Deterministic and stochastic views of turbulence

VIII Brazilian Micrometeorology Workshop Santa Maria RS

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Thanks,

For the invitation, for the attention, and for the kindness.

It is an honor.





Motivation and Introduction

This presentation is about two questions that I have always asked myself (and a few other people), for which I never obtained statisfactory answers:

- 1. Why do we generate random numbers in a computer in a completely deterministic way, and still "get away" with it?
- 2. Why do we take averages and moments of the quantitities in the Navier-Stokes and scalar transport equations, and, again, "get away" with the statistics?





The dichotomy Random \times Deterministic

is deeply ingrained. For example, Breuer and Petruccione (1992):

It is well known that models of homogeneous turbulence often rely upon statistical tools [1,2]. In principle, statistical concepts are introduced in the theory only by considering random initial ensembles of velocitiy fields. However, the time evolution of each member of the ensemble is governed by the deterministic Navier-Stokes equation.

In this letter, a mesoscopic approach ... which in contrast to the classical theory, regards the velocity itself as a discrete stochastic process. ... In doing so, an inherently stochastic model of turbulence can be formulated. An initial ensemble of velocity fields evolves probabilistically in time.





In summary:

- Navier Stokes ⇒ Deterministic evolution in time.
- Stochastic Process ⇒ Probabilistic evolution in time.

As we shall see, this is not necessarily true!





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This is by no means a criticism against Breuer and Petruccione (1992); rather, their view is probably the prevalent one.

In this view, randomness accompanies the stochastic process "along the way": at each time t, the future remains "random".

Does it? In this presentation, I will try to convince you that this dichotomy does not really exist.





Main sources for this presentation are

- 1. J. L. Lebowitz and O. Penrose (1973) Modern ergodic theory. Physics Today **2(26)**, 23–29.
- 2. P. Collet (2010) Dynamical Systems and Stochastic Processes, http://escuelainvierno.cimfav.cl/documentos/pdf/NotesP_Collet.pdf





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A classical random number generator

The map

$$f(x) = (16807 x) \mod (2^{31} - 1).$$

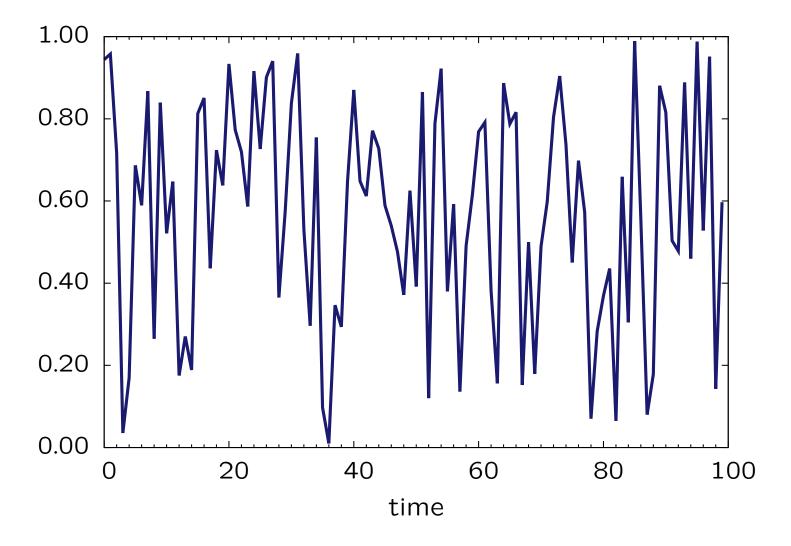
generates a sequence of pseudorandom numbers "uniformly" distributed on [0, 1]. Here is a program for generating 10000 values:

```
1 #!/usr/bin/python
2 from math import floor
3 \text{ deno} = 2**31
4 \text{ denu} = 2**31 - 1
5 \times 0 = 0.9439494030244930249
6 \text{ no} = \text{int}(xo * deno)
7 fou = open('rnum2.out','wt')
8 fou.write("%8.6f_{\perp}%8.6f_{n}" % (float(0),xo))
9 n = 10000
10 <u>for</u> i <u>in</u> range(1,n):
  nn = 16807*no % denu
11
   xn = float(nn)/deno
12
    fou.write("\%8.4f_{11}\%8.6f\n" % (float(i),xn))
13
      no = nn
14
15 fou.close()
```





