CHAPTER

UNCERTAIN FORECASTS FROM DETERMINISTIC DYNAMICS

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1.1 SENSITIVITY TO INITIAL CONDITIONS, OR "CHAOS"

In a startling paper that was published more than a half-century ago, Lorenz (1963) demonstrated that solutions to systems of deterministic nonlinear differential equations can exhibit sensitive dependence on initial conditions. That is, even though deterministic equations yield unique and repeatable solutions when integrated forward from a given initial condition, integrating systems exhibiting sensitive dependence from very slightly different initial conditions eventually yields computed states that diverge strongly from each other. Twelve years later, Li and Yorke (1975) coined the name "chaotic" dynamics, although this label is somewhat unfortunate in that it is not descriptive of the sensitive-dependence phenomenon.

The system of three coupled ordinary differential equations used by Lorenz (1963), and originally derived by Saltzman (1962), is deceptively simple:

$$\frac{dX}{dt} = -10X + 10Y \tag{1.1a}$$

$$\frac{dY}{dt} = -XZ + 28X - Y \tag{1.1b}$$

$$\frac{dZ}{dt} = XY - \frac{8}{3}Z \tag{1.1c}$$

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This system is a highly abstracted representation of thermal convection in a fluid, where X represents the intensity of the convective motion, Y represents the temperature difference between the ascending and descending branches of the convection, and Z represents departure from linearity of the vertical temperature profile. Despite its low dimensionality and apparent simplicity, the system composed of Eqs. (1.1a)–(1.1c) shares some key properties with the equations governing atmospheric flow, in particular an apparently erratic behavior whose characterization is at the heart of dynamical weather prediction. Accordingly, Lorenz (1963, p. 141) concluded that his results "indicate that prediction of the sufficiently distant future is impossible by any method, unless the present conditions are known exactly. In view of the inevitable inaccuracy and incompleteness of weather observations, precise very-long-range forecasting would seem to be nonexistent."

Palmer (1993) points out that in addition to sensitive dependence, the simple Lorenz system and the equations governing atmospheric motion also exhibit regime structure, multiple distinct time scales, and state-dependent variations in predictability. Because the Lorenz system has only three prognostic variables, these three properties, as well as their sensitive dependence on initial conditions, can be visualized in terms of trajectories on the system's phase-space attractor. A phase space is an abstract geometrical space, each of the coordinate axes of which corresponds to one of the prognostic variables in a dynamical system. The phase space for the Lorenz system (Eqs. 1.1a–1.1c) is therefore a three-dimensional volume. The attractor of a dynamical system is a geometrical object within the phase space toward which trajectories are attracted in the course of time, each point on which represents a dynamically self-consistent state, jointly for all of the prognostic variables. The understanding of the specific geometry and the dynamical properties of this type of attractor is the subject of the ergodic theory of chaos and of strange attractors (e.g., Eckmann & Ruelle, 1985).

Fig. 1.1, from Palmer (1993), shows an approximate rendering of the Lorenz attractor, projected onto the X–Z plane. The figure has been constructed by numerically integrating the Lorenz system

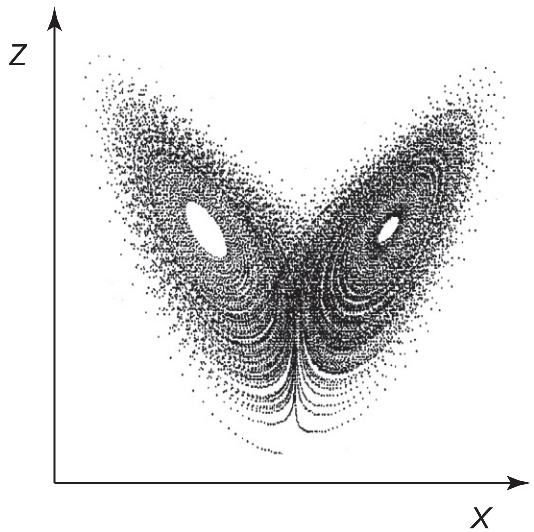

FIG. 1.1

Projection of a finite rendering of the Lorenz attractor onto the X–Z plane, yielding the Lorenz "butterfly."

