An information-theoretic framework for improving imperfect predictions via Multi Model Ensemble forecasts

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Abstract
This work focuses on elucidating issues related to an increasingly common prediction technique which exploits Multi Model Ensemble (MME) forecasts in order to improve the statistical accuracy of imperfect predictions through combining information from a collection of reduced-order models. Despite some operational evidence in support of the use of the MME strategy for mitigation of model error in imperfect predictions, the mathematical framework justifying this approach is largely non-existent. In particular, it is not obvious how to measure the prediction error, which imperfect models should be included in the ensemble forecast and what weights to assign to the individual models in MME. The main emphasis of the analysis here is on uncertainty quantification and systematic understanding of the benefits and limitations associated with the MME approach, as well as on the development of practical guidelines and design principles for constructing multi model ensembles with improved predictive performance. This problem is considered within a stochastic-statistical framework which exploits tools from information theory and is capable of systematically addressing the issue of statistical fidelity of imperfect predictions. Based on these information-theoretic considerations, a simple condition is derived which guarantees improvement of statistical predictions within the MME framework relative to the single model predictions; this sufficient condition stems from the convexity of the relative entropy which is used here as a measure of the lack of information in the imperfect models relative to the resolved characteristics of the truth dynamics. Apart from considering various time-asymptotic cases, it is also shown how this sufficient condition can be practically implemented with the help of the fluctuation-dissipation theory to improve imperfect predictions of the forced response of the truth equilibrium dynamics to external perturbations. Moreover, this framework allows us to formulate and understand the necessary conditions for reducing the information barriers to predictive skill improvement via the MME approach for a given family of imperfect models; this is illustrated on a simple but revealing example in the context of forced response predictions. The general theoretical results are validated and illustrated using exactly solvable Gaussian and non-Gaussian test models.

1 Introduction
Predicting complex high-dimensional turbulent systems based on imperfect models and sparse observations of a small subset of coarse-grained system variables is a notoriously difficult problem which is, nevertheless, essential in practical applications in areas ranging from climate-atmosphere science [16, 63] to materials [12, 34], neuroscience [64], and to systems biology and biochemistry [59, 68, 14, 18, 33]. In all these scientific areas statistically accurate predictions of the coarse-grained characteristics are important for gaining insight into the characteristics of the complex truth dynamics which cannot be fully captured due to its high-dimensional, multi-scale nature. Ever since the times of von Neumann [72], increasing computing power combined with theoretical insight has allowed for developing and implementing a plethora of reduced-order models (e.g., [17, 16, 58, 63]), as well as combining the model prediction with assimilation of available measurements (e.g., [4, 32, 31, 19, 54, ?]). Various ways of minimizing the uncertainties in imperfect predictions and validating the reduced-order models have been developed (e.g., [51, 43, 52, 10, 50]). Data assimilation aside, one of the most important challenges in improving imperfect
predictions concerns the mitigation of model error in imperfect, reduced-order models of the truth dynamics (e.g., [48]). Recent theoretical developments provide new techniques aimed at improving imperfect predictions using reduced-order models, including the stochastic superparameterization approach [28, 53] and reduced subspace closure techniques [66, 67, 65]. This work focuses on elucidating issues which are related to an increasingly common technique of Multi Model Ensemble (MME) predictions, which has been particularly popular in the climate and atmospheric sciences (e.g., [62, 69, 15, 73, 74, 70, 71]). The heuristic idea behind MME prediction framework is simple: given a collection of imperfect models, consider the prediction obtained through the linear superposition of the individual forecasts in the hope of mitigating some of the errors intrinsic to the respective models. While there is some evidence in support of the MME approach to improving imperfect predictions (e.g., [69, 29, 73, 74, 71]), the systematic mathematical framework justifying this approach is essentially non-existent. In particular, it is not obvious which imperfect models should be included in the ensemble forecast and what weights to assign to the individual models in MME in order to achieve the best predictive performance in this framework; this issue is particularly problematic in practical applications. Consequently, virtually all existing operational Multi Model Ensemble prediction systems for weather and climate are based on equal-weight ensembles [29, 73, 70, 74, 71] which are likely to be far from optimal [15].