The first 100

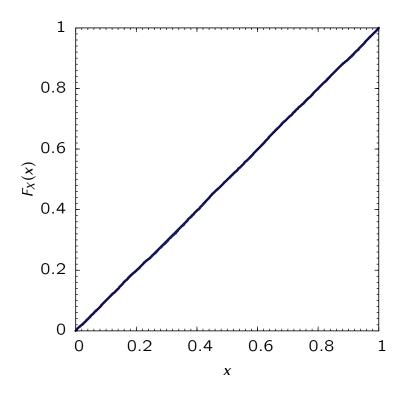


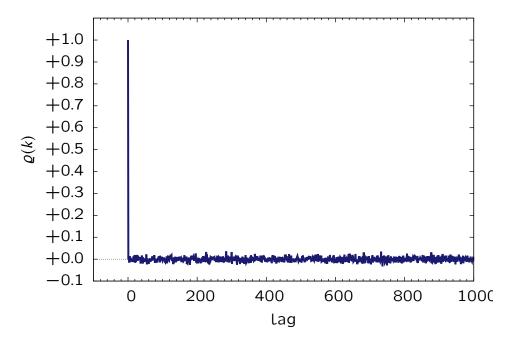




Checking

How good are they? We should check: the marginal cumulative distribution (left), and the apparent independence between consecutive values via the autocorrelation function (right).



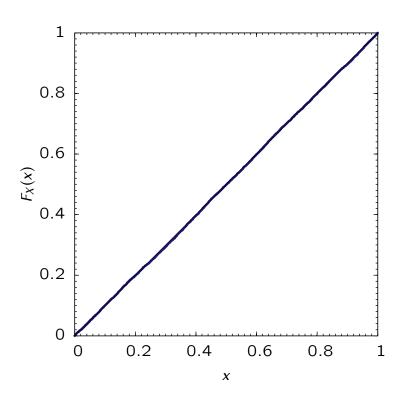


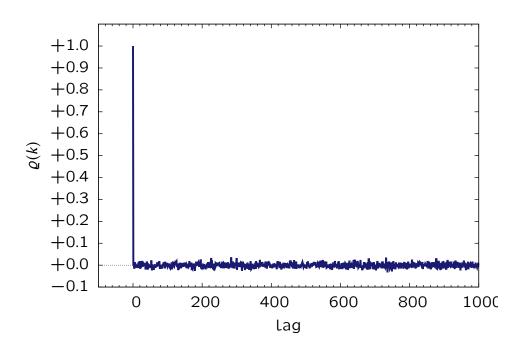




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The 10000 pseudorandom numbers will look like 10000 independent realizations of $X \sim U[0, 1]$. But they were generated deterministically!





Averaging physical equations

We are all very used to Reynolds' decomposition and averaging equations, and treating the fluctuations as random variables:

$$\frac{\partial \Theta}{\partial t} = -\frac{\partial (U_k \Theta)}{\partial x_k} + \nu_\theta \frac{\partial^2 \Theta}{\partial x_k \partial x_k},$$

$$\Theta = \langle \Theta \rangle + \theta, \qquad U_k = \langle U_k \rangle + u_k,$$

$$\vdots$$

$$\frac{\partial \theta}{\partial t} = -\frac{\partial}{\partial x_k} \left[\langle U_k \rangle \theta + u_k \langle \Theta \rangle + u_k \theta - \langle u_k \theta \rangle \right] + \nu_\theta \frac{\partial^2 \theta}{\partial x_k \partial x_k},$$

$$\vdots$$

$$\frac{\partial \langle \theta \theta \rangle}{\partial t} = -\langle U_k \rangle \frac{\partial \langle \theta \theta \rangle}{\partial x_k} - 2\langle u_k \theta \rangle \frac{\partial \langle \Theta \rangle}{\partial x_k} - \frac{\partial \langle u_k \theta \theta \rangle}{\partial x_k} - 2\nu_\theta \langle \frac{\partial \theta}{\partial x_k} \frac{\partial \theta}{\partial x_k} \rangle$$





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But can we really do it?





Averaging ensembles

The equation

$$f(x) = (16807 x) \mod (2^{31} - 1).$$

is a simple example of a *dynamical system*. At the end of the 19th century, physicists — and engineers! — were taking liberties and mixing deterministic and stochastic approaches. A very nice review is given in J. L. Lebowitz and O. Penrose, "Modern Ergodic Theory", *Physics Today* 26(2), 26–29, 1973, from which we quote extensively:

The founding fathers of statistical mechanics, Boltzmann, Maxwell, Gibbs and Einstein, invented the concept of ensembles to describe equilibrium and none-quilibrium macroscopic systems. In trying to justify the use of ensembles, and to determine whether the ensembles evolved from nonequilibrium to equilibrium, they introduced further concepts such as "ergodicity" and "coarse graining". The use of these concepts raised mathematical problems that they could not solve, but like the good physicists they were they assumed that everything was or could be made all right mathematically and went on with the physics.





