Efficient Investigation of the Feasible Parameter Set for Large Models

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EXTENDED ABSTRACT

In model identification, calibration or sensitivity analysis, the model-parameter values may be required to yield model-output values that satisfy specified constraints, for given initial conditions and forcing. Inequality constraints on scalar functions of the model outputs (henceforth called output bounds) confine the parameters to their *feasible set.* Output bounds are fundamental to regional sensitivity analysis and a desirable addition to multi-objective calibration.

In large simulation models, there is limited prior knowledge of how such output bounds translate into parameter bounds, so the nature of the feasible set is largely unknown. The simplest way to locate and explore the feasible set is to run the model for each of a large number of samples of the parameter values and note those that meet the output bounds. However, the feasible set may be almost in a subspace of the parameter space and may be fragmented into feasible subregions, some perhaps small. In such cases brute-force search, sampling from a uniform distribution or over a regular grid, is impracticable, as very few samples prove feasible. A more efficient approach is presented here. It fits ellipsoids to samples satisfying individual pairs of output bounds, using Khachiyan's algorithm, which approximates the ellipsoid most tightly bounding the convex hull of an arbitrary collection of points.. A minimum-volume ellipsoidal outer bound is then fitted to the intersection of two such ellipsoids by an algorithm described by Maksarov and Norton. The rest of the ellipsoids are incorporated one by one in successive applications of the algorithm, until the final ellipsoid approximates the feasible set.

The technique is tested on a demanding synthetic example and on the IHACRES rainfall-runoff model. In the former it approximates the feasible set well even when no sampled parameter-vector value is feasible. In the latter, the feasible set is defined by bounds on three complementary objective functions. Useful approximations of the non-convex feasible set are found. Simple bound relaxation is effective in reducing the number of trials needed to produce enough parameter-vector values meeting single-objective bounds to allow use of Khachiyan's algorithm.

There is scope for refining the procedure by exploring for feasible points about each ellipsoid as soon as it is fitted. Further experience with larger models, where efficiency is critical to the practicability of sampling-based investigation of the feasible set, is required.

1. INTRODUCTION

This paper addresses a problem that arises in sensitivity assessment (SA) of large simulation models and constrained multi-objective (MO) optimization (Fonseca and Fleming 1998) for model identification or calibration of an existing model. Regional sensitivity analysis (RSA) (Spear *et al*. 1994) investigates the *feasible set* of all model-parameter values yielding, for given initial conditions and forcing, model outputs that meet requirements expressed as scalar inequality constraints, henceforth called output bounds. The feasible set must also be identified if output bounds are to be applied in MO calibration or identification. Such bounds impose hard objectives to be attained before optimizing soft objectives. SA and MO model development are becoming recognised as essential for complex models.

In principle, the feasible set may be found either by inverting the output bounds analytically through the model to yield parameter bounds or simply by noting which parameter values in a large number of samples give outputs which fall within the output bounds, as in RSA. The former is seldom practicable for large non-linear models, although methods exist for smaller models (Jaulin *et al.* 2001; Milanese and Novara 2004). In RSA of large models, the feasible set is found typically to lie almost in a lower-dimension manifold in parameter space (Spear *et al.* 1994). The cause is over-parameterization of models of complex and/or distributed processes with aggregate behaviour simple enough to be approximated well by a reduced model; such models are often preferred as they can incorporate knowledge of physical processes (Reichert and Omlin 1997). The feasible set then fills very little of the region explored, few of the parameter values tested are feasible, and sampling is inefficient. It may well miss portions of the feasible set, especially if they are disjoint, as in an example below.

The problem of inverting a model to translate output bounds into parameter (or state or input) bounds is *set inversion*: subjecting a set to an implicit inverse mapping. Identifying the feasible set by forward runs with parameter values from dense random sampling or on a fine grid is impracticable for high-dimension spaces. Indeed, even for a few parameters the computing load of running a large simulation model may so restrict sampling as to make the feasible set hard to identify. A more economical way to find feasible points is needed. The approach presented here fits ellipsoids, first to parameter samples satisfying successive subsets of the output bounds, then to intersections of those ellipsoids, and ultimately to the feasible set. Existing ellipsoid-fitting algorithms (Milanese *et al*., 1996; Maksarov and Norton, 1996) are used. Advantages of ellipsoids for bounding include simple specification (by centre and symmetric describing matrix), relatively easy checking whether two of them intersect or one contains the other (Norton, 2005) and ability to minimize their size *via* the trace or determinant of the describing matrix (Schweppe 1968, Chernous'ko 1994, Durieu *et al.* 1996, Maksarov and Norton 1996). Other bounding objects, e.g. parallelotopes (Chisci *et al*. 1996) or limited-complexity polytopes (Veres *et al*. 1999), are as simple to specify but rather more complicated to fit, check and optimize. A limitation is that ellipsoids cannot tightly fit asymmetric or non-convex sets.

