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Predictability Theory4. Structure of Errors

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Structure of errors

(Legras, B., and R. Vautard, 1996: A guide to Lyapunov vectors. *Proceedings of the ECMWF seminar on predictability.* September 4-8, 1995, Reading, UK, Vol. 1, 143-156.)

Recall that the squared-amplitude of the error at time t_2 is

 $\mathbf{x}(t_2)^T \mathbf{x}(t_2) = \mathbf{x}(t_1)^T \mathbf{A}(t_2, t_1)^T \mathbf{A}(t_2, t_1) \mathbf{x}(t_1) \cdot$

The matrix $\mathbf{A}^T \mathbf{A}$ is symmetric positive-definite and possesses *M* real positive eigenvalues σ_i^2 and orthogonal eigenvectors \mathbf{v}_i . Both the eigenvalues and eigenvectors depend on the time interval (t_1, t_2) .

The structure of the evolving errors is provided by the eigenvectors of the matrix $\mathbf{A}^T \mathbf{A}$. The eigenvectors \mathbf{v}_i describe the axes of inertia of the error growth. If the errors are on a sphere of unit radius at time t_1 , then, at time t_2 , they lie on an ellipsoid whose axes are along the vectors $\mathbf{A}(t_2,t_1)\mathbf{v}_i$ with lengths σ_i .

Because of the continuous change in the orientation of the ellipsoid, the phase space direction corresponding to a particular eigenvalue varies in a complex manner.

The error growth is better described by the singular structure of the error matrix A.

Singular vectors

Any matrix can be expressed in terms of two orthogonal matrices U and V by singular value decomposition (SVD):

 $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^T$

where U and V are $M \times M$ orthogonal matrices, S is a diagonal matrix containing the singular values of A,

$$\mathbf{S} = \begin{pmatrix} \boldsymbol{\sigma}_1 & \boldsymbol{0} & \cdots & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\sigma}_2 & \cdots & \boldsymbol{0} \\ \vdots & \vdots & & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & \boldsymbol{\sigma}_M \end{pmatrix}$$

$$\mathbf{U}\mathbf{U}^T = \mathbf{I}$$

 $\mathbf{V}\mathbf{V}^T = \mathbf{I}$

AV = US i.e.,
$$\mathbf{A}(\mathbf{v}_1, \dots, \mathbf{v}_M) = (\sigma_1 \mathbf{u}_1, \dots, \sigma_M \mathbf{u}_M)$$

$$\mathbf{A}^T \mathbf{U} = \mathbf{V} \mathbf{S}$$
 i.e., $\mathbf{A}^T (\mathbf{u}_1, \dots, \mathbf{u}_M) = (\sigma_I \mathbf{v}_1, \dots, \sigma_M \mathbf{v}_M)$

where \mathbf{u}_i and \mathbf{v}_i are columns of U and V respectively.

Note that

 $\mathbf{A}^T \mathbf{A} \mathbf{V} = \mathbf{V} \mathbf{S}^2$

 $V = (v_1, ..., v_M)$ are the <u>right singular vectors</u> or <u>forward singular vectors</u>.

 $\mathbf{v}_1, \dots, \mathbf{v}_M$ are also orthogonal eigenvectors of $\mathbf{A}^T \mathbf{A}$ with eigenvalues $\sigma_1^2, \dots, \sigma_M^2$ and, as discussed earlier, describe the evolution of a sphere of perturbations at time t_1 to an ellipsoid at time t_2 .

The errors lie on the ellipsoid whose axes are along the vectors $A(t_2, t_1)v_i$ with lengths σ_i .

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Also, $AA^TU = US^2$

 $\mathbf{u}_1, \dots, \mathbf{u}_M$ are also orthogonal eigenvectors of $\mathbf{A}\mathbf{A}^T$ with eigenvalues $\sigma_1^2, \dots, \sigma_M^2$.

 $\mathbf{U} = (\mathbf{u}_1, \dots, \mathbf{u}_M)$ are the <u>left singular vectors</u> or <u>backward singular vectors</u>.