Even so!

(maybe I am a bad physicist or engineer :-))

I would like a little justification for mixing the deterministic and stochastic approaches.

This dates back to my bewilderment, as a student, at the need for an equation for turbulence kinetic energy.





A brief chronology

1871 Boltzmann introduces the ergodic hypothesis.

1867 Maxwell (1867) averages equations of motion for gas molecules.

1895 Clearly influenced by Maxwell's paper — but without mentioning Maxwell's name! — Reynolds introduces his decomposition, $u = \overline{u} + u'$, which we still use today; he tries to found his equations on *statistical mechanics*, and explicitly mentions at the introduction (Reynolds, 1895) the "kinetic theory of matter". Reynolds derives the mean equations, and the equation for turbulence kinetic energy, by averaging essentially in the same way as we did for $\langle \theta \theta \rangle$ in the introduction! However, ensemble averaging is not explicit; instead there is a mix of space and time averages.





(continued)

- **1905** Einstein's 1905 theory of Brownian motion. Averaging equations of motion is not very explicit, but deterministic and probabilistic ideas are freely mixed (see Einstein, 1956).
- 1908 Langevin's 1908 paper on Brownian motion. Equations of motion are explicitly averaged (see Lemons and Gythiel, 1997).
- 1927 Birkhoff's 1931 proof of the Ergodic Theorem.
- **1933** Kolmogorov's 1933 book on the "Foundations of probability theory".





Four Perspectives on Probability

http://www.ma.utexas.edu/users/mks/statmistakes/probability.html

- 1. Classical (sometimes called "A priori" or "Theoretical"): If we have a situation (a "random process") in which there are n equally likely outcomes, and the event A consists of exactly m of these outcomes, we say that the probability of A is m/n. This is circular reasoning!
- 2. **Empirical** (sometimes called "A posteriori" or "Frequentist") This idea is formalized to define the probability of the event A as P(A) = 1 the limit as n approaches infinity of m/n, where n is the number of times the process (e.g., tossing the die) is performed, and m is the number of times the outcome A happens.

3. Subjective

Subjective probability is an individual person's measure of belief that an event will occur.

4. Axiomatic

This is Kolmogorov (1933)'s book.





Kolmogorov's definitive Probability

A probability triple, or probability space, is a triple (Ω, \mathcal{F}, P) , where:

- Ω is any non-empty set;
- \mathscr{F} is a σ -field, a collection of subsets of Ω obeying special conditions.
- P is a function from \mathscr{F} to [0, 1]

Several probability axioms hold, including the usual

$$P\{\emptyset\} = 0,$$

$$P\{\Omega\} = 1,$$

$$A_i \cap A_j = \emptyset \Rightarrow P\left\{\bigcup_{i=1}^{\infty} A_i\right\} = \sum_{i=1}^{\infty} P\{A_i\}$$
 (countable additivity).



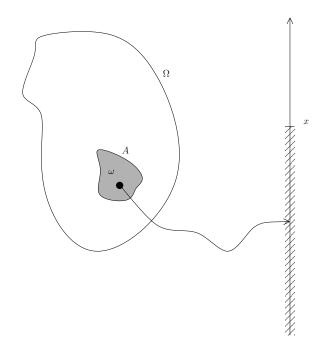


Random variables

A random variable is a function $X:\Omega\to\mathbb{R}$ such that

$$\{\omega \in \Omega \mid X(\omega) \leq x\} \in \mathscr{F}.$$

X is a measurable function.



