THE UNIVERSITY OF AUCKLAND

FIRST SEMESTER, 2012 – 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 page at the end of the test script for scratch work, which will not be marked.

Section:	**A**	**B**	**C**	**D**	Total
Possible marks:	10	20	10	10	50
Awarded marks:					

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FIRSTNAME:

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Section A: Linear Systems, SVD, PCA (10 marks)

1. What decompositions $\mathbf{A} = \mathbf{BC}$ of a given ordinary matrix $\mathbf{A}$ are done by Gauss elimination and Gram-Schmidt orthogonalisation? Write down standard notations for the matrices $\mathbf{B}$ and $\mathbf{C}$ and types and shapes of the matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$, which appear in both the cases.

   Hint: Notations: $\mathbf{L}$, $\mathbf{Q}$, $\mathbf{R}$, or $\mathbf{U}$; shapes: square $m \times m$ or rectangular $m \times n$; types: lower triangular, orthonormal, or upper triangular. [3 marks]

   Gauss: _____ decomposition of a _____ ___ × ___ matrix $\mathbf{A}$

   _____ is a _____ ___ × ___ matrix

   _____ is a _____ ___ × ___ matrix

   Gram-Schmidt: _____ decomposition of a _____ ___ × ___ matrix $\mathbf{A}$

   _____ is a _____ ___ × ___ matrix

   _____ is a _____ ___ × ___ matrix

2. The Singular Value Decomposition (SVD) of a given ordinary $m \times n$ matrix $\mathbf{A}$, $m > n$, is represented by a product, $\mathbf{A} = \mathbf{UDV}^\mathsf{T}$, of three matrices with special properties. In particular, $\mathbf{U}$ is an $m \times n$ column-orthogonormal matrix with the following properties: its n columns are the n top-rank eigenvectors $\mathbf{u}_1,\ldots,\mathbf{u}_n$ of the $m \times m$ symmetric matrix $\mathbf{AA}^\mathsf{T}$, i.e. the only n eigenvectors that can have non-zero eigenvalues. Specify the properties of the matrices $\mathbf{D}$ and $\mathbf{V}$.

   Hint: Consider the eigenvectors and eigenvalues $\{(\mathbf{v}_i, \lambda_i) : i = 1,\ldots,n\}$ of the $n \times n$ matrix $\mathbf{A}^\mathsf{T}\mathbf{A}$. [4 marks]

   $\mathbf{V}$ –

   $\mathbf{D}$ –

3. Let $\mathbf{A} = [\mathbf{a}_1,\ldots,\mathbf{a}_n]$; $m \ll n$, be an $m \times n$ matrix, which is built from n centred $m \times 1$ vectors $\mathbf{a}_i$; $i = 1,\ldots,n$, of measurements. Let $\mathbf{u}_1$ and $\mathbf{u}_2$ be two principal components, i.e. two eigenvectors of the $m \times m$ covariance matrix of the measurements, $\mathbf{\Sigma}_n = \frac{1}{n-1}\mathbf{AA}^\mathsf{T}$, with the largest eigenvalues. Write down the projection matrix $\mathbf{P}_2$, which projects the measurement vectors (i.e. the columns of $\mathbf{A}$) to the principal subspace of the eigenvectors $\mathbf{u}_1$ and $\mathbf{u}_2$. [4 marks]

   $\mathbf{P}_2 =$

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Section B: Root Finders, Optimisation, Least Squares (20 marks)

4. Explain how the root of the non-linear function $g(x) = x^4 + 2x^2 - 25$ is being searched for with the **modified Newton method** starting from the first approximation $x^{[0]} = 2$ and derive the approximate root value $x^{[1]}$ at the first step of the search.

   Hint: In this case the Jacobian $J(x)$ of the function $g(x)$ is the first derivative $J(x) = \frac{dg(x)}{dx}$ at point x. The **non-modified Newton method** chooses at each iteration t the root $x^{[t+1]}$ of the linear approximation $g_{\text{app:}t}(x) = g(x^{[t]}) + J(x^{[t]})\left(x - x^{[t]}\right)$, i.e. $g_{\text{ap:}t}(x^{[t+1]}) = 0$. Recall what the **modified** one differs in. [5 marks]

5. At each iteration of unconstrained gradient maximisation of a scalar bivariate function $f(x, y)$, the gradient, $\nabla f(x, y) = \left(\frac{\partial f(x,y)}{\partial x}, \frac{\partial f(x,y)}{\partial y}\right)$, is computed at the current point (x_i, y_i), and the next point, (x_{i+1}, y_{i+1}), is selected along a line $L_i(t) = (x_i + tu_i, y_i + tv_i)$ through (x_i, y_i) in the gradient direction $\left(u_i = \left.\frac{\partial f(x,y)}{\partial x}\right|_{x=x_i,y=y_i}, v_i = \left.\frac{\partial f(x,y)}{\partial y}\right|_{x=x_i,y=y_i}\right)$. Write down in the general form the condition for selecting the next steepest ascent point (x_{i+1}, y_{i+1}). [4 marks]

