Sensitivity Analysis When Model Outputs Are Functions

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Abstract: When outputs of computational models are time series or functions of other continuous variables like distance, angle, etc., it can be that primary interest is in the general pattern or structure of the curve. In these cases, model sensitivity and uncertainty analysis focuses on the effect of model input choices and uncertainties on the overall shapes of such curves. We explore methods for characterizing a set of functions generated by a series of model runs for the purpose of exploring relationships between these functions and the model inputs.

Keywords: functional sensitivity analysis**,** functional data analysis, basis functions

1. INTRODUCTION

The outputs of computational models are often time series or functions of other continuous variables like distance, angle, etc. Following Campbell [1], we propose that sensitivity analysis of such outputs be carried out by means of an expansion of the functional output in an appropriate functional coordinate system, i.e., in terms of an appropriate set of basis functions, followed by sensitivity analysis of the coefficients of the expansion using any standard method. The principal new problem, therefore, is choosing an appropriate coordinate system in which to apply the selected sensitivity analysis methods. We consider both pre-defined basis sets and data-adaptive basis sets, with their associated advantages and disadvantages. We devote only passing mention to some related, but important problems, such as increasing the interpretability of the results by appropriate preprocessing of the functional outputs (in particular, alignment or registration of curves), and by enforcing some degree of smoothness when data-adaptive bases are used.

We will use a simple made-up example for explaining ideas. Fig. 1 shows a sample of curves generated by varying the four parameters, *a*, *b*, *c* and *d* in the "model"

$$f(\theta) = 10 + a \exp\left(-\frac{(\theta - b)^2}{K_1 a^2 + c^2} \right) + (b + d) \exp\left(K_2 \, a \, \theta \right). \tag{1}$$

We interpret these functions as model output from a problem where the independent variable θ is a polar angle ranging from -90º to 90º. The model was run 81 times, using a complete 3^4 factorial design for the four input parameters.

In analyzing this "model output" we are typically less interested in what affects the values at, say, 45º, than in questions such as: What shifts the curves up and down or moves them left or right? What makes the central peak wider or narrower? What makes the right-hand tail higher or lower? We could, of course, pick some appropriate functionals for answering these questions. The last, for example, we might address by examining the sensitivity of the values at 90º to the four input parameters. In order to address questions such as peak width we could devise some surrogate measurement that could be computed on each curve and then study its sensitivity to the input parameters. However, such choices are highly problem specific.

