Stochastic Mode Reduction -- Beyond Standard Averaging

Tuesday, April 14, 2009
12:02 PM

Homework 3 due Tuesday, April 21 at 12 PM.

Picking up from last time, one can show that the following system

could also depend explicitly on time under certain conditions

$$d\vec{X} = \vec{a}(\vec{X}, \vec{Y})\,dt$$

$$d\vec{Y} = \frac{1}{\varepsilon}\vec{b}(\vec{X}, \vec{Y})\,dt + \frac{1}{\sqrt{\varepsilon}}\mathcal{L}(\vec{X}, \vec{Y})\,d\vec{W}(t)$$

The method of averaging (see Arnold) shows that for $\varepsilon \ll 1$ and $t \lesssim O(1)$

$$\vec{X}(t) \approx \vec{X}^{\#}(t) + \sqrt{\varepsilon}\,\vec{\rho}(t) + O(\varepsilon)$$

$$d\vec{X}^{\#}(t) = \vec{a}^{\#}(\vec{X}^{\#}(t))$$

$$d\vec{\rho} = \vec{\rho}(t)\cdot\vec{\nabla}\vec{a}^{\#}(\vec{X}^{\#}(t))\,dt + \sigma(\vec{X}^{\#}(t))\,d\vec{W}(t)$$

$$\vec{a}^{\#}(\vec{x}) = \int \vec{a}(\vec{x}, \vec{y})\, p^{(s)}_{\vec{Y}|\vec{X}}(\vec{y}\,|\,\vec{x})\,d\vec{y}$$

Kubo formula

$$\sigma(\vec{x})\,\sigma^{T}(\vec{x}) = \lim_{T\to\infty}\frac{1}{T}\int_0^T\!\!\int_0^T \mathrm{Cov}\left(\vec{a}(\vec{x}, \vec{Y}_x(t)), \vec{a}(\vec{x}, \vec{Y}_{\vec{x}}(s)\right)\,ds\,dt$$

$$d\vec{Y}_x = \frac{1}{\varepsilon}\,b(\vec{x}, \vec{Y}_x)\,dt + \frac{1}{\sqrt{\varepsilon}}\mathcal{L}(\vec{x}, \vec{Y})\,d\vec{W}$$

This averaging framework is good when the leading order solution is nontrivial, but in many cases (like our Brownian motion example), we have that

$$\vec{a}^{\#}(\vec{x}) = \vec{0}$$

The reason this happens in Brownian motion example is that we had:

$$\vec{X} \to \vec{X}$$

$$\vec{Y} \to \vec{V} \qquad\qquad \vec{a}(\vec{x}, \vec{v}) = \vec{v}$$

$$p^{(s)}_{\vec{V}|\vec{X}} = e^{-\frac{1}{2}m|\vec{v}|^2/k_B T}$$

$$\vec{a}^{\#}(\vec{x}) = \int \vec{v}\, e^{-\frac{1}{2}m|\vec{v}|^2/k_B T}\,d\vec{v}$$

$$= \vec{0}$$

In this situation, the method of averaging tells us that

$$\vec{X}(t) \approx \sqrt{\varepsilon}\,\vec{\xi}(t) + O(\varepsilon)$$

This just says that the slow variables change by a slow amount over the O(1) time scale on which the method of averaging is valid. To see interesting behavior for the slow variable X one needs to go to even longer time scales by another factor of $1/\varepsilon$

$$t' = \varepsilon t$$

$$d\vec{X}(t') = \frac{1}{\varepsilon}\,\vec{a}(\vec{X},\vec{Y})\,dt'$$

$$d\vec{Y}(t') = \frac{1}{\varepsilon^2}\,\vec{b}(\vec{X},\vec{Y})\,dt' + \frac{1}{\varepsilon}\,\sigma(\vec{X},\vec{Y})\,d\vec{W}(t')$$

This was the way we nondimensionalized our Brownian motion system. This is nondimensionalizing on a "diffusive" time scale which is longer than the more obvious "advective" time scale.

