Ensemble Methods

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Goals of Lecture

- Describe a mathematical framework for ensemble methods to estimate Lyapunov exponents/vectors of a dynamical system, and/or to perform data assimilation, without explicitly linearizing the dynamics.
- Discuss work with Cecilia González-Tokman (Physica D 2012) proving that these methods "work" in an appropriate limit for hyperbolic dynamical systems.

Motivation

- For high-dimensional systems, computing the derivative of the system can be very time-consuming.
- An ensemble of nearby trajectories provides discrete information about the derivative.
- Ensemble methods can treat the system as a “black box”.

Lyapunov Exponents

- Given a trajectory of a dynamical system, the “tangent linear model” (TLM) describes the evolution of infinitesimal perturbations from that trajectory.
- Lyapunov exponents/vectors (Oseledec 1968) correspond to asymptotically exponential solutions of the TLM.
- Chaos: at least one positive Lyapunov exponent.

Data Assimilation

- Given a forecast model for a physical system and an ongoing time series of observations, data assimilation is an iterative procedure to:
- Synchronize the model state with the physical state, and thereby…
- Estimate the current state of the system based on current and past observations.

Data Assimilation Cycle

- Run a weather forecast model.
- Gather atmospheric observations over a 6-hour time interval.
- Adjust the 6-hour forecast state to better fit the observations.
- Use the adjusted model state as the initial conditions for a new forecast.
- Repeat this cycle every 6 hours.

Notation and Terminology

- "Forecast model": a discrete-time dynamical system:

$$x_n = f(x_{n-1}), \quad x \in R^m$$

- "δ-pseudotrajectory": $\{x_n\}$ for which

$$| x_n - f(x_{n-1}) | \leq \delta$$

- "Background ensemble": $\{ x_n^{b(i)} \}$
- "Analysis ensemble": $\{ x_n^{a(i)} \}$

Ensemble Methods

- Forecast step:

$$x_n^{b(i)} = f(x_{n-1}^{a(i)}), \quad i = 1, 2, \ldots, k$$

- Adjustment step:

$$\{ x_n^{a(i)} \} = g(\{ x_n^{b(i)} \}, y_n), \qquad y \in R^{\ell}$$

- Preserve "ensemble space":

$$\bar{x}_n^{a} + \text{Span}\{ x_n^{a(i)} - \bar{x}_n^{a} \}$$

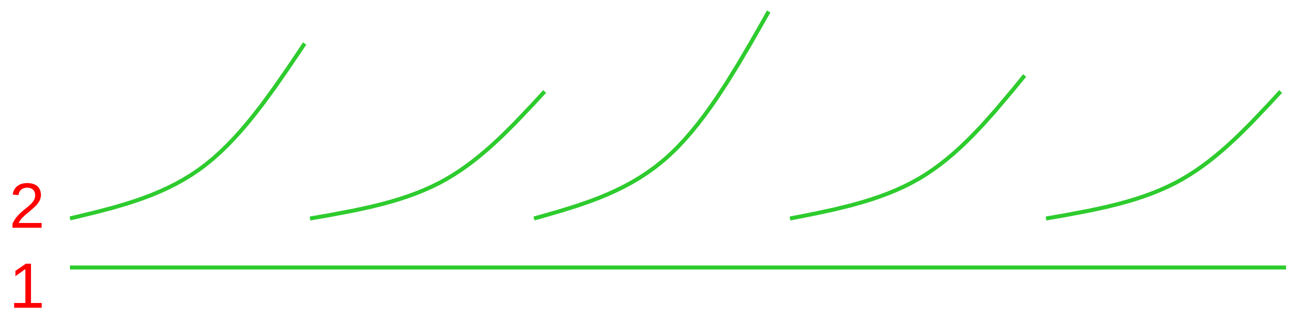
$$= \bar{x}_n^{b} + \text{Span}\{ x_n^{b(i)} - \bar{x}_n^{b} \}$$

Example 1: Breeding

- Adjustment step:

$$x_n^{a(1)} = x_n^{b(1)}$$

$$x_n^{a(2)} = x_n^{b(1)} + \frac{\beta \, (x_n^{b(2)} - x_n^{b(1)})}{|\, x_n^{b(2)} - x_n^{b(1)} \,|}$$



Uses for Breeding

- With small β, approximate leading Lyapunov exponent/vector.
- With β representing the size of uncertainty in initial condition, assess forecast uncertainty (Toth & Kalnay, 1993).

Ensemble Data Assimilation

- Given: observations $\{y_n\}$ and a "forward operator" h such that

  $$y_n = h(x_n^t) + \varepsilon_n$$

  where the "truth" $\{x_n^t\}$ is a pseudotrajectory and the "error" ε_n is usually small.
- Goal: design the ensemble adjustment operator g so that the ensemble approximates the truth well.

Ensemble Kalman Filtering

- Introduced by G. Evensen (1994).
- Many variations, e.g. pert. obs. EnKF (Burgers et al. 1998, Houtekamer & Mitchell 1998), EAKF (Anderson 2001), EnSRF (Whitaker & Hamill 2002).
- Formulation here based on LETKF (Hunt et al. 2007), drawing on LEKF (Ott et al. 2004) and ETKF (Bishop et al. 2002).

Ensemble Kalman Filter

- Assume (pretend) $\varepsilon_n \sim N(0,R)$ i.i.d.
- Consider $\bar{x}_n^b$ to represent the "most likely" true state given past data; $\bar{x}_n^a$ likewise but given current data too.
- Consider each ensemble to represent a Gaussian distribution with the same (sample) mean and covariance.

Ensemble Kalman Filter, cont.

