Influence of database noises to machine learning for spatiotemporal chaos

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A new strategy, namely the “clean numerical simulation” (CNS), was proposed (J. Computational Physics, 418:109629, 2020) to gain reliable/convergent simulations (with negligible numerical noises) of spatiotemporal chaotic systems in a long enough interval of time, which provide us benchmark solution for comparison. Here we illustrate that machine learning (ML) can always give good enough fitting predictions of a spatiotemporal chaos by using, separately, two quite different training sets: one is the “clean database” given by the CNS with negligible numerical noises, the other is the “polluted database” given by the traditional algorithms in single/double precision with considerably large numerical noises. However, even in statistics, the ML predictions based on the “polluted database” are quite different from those based on the “clean database”. It illustrates that the database noises have huge influences on ML predictions of some spatiotemporal chaos, even in statistics. Thus, we must use a “clean” database for machine learning of some spatiotemporal chaos. This surprising result might open a new door and possibility to study machine learning.

It was first discovered by Poincaré \textsuperscript{1} that noises (or uncertainty) increase exponentially for chaotic dynamic systems due to the sensitivity dependence on initial conditions (SDIC). The same phenomena was rediscovered by Lorenz \textsuperscript{2} in 1963 with a more popular name “butterfly-effect”: for a chaotic system, a tiny variation of initial condition might lead to a huge difference of numerical simulations after a long enough time \textsuperscript{3,4}. Furthermore, Lorenz \textsuperscript{5} discovered that computer-generated simulations of a chaotic system given by traditional methods (such as Runge-Kutta method and so on) in single/double precision are sensitive not only to initial conditions but also to numerical algorithms.

To overcome the above-mentioned limitations of traditional algorithms for chaotic systems, Liao \textsuperscript{6,7} proposed a new numerical strategy, called the “Clean Numerical Simulation” (CNS). The CNS can greatly reduce the global numerical noises to a required tiny level so that a reliable (replicable) simulation can be obtained in the whole spatial domain within a controllable interval of time \(0 \leq t \leq T_c\), where \(T_c\) is called “critical predictable time”. Thus, the CNS can provide us a reliable, true simulation of chaos in a long enough interval of time, which can be used as a benchmark solution. The CNS has been successfully applied to gain reliable computer-generated simulations of many chaotic systems, such as Lorentz system \textsuperscript{8,9}, three-body systems \textsuperscript{9,12}, some spatiotemporal chaotic systems \textsuperscript{13,15}, two-dimensional Rayleigh-Bénard turbulence \textsuperscript{16}, and so on. All of these illustrate the validity of the CNS.

Currently, machine learning (ML) \textsuperscript{17,28} has been successfully applied in predicting evolution of many nonlinear dynamic system. Particularly, the reservoir computing (RC) \textsuperscript{20,28} has shown significant success in modelling chaotic systems, which can alleviate the difficulty in learning recurrent connections of recurrent neural networks (RNNs) and besides decrease training cost.

However, all computer-generated chaotic simulations, which were used as database to evaluate performance of machine learning before, were given by the traditional algorithms in single/double precision, so that they contain considerably large numerical noises and thus unavoidably have great deviations from their corresponding “true” trajectories, due to the butter-effect of chaos. In other words, these databases contain large artificial noises: they are “polluted database” for machine learning. On the other side, using the CNS, one can gain a true/reliable simulation of chaos in a long enough interval of time, which as a benchmark solution can provide us a “clean database” for machine learning. These two computer-generated chaotic simulations of the same equation under the same initial/boundary conditions provide us two different training sets for machine learning. Obviously, we can use the “clean database” as a benchmark to investigate whether or not the ML predictions based on the “polluted database” have huge differences from those based on the “clean database”. This can reveal the influence of database noise to machine learning, which has been almost neglected by the ML community.

Without loss of generality, let us consider here the Kuramoto-Sivashinsky (KS) equation

\[
U_t + U U_x + U_{xx} + U_{xxxx} = 0, \quad 0 \leq x \leq L, \tag{1}
\]

which is a prototypical model of spatiotemporal chaos. Like Khellat and Vasegh \textsuperscript{29}, we choose the initial condition

\[
U(x, 0) = -\sin (\alpha x) + \cos (\alpha x) + \sin (2\alpha x) - \cos (2\alpha x) \tag{2}
\]

and the periodic boundary condition \(U(0, t) = U(L, t)\), where \(\alpha = 2\pi/L\). Following Lu \textit{et al.} \textsuperscript{31} and Lin &
as long as the mode-number form (FFT) algorithm is used. Thus, we can obtain an error. Here, the fast Fourier transforms is large enough. In this way, the spatial truncation error can be reduced to a required tiny level, too. For them by $m$, we have

