POLYNOMIAL REPRESENTATIONS FOR RESPONSE SURFACE MODELING

By Norman R. Draper¹ and Friedrich Pukelsheim^{1,2}

University of Wisconsin and University of Washington

In response surface models the expected response is usually taken to be a low degree polynomial in the design variables that are coded from the factor settings. We argue that an overparameterized polynomial representation of the expected response offers great economy and transparency. As an illustration, we exhibit a constructive path of design improvement relative to the Kiefer design ordering, for polynomial regression up to degree three when the experimental domain is a ball.

1. Introduction. We overview some of the recent work on design optimality for response surface models and polynomial regression. However, our emphasis is not on scalar optimality criteria. Any such criterion singles out one—or a few—designs as being optimal, while saying little or nothing about all the other designs that are nonoptimal.

Rather, we concentrate on the Kiefer design ordering. We show that under this partial ordering there is a constructive path of design improvement. Starting with an arbitrary design, good or bad, we are lead to a small design class that turns out to be minimal complete. This is carried out for first-, second-, and third-degree polynomial response surface models when the experimental domain is a ball.

The Kiefer design ordering does not depend on how the polynomials are represented. This opens the way to write the regression function in a form that is deemed most convenient. We argue that the Kronecker product offers attractive symmetry, compact notation, and great transparency. The present paper offers a short-cut access by just verifying the results. The underlying theory for deriving these results is available in greater detail elsewhere in the literature.

A brief review of the literature is as follows. Pukelsheim (1993, p. 354) introduced the Kiefer ordering, thus extending Kiefer's (1975, p. 336) notion of universal optimality to general design settings. The Kiefer ordering combines two steps, increase in symmetry is followed by the usual enlargement of the moment matrix of a design. Kiefer (1975)

 $^{^1}$ Supported in part by the Alexander von Humboldt-Stiftung, Bonn, through a Max Planck-Award for cooperative research.

 $^{^2}$ Supported in part by the Volkswagen-Stiftung, Hannover, while on leave from the University of Augsburg.

Received July 1997; revised January 1998.

AMS 1991 subject classifications. Primary 62K15, 62J05; secondary 15A69, 15A45.

Key words and phrases. Box-Hunter representation, cubic regression, design admissibility, Kiefer design ordering, Kronecker product, minimal complete design classes, quadratic regression, rotatable designs, tensor product.