From Palmer, T. N. (1993). Extended-range atmospheric prediction and the Lorenz model. Bulletin of the American Meteorological Society, 74, *49–65.*

forward for an extended time, with each dot representing the system state at a discrete time increment. The characteristic shape of this projection of the Lorenz attractor has come to be known as the Lorenz "butterfly." In a sense, the attractor can be thought of as representing the "climate" of its dynamical system, on which each point represents a possible instantaneous "weather" state. A sequence of these states then traces out a trajectory in the phase space, along the attractor.

Each wing of the attractor in Fig. 1.1 represents a regime of the Lorenz system. Trajectories in the phase space consist of some number of clockwise "laps" around an unstable fixed point of the dynamical equations on the left-hand ($X < 0$) wing of the attractor, followed by a shift to the right-hand ($X > 0$) wing of the attractor where some number of counterclockwise laps are executed around a second unstable fixed point, until the trajectory shifts again to the left wing, and so on. The transition from one wing to the other is performed in the vicinity of the third unstable fixed point of the dynamical equations. Circuits around one or the other of the wings occur on a faster time scale than residence times on each wing. The traces in Fig. 1.2, which are example time series of the X variable, illustrate that the fast

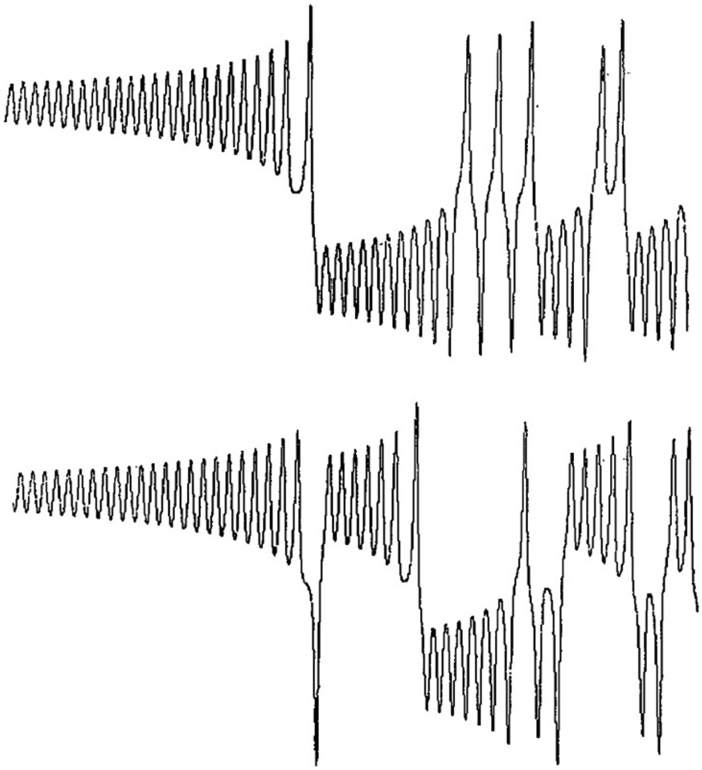

FIG. 1.2

Example time series for the *X* variable in the Lorenz system. The two time series have been initialized at nearly identical values.

From Palmer, T. N. (1993). Extended-range atmospheric prediction and the Lorenz model. Bulletin of the American Meteorological Society, 74*, 49–65.*

oscillations around one or the other wings are variable in number, and that transitions between the two wing regimes occur suddenly. The two traces in Fig. 1.2 have been initialized at very similar points, and the sudden difference between them that begins after the first regime transition illustrates the sensitive-dependence phenomenon.

An especially interesting property shared by the Lorenz system and the real atmosphere is their state-dependent variations in predictability. That is, forecasts initialized in some regions of the phase space (corresponding to particular subsets of the dynamically self-consistent weather states) may yield better predictions than others. Fig. 1.3 illustrates this idea for the Lorenz system by tracing the trajectories of loops of initial conditions initialized at different parts of the attractor. The initial loop in Fig. 1.3a, on the upper part of the left wing, illustrates extremely favorable forecast evolution. These initial points remain close together throughout the 10-stage forecast (although of course they would eventually diverge if the integration were to be carried further into the future). The result is that the forecast from any one of these initial states would produce a good forecast of the trajectory from the (unknown) true initial condition, which might be located near the center of the initial loop. In contrast, Fig. 1.3b shows forecasts for the same set of future times when the initial conditions are taken as the points on the loop that is a little lower on the left wing of the attractor. Here, the dynamical predictions are reasonably good through the first half of the forecast period, but they diverge strongly toward the end of the period as some of the trajectories remain on the left-hand wing of the attractor while others undergo the regime transition to the right-hand wing. The result is that a broad range of the prognostic variables might be forecast from initial conditions near the unknown true initial condition, and there is no way to tell in advance which of the trajectories might represent good or poor forecasts.

