Estimating the State of Large Spatiotemporally Chaotic Systems

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Data assimilation refers to the process of obtaining an estimate of a system’s state using a model for the system’s time evolution and a time series of measurements that are possibly noisy and incomplete. However, for practical reasons, the high dimensionality of large spatiotemporally chaotic systems prevents the use of classical data assimilation techniques. Here, via numerical computations on the paradigmatic example of large aspect ratio Rayleigh-Bénard convection, we demonstrate the applicability of a recently developed data assimilation method designed to circumvent this difficulty. In addition, we describe extensions of the algorithm for estimating unknown system parameters. Our results suggest the potential usefulness of our data assimilation technique to a broad class of situations in which there is spatiotemporally chaotic behavior.

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Estimation of the state of an evolving dynamical system from measurements that are possibly noisy and incomplete is a prerequisite for prediction and control in many situations. Furthermore, scientific investigations of dynamical processes often require inference of an evolving system state from data. The term ‘data assimilation’ refers to the case where a model for the time evolution of the system is available and is used in conjunction with incoming measurements to estimate the evolving system state. The Kalman filter [1, 2] optimally solves the data assimilation problem for systems with linear dynamics. The classical adaptation of the Kalman filter to non-linear systems is called the extended Kalman filter [3]. However, it requires inversion of $N \times N$ matrices, where $N$ is the number of model variables [4]. As a consequence, the application of such a technique to large, dynamically high-dimensional spatiotemporally chaotic systems is infeasible because no existing computers are large or fast enough to do the required matrix inversions. Despite these difficulties, recent developments from the field of numerical weather prediction [5, 6, 7, 8, 9, 10] suggest the possibility of achieving good accuracy (as in a Kalman filter), but in a way that is computationally feasible for large systems.

The purpose of this Letter is to use numerical simulations to demonstrate the potential usefulness of a new, weather-inspired data assimilation method, the local ensemble transform Kalman filter (LETKF), to a broad class of high dimensional spatiotemporally chaotic physical processes. For specificity we employ a particular paradigmatic example: spatiotemporally chaotic Rayleigh-Bénard convection. Flows such as spiral defect chaos [12, 13] in the Rayleigh-Bénard problem are, perhaps, the best studied experimental examples of spatiotemporal chaos; nevertheless, many general aspects of spatiotemporal chaos remain poorly understood.

The LETKF is motivated by the observation that, in typical examples of spatiotemporal chaos, spatial regions much smaller than the system size are accurately described by many fewer degrees of freedom than the full system. With this in mind, the LETKF employs many independent data assimilations in a large set of heavily overlapping regions. Because these regions are relatively small, the individual regional computations are not prohibitive. In addition, the regional data assimilation computations are independent of each other and can thus be done in parallel. Furthermore, by use of a simple example [14, 15] it was indicated that, if the size of the individual regions employed in LETKF is not too small (but still small compared to the total system size), then state estimates with accuracies virtually the same as those for a classical Kalman filter technique (thus presumably of near optimal accuracy) can be achieved. For details of the LETKF algorithm we refer the interested reader to Refs. [14, 15, 16].

In Rayleigh-Bénard convection, a horizontal fluid layer of thickness $d$ is confined between a heated lower plate and a cooled upper plate. The onset of fluid motion occurs when buoyancy overcomes viscous dissipation and thermal diffusion as the temperature difference between the plates $\Delta T$ is raised above a critical value $\Delta T_c$. Rayleigh-Bénard convection is typically modeled using the Boussinesq equations [17], which are commonly nondimensionalized with temperature scaled by $\Delta T_c$, length scaled by $d$, and time scaled by the vertical diffusion time $d^2/\kappa$, where $\kappa$ is the thermal diffusivity. This system of units is used throughout this Letter. We numerically solve the Boussinesq equations [18] applying realistic boundary conditions $u = 0$ and $T = 0$ (conducting) on the walls of the region boundary ($x^2 + y^2 \leq \Gamma^2$, $|z| \leq \frac{1}{2}$). We denote the temperature deviation from the conducting static solution (which is linear in $z$) as $T$ and the fluid velocity as $u$.

