Inverse prediction is important in a variety of scientific and engineering contexts such as geophysical (Krasnopolsky and Schiller (2003), Sun (1994)), nuclear forensics (Moody et al. (2015), Anderson-Cook et al. (2015a, b), chemometrics (Martens and Naes (1987), Haaland and Thomas (1988)), and medical applications (Messinger-Rapport and Rudy (1986)). The motivation and major application for the methods described in this paper is inverse prediction using experimentally based models (e.g., see Anderson-Cook et al. (2015a, b) and Nel-

Key Words: Calibration; Errors in Variables; Glass Composition; Nuclear Forensics; Total Least Squares.

1. Introduction

Inverse prediction is important in a wide variety of scientific and engineering contexts such as geophysical (Krasnopolsky and Schiller (2003), Sun (1994)), nuclear forensics (Moody et al. (2015), Anderson-Cook et al. (2015a, b), chemometrics (Martens and Naes (1987), Haaland and Thomas (1988)), and medical applications (Messinger-Rapport and Rudy (1986)). The motivation and major application for the methods described in this paper is inverse prediction using experimentally based models (e.g., see Anderson-Cook et al. (2015a, b) and Nel-

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son et al. (1986)). However, the approach presented here can also relate to a variety of scientific and engineering contexts that involve the use of science-based computational models (e.g., see Taflove and Hagness (2005)).

The existence of one or more forward causal models is assumed (see Figure 1). Each model operates on one or more factors (inputs) to yield one or more responses (outputs). The models could be experimentally based and/or science based. In the case of an experimentally based model, the model parameters (and often the form of the model) are estimated using outputs that are observed for a series of experimental trials in which the inputs are controlled. This process is sometimes referred to as calibration, model fitting, or simply “fitting”. A sensible experimental strategy for the fitting process is one that allows for efficient estimation of forward model parameters such that the factor space of interest in the study is appropriately spanned (where inverse prediction is to be applied) and accurate forward models can be estimated. Note that, in the case of science-based computational models, some of the model parameters might be the same as the inputs. For example, Thomas et al. (2010) refer to a science-based computer model that requires the thickness of lead shielding (which is a model parameter) as an input. Inverse prediction has to do with the process of inferring the factors (or, in the case of a science-based model, inferring the model parameters) based on the responses. Inverse prediction is inherently more difficult than fitting. For example, there is no guarantee of a unique inverse solution (e.g., see Aster et al. (2013)). The utility of an inverse prediction process depends on the nature of the forward models and whether the collective set of responses can yield accurate, precise, and unconfounded predictions of each of the factors of interest, so as to be sufficiently informative and discriminating.

To illustrate inverse prediction, consider a chemist who uses the measured absorbance \( y \) of a solution at a particular wavelength to infer the concentration \( x \) of a particular chemical species in that solution. The forward model in this case, relating absorbance to concentration, might be of the form 
\[
 y = a + b \cdot x + \varepsilon ,
\]
where \( x \) is the factor, “\( a \)” and “\( b \)” are the model parameters, and \( \varepsilon \) is a measurement error. By using estimates of the model parameters \( \hat{a} \) and \( \hat{b} \), the fitted forward model is inverted to predict \( x \) given a new \( y \) via
\[
 \hat{x}_{\text{new}} = (y_{\text{new}} - \hat{a})/\hat{b} .
\]  

Krutckhoff (1967) refers to this as classical calibration. Inverse calibration relates to the case where \( x \) is modeled as a function of \( y \), i.e., 
\[
 x = \hat{c} + \hat{d} \cdot y .
\]
This fitted inverse model is used directly to predict \( x \) given a new \( y \) via
\[
 \hat{x}_{\text{new}} = \hat{c} + \hat{d} \cdot y_{\text{new}} .
\]

Other situations involve multiple forward models relating multiple measurements (a multivariate response) to multiple factors. Not surprisingly, there are additional complexities, options, and advantages when predicting material properties from measurements when the response space and/or factor space are multidimensional (e.g., see Martens and Naes (1987)). In some cases, when the response is highly dimensional (e.g., near-infrared spectroscopy), regularization methods (e.g., based on dimension reduction and inverse calibration) such as partial least squares (PLS) and principal component regression (PCR) are used to construct separate direct predictive models for each characteristic of interest (e.g., see Haaland and Thomas (1988)). Such methods are needed in these cases due to the high degree of collinearity among the response variables. In these cases, there is often only incomplete knowledge of the causal factors; hence, there is no ability to construct accurate forward models. Note that we are not focusing on such situations here. Rather, we focus on cases involving a moderate number of response variables (perhaps 5 to 20) and a small number of factors (perhaps 2 to 5). Further, each response is associated with a separate forward model. In such cases, inverse prediction is based on the collective multivariate response in combination with the set of associated forward models. For example, Anderson-Cook et al. (2015b) discuss inverse prediction in such a situation in the context of nuclear forensics in which physical and chemical measurements from interdicted ma...
terial are to be used to infer information relating to how the material was prepared and processed (factors such as reagent concentrations and processing temperatures) and thus indicate what facilities might have produced the material. Their recommendation is to develop forward models for a wide range of potentially useful responses in the calibration stage of a study. However, because of possible limitations regarding the amount of interdicted material available for testing and the destructive nature of testing, the number of responses that can be acquired during inverse prediction may be constrained. Hence, it would be useful (in this situation and many others) to have a strategy for down selecting an informative and discriminating subset of responses from among candidate responses. A discriminating subset of responses allows for potentially unconfounded inverse prediction of each of the factors.

The remainder of this paper explores, via analysis and two main examples, inverse prediction and means to assess the capability of a multivariate response with regard to being informative and discriminating in the context described. Section 2 provides notation, a general framework, and methodology for performing inverse prediction based on a multivariate response and an associated set of forward models. The methodology involves multifactor optimization with a least-squares objective function that incorporates multiple sources of prediction uncertainty, including the estimated parameters of the forward models. In order to streamline this exposition and make the associated guidance practical, various simplifications of the objective function are suggested when one or more of the sources of variation are considered to be relatively unimportant. Section 3 describes example 1, in which the composition of glass is predicted based on a set of six physical measurements and an associated set of simple first-order linear forward models involving three factors. The utility of selected subsets of the response variables is examined by analyzing the associated covariance of the inverse prediction errors. This analysis shows the benefit of including certain responses (e.g., density) for predicting certain compositional constituents (e.g., barium oxide). Specific criteria for a multivariate response being “informative and discriminating” based on the estimated covariance matrix of the inverse prediction errors are proposed. Section 4 considers a more general context for assessing the predictive capability of subsets of response variables where the forward models are assumed to be continuous parametric functions of the factors.

Further, the forward models are assumed not to be highly nonlinear so that the local first-order linear approximations used throughout the paper are accurate. Analysis of the first-order partial derivatives of the fitted forward models with respect to the factors is used to refine the criteria for being “informative and discriminating”. This more general context is illustrated with example 2, a synthetic example involving a set of 16 responses represented by quadratic surfaces defined by two factors. The example shows how the ability of inverse prediction to be informative and/or discriminating can vary widely depending on the subset of responses used as well as the location in the factor space where inverse prediction is performed. Thus, the proposed criteria provide a basis for down selecting a subset of responses with predictive ability from among candidate subsets. Concluding remarks are given in Section 5.

