2 := f(x_2)$. Compute a 'best guess' for the parameters α and β given the points (x_1, y_1) and (x_2, y_2).
   - Return (Output): α and β.
3. a function called `test_g`.
   - Arguments (Input): Parameters α and β.
   - Functionality: Randomly pick N points in $[0, 1]$. For each point, x_k, evaluate $f(x_k)$ and $g(x_k; \alpha, \beta)$. Compute the average error from the N points as defined by
   $$E_N = \frac{1}{N} \sum_{k=1}^{N} \Big(f(x_k) - g(x_k, \alpha, \beta) \Big)^2$$
   - Return (Output): E_N

Someone proposes that the variance is so big that it makes the linear model unusable. They suggest that we should approximate f by a constant function $h(x; \alpha)$. Compute the new bias, and the estimate the new total error.

7 Nearest neighbors can be very far away. Curse of dimensionality

In Progress.