Here, we consider the problem of MME prediction within a stochastic-statistical framework which exploits tools from information theory and we focus on the fidelity of imperfect statistical predictions of the truth dynamics via the MME approach. The statistical prediction framework can be utilized in two different contexts: First, when dealing with deterministic imperfect models, one can consider a time-dependent probability density function (PDF) constructed by initializing the model from a given distribution of initial conditions. Second, the statistical prediction framework arises naturally when using stochastic reduced-order models in imperfect predictions of the resolved truth dynamics; in this increasingly common approach (e.g., [17, 61, 62, 49, 47]) aimed at mitigating model error in reduced-order modeling of high-dimensional, multi-scale, turbulent systems the issue of quantifying discrepancies between different PDFs arises naturally, even for deterministic initial conditions. The use of statistical descriptions is not new and goes back to early predictability studies for simplified atmosphere models [39, 40, 41, 17]. The main focus of the present work is on a systematic understanding of the benefits and limitations associated with the Multi Model Ensemble approach to imperfect predictions, as well as on the development of guidelines and design principles for constructing the MME with improved predictive performance in practical situations; the important topical issues in this context are the following:

1. **What are the advantages/disadvantages of the MME framework relative to using a single model predictions with an ensemble of initial conditions?** In particular,
   - Is there a condition guaranteeing the improvement of prediction skill (i.e., statistical accuracy) of MME predictions relative to the single model predictions? What tests need to be carried out to clarify what approach is better in which circumstances?
   - How to measure the skill of MME predictions relative to the single model predictions?

2. **How to construct the MME for best prediction skill at short, medium and long time ranges?** Additionally,
   - Can one particular MME have best predictive skill at all ranges?
   - What characteristics of the MME, if any, lead to uncertainty reduction relative to the single imperfect model?
   - Does combining imperfect models with different equilibria or different sensitivities to external perturbations help improve the prediction skill?

The goal of this paper is to set out an information-theoretic framework capable of addressing the above issues in a systematic fashion; in particular, we focus on

1. quantification of uncertainty and improving the imperfect predictions via the MME approach;
2. providing practical guidelines for constructing the best possible Multi Model Ensemble given a small collection of available models.
The latter issue is particularly important in applications since most operational forecasts can be obtained, in the best case scenario, through a weighted superposition of individual forecasts from imperfect models which are not easily tunable (e.g., [29, 73, 70, 74, 71]). Although we focus here on mitigating model error through the Multi Model Ensemble forecasting, it is worth stressing that the ultimate goal in imperfect reduced-order prediction should involve a synergistic approach that combines MME forecasting, data assimilation, and improving individual models through various stochastic parameterization, and reduced subspace closure techniques as mentioned above. In this work we show that, despite many important subtleties, it is possible to obtain relatively simple conditions which guarantee gain in skill of statistical predictions within the MME framework. These conditions stem from the information-theoretic approach to the prediction problem and they exploit the convexity of relative entropy (e.g., [49, 13]) which is used here as a measure of the lack of information in the imperfect models relative to the resolved characteristics of the truth dynamics. We show that these conditions can be practically implemented with the help of the fluctuation-dissipation theorem (e.g., [49, 38, 2, 44, 27, 52, 42]) when considering improvements in imperfect prediction of the forced response of the truth equilibrium dynamics to external perturbations. Practical implementation of the condition for skill improvement through MME in the context of the initial value problem is more involved but we show how techniques similar to those discussed in [23, 24, 25] could be used to effectively evaluate this condition. The use of information theory and the fluctuation-dissipation theorem in the context of improving imperfect predictions in the presence of model error has been extensively studied recently in the 'single model' setup (see, for example, [35, 45, 36, 51, 43, 22, 10, 50]); here we extend this framework to the Multi Model Ensemble case which provides a concise and much needed mathematical framework for assessing the predictive skill improvement through the MME approach.

