Name	

## Midterm 1

Due Tuesday, March 6, 2018 (in class and R Markdown file submitted to Moodle before class)

- The exam is open notes and open book. You may use the internet and library to look things up, but of course you should cite any reference you use that is not the textbook.
- It is not okay to talk to each other or anyone else about the exam! This of course includes discussing how you solve problems, but it even includes things like asking, "how is it going?" or "which problem are you working on?" or making comments like "problem 5 is easy."
- Please show and explain all of your work so that I can give you as much partial credit as possible. However, do not turn in information that is not germane to your solution.
- You are welcome to use any of the R functions in 365Functions.r
- The first 5 problems may be hand-written on this answer sheet.
- The 6th problem should be typed up in LaTeX. You should use the template provided.
- The last two problems should be submitted as a knitted html or pdf document coming from an R Markdown file that contains your code, relevant calculation output, plots, as well as your written explanations. Make sure that this file is readable and clear. You should use the R Markdown template provided. You must submit this file in Moodle as well as make a print-out as discussed below.
- All three of these documents (your handwritten answer sheet for problems 1-5, your LaTeX essay, and your html R Markdown document) should be printed out and stapled together.
- Hints: I may give a small hint or a little help with R for free. If you are stuck, I may sell a hint for points so that you can move forward. I will warn you of the point value before I sell you anything.
- I may reserve some "style" points for the clarity of your work and the quality of your computation. That is, I may possibly take some points off if you get the right answer, but do it in a confusing or clumsy or inefficient way. (It is still true, though, that it's okay to use a loop even if vectorization is possible).

Problem	Point Value	Your Score
1	7	
2	10	
3	8	
4	16	
5	8	
6	17	
7	14	
8	20	
Total	100	

Please sign the following (if you are able) and be sure to turn in this cover sheet with your exam:

I pledge my honor that I have not participated in any dishonest work on this exam, nor do I know of dishonest work done by other students on this exam.

(signature)	

- 1. (7 points) For all parts of this problem, I am using the same computer and software. I have a  $1000 \times 1000$  symmetric positive definite matrix A. On this machine, I solve  $A\mathbf{x} = \mathbf{b}$  for a particular choice of  $\mathbf{b}$  in 10 seconds.
  - (a) (4 points) I would also like to solve a second problem  $B\mathbf{y} = \mathbf{c}$  on the same machine, where B is a dense  $100000 \times 100000$  matrix without any particularly nice structure and  $\mathbf{c}$  is a  $100000 \times 1$  vector. Approximately how many hours will it take to solve  $B\mathbf{y} = \mathbf{c}$ ?

(b) (3 points) I have a third matrix C that is a  $1000 \times 1000$  dense matrix without any particularly nice structure, and I would like to solve  $C\mathbf{z} = \mathbf{d}$  for one hundred different values of  $\mathbf{d}$ . How long should I expect it to take to solve the 100 problems

$$C\mathbf{z} = \mathbf{d}_1, \quad C\mathbf{z} = \mathbf{d}_2, \quad C\mathbf{z} = \mathbf{d}_2, \quad \dots \quad , \quad C\mathbf{z} = \mathbf{d}_{100}$$

with the same C matrix and 100 different  $\mathbf{d}$  vectors, as efficiently as possible? (Just circle one answer. No justification is necessary.)

- (i) Approximately 10 seconds
- (ii) Approximately 100 seconds
- (iii) Approximately 1,000 seconds
- (iv) Approximately 10,000 seconds
- (v) Approximately 100,000 seconds
- (vi) Approximately 1,000,000,000,000 seconds

2. (10 points) Before the iPhone, there was the hPhone. Unfortunately, the hPhone had a serious design flaw. While the rest of the world was designing 32-bit and 64-bit phones, the hPhone was a 16-bit machine that used one bit for the sign, 8 bits for the mantissa, and 7 bits for the exponent:

$\pm$	m	а	ı	n 1	t :	i	S	S	a		е	X	р	
													•	

(a) (3 points) An exponent bias of 63 is used in this system, so 63 is subtracted from the stored value to get the actual exponent, or 63 is added to the actual exponent before it is stored. We are then able to store exponent values from -62 to +63 (saving -63 and +64 for subnormal numbers and INF, respectively).

Which number below is the best approximation of the largest (finite) exactly representable number on the hPhone? (Just circle one answer. No justification is necessary.)

- (i)  $10^6$
- (ii)  $10^{10}$
- (iii)  $10^{18}$
- (iv)  $10^{31}$
- $(v) 10^{63}$
- (vi)  $10^{307}$
- (b) (4 points) The decimal number -45.4375 converts to binary as -101101.0111. How will this number be stored in your machine? Make sure to show how you calculated your answer.

