THE UNIVERSITY OF AUCKLAND

FIRST SEMESTER, 2013 — MID-SEMESTER TEST
Campus: City

COMPUTER SCIENCE

Computational Science

(Time allowed: 50 minutes)

NOTE: Attempt *all* questions

Use of calculators is NOT permitted.

Put your answers in the answer boxes provided below each question. You may use the blank pages at the end of the exam script for scratch work, which will not be marked.

52 Marks in total. For grading purposes, 50 marks will be considered 100%.

SURNAME:

FIRSTNAME:

ID:

ID: ______________________________

1. The bisection method and Newton's method are both methods for finding the roots of a function, $f(x)$. [7 marks total]

   (a) What does it mean for x to be a root of f? [**1** mark]

   x is a root of f when $f(x) = 0$.

   (b) What is one reason to choose the bisection method over Newton's method? [**1** mark]

   A few reasons: certain to converge, good stability, no need to calculate derivative of f.

   (c) What is one reason to choose Newton's method over the bisection method? [**1** mark]

   Faster convergence (more efficient).

   (d) Suppose we are using Newton's method to find the roots of $f(x) = x^2 - 2$. If $x_0 = 0.5$, calculate x_1, the approximation found after one iteration of Newton's method. [**4** marks]

   Newton's method is $x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$. Here, $f'(x) = 2x$ so

   $$x_1 = 0.5 - \frac{0.5^2 - 2}{2 \cdot 0.5} = 2.25$$

2. Suppose $\mathbf{A}$ is the square matrix $\mathbf{A} = \mathrm{diag}(a_1, \ldots, a_n)$. [5 marks total]

   (a) What is the determinant of $\mathbf{A}$, $\det(\mathbf{A})$? [**1** mark]

   $\det(\mathbf{A}) = a_1 \times a_2 \times \ldots \times a_n = \prod_{i=1}^n a_i$.

   (b) What condition on $\det(\mathbf{A})$ tells us that $\mathbf{A}^{-1}$ exists? If $\mathbf{A}^{-1}$ exists, what can we say about each a_i? [**2** marks]

   $\mathbf{A}^{-1}$ exists if and only if $\det(\mathbf{A}) \neq 0$. In this case, $\det(\mathbf{A}) \neq 0$ if and only if $a_i \neq 0$ for all i.

ID: ______________________________

(c) Assuming $\mathbf{A}^{-1}$ exists, what is it? [**2** marks]

$\mathbf{A}^{-1} = \text{diag}(\frac{1}{a_1}, \ldots, \frac{1}{a_n})$

3. Suppose $\mathbf{A}$ is a square matrix. [4 marks total]

(a) What does it mean for $\mathbf{A}$ to be orthonormal? [**2** marks]

$\mathbf{A}$ is orthonormal if the columns of $\mathbf{A}$ are mutually orthogonal unit vectors. Equivalently, $\mathbf{A}$ is orthonormal if $\mathbf{A}\mathbf{A}^T = \mathbf{I}$

(b) If $\mathbf{A}$ is orthonormal, what is the solution to $\mathbf{Ax} = \mathbf{b}$ where $\mathbf{x}$ is unknown? [**2** marks]

$\mathbf{x} = \mathbf{A}^{\mathbf{T}}\mathbf{b}$.

4. Suppose we wish to solve the over-determined linear system represented by $\mathbf{Au} = \mathbf{b}$ where $\mathbf{A}$ is an $m \times n$ matrix and $\mathbf{u}$ is an unknown $n \times 1$ vector and $\mathbf{b}$ is known. [12 marks total]

(a) Given that $\mathbf{A}$ is over-determined, what is the relationship between m and n? [**1** mark]

$m > n$. That is, there are more columns (equations) than rows (parameters).

(b) Write down the normal equation that we solve to find the least squares solution to this problem. [**2** marks]

The normal equation is $\mathbf{A}^{\mathsf{T}}\mathbf{Au} = \mathbf{A}^{\mathsf{T}}\mathbf{b}$.

(c) Let $\mathbf{A} = \mathbf{QR}$ be a QR-decompostion of $\mathbf{A}$. What are the dimensions and properties of $\mathbf{Q}$ and $\mathbf{R}$? [**4** marks]

$\mathbf{Q}$ is an $m \times n$ matrix with n orthonormal columns and $\mathbf{R}$ is an $n \times n$ upper triangular matrix.

ID: ____________________

(d) Show how the QR decomposition is used to simplify the normal equation. Why is the resulting equation easy to solve? [**5** marks]

$$\begin{aligned}
\mathbf{A}^\mathsf{T}\mathbf{A}\mathbf{u} &= \mathbf{A}^\mathsf{T}\mathbf{b} \\
\implies (\mathbf{Q}\mathbf{R})^\mathsf{T}\mathbf{Q}\mathbf{R}\mathbf{u} &= (\mathbf{Q}\mathbf{R})^\mathsf{T}\mathbf{b} \\
\implies \mathbf{R}^\mathsf{T}\mathbf{Q}^\mathsf{T}\mathbf{Q}\mathbf{R}\mathbf{u} &= \mathbf{R}^\mathsf{T}\mathbf{Q}^\mathsf{T}\mathbf{b} \\
\implies \mathbf{R}^\mathsf{T}\mathbf{R}\mathbf{u} &= \mathbf{R}^\mathsf{T}\mathbf{Q}^\mathsf{T}\mathbf{b} \text{ since } \mathbf{Q}^T\mathbf{Q} = \mathbf{I} \\
\implies \mathbf{R}\mathbf{u} &= \mathbf{Q}^\mathsf{T}\mathbf{b}.
\end{aligned}$$

This is easy to solve via back-substitution, since $\mathbf{R}$ is upper triangular.