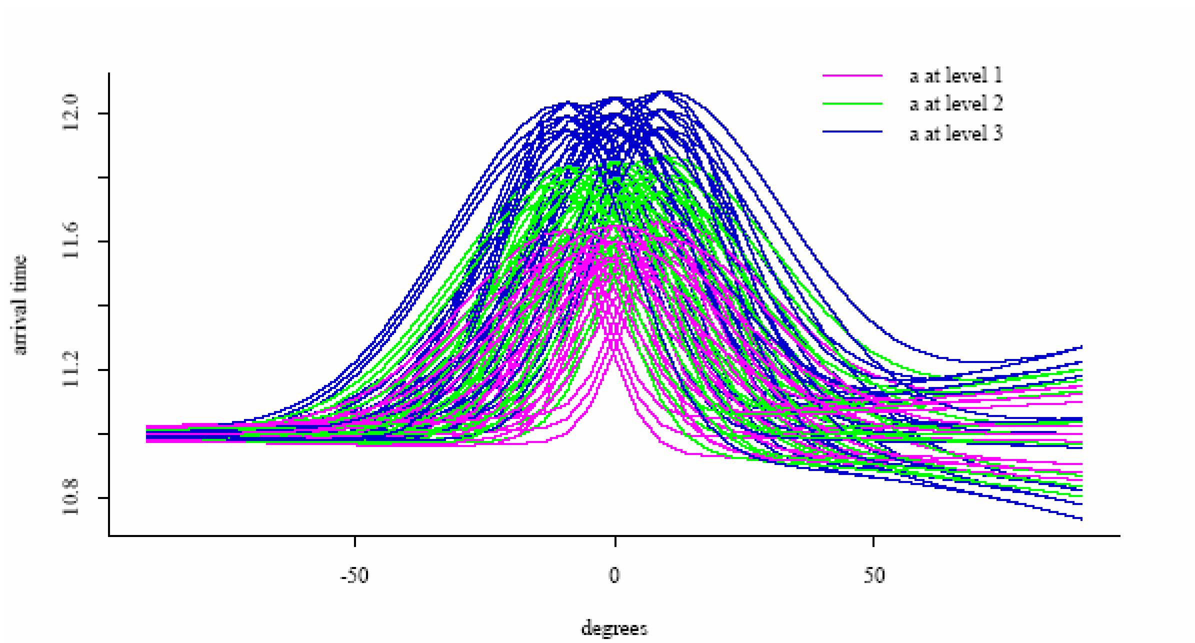

Figure 1. Functional output from 81 runs of the example model

2. TRANSFORMING FUNCTIONAL DATA

It might seem natural to regard functions provided on a grid of T points as T dependent variables for the purposes of sensitivity analysis. However, this approach can be unsatisfactory for many reasons:

- The T variables are highly correlated with one another, so this natural coordinate system is inefficient for statistical methods like discriminant analysis, sensitivity analysis, or almost anything other than multivariate statistical methods. Results are redundant from one value of θ to another.
- The pointwise results can be difficult to interpret for the underlying physical or modeling problem. In particular, information about the global functioning of the model or physical system contained in such curve features as location, scale and phase shifts, as well as in localized fluctuations including tail behavior, cannot generally be extracted from individual univariate analyses.

- Even though the data are the output of a computer model, the different runs may not have generated outputs at the same times or points θ. Alternatively, identical model output times may not be physically comparable because, as a function of the input parameters, the modeled process may be evolving faster in one run than another. So we may need to register the output curves (rescale time) in some physically more interpretable manner before proceeding with analysis.

All of these problems can be addressed by transforming the functional output in one way or another. For sensitivity analysis, the most useful approach is expanding the output functions in terms of some basis functions (after rescaling time, if necessary) and then applying the statistical method of interest—in our case, a sensitivity analysis method—to the coefficients of that expansion. Different types of bases can be considered. There are familiar, predefined bases such as Legendre polynomials or other orthogonal polynomials, trigonometric functions, Haar functions, or wavelet bases. Adaptive basis functions include principal components and partial least squares components. Ramsay and Silverman [2] provide a detailed treatment of functional data analysis methodology. In the remainder of this section, we highlight the techniques that are directly relevant to the application of Section 1.

If the columns of $\Phi_{T\times K}$ ($K \le T$) are a proposed set of basis functions, then the original functional output from N model runs, an $N \times T$ matrix Y, can be rewritten as

$$Y - \overline{Y} \approx H\Phi^T \, , \tag{2}$$

where $\overline{Y} = N^{-1}11^T Y$ with 1 the N-vector of ones, or

$$y_i(t) - \overline{y}(t) \approx \sum_{k=1}^{K} h_{ik}\varphi_k(t) \quad \text{for } 1 \le i \le N \, ,$$

where the mean function $\overline{y}(t)$ is computed as the mean of the $y_i(t)$ for each t. Equality holds in (2) if and only if the row space of $Y - \overline{Y}$ is a subspace of the column space of Φ.