$\pm$	m	a	n	t	i	S	$\mathbf{S}$	a	e x p

- (c) (3 points) On the hPhone, the distance between 2<sup>8</sup> and the next largest exactly representable number after 2<sup>8</sup> is: (Just circle one answer. No justification is necessary.)
  - (i) less than the distance between 1 and the next largest exactly representable number after 1
  - (ii) the same as the distance between 1 and the next largest exactly representable number after 1
  - (iiii) greater than the distance between 1 and the next largest exactly representable number after 1

3. (8 points) Inspired by questions from the class, I went home last weekend and developed a new iterative root-finding algorithm, which I'm currently referring to as the Ziegelmeier 365i (i for ingenious). I used it to approximate the root of the function  $f(x) = (x-3)x^4$  with a starting guess of  $x^{(0)} = 0.9$ . Here is the sequence of approximations  $\left\{x^{(k)}\right\}_{k=0,1,\ldots,9}$  it generated:

k	$x^{(k)}$
0	$9.00 \cdot 10^{-1}$
1	$6.83 \cdot 10^{-1}$
2	$4.52 \cdot 10^{-1}$
3	$2.43 \cdot 10^{-1}$
4	$9.57 \cdot 10^{-2}$
5	$2.37 \cdot 10^{-2}$
6	$2.92 \cdot 10^{-3}$
7	$1.26 \cdot 10^{-4}$
8	$1.13 \cdot 10^{-6}$
9	$9.63 \cdot 10^{-10}$

(a) (4 points) What is the rate of convergence of my algorithm for this specific problem: worse than linear, linear, superlinear, quadratic, or faster than quadratic? Explain your answer.

(b) (4 points) How does this compare to the rate of convergence for Newton's method on this problem? How about the bisection method? Explain your answers.

Hint: You should NOT have to do any computations to answer this part (b).

- 4. (16 points) Let  $A = \begin{bmatrix} 1 & -1 & -1 & -1 & \dots & -1 \\ 0 & 1 & -1 & -1 & \dots & -1 \\ 0 & 0 & 1 & -1 & \dots & -1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$ .
  - (a) (5 points) Show that  $||A||_2 \ge \sqrt{n}$ . Hint: For this problem and the next you might find the standard basis vector  $\vec{\mathbf{e}}_n = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}$  useful.

(b) (5 points) Give a lower bound for  $\kappa_2(A)$  (the matrix condition number in the 2-norm).

- (c) (4 points) Would you say that the  $n \times n$  matrix A is a well-conditioned matrix (for large n)? **Yes or No (Circle one)**. Briefly justify your answer below.
- (d) (2 points) How does your previous answer relate to the error in computing  $A\mathbf{x} = \mathbf{b}$ ?

5. (8 points) We are trying to solve a system of equations Ax = b, where A is a  $10000 \times 10000$  matrix that has been generated with the following code:

```
> N=10000
> A <- spMatrix(nrow=N,ncol=N,i=c(1:N,1:N),j=c(1:N,N:1),x=c(rep(-2*N,N),1:N))
> A[2:(N-1),1] <- A[2:(N-1),N] <- 1
> A[1,2:(N-1)] <- A[N,2:(N-1)] <- 1</pre>
```

- (a) (4 points) Since A is a large matrix, I am going to try an iterative method. Which of the following best describes the computational complexity of a single iteration of the Jacobi method to solve Ax = b, where A has the structure described in the code above for large values of N (say 10,000 or higher)? Note that I've omitted constants that do not depend on N. Circle one and briefly justify your answer below.
  - (i)  $\mathcal{O}(N)$
  - (ii)  $\mathcal{O}(N \log N)$
  - (iii)  $\mathcal{O}(N^2)$
  - (iv)  $\mathcal{O}(N^3)$
- (b) (4 points) Which of the following statements is true? Circle one and briefly justify your answer below.
  - (i) There is no choice of b for which Jacobi's method will converge.
  - (ii) Jacobi's method will converge for any choice of b.
  - (iii) Jacobi's method may or may not converge. It will depend on the choice of b.
  - (iv) Jacobi's method may or may not converge, but it will not depend on the choice of b.

6. (17 points) In this problem, you will write an essay on sparse matrix storage formats. Use an internet search engine to find what is available/popular, but your essay must be in your own words. List three different storage formats for sparse matrices and compare their advantages and disadvantages (or main features) in storage and matrix-vector multiplications. Choose one of the storage formats you discuss and write a pseudocode for matrix-vector multiplication using this storage format. Your essay should be written in LaTeX. You may use the technical report template. I am willing to give LaTeX help. Your essay should include an abstract, introduction, and conclusion as well as citations for the resources that you reference.

