Final test (Tuesday 17 December 2024, 15:00-17:00 CET)
Elements of Mathematics – Master in Bioinformatics for Health Sciences

1. Consider the matrix $A = BB^t$ where
$$B = \begin{bmatrix} 1 \\ 3 \\ 0 \end{bmatrix}.$$

   (a) **(0.5 point)** Provide a basis of the column space of A.
   Answer: The columns of A are linear combinations of the only column of B. Thus $\mathcal{C} = \{(1,3,0)\}$ is a basis of column space of A.

   (b) **(0.5 points)** Provide a basis of the null space of A.
   Answer: You can reason by Gauss-Jordan elimination with the matrix A. A more direct approach is to note that $N(A)$ is the set of vectors that are orthogonal to $R(A)$, which is generated by $v = (1,3,0)$. Then $N(A)$ is the set of vectors in $\mathbb{R}^3$ that are orthgonal to v, i.e.
$$N(A) = \{(x,y,z) \in \mathbb{R}^3 \mid x + 3y = 0\}.$$
   Since $\dim(N(A)) = 2$, in order to find a basis of $N(A)$ it is enough to find two linearly independent vectors that are orthogonal to v. Following this argument, $\mathcal{N} = \{(3,-1,0),(0,0,1)\}$ is a basis of $N(A)$.

2. **(1 point)** Let $H \subset \mathbb{R}^3$ be the vector space of solutions of the equation $x + y + z = 0$. Compute an orthonormal basis of H.

   Answer: H is the null space of the rank 1 matrix
$$A = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}$$
   which can be seen as the set of vectors in $\mathbb{R}^3$ that are orthogonal to $w = (1,1,1)$. Since $\dim(H) = 2$, in order to find a basis it is enough to find two linearly independent vectors that are orthogonal to w. Following this argument, $\{u_1 = (1,-1,0), u_2 = (0,1,-1)\}$ is a basis of H, but this is not an orthonormal basis. Let's do two steps of the Gram-Schmidt orthogonalization algorithm. First, let's choose one of the vectors, say u_1, and we re-scale it so that it yields a length 1 vector,
$$v_1 = \frac{u_1}{\|u_1\|} = \frac{1}{\sqrt{2}}(1,-1,0)$$
   Then define,
$$\tilde{v}_2 = u_2 - (u_2 \cdot v_1)v_1 = (0,1,-1) + \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}(1,-1,0) = (1/2,1/2,-1).$$
   Re-scaling so that it yields a length 1 vector,
$$v_2 = \frac{1}{\sqrt{3/2}}(1/2,1/2,-1) = \frac{1}{\sqrt{6}}(1,1,-2).$$
   The basis $\mathcal{N} = \{v_1, v_2\}$ meets the requirements of the exercise.

3. Consider the following vectors in $\mathbb{R}^3$:
$$u = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} \quad v = \frac{1}{\sqrt{6}}\begin{bmatrix} 1 \\ 1 \\ -2 \end{bmatrix} \quad w = \frac{1}{\sqrt{3}}\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}.$$
   The matrix of a linear transformation f in coordinates the basis $\mathcal{B} = \{u, v, w\}$ is:
$$A = \begin{bmatrix} \cos(\pi/6) & -\sin(\pi/6) & 0 \\ \sin(\pi/6) & \cos(\pi/6) & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

(a) **(0.5 points)** Is $\mathcal{B}$ an orthonormal basis of $\mathbb{R}^3$?
Answer: $u \cdot v = u \cdot w = v \cdot w = 0$ and $\|u\| = \|v\| = \|w\| = 1$.

(b) **(0.5 point)** Compute the inverse of the decoding matrix $C = [u|v|w]$ which has as columns the vectors of $\mathcal{B}$.
Answer: Because $\mathcal{B}$ is orthonormal, the resulting decoding matrix C is orthogonal, therefore

$$C^{-1} = C^t = \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 1/\sqrt{6} & 1/\sqrt{6} & -2/\sqrt{6} \\ 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \end{bmatrix} = \frac{1}{\sqrt{6}} \begin{bmatrix} \sqrt{3} & -\sqrt{3} & 0 \\ 1 & 1 & -2 \\ \sqrt{2} & \sqrt{2} & \sqrt{2} \end{bmatrix}$$