2. Inverse Prediction

Recall that, in our context, inverse prediction depends on a set of forward models that are based on well-understood science and/or one or more controlled experiments. One main purpose of a controlled experiment is to provide a basis for understanding the relationships between the response variables and the causal factors. Here it is assumed that, for each of $q$ response variables, a forward model can be fit that adequately relates the response variable to the set of $p$ causal factors. Model estimation uncertainty can have adverse effects on both inverse prediction and the down-selection process, depending on its magnitude. The proposed approach also assumes that $q \geq p$ so that inverse prediction can produce a unique solution. Otherwise, auxiliary information distinct from the available measurements (e.g., from experts) would be needed to obtain a unique solution. The use of additional response variables beyond the required minimum (i.e., $q > p$) can improve the precision of the inverse prediction solution. Collectively, the forward models also need to be sufficiently dissimilar in character (e.g., models cannot just be simple translations of one another) so that a unique solution can be obtained. The success of the inverse prediction process depends on how well the individual responses complement each other. The ability to measure the complementary nature of a candidate set of responses can be adversely affected by relatively large model estimation uncertainty. It is also assumed that the forward models are continuous and not highly nonlinear so that the local first-order linear approximations, which are used
in the down-selection process, are useful. Otherwise, conclusions developed from using the down-selection process could be distorted or inappropriate.

The model form and vector of estimated model parameters associated with the ith response variable are denoted by \( f_i \) and \( \hat{\beta}_i \), respectively. Given that the models provide an adequate fit, \( f_i(\hat{\beta}_i; \mathbf{x}) \approx y_i \) for each of the \( i = 1 : q \) response variables and for each trial of the controlled experiment. Here, \( \mathbf{x} \) is a vector representing the levels of the factors (assumed throughout to have been set with negligible error) and \( y_i \) represents the observed value of the ith response variable for a single experimental trial. The forward models derived from controlled experiments are often (but not necessarily) expressed in terms of a low-order polynomial, which can be thought of as a Taylor-series approximation to the true underlying relationship. As an aside, note that forward models are sometimes science-based and can also be represented by \( f_i(\beta_i; \mathbf{x}) \). In these cases, models can be quite complex (e.g., see Mitchell et al. (2014)) and take a wide variety of forms. Even more broadly, the set of models could include a mix of experimentally based and science-based models.

The multivariate response obtained by measuring a new object is used to predict the levels of the causal factors (unknown, but represented by \( \mathbf{x}^* \)) associated with the new object. Let

\[
y^* = \{y_i^* = \mu_i^* + \epsilon_i^*, \; i = 1 : q\}
\]

denote the observed response associated with a new object (\( * \)), where \( \mu_i^* = f_i(\beta_i; \mathbf{x}^*) \) is the true (expected) value of the ith response variable and \( \epsilon_i^* \) is the random measurement error of the ith response variable. The covariance of the collective set of measurement errors is denoted by \( \mathbf{V}_\varepsilon = \text{Cov}(\epsilon_i^*, \; i = 1 : q) \). Note that measurement errors exhibiting constant bias, independent of the true value, can be absorbed into fitted constants and so do not impact the ability to infer \( \mathbf{x}^* \). Measurement errors exhibiting constant relative bias are also possible, but are beyond our scope here, unless simple data transformations are adequate. Next, let

\[
\hat{y}^* = \{\hat{y}_i^* = f_i(\hat{\beta}_i; \hat{x}), \; i = 1 : q\}
\]

denote the predicted response derived from underlying models developed during the calibration process. These models are given in terms of estimated model parameters (\( \hat{\beta}_i \)) and a candidate solution (\( \hat{x} \)). In the case of the ith response, the difference between the predicted and observed response is

\[
d_i = \hat{y}_i^* - y_i^* = f_i(\hat{\beta}_i; \hat{x}) - f_i(\beta_i; \mathbf{x}^*) - \varepsilon_i^*, \quad (5)
\]

where \( f_i(\hat{\beta}_i; \hat{x}) \) is the predicted response using the estimated forward model evaluated at \( \hat{x} \). This difference can be re-expressed in terms of fundamental effects as

\[
d_i = \hat{y}_i^* - y_i^* = [f_i(\hat{\beta}_i; \hat{x}) - f_i(\beta_i; \mathbf{x}^*)] + [f_i(\beta_i; \mathbf{x}) - f_i(\beta_i; \mathbf{x}^*)] - \varepsilon_i^*. \quad (6)
\]

Let \( \lambda_i = [f_i(\hat{\beta}_i; \hat{x}) - f_i(\beta_i; \mathbf{x}^*)] \) and \( \omega_i = [f_i(\beta_i; \mathbf{x}) - f_i(\beta_i; \mathbf{x}^*)] \) represent effects due to imprecise estimation in the forward model parameters and uncertainty in the candidate solution (\( \hat{x} \)), respectively. This form of re-expression is useful to provide understanding of the various components of \( \mathbf{V} = \text{Cov}(d) \), where \( d_i, \; i = 1, 2, \ldots, q \). As will be seen in Sections 3 and 4, knowledge of the components of \( \mathbf{V} \) is necessary for estimating the covariance of \( \hat{x} \). The covariance of \( \hat{x} \) can be estimated for different subsets of responses and hence provide a basis for down-selecting an informative and discriminating subset of responses from among candidate subsets.

Assuming that the model form is properly specified and that the candidate solution is unbiased, the expected value of \( d_i \) is zero. Furthermore, based on Equation (6),

\[
\mathbf{V} = \mathbf{V}_\lambda(\hat{x}) + \mathbf{V}_\omega(\hat{x}) + 2\text{Cov}_\lambda(\hat{x}) + \mathbf{V}_z, \quad (7)
\]

where \( \mathbf{V}_\lambda(\hat{x}) = \text{Cov}(\lambda_i, \; i = 1 : q), \; \mathbf{V}_\omega(\hat{x}) = \text{Cov}(\omega_i, \; i = 1 : q), \) and \( \text{Cov}_\lambda(\hat{x}) \) represents the covariance between \( \{\lambda_i\} \) and \( \{\omega_i\} \).

The measurement error covariance, \( \mathbf{V}_\varepsilon \), can be estimated as \( (\mathbf{V}_\varepsilon) \) by using knowledge of the measurement processes (e.g., obtained from a measurement capability study) or indirectly by the empirical covariance of the residuals from model fitting. The latter strategy is possible if the data acquired from a common set of experimental trials are used for fitting the forward models for each of the potential responses. Further, if the number of responses (\( q \)) is relatively large compared with the number of observations used for fitting, it may be advisable to use a shrinkage estimator of the covariance matrix (e.g., see Daniels and Kass (2001)).

Estimates of the diagonal elements of \( \mathbf{V}_\lambda \), denoted by \( \{\text{Var}(\lambda_i), \; i = 1 : q\} \), can be obtained as follows. In the case of the ith response variable, the errors in the estimated model parameters (\( \hat{\beta}_{i1}, \hat{\beta}_{i2}, \ldots, \hat{\beta}_{im} \)) are denoted by \( \{\delta_{i1}, \delta_{i2}, \ldots, \delta_{im}\} \). The values of \( \delta_{ij} \)
are assumed to be distributed with \( E(\delta_{ij}) = 0 \), \( \text{Var}(\delta_{ij}) = \sigma_{ij}^2 \), and \( \text{Cov}(\delta_{ij}, \delta_{ij'}) = c_{ij} \), \( j \neq j' \). Then, by using a first-order approximation,

\[
\text{Var}(\lambda_i) = \sum_{j=1}^{m_i} \left( \frac{\partial \hat{g}_j}{\partial \beta_{ij}} \right)^2 \sigma_{ij}^2 \\
+ 2 \sum_{j'=j}^{m_i} \left( \frac{\partial \hat{g}_j}{\partial \beta_{ij}} \right) \left( \frac{\partial \hat{g}_{j'}}{\partial \beta_{ij'}} \right) c_{jj'}. \tag{8}
\]

We suggest that the off-diagonal elements of \( \hat{V}_\lambda \) be assumed to be zero unless the measurement errors across the responses are highly correlated.