To interpret the meaning of U, consider the error growth backward in time:

 $\mathbf{x}(t_1) = [\mathbf{A}(t_2, t_1)]^{-1} \mathbf{x}(t_2)$

The squared-amplitude of the error at time t_1 is

$$\mathbf{x}(t_1)^T \mathbf{x}(t_1) = \mathbf{x}(t_2)^T [\mathbf{A}(t_2, t_1) \mathbf{A}(t_2, t_1)^T]^{-1} \mathbf{x}(t_2)$$

If the errors are on a sphere of radius ε at time t_2 , then

 $\mathbf{x}(t_1)^T \mathbf{x}(t_1) = \mathbf{S}^{-2} \varepsilon^2$

ie., the errors lie on an ellipsoid at time t_1 along the axes $\mathbf{A}^T \mathbf{u}_i$ with lengths $1/\sigma_i$.

Asymptotic behavior

The asymptotic behavior of the eigenvalues and eigenvectors of $A^T A$ are governed by an important theorem in dynamical systems called the *Oseledec theorem*.

(1) For any vector **e**, there exists an exponent

$$\lambda(\mathbf{e}) = \lim_{t_2 \to \infty} \frac{1}{t_2 - t_1} \ln\left(\frac{\|\mathbf{A}(t_2, t_1)\mathbf{e}\|}{\|\mathbf{e}\|}\right)$$

which is finite and does not depend on t_1 . There are *M* such exponents $\lambda_1 > \lambda_2 > \cdots > \lambda_M$ called the *Lyapunov exponents*.

(2) The limit operator

$$\mathbf{B}_{\infty}(t_1) = \lim_{t_2 \to \infty} \frac{1}{t_2 - t_1} \left[\mathbf{A}(t_2, t_1)^{\mathrm{T}} \mathbf{A}(t_2, t_1) \right]^{\frac{1}{2(t_2 - t_1)}}$$

exists.

This limit operator depends on t_1 or on the initial point $\mathbf{X}(t_1)$. The eigenvectors $\mathbf{v}_i(t_1)$ of $\mathbf{B}_{\infty}(t_1)$ are called the <u>Lyapunov vectors</u> and are orthogonal.

Lyapunov exponents and dimension

The error matrix **A** is multiplicative. However, it does not mean that the singular values of $\mathbf{A}(t_3,t_1)$ are products of the singular values of $\mathbf{A}(t_3,t_2)$ and $\mathbf{A}(t_2,t_1)$. It is even possible $\mathbf{A}(t_3,t_2)$ and $\mathbf{A}(t_2,t_1)$ may each possess a singular value greater than one, while $\mathbf{A}(t_3,t_1)$ may not. The growth of small errors along a trajectory in the attractor varies continuously.

The ultimate growth or decay of small errors, as opposed to temporary growth or decay, is investigated by considering the initial error in the zero limit along with the time interval approaching a large limit.

The limiting values

$$l_i = \lim_{t \to \infty} \sigma_i^{1/(t-t_0)}$$

are called the Lyapunov numbers of the system, while their logarithms

$$\lambda_i = \lim_{t \to \infty} \left(\frac{\ln \sigma_i}{t - t_0} \right)$$

are called the *Lyapunov exponents*.

For an *M*-dimensional dynamical system, there are *M* Lyapunov exponents representing the average exponential rate of growth or decay of small errors (i.e., *M* axes of the error ellipsoid).

The positive exponents represent the axes that are expanding on the average, whereas the negative ones are related to the contracting axes.

Let $\lambda_1 > \lambda_2 > \ldots > \lambda_M$.

The signs of the Lyapunov exponents indicate the qualitative nature of the attractor.

If an attractor possesses one or more positive exponents, it is chaotic. For an attractor to be chaotic, it is sufficient that $\lambda_1 > 0$.

For a periodic attractor, $\lambda_1 = 0$ and the rest are negative. For a steady state attractor, all the exponents are negative.

Except for steady state attractors, at least one Lyapunov exponent is always zero and corresponds to the direction of the flow (principal axis tangent to the flow) where the perturbations stay at about the same level.

For many well behaved systems, the exponents are independent of initial time (*Oseledec theorem*).

The magnitudes of the Lyapunov exponents quantify the attractor's dynamics.