2. PROCEDURE TO SEEK FEASIBLE SET

In the absence of prior information, parameter values are sampled from a uniform distribution. Then, for each pair of upper and lower output bounds in turn, an ellipsoidal outer bound is fitted, by the algorithm of Khachiyan (1996), around parameter-space points found to be feasible with respect to those bounds alone. Each ellipsoid excludes no feasible point found but may include infeasible ones. Next, another established algorithm (Maksarov and Norton, 1996) is used to find the minimum-volume ellipsoid, from a parametric family, containing the intersection of two ellipsoids. In successive stages it outer-bounds the intersection of 2, 3, ..., all of the initial ellipsoids. Thus it outer-bounds all samples (if any) meeting all bounds, but may exclude feasible points not yet found. As the new ellipsoids include some infeasible segments, the end result is suboptimal. Disjoint ellipsoids at any stage may indicate a need to loosen incompatible bounds.

This procedure exploits the fact that the feasible set taking all bounds together has abrupt changes in boundary gradient where bounds join and may also be small and/or fragmented, yet the feasible sets for single bound pairs are larger, have smoother boundaries easier to approximate, and will be less fragmented. Hence, they generally take far fewer samples each to characterise than the feasible set for all bounds. Moreover, the intersection of the fitted one-bound-pair sets may be a useful guide to the overall feasible set even if no sample point meets all bounds. The procedure requires, of course, enough samples to define each one-bound-pair set adequately. Even then, its effectiveness in reducing the region to be explored for values feasible overall depends on how well the one-bound-pair ellipsoids fit those sets.

Khachiyan's algorithm requires at least n+1 points to find the minimum-volume n-dimensional circumscribing ellipsoid. If the feasible region for a single bound pair is small, dense sampling may be needed to find enough feasible parameter values. Instead, if initial sampling fails to find n+1 points, bound relaxation is initiated. Let the bounds on a scalar function of outputs $\boldsymbol{y}$ be $L \leq f(\mathbf{y}) \leq U$. They are relaxed in steps δx until m samples meet $L\text{-}k\delta x \leq f(\mathbf{y}) \leq U+k\delta x$. The m points are then evolved to satisfy the original bounds, using the MOCOM-UA genetic algorithm (Yapo *et al*. 1998). Points closer to meeting the original bounds are given better fitness ranks. The bounds are then tightened in steps δx, points meeting $L\text{-}i\delta x \leq f(\mathbf{y}) \leq U+i\delta x$ but no tighter bounds being given fitness rank i. The coarse fitness quantisation may assign all points equal fitness, causing MOCOM-UA to terminate prematurely unless the rank is zero. If so, the outermost bound is contracted until at least one point is infeasible, but not all m. At least one point then has rank differing from the others', and fitness assignment as above is repeated.

3. EXAMPLES

3.1. An Artificial Example

The first example finds the feasible set of an instantaneous, 2-parameter, 2-output model subject to linear and quadratic output constraints. The model is $y_1 = 2x_1x_2;\ \ y_2 = \dfrac{1}{2-x_1} + \dfrac{2+x_1}{3-2x_2}$ with parameters $x_1 \in [2,22]$ and $x_2 \in [0,1]$. The problem is to find all (x_1, x_2) such that $(y_1-2)^2 + (y_2-4)^2 \leq 3$ and either $(y_1-3)^2 + (y_2-5)^2 \leq 1$ or both $2.4 \leq y_1 \leq 2.8$ and $2 \leq y_2 \leq 3$. The parameter bounds are quite complicated, with two distinct feasible regions.