The values in \( \hat{V}_w \) can be approximated as follows. First, assume that each of the \( q \) forward models, \( \{f_i(\beta; \mathbf{x}), i = 1 : q\} \), is continuous in terms of the factors, and let \( \mathbf{J} \) be the Jacobian matrix where the \( ij \)th element of \( \mathbf{J} \) is

\[
J_{ij}(\mathbf{x}) = \{x_1, x_2, \ldots, x_p\} = \frac{\partial f_i(\beta; \mathbf{x})}{\partial x_j}. \tag{9}
\]

A first-order approximation to \( f_i(\beta; \hat{\mathbf{x}}) \) in the vicinity of \( \mathbf{x}^* \) is given by

\[
f_i(\beta; \mathbf{x}^*) + \sum_{j=1}^{p} \hat{J}_{ij} \cdot (\hat{x}_j - x_j^*), \tag{10}
\]

where

\[
\hat{J}_{ij} = \frac{\partial f_i(\hat{\beta}; \hat{\mathbf{x}})}{\partial x_j}.
\]

Thus, \( \omega_i \approx \sum_{j=1}^{p} \hat{J}_{ij} \cdot (\hat{x}_j - x_j^*) \) and

\[
\text{Var}(\omega_i) \approx \sum_{j=1}^{p} \hat{J}_{ij}^2 \cdot \text{Var}(\hat{x}_j - x_j^*) \\
+ 2 \sum_{j > j'} \hat{J}_{ij} \hat{J}_{ij'} \cdot \text{Cov}(\hat{x}_j - x_j^*, \hat{x}_{j'} - x_{j'}^*). \tag{11}
\]

Furthermore,

\[
\text{Cov}(\omega_i, \omega_{i'}) \approx \sum_{j=1}^{p} \hat{J}_{ij} \hat{J}_{ij'} \text{Var}(\hat{x}_j - x_j^*) \\
+ \sum_{j \neq j'} \hat{J}_{ij} \hat{J}_{ij'} \cdot \text{Cov}(\hat{x}_j - x_j^*, \hat{x}_{j'} - x_{j'}^*). \tag{12}
\]

The goal of inverse prediction is to find an “optimal” solution such that predicted values of the responses are close to those observed, namely that \( \hat{y}_i^* \approx y_i^* \) \( \forall i \). In general, an iterative approach involving nonlinear optimization can be used to find a good estimate for \( \mathbf{x}^* \), here denoted by \( \hat{\mathbf{x}}^* \). Software modules for performing this optimization include \textit{nlmiser} (R) and \textit{fminsearch} (MATLAB). Our iterative approach requires the set of forward model parameter estimates \( \{\hat{\beta}_i, i = 1 : q\} \), an estimate of \( \hat{V} \) based on its components, and an initial guess for the solution (\( \mathbf{x}_{\text{init}} \)). Here, to simplify, we focus on two of the components, \( \hat{V}_w(\mathbf{x}) \) and \( \text{Cov}_{\lambda}(\mathbf{x}_{\text{init}}) \). We believe that, when inverse prediction is suitably overdetermined (\( q \) is sufficiently larger than \( p \)), \( \hat{V}_w(\mathbf{x}) \) and \( \text{Cov}_{\lambda}(\mathbf{x}_{\text{init}}) \) will contribute negligibly to \( \hat{V} \). That is, the uncertainty in \( \mathbf{x} \) can be quite small in such cases and vanish as \( q \to \infty \) (see e.g., Thomas (1991)). Therefore, we simplify Equation (7) by letting

\[
\hat{V} = \hat{V}_\lambda(\mathbf{x}_{\text{init}}) + \hat{V}_\varepsilon. \tag{13}
\]

Conditioned on the initial guess (\( \mathbf{x}_{\text{init}} \)), we search for a \( p \)-dimensional \( \mathbf{x}_{\text{update}} \) such that \( Q = d^T \hat{V}^{-1} d \) is minimized. As described, \( \hat{V} \) should be invertible. If another method is used to estimate \( \hat{V} \), it would be prudent to confirm that it is invertible. Shrinkage methods (e.g., see Daniels and Kass (2001)) could be used to modify \( \hat{V} \) if it is found not to be invertible or to have an unstable inverse due to being poorly conditioned. The minimization of \( Q \) results in an updated predicted response,

\[
\hat{y}_{\text{update}}^* = \{f_i(\hat{\beta}_i; \hat{\mathbf{x}}_{\text{update}}), i = 1 : q\}
\]

and an updated estimated covariance,

\[
\hat{V} = \hat{V}_\lambda(\mathbf{x}_{\text{update}}) + \hat{V}_\varepsilon.
\]

The iterative process continues to update both \( \hat{\mathbf{x}} \) and \( \hat{V} \) in this way until the updated version of \( \hat{\mathbf{x}} \) becomes indistinct from the previous version of \( \hat{\mathbf{x}} \). This process is illustrated with example 1 in Section 3. Depending on the nature of the forward models, the efficiency of the calibration experiment, and the specific unknown levels of the causal factors \( \mathbf{x}^* \), \( \hat{V}_\lambda \) may or may not contribute a significant amount to \( \hat{V} \). If \( \mathbf{x}^* \) is well within the design space used to construct the forward models, then \( \hat{V}_\lambda \) will likely not contribute a significant amount to \( \hat{V} \). In that case, the iterative process may converge immediately. Conversely, if \( \mathbf{x}^* \) is outside of the design space, \( \hat{V}_\lambda \) could be a significant contributor due to model extrapolation. Additionally, note that other minimization criteria (e.g., emphasizing robustness) could be used.

It is important to restate that the iterative approach presented here considers the uncertainty in the predicted response (induced by uncertainty in the forward model parameters). In the inverse prediction
context, one might view the forward model parameters as “regressors” and the components of $\mathbf{x}^*$ as parameters to be estimated. The errors in the estimated model parameters are analogous to measurement errors in the regressors. Hence, the approach presented here is connected to models and methods discussed in the errors-in-variables and total least-squares literature (e.g., see Fuller (1987), Van Huffel and Vandervalle (1991), and Thomas (1991)). Alternatively, a Bayesian approach that also recognizes the uncertainty in the forward model parameters in the context of inverse prediction is presented by Anderson-Cook et al. (2015a).

Finally, note that the approach presented here for inverse prediction (with some slight modifications) could relate to inverse problems involving science-based forward models. For example, Thomas et al. (2010) describe an example of inverse prediction where the goal is to infer two parameters of a physics-based radiation transport model from an observed high-dimensional gamma spectrum. The two model parameters are the radius of a plutonium sphere and the thickness of lead shielding surrounding it. In many cases of science-based forward models, the partial derivatives (describing the sensitivity of model outputs to changes in the model parameters) cannot be expressed analytically. In such cases, these partial derivatives can be approximated numerically. The estimated variance of $\hat{\mathbf{y}}^*$ due to uncertainty in the model parameters is then based on this numerical approximation.

3. Example 1: Prediction of Glass Composition from Physical Properties

A study was performed at Sandia National Laboratories to investigate how glass properties varied as a function of composition (Nelson et al. (1986)). A secondary purpose of the study was to assess the ability to detect batching errors (resulting in off-target composition of the finished glass) based on the physical properties. The basis of this study was a controlled experiment in which various target glass compositions were batched. The glass composition can be described in terms of a mixture of four components: $\text{P}_2\text{O}_5$, $\text{Na}_2\text{O}$, $\text{BaO}$, and $\text{Al}_2\text{O}_3$. Measurements of six physical properties were acquired from the materials that were produced during the controlled experiment. These properties included thermal expansion coefficient ($\alpha$), softening temperature ($T_s$), glass transition temperature ($T_g$), crystallization temperature ($T_x$), density ($\rho$), and index of refraction ($n$).