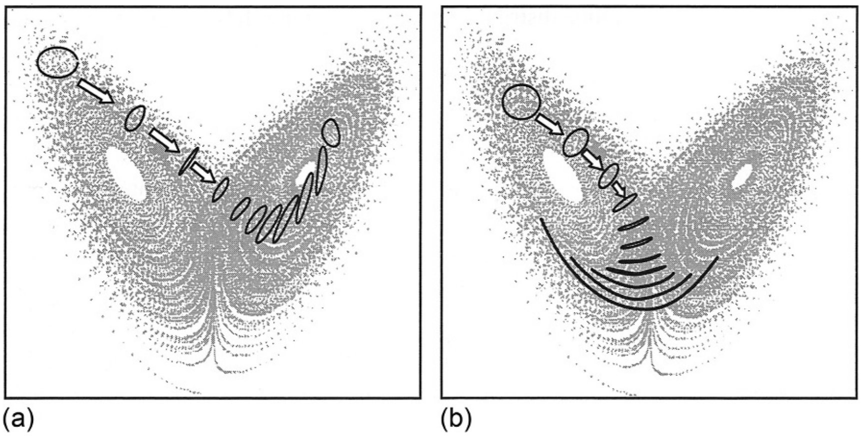

FIG. 1.3

Collections of forecast trajectories for the Lorenz system, initialized at (a) a high-predictability portion of the attractor, and (b) a moderate-predictability portion of the attractor. Any of the forecasts in panel (a) would likely represent the unknown true future state well, whereas many of the results in panel (b) would correspond to poor forecasts.

From Palmer, T. N. (1993). Extended-range atmospheric prediction and the Lorenz model. Bulletin of the American Meteorological Society, 74*, 49–65.*

This high sensitivity is related to the divergence along the unstable direction on both sides of the saddle node present at the center of the attractor. The inhomogeneity of the predictability of the flow on the attractor is a property shared by many low-order systems such as the Lorenz model, as well as by higher complexity models up to and including operational forecasting systems, as discussed in two recent reviews (Vannitsem, 2017; Yoden, 2007).

1.2 UNCERTAINTY AND PROBABILITY IN “DETERMINISTIC” PREDICTIONS

In the middle of the past century, when dynamical weather prediction was not yet an operational tool but rather a research curiosity, Eady (1951) wrote:

> [T]he initial state of motion is never given precisely and we never know what small perturbations may exist below a certain margin of error. Since the perturbations may grow at an exponential rate, the margin of error in the forecast (final) state will grow exponentially as the period of forecast is increased, and this possible error is unavoidable whatever our method of forecasting… [T]he set of all possible future developments consistent with our initial data is a divergent set and any direct computation will simply pick out, arbitrarily, one member of the set. Clearly, if we are to glean any information at all about developments beyond the limited time interval, we must extend our analysis and consider the properties of the set or “ensemble” (corresponding to the Gibbs-ensemble of statistical mechanics) of all possible developments. Thus, long-range forecasting is necessarily a branch of statistical physics in its widest sense: both our questions and answers must be expressed in terms of *probabilities*.

Of course Eady could not have been aware of what today is called chaotic dynamics, but he realized that amplification of initial-condition errors would inevitably lead to uncertainty in dynamical forecasts, and that those uncertainties should be expressed in the language of probability.