The Boussinesq equations have two dimensionless parameters, the reduced Rayleigh number $\epsilon$ and the Prandtl
Here \( R = \text{Rayleigh number} \), \( R_c \) is the critical Rayleigh number at convective onset, \( g \) is gravitational acceleration, \( \alpha \) is the thermal expansion coefficient, and \( \nu \) is the kinematic viscosity. Fluid convection arises when \( \epsilon > 0 \). In addition, the radius \( r \) of the disk in units of the cell depth \( d \), also referred to as the aspect ratio, specifies the geometry. We focused our studies on \( r = 20, \epsilon = 1, Pr = 1 \) [19].

In experiments, flows are visualized using the shadowgraph method [20], an indirect measurement of the fluid’s spatial temperature variation. In typical experiments, due to its difficulty, measurement of the fluid velocity field is not performed. The so-called mean flow, defined here as \( \bar{u}(x, y) \equiv \int u(x, y, z) \, dz \) (though see [21] for a more complete description), has been shown, through the use of simulations, to play a significant role in the dynamics [21]. Here \( u \) denotes the horizontal component of the fluid velocity \( u = u_x + u_z \). Our goal is to determine the full fluid state \((T(x, y, z), u(x, y, z))\), from a time series of shadowgraph measurements at a finite number of horizontal (pixel) locations, and we view this as a test case investigation of the general usefulness of our technique for laboratory experiments on spatiotemporal chaos.

We begin by considering a system state vector \( \xi \) with \( N \) components, for which we have a dynamical model, \( \xi_{j+1} = G(\xi_j) \). Our \( G(\cdot) \) is an integration of the Boussinesq equations [18] from a time \( t_j \) to \( t_{j+1} \) where \( t_j \equiv j \Delta t \) and \( t_1, t_2, \ldots \) are the times at which state estimates are constructed (also the times at which a measurement is taken). The model state \( \xi \) consists of the variables \( T \) and \( u \) defined on the grid points of the cylindrical mesh used by the model.

We map the temperature field to the shadowgraph light intensity \( I(x, y) \) with a map \( M \) using a relation derived from geometric optics [20, 22]

\[
I(x, y) = \frac{I_o(x, y)}{1 - a \nabla^2 T(x, y)} \equiv M[T(x, y, z)].
\]

Here, \( \nabla^2 \equiv \partial^2 / \partial x^2 + \partial^2 / \partial y^2 \) is the horizontal Laplacian, and the temperature field \( \nabla T(x, y) \equiv \int T(x, y, z) \, dz \) is vertically averaged. \( I_o(x, y) \) is the incident light intensity and \( a \equiv 2z_1|dn/dT| \), where \( n \) is the index of refraction of the fluid, \( z_1 \) is the optical path length from the mid-plane of the fluid layer to the image plane (in units of \( d \)), and \( dn/dT \) is evaluated at the average fluid temperature. Note that for \( M \) to be a good approximation to a more correct physical optics treatment [23] we require \( \|a \nabla^2 T\| \ll 1 \), thus \( M[\cdot] \) is only weakly nonlinear in \( T(x, y, z) \). We assume that shadowgraph measurements are of the form \( M[T]_{mn} + \epsilon_{mn} \) where \( M[T]_{mn} \) denotes the value of \( M[T(x, y, z)] \) at the location of pixel \((m, n)\), and the quantities \( \epsilon_{mn} \) denote the errors in the measurement (noise), which we take to be zero mean iid Gaussian random variables with variance \( \sigma^2 \).

Most data assimilation algorithms are iterative, cycling between a predict and update step once every time interval \( \Delta t \). In the update step, current measurements are used to update (or correct) the prediction. The predict step then propagates the updated state, via the model, to the next measurement time (i.e., it is a short term forecast). If the method works as intended, this process will closely synchronize the experiment and the model by coupling them via the measurements. The LETKF operates on this basic principle [14, 15, 16].