Figure 1 shows the results of ellipsoidal bounding and compares them with the exact solution. Although only 35 of 200 parameter points sampled from a uniform distribution satisfy one or more bounds and none meets all of them, the procedure discovers that there are two distinct feasible regions and estimates their sizes and locations. This is despite the output bounds yielding asymmetric, non-convex feasible subsets, which ellipsoids cannot fit well. Aspects of the algorithm needing refinement also emerge. First, an ellipsoid fitted to random points meeting a subset of bounds tends to exclude narrow, extreme, unexplored parts of the feasible region. As a result, the ellipsoids that bound regions feasible for subsets may not enclose the joint feasible set. In future, each ellipsoid could be refined, e.g. by exploring around the ends of its axes. Second, the smallest ellipsoid fitted to samples from a non-convex set may greatly overestimate its volume. Poor fits could be noted and costlier fitting initiated, e.g. fitting ellipsoids to subsets of the points and taking their union.

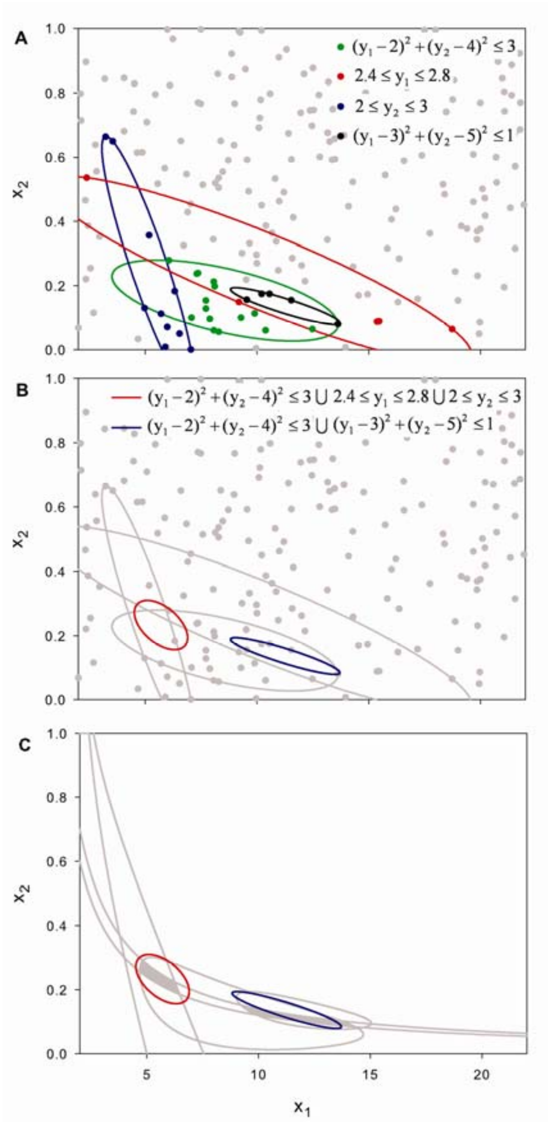

Figure 1. Example I. A: minimum-volume ellipsoids fitted around points meeting each objective's bounds. B: approx. bounds on feasible set, i.e. minimum-volume ellipsoids (coloured) containing intersection of ellipsoids in A. C: compares results B with exact solutions. Single-output bounds light grey lines, feasible set shaded grey.

3.2. IHACRES Rainfall-runoff Model

Next, the procedure finds the feasible set for the IHACRES model (Jakeman *et al*. 1990). Coupling it to MOCOM-UA then shows how it can speed up finding the Pareto set in MO calibration.

The IHACRES model was calibrated for the 105 km^2 Murrindindi catchment in Victoria, Australia. IHACRES is a conceptual-empirical model with a non-linear loss module to convert daily rainfall and temperature into effective rainfall and a linear routing module converting effective rainfall into stream flow. Each module has three parameters (Table 1), with loose prior bounds known. Daily records from 1976 to 1996 are available, split for this study into sets A, B and C, each spanning seven years.

Calibration uses three objective functions: mean error $bias = \frac{1}{n}\sum_{i=1}^{n}(Q_{Oi} - Q_{Mi})$ in flow volume,

proportional reduction $R^2 = 1 - \frac{\sum_{i=1}^{n}\left(Q_{Oi} - Q_{Mi}\right)^2}{\sum_{i=1}^{n}\left(Q_{Oi} - \overline{Q_O}\right)^2}$ in

mean square flow error and

$$R_{inv}^2 = 1 - \frac{\sum_{i=1}^{n}\left(\frac{1}{Q_{Oi}+\varepsilon} - \frac{1}{Q_{Mi}+\varepsilon}\right)^2}{\sum_{i=1}^{n}\left(\frac{1}{Q_{Oi}+\varepsilon} - \frac{1}{Q_{Mi}+\varepsilon}\right)^2}$$ where Q is

flow, subscripts O and M denote observed and modelled values and ε is a small number to avoid overflow when Q is zero. The objectives yield different parameter estimates and hydrographs. R^2 tends to highlight peak-flow errors while R_{inv}^2 gives most weight to low flows. The intersection of the bounds relating to all three determines the feasible set.