The experiment was designed such that responses would be obtained in a balanced configuration of the factor space illustrated in Figure 2. The experimental space was defined in terms of mole ratios in order to accommodate the constraint that the proportions of all mixture components must sum to one. The quantity of $\text{P}_2\text{O}_5$ is used in the denominator in the set of mole ratios because it is the dominant component in the nominal glass composition and because its targeted relative variation was relatively small. Table 1 summarizes the measured glass properties associated with each composition. Note that the actual compositions of the glass materials (although precisely measured by wet chemical methods) differ somewhat from the original target compositions (particularly in the case of sample 2-1).

Based on the experimental data, simple forward models (relating glass properties to composition) were constructed via least-squares regression. These models are of the form,

$$\hat{\mathbf{y}} = \hat{\mathbf{b}}_0 + \hat{\mathbf{b}}_1 \cdot \mathbf{x}_1 + \hat{\mathbf{b}}_2 \cdot \mathbf{x}_2 + \hat{\mathbf{b}}_3 \cdot \mathbf{x}_3,$$

where $\mathbf{x}_1 = \text{Na}_2\text{O}/\text{P}_2\text{O}_5$, $\mathbf{x}_2 = \text{BaO}/\text{P}_2\text{O}_5$, and $\mathbf{x}_3 = \text{Al}_2\text{O}_3/\text{P}_2\text{O}_5$. Measurements from sample 2-1 were not used to construct the models. A few other measurements ($T_s$ from sample 1-1, $n$ from sample 1-2, and $T_s/T_g$ from sample 1-8) were also deemed to be anomalous and were not used when constructing the forward models. Table 2 provides the estimated model parameters obtained by least squares (as the errors in the assayed compositions were negligible). In addition, Table 2 provides $\hat{\sigma}_e$ (the square root of
### TABLE 1. Measured Composition (Mole Ratios) and Properties of Glass Materials

<table>
<thead>
<tr>
<th>Sample</th>
<th>Na$_2$O/P$_2$O$_5$</th>
<th>BaO/P$_2$O$_5$</th>
<th>Al$_2$O$_3$/P$_2$O$_5$</th>
<th>$\alpha$</th>
<th>$T_s$ °C</th>
<th>$T_g$ °C</th>
<th>$T_x$ °C</th>
<th>$\rho$ g/cc</th>
<th>$n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-1</td>
<td>0.679</td>
<td>0.474</td>
<td>0.101</td>
<td>179</td>
<td>499</td>
<td>350</td>
<td>473</td>
<td>3.12</td>
<td>1.542</td>
</tr>
<tr>
<td>1-2</td>
<td>0.647</td>
<td>0.476</td>
<td>0.043</td>
<td>196</td>
<td>358</td>
<td>325</td>
<td>481</td>
<td>3.09</td>
<td>1.543</td>
</tr>
<tr>
<td>1-3</td>
<td>0.652</td>
<td>0.318</td>
<td>0.108</td>
<td>182</td>
<td>395</td>
<td>343</td>
<td>516</td>
<td>2.96</td>
<td>1.531</td>
</tr>
<tr>
<td>1-4</td>
<td>0.629</td>
<td>0.321</td>
<td>0.046</td>
<td>188</td>
<td>354</td>
<td>324</td>
<td>452</td>
<td>2.92</td>
<td>1.523</td>
</tr>
<tr>
<td>1-5-a</td>
<td>0.489</td>
<td>0.474</td>
<td>0.108</td>
<td>165</td>
<td>427</td>
<td>359</td>
<td>564</td>
<td>3.12</td>
<td>1.545</td>
</tr>
<tr>
<td>1-5-b</td>
<td>0.469</td>
<td>0.471</td>
<td>0.111</td>
<td>169</td>
<td>415</td>
<td>376</td>
<td>551</td>
<td>3.10</td>
<td>1.542</td>
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<tr>
<td>1-6</td>
<td>0.462</td>
<td>0.472</td>
<td>0.039</td>
<td>177</td>
<td>367</td>
<td>336</td>
<td>509</td>
<td>3.08</td>
<td>1.538</td>
</tr>
<tr>
<td>1-7</td>
<td>0.477</td>
<td>0.331</td>
<td>0.107</td>
<td>166</td>
<td>414</td>
<td>374</td>
<td>530</td>
<td>2.95</td>
<td>1.533</td>
</tr>
<tr>
<td>1-8</td>
<td>0.418</td>
<td>0.338</td>
<td>0.051</td>
<td>178</td>
<td>356</td>
<td>323</td>
<td>508</td>
<td>2.95</td>
<td>1.527</td>
</tr>
<tr>
<td>2-1</td>
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<td>0.365</td>
<td>0.179</td>
<td>200</td>
<td>408</td>
<td>374</td>
<td>445</td>
<td>2.97</td>
<td>1.526</td>
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<td>0.042</td>
<td>189</td>
<td>367</td>
<td>342</td>
<td>480</td>
<td>2.98</td>
<td>1.529</td>
</tr>
<tr>
<td>2-3</td>
<td>0.535</td>
<td>0.395</td>
<td>0.074</td>
<td>173</td>
<td>385</td>
<td>340</td>
<td>484</td>
<td>3.01</td>
<td>1.534</td>
</tr>
<tr>
<td>2-4</td>
<td>0.540</td>
<td>0.324</td>
<td>0.076</td>
<td>175</td>
<td>387</td>
<td>349</td>
<td>501</td>
<td>2.92</td>
<td>1.527</td>
</tr>
<tr>
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<td>0.077</td>
<td>181</td>
<td>387</td>
<td>338</td>
<td>495</td>
<td>3.00</td>
<td>1.533</td>
</tr>
<tr>
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<td>0.424</td>
<td>0.072</td>
<td>172</td>
<td>400</td>
<td>355</td>
<td>507</td>
<td>3.04</td>
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<td>2-7</td>
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<td>0.422</td>
<td>0.084</td>
<td>180</td>
<td>394</td>
<td>356</td>
<td>512</td>
<td>3.05</td>
<td>1.537</td>
</tr>
<tr>
<td>c-p-a</td>
<td>0.549</td>
<td>0.406</td>
<td>0.071</td>
<td>182</td>
<td>383</td>
<td>347</td>
<td>481</td>
<td>3.02</td>
<td>1.534</td>
</tr>
<tr>
<td>c-p-b</td>
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<td>0.402</td>
<td>0.077</td>
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<td>1.534</td>
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<td>0.386</td>
<td>0.074</td>
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<td>380</td>
<td>353</td>
<td>505</td>
<td>3.00</td>
<td>1.533</td>
</tr>
</tbody>
</table>