This paper is structured as follows: First, in section 2 we provide some motivation for more systematic analysis; this is done with the help of two simple examples illustrating common characteristics of MME prediction, including the dependence of the MME skill on the characteristics of individual models in the ensemble, as well as the sensitivity of the MME skill to the unresolved truth dynamics. In section 3 we derive the sufficient condition for improving the skill of MME predictions relative to single model predictions; this is achieved through some simple convexity arguments by extending the information-theoretic framework for improving imperfect predictions to the MME configuration. A set of particularly useful results is derived and discussed in §3.3 in the Gaussian framework which utilizes Gaussian models in the Multi Model Ensembles; this approach provides useful intuition and guidelines in more complex cases for the general results of §3. Section 5 combines the analytical estimates of §3 with simple numerical tests based on statistically exactly solvable models described in §4. We conclude in §6 by summarizing the most important results and discuss directions for further research in this area, including extensions to multi model approach to data assimilation. Finally, the technical details associated with the analytical estimates derived in §3 are presented in extensive Appendices.

2 Motivating examples

In order to focus attention and motivate the subsequent analysis of the performance of MME predictions, we consider two examples of imperfect statistical predictions of the truth dynamics using reduced-order models; more precisely, we attempt to predict - in a statistically accurate fashion - the evolution of the resolved characteristics of the truth dynamics using one or more imperfect reduced-order models which approximate or neglect the interaction between the resolved and unresolved dynamics. In general, the dynamics of high-dimensional, multi-scale systems for the resolved dynamics of sufficiently large-scale and low-frequency processes is affected by unresolved processes which cannot be directly observed or even correctly modeled (e.g., [46]). As already discussed in the Introduction, we focus here solely on the possibility of mitigating model error in imperfect predictions via the MME approach; that is, we do not consider improving the individual imperfect models.

Assume that the state vector of dynamical variables in the true high-dimensional system decomposes as \( \mathbf{v} = (\mathbf{u}, \mathbf{v}) \), where \( \mathbf{u} \in \mathbb{R}^K \) denotes the resolved variables and \( \mathbf{v} \in \mathbb{R}^N \) denotes the unresolved variables;
we tacitly assume that $K \ll N$ and $K + N \gg 1$ which is natural when considering turbulent dynamical systems such as geophysical flows (e.g., [46]). Moreover, we assume that the truth dynamics has a statistical equilibrium state which is sufficiently complex to be described by a probability density function that is smooth at least in the subspace of resolved dynamical variables $u$. The lack of information at time $t$ between the MME and the truth statistics on the resolved subspace of variables $u$ by using the the Multi Model Ensemble (MME) of imperfect models with the probability density given by the linear convex superposition of the individual imperfect model densities

$$\pi^\text{MME}_t(u) = \sum_{i=1}^{\mathcal{M}} \alpha_i \pi^m_i(u), \quad \int du \pi^\text{MME}_t(u) = 1, \quad \sum_{i=1}^{\mathcal{M}} \alpha_i = 1, \alpha_i \geq 0,$$

where $\pi^m_i$ represent probability densities associated with the imperfect models $m$ in some class $\mathcal{M}$ of available models. The lack of information at time $t$ between the MME and the truth statistics on the resolved subspace of variables is measured using the relative entropy

$$\mathcal{P}(\pi_t, \pi^\text{MME}_t) = \int du \pi_t \ln \frac{\pi_t}{\pi^\text{MME}_t}.$$  

This is a well-known information-theoretic functional with metric-like properties including non-negativity and the fact that $\mathcal{P}(\pi_t, \pi^\text{MME}_t) = 0$ only when $\pi_t = \pi^\text{MME}_t$ (e.g., [37, 49, 10, 50]); moreover, the relative entropy is invariant under general changes of variables [45, 46] which is a desirable property for a measure of model uncertainty in practical applications involving various physical quantities.