$$U^m(x_k, t) = \frac{1}{m!} \frac{\partial^m U(x_k, t)}{\partial t^m}.$$  

Obviously, the temporal truncation error can be reduced to a required tiny level as long as $M$ is large enough and $\Delta t$ is reasonably small. Differentiating $(m - 1)$ times on both sides of Eq. (1) with respect to $t$ and then dividing them by $m!$, we have

$$U^m(x_k, t) = \frac{1}{m} \left[ \sum_{j=0}^{m-1} U^j(x_k, t) U^{m-1-j}(x_k, t) \right] + U^{m-1}(x_k, t) + U^{m-1}(x_k, t),$$

where $m \geq 1$, $U^0(x_k, t) = U(x_k, t)$ and

$$U^j(x_k, t) = \frac{\partial U^j}{\partial t}|_{x=x_k} U^j(x_k, t) = \frac{\partial^2 U^j}{\partial x^2}|_{x=x_k}$$

and so on. In the frame of the CNS, the spatial derivatives, such as $U^j_x(x_k, t)$, $U^j_{xx}(x_k, t)$, and $U^j_{xxx}(x_k, t)$ in Eq. (1), are calculated in rather high accuracy by means of the Fourier series of $U(x, t)$ in space, so as to reduce the spatial truncation error. Here, the fast Fourier transform (FFT) algorithm is used. Thus, we can obtain an accurate enough approximation of the spatial derivatives as long as the mode-number $N$ of the spatial Fourier series is large enough. In this way, the spatial truncation error can be reduced to a required tiny level, too. For details, please refer to Hu & Liao [13].

In addition, unlike traditional algorithms that mostly use single/double precision, the multiple-precision [32] with a large number of significant digits is employed in the frame of the CNS for all physical/numerical variables and parameters so as to reduce the round-off error to a required tiny level. In practice, in order to gain simulations more efficiently, the variable step-size (VS) scheme [33] is applied in the temporal dimension with a given allowed tolerance $tol$ of the governing equations. Besides, since the round-off error should be in the same level of the (temporal) truncation error, we always set the allowed tolerance $tol = 10^{-N_s}$, where $N_s$ is the number of significant digits in multiple precision [32]. In this way, we can globally control the spatial and temporal truncation errors by choosing a large enough mode-number $N$ of the spatial Fourier series and a large enough number $N_s$ of significant digits for multiple precision [32], which corresponds to a small enough temporal allowed tolerance $tol = 10^{-N_s}$ of the governing equation by means of the VS scheme [33]. For details, please refer to Hu & Liao [13].

Furthermore, to guarantee the reliability of a computer-generated simulation given by the CNS, an additional simulation with even smaller numerical noises is required to determine the so-called “critical predictable time” $T_c$ by means of comparing them with each other.
so that both of them have no distinct differences in $0 \leq t \leq T_c$ within the whole spatial domain, as illustrated in [13]. Solving the KS equation (1) by the CNS using different values of the mode-number $N$ and the significant digit number $N_s$ for the multiple precision [32], we gained the linear relationship

$$T_c \approx \min \{18.6N - 387, 46.4N_s - 222\}. \quad (5)$$

Thus, for a given value of $T_c$, we can always find the corresponding mode-number $N$ of the spatial Fourier expansion and the significant digit number $N_s$ for multiple precision so as to gain a reliable chaotic numerical simulation of Eq. (1) in $0 \leq t \leq T_c$ within the whole spatial domain $x \in [0, L]$. Therefore, according to (5), we have $T_c \approx 4186$ in the case of $N = 256$, $N_s = 95$ and tol $= 10^{-95}$, which provides us a reliable simulation (marked as CNS) of the KS equation (1) in $0 \leq t \leq 4000$. It also provides us the “clean database” for the machine learning, which is used here as a benchmark to investigate the influence of database noises.

On the other side, following [31], we solved the KS equation (1) with the same initial condition (2) and the same physical parameters in $0 \leq t \leq 4000$ by means of the 4th-order exponential time-differencing Runge-Kutta method [34, 35] in double precision with the mode-number $N = 108$ of the spatial Fourier expansion and time-step $\Delta t = 10^{-3}$. This provides us another numerical simulation (marked as ETDRK4wD) with considerably large numerical noises, i.e. the “polluted database”.