### TABLE 2. Estimated Forward Model Parameters (Standard Errors), $\hat{\sigma}_e$, and $R^2$

<table>
<thead>
<tr>
<th>Property: $i = 1 : 6$</th>
<th>$\hat{\beta}_0$</th>
<th>$\hat{\beta}_1$</th>
<th>$\hat{\beta}_2$</th>
<th>$\hat{\beta}_3$</th>
<th>$\hat{\sigma}_e$</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Coefficient of thermal expansion ($\alpha$)</td>
<td>155.8</td>
<td>70.59</td>
<td>—</td>
<td>$-216.5$</td>
<td>3.12</td>
<td>0.86</td>
</tr>
<tr>
<td>2. Softening temperature ($T_s$)</td>
<td>392.7</td>
<td>$-104.7$</td>
<td>—</td>
<td>694.6</td>
<td>5.73</td>
<td>0.93</td>
</tr>
<tr>
<td>3. Glass transition temperature ($T_g$)</td>
<td>374.8</td>
<td>$-104.5$</td>
<td>—</td>
<td>412.1</td>
<td>6.39</td>
<td>0.82</td>
</tr>
<tr>
<td>4. Crystallization temperature ($T_x$)</td>
<td>570.5</td>
<td>$-219.5$</td>
<td>—</td>
<td>709.8</td>
<td>14.7</td>
<td>0.74</td>
</tr>
<tr>
<td>5. Density ($\rho$)</td>
<td>2.534</td>
<td>1.113</td>
<td>0.484</td>
<td>0.0119</td>
<td>0.97</td>
<td></td>
</tr>
<tr>
<td>6. Index of refraction ($n$)</td>
<td>1.498</td>
<td>$-0.0097$</td>
<td>0.0834</td>
<td>0.1036</td>
<td>0.00113</td>
<td>0.97</td>
</tr>
</tbody>
</table>
the mean-squared-residual obtained from the regression analysis) and $R^2$. Here, disregarding model misspecification, $\hat{\sigma}_\epsilon$ is also used as an estimate of the standard deviation of the measurement error for each property. Figure 3 illustrates the fitted surfaces. It is interesting to examine the magnitude of $\hat{\sigma}_\epsilon$ relative to the ranges of the fitted responses over the factor space of interest. Smaller measurement errors relative to the ranges of the responses over the factor space of interest enable more precise inverse predictions.

Next, we follow the approach for inverse prediction outlined in Section 2. It is assumed that the measurement errors are independent so that an estimate of the measurement error covariance is $\mathbf{V}_\epsilon = \text{diag}(\hat{\sigma}^2_1, \hat{\sigma}^2_2, \ldots, \hat{\sigma}^2_6)$. An analysis of the

![Figure 3. Fitted Response Surfaces (see Table 1 for Measurement Units).](image-url)
residuals associated with the fitted forward models supports this assumption. For the \( i \)th response variable, the errors in the estimated model parameters \( (\hat{\beta}_{i0}, \hat{\beta}_{i1}, \hat{\beta}_{i2}, \hat{\beta}_{i3}) \) are denoted by \( (\delta_{i0}, \delta_{i1}, \delta_{i2}, \delta_{i3}) \). It is assumed that the values of \( \delta_{ij} \) are distributed with \( E(\delta_{ij}) = 0 \), \( \text{Var}(\delta_{ij}) = \sigma^2_{ij} \), and \( \text{Cov}(\delta_{ij}, \delta_{ij'}) = c^i_{jj'} \), \( j \neq j' \). If the \( j \)th effect is not included in the forward model, then by definition \( \hat{\beta}_{ij} = 0 \), \( \text{Var}(\delta_{ij}) = 0 \), and \( \text{Cov}(\delta_{ij}, \delta_{ij'}) = 0 \). Thus, \( \lambda_i = y_i - \mu_i \) has an expected value of zero and variance

\[
\text{Var}(\lambda_i) = \sigma^2_{i0} + \sum_{j=1}^{3} \left( \frac{\partial \hat{y}_i}{\partial \beta_{ij}} \right)^2 \sigma^2_{ij} \\
+ 2 \cdot \sum_{j=1}^{3} \left( \frac{\partial \hat{y}_i}{\partial \beta_{ij}} \right) c^i_{ij} \\
+ 2 \cdot \sum_{j'=j+1}^{3} \left( \frac{\partial \hat{y}_i}{\partial \beta_{ij}} \right) \left( \frac{\partial \hat{y}_i}{\partial \beta_{ij'}} \right) c^i_{jj'}.
\]

(15)

Given the simple nature of the forward models in this case,

\[
\text{Var}(\lambda_i) = \sigma^2_{i0} + \sum_{j=1}^{3} (\hat{x}_j)^2 \cdot \sigma^2_{ij} + 2 \cdot \sum_{j=1}^{3} \hat{x}_j \cdot c^i_{oj} \\
+ 2 \cdot \sum_{j'=j+1}^{3} \hat{x}_j \cdot \hat{x}_{j'} \cdot c^i_{jj'}.
\]

(16)

An estimate of \( \text{Var}(\lambda_i) \) can be obtained by substituting estimates for \( \sigma^2_{ij} \) and \( c^i_{jj'} \) into the above expression. These estimates are obtained easily from the analysis used to develop the forward models (least-squares regression). Assuming independence of the \( \lambda_i \)s, \( \mathbf{V}_\lambda(\hat{x}^*) = \text{diag}(\text{Var}(\lambda^*_1), \text{Var}(\lambda^*_2), \ldots, \text{Var}(\lambda^*_q)) \), where \( \text{Var}(\lambda^*_i) \) is the estimate of \( \text{Var}(\lambda_i) \). The apparent independence of measurement errors across the set of responses supports this assumption.

Without an initial guess at the solution \( \hat{x}^* \), the iterative process (as described in Section 2) is initiated with \( \mathbf{V}_\lambda = 0 \). Recall from Section 2 that the main goal is to search for \( \hat{x}^* \), and we do so by seeking \( \hat{x}^* \) such that \( Q = \mathbf{d} \mathbf{V}^{-1} \mathbf{d} \) is minimized, where \( \mathbf{d} = \hat{y}^* - \mathbf{y}^* \), \( \hat{y}^* = \{f_i(\beta_i; \hat{x}^*) \}, i = 1 : q \) and \( \mathbf{V} = \mathbf{V}_\lambda + \mathbf{V}_\epsilon \). For this particular example, a sensible estimate/prediction for \( \hat{x}^* \) is obtained as follows. First, let \( z_i = y_i^* - \hat{\beta}_{i0} \), for \( i = 1, 2, \ldots, 6 \), and \( \hat{\beta}_{ij} = \hat{\beta}_{ij} \), for \( i = 1, 2, \ldots, 6 \), and \( j = 1, 2, 3 \). Let the \( z_i \) form a column vector \( \mathbf{z} \) with six elements and the \( \hat{\beta}_{ij} \) form a matrix \( \mathbf{B} \) with six rows and three columns. Using the iterative procedure described in Section 2, it follows from weighted least-squares regression that \( \hat{x}^* = (\mathbf{B}^T \mathbf{V}^{-1} \mathbf{B})^{-1} \mathbf{B}^T \mathbf{V}^{-1} \mathbf{z} \) minimizes \( Q \) at each iteration. The estimated covariance matrix of \( \hat{x}^* \) is

\[
\hat{\mathbf{C}}_{\hat{x}^*} = (\mathbf{B}^T \mathbf{V}^{-1} \mathbf{B})^{-1}.
\]

(17)

Thus, inverse prediction here is equivalent to regression of the \( q = 6 \) adjusted property measurements on the estimated forward model parameters, where errors in the estimated forward model parameters are accounted for by \( \mathbf{V}_\lambda \) (as a component of \( \mathbf{V} \)). Hence, this is analogous to a linear errors-in-variables problem. Note that the column dimension of \( \mathbf{B} \) refers to the dimension of \( \hat{x}^* \) (which is \( p = 3 \)) and not to the number of terms in the forward models (which can vary from model to model). Also note that, in this case, \( q \geq p \), which is necessary, but not sufficient, for all \( p \) elements of \( \hat{x}^* \) to be properly determined (not only in this case, but in general). Ultimately, the utility of the \( q \)-dimensional multivariate response for inverse prediction also depends on how well the individual responses complement one another. Figure 4 illustrates the results of applying this method for predicting the composition of the samples listed in Table 1 (excluding samples with anomalous measurements; 1-1, 1-8, and 2-1) based on the measured properties. Predictions converged within two iterations. Only minor changes in predictions were observed between iterations (suggesting that \( \mathbf{V}_\lambda \) is negligible). In fact, depending on the location of the particular observation within the design space used to develop the forward models, elements of \( \mathbf{V}_\lambda \) were typically about 30\% the magnitude of the corresponding elements of \( \mathbf{V}_\epsilon \).