- Analysis (posterior) distribution determined by Bayes' rule from the background (prior) and observation error distributions, linearizing h in ensemble space.
- Qualitatively, the adjustment step moves the ensemble toward the background members that best match the data and reduces its covariance (new information $\rightarrow$ less uncertainty).

Ensemble Kalman Filter, cont.

- Formally (square brackets $\rightarrow$ form matrix):

$$\bar{x}_n^{\,a} = \bar{x}_n^{\,b} + [x_n^{b(i)} - \bar{x}_n^{\,b}]L_n(y_n - \overline{h(x_n^{b})}),$$

$$[x_n^{a(i)} - \bar{x}_n^{\,a}] = [x_n^{b(i)} - \bar{x}_n^{\,b}]T_n,$$

$$L_n = L(\{h(x_n^{b(i)})\}, R),$$

$$T_n = T(\{h(x_n^{b(i)})\}, R)$$

- Remark: Breeding can also be formulated this way with appropriate y, h, L, T.

ETKF specifics

- Use

$$L_n = T_n^{2} Y_n^{T} ((k-1)R)^{-1},$$

$$T_n = (I + Y_n^{T} ((k-1)R)^{-1} Y_n)^{-1/2}$$

where

$$Y_n = [h(x_n^{b(i)}) - \overline{h(x_n^{b})}].$$

- Among all T_n that give the correct analysis covariance, this minimizes distance from background to analysis ensemble.

Takens Embedding Theorem

- If $f : R^m \to R^m$ is the time 1 map of a C^2 flow with no orbits of integer period up to $2m+1$, and all of whose fixed points have simple eigenvalues different from 1, then for generic C^2 $h : R^m \to R$, the map

$$x \to (h(x), h(f^{-1}(x)), \ldots, h(f^{-2m}(x)))$$

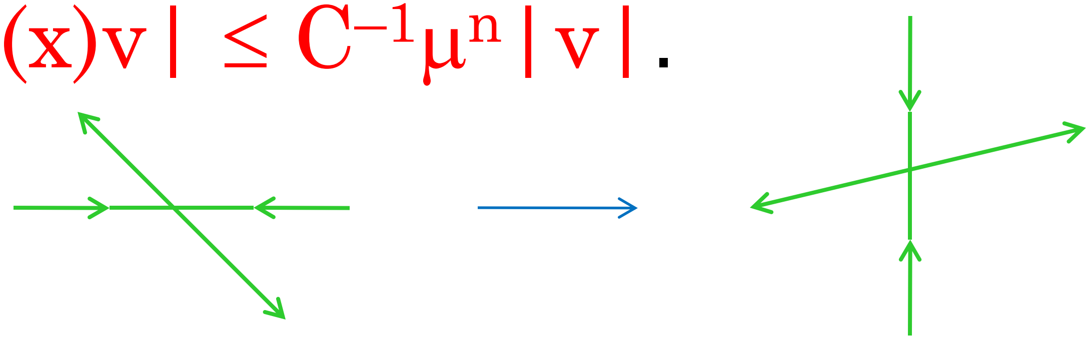
is an embedding (one-to-one and its derivative has full rank everywhere).

Embedding Theorem, cont.

- True for diffeomorphisms more generally, and for “prevalent” h.
- For a d-dimensional attractor, the number of observations only has to exceed $2d$ (Sauer, Yorke, Casdagli 1991; following Takens 1981).
- Attractor: a compact invariant set that attracts nearby initial conditions.

Hyperbolicity

- We say an attractor A of a C^1 diffeomorphism $f : R^m \to R^m$ is hyperbolic if $\exists\ C > 0$, $\lambda > 1 > \mu$, and $\forall\ x \in A$, $\exists$ subspaces $E^+(x)$ and $E^-(x)$ s.t. $Df\ E^{\pm}(x) = E^{\pm}(f(x))$ and $\forall v \in E^+(x)$ and $n > 0$ we have $|Df^n(x)v| \geq C\lambda^n|v|$, while $\forall v \in E^-(x)$ and $n > 0$ we have $|Df^n(x)v| \leq C^{-1}\mu^n|v|$.



Results (w/ C. González Tokman)

- Proposition: Let f and h be as in Takens' Theorem, and A be a hyperbolic attractor w/ $<k$ unstable directions. Then $\exists\ C, \delta_0 > 0$ s.t. if $\delta \leq \delta_0$, $\{x_n^t\}$ is a δ-pseudotrajectory, and $|\varepsilon_n| \leq \delta$, then k-member ETKF has the following property. For an open set of initial ensembles, the ensemble stays within $C\delta$ of the truth.
- The ensemble spread in the unstable directions stays $\geq C^{-1}\delta$.

Lyapunov Exponents from ETKF

- Recall: $[x_n^{a(i)} - \bar{x}_n^{a}] = [x_n^{b(i)} - \bar{x}_n^{b}]T_n$
- Corollary: If the ensemble covariance remains bounded (above and below), the positive Lyapunov exponents/vectors of the attractor can be estimated to order δ from the matrices T_n (we proved this for the largest Lyapunov exponent).
- Caveat: for high-dimensional systems, we can only practically estimate finite-time Lyapunov exponents/vectors.

Remarks

- For weather models, we use ensembles that are smaller than the global number of unstable directions. This works only because in LEKF/LETKF we use "localization": assimilate in local regions.
- With similar hypotheses, we should be able to prove that for δ sufficiently small, for generic initial perturbations, breeding approximates the largest Lyapunov exponent/vector to within order δ.

Conclusions

- Ensemble methods provide a discrete analogue to algorithms that use the derivative of a dynamical system (e.g., standard methods for computing Lyapunov exponents, Extended Kalman Filter, 4D-Var).
- We can prove convergence results for ensemble methods in hyperbolic systems…and beyond??