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6. You have to maximise the function $f(x, y) = x^3 - x^2y + 4xy^2 + y^3$ subject to the constraint $x^2 + y^2 = 4$. Write down the Lagrangian $F(x, y, \lambda)$ and derive the system of equations that give all the stationary (i.e. maximum, minimum, and saddle) points of the Lagrangian.
   Note that you need not solve this system. [5 marks]

7. You have to solve an overdetermined system $\mathbf{Ax} = \mathbf{a}$ of m linear equations with $n \times 1$; $n \ll m$, vector $\mathbf{x}$ of unknowns, provided that the $m \times n$ matrix $\mathbf{A}$ and the $m \times 1$ vector $\mathbf{a}$ are known and the matrix $\mathbf{A}$ has n linearly independent columns.

   Derive the "normal" equation and the least squares solution for this system.

   Hint: Consider the residual error vector $\mathbf{e_x} = \mathbf{Ax} - \mathbf{a}$ and recall that the least squares solution $\mathbf{x}^*$ minimises the total squared error $E(\mathbf{x}) = \mathbf{e_x^T e_x}$. [6 marks]

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Section C: Taylor Series, Finite Differences (10 marks)

8. Approximate the function $f(x) = \mathrm{e}^x$ in the neighbourhood of point $x = 1$ with the first four terms of the Taylor series (that is, with the terms involving up to the third derivative $f^{[3]}(x)$ at $x = 1$.

   Hint: The derivatives in this case are equal to the function: $\frac{d^k}{dx^k}\mathrm{e}^x = \mathrm{e}^x$ for any $k = 1, 2, \ldots$. [3 marks]

9. Assuming only integer values of x, derive the centred finite difference approximation for the first derivative of function $u(x) = x^4$ and compare it to the exact derivative $\frac{d}{dx}u(x)$ at point $x = 2$.

   Hint: Recall that $(a \pm b)^4 = a^4 \pm 4a^3b + 6a^2b^2 \pm 4ab^3 + b^4$ and $\frac{dx^n}{dx} = nx^{n-1}$. [3 marks]

10. Assuming integer arguments $x = 0, 1, 2, \ldots$, and the forward difference approximation of the first derivative, deduce and solve the finite difference equation for the first-order differential equation $\frac{d}{dx}u(x) = 2u(x)$ with the boundary condition $u(0) = 1$. [4 marks]

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Section D: Dynamic Programming, Search Methods (10 marks)

11. Consider discrete global minimisation of an objective function $F(x_1, \ldots, x_n) = \sum_{i=2}^{n} \varphi_i(x_{i-1}, x_i)$ of n integer state variables, taking values from a finite set $\mathbb{X} = \{0, 1, \ldots, X-1\}$:

$$(x_1^*, \ldots, x_n^*) = \arg \min_{(x_1,\ldots,x_n)\in\mathbb{X}^n} F(x_1, \ldots, x_n); \quad F^* = F(x_1^*, \ldots, x_n^*)$$

To find the desired minimum F^* and the minimiser $(x_1^*, \ldots, x_n^*)$, discrete dynamic programming computes for each state $x_i \in \mathbb{X}$ at each step $i = 2, \ldots, n$ of the forward pass a potentially optimal solution, $\Phi_i(x_i)$, and a candidate backward pointer $B_i(x_i)$ to the preceding candidate state.

Complete Bellman equations, specifying $\Phi_i(x_i)$ and $B_i(x_i)$, as well as equations for the backward pass (backtracking), which reconstructs the minimiser. [7 marks]

Bellman equation for $i = 1, \ldots, n-1$ and each $x_i \in \mathbb{X}$:

$$\begin{cases} \Phi_i(x_i) &= \min\limits_{x_{i-1}\in\mathbb{X}} \left\{ \_\_\_\_\_ + \varphi_i(x_{i-1}, x_i) \right\} \\ B_i(x_i) &= \arg\min\limits_{x_{i-1}\in\mathbb{X}} \left\{ \_\_\_\_\_ \right\} \end{cases}$$

Brief explanation:

Backtracking:

$$\begin{cases} F^* &= \min\limits_{x_n\in\mathbb{X}} \Phi_n(x_n); \quad x_n^* = \_\_\_\_\_; \\ x_{i-1}^* &= \_\_\_\_\_; \quad i = n-1, \ldots, 2 \end{cases}$$

Brief explanation:

12. What search via a graph of solutions is performed by backtracking and branch-and-bound methods?
Hint: Consider the breadth-first search (BFS) or the depth-first search (DFS) options. [3 marks]

Backtracking:

Branch-and-bound:

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