By considering Figure 4, it is clear that the utility of the collective set of glass properties for predicting the various constituents of composition varies across the constituents. The correlation between the predicted and measured values for each of the molar-ratio constituents is 0.81 for Na\(_2\)O/P\(_2\)O\(_5\), 0.97 for BaO/P\(_2\)O\(_5\), and 0.89 for Al\(_2\)O\(_3\)/P\(_2\)O\(_5\). In contrast with the apparent mediocre ability to predict the Na\(_2\)O/P\(_2\)O\(_5\) molar ratio, the collective set of properties seems to provide a good basis for predicting both the Al\(_2\)O\(_3\)/P\(_2\)O\(_5\) and BaO/P\(_2\)O\(_5\) molar ratios. We point out that the strongest forward models (measured by \( R^2 \)) relate to density and index of refraction. Density is certainly most responsible for the relatively precise predictions of BaO/P\(_2\)O\(_5\) by virtue of barium’s unusually large density relative to the other constituents. Note in Table 2 that the forward model for density does not involve Na\(_2\)O/P\(_2\)O\(_5\). This is not surprising because the densities of Na\(_2\)O and P\(_2\)O\(_5\) are quite similar (i.e., substitution of Na\(_2\)O by
for the "index of refraction" depends only weakly on
found to be negligible, we further simplify Equation
positive notion that one must have a sufficient collection
tween errors associated with predicting Na
prediction.
also, note that the forward model for the "index of refraction" depends only weakly on Na$_2$O/P$_2$O$_5$. Thus, this is consistent with the intuitive notion that one must have a sufficient collection of strong forward models to obtain effective inverse prediction.

Figure 5 displays the relationship between the prediction errors ($\hat{x}_j^* - x_j^*$) associated with the three compositional constituents. There is a moderate level of negative correlation between the errors associated with predicting BaO and each of the other two constituents. There is very high positive correlation between the errors associated with predicting Na$_2$O and Al$_2$O$_3$. This behavior can be easily deduced through some simple analysis. Given that $\mathbf{V}_\lambda$ was found to be negligible, we further simplify Equation (17), resulting in

$$\mathbf{C}_{x^*} = (\mathbf{B}^\top \mathbf{V}_e^{-1} \mathbf{B})^{-1}$$

The associated correlation matrix of $\hat{x}^*$ is

$$\hat{\mathbf{R}}_{x^*} = \begin{bmatrix} 1.00 & -0.68 & 0.94 \\ -0.68 & 1.00 & -0.75 \\ 0.94 & -0.75 & 1.00 \end{bmatrix}.$$  

For purposes of inverse prediction, we regard the multivariate response as being informative if the diagonal elements of $\mathbf{C}_{x^*}$ are sufficiently small and discriminating if the off-diagonal elements of $\mathbf{C}_{x^*}$ are sufficiently small. An examination of the various elements of $\mathbf{C}_{x^*}$ (and $\hat{\mathbf{R}}_{x^*}$) allows for such an assessment. The off-diagonal elements of $\hat{\mathbf{R}}_{x^*}$ suggest correlations of 0.94 between errors associated with predicting Na$_2$O/P$_2$O$_5$ and Al$_2$O$_3$/P$_2$O$_5$ and −0.68 between errors associated with predicting Na$_2$O/P$_2$O$_5$ and BaO/P$_2$O$_5$. This level of correlation is consistent with what is observed in Figure 5. An examination of the diagonal elements of $\mathbf{C}_{x^*}$ suggests the root mean-squared prediction error associated with Na$_2$O/P$_2$O$_5$, BaO/P$_2$O$_5$, and Al$_2$O$_3$/P$_2$O$_5$ to be 0.08, 0.013, and 0.018, respectively.

Next, consider a subset of the multivariate responses that excludes density. If density is not used to help predict composition, then

$$\hat{\mathbf{C}}_{x^*} = \begin{bmatrix} 6.81 \times 10^{-3} & -1.02 \times 10^{-3} & 1.46 \times 10^{-3} \\ -1.02 \times 10^{-3} & 3.95 \times 10^{-4} & -2.65 \times 10^{-4} \\ 1.46 \times 10^{-3} & -2.65 \times 10^{-4} & 3.50 \times 10^{-4} \end{bmatrix}.$$  

This analysis suggests the root mean-squared prediction errors associated with Na$_2$O/P$_2$O$_5$ and Al$_2$O$_3$/P$_2$O$_5$ are still approximately 0.08 and 0.018, respectively. Thus, the effects of not using density to help predict these two constituents is inconsequential. However, by not using density, this analysis suggests that the root mean-squared prediction error for predicting BaO/P$_2$O$_5$ increases from 0.013 to about 0.020. Thus, density is very important for predicting BaO/P$_2$O$_5$. The suggested correlation structure remains similar. Clearly, the multivariate response is less informative for predicting BaO/P$_2$O$_5$ when excluding density.

Similar analyses could be performed to evaluate the potential predictive utility of any subset of the six response variables. In a different context, such an analysis might be useful for selecting the most valuable measurements to acquire during the prediction phase of a study when the number of measurements possible is limited by difficulty, expense,
and/or availability of material (perhaps due to the destructive nature of testing). In addition, one could use simulation and/or simple trial and error to examine the predictive capability of each candidate subset of the six responses, but our analysis and criteria provide insight into the relative merits of each candidate subset.

4. Inverse Prediction with More Complex Forward Models

The forward models used in the previous section each had a very simple form. For that reason, the required analysis was also simple. Sensible inverse predictions were obtained by using weighted least-squares regression. Here, a more general context is considered in which the forward models are assumed to be continuous parametric functions of the factors and are not highly nonlinear. We seek to provide additional insight and criteria regarding predictive utility in this more general context. This can then be used to develop a strategy for down selecting an informative and discriminating subset of responses. A synthetic example involving a candidate set of 16 response surfaces is used to illustrate the strategy.

In order to explore the characteristics of an informative and discriminating multivariate response, it is useful to make the following simplifying assumptions. First, assume that there is a unique solution, meaning that there is a unique $\hat{x}^*$ for a given $y^*$. Following the assumptions and notation in Section 2, we assume that each of the $q$ forward models, \{$f_i(\beta; x)$, $i = 1 : q$\}, is continuous in terms of the factors. While a complex model may be required to represent a given response over the whole region of inter-

![Figure 5. Scatterplot Matrix of Prediction Errors.](image-url)
est, a local first-order approximation can accurately reflect the response’s behavior within a small region. Thus, to further simplify and facilitate our analysis, we consider local first-order approximations to \( \{ f_i(\beta_i; x), i = 1 : q \} \) in the vicinity of \( x^* \) given by

\[
\hat{f}_i(\beta_i; x^*) + \sum_{j=1}^{p} \hat{J}_{ij}(x^*) \cdot (x_j - x_j^*),
\]

where

\[
\hat{J}_{ij}(x^*) = \frac{\partial}{\partial x_j} f_i(\beta_i; x^*)
\]

are the elements that form the \( q \) by \( p \) Jacobian matrix, \( \hat{J}(x^*) \). Note that the level of collinearity in \( \hat{J}(x^*) \) provides a good indicator of the discriminating ability of the multivariate response at \( x^* \). For example, a high level of collinearity is indicative of poor discrimination (and possible redundancy) because, in such cases, the effects of the factors on the various responses are not sufficiently dissimilar.