The linear extent of the ellipsoid grows as $\exp(\lambda_1 t)$, the area defined by the first two principal axes grows as $\exp[(\lambda_1 + \lambda_2)t]$, and so on.

The sum of the first j exponents represent the long term exponential growth rate of a j-volume element.

The sum of all the Lyapunov exponents is the time-averaged divergence of the phase space. Recall the earlier discussion of the rate of change of volume of a phase space in terms of the dissipation parameter. Any dissipative system will have at least one negative exponent and the sum of all exponents is negative.

Based on a conjecture by Kaplan and Yorke (1979), the fractional dimension of the attractor is expressed in terms of the Lyapunov spectrum. The Lyapunov dimension d of an attractor is

$$d = L + \frac{1}{\left|\lambda_{L+1}\right|} \sum_{j=1}^{L} \lambda_j$$

where L is the number of all the largest exponents that can be added to yield a nonnegative sum. The Lyapunov dimension is less than the phase-space dimension of the system. The Lyapunov dimension of a chaotic attractor is greater than 2, and is typically not an integer.

Lyapunov vectors

The Lyapunov vectors are the limits when $t_2 \rightarrow \infty$ of the forward singular vectors $\mathbf{v}_i(t_2, t_1)$ while t_1 is fixed. These may also be referred to as the *forward Lyapunov vectors*.

Similarly, from the time symmetry, we can define <u>backward Lyapunov vectors</u> as the backward singular vectors $\mathbf{u}_{i}(t_{2},t_{1})$ when $t_{1} \rightarrow -\infty$ while t_{2} is fixed and $\mathbf{A}\mathbf{A}^{\mathrm{T}}$ is considered in the limit operator.

As $t_2 - t_1 \rightarrow \infty$, any random perturbation $\mathbf{e}(t_1)$ starting from time t_1 will converge to $\mathbf{u}_1(t_2)$, the first backward Lyapunov vector.

Ensemble forecasting

A single forecast can depart quite rapidly from the real atmosphere if the error in the analysis (i.e., observation) happens to project strongly on a leading singular vector. However, if the initial error does not project strongly, then a forecast could be reliable. Therefore, the quality of the forecast could vary wildly from day to day with no prior knowledge of which forecasts are likely to be good. The approach taken to provide some information about the likely uncertainty in the forecast is called **ensemble forecasting**.

The control forecast (the one made starting from the analysis) is supplemented by a number (ensemble) of other forecasts starting from analysis plus a small perturbation. The single trajectory of forecast is replaced by a "cloud" of trajectories.

If the cloud grows quickly with many possible outcomes (weather states) after a few days, there is a warning that any single forecast may be unreliable. The deterministic forecast is replaced by a probabilistic one with more than one type of weather state.

It is also possible that the sampling of the state space near the analysis may include the correct initial state.

For a meaningful probabilistic forecast that includes proper upper bounds of uncertainty, the ensemble approach requires that the rapidly growing (leading) singular vectors are sampled reasonably. Otherwise, the ensemble of forecast trajectories may stay close together, with all of them being wrong.

Initial perturbations

The number of rapidly growing singular vectors is quite small compared to the dimension of the system. Some care must be taken to choose the initial perturbations to include the rapidly growing modes. Adding a number of random errors may be easier, but may miss the growing directions completely. There are two approaches to include rapidly growing directions in the initial ensemble: (1) singular vector and (2) bred vector.

Singular vectors

In this approach, the perturbations are projected onto the fastest growing directions over a finite period of time. The singular vectors are computed by linearizing the equations about the initial state (analysis) and integrating the linearized equations over finite forward time (optimization time). These **forward singular vectors** are used to add a cloud of small perturbations to the analysis. These perturbed states are expected to evolve along most rapidly growing directions. In the large time limit, the forward singular vectors are the forward Lyapunov vectors. The singular vector approach for ensemble forecasting was used by

Buizza, R., and Palmer, T., 1995: The singular vector structure of the atmospheric general circulation. J. Atmos. Sci., 52, 1434-1456,

Buizza, R., Tribbia, J., Molteni, F., and Palmer, T., 1993: Computation of optimal unstable structures for a numerical weather prediction model. Tellus, 45A, 388-407.

