Optimization in the Context of Data Assimilation: I

Parameter Estimation and Model Validation in Nonlinear Dynamical Networks
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Abstract

Data assimilation takes discrete time observations $y_l(t_n)$; $l = 1, \ldots, L$; $n = 0, \ldots, m$, and uses information in the measurements to estimate properties of a dynamical model of the system producing the data. If the states of the model $x_a(t_n)$; $a = 1, \ldots, D$ $(D \geq L)$ satisfy $x_a(n+1) = f_a(\mathbf{x}(n), \mathbf{p})$ with fixed parameters $\mathbf{p}$, then answers to data assimilation questions such as the mean state during observations and covariances about that mean, are given by an integral along the $(m+1) \times D$ dimensional path $\mathbf{X} = [x_1(t_n), x_2(t_n), \ldots, x_D(t_n)]$ of the form:

$$E[F(\mathbf{X})] = \int d\mathbf{X} F(\mathbf{X}) \exp[-A_0(\mathbf{X})],$$

where the action $A_0(\mathbf{x})$ receives contributions from three sources: (i) the dynamical movement $\mathbf{x}(n) \to \mathbf{x}(n+1)$ (ii) the measurements process, and (iii) knowledge of the state at t_0.

The saddle-path estimate of this integral is the numerical optimization problem for the path $\mathbf{S}$ that satisfies

$$\frac{\partial A_0(\mathbf{X})}{\partial \mathbf{X}}|_{\mathbf{X}=\mathbf{S}} = 0.$$

Another formulation of the estimation is to change variables from the path $\mathbf{X}$ to the mean state ϕ, giving the effective action $A(\phi)$ as

$$A(\phi) = \log\left\{\int d\mathbf{X} \exp[-A_0(\mathbf{X}) + \mathbf{K}\cdot(\mathbf{X}-\phi)\right\}, \quad \text{where} \quad \mathbf{K} = \frac{\partial A_0(\mathbf{X})}{\partial \mathbf{X}}.$$

An expansion of the integral in powers of the number of "loops" results in an expression for $A(\phi)$ that sums up an infinite number of terms in the nonlinearities in the dynamics $\mathbf{f}(\mathbf{x}(n), \mathbf{p})$. This expression yields the mean state $E[\mathbf{x}_a(n)]$ and the covariance about this mean state as

$$E[x_a(n)] = \frac{\partial A(\phi)}{\partial \phi_a(n)} = 0, \quad \text{and} \quad E[(x_a(n) - E[x_a(n)])(x_b(m) - E[x_b(m)])] = \left\{\frac{\partial^2 A(\phi)}{\partial \phi_a(n)\, \partial \phi_b(m)}\right\}^{-1}.$$

Higher covariances are also expressed as derivatives of the effective action.

The determination of all the information in the exact expression of data assimilation questions embodied in the integral can thus be cast as an optimization problem involving the extrema of the effective action $A(\phi)$. State-of-the-art numerical optimization routines, including `SNOPT` and `IPOPT` have been used to solve the associated numerical optimization problems.

The power of the statistical physics formulation of data assimilation, and the numerical optimization approaches we have developed allow a systematic and accurate solution to many uncertainty quantification problems associated with DOE programs that range from stockpile stewardship to climate-change predictions.