7. (14 points) In this problem, we are going to use sparse matrices to represent chemical graphs of organic molecules, and then use eigenvalues to analyze where two molecules might bridge (connect).<sup>1</sup>

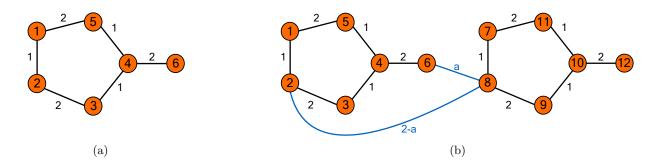


Figure 1: (a) Voltage graph for a single fulvene molecule. (b) Two fulvene molecules connected with two extra edges.

Figure 1(a) shows the voltage graph for a single fulvene molecule. The graphs for two individual molecules can be bridged by adding one or more edges connecting a vertex from each graph. As an example, in Figure 1(b), we consider adding two new edges (shown in blue), each connecting vertices from each of the initial graphs. The resulting weighted, undirected graph in Figure 1(b) features 12 vertices, labeled 1 through 12. The edges of the graph connecting vertices on the same organic molecule retain their initial edge weights. The two new connecting edges have weights of a (connecting vertices 6 and 8) and 2-a (connecting vertices 2 and 8), where a is some number between 0 and 2. The weighted adjacency matrix W for this bridged graph is a  $12 \times 12$  matrix, with the  $(i,j)^{th}$  entry  $W_{ij}$  equal to 0 if there is no edge connecting vertices i and j, and equal to the weight of the edge connecting vertices i and j otherwise.

- (a) (2 points) Let a = 1. Create the sparse matrix W. Run the command image(W) to make sure your W has the correct sparsity (nonzero) pattern.
- (b) (6 points) The weighted adjacency matrix W has both negative and positive eigenvalues. The spectral gap of W is the difference between the negative eigenvalue closest to 0 and the positive eigenvalue closest to 0. For example, when a=1, the negative eigenvalue closest to 0 is -0.755, and the positive eigenvalue closest to 0 is 1.344. So the spectral gap is  $2.099.^2$

We are going to let a vary, and see how it affects the spectral gap. Create a function sg(a) that takes as input a choice of a between 0 and 2, and returns the spectral gap of the graph shown above in Figure 1(b), for the given value of a. Plot the function  $sg(\cdot)$  on the interval [0,2].

(c) (6 points) Now we want to determine for which value of a the spectral gap of the graph shown in Figure 1(b) is maximized. First, use the finite difference derivative function D from Technical Report 1 (you can use yours or mine, which is called FDDeriv) to generate a function g that is the numerical derivative of the  $sg(\cdot)$  function. Plot the function  $g(\cdot)$  on the interval [0,2]. Then use your favorite root-finding method to find the value of a on the interval [0,2] that maximizes the spectral gap of W. For your answer to this question, include a single code block with all of your code. On the last line, execute the command

paste("Root =",as.character(root))

where root is a variable containing your approximation of the root.

<sup>&</sup>lt;sup>1</sup>This is an idea discussed in a recent paper here: https://arxiv.org/abs/1611.06959. You are welcome to read this article, but you do not have to look at it at all in order to do this problem. Full disclosure: I have not yet run this application by a chemist. So while the math and computing are sure to be interesting, the interpretations may not be chemically accurate due to my desire to simplify the problem and use tools we know

<sup>&</sup>lt;sup>2</sup>According to the paper at https://arxiv.org/abs/1611.06959, this gap represents the difference between the energy of the lowest unoccupied molecular orbital and the energy of the highest occupied molecular orbital. A larger gap implies higher kinetic stability.

8. (20 points) Brownian motion is a simple continuous stochastic process that is widely used in physics and finance for modeling random behavior that evolves over time. Quantitative Finance uses a version called "Geometric Brownian Motion" (GBM) to predict pricing options. The general model we use to determine the future behavior of an asset is:  $S_t = S_0 + e^{(\mu - \frac{\sigma^2}{2})t + \sigma W_t}$ , where  $S_t$  is the price at time t,  $S_0$  is the initial price,  $\mu$  is the expected return, and  $\sigma$  is the standard deviation of the return.