The connection between uncertainty, probability, and dynamical forecasting can be approached using the phase space of the Lorenz attractor as a low-dimensional and comprehensible metaphor for the millions-dimensional phase spaces of realistic modern dynamical weather prediction models. Consider again the forecast trajectories portrayed in Fig. 1.3. Rather than regarding the upper-left loops as collections of initial states, imagine that they represent boundaries containing most of the probability, perhaps the 99% probability ellipsoids, for probability density functions defined on the attractor. When initializing a dynamical forecast model we can never be certain of the true initial state, but we may be able to quantify that initial-condition uncertainty in terms of a probability distribution, and that distribution must be defined on the system’s attractor if the initial state is to be dynamically consistent with the governing equations. In effect, those governing equations will operate on the probability distribution of initial-condition uncertainty, advecting it across the attractor and distorting its initial shape in the process. If the initial probability distribution is a correct representation of the initial-condition uncertainty, and if the model’s equations are a correct representation of the dynamics of the true system, then the subsequent advected and distorted probability distributions will correctly quantify the forecast uncertainty at future times. This uncertainty may be larger (as represented by Fig. 1.3b) or smaller (Fig. 1.3a), depending on the intrinsic predictability of the states in the initial region of the attractor. (To the extent that the forecast model equations are not complete and correct representations of the true dynamics, which is inevitable in atmospheric modeling, then additional uncertainty will be introduced.)

Using this concept of a probability distribution that quantifies the initial-condition uncertainty, Epstein (1969) proposed the method of stochastic-dynamic prediction. The historical and biographical background leading to this important paper has been reviewed by Lewis (2014). Denoting the (multivariate) uncertainty distribution as φ and the vector $\dot{\mathbf{X}}$ as containing the total derivatives with respect to time of the prognostic variables defining the coordinate axes of the phase space, Epstein (1969) begins with the conservation equation for total probability, φ,

$$\frac{\partial \varphi}{\partial t} + \nabla \cdot \left(\dot{\mathbf{X}}\varphi\right) = 0 \tag{1.2}$$

Eq. (1.2), also known as the Liouville equation (Ehrendorfer, 1994a; Gleeson, 1970), is analogous to the more familiar continuity (i.e., conservation) equation for mass. As noted by Epstein (1969),

> It is possible to visualize the probability density in phase space, as analogous to mass density (usually ρ) in three-dimensional physical space. Note that $\rho \geq 0$ for all space and time, and $\int\int\int (\rho/M) dxdydz = 1$ if M is the total mass of the system. The "total probability" of any system is, by definition, one.

Eq. (1.2) states that any change in the probability contained within a small (hyper-) volume surrounding a point in phase space must be balanced by an equal net flux of probability through the boundaries of that volume. The governing physical dynamics of the system (e.g., Eqs. 1.1a–1.1c for the Lorenz system) are contained in the time derivatives $\dot{\mathbf{X}}$ in Eq. (1.2), also known as tendencies. Note that the integration of Eq. (1.2) is deterministic, in the sense that there are no random terms introduced on the right-hand sides of the dynamical tendencies. The Liouville equation is, in fact, the limiting case (drift-only case) of a more general approach in which stochastic diffusion forcings and jump processes are incorporated, known as the Chapman-Kolmogorov equation (e.g., Gardiner, 2009). Thus the terminology used by Epstein (1969) should not be confused with the current notion of a stochastic system.

Epstein (1969) considered that direct integration of Eq. (1.2) on a set of gridpoints within the phase space was computationally impractical, even for the idealized 3-dimensional dynamical system he used as an example. Instead he derived time-tendency equations for the elements of the mean vector and covariance matrix of φ (in effect, assuming multivariate normality for this distribution initially and at all forecast times) yielding a system of nine coupled differential equations (three each for the means, variances, and covariances), by assuming that the third and higher moments of the forecast distributions vanished. In addition to providing a (vector) mean forecast, the procedure characterizes state-dependent forecast uncertainty through the forecast variances and covariances that populate the forecast covariance matrix, the increasing determinant ("size") of which at increasing lead times can be used to characterize the increasing forecast uncertainty.

Stochastic-dynamic prediction in the phase-space in terms of the first and second moments of the uncertainty distribution, or related approaches to integration of Eq. (1.2) (Ehrendorfer, 1994b; Thompson, 1985), are even today computationally impractical when applied to realistic forecast models. Furthermore, forecasts of forecast uncertainty based on Eq. (1.2) assume that the system dynamics encoded in the elements of $\dot{\mathbf{X}}$ are correct and complete, whereas the violation of this assumption in realistic weather forecast models adds uncertainty to any forecast.