The ellipsoidal-bounding procedure was first applied to the linear module. Effective rainfall as input was obtained from the pre-calibrated non-linear module. The objectives were bounded by $-20 \le bias \le 20$, $0.3 \le R^2 \le 1$ and $0.3 \le R_{inv}^2 \le 1$. For each data set, ellipsoidal bounding used 100 parameter-vector samples from a uniform distribution. Figures 2, 4 and 6 and Table 2 show the results. They differ between the three data sets. For set A, containing the driest seven-year period, a smaller range of parameter values meets the bounds on *bias* than for set B or C. Thus, the IHACRES model is more sensitive at low flows to linear-module parameter changes. The small proportion of samples meeting the R_{inv}^2 bounds, which give more weight to low flows, supports this. For set C, the parameter ranges meeting the R^2 and R_{inv}^2 bounds are much smaller than for set A or B. The years spanned by set C have most variation in rainfall and stream flow, so the model's ability to fit highly fluctuating stream flows is sensitive to changes in the linear-module parameters. This is expected, as IHACRES tends to underestimate flow peaks and overestimate low flows. For data set A, Figure 3 compares the ellipsoidal approximation to the feasible set with feasible points from dense sampling; the ellipsoid locates the feasible region but underestimates its volume.

For set B, no sample points meet all the bounds. Even so, the ellipsoid successfully identifies the existence and location of the feasible region. As seen in Figure 4, the feasible region is non-convex, so the ellipsoid overestimates its volume. Figure 5 compares the ellipsoid with a set of feasible points found, at high computational cost, by dense sampling from a uniform distribution.

The feasible region for data set C is small and hard to find since it lies at the intersection of extreme sections of the individual bound regions. Again, no points satisfy all bounds. The resulting ellipsoidal bound (Figure 7) is comparable in size to the feasible set but does not intersect it.

Table 1. Parameters of the IHACRES model, with their initial uncertainty.

Module	Parameter	Physical interpretation	Prior bounds
Linear	T_w	Drying rate at reference temperature	$1 < T_w < 100$
	f	Temperature dependence of drying rate	$0 < f < 10$
	c	Mass-balance term (a scaling factor)	$0 < c < 0.01$
Non-linear	T_q	Quick-flow time constant	$0 < T_q < T_s$
	T_s	Slow-flow time constant	$T_q < T_s < 500$
	V_s	Slow-flow volume proportion	$0 < V_s < 1$

Table 2. Number of parameter samples, out of 100, meeting output bounds.

Data set	No. of samples meeting single-objective bounds			No. of samples meeting all bounds
	bias $\in$ [-20,20]	$R^2 \in$ [0.3,1]	$R_{inv}^2 \in$ [0.3,1]	
A	15	13	6	6
B	64	19	27	0
C	34	4	4	0

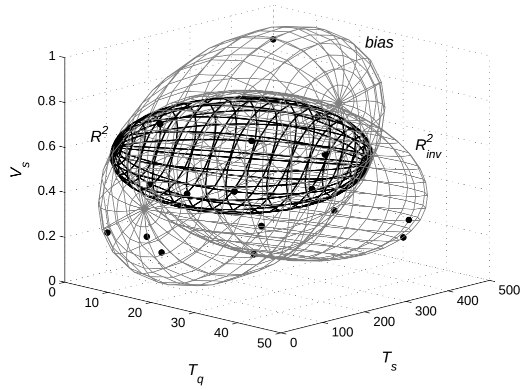

Figure 2. Data set A. Minimum-volume ellipsoids for bounds on single objectives (grey) and ellipsoid containing their intersection (black). All points meeting R_{inv}^2 bounds also meet those on R^2 and bias, so ellipsoid of intersection coincides with ellipsoid meeting R_{inv}^2 bounds.