Graphical representation of the event $X(\omega) \leq x$





Integration

With Kolmogorov's axiomatic approach, things quickly fall into place. The distribution function of X is

$$F_X(x) \equiv P\{\omega \mid X(\omega) \leq x\};$$

with different degrees of sophistication and difficulty, one can now calculate moments, such as the *expected value*

$$\langle X \rangle = \int_{\Omega} X(\omega) \, \mathrm{d}P(\omega).$$

Even better, a *change of variable* theorem (Rosenthal, 2008, Theorem 6.1.1) allows to do the same "without Ω ": for any measurable function $g: \mathbb{R} \to \mathbb{R}$,

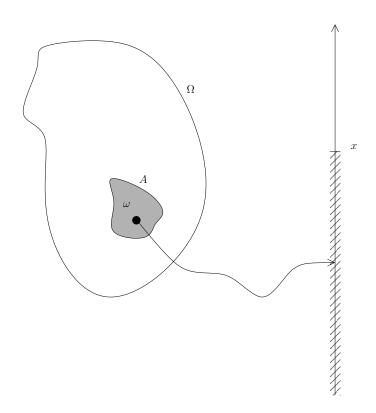
$$\int_{\Omega} g(X(\omega)) dP(\omega) = \int_{\mathbb{R}} g(t) dF_X(t).$$





The "sample bag"

Learning all this is hard; it is often good enough to think about it as the sample bag Ω from which we draw numbers, beads, of any other concrete representation of $X(\omega)$. Here it is again:



But Kolmogorov did not — and neither anybody else ever since — ever teach us how to draw an ω from the bag!