The following general questions arise in the context of improving imperfect predictions via the MME approach:

- What characteristics of MME lead to uncertainty reduction relative to the single imperfect model?
- How to measure the improvement in the skill of MME predictions relative to single model predictions?
- Can a single MME provide the optimal skill improvement at all time ranges?
- How to construct MME for best prediction at short, medium and long ranges?
Figure 2: Dependence of the prediction skill improvement via MME approach on the nature of the resolved and unresolved non-Gaussian truth dynamics (given by (39) in §4.2); the MME mixture density in (1) contains Gaussian models (23) with correct initial conditions and correct second-order marginal equilibrium statistics. (Left) Example of model error via relative entropy in (2) for predicting the resolved non-Gaussian dynamics with symmetric fat-tailed equilibrium density starting from initial conditions in a stable regime of the truth dynamics. (middle) Example of model error for predicting the resolved non-Gaussian dynamics with symmetric equilibrium density starting from initial conditions in an unstable regime, (right) Model error for predicting the resolved non-Gaussian dynamics with skewed equilibrium density starting from initial conditions in a stable regime. The bottom insets show the weights in the equal-weight and optimal weight MME; the optimal-weight MME is determined by minimizing the relative entropy in (2) for all time by adjusting weights in the ensemble. Note that the structure of the optimal MME and the benefits of using the MME approach depend strongly on the nature of the marginal truth dynamics.

The issues of improving predictions of a single imperfect model within the information-theoretic framework used here were discussed in [43, 52, 47, 10, 50]. In the remainder of this paper we show that the information-theoretic approach to the imperfect prediction problem is very useful in the MME context as well and, despite many important subtleties discussed in the subsequent sections, it is possible to obtain a relatively simple condition which guarantees a gain in skill of statistical predictions within the MME framework. However, before embarking on the detailed analysis some motivating examples are presented below.

In figures 1 and 2 we illustrate two different scenarios of evolution of model error in imperfect statistical predictions of partially observed truth dynamics; the model error is quantified via the relative entropy (2) and the predictions are carried out using a single imperfect model or MME with correct statistical initial conditions and correct equilibrium statistics. The first example in figure 1 shows the dependence of model error on the structure of the MME which is encoded in the characteristics of the imperfect models used in the ensemble. The second example, shown in figure 2, illustrates a subtle interplay between the potential gain in predictive skill due to the MME approach and the nature of the truth dynamics and, in particular, its unresolved component All of these issues are discussed in detail in the following sections (see, in particular, §3 and §5).

Figure 1 shows that not every MME prediction is superior to the single model predictions. In the three insets shown in this figure both the truth dynamics and the imperfect models are linear and Gaussian with correct statistical initial conditions and correct marginal statistical equilibrium of the resolved dynamics $u(t)$. However, the Gaussian truth dynamics in this example is two-dimensional and it linearly couples the resolved and unresolved processes, $u(t)$ and $v(t)$, while the imperfect predictions of the resolved dynamics are carried out using Gaussian models which neglect the coupling between the resolved and unresolved variables. (The model used to generate the ‘truth’ dynamics is described later in §4.1 and the reduced-order imperfect Gaussian models are described in §3.3.) Model error in 9-member MME

\[ \tau^{\text{truth}} \]
prediction is computed via the relative entropy \( \mathcal{P}(\pi_t, \pi_t^{\text{MME}}) \) in (2) for the marginal statistics of the resolved variable \( u(t) \). Here, the optimal-weight MME (magenta) is determined by minimizing the lack of information in (2) between the truth and the MME for all time by adjusting weights \( \alpha_i \) in the mixture density (1) which contains models \( M_i \) with different correlation times, \( \tau_M^i \), for the resolved dynamics (see §4.3 and (44) for details): in the first configuration (left inset in figure 1) all models \( M_i \) in MME have longer correlation times (i.e., \( \tau_M^i > \tau_M^0 \)) than the single model \( M_0 \) (green) which has correct correlation time for the resolved dynamics, i.e., \( \tau_M^0 = \tau_{\text{truth}} \); in the second case (middle inset) the correlation times of the imperfect models in the MME are evenly distributed around the correct correlation time; finally, in the last case (right inset in figure 1) all imperfect models have shorter correlation times (i.e., \( \tau_M^i < \tau_M^0 \)) than the single model with correct correlation time. Clearly, the potential predictive skill gain within the MME framework is sensitive to the structure of the ensemble relative to the single model; in the particular case shown in figure 1 there is no predictive skill gain due to MME approach when using ensembles of imperfect models with correlation times smaller than the correlation time of the single imperfect model.