1.3 ENSEMBLE FORECASTING

Even though the stochastic-dynamic approach to forecasting as proposed by Epstein (1969) is out of reach computationally, it is theoretically sound and conceptually appealing. It provides the philosophical basis for addressing the problem of sensitivity to initial conditions in dynamical weather and climate models, which is currently best achieved through ensemble forecasting. Rather than computing the effects of the governing dynamics on the full continuous probability distribution of initial-condition uncertainty, ensemble forecasting proceeds by constructing a discrete approximation to this process. That is, a collection of individual initial conditions (each represented by a single point in the phase space) is chosen, and each is integrated forward in time according to the governing equations of the dynamical system. Ideally, the distribution of these states in the phase space at future times, which can be mapped to physical space, will then represent a sample from the statistical distribution of forecast uncertainty.

Ensemble forecasting is an instance of Monte-Carlo integration, (Metropolis & Ulam, 1949), the use of which in meteorology was foreshadowed by the quotation from Eady (1951) reproduced at the beginning of Section 1.2. Ensemble forecasting in meteorology appears to have been first proposed explicitly in a conference paper by Lorenz (1965):

> The proposed procedure chooses a finite ensemble of initial states, rather than the single observed initial state. Each state within the ensemble resembles the observed state closely enough so that the differences might be ascribed to errors or inadequacies in observation. A system of dynamic equations previously deemed to be suitable for forecasting is then applied to each member of the ensemble, leading to an ensemble of states at any future time. From an ensemble of future states, the probability of occurrence of any event, or such statistics as the ensemble mean and ensemble standard deviation of any quantity, may be evaluated.

Ensemble forecasting was first implemented in a meteorological context by Epstein (1969) as a means to provide representations of the true forecast distributions to which his (truncated) stochastic-dynamic calculations could be compared. He explicitly chose initial ensemble members as independent random draws from the initial-condition uncertainty distribution:

> Discrete initial points in phase space are chosen by a random process such that the likelihood of selecting any given point is proportional to the given initial probability density. For each of these initial points (i.e. for each of the sample selected from the ensemble) deterministic trajectories in phase space are calculated by numerical integration… Means and variances are determined, corresponding to specific times, by averaging the appropriate quantities over the sample.

Forecasts entailing more or less uncertainty are then characterized by larger or smaller ensemble variances. A more detailed exposition of the procedure was provided in the influential paper by Leith (1974).

In addition to computational tractability, an advantage of ensemble forecasting is that it permits bi- or multi-modal forecast distributions as ensemble members diverge, allowing representation of possible regime shifts. Lorenz (1965) specifically considered this attribute in his proposal for the method. In contrast, Epstein's (1969) truncated stochastic-dynamic formulation is limited in the allowed mathematical form of its predictive distributions because of its formulation in terms of distribution moments, so that only unimodal predictive distributions can be computed. This problem of multimodality was nicely addressed in the context of the atmospheric Lorenz 3-variable model through the development of a stochastic equation for the error growth by Nicolis (1992).

Both the stochastic-dynamic and ensemble approaches to representing the effects of initial-condition uncertainty initially assumed that the equations governing the physical dynamics were complete and correct. Of course, in practice dynamical weather forecast models are not perfect, and errors are introduced through spatial and temporal discretization, and through empirical formulations for unresolved processes. Pitcher (1974, 1977) represented the effects of these structural model errors through addition of random forcing terms to the prognostic equations following approaches developed in the context of stochastic modeling (e.g., Gardiner, 2009), and Leith (1974) suggested applying the same approach to ensemble forecasts.

This "stochastic parameterization" approach was first introduced into operational ensemble weather forecasting practice at the European Centre for Medium Range Weather Forecasts (ECMWF, Buizza, Miller, & Palmer, 1999), although the issue is not considered solved and research in this area is ongoing both from a practical forecasting side (e.g., Christensen, Lock, Moroz, & Palmer, 2017), and from a more theoretical perspective through the development of techniques deduced from first principles (e.g., Demaeyer & Vannitsem, 2017; Majda, Timofeyev, & Vanden Eijnden, 2001; Wouters & Lucarini, 2012).

Stochastic approaches for the representation of uncertainties are also very popular in the context of climate (e.g., Hasselman, 1976) and hydrological modeling (Bras & Rodriguez-Iturbe, 1984), due to a larger number of sources of uncertainties than in atmospheric modeling for weather forecasting. For climate modeling, many forcings influence the atmosphere that are either not fully understood or too expensive to incorporate at the current stage of development of climate models. In hydrology, both external forcings essentially coming from the atmosphere and the description of (small-scale) surface processes display important uncertainties. In both cases, these uncertainties are often best described with stochastic forcings.