Here is how I drew an ω in my program:

```
#!/usr/bin/python
from math import floor
deno = 2**31
denu = 2**31 - 1
xo = 0.9439494030244930249
no = int(xo * deno)
fou = open('rnum2.out','wt')
fou.write("%8.6f %8.6f\n" % (float(0),xo))
n = 10000
for i in range(1,n):
   nn = 16807*no
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In other words, I drew it myself! This is what we all call the "seed" of the random number generator.





The stochastic process

Kolmogorov would not stop. From Todorovic (1992):

A stochastic process is a family of random variables X(t), $t \in T$, defined on a *common* probability space (Ω, \mathcal{F}, P) , $T \subset \mathbb{R}$

That is:

$$X: \Omega \times T \to \mathbb{R},$$

$$(\omega, t) \mapsto x = X(\omega, t)$$

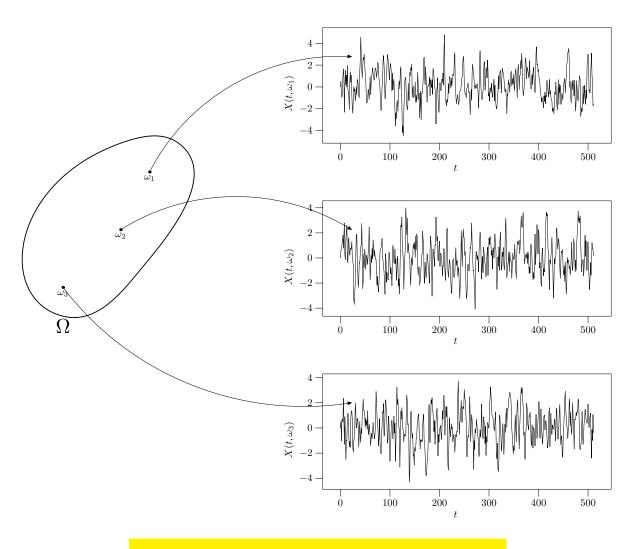
The really important point to be made is this:

Once ω is chosen, X(t) is deterministic: an ordinary function like any other!





A "bag" for stochastic processes, too



A single ω for each x(t)!





Reconciling divorcees

Now the random number generator is beginning to look like a stochastic process!

We can almost "see" the trick: if the function $f(x) = (16807 x) \mod (2^{31} - 1)$ is "measurable" in some sense, then a single ω may spawn a multidimensional vector $\mathbf{X}(\omega)$, which we may call, perhaps at the same time, a stochastic process and a dynamical system.





Theorems of statistical mechanics and ergodic theory

Let us extend — and change — nomenclature a little bit. Let us call Ω the state space (also!). Let

$$\omega \equiv x_0 \in \Omega$$
,

with

$$\phi_t: \Omega \to \Omega,$$

$$x_0 \mapsto x(t) = \phi_t(x_0).$$

Above, t can be either discrete ("maps") or continuous ("flows"). We have

$$\phi_{t+s} = \phi_s \circ \phi_t$$
.





Def of a dynamical system

A definition of a dynamical system is now the triple (Ω, \mathcal{F}, P) together with ϕ_t .

This definition is essentially identical at first sight to that of a stochastic process, but we must look at the conditions on ϕ_t and P for the equality to hold.





Measures

As we already know from Kolmogorov's axiomatic probability approach, the measure (probability) of a set A in Ω is

$$P(A) = \int_{x \in A} dP(x).$$

Let us say that ϕ_t is, in some sense, a measurable function. Then, if P is a probability measure on Ω , then ϕ_t induces a new probability measure in Ω , by means of:

$$P(\phi_t(A)) \equiv P(A)$$
 (forward).

This is often done the other way around:

$$P(A) \equiv P(\phi_{-t}(A))$$
 (backward).

If the above holds for all measurable $A \in \Omega$, we say that P is invariant under ϕ_t .





The Côup de grâce

From:

Dynamical Systems and Stochastic Processes

(P. Collet, 2010)

http://escuelainvierno.cimfav.cl/documentos/pdf/ NotesP_Collet.pdf

Given a probability measure μ (read P) on the phase space Ω and the time evolution map T (or a (semi)-flow) (read ϕ_t), we are **exactly** in the setting of stochastic processes.

This is because, given the dynamical system ϕ_t , and a measurable function g on Ω , we can define a stochastic process X(t) by means of

$$X(\omega, t) \equiv g(\phi_t(\omega))$$
.





Could it be any clearer?

Yes!





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Yes!

Collet (2010):

The fact which may look a little unusual for a Probabilist is that the probability is given on the initial condition, and there is no randomness appearing in the time evolution (my emphasis). However the points on the phase space completely characterize the orbits, and we can think of μ (read P) as a probability measure on the orbits, the time evolution being the shift.

In that sense, any stochastic process is a dynamical system (a not very useful remark in practice).





Ergodicity, and Birkhoff's theorem

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T g(\phi_t(x_0))\,\mathrm{d}t = L \stackrel{\text{if ergodic}}{=} \int_\Omega g(\omega)\,\mathrm{d}\omega$$

Remark: $X(x_0, t) = g(\phi_t(x_0))$ is a single realization of a stochastic process from the initial condition x_0 . The rightmost expression is independent of x_0 , and only then is the process ergodic.

Moreover, (Lebowitz and Penrose, 1973):

Stated precisely, this means that a system is ergodic on S (read Ω) if and only if all regions R of S (read Ω) left invariant by the time evolution, $\phi_t(R) = R$ either have zero area or have an area equal to the area of S (read either have zero probability measure, or have P(R) = 1).





Being more accurate,