While the trend for improvement of prediction skill through the use of MME consisting of underdamped imperfect models (\( \tau_M^i > \tau_M^0 \)) appears to be relatively common, the general case is much more subtle. Figure 2, which motivates the need for more detailed analysis (see §3 and §5), illustrates the evolution of model error via the relative entropy (2) in predictions of more complex nonlinear and non-Gaussian dynamics; the model used to generate the non-Gaussian ‘truth’ in this example is described later in §4.2 and it is used in more detailed numerical tests in §5. In this case the predictive performance varies depending on the characteristics of the truth dynamics rather than on the structure of MME. As in the previous example, the statistical initial conditions and the marginal equilibrium for the resolved dynamics in the imperfect models \( M_i \) are correctly tuned; however, the correlation times \( \tau_M^i \) in the MME models are symmetrically distributed about the correct correlation time \( \tau_{\text{truth}} \) (as in figure 1b). The difference between the configuration in figure 2a and 2b lies in the initial statistical conditions for the unresolved dynamics. In figure 2b the initial conditions in the unresolved dynamics are far from the (globally stable) statistical equilibrium which induces a rapid transient in the truth dynamics accompanied by a phase of intermittent instabilities in the path-wise dynamics (see [10] for more details), while the configuration in figure 2a corresponds to the evolution of the truth from initial conditions which are much closer to the stable statistical equilibrium of the truth dynamics. The last configuration shown in figure 2c shows model error in imperfect predictions of the resolved non-Gaussian dynamics in the case when the truth equilibrium statistics is significantly skewed in the resolved subspace. Note that the skill of MME prediction (blue and magenta) relative to the single model prediction (green) varies significantly depending on the properties of the truth dynamics; moreover, in the configurations (b) and (c), the optimal MME (magenta) obtained by minimizing the model error through adjusting the weights in (1) contains only models with short correlation times \( \tau_M^i \leq \tau_M^0 \) which is different than the case shown in figure 1; in fact, the case in figure 2c has only a single model in the optimal MME. Clearly, the benefits of using the MME approach for improving imperfect predictions depend on both the structure of MME and on the nature of the truth dynamics.

The above examples highlight the fact that more analytical insight is necessary for understanding the essential features of the Multi Model Ensemble (MME) method for prediction and the conditions for obtaining improved predictions through such an approach. In the next section we focus solely on this topic and we obtain a general sufficient condition for prediction improvement via the MME approach; this sufficient condition involves the information-theoretic measure of the model error in imperfect statistical predictions given by the relative entropy in (2) and the derivation exploits the convexity of the relative entropy with respect to the imperfect model density. The general theoretical results derived in §3 are discussed further in §5 based on two simple but revealing test models described in §4.

3 Information-theoretic estimates of the predictive skill of MME

Here, we present the general framework for assessing the potential improvement of predictive skill through the Multi Model Ensemble (MME) approach; the information-theoretic framework for improving imperfect single-model predictions was discussed in [43, 52, 47, 10, 50]. All the estimates within this analytical
framework exploit the convexity of the relative entropy (2) between the truth and the MME density in (1); the relative entropy represents an information-theoretic measure of lack of information in the model density relative to the truth (e.g., [13, 49]). First, in §3.1 we derive the sufficient condition for improving the predictive skill via MME; it turns out that this condition requires evaluating only certain least-biased estimates of the truth which makes it more practical in applications, especially when considering improvements of the forced response prediction via the MME approach. Subsequently, in §3.2 we discuss the insight provided by the general condition and its implications for both the initial value problem and forced response prediction; more insight can be gained by restricting the problem to the Gaussian mixture MME which is discussed in §3.3. Further details, along with some simple proofs of the facts established below, are relegated to Appendix A.

