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HGEN 48800 (2024 spring)
Problem Set #4

Problem 1 (10 points) Consider the propagated data error in evaluating function $\sin(x)$, i.e., the error in the function value due to a perturbation h in the argument x. Estimate the condition number for this problem. For what values of the argument x is this problem highly sensitive?

Problem 2 (25 points) Consider the evolution of DNA sequences in two species. Suppose the divergence time between two sequences is t, and the rate of substitution is α. Under the Jukes-Canter model of DNA evolution, the probability of a nucleotide being substituted is $s_t = 3 \times (\frac{1}{4} - \frac{1}{4}e^{-4\alpha t/3})$, and the probability of a nucleotide being conserved is: $r_t = 1 - s_t = \frac{1}{4} + \frac{3}{4}e^{-4\alpha t/3}$.

(a) (5 points) Given a pair of DNA sequences, let t be the divergence time from one sequence to the other. Since α and t are coupled, we can set α to 1. Write the log-likelihood function of t in terms of the number of nucleotide substitution pairs n_S and the number of conserved nucleotide pairs n_C.

(b) (10 points) Implement the Newton's method to give the maximum likelihood estimate of t when $n_S = 5$ and $n_C = 25$. Specifically, solve the equation that the derivative of the log-likelihood function is equal to 0.

(c) (10 points) Check if the solution is a local maximum, minimum or saddle point. Plot the function and verify the results visually.

Problem 3 (25 points) Consider the function $f : \mathbb{R}^2 \to \mathbb{R}$, defined by

$$f(x, y) = 2x^3 - 3x^2 - 6xy(x - y - 1)$$

(a) (5 points) Determine all of the critical points of f analytically.

(b) (5 points) Classify each critical point as local maximum, minimum or saddle point, again analytically.

(c) (5 points) Verify your results visually by creating a contour plot of f over the region $-2 \le x \le 2, -2 \le y \le 2$.

(d) (10 points) Use a library routine to find the minimum of both f and $-f$. Experiment with various starting points.

Problem 4 (20 points) Let A be $n \times n$ real symmetric matrix. Consider the quadratic form defined on A: $f(x) = x^T Ax$, where $x \in \mathbb{R}^n$, and is subject to the constraint that its norm is 1, i.e. $x^T x = 1$. Using the Lagrange multiplier method to show that the maximum and minimum of f is the largest, and smallest eigenvalue of A. Hint: it may be helpful to read about matrix calculus. See a reference here: `https://www.dropbox.com/s/4n6m48iiotbr2p9/matrix-calculus-R.pdf?dl=0`. But it is also possible to solve this problem just using the definition of quadratic forms.