(c) **(1 point)** Compute the matrix of f in coordinates of the canonical basis.
Answer: The matrix sought is $R = CAC^{-1}$, which can be read from right to left as: 1) change coordinates to the new basis $\mathcal{B}$ (encode), 2) apply linear transformation in said coordinate system, 3) change coordinates back to the canonical basis. Let's compute:

$$R = \frac{1}{6} \begin{bmatrix} \sqrt{3} & 1 & \sqrt{2} \\ -\sqrt{3} & 1 & \sqrt{2} \\ 0 & -2 & \sqrt{2} \end{bmatrix} \begin{bmatrix} \cos(\pi/6) & -\sin(\pi/6) & 0 \\ \sin(\pi/6) & \cos(\pi/6) & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \sqrt{3} & -\sqrt{3} & 0 \\ 1 & 1 & -2 \\ \sqrt{2} & \sqrt{2} & \sqrt{2} \end{bmatrix} =$$

$$= \frac{1}{6} \begin{bmatrix} \sqrt{3} & 1 & \sqrt{2} \\ -\sqrt{3} & 1 & \sqrt{2} \\ 0 & -2 & \sqrt{2} \end{bmatrix} \begin{bmatrix} \sqrt{3}/2 & -1/2 & 0 \\ 1/2 & \sqrt{3}/2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \sqrt{3} & -\sqrt{3} & 0 \\ 1 & 1 & -2 \\ \sqrt{2} & \sqrt{2} & \sqrt{2} \end{bmatrix} =$$

$$= \frac{1}{6} \begin{bmatrix} 2 & 0 & \sqrt{2} \\ -1 & \sqrt{3} & \sqrt{2} \\ -1 & -\sqrt{3} & \sqrt{2} \end{bmatrix} \begin{bmatrix} \sqrt{3} & -\sqrt{3} & 0 \\ 1 & 1 & -2 \\ \sqrt{2} & \sqrt{2} & \sqrt{2} \end{bmatrix} = \frac{1}{3} \begin{bmatrix} 1+\sqrt{3} & 1-\sqrt{3} & 1 \\ 1 & 1+\sqrt{3} & 1-\sqrt{3} \\ 1-\sqrt{3} & 1 & 1+\sqrt{3} \end{bmatrix}$$

4. We are analyzing a dataset $\mathcal{D}$ of standardized gene expression values of 5 genes across 100 cells sampled from a tissue and sequenced. We carried out the eigendecomposition of Ω, the covariance matrix of the dataset $\mathcal{D}$, and obtained the following results:

(a) The eigenvalues of Ω are $\lambda_1 = 4$, $\lambda_2 = 3$, $\lambda_3 = 2$, $\lambda_4 = 0.5$, $\lambda_5 = 0.5$

(b) The respective eigenvectors are:

$$u_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \quad u_2 = \frac{1}{\sqrt{6}} \begin{bmatrix} -1 \\ 2 \\ 0 \\ 0 \\ 1 \end{bmatrix} \quad u_3 = \frac{1}{2\sqrt{3}} \begin{bmatrix} -1 \\ -1 \\ 3 \\ 0 \\ 1 \end{bmatrix} \quad u_4 = \frac{1}{2\sqrt{5}} \begin{bmatrix} -1 \\ -1 \\ -1 \\ 4 \\ 1 \end{bmatrix} \quad u_5 = \frac{1}{\sqrt{5}} \begin{bmatrix} -1 \\ -1 \\ -1 \\ -1 \\ 1 \end{bmatrix}$$

(a) **(0.25 points)** What is the proportion of variance explained by the first 3 principal components?
Answer: The eigenvalues represent the variance in each principal direction. The total variance $T = \text{trace}(\Omega)$ is invariant with respect of coordinate changes, hence it can be computed as $T = \lambda_1 + \ldots + \lambda_5 = 10$. The proportion of variance explained by the 3 principal components is $(\lambda_1 + \lambda_2 + \lambda_3)/T = 0.9$.

(b) **(0.25 points)** What are the loadings of the second principal component?
Answer: The loadings of the second principal component are the entries of u_2.

(c) **(0.5 points)** After centering and scaling the standardized gene expression values, one of the cells has the following feature values: $c = (1, 0, 0, 0, 0)$. What are the scores of this cell in the coordinate system of the principal components?
Answer: We can compute the scores simply by multiplying c with the encoding matrix V^t which has the vectors $u_1, \ldots, u_5$ as rows. In this particular case, this gives us the first column of V^t:

$$s = V^t c = \left(\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{6}}, \frac{-1}{2\sqrt{3}}, \frac{-1}{2\sqrt{5}}, \frac{-1}{\sqrt{5}} \right)$$

5. **(1 point)** Find the second order Taylor approximation of $f(x) = (1-c)\log(1-x) + c\log(x)$ at $a = 1/2$.