However, the equality $\phi_t(R) = R$ in Lebowitz and Penrose (1973)'s statement is somewhat *imprecise*! Given the *symmetric difference* between two sets.

$$A \triangle B \equiv (A \cup B) - (A \cap B),$$

then, in terms of probability measure, the corresponding statement is.

$$P(A \triangle \phi_{-t}(A)) = 0 \Leftrightarrow P(A) = 0 \text{ or } P(A) = 1.$$

My simple-minded interpretation: in an ergodic system, the map ϕ_t makes any realization eventually wander over almost all of Ω (P(A) = 1), or almost none of it at all (P(A) = 0).





Example: a non-ergodic process

The stochastic process

$$X(\omega, t) = U(\omega)$$

with U uniformly distributed on [0, 1] is stationary, but it is not ergodic. Indeed, for instance,

$$E\{X(t)\} = E\{U\} = 1/2$$
, etc.

but

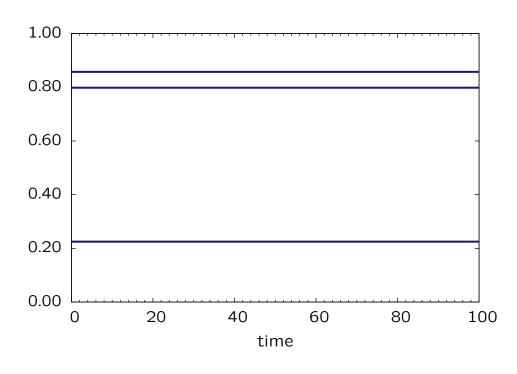
$$\lim_{T \to \infty} \frac{1}{T} \int_0^T X(t) dt = X(0) \neq 1/2 \text{ in general.}$$





Picture of this non-ergodic process

3 realizations:



What is the problem? This process has *infinite* memory, and it does not wander all over Ω .





The mixing condition

implies (is a sufficient condition for) ergodicity:

$$\lim_{\tau \to \infty} \int_{\Omega} f(x)g(\phi_{\tau}(x)) dP(x) = \int_{\Omega} f(x) dP(x) \int_{\Omega} g(x) dP(x)$$

But

$$C_{fg}(\tau) \equiv \langle f(x)g(\phi_{\tau}(x))\rangle - \langle f(x)\rangle \langle g(x)\rangle$$

is the τ -covariance function; therefore,

If the τ -covariance function goes go to zero, the process is ergodic.

But this does not even guarantee that the process has finite variance. For more regularity, more conditions are needed.





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The most common is the existence of integral scales.





Ergodic, but nonstationary, and non-mixing

The harmonic oscillator is

$$X(\omega, t) = A(\omega) \cos t + B(\omega) \sin t,$$

$$\dot{X}(\omega, t) = -A(\omega) \cos t + B(\omega) \cos t$$

The state space is the circle

$$\Omega: X^2 + \dot{X}^2 = R^2; \qquad X(\omega, 0) = A(\omega), \ \dot{X}(\omega, 0) = B(\omega).$$

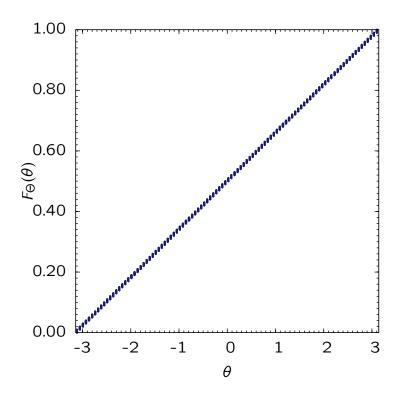
Without loss of generality, $R^2=1$. We randomly pick a point $(A(\omega), B(\omega))$ on the unit circle, and it will go round and round forever on it. The random point actually corresponds to a uniform distribution of $\Theta(\omega)=\arctan(2(B,A))$ on (say) $[-\pi,+\pi]$.

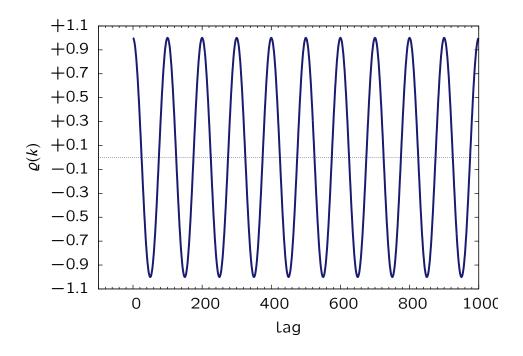




Numerical test of the harmonic oscillator

X(t) and $\dot{X}(t)$ wander all over Ω , and the cdf of Θ is recovered empirically: this is an indication that the process is *ergodic*. However, the autocorrelation function does not $\to 0$ as $\tau \to \infty$: the process is non-mixing. Moreover, it is not stationary.









Example: the AR-1 process

A multivariate random variable is a stochastic process. An n-uple $(U_1, U_2, ..., U_n, ...)$ of zero-mean (without loss of generality), independent and identically distributed random variables with variance σ^2 is a stochastic process, if we look at it as:

$$\mathbf{U}(\omega) = (U_1(\omega), U_2(\omega), \dots, U_n(\omega), \dots).$$

Then this process can be used to build another one. For instance, an autoregressive, order 1 process

$$X_1 = U_1$$

$$X_{n+1} = \rho X_n + \sqrt{1 - \rho^2} U_{n+1}$$

can now be seen as

$$\mathbf{X}(\omega, n) = (X_1(\omega), X_2(\omega), \dots, X_n(\omega), \dots).$$





Interpretation

This is contrary to the usual first impression that in such a process there is a "deterministic" component (ρX_n) and randomness introduced at each time step $(\sqrt{1-\rho^2}U_{n+1})$: we can alternatively think of all the "randomness" being drawn from the bag "instantaneously" $(\mathbf{U}(\omega))$ and a deterministic function $X(\omega, n)$ being defined once ω has been drawn.





Conclusions

- To a large extent, stochastic processes and dynamical systems can be given a unified treatment. There are technicalities, like the nature of the measures, and the sigma-fields involved, etc..
- At any rate, this unified approach justifies the liberties taken for instance in averaging turbulent flows both analytically and in the laboratory/field.
- A long way lies ahead, however. For instance: are the Navier-Stokes equations ergodic? How about mixing?
- Reynolds' approach in averaging the Navier-Stokes equations antedates important and seminal work on Statistical Mechanics and Ergodic Theory. It remains far-reaching and an important tool to this day.





That's it

Thank you very much for the attention: questions?





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