1.4 POSTPROCESSING INDIVIDUAL DYNAMICAL FORECASTS

Statistical postprocessing of dynamical weather forecasts has a history that is almost as long as the history of dynamical weather forecasting itself. Operational dynamical forecasting began in 1956 in the U.S. (Fawcett, 1962), and dissemination to the public of products derived from statistically post-processed dynamical forecasts (Klein & Lewis, 1970) was initiated in 1968 (Carter, Dallavalle, & Glahn, 1989). These early forecasts were based on a technique known as "perfect prog" (e.g., Wilks, 2011), which required no training data from the dynamical model. Shortly thereafter, the preferred model output statistics (MOS, Glahn & Lowry, 1972) method began to be used when sufficient dynamical-model training data became available.

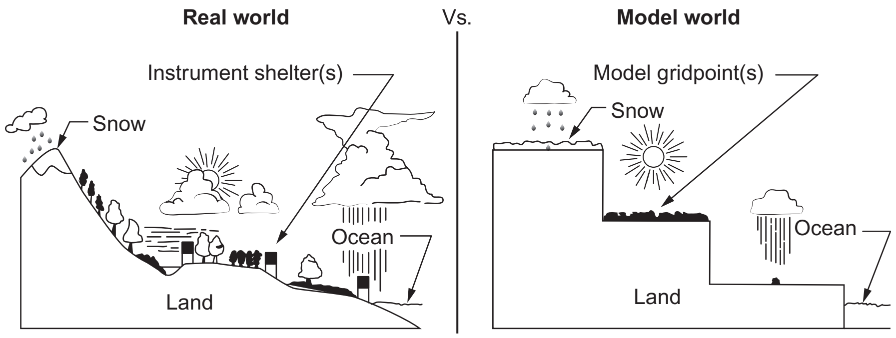

FIG. 1.4

Cartoon illustration of representativeness error inherent in making forecasts for small-scale variations in the real-world (left) on the basis of coarse grid-cell dynamical forecasts (right).

From Karl, T. R., Schlesinger, M. E., & Wang, W. C. (1989). A method of relating general circulation model simulated climate to the observed local climate. I. Central tendencies and dispersion. In: Preprints, sixth conference on Applied Climatology, American Meteorological Society *(pp. 188–196).*

The MOS approach continues to be preferred because it relates past forecasts from a particular dynamical forecast model to the subsequent weather elements of interest, and so is able to correct biases deriving from structural errors that are specific to that particular dynamical model. MOS methods also adjust for "representativeness errors," notably mismatches between grid-cell-scale dynamical forecast output and the local instrumental observations that are of primary interest to many forecast users, the correction of which is known in the climate-change literature as "downscaling" (e.g., Wilby & Wigley, 1997). These mismatches are illustrated by the cartoon in Fig. 1.4.

The original MOS forecast systems operated on the single-integration dynamical forecasts available at the time, and were nearly all structured as multiple linear regressions:

$$y_t = a + b_1 x_{t,1} + b_2 x_{t,2} + \cdots + b_m x_{t,m} + \varepsilon_t \tag{1.3}$$

where y_t, $t = 1, \ldots, n$, are the values to be predicted in a set of training data, the $x_{t,k}$ are any relevant predictor variables, and the regression coefficients b_k, $k = 1, \ldots, m$, are estimated by minimizing the sum of the squared residuals ε_t^2 over the n training samples. Often one of the predictor variables corresponds to the quantity y of interest if it is available as a prognostic variable in the dynamical model. However, due to the lower quality of the early dynamical models relative to those of the present day, these equations sometimes included 10 or more additional predictors (Glahn, 2014), such as other dynamical prognostic variables, recent surface observations, climatological values, and (trigonometric transformations of) the day of the year in order to represent some aspects of seasonality (e.g., Jacks et al., 1990).