3.1 Improving predictions through MME framework

We are interested in improving the imperfect statistical predictions the truth dynamics on the subspace of resolved variables $u \in \mathbb{R}^K$ by using the the Multi Model Ensemble (MME) with density given by (1); the full vector dynamical variables is denoted by $v = (u, v)$, where $v \in \mathbb{R}^N$, $N \gg K$, denotes the unresolved variables in the high-dimensional phase space with $N + K \gg 1$. As in §2, we assume that the truth dynamics has a statistical equilibrium state which is sufficiently complex to be described by a non-trivial probability density function denoted by $p_t(\pi)$ and the corresponding marginal density on the resolved subspace is $p_t(u) = \int p_t(\pi, u, v)dv$. Given some class $\mathcal{M}$ of reduced-order models for the resolved dynamics $u(t)$, the best single model, $M_\ast$, for making predictions at time $t$ is given by

$$P(\pi, \pi^M) = \min_{M \in \mathcal{M}} P(\pi, \pi^M),$$

where $\pi_t^M$ represents the probability density associated with models $M \in \mathcal{M}$, and the relative entropy $P(\pi_t, \pi^M)$ measures the lack of information in $\pi^M$ relative to the truth marginal density $\pi$ (see [51, 43, 52, 10, 50]). Similarly, the best single model $M^\ast \in \mathcal{M}$ for making predictions over the time interval $[0, T], T \neq 0$, is given by

$$P_T(\pi, \pi^M) = \min_{M \in \mathcal{M}} P_T(\pi, \pi^M),$$

where $P_T(\pi, \pi^M) = \frac{1}{T} \int_0^T P(\pi, \pi^M)dt$ measures the net lack of information over the time interval $[0, T]$. In general $M_\ast$ and $M^\ast_T$ are not the same which has important consequences for the robustness of MME predictions as outlined below. Given the definitions (3) and (4), we will refer to $P(\pi, \pi^M)$ as the local-in-time information barrier, and to $P_T(\pi, \pi^M)$ simply as the information barrier associated with the class of models $\mathcal{M}$ (see [52, 48, 50] for more details); these information barriers correspond to the minimum lack of information in the imperfect predictions achievable within the given class of models $\mathcal{M}$.

In order to systematically study the performance of the MME prediction relative to the single-model prediction, we introduce the following measures of information gain through the MME framework relative to the single imperfect model $M_0 \in \mathcal{M}$:

$$a) \, P_{M, t}^{MME, M_0} = P(\pi, \pi^M) - P(\pi, \pi^{M_0}), \quad b) \, P_{M, t}^{MME, M_0} = \frac{1}{T} \int_0^T \left( P(\pi, \pi^M) - P(\pi, \pi^{M_0}) \right) dt;$$

note that the imperfect model $M_0$ does not have to coincide with the best (imperfect) models $M^\ast$ or $M^\ast_T$, which are both unknown in practice. We say that the MME prediction at time $t$ is more skillful than the single model prediction using $M_0$ when $P_{M, t}^{MME, M_0} < 0$, and that MME prediction is more skillful over the time interval $[0, T]$ if $P_{M, t}^{MME, M_0} < 0$.

The two useful facts stated below in the context of MME prediction are a direct consequence of the convexity of the relative entropy in (2) in the second argument (e.g., [13, 49])

$$P(\pi, \sum a_i \pi_i) \leq \sum a_i P(\pi, \pi_i), \quad a_i \geq 0, \, \sum a_i = 1.$$
FACT 1. Assume that $M^*$ is the best model in the sense (3) within the class $M$ of available models for the resolved dynamics $u(t)$. Unless $M^*$ is the perfect model for the resolved dynamics, the predictive skill in (5a) of MME with $\{M_i\} \in M$ can be superior to the skill of the best single model $M^*$, i.e., $\mathcal{F}_{a,M,t}^{MME,M^*} < 0$. Similarly, given the best imperfect model $M^*_T$ in the sense (4) for predicting the resolved truth dynamics over the interval $[0 \ T]$, the MME prediction can be superior to the predictive skill of $M^*_T$, i.e., $\mathcal{F}_{a,M,T}^{MME,M^*} < 0$.