Bred vectors

In this method, with an initial small random perturbation (random seed), the nonlinear model is integrated a long time before the target time of the forecast. The perturbations are rescaled over short cycles and grown again. At the end of this "breeding" process, all perturbations are scaled to desired amplitude.

With an evolving flow (e.g., a long model run), start a breeding cycle by introducing a <u>random</u> initial perturbation of a certain size (usually not small). This random seed is introduced only once.

The same nonlinear model is integrated from the control (unperturbed) initial condition and from the perturbed initial condition.



(Kalnay, E., 2003: Atmospheric modeling, data assimilation and predictability)

At fixed time intervals (say every 6 hours), the control forecast is subtracted from the perturbed forecast. The difference (evolved error) is scaled down so that it has the same amplitude as the initial perturbation and the scaled error is added to the new analysis or model state.

The procedure is repeated for several cycles and the perturbations generated in these breeding cycles are called *bred vectors*. The bred vectors supposedly acquire large growth rates.

Since the initial errors are of finite size, this method is considered a nonlinear generalization of the method used to construct Lyapunov vectors. Since the bred vectors are generated after integrating the model for a long time before the target time of forecast, they are considered somewhat similar to backward Lyapunov vectors.

However, because of the large size of the initial perturbations, this method assumes the saturation of small-scale modes such as convective modes. The similarity of the bred vectors to backward Lyapunov vectors may be in large spatial scales.

Error Growth in low-order systems

Computation of local error growth

When a sphere of small initial errors evolves into an ellipsoid, the problem of determining the growth or decay of errors in terms of the lengths of the semi-axes of the ellipsoid reduces to finding the singular values of the error matrix \mathbf{A} or the eigenvalues of the matrix $\mathbf{A}\mathbf{A}^{T}$.

Consider the *M*-dimensional dynamical system

$$\frac{d\mathbf{X}}{dt} = \mathbf{F}(\mathbf{X})$$

and the solution of the linear tangent equation

$$x_i(t_2) = \sum_{j=1}^M a_{ij}(t_2, t_1) x_j(t_1), \quad i = 1, \dots, M$$

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To evaluate $A(t_2,t_1)$, first choose the initial basic state $X(t_1)$ and numerically integrate dynamical equation from t_1 to t_2 and obtain the basic state $X(t_2)$.

Next, by choosing a new state $\mathbf{X'}(t_1)$ at time t_1 which differs from the basic solution $\mathbf{X}(t_1)$ in only one component, say

 $x_i(t_1) = \varepsilon \delta_{ik} \,,$

where ε is small, we obtain

 $x_i(t_2) = \varepsilon a_{ik}(t_2, t_1).$

When the basic solution is subtracted from the perturbed solution at time t_2 , the result is ε times the *k*th column of $\mathbf{A}(t_2,t_1)$. By repeating this process for *M* times for different values of *k*, the matrix $\mathbf{A}(t_2,t_1)$ is evaluated.

Once $\mathbf{A}(t_2,t_1)$ has been computed, the length of the semi-axes of the ellipsoid, $\sigma_1, \ldots, \sigma_M$, can be determined by a singular value decomposition of $\mathbf{A}(t_2,t_1)$ or by an eigenanalysis of $\mathbf{A}(t_2,t_1) \mathbf{A}^T(t_2,t_1)$.

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Lorenz's 3-variable model

 $\sigma = 10, \ b = 8/3 = 2.67, r = 28$

A sphere of errors, introduced at the beginning of each time interval, evolves into an ellipsoid. The value of σ_1 varies considerably and is sometimes less than one. The longest axis is growing most of the time.

