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OPTIMAL DESIGN FOR NEURAL NETWORKS

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In this paper the statistical principles underlying hidden-layer feed-forward neural networks are introduced and are invoked to develop strategies for the construction of appropriate optimal experimental designs. The ideas are illustrated by means of a simple network involving single input and output neurons and two neurons in the hidden layer. Locally and Bayesian optimal designs are obtained for the underlying nonlinear model and in particular it is shown that the relevant Bayesian criteria can be estimated from samples generated using Markov chain Monte Carlo methods.

1. Introduction. Neural networks are models abstracted from certain functions of the brain, and are proving to be valuable and exciting tools for solving problems in a diversity of areas such as economics, medicine, and psychology. The focus of the present paper is on hidden-layer feed-forward neural networks which are used extensively to model regression and classification data and, in particular, on the issue of choosing experimental data for these networks so that the fitted curve or surface is in some sense optimal. This problem of optimal design, also referred to within the neural network literature as "active data selection" and "query-based learning", is of some current interest. For example, Baum (1991) and Hwang, Choi, Oh and Marks (1991) provide heuristic procedures for sequentially selecting data, while MacKay (1992a, b), Plutowski and White (1993), Williams, Qazaz, Bishop and Zhu (1995) and Cohn (1996) draw closely on statistical notions to develop optimal strategies in which points are added "one-at-a-time" to the existing data. In addition Sollich (1994) provides a broad and fascinating framework for design within the context of statistical physics.

The aim of the present study is to construct optimal designs for nonlinear regression models describing hidden-layer feed-forward neural networks. Some necessary statistical insights are provided in Section 2 and designs for a specific example which are optimal in a classical and in a Bayesian sense are presented in Sections 3 and 4 respectively. Some broad conclusions and pointers for future research are given in Section 5.

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