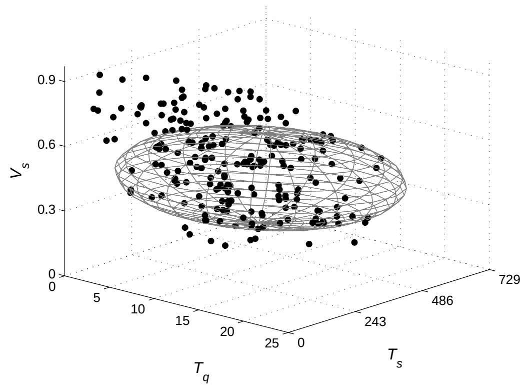

Figure 3. Data set A. Ellipsoid of intersection and 221 feasible points by dense u.d. sampling.

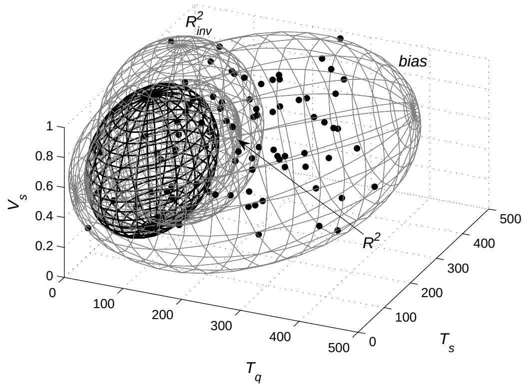

Figure 4. Data set B. Minimum-volume ellipsoid for single-objective bounds (grey) and ellipsoid containing their intersection (black).

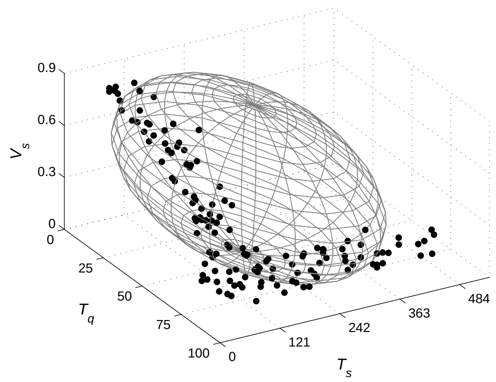

Figure 5. Ellipsoid of intersection for data set B and 138 feasible points by dense u.d. sampling.

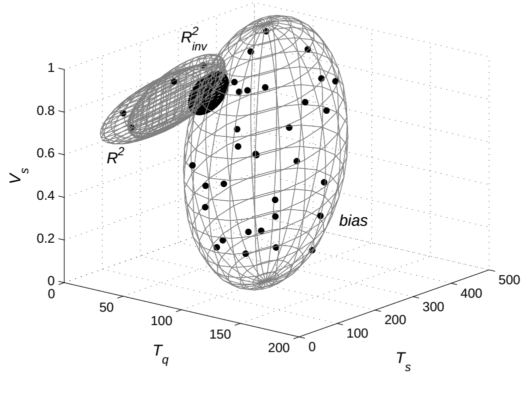

Figure 6. Data set C. Minimum-volume ellipsoids for a single-objective bound pairs (grey) and ellipsoid containing their intersection (black). No points meet all bounds simultaneously.

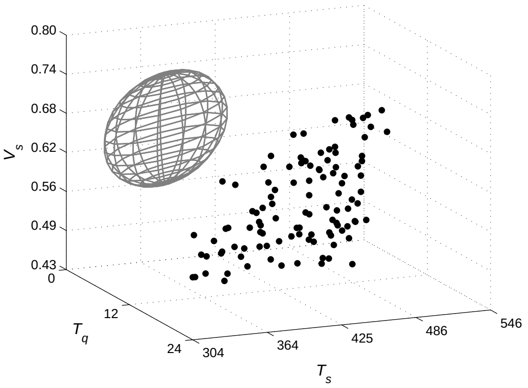

Figure 7. Ellipsoid of intersection for data set C and 109 feasible points by dense u.d. sampling.

