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AUTOMATIC MODEL SELECTION FOR VERIFICATION

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The usual approach for code or solution verification uses an a priori choice of a model for an error with a power law being the standard [1]. Other models have been considered, but always chosen prior to any analysis. Here we explore a different concept where the first stage of the analysis of solutions involves the automatic selection of the error model using techniques adapted from statistics and signal processing. We then use the results of the analysis to define the proper model to continue the full analysis of the results and produce the error estimates from a defined mesh sequence. The key is that rather than assuming the power law error ansatz holds a priori, we find the model that best fits the data without the assumption.

In 1996 Tibisharani [Tib96,2] introduced the LASSO, which was structured like least squares with ridge regression, but used a L1 based penalty to regularize the system. The penalty can be varied to systematically discover the relative importance of various terms in the model of a data set. During the same period a L1 minimization method was used to define basis sets for reconstructing signals known as basis pursuit [Chen,3]. This field was then extended to form the foundation of compressed sensing using the same fundamental approach [Donoho,4]. The primary difference is nature of the system, where LASSO is applied to over-determined systems, and basis pursuit and compressed sensing applied to under-determined systems. Using the LASSO we can effectively combine the approaches to produce a model selection approach. The one catch is that these methods are applied to linear models, and the error estimation is invariably interested in nonlinear models. Undeterred we will move forward applying the basic methodology developed for linear models to the nonlinear models we desire. This follows the same lines of development for linear regression's extension to nonlinear regression although our implementation is applied within an optimization context.

We provide an example of the approach we will include a number of potential models for the numerical error including the standard power law form, parts of polynomials, and several transcendental functions (exponential, logarithm and sine). We also include the inverse of these functions providing a diversity of behavior away from the limit of vanishing mesh size. All the functions are developed and structured to vanish appropriately for a vanishingly small mesh size. It is the behavior away from zero that will determine any selection utlimately. These will be deciphered for their dominance given several data sets from calculations. Once the leading terms for the model are found, we apply the robust multi-regression approach (where the LASSO is used as a regularized regression technique). This will then provide the error estimate. Our example is based on the putative second-order solution of an ordinary differential equation.

Our methodology removes key concerns with the a priori definition of the error form without appropriate consideration of alternatives. We present a systematic and rigorous approach to providing alternatives, or likewise a stern defense of the axiomatic choice. We have seen that the best model depends on the data itself, sometimes being the standard, and sometimes not. In the end this procedure will produce better errors.

We will derive and compare the error models on a number of data sets. We begin with ideal data using "clean" solvers with analytical problems suitable for code verification. We then extend our results to problems arising from more practical engineering problems including the diverse problem areas of thermal analysis with adaptivity, large eddy simulation and neutron transport. In each case we find significant support for the utility of the model selection. In many cases we find that the a priori model selection to be justified, while in other cases this model is too restrictive.

REFERENCES

[1] W. L. Oberkampf and C. Roy, Verification and Validation in Scientific Computing, Cambridge, 2011.

[2] Tibshirani, Robert. ". Journal of the Royal Statistical Society, Series B 58 (1): 267–288. 1996.

[3] Scott Shaobing Chen, David L. Donoho, Michael, A. Saunders.Atomic decomposition by basis pursuit", by SIAM Journal on Scientific Computing, Vol 28, pp. 33-61, 1998, or SIAM REVIEW Vol.43(1), pp.129–159

[4] Donoho, D.L. (2006). "Compressed sensing". IEEE Transactions on Information Theory 52 (4): 1289. doi:10.1109/TIT.2006.871582