Time	$\sigma_{ t l}$	$\sigma_{_2}$	$\sigma_{\scriptscriptstyle 3}$
5000-5010	1.0094	0.7698	0.3281
5010-5020	1.3513	0.7688	0.2454
5020-5030	1.7128	0.7697	0.1934
5030-5040	2.0157	0.7759	0.1630
5040-5050	2.1206	0.8013	0.1501
5050-5060	1.7324	0.8737	0.1684
5060-5070	1.0740	0.8867	0.2677
5070-5080	0.9324	0.7728	0.3539
5080-5090	1.2117	0.7662	0.2746
5090-5100	1.5855	0.7659	0.2099
5100-5110	1.9545	0.7659	0.1703
5110-5120	2.2851	0.7659	0.1457
5120-5130	2.5660	0.7659	0.1297
5130-5140	2.7970	0.7660	0.1190
5140-5150	2.9812	0.7663	0.1116
5150-5160	3.1091	0.7685	0.1067

Lorenz's 3-variable model

 $\sigma = 10, \ b = 8/3 = 2.67, \ r = 28$

A sphere of errors evolving into an ellipsoid for combined time intervals.

Time	σ_1	σ_2	σ_3
5000-5020	1.3363	0.5850	0.0832
5020-5040	3.3802	0.6062	0.0317
5040-5060	3.0535	0.7949	0.0268
5060-5080	0.9824	0.6329	0.1045
5080-5100	1.9081	0.5863	0.0581
5100-5120	4.4041	0.5866	0.0252
5120-5140	6.8485	0.5867	0.0162
5140-5160	8.6159	0.5900	0.0128
Time	σ_1	σ_2	σ_3
5000-5040	4.4056	0.3606	0.0027
5040-5080	1.7418	0.7155	0.0034
5080-5120	8.3917	0.3439	0.0015
5120-5160	54.9143	0.3465	0.0002

Some of the eigenvalues of become much larger than others. The ellipsoid becomes extremely elongated in a few directions.

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Lorenz's 28-variable model

Lorenz, E. N., 1965: A study of the predictability of a 28-variable atmospheric model. *Tellus*, **17**, 321-333.

Lorenz studied the growth of small errors in a 28-variable model derived from the two-layer quasi-geostrophic model. For suitable values of the parameters of the model, the attractor is chaotic. A sphere in the model's phase space becomes a 28-dimensional ellipsoid. There are several growing principal axes, and there is considerable variation from one four-day period to another.

i	λ,	λ_2	λ3	λ_{4}	λ₅	λ,	λ,
0	6.3	4.2	2.9	1.3	1.3	0.9	0.4
4	93.8	2.5	1.5	0.9	0.6	0.4	0.1
8	25.1	5.3	3.9	2.3	1. 1	0.7	0.5
12	10.0	7.0	4.9	2.6	1.6	1.3	0.8
16	7.1	3.1	1.8	1.3	0.8	1.0	0.2
20	7.2	4.9	3.7	2.4	1.3	0.7	0.6
24	8.5	4.5	3.9	3.0	2.0	1.2	0.5
28	3.7	2.5	2.1	1.8	1.2	1.0	0.6
32	10.8	7.6	6.5	3.3	1.6	1.2	0.7
36	7.1	3.7	2.1	1.8	1.6	1.3	0.6
40	38.5	7.4	5.1	2.0	1.0	0.6	0.5
44	6.7	4.3	0.2	1.2	1.0	0.8	0.4
48	126.3	2.5	2.2	0.9	0.6	0.4	0.1
52	5.4	• 2.9	2.4	1.8	1.3	1.0	0.6
56	16.4	11.0	9.1	6.1	3.7	0.9	0.7
60	8.0	5.6	3.8	2.5	1.2	1.1	0.7

TABLE 1. Square roots $\lambda_1, ..., \lambda_7$ of seven largest eigenvalues of matrices $A(t_{i+4}, t_i)A^T(t_{i+4}, t_i)$, for 16 successive 4-day periods.

Computation of Lyapunov exponents

(Wolf, A., J. B. Swift, H. L. Swinney, and J. A. Vatsano, 1985: Determining Lyapunov exponents from a time series. *Physica D*, **16**, 285-317.)

Lyapunov exponents are the long-term averages of the semi-axes of the error ellipsoid. If the ellipsoid evolves for a long time, the magnitudes of the principal axes diverge, and also, the axes tend to fall along the local direction of most rapid growth making it difficult to distinguish them. These problems are solved by repeated use of Gram-Schmidt reorthonormalization (GSR) on the vector frame.