Nearly all MOS forecasts based on single-integration dynamical forecasts were, and continue to be disseminated in nonprobabilistic formats, although some of the computations underlying these forecasts are probabilistic. For others, issued forecasts correspond to Eq. (1.3), operating on new predictor data $x_{t,k}$ with $\varepsilon_t = 0$, with no expression of uncertainty and so yielding an estimate of the conditional expectation for y given current values of the $x_{t,k}$. Although a probabilistic forecast can be constructed using Eq. (1.3), by assuming a Gaussian predictive distribution centered on y_t, with variance related to the regression mean-squared error (e.g., Glahn et al., 2009; Wilks, 2011), case-to-case (i.e., state-dependent) variations in forecast uncertainty are not represented. However, extension of this MOS concept to postprocessing of ensemble forecasts allows both correction of biases due to model errors as well as representation of variations in uncertainty based on variations in ensemble spread.

1.5 POSTPROCESSING ENSEMBLE FORECASTS: OVERVIEW OF THIS BOOK

Operational ensemble forecasting began in 1992 at both ECMWF and the U.S. National Meteorological Center (Molteni, Buizza, Palmer, & Petroliagis, 1996; Toth & Kalnay, 1993). As expected from prior research, ensemble-mean forecasts outperformed traditional high-resolution single-integration dynamical forecasts in terms of such metrics as mean-squared error, but the primary aim was to characterize and forecast the uncertainty on the basis of ensemble spread. Initially, relative frequency within each forecast ensemble was regarded as a rough estimate of the corresponding outcome probability, but it became quickly evident that these probability estimates were typically biased. In particular, the raw dynamical ensembles exhibited insufficient dispersion (e.g., Buizza, 1997; Hamill, 2001), which imparted overconfidence to their uncertainty forecasts (e.g., Wilks, 2011).

Evidently, ensemble forecasts require the same kinds of statistical postprocessing for bias correction as their traditional single-integration counterparts. Indeed, the same computer code is executed for both. But in addition, forecast ensembles require statistical postprocessing to adjust their dispersion to yield properly calibrated forecast probabilities. Ensemble-MOS methods thus aim to correct forecast errors deriving from both structural deficiencies in the dynamical models and forecast sensitivity to uncertain initial conditions. These methods began to be developed early in the present century, and a comparison among the first approaches to be proposed is provided in Wilks (2006). The past decade has seen an explosion of interest in the statistical postprocessing of ensemble forecasts, and the purpose of this book is to document the progress to date in this rapidly expanding field.

In Chapter 2, Buizza (2018) concludes the introductory section of this book by reviewing the construction of ensemble prediction systems, with a particular focus on operations at ECMWF, and underscores their need for postprocessing.

The second section of the book is devoted to exposition of the methods available for statistical postprocessing of ensemble forecasts. In Chapter 3, Wilks (2018) reviews univariate ensemble postprocessing, where forecasts for a single weather element, at one location and for one time in the future, are considered. Chapter 4, by Schefzik and Möller (2018), extends these methods for multivariate forecasts, where the postprocessed forecasts for multiple weather elements are meant to be statistically consistent with each other. Such methods are important where spatial and/or temporal coherence of the forecasts are important to the management of weather-sensitive enterprises. In Chapter 5, Friederichs, Wahl and Buschow (2018) consider the specialized perspective necessary for postprocessing forecasts for extreme, and therefore rare, events. The section concludes with the discussion in Chapter 6, by Thorarinsdottir and Schuhen (2018), of the methods of forecast verification devised specifically for evaluation of postprocessed ensemble forecasts.

Section three of this book is devoted to applications of ensemble postprocessing. Practical aspects of ensemble postprocessing are detailed by Hamill (2018) in Chapter 7, including an extended and illustrative case study. In Chapter 8, Hemri (2018) discusses ensemble postprocessing specifically for hydrological applications, where the spatial correlations among the forecast elements must be represented correctly if the forecasts are to have real-world utility. Pinson and Messner (2018) treat postprocessing in support of renewable energy applications, where the conversion of meteorological variables into power generation imposes additional challenges, in Chapter 9. Chapter 10, by Van Schaeybroeck and Vannitsem (2018), discusses postprocessing of monthly, seasonal, and interannual forecasts, which is especially difficult because for these lead times the predictable signal is typically small relative to the intrinsic uncertainty. Finally, in Chapter 11 Messner (2018) provides a guide to the ensemble-postprocessing software available in the R programming language, that should greatly help readers implement many of the ideas presented in this book.

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