In order to assess how well the LETKF is performing, we will compare it to a more naive approach that we call Direct Insertion (DI). At the time \( t_j \) of the shadowgraph measurement \( I_j(x, y) \), the DI method updates the predicted temperature field \( T^p_j(x, y, z) \) by adding a correction \( \delta T_j(x, y, z) \) that is the unique field that is quadratic in \( z \), matches the boundary conditions at \( z = \pm \frac{d}{2} \), and for which the updated field \( T^u_j(x, y, z) = T^p_j(x, y, z) + \delta T_j(x, y, z) \) satisfies \( M[T^u_j(x, y, z)] = I_j(x, y) \). This gives the update

\[
\delta T_j(x, y, z) = (\bar{T}^u_j(x, y) - \bar{T}^p_j(x, y)) \left( \frac{3}{2} - 6z^2 \right),
\]

where \( \bar{T}^u_j(x, y) \) is found by solving a Poisson equation,

\[
\nabla^2 \bar{T}^u_j(x, y) = \frac{1}{a} \left[ 1 - \frac{I_o(x_c, y_c)}{I_j(x_c, y_c)} \right],
\]

and \((x_c, y_c)\) is the location of the closest pixel to \((x, y)\) that is observed. Note that with DI the velocity is not updated, \( (u^u_j(x, y, z) = u^p_j(x, y, z)) \); rather, it develops via coupling with the temperature during the simulation step. The predicted field (which has a proper \( z \)-dependence) is only slightly affected since, if the method is working properly and measurements are sufficiently frequent, the correction \( \delta T_j(x, y, z) \) is small. This method is the most successful data assimilation technique we have tested that does not use an update based on the Kalman filter. It is meant to represent what one might try without knowledge of the techniques described in Ref. [14, 15, 16].

Now we describe so-called perfect model tests in which a time series of states, generated from a Boussinesq simulation of one particular initial condition, serves as a proxy for the evolution of an experimental system whose state we wish to infer. Simulated shadowgraph measurements of this time series are generated every \( \Delta t = 1/4 \) using [24] with the parameters \( a = 0.08 \), \( I_o(x, y) = 0.5 \), and adding noise of variance \( \sigma^2 \) as previously described. Measurements are made sparse by removing shadowgraph pixels, leaving only those that lie on observation locations. We introduce the measurement density \( \rho = s/(\pi \Gamma^2) \), where \( s \) is the number of observation locations. When \( \rho \) is not small \((\rho > 5)\) we randomly and uniformly distribute observation locations over the disk; while at low density
(\(\rho \leq 5\)) the observation locations are placed on a Cartesian grid covering the disk \(x^2 + y^2 \leq \Gamma^2\) (giving more repeatable results when using sparse measurements). The observation locations are fixed for the entire data assimilation process.

We apply the LETKF and DI methods to our simulated shadowgraphs to approximately reconstruct the original time series of true states. Here we document their performance as a function of measurement noise \(\sigma\) and measurement density \(\rho\). Simulated shadowgraphs are assimilated at times \(t_j, j = 1 \ldots J\). During this process the DI and LETKF converge on an estimate of the system state (J chosen large enough to ensure convergence). At time \(t_J\) assimilation is turned off and the final updated state estimate is used as an initial condition for a long term forecast.

Performance is quantified via the RMS relative error of the temperature and mean flow, \(E_T(t) = \left[ \langle |T - \bar{T}|^2 \rangle / \langle |\bar{T}|^2 \rangle \right]^{1/2}\) and \(E_u(t) = \left[ \langle |\bar{u} - \tilde{u}|^2 \rangle / \langle |\tilde{u}|^2 \rangle \right]^{1/2}\). Here, \(T(x, y, z, t)\) and \(\bar{u}(x, y, t)\) are the true temperature and mean flow from the proxy experiment, and \(\langle \cdot \rangle\) indicates a spatial average. The fields \(T(x, y, z, t)\) and \(\tilde{u}(x, y, t)\) are the long term forecast fields from either DI or LETKF. Note that, in contrast with the case of a real physical experiment, the perfect model set-up used here has the advantageous property that the exact true fields \(\bar{u}\) and \(T\) are known and hence available for evaluating the actual error \(E_T\) and \(E_u\).