Most standard basis systems are orthonormal. For example, the Legendre polynomials are orthonormal with respect to Lebesgue measure on [-1, 1]. But the Legendre polynomials in sin(t), which are used in the example below, are not orthonormal with respect to ordinary Lebesgue measure $d\theta$, but only with respect to a weighted measure $\cos\theta d\theta$. Adaptive bases functions may be orthonormal by construction, or not. Orthonormality of the basis functions is a nice property, since then the total variance is naturally partitioned among the variances of the coefficients:

$$\begin{aligned} \sum_{i=1}^{N} \left\| y_i - \overline{y} \right\|^2 &= \sum_{i=1}^{N} \left(\sum_{t=1}^{T} \left(y_i(t) - \overline{y}(t) \right)^2 \right) \\ &\approx \sum_{k=1}^{K} \left(\sum_{i=1}^{N} h_{ik}^2 \right) \\ &= \sum_{k=1}^{K} \left\| h_k \right\|^2 \quad . \end{aligned} \tag{3}$$

(Usually the basis functions are ordered so that the first few capture most of the total variance.) However, even when the basis functions are not orthonormal, the total variance captured by the expansion in terms of the first k ($k \leq K$) basis functions can be computed, and orthonormality may be less important than some other features when it comes to sensitivity analysis.

3. LEGENDRE POLYNOMIAL BASES

Since the example is being interpreted as a set of functions of angles from -90º to +90º, the Legendre expansion in sin(t) is a natural choice among standard expansions. Fig. 2 shows how the coefficients $\{h_{ik}\}$ of the expansions of the (N =) 81 functional outputs depend on the parameters, for k = 1, 2, ..., 6 (= K). The Legendre polynomials are alternately symmetric and anti-symmetric around zero, as shown in the top row of Fig. 2. The first k polynomials define a k-dimensional subspace of the (T =) 41-dimensional space in which the output functions are vectors. The percentages at the top show how much of the total variance in the original family of functions lies in this subspace for k up to 6. Note for future reference that the six-dimensional subspace defined by the first six polynomials still includes less than 90% of the total variance.