Note that the ETDRK4wD simulation is given by the Runge-Kutta method in double precision (corresponding to $N_s = 16$) using the mode number $N = 108$, which are much smaller than the significant digit number $N_s = 95$ and the mode number $N = 256$ for the CNS simulation, respectively. So, the numerical noises of the ETDRK4wD simulation should be much larger than that of the benchmark solution given by the CNS. Thus, due to the butterfly-effect of chaos, the ETDRK4wD simulation should quickly become unreliable. This is indeed true. As shown in Fig. 1 and Fig. 2, the trajectories of $U(x, t)$ and the total energy $E(t) = \frac{1}{2L} \int_0^L U^2(x, t)dx$ given by the ETDRK4wD simulation agree with those of the benchmark solution (given by the CNS) only in a short time $0 \leq t \leq 560$: the difference between the two simulations becomes distinct at $t = 600$. Thereafter, the numerical noises of the ETDRK4wD simulation quickly increase to the same level of the “true” solution so that it has obvious deviations from the benchmark result given by the CNS.

Following Jaeger [17], Jaeger & Haas [20] and Pathak et al. [23], we employ one widely used technique of machine learning (ML), i.e. the reservoir computing (RC), to these two computer-generated simulations (of the KS equation in the same case) given by the ETDRK4wD and CNS, respectively, corresponding to the “polluted database” and the “clean database”. For the sake of simplicity, we designate the ML system based on the “clean database” as ML-CNS, and the ML system based on the “polluted database” as ML-ETDRK4wD, respectively. We choose the observation time step $\Delta t = 0.1$, and use the results of the first 38000 time steps, i.e. $t \in (0, 3800)$, as the training data. The numbers of observation spatial grid of the training data are 128 and 108 for the ML-CNS and ML-ETDRK4wD, respectively. The basic ideas of the reservoir computing (RC) are briefly described in
the supplement, together with the corresponding hyperparameters for the ML-CNS and ML-ETDRK4wD.

Predictions are made respectively by these two ML systems in \( t \in [3800, 7800] \) with \( \Delta t = 0.1 \). Fig. 5 and Fig. 6 show the ML predictions (middle panel) of the spatiotemporal trajectories given by the ML-CNS (based on the “clean database”) and ML-ETDRK4wD (based on the “polluted database”), respectively, along with their corresponding actual values (top panel) and deviations between the actual values and ML predictions (bottom panel). In addition, Fig. 5 shows the comparisons of the total energy \( E(t) \) predicted by the ML-CNS and ML-ETDRK4wD with their corresponding actual values. The ML predictions of the spatiotemporal trajectories and the total energy given by the ML-CNS (based on the “clean database”) agree well to their corresponding actual values in \( t \in [3800, 3950] \) (about 6 Lyapunov time). So do the ML predictions by the ML-ETDRK4wD (based on the “polluted database”) in \( t \in [3800, 3950] \), too. However, it must be emphasized that, the ML predictions of the spatiotemporal trajectories and the total energy based on the “polluted database” have the distinct deviations from those based on the “clean database”. It illustrates that data noises have a great influence on the ML predictions of the spatiotemporal trajectories and the total energy.

How about the statistic properties of the ML predictions? Write
\[
U(x, t) = \sum_{n=-N/2}^{N/2-1} a_n(t) e^{inx},
\]
where \( a_n(t) \) is the evolution of the Fourier mode. As shown in Fig. 6(a), the autocorrelation function (ACF) of the real part of \( a_2(t) \) given by the ML-ETDRK4wD prediction (based on the “polluted database”) in \( t \in [3800, 7800] \) agrees well with that by the actual ETDRK4wD simulation. Similarly, the ACF of the real part of \( a_2(t) \) given by the ML-CNS prediction (based on the “clean database”) also agrees well with that by the actual CNS result. For each database, unlike the ML predictions of the spatiotemporal trajectories and the total energy that agree well with the corresponding actual values only in about six Lyapunov’s times \( t \in [3800, 3950] \), the ML predictions of the ACF (as a statistic result) are accurate enough in a much larger interval of time \( t \in [3800, 7800] \).

In other words, the statistic predictions given by the machine learning for the spatiotemporal chaotic system are valid in a much longer interval of time than the ML pre-
dictions of the spatiotemporal trajectories and the evolution of the total energy $E(t)$. However, the ACF of the real part of $a_2(t)$ given by the ML prediction based on the “polluted database” significantly deviates from that by the ML prediction based on the “clean database”.

In a similar way we can investigate the ACFs of the ML prediction of $U(0, t)$. It is found that the ACF of $U(0, t)$ given by the ML prediction based on the “polluted database” also significantly deviates from that by the ML prediction based on the “clean database”, as shown in Fig. 6(b). These illustrate that the database noises might have huge influences on the ML predictions even in statistics.

Machine learning (ML) [17-28] is indeed a very promising tool that has many exciting applications in science and engineering. However, for machine learning of some spatiotemporal chaos, database noises might lead to huge deviations from the true simulation, even in statistics. Thus, we must use a “clean” database for machine learning of such kind of spatiotemporal chaos, otherwise the ML predictions might lead to huge misunderstandings. This surprising result might open a new door and possibility to study machine learning. Certainly, there are lots of work to do in future.

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