We define the ideal scenario as measuring a shadowgraph with \(\rho = 127\) (corresponding to a 451 \(\times\) 451 shadowgraph image) and \(\sigma = 0.01\) (this situation can be achieved in an experiment). Under these conditions the DI and LETKF converge on a state estimate within a few vertical diffusion times. Both DI and the LETKF are effective for estimation of the (unobserved) mean flow \(\bar{u}(x, y)\); however, the LETKF achieves an initial error \(E_u\) that is less than half that of DI. The forecast error for a typical state estimate is shown in Figs. 1 and 2. The general character of the forecasts is near-perfect agreement with the true state, followed by rapid divergence due to local error growth at the location of a defect. It is clear that the LETKF forecast is far superior to DI’s, as measured by the predictability time \(t_p\), defined as the time when the forecast error \(E_T\) first crosses the (somewhat arbitrary) value of 0.15.

Under non-ideal conditions the LETKF proves much more robust than DI. Results for sparse measurements, shown in Fig. 3, demonstrate the large range of \(\rho\) for which the LETKF converges. One can observe the existence of a critical density of observations (\(\rho \approx 1.3\)) below which it fails to converge. DI on the other hand exhibits a rapidly deteriorating forecast when even a few observation locations are removed.

We investigated performance as measurement noise was increased. The meaningful signal to noise ratio is \(\sigma_{sg}/\sigma\), where \(\sigma_{sg} = \langle I(x, y) - \langle I(x, y) \rangle \rangle\) is the RMS intensity of a typical shadowgraph (\(\sigma_{sg} = 0.123\) when \(a = 0.08\) and \(I_s(x, y) = 0.5\)). DI relies on the Poisson solve which is fundamentally insensitive to noise (it smooths the right hand side). However, this insensitivity competes with the sensitivity of the chaotic system dynamics when producing forecasts. The net result, in Fig. 4, indicates that DI forecasts are only reliable for a few vertical diffusion times when \(\sigma > 0.4\sigma_{sg}\), whereas the LETKF yields accurate forecasts up to and exceeding \(\sigma = \sigma_{sg}\).

Finally, we note that it is common for model parameters to be unknown, and that one of the advantages of the Kalman filter methodology is that it can be utilized to infer unknown system parameters from measured time series. In particular, let \(p\) denote the vector of unknown system parameters; with the model now determined by \(\xi_{j+1} = G(\xi_j, p)\). One can then introduce an extended state space vector having the form \(\gamma = [\xi \ p]^T\), where \(p\) is treated as a state variable with no time dependence. The extended model evolves as

\[
\gamma_{j+1} = \begin{bmatrix} \xi_{j+1} \\ p_{j+1} \end{bmatrix} = \begin{bmatrix} G(\xi_j, p_j) \\ p_j \end{bmatrix} = \tilde{G}(\gamma_j).
\]

By now regarding the system model as \(\tilde{G}\), estimates of
Essentially, a Kalman filter uses the model to find an optimal fitting of the current system state to current and past measurements.

FIG. 3: Comparison of DI and the LETKF; the predictability time $t_p$ is shown as the density of observations $\rho$ is reduced, demonstrating the superiority of the LETKF.

\[ \sigma = \text{[0.01, 0.05, 0.08]} \text{ for DI and } \sigma = \text{[0.01, 0.05, 0.2]} \text{ for the LETKF.} \]

In conclusion, our results support the potential effectiveness of the LETKF at estimating the fluid state in laboratory Rayleigh-Bénard convection experiments. We believe that the method we have presented is applicable to a large class of spatiotemporally chaotic systems, and offers the possibility of bridging gaps between experiment and theory in the study of spatiotemporal chaos [24].

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measurements from a laboratory Rayleigh-Bénard experiment.