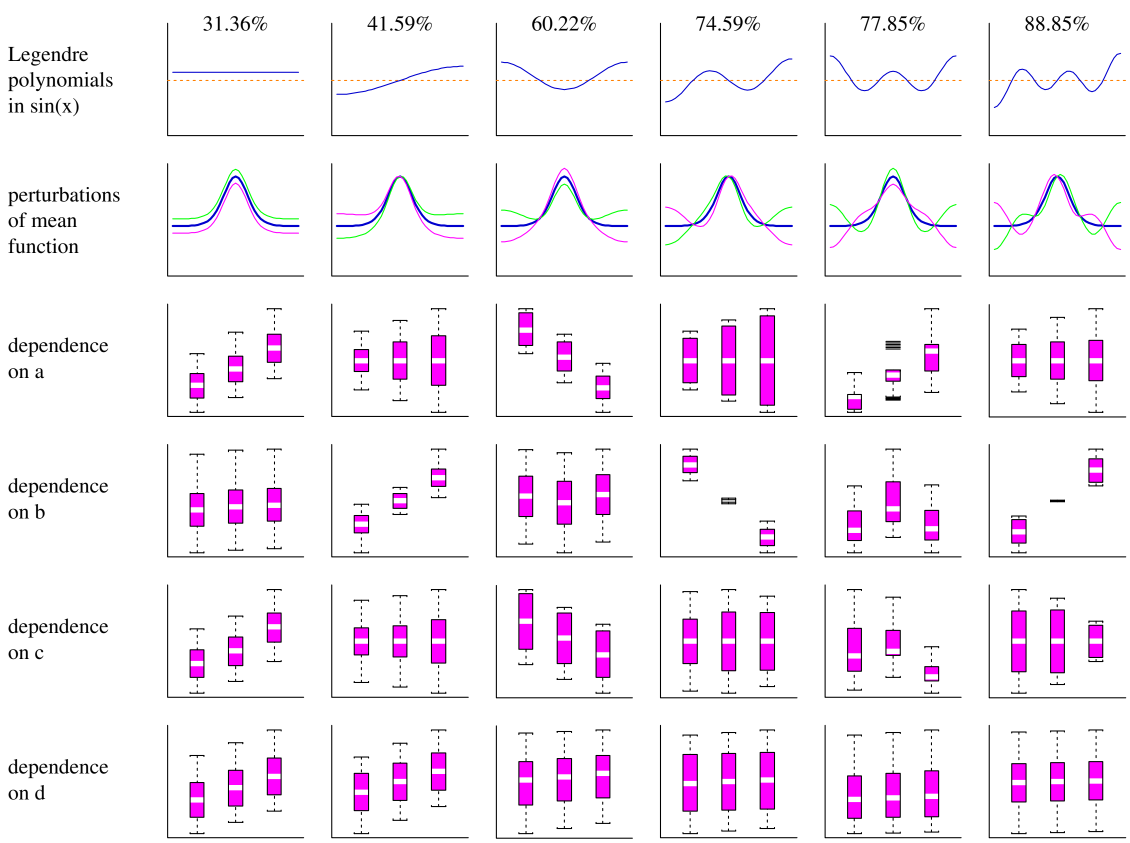

Figure 2. Dependence of the coefficients of the Legendre expansion on the parameters

In the second row, the Legendre polynomials are interpreted as perturbations of the overall mean of the 81 output functions. The mean function is the darker line. The mean plus and minus a multiple of the Legendre polynomial are the lighter lines.

The remaining rows contain box plots showing dependencies of the coefficients on the four parameters. Of course, we are not proposing sensitivity analysis by inspection-only as a serious method, but sensitivity analysis methodology is not the main goal of this paper. The figures are intended to suggest what more formal sensitivity analysis methods, such as described by McKay [3] and in Saltelli et al. [4], would indicate.

Variability in the coefficients of the Legendre polynomials of even order is controlled largely by a, although c and d influence the constant, zero-order term. The odd orders are controlled mostly by b with some influence of d on the first-order term.

An advantage of Legendre polynomials and other standard expansions is that they are well understood by many modelers. The other main advantage of using a consistent, non-adaptive basis system arises when a series of problems is being considered. The differences among corresponding analyses are then localized to the coefficients, instead of being partitioned out between the coefficients and the basis functions themselves.

The disadvantages arise in the case where the selected basis functions are not particularly well suited to the problem at hand. The Legendre polynomial basis, for example, is not a particularly good choice for a problem in which one of the main effects is neither symmetric nor antisymmetric, as in our example. The dispersion in the right-hand tail by comparison with the tight left-hand tail is not well captured by any single polynomial but spread out over several of them. The other disadvantage is that a relatively simple effect may be spread over several terms. For example, in this problem the effect of b, responsible for the left-right shift of the main peak, is spread out over all polynomials of odd order.

4. ADAPTIVE BASES COMPUTED BY PRINCIPAL COMPONENTS ANALYSIS

The principal components of Y, considered as N observations in a T-dimensional space, are themselves T-vectors, and are the eigenvectors of the $T \times T$ sample covariance matrix. They form an orthonormal basis for the T-dimensional space (or for a subspace of T-dimensional space, if $N < T$) that is specifically adapted to maximize the variance of the projection of the data onto the first basis vector, then onto the subspace spanned by the first and second basis vectors, etc. Thus expansions in the principal component basis for sensitivity analysis should at least achieve some information aggregation, avoiding one of the more serious problems with the Legendre polynomial, namely the allocation of a fairly simple effect (e.g., width changes or left-right shifts) to several components.

The principal component analysis (PCA) is shown in Fig. 3. For the family of curves in Fig. 1, the first principal component is basically an up-down shift, but unlike the first Legendre function this shift is not constant across all angles. The subspace spanned by this one function accounts for about 46% of the total variance in the family of curves, compared with about 31% for the Legendre polynomial of order zero. Like the zero-order Legendre coefficient, the coefficient of the first principal component depends on all four parameters. The second principal component for this example is a left-right shift accounting for another 34% of the total variance and controlled primarily by the b parameter. A similar amount of the total variance was spread across the Legendre polynomials of odd orders. The third principal component is devoted explicitly to the right-hand tail and accounts for 11% of the total variance. It is clearly controlled by the *d* parameter, something that could not be extracted from the Legendre analysis.