Choose an initial set of orthonormal vectors and let it evolve according to the linear tangent equation to become the set $(\mathbf{w}_1, \dots, \mathbf{w}_M)$. Then an application of GSR results in the orthonormal set $(\mathbf{w}'_1, \dots, \mathbf{w}'_M)$ given by

$$\mathbf{w}_{1}^{\prime} = \frac{\mathbf{w}_{1}}{\|\mathbf{w}_{1}\|},$$

$$\mathbf{w}_{2}^{\prime} = \frac{\mathbf{w}_{2} - \langle \mathbf{w}_{2}, \mathbf{w}_{1}^{\prime} \rangle \mathbf{w}_{1}^{\prime}}{\|\mathbf{w}_{2} - \langle \mathbf{w}_{2}, \mathbf{w}_{1}^{\prime} \rangle \mathbf{w}_{1}^{\prime}\|}$$

$$\vdots$$

$$\mathbf{w}_{M}^{\prime} = \frac{\mathbf{w}_{M} - \langle \mathbf{w}_{M}, \mathbf{w}_{M-1}^{\prime} \rangle \mathbf{w}_{M-1}^{\prime} - \dots - \langle \mathbf{w}_{M}, \mathbf{w}_{1}^{\prime} \rangle \mathbf{w}_{1}^{\prime}}{\|\mathbf{w}_{M} - \langle \mathbf{w}_{M}, \mathbf{w}_{M-1}^{\prime} \rangle \mathbf{w}_{M-1}^{\prime} - \dots - \langle \mathbf{w}_{M}, \mathbf{w}_{1}^{\prime} \rangle \mathbf{w}_{1}^{\prime}\|}$$

where < , > denotes an inner product.

The GSR is applied at frequent intervals such that the magnitudes and directions of the vectors do not diverge. The GSR preserves the orientation of the vectors.

The first vector, which is unaffected by the GSR, tends to fall along the most rapidly growing direction in the tangent space.

The second vector is normalized after its component along the direction of the first vector is removed.

The vectors w_1' and w_2' span the same two-dimensional subspace as w_1 and w_2 , and represent the two-dimensional space that is most rapidly growing.

The length of the vector w_1 is proportional to $exp(\lambda_1 t)$ while the area defined by w_1 and w_2 is proportional to $exp[(\lambda_1 + \lambda_2)t]$.

The volume defined by *M* vectors evolve as $\exp[(\lambda_1 + ... + \lambda_M)t]$.

The long-term averages of the norms of w_1', \ldots, w_M' provide the values of the Lyapunov exponents $\lambda_1, \ldots, \lambda_M$.

Lorenz's 3-variable Model Lyapunov Exponents and Lyapunov dimension

 $\sigma = 10, \ b = 8/3 = 2.67$

r	λ_1	λ_2	λ_3	$\lambda_1 + \lambda_2 + \lambda_3$	- (<i>σ</i> + <i>b</i> +1)	d
Steady	1	2	J	1 2 3		
0.5	-0.48	-2.67	-10.52	-13.67	-13.67	0.00
10.0	-0.60	-0.60	-12.48	-13.67	-13.67	0.00
Periodic						
100.5	0.00	-1.74	-11.93	-13.67	-13.67	1.00
150.0	0.00	-0.66	-13.01	-13.67	-13.67	1.00
320.0	0.00	-0.13	-13.55	-13.68	-13.67	1.00
Chaotic						
28.0	0.90	0.00	-14.57	-13.67	-13.67	2.06
45.0	1.22	0.00	-14.88	-13.67	-13.67	2.08
90.0	1.37	0.00	-15.03	-13.67	-13.67	2.09
120.0	1.55	0.00	-15.22	-13.67	-13.67	2.10
200.0	1.46	0.00	-15.13	-13.67	-13.67	2.10

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Lorenz's 28-variable model

(Krishnamurthy, V., 1993: A predictability study of Lorenz's 28-variable model as a dynamical system. *J. Atmos. Sci.*, **50**, 2215-2229)

Lyapunov exponents for chaotic attractors at various values of forcing θ_0^* shows that the number of positive exponents and the value of the largest exponent increase as the forcing increases. The Lyapunov dimension also increases with the forcing indicating that the degree of chaos and the measure of predictability vary.