The procedure was also used to seek the feasible set of the full 6-parameter IHACRES model with objective bounds $-5 \le bias \le 5$, $0.3 \le R^2 \le 1$ and $0.3 \le R^2_{inv} \le 1$. Of 3000 u.d. parameter samples, 15 meet the *bias* bounds, 8 those on R^2 and 10 those on R^2_{inv}. Ten samples meet all the bounds. Figures 8 and 9 show the ellipsoid of intersection and 100 feasible points obtained by dense u.d. sampling. To help visualize the fit of the 6-dimensional ellipsoid to the feasible set, the figures show 3-dimensional projections of the ellipsoid with the parameters of the non-linear and linear module respectively set at the ellipsoid centre. As an indication, 18 of 100 feasible points in a larger sample lie within the 6-dimensional ellipsoid. The feasible set is non-convex, so an ellipsoidal bound on it cannot be tight, yet the ellipsoid approximately locates the feasible set.

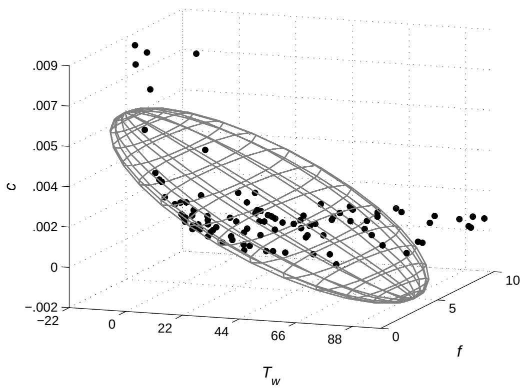

Figure 8. Projection of intersection ellipsoid onto space spanned by parameters of non-linear IHACRES module. Ellipsoid is compared with 100 feasible points.

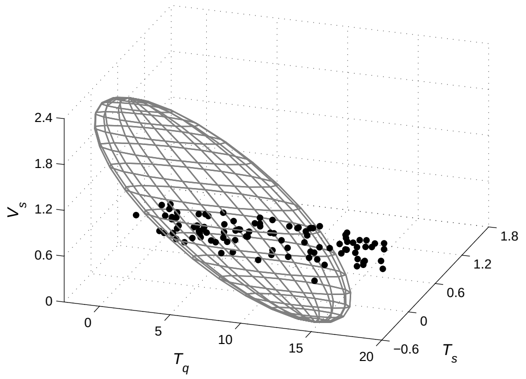

Figure 9. As for Figure 8 but for linear-module parameters.

Bound relaxation results for linear IHACRES module: Recall that Khachiyan's algorithm requires at least n+1 points to find the minimum-volume ellipsoid circumscribing them. The full IHACRES model required a large sample to find enough points meeting each bound pair. Bound relaxation to reduce the number required was first employed for the linear module of IHACRES. The objectives were bounded by $-20 \le bias \le 20$, $0.3 \le R^2 \le 1$ and $0.3 \le R^2_{inv} \le 1$ and 20 parameter samples drawn. The experiment was repeated 100 times with independent samples and the average number of feasible points calculated. Bound relaxation generated an average of 13 new points in finding a minimum of 4 points satisfying each bound pair, giving an average total sample size of 33. In comparison, a u.d. random sample of 33 points generally found too few points satisfying each bound pair (Table 3).

Table 3. Average number of samples satisfying each bound pair, with and without bound relaxation.

Bound relax -ation	Mean no. of samples within individual bound pairs			Total no. of samples within at least one bound pair
	Bias ∈ [-20,20]	$R^2 \in$ [0.3,1]	$R^2_{inv} \in$ [0.3,1]	
Yes	13.51	9.26	4.69	33.14
No	4.32	3.36	1.41	33

Bound relaxation results for full IHACRES model: Above, a u.d. sample of 3000 points was required for a high probability of generating enough points meeting each bound pair in the full IHACRES model. The efficacy of bound relaxation is demonstrated by a sample of just 200 u.d. points in the 6-dimensional parameter space. On average, only one point satisfies any of the bound pairs, that on *bias*. To find a minimum of

n+1 = 7 points meeting each bound, bound relaxation needs an average of only 49 new points.

4. CONCLUSION

A method of approximately bounding sections of the feasible parameter set of complex models, using ellipsoids, has been presented. It needs no prior knowledge of the feasible set. In examples, the feasible set is approximated usefully even when no trial parameter values prove feasible for all output bounds. The procedure can identify disjoint regions of the feasible set without resorting to cluster analysis. However, further work is desirable to develop a means of refining the size and shape of the ellipsoids employed.

Application to constrained MO hydrological modelling was demonstrated for an IHACRES model, chosen because it is well understood and relatively easily analysed. Future work should apply the technique to more complex models.

5. ACKNOWLEDGMENTS

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