These first three terms capture over 90% of the total variance, compared to seven terms required by the Legendre analysis. The fourth component, which accounts for another 5% of the total variance, is a symmetric kurtosis or tail-fattening component depending most strongly on *a* and *c*.

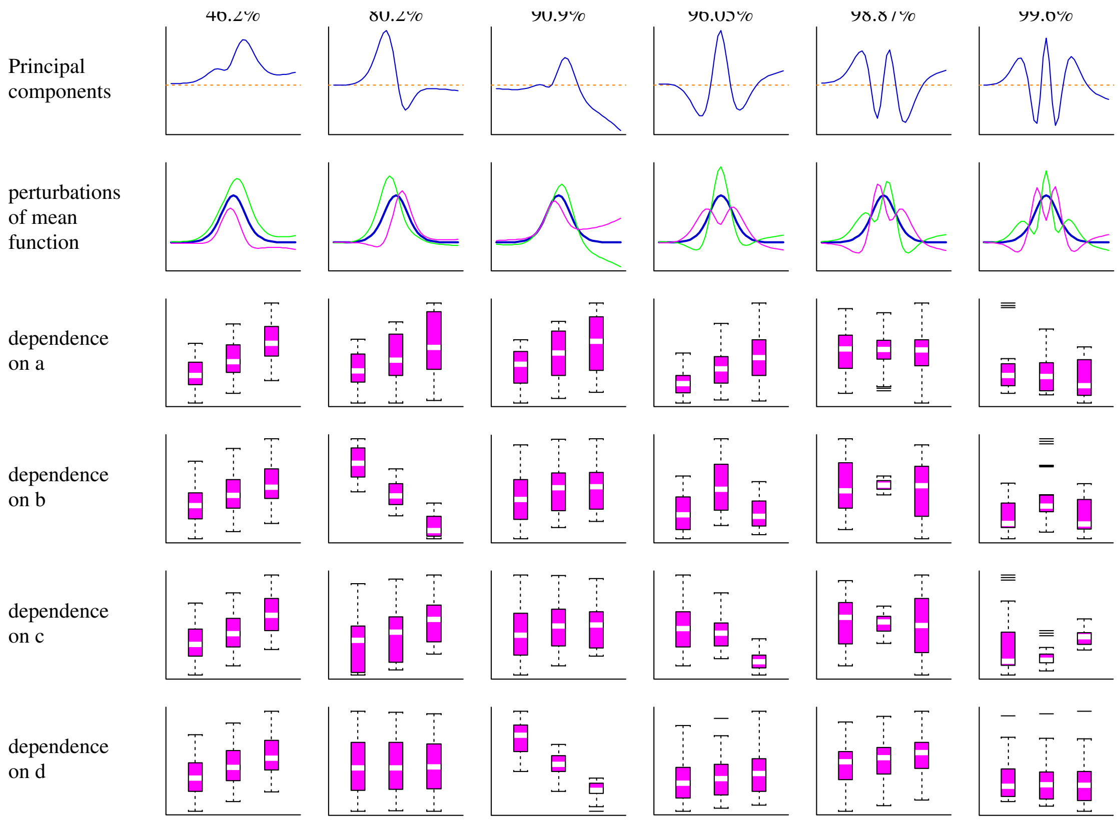

Figure 3. Dependence of the coefficients of PCA expansion on the parameters

5. ADAPTIVE BASES COMPUTED BY PARTIAL LEAST SQUARES

Partial least squares (PLS) regression was invented to handle near-collinearity among the independent variables, which is not usually a problem in analyzing computer experiments, assuming a reasonable experimental design. Thus, PLS is really a technique for decomposing the design matrix. (For a review of PLS regression, see Frank and Friedman [5].) However, PLS simultaneously provides a transformation of the dependent variables in such a way that the first PLS component of the dependent variables has the maximum variance that can be predicted by a linear combination of the independent variables. The second PLS component is computed using the residuals from the prediction of the first, and has the maximum variance that can be predicted by a second, orthogonal component of the independent variables, etc. So one might think of PLS as "peeking" at the explanatory variables while doing something that is similar to a PC analysis of the dependent variable. Note that while the PLS components of the independent variables are orthogonal, the PLS components of the dependent variables are not, in general.

While there is no *a priori* guarantee that PLS results will be interesting for functional sensitivity analysis, we discuss them because they often seem to be fairly revealing. In particular, in the example they pull out some dependencies that were overshadowed by more important terms in both Legendre and principal component analyses.