5. Let $\mathbf{A} = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 1 & 0 \end{bmatrix}$. [14 marks total]

(a) The eigenvectors of $\mathbf{A}^\mathsf{T}\mathbf{A}$ are

$$\frac{1}{\sqrt{2}}\begin{bmatrix} -1 \\ 1 \end{bmatrix} \text{ and } \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

Find the corresponding eigenvalues. [**6** marks]

$$\mathbf{A}^\mathsf{T}\mathbf{A} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

If $\mathbf{u}$ is an eigenvector, $\mathbf{A}\mathbf{u} = \lambda\mathbf{u}$ where λ is the associated eigenvalue. So

$$\frac{1}{\sqrt{2}}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}\begin{bmatrix} -1 \\ 1 \end{bmatrix} = \frac{\lambda}{\sqrt{2}}\begin{bmatrix} -1 \\ 1 \end{bmatrix} \implies -1 = -1 \cdot \lambda \implies \lambda = 1.$$

Similarly, the eigenvalue associated with $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ is 3.

ID: ______________________________

(b) The eigenvectors of $\mathbf{A}\mathbf{A}^\mathsf{T}$ corresponding to the two largest eigenvalues are (in order of descending eigenvalues)

$$\frac{1}{\sqrt{6}}\begin{bmatrix}1\\2\\1\end{bmatrix} \text{ and } \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\\-1\end{bmatrix}.$$

What are the corresponding eigenvalues? *Hint: don't calculate them directly!* [**2** marks]

They eigenvalues of $\mathbf{A}\mathbf{A}^\mathsf{T}$ are the same as the eigenvalues of $\mathbf{A}^\mathsf{T}\mathbf{A}$ so the associated eigenvalues are 3 and 1, respectively.

(c) Find the singular value decomposition of $\mathbf{A}$. Ensure that the singular values in matrix $\mathbf{D}$ are ordered from largest to smallest. [**3** marks]

The singular value decomposition is $\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^\mathsf{T}$ where $\mathbf{D}$ is the diagonal matrix of singular values ordered from largest to smallest, $\mathbf{U}$ is the matrix with columns the normalised eigenvectors of $\mathbf{A}\mathbf{A}^\mathsf{T}$ and $\mathbf{V}$ is the matrix with columns the normalised eigenvectors of $\mathbf{A}\mathbf{A}^\mathsf{T}$. So

$$\mathbf{A} = \underbrace{\begin{bmatrix}1/\sqrt{6} & 1/\sqrt{2}\\ 2/\sqrt{6} & 0\\ 1/\sqrt{6} & -1/\sqrt{2}\end{bmatrix}}_{\mathbf{U}}\underbrace{\begin{bmatrix}\sqrt{3} & 0\\ 0 & 1\end{bmatrix}}_{\mathbf{D}}\underbrace{\begin{bmatrix}1/\sqrt{2} & 1/\sqrt{2}\\ -1/\sqrt{2} & 1/\sqrt{2}\end{bmatrix}}_{\mathbf{V}^\mathsf{T}}.$$

(d) Write an expression for an approximation, $\widehat{\mathbf{A}}_1$, of $\mathbf{A}$ using only its largest singular vectors and singular value (you can leave it in the form of a vector product). [**3** marks]

$$\widehat{\mathbf{A}}_1 = \sigma_1\mathbf{u}_1\mathbf{v}_1^\mathsf{T} = \sqrt{3}\cdot\tfrac{1}{\sqrt{6}}\begin{bmatrix}1\\2\\1\end{bmatrix}\cdot\tfrac{1}{\sqrt{2}}[1\ \ 1] = \tfrac{1}{2}\begin{bmatrix}1\\2\\1\end{bmatrix}[1\ \ 1]$$

6. Suppose we have a method of generating Bernoulli random variables with probability of success p for any $0 < p < 1$. [10 marks total]

(a) How would we generate geometric random variables with parameter p? [**2** marks]

Generate Bernoullis until the first success and count the number of failures.

ID: ____________________

(b) How would we simulate the position of a random walker after 200 steps where the walk started at 0 and steps in the positive direction with probability p? [**2** marks]

> Generate 200 Bernoulli variates, taking values 1 on a success and -1 on a failure. Sum the 200 variates to get the position of the walker.

(c) How would we generate binomial random variables? [**3** marks]

> Generate Binomial(n, p) by generating n Bernoulli r.v.s with success probability p and count the number of successes.

(d) If we also had a method of simulating the Poisson process with rate $\lambda_1 = 5$, how could we couple this with our Bernoulli generator to simulate the Poisson process with rate $\lambda_2 = 2$? [**3** marks]

> Split the λ_1 Poisson process by thinning it. Generate an arrival in the λ_1 Poisson process and generate a Bernoulli variable X with $p = \frac{\lambda_2}{\lambda_1} = \frac{2}{5}$. If X is a success, the arrival is an arrival in the λ_2 Poisson process, if X is a failure, discard it.

ID: ______________________________

Blank page 1 — will not be marked

ID: ______________________________

Blank page 2 — will not be marked