Updating uncertainty in HYCOM's parameters

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This note discusses how data might be used to correct the input uncertainties used for polynomial chaos expansions. At the heart of the correction is the usual Bayesian formalism, but this note attempts to bypass much ofthe details of that formalism and get to the aspects that are essential in actual computations. For concreteness and simplicity the focus here is on a single parameter, the drag coefficient, and on the use of axbt data to provide information about its likely values. The generalization to other or more parameters and to other data is straightforward.

First, it is useful to establish notation. The axbt data d_i are values of oceanic temperature at discrete points (x_i, y_i, z_i, t_i), $i = 1, \ldots, I$, where x denotes longitude, y latitude, z depth, and t time. The drag coefficient, which can be denoted as θ, is presumed to be between between $\theta_{\min}$ and $\theta_{\max}$. Its probability density, which is assumed to be uniform on this interval, can be regarded as uninformative when the interval is sufficiently large as to encompass all reasonable values. To evaluate the polynomial-chaos expansion coefficients, HYCOM is run for particular values of the drag coefficient θ_q, $q = 1, \ldots, Q$ dictated by the quadrature points used for evaluating integrals. In order to infer a posterior distribution for θ, it is necessary to compare the axbt data with their counterparts from HYCOM. Thus, PCE coefficients are needed for the HYCOM counterparts of d_i; these simulated data s_i depend on the drag coefficient: $s_{i,q} = s_i(\theta_q)$. Once the coefficients have been evaluated, the polynomial expansions can be used to emulate the axbt data for any value of θ, so let $e_i(\theta)$ denote the emulated values.

The next step is to specify a statistical model for the axbt data, given a HYCOM model with drag coefficient θ. If the model does a good job at characterizing the data, it is reasonable to assume that the errors are normally distributed. This leads to the possibility of determining the optimal values of θ by (weighted) least squares., i.e., by minimizing:

$$J(\theta) = \frac{1}{2}(d - e(\theta))^T D^{-1}(d - e(\theta)) , \tag{1}$$

where d and e are column vectors containing the data and their emulated counterparts and D is a covariance matrix. Minimizing J is equivalent to assuming that the probability density for the data axbt given HYCOM with drag coefficient θ has the form:

$$p_d(d|e(\theta)) \propto \exp\left(-J(\theta)\right) . \tag{2}$$

From the Bayesian perspective, minimizing J is equivalent to maximizing a likelihood function that is proportional to the probability density for θ given the axbt data:

$$L((\theta)) = p_d(d|e(\theta))p_e(e(\theta)|\theta)p_\theta(\theta)\ . \tag{3}$$

The last factor is simply a constant, as the prior density for θ has been assumed to be uniform. The middle factor drops out, because $e(\theta)$ provided by the polynomial-chaos expansions is completely certain, so the joint density for the counterparts of all the axbt data is generated from the uniform density for θ. Thus, $L(\theta)$ is given by the right-hand side of (2) minimizing J is equivalent to maximizing L when $e(\theta)$ is given by the polynomial expansions.

The minimization of J can be done in two different ways. The first is to exploit the polynomial expressions for $e(\theta)$ and solve $dJ/d\theta = 0$. This would determine the optimal value of the drag coefficient to be $\theta = \theta_{\text{opt}}$ at the maximum of the posterior density . Then the spread of the posterior density could be approximated as the standard deviation of a Gaussian centered on the optimum and having the same second derivative: $1/\sqrt{d^2J/d\theta^2}$. The second is to evaluate $\exp(-J(\theta))$ for values of θ uniformly distributed over the allowed interval to generate the posterior density for the drag coefficient. Plotting this posterior density will show how it differs from a Gaussian and whether the median or mean might be preferable to the mode (maximum Likelihood) as a preferred value for the drag coefficient.

The utility of the polynomial expansions is principally in their computational savings. If expense were no object, then the emulated values $e(\theta)$ might be replaced by simulated values $s(\theta)$, which would be evaluated using HYCOM integrations for a large number of values of the drag coefficient. As the simulated values have no easily evaluated expression, the first method would require either an adjoint code or divided differences to approximate $dJ/d\theta$ and a descent algorithm to compute the optimal drag coefficient. The second method (Monte Carlo) would require many expensive HYCOM simulations in the place of the more economical emulations.

The approach outlined above can be compared with data assimilation, which is commonly based on minimizing an objective function like $J(\theta)$. There are two differences that are immediately seen. First, in the place of a single parameter θ the objective function would depend on HYCOM's entire initial state and might also depend on it's surface or lateral boundary conditions, so there would be an extremely large number of uncertain variables characterizing these fields. Second, because the axbt data are far fewer in number than the variables to be updated, the objective function would contain and additional term, generally referred to as the background term, characterizing the uncertainties in the absence of the axbt data. This term reflects a non-uniform, often Gaussian, prior probability density for the fields to be updated, which would correspond to the third factor on the right-hand side of (3), so prior information about the drag coefficient is easily accommodated. There is a third aspect of data assimilation that has been neglected in the above discussion, namely the uncertainties associated with the inadequacies of HYCOM, which are often called process errors. When these are neglected, HYCOM would be regarded as providing a "strong constraint', but "weak-constraint" methods like the Kalman filter do account for process errors. As the middle factor on the right-hand side of (3) reflects these uncertainties, the approach outlined above can be expanded to handle both the inadequacies of HYCOM and of the polynomial interpolation, if an appropriate density is used.

Most important is that all the additional inputs to HYCOM, whose uncertainties have been neglected, should have reasonable values. In other words, their simulated and emulated counterparts should resemble the axbt data. After the optimal drag coefficient has been determined, any systematic differences between the data and their counterparts would point to an inadequacy in their simulation or emulation. Subsequent determination of additional parameters might improve the fit, but care should be taken to insure that HYCOM is provided with reasonable initial fields, surface winds, etc. Thus, before attempting to find the optimal input, plots comparing the axbt data with their simulated counterparts based on commonly used parameters, including the drag coefficient, should be carefully examined to insure that HYCOM is capable of hitting the target. Then, the simulated values from the quadrature runs should be examined to get a first impression of how changing the drag coefficient might improve agreement with the axbt data. Finally, after determining the optimal value and the posterior density, similar plots should be examined to see how much the agreement has actually been improved and whether there are systematic disagreements that might be improved by updating a second parameter.