The PLS components (Fig. 4) are somewhat more readily interpretable than the PCA components (Fig. 3). The first component is an up-down shift of the middle of the curve, depending as before on all four parameters. (The first PLS component should be the same as the first PCA component if the independent variables are standardized, which is to be recommended; it is only with the extraction of the second component that the algorithms diverge.) The second PLS component is a left-right shift, almost entirely a function of *b*, compared to the second PCA component which had more substantial contributions from *a* and *c* as well. The third PLS component is pure right-hand tail, dependent on *d*. The fourth is primarily a widthing term, although it also includes a small left-right shift component, and depends on *a* and *c*. As there are only four input parameters, the PLS algorithm can provide only four component vectors, but this four-dimensional subspace captures almost 96% of the total variability in this family of curves, which is almost as much as the first four PCA components. By comparison, the first four Legendre components captured only about 75% of the total variance.

The advantages and disadvantages of adaptive bases are pretty much the inverse of those for standard bases. The main advantage is good compaction or aggregation of the information; it is usually necessary to do sensitivity analysis on only the first few coefficients. The basis functions are also frequently more interpretable in physical terms. In a series of related problems, it may be interesting to study how the shapes of the component functions (as well as their coefficients) evolve. Of course, the down side to this is that shapes and coefficients are evolving simultaneously, which may lead to interpretation problems. In some cases it may make sense to pool all of the output functions for the series to extract a common set of PC or PLS components, so that the evolution of their coefficients through the series can be studied in the same way as the evolution of the coefficients of a fixed basis set, such as Legendre polynomials, could be examined.

6. OTHER CONSIDERATIONS

Penalty methods can be used to enforce a degree of smoothness on adaptive basis functions. Orthonormality is lost when this is done, but the results are probably more interpretable, and curve comparison across problems, or between model output and noisy data, becomes easier. Ramsay and Silverman [2] discuss the enforcement of smoothness in PCA (Chapter 7), and the technique is readily extended to PLS.