Under this nondimensionalization, one can again derive an effective equation fo r the slow variables X alone on this longer diffusive time scale, but the computation is more complicated, follows the same structure as our computation for Brownian motion. One finds...

(valid for $t' \lesssim O(1) \Leftrightarrow t \lesssim O(1/\varepsilon)$)

$$\vec{X}(t') \approx \vec{X}^{\#}(t') + O(\varepsilon)$$

$$d\vec{X}^{\#}(t) = \vec{a}^{\#}(\vec{X}^{\#}(t'))\,dt' + \Sigma(\vec{X}^{\#}(t'))\,d\vec{W}(t')$$

where the coefficients $\vec{a}^{\#}, \Sigma$

have more complicated expressions in terms of again the statistics of the fast variables $\vec{Y}$ with the slow variables X held frozen.

The detalis can be found in the optional reading by E, Liu, Vanden-Eijnden

The analytical framework for stochastic mode reduction can be carried out purely theoretically for cases where the leading or der operator in the Fokker-Planck equation is explicitly invertible (solvable), as it is for our Brownian motion case and for the example on microfluid simulations in the paper by K and Majda.

Another interesting field in which the analytical approach was adopted was by Majda, Timofeyev, Vanden-Eijnden in weather/climate simulation models involving geophysical fluid dynamic equations. See references for details. The basic idea is to add noise to the equations for the unresolved variables, then coarse-grain rigorously to obtain effective stochastic differential equations for large scale modes.

What can we do, though, when the fast dynamics are not so simple they can be exactly solved? (The key operator in the fokker-Placnk equation associated to the fast variables -- suppose we don't know how to invert it analytically as in the above examples.)

This brings us into the domain of "multiscale computing" and particularly the version known as "heterogeneous multiscale method." The basic concept has a wide range of implementations by a wide number of people -- we'll focus on just the particular framework for systems of stochastic differential equations which is summarized in the paper by E, Liu, Vanden-Eijnden

This idea is also extended to partial differential equations and chemical kinetics -- see more papers by E and Vanden-Eijnden.

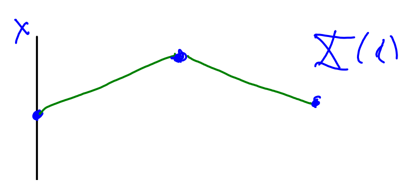
How the heterogeneous multiscale method works is that you compute the averaged coefficients for the effective SDE for the slo w variable by doing some direct simulation of the dynamics of the fast variable Y_x and extracting the necessary statistics.

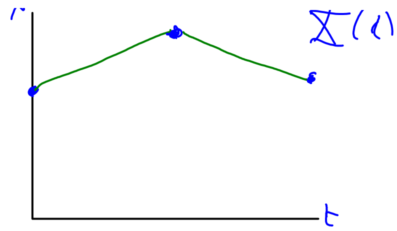
How do you extract statistics from a simulated trajectory -- this is the subject of parameter estimation; see recent papers by Andrew Stuart and now Ilya Timofeyev is in the action and will present a talk on this

Thursday, April 16 at 4 PM in Amos Eaton 214

Heterogeneous multiscale methods come in two flavors:

- sequential coupling (precompute all the fast statistics -- important to use sampling techniques (Weinan E))
- concurrent coupling (the computations of the fast variables are done on the fly as needed)

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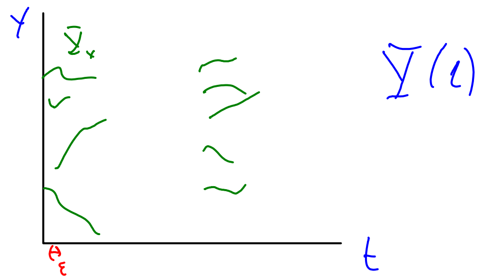
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