   Answer: We must compute $f(a)$, $f'(a)$ and $f''(a)$.

$$f(a) = \log(a) = \log(1/2) = -\log(2)$$

$$f'(x) = -\frac{1-c}{1-x} + \frac{c}{x} \Rightarrow f'(a) = -\frac{1-c}{a} + \frac{c}{a} = \frac{2c-1}{a} = 4c-2$$

$$f''(x) = -\frac{1-c}{(1-x)^2} - \frac{c}{x^2} \Rightarrow f''(a) = \frac{-1}{a^2} = -4$$

   Therefore the Taylor approximation sought is:

$$T(x) = f(a) + f'(a)(x-a) + \frac{1}{2}f''(a)(x-a)^2 = -\log(2) + (4c-2)(x-1/2) - 2(x-1/2)^2$$

6. If b is a positive real number, the *logarithm of x to base b*, denoted $\log_b(x)$, is a function that satisfies the identity $\log_b(b^z) = z$. The *natural logarithm*, which we simply denote $\log(x)$, is the logarithm to base e (Euler's number).

   (1 point) Use the definition of logarithm to base b and the identity $b^x = e^{\log(b)x}$ to provide an expression of the derivative of $\log_b(x)$.

   Answer: Using the definition of $\log_b(x)$ and the identity, we have $x = b^{\log_b(x)} = e^{\log(b)\log_b(x)}$. Taking derivatives in both members of the equation and applying the chain rule,

$$1 = e^{\log_b(x)\log(b)}\log_b \log_b'(x) = x\log(b)\log_b'(x).$$

   From this equation we can infer an expression for the derivative of $\log_b(x)$:

$$\log_b'(x) = \frac{1}{x\log(b)}$$

7. A *quadratic form* is a function $f : \mathbb{R}^n \to \mathbb{R}$ with the form $f(z) = \frac{1}{2}z^tAz + b^tz + c$, where $A \in \mathbb{R}^{n\times n}$ is a matrix, $b \in \mathbb{R}^n$ is a vector and $c \in \mathbb{R}$ is a scalar. Consider the quadratic form $f : \mathbb{R}^2 \to \mathbb{R}$ with

$$A = \begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix} \quad b = \begin{bmatrix} 2 \\ -8 \end{bmatrix} \quad c = 0$$

   (a) **(0.5 points)** Compute the gradient of f.

   Answer: Note that the gradient of f is the vector $\nabla f(z) = Az + b$. This can be seen by making explicit the expression of f. For example, if $z = (x, y)$ we obtain the following expression for f:

$$f(x,y) = \frac{1}{2}\begin{bmatrix} x & y \end{bmatrix}\begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} + \begin{bmatrix} 2 & -8 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} + 0$$

   Doing the matrix-vector multiplications:

$$f(x,y) = \frac{1}{2}\left(3x^2 + 2xy + 2xy + 6y^2\right) + 2x - 8y$$

$$f(x,y) = \frac{3}{2}x^2 + 2xy + 3y^2 + 2x - 8y$$

   The gradient of f is:

$$\nabla f(x,y) = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{bmatrix} = \begin{bmatrix} 3x + 2y + 2 \\ 2x + 6y - 8 \end{bmatrix}$$

(b) **(1 points)** Find the critical points f.

Answer: The critical points of f are the points P where the gradient vanishes, i.e. such that $\nabla f(P) = AP + b = \vec{0}$.

$$A = \begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -2 \\ 8 \end{bmatrix} \Leftrightarrow x = -2,\ y = 2$$

Therefore $P = (-2, 2)$ is the only critical point of f

(c) **(0.5 points)** Compute the Hessian of f at the critical points.

Answer: The Hessian matrix of f is given by:

$$Hf(x,y) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix}$$

In other words, the Hessian matrix of f is constant and equal to A.

(d) **(1 points)** Classify the critical points of f.

Answer: Classifying the only critical point of f is equivalent to study the sign of the eigenvalues of A, which are the roots of the characteristic polynomial of A:

$$Q_A(t) = \det(A - tI) = \begin{vmatrix} 3-t & 2 \\ 2 & 6-t \end{vmatrix} = t^2 - 9t + 14$$

Finding the roots of $Q_A(t)$ using the quadratic equation formula or simply noting that the roots λ_1, λ_2 of $Q_A(t)$ must satisfy

$$\lambda_1 \lambda_2 = \det(A) = 14$$

$$\lambda_1 + \lambda_2 = \mathrm{trace}(A) = 9$$

we can conclude that the matrix A has eigenvalues $\lambda_1 = 7$, $\lambda_2 = 2$. Since both eigenvalues are positive, P is a minimum.