Covariance in Uncertainty Quantification of Experimental Analyses

S. P. Smith, General Atomics
smithsp@fusion.gat.com
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Challenge

The range of uncertainties placed on experimental analysis outputs provide bounds within which the inputs of codes can be varied to determine if the codes are valid. It is unclear if current practices used to obtain the range of uncertainties correctly propagate the covariant uncertainties of all data inputs to the experimental analysis.

Current approach

For measured data, an experimentalist can obtain a mean and standard deviation of the mean as the uncertainty. However, most profile "measurements" involve the measurement of spectra and fitting of the spectra with a model, such that the fitting parameters now have the fundamental information of covariance. This is also true of equilibrium reconstructions, where the various magnetic probe, MSE, and flux loops contribute to the overall characterization of the reconstruction, but no information on the covariance of the reconstruction parameters is output (and for EFIT, the parameters themselves are not routinely output). The profile "measurements" are then fit in normalized toroidal flux space based on the equilibrium reconstruction, where again, the covariance on the profile fit parameters is provided by some tools, but not all tools, and there is not any covariance of equilibrium reconstruction parameters and profile fit parameters. The profile fits and equilibrium reconstructions are fed to a transport code to determine the "experimental" heat, particle, and momentum fluxes, which will be the basis for comparison to code outputs. The transport code knows nothing about uncertainties or their covariances. One approach to quantify the overall range of uncertainties has been to vary the data points individually within their range of uncertainty in a monte carlo type approach to obtain a final result with some uncertainty.

Suggested approach

This paper's suggested approach is to propagate uncertainties and their covariances appropriately. My interpretation of appropriate is based on the python uncertainties package [1] and its propagation of covariances of uncertainties. A separate interpretation of appropriate would be Bayesian methods as outlined in [2] and references therein.

Example workflow

1. Start with the EFIT code to produce an equilibrium reconstruction. One of its outputs is the value of psi (poloidal flux) on an R,Z grid. It also puts out the safety factor, q, and the pressure, p, as a function of normalized psi from the magnetic axis to the last closed flux surface. It is desirable for psi, q, and p to be output with some uncertainty based on the uncertainties of the fitting parameters that resulted from the chi-squared minimization for the reconstruction. Depending on the choice of basis function, the fitting parameters in EFIT are the coefficients of a polynomial expansion or the values at tension spline knots for the pprime and ffprime flux functions. Presumably the parameters are not independent, and so have some covariance in their uncertainty.

2. Once we have an equilibrium reconstruction, this is fed to a profile fitting algorithm that first maps the experimental data points from R,Z to normalized toroidal flux, rho. The uncertainty in the reconstruction would provide some uncertainty in the rho value of the data points, but that uncertainty for each point is presumably not independent. A fitting algorithm could produce a least squares fit to the data points, which now have x and y uncertainties, based on some parameterization of the profile (spline, tanh, scale length), and the fit parameters would have some covariance. But how do we appropriately propagate the covariances from the equilibrium reconstruction into the profile fit parameter covariances?
3. The profile fits and equilibrium reconstruction are fed into a power balance code where the sources of heat, particles, and momentum are calculated based on the uncertainties in the equilibrium parameters and the profile fitting parameters.
    a. For Electron Cyclotron Heating (ECH), the resonance layer where the heat is deposited depends sensitively on the local magnetic field strength and electron density. The ECH deposition should have an uncertainty associated based on the uncertainties in those quantities, instead of sending a variety of similar waves into the plasma to represent how a single wave encounters the natural fluctuations (uncertainties) in a plasma.
    b. Neutral beam injection deposition should be calculated taking into account the uncertainties in the profiles and equilibrium. Usually beam deposition is calculated by a monte carlo process. Perhaps uncertainties can be folded into the monte carlo process.
    c. The calculated bootstrap current is very sensitive to the gradients (radial derivatives) of the profiles, where the covariance of the fitting parameters better constrains the derivatives.

Impact

The "validation" of a given model can be more robustly quantified, by providing tighter bounds for the ranges of inputs that can be given to the model, and not allowing those inputs to be varied independently.

[1] http://pythonhosted.org/uncertainties/

[2] http://arxiv.org/pdf/1403.1321.pdf