Recall from Section 2 that we proposed that an iterative approach involving nonlinear optimization can be used to obtain an estimate of \( x^* \), given by \( \hat{x}^* \). To estimate the covariance of \( x^* \) obtained in this manner, we rely on the assumption that the local first-order approximations to \( \{ f_i(\beta_i; x), i = 1 : q \} \) are sufficiently accurate. We further assume that the measurement errors are negligible relative to the magnitude of the elements of the Jacobian. Given these assumptions, it follows that a reasonable estimate of the covariance matrix of \( \hat{x}^* \) is given by

\[
\hat{C}_{\hat{x}^*} = (\hat{J}^T(\hat{x}^*)\hat{V}^{-1}\hat{J}(\hat{x}^*))^{-1},
\]

(19)

where \( \hat{V} = \hat{V}_0(\hat{x}^*) + \hat{V}_e \). However, if one or more of the forward models is highly nonlinear in the region of \( x^* \), the viability of \( \hat{C}_{\hat{x}^*} \) could be adversely affected. Thus, it is important for users of this methodology to establish that this is not the case. It is important to note that Equation (19) is a simple generalization of Equation (17). The elements of \( \hat{B} \) (in Equation 17) are equivalent to the elements of the estimated Jacobian of a set of forward models that consist exclusively of simple main effects. However, note that, in the case of more complex models, the elements of the Jacobian can depend on \( x^* \). Thus, even if we assume that \( \hat{V}_0(\hat{x}^*) \) is largely unimportant, for this more general case, the previously mentioned criteria for being informative and discriminating needs to be amended so as to be conditional on the location of \( x^* \).

### 4.1. Example 2: Synthetic Example

To make this discussion less abstract, we consider a synthetic example with a candidate set of 16 response surfaces (\( q = 16 \)) that each depend on two factors (\( p = 2 \)) over the input space \( x_1 \in [-1, 1] \times x_2 \in [-1, 1] \). The response surfaces are chosen to be of quadratic order (or less). Each can be characterized by the general model form

\[
y_i = \beta_{i0} + \beta_{i1} \cdot x_1 + \beta_{i2} \cdot x_2 + \beta_{i12} \cdot x_1 \cdot x_2 + \beta_{i11} \cdot x_1^2 + \beta_{i22} \cdot x_2^2.
\]

(20)

We show how the capability of inverse prediction depends not only on the particular subset of responses used but also on where \( x^* \) is positioned in the factor space. Table 3 provides the specific coefficients for each response surface. Figure 6 displays the surfaces. In industrial and other applications, quadratic response surface models are sufficient in complexity to represent a wide variety of responses (Box and Draper (1987), Myers et al. (2009)). We believe that such surfaces are representative of forward models used as a basis for inverse prediction in applications such as nuclear forensics. The set of surfaces considered here consists of four general types. Surfaces 1–4 involve a “peak”. Surfaces 5–8 represent “hillsides”. Surfaces 9–12 each represent a “rising ridge”. Surfaces 13–16 each represent a “saddle”. The vari-

<table>
<thead>
<tr>
<th>Surface (i)</th>
<th>( \beta_{i0} )</th>
<th>( \beta_{i1} )</th>
<th>( \beta_{i2} )</th>
<th>( \beta_{i12} )</th>
<th>( \beta_{i11} )</th>
<th>( \beta_{i22} )</th>
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lations of each surface type are essentially rotations of one another. In the context of these and other more complex forward models, the general iterative approach for inverse prediction involving nonlinear optimization described in Section 2 can be used to estimate the $p$ dimensions of $\mathbf{x}^*$. In general, this approach does not reduce to weighted linear regression, as was the case of the example in Section 3 with simple first-order linear forward models.

In the cases involving the quadratic forward models in two factors ($x_1$ and $x_2$),

\[
\begin{align*}
\hat{J}_{i1} &= \hat{\beta}_{i1} + \hat{\beta}_{i12} \cdot x_2 + 2 \cdot \hat{\beta}_{i11} \cdot x_1 \\
\hat{J}_{i2} &= \hat{\beta}_{i2} + \hat{\beta}_{i12} \cdot x_1 + 2 \cdot \hat{\beta}_{i22} \cdot x_2.
\end{align*}
\]  

(21)

In these cases, with $p = 2$, a local first-order approximation to $f_i(\beta_i; \mathbf{x})$ is

\[
\begin{align*}
f_i(\hat{\beta}_i; \mathbf{x}^*) + \hat{J}_{i1} \cdot (x_1 - x_1^*) + \hat{J}_{i2} \cdot (x_2 - x_2^*). \quad (22)
\end{align*}
\]

Hence, an estimate for the covariance matrix of $\mathbf{x}^*$ is given in Equation 19.

To simplify the illustrative example for purposes of clarity, we assume that $\mathbf{V}_{\lambda} = 0$ and $\mathbf{V}_{\epsilon} = \mathbf{V}_e = \sigma^2 \cdot \mathbf{I}$. Furthermore, without loss of generality, we also assume that $\sigma^2 = 1$. With these assumptions, Equation (19) simplifies to $\hat{\mathbf{C}}_{\mathbf{x}^*} = (\hat{\mathbf{J}}^T(\mathbf{x}^*) \hat{\mathbf{J}}(\mathbf{x}^*))^{-1}$. Here, we use $\hat{\mathbf{C}}_{\mathbf{x}^*}$ evaluated at $\mathbf{x}^*$ and the true forward parameter values as the basis for assessing the performance of inverse prediction. In practice, as in...
SELECTING AN INFORMATIVE/DISCRIMINATING MULTIVARIATE RESPONSE FOR INVERSE PREDICTION  241

the case of example 1 in Section 3, one would use estimates of both \( x^* \) and the forward parameter values to assess performance. This performance assessment would be adversely affected by poor estimates of \( x^* \) and/or the forward parameter estimated values. Note that, by including (or excluding) certain rows of \( J \), it is straightforward to evaluate and understand the performance of inverse prediction when using any subset \( (S) \) of the available response variables. Note that this evaluation could also be performed by brute force simulation using a candidate subset. A general understanding regarding the characteristics of an informative and discriminating multivariate response can be obtained by comparing inverse prediction performance when using various subsets of the responses represented in Table 3. The aspects of performance that will be considered are

\[
\sigma_1 = \sqrt{\hat{C}_{x^*}(1,1)}, \quad \sigma_2 = \sqrt{\hat{C}_{x^*}(2,2)}
\]

and

\[
\rho_{12} = \frac{\hat{C}_{x^*}(1,2)}{\sqrt{\hat{C}_{x^*}(1,1) \cdot \hat{C}_{x^*}(2,2)}}
\]

where \( \hat{C}_{x^*}(i,j) \) is the \( ij \)th element of \( \hat{C}_{x^*} \). The measures reflect the root mean-squared error of predicting the elements of \( x^* \) and the correlation between prediction errors. Due to the fact that \( J \) depends on \( x^* \), it is important to consider these quantities over the input space of interest for each of the four responses

\[
\{x_1, x_2\} = \{-0.2, 0.4\}
\]