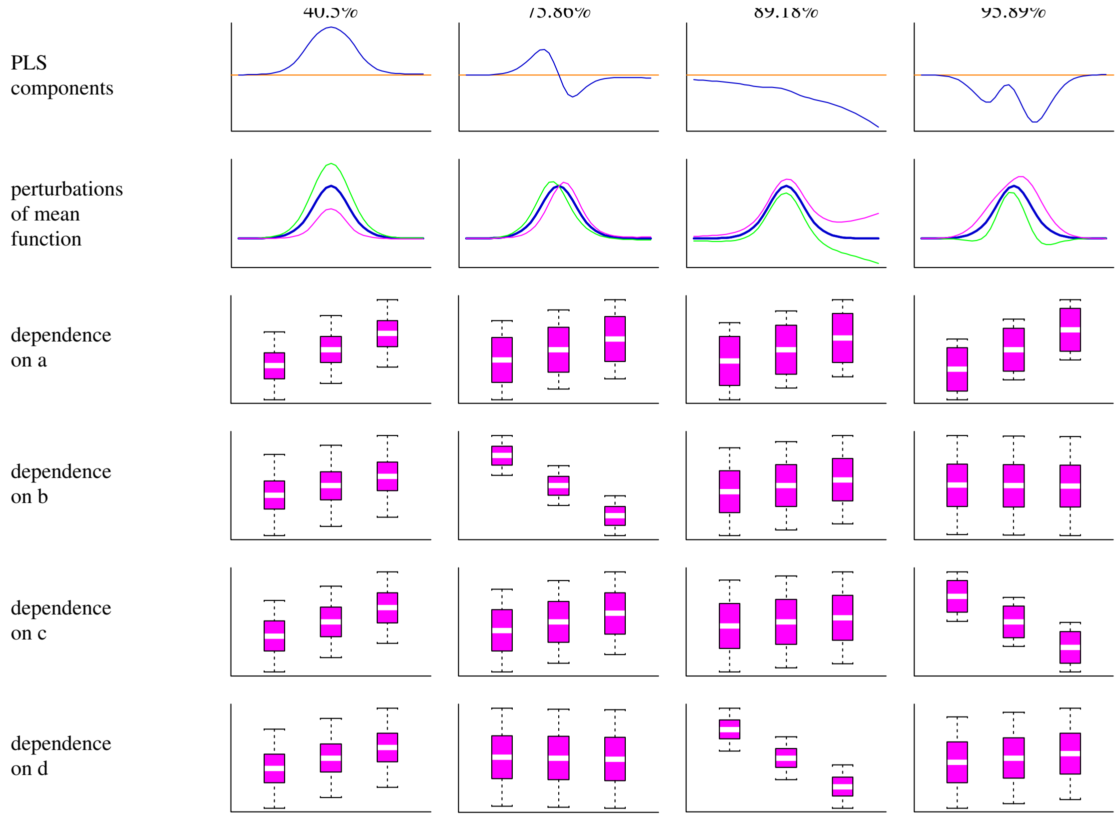

Figure 4. Dependence of the coefficients of PLS expansion on the parameters

Curve registration may be needed or advisable when the parameters affect the time- or space-scale or when the functions are not sampled at identical times in different runs. We would likely be interested in studying the sensitivity of the scaling and shifting to the input parameters, independently of the variability in the functional outputs after adjusting for these effects. Again, Ramsay and Silverman [2] address this problem in detail, proposing a series of methods from parametric location and/or scale change, through feature or landmark registration methods, to the estimation of general monotonic transformation.

7. SUMMARY

The purpose of this paper has been to suggest that sensitivity analysis for functional computer model outputs, correctly performed, is not significantly more difficult than for scalar outputs. The basic method is the expansion of the functional outputs in an appropriate functional coordinate system, i.e., in terms of an appropriate set of basis functions, followed by sensitivity analysis of the coefficients of the expansion using any standard method. The main art, then, is in choosing the appropriate coordinate system. We have considered both standard, pre-defined basis sets and data-adaptive basis sets. The example tends to favor the latter because of the aggregation and interpretability of the results, but the former may have value, depending on the problem or set of problems and the customer.

REFERENCES

1. Campbell K. “Functional sensitivity analysis of computer model output.” In: *Proc 7th Army Conf on Statistics*, Santa Fe, NM, 2001.
2. Ramsay JO, Silverman BW. *Functional data analysis*. Springer, New York 1997.
3. McKay MD. “Nonparametric variance-based methods of assessing uncertainty importance.” *Reliability Engineering and System Safety 1997*; *7*: 67-279.
4. Saltelli A, Chan K, Scott EM. (Eds.). *Sensitivity analysis*. John Wiley and Sons, Ltd. 2000.
5. Frank IE. Friedman JH. “A statistical view of some chemometrics regression tools.” *Technometrics* 1993;**35**: 109-135.