The R implementation of the solution is shown below (no changes need to be made to this code, but look it over carefully to see what it does.):

```
GBM <- function(N, sigma, mu, SO, Wt = NULL) {
  # Creates a single asset path of daily prices using Geometric Brownian Motion.
 # One year is 252 days since that is about how many trading days are in any
  # given year.
  # Inputs:
  #
      N: Number of days in the path.
  #
      sigma: Standard deviation of daily continuously compounded
  #
             returns (known as volatility).
  #
      mu: Average daily continuously compounded returns (known as drift).
  #
      SO: The initial price of the asset.
  #
      Wt: The cumulative Brownian motion of the model. This can be supplied or
  #
          left as NULL. In the case that it is NULL, a vector will be provided.
  #
          If you include this argument, it must be a vector of length N of the
  #
          cumulative sum of a random variable to work properly. (Steps i.-iii. below
  #
          create this.)
  # Returns:
  #
      A vector of length N containing the asset prices generated by the specified
  if (is.null(Wt)) {
   Wt <- cumsum(rnorm(N, 0, 1))
 t <- (1:N)/252
 p1 <- (mu - 0.5*(sigma*sigma)) * t
 p2 <- sigma * Wt
 St = S0 * exp(p1 + p2)
 return(St)
}
```

- (a) (6 points) We are going to simulate the prices of several correlated assets over time, using Correlated GBM. Imagine we have assets that are dependent on each other. Our goal is to predict future asset values taking into consideration correlation of past asset values. The simulation process starts with an  $n \times n$  correlation matrix C, which shows the correlation between n stocks. The following is the procedure for generating correlated random variables:
  - i. Perform Cholesky Decomposition of correlation matrix C to obtain upper triangular matrix R.
  - ii. Generate a random matrix X with n columns following a standard normal distribution with mean = 0 and variance = 1.
  - iii. Obtain a correlated random matrix Wt = XR. This generates a matrix that encodes both randomness and correlation within the problem.
  - iv. Use the above GBM function to generate the daily price path for each asset.

Implement the algorithm described above. Below is a starter of the function:

```
CorrelatedGBM <- function(N, S0, mu, sigma, cor.mat) {
    # Creates a matrix of correlated daily price paths using Geometric
    # Brownian Motion.
    #
    # Inputs:
    # N: Number of days in the path.
    # mu: A vector of drift or average daily continuously compounded returns.
    # sigma: A vector of volatility or standard deviation of daily continuously compounded return
    # S0: A vector of initial prices of the assets.
    # cor.mat: The correlation matrix of the daily continuously compounded
    # returns.</pre>
```

```
# Returns:
# A matrix of simulated daily price paths of length N having the same number
# of assets as in the mu and sigma vectors. Note that mu and sigma must have
# the same dimensions.

GBMs <- matrix(nrow = N, ncol = length(mu)) # Generate empty GBM vector for return

# Fill in code below for Step i.

# Step ii. (done for you):
X <- matrix(rnorm(N * length(mu), 0, 1), ncol = length(mu)) # Generate the Nxn random matrix
X <- apply(X, 2, cumsum) # cumulate value from random matrix to reflect compounded return.

# Fill in code below for Step iii.

# Fill in code below for Step iv. and store it in GBMs:
return(GBMs)
}</pre>
```

- (b) (10 points) Delta, United, and American Airlines are the three biggest airlines in the U.S. airlines market. They are top choices for investors who love aviation. The dataset AirlineStockPrices.csv records the stock price for these three stocks starting from July 1, 2007. In order to simulate the stock prices, we need to determine the inputs for the function CorrelatedGBM. Here are the steps you can follow to generate every piece of information you'll need:
  - i. Generate a return matrix by calculating the daily log return. For example,  $r_{i,j} = log(\frac{S_{i+1,j}}{S_{i,j}})$  where  $r_{i,j}$  denotes the return while  $S_{i,j}$  denotes the price for stock j in the  $i^{th}$  day.<sup>3</sup>
  - ii. Use the cor() function to calculate the correlation matrix cor.mat on the return matrix.
  - iii. Calculate the column mean of the return matrix to create the vector of average returns mu.
  - iv. Calculate the standard deviation of each column of the return matrix to create the vector of standard deviations sigma. (HINT: sd() is a function that computes standard deviation. You may find the function apply() useful, but it is not required to use it).
  - v. Generate the vector that represents the current price value S0 (that is, the last price available).
- (c) (2 points) We would like to simulate the price of these stocks over the next 3 years (remember there are only 252 trading days in a year). Use the CorrelatedGBM function to construct the three paths of these stock prices. Plot the path of these stocks over 3 years using the code below:

(d) (2 points) What do you observe about the stock prices? How will you invest based on the simulation?

<sup>&</sup>lt;sup>3</sup>If you are curious to know why this works, check out this link.