for each \( J \). Figure 7 displays \( \sigma_1, \sigma_2, \) and \( \rho_{12} \) across the space of interest for several cases. In the first case, all \( q = 16 \) responses are used to predict \( x^* \) (i.e., \( S = \{1, 2, \ldots, 16\} \)). The other cases pertain to subsets, \( S = \{3, 7, 9, 13\} \) and \( S = \{9, 10, 11, 12\} \). When all 16 responses are used, the prediction errors (for both \( x_1^* \) and \( x_2^* \)) are expected to be largest in the center of the space of interest. This can be anticipated by noting that some of the surfaces (1, 2, 3, 4, 13, 14, 15, and 16) have relatively “flat spots” with little sensitivity to \( x_1 \) and \( x_2 \) near the center of the space of interest. The correlation of the prediction errors is relatively modest (typically between −0.4 and 0.4) over the space of interest. From Figure 7, it is clear that \( S = \{3, 7, 9, 13\} \) is a particularly bad choice for making an inference about \( x^*_1 \) when \( x^* \) is in the vicinity of \( \{x_1, x_2\} = \{-0.2, 0.4\} \). This is a consequence of the fact that \( |J_{11}(x)| \) is relatively small in the vicinity of \( \{x_1, x_2\} = \{-0.2, 0.4\} \) for each of the four responses in \( S = \{3, 7, 9, 13\} \). In contrast, \( |J_{12}(x)| \) is relatively large (in general) across the space of interest for each

of the four responses in $S = \{3, 7, 9, 13\}$. This leads
to relatively good predictions of $x_2^*$ across the space
of interest. The correlation of the prediction errors
varies considerably over the space of interest and is
most extreme when $\{x_1, x_2\} \approx \{-1.0, 1.0\}$. It is clear
that $S = \{9, 10, 11, 12\}$ is a good choice for making
an inference about both $x_1^*$ and $x_2^*$ across the
space of interest. This is largely a consequence of the
wide range of the values of these four response vari-
ables across the space of interest. In addition, the
response variables in $S = \{9, 10, 11, 12\}$ complement
each other well with steep contours in each of the two
dimensions throughout the space of interest for one
or more of the responses. In a relative sense, prediction
performance is worst around the center of the space
of interest where the contours are less steep.
The correlation of the prediction errors is most ex-
treme when $\{x_1, x_2\}$ is near the corners of the space
of interest.

Next, consider the case where $S = \{7, 8\}$. In the
absence of model and measurement errors, $y_8$ is a
perfect predictor of $x_1^*$ and $y_7$ is a perfect predic-
tor of $x_2^*$. Thus, by itself, the combination of $y_7$ and
$y_8$ should be useful for predicting $x^*$. In this case,
$\sigma_1, \sigma_2 = 0.0286$ and $\rho_{12} = 0$ are constant
over the space of interest. By comparing the results from
$S = \{1, 2, \ldots, 16\}$ and $S = \{7, 8\}$, it is clear that
the additional 14 responses from $S = \{1, 2, \ldots, 16\}$
may improve precision, particularly near the perimeter
of the space of interest. This is due to the fact that $|\lambda_{ij}(x)|$ tends to be larger around the perim-
eter (when compared with the center of the space of
interest) for some of these 14 additional responses.

A good subset of responses for inverse prediction
could be based on an I-optimality–like criterion (e.g.,
see Anderson-Cook et al. (2009)). That is, one might
seek to find a subset of responses of a given size
that minimizes the average inverse prediction vari-
ance over the space of interest. This approach could
be applied separately to each of the $p$ dimensions to
be predicted. Or, given an appropriate utility function,
one could apply this approach to some weighted
combination of the inverse prediction variance of the
$p$ dimensions while taking into account the correla-
tion in the prediction errors across the various di-
dimensions. For this example, we consider the aver-
age inverse prediction variance separately for $x_1^*$
and $x_2^*$. Table 4 compares the square root of the average
prediction variance of $\hat{x}_1^*$ and $\hat{x}_2^*$ across the response
subsets that were considered as examples. One could
easily consider other subsets of response variables.

Table 4 shows clearly that $S = \{9, 10, 11, 12\}$ is
an efficient subset of responses to use for inverse pre-
prediction. The summary measure of prediction ability
presented in Table 4 is useful for quickly comparing
the relative capability of various subsets of responses.
In cases with a large number of candidate responses,
this summary measure could be used as the basis
(“fitness function”) for selecting responses using a
structured search approach like genetic algorithms
e.g., see Goldberg (1989) and Thomas (1993)). How-
ever, it is important to recognize that prediction abil-
ity can vary widely across the space of interest (e.g.,
see Figure 7). It is also important to consider the
correlation of prediction errors across the various di-
ensions. In practice, one might also want to con-
sider model error in the analysis (i.e., not assume
$\lambda = 0$) and the possibility of using replicate mea-
urements. Finally, the selection of an informative
subset of response variables should naturally involve
subject-matter knowledge and economics (cost to ob-
tain the responses).

5. Conclusion

This paper considers inverse prediction based on
a multivariate response with an associated set of
forward models. In order for the multivariate re-
response to be useful for inverse prediction across all
input factor dimensions, one condition is that the
estimated forward models need to be accurate and
precise across the space of interest. A sensible ex-
perimental strategy for ensuring this during calibra-
tion requires that the factor space be appropriately
spanned with sufficient replication and number of
levels per factor. Furthermore, a second condition is
that the dimension of the multivariate response must
equal or surpass the number of factors to be pre-
dicted. Finally, for the multivariate response to be
useful for inverse prediction, it is also necessary that
the collection of forward models must be informative
and discriminating with respect to the individual fac-

tor dimensions over the space of interest. The causal

<table>
<thead>
<tr>
<th>Response subset</th>
<th>$\sqrt{\text{var}_{\text{avg}}(\hat{x}_1^*)}$</th>
<th>$\sqrt{\text{var}_{\text{avg}}(\hat{x}_2^*)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S = {1, 2, \ldots, 16}$</td>
<td>0.0075</td>
<td>0.0075</td>
</tr>
<tr>
<td>$S = {7, 8}$</td>
<td>0.0286</td>
<td>0.0286</td>
</tr>
<tr>
<td>$S = {3, 7, 9, 13}$</td>
<td>0.0291</td>
<td>0.0154</td>
</tr>
<tr>
<td>$S = {9, 10, 11, 12}$</td>
<td>0.0121</td>
<td>0.0121</td>
</tr>
</tbody>
</table>
relationships between factors and responses are dictated by nature and cannot be controlled by the experimenter. However, once the forward models have been developed, the experimenter can evaluate both the collective value of a set of responses as well as the incremental benefit of each additional response (individually) with regard to achieving useful inverse predictions associated with new observations.

This paper provides guidance to the practitioner for assessing the capability of a particular set of responses (and associated forward models) for providing adequate information and discrimination during inverse prediction. The method is based on the computation of the Jacobian matrix, consisting of all first-order partial derivatives of the estimated forward models with respect to each of the causal factors. The level of collinearity within the Jacobian provides a good indicator of the discriminating ability of the multivariate response. In general, the Jacobian varies depending on the location of the particular point in the space of interest that is being considered. Based on the Jacobian and estimates of the measurement error covariance and modelling error covariance, one can assess the level of uncertainty associated with inverse prediction at a particular point in the factor space. In cases where the number of response variables that can be acquired is limited by difficulty, expense, and/or availability of material, the assessed inverse prediction variance together with subject-matter knowledge can be used to help select a set of response variables from among various candidates. Thus, the methods described here can be helpful for implementing inverse prediction in cases where one needs to down select from a candidate pool of responses.

Finally, note that the discussion presented in this paper relates directly to a wide variety of inverse prediction problems, including those using science-based forward models. In such cases, one might use multivariate observational data to infer values of the parameters associated with science-based forward models.

References