FACT 2. Consider the optimal-weight MME for a given class $M$ of imperfect models which is defined analogously to the best single model $M^*$ in (3) or $M^*_T$ in (4), so that

$$
\mathcal{P}(\pi_t, \pi_t^{MME*}) = \min_\alpha \mathcal{P}(\pi_t, \pi_t^{MME}), \quad \mathcal{P}_T(\pi, \pi^{MME*}_T) = \min_\alpha \mathcal{P}_T(\pi, \pi^{MME}_T),
$$

where $\alpha$ is the vector of weights in the MME mixture density (1) containing the models $m \in M$. Improving the skill of imperfect predictions via the MME approach is not equivalent to reducing the single model information barriers, $\mathcal{P}(\pi_t, \pi_t^{M_0})$ in (3) or $\mathcal{P}_T(\pi, \pi^{M_0})$ in (4), for the given class of imperfect models $M$. Moreover, if the predictive skill cannot be improved within the MME framework, then either $\pi_t^{MME} = \pi_t^{M^*}$ or $\pi_t^{MME*} = \pi_t^{M^*_T}$, and the model error of the optimal-weight MME (7) is equal to the respective information barrier for single model prediction.

Simple justification of the above facts is illustrated in figure 3 and it follows immediately from the convexity of the relative entropy in (6). Fact 1 becomes obvious upon considering the configuration in figure 3a and noticing that the prediction error via the relative entropy (2), $\mathcal{P}(\pi_t, \pi_t^{M_0})$ or $\mathcal{P}_T(\pi, \pi^{M_0})$, in the single model prediction with model $M_0$ can be reduced in MME prediction, provided that $M_0 \neq M^*$ or $M_0 \neq M^*_T$ respectively. Fact 2 is established by considering the two distinct configurations in figures 3a and 3b. In both cases the error, $\mathcal{P}(\pi_t, \pi_t^{M_0} + \pi_t^{M^*})$, in the MME prediction containing imperfect models $M_0 \neq M^*$ and $M_1$ is smaller than the error, $\mathcal{P}(\pi_t, \pi_t^{M^*})$, in the single model prediction. However, in the configuration shown in figure 3b the MME information barrier (7) at time $t$ (gray shaded) is the same as that of the single model prediction and equal to $\mathcal{P}(\pi_t, \pi_t^{M_1})$, while the MME information barrier of MME at $t$ (magenta shaded) is reduced to $\mathcal{P}(\pi_t, \pi_t^{M_0} + \pi_t^{M^*}) < \mathcal{P}(\pi_t, \pi_t^{M^*})$. Clearly, the choice of the imperfect models in MME is important for its improved performance over the single model $M_0$. (Examples of prediction improvement via MME without reducing the single model information barrier are shown in different configurations in figures 2c, 4, 5, 8 and 11; these are discussed in the subsequent sections.)

A more intricate issue which is related to the above general facts and is important in practical prediction problems concerns:

(i) the assessment of prediction improvement for a given MME containing a discrete collection $\{M_i\} \in M$ of imperfect models,

(ii) the issue of constructing MME given a class $M$ of tunable imperfect models in a way that would guarantee the improvement in predictions in the absence of the knowledge of the truth.

It turns out that a significant insight into the above issues and practical techniques can be derived within the information-theoretic framework by exploiting the convexity of the relative entropy in (6) which leads to the following simple and sufficient condition for improving imperfect statistical predictions at time $t$ via the MME approach relative to the statistical predictions with single model $M_0$

$$
\mathcal{P}(\pi_t, \pi_t^{M_0}) > \sum_{i \neq 0} \beta_i \mathcal{P}(\pi_t, \pi_t^{M_i});
$$

assuming that $M_0, M_i \in M$, the weights in (8) are related to the weights $\alpha_i$ in the MME mixture density $\pi_t^{MME}$ in (1) via

$$
\beta_i = \frac{\alpha_i}{1 - \alpha_0}, \quad \sum_{i \neq 0} \beta_i = 1.
$$

One should note that the true marginal density $\pi_t$ in (8) is generally not known; however, it is shown in Appendix A that the condition (8) can be rewritten as

$$
\mathcal{P}(\pi_t^L, \pi_t^{M_0}) > \sum_{i \neq 0} \beta_i \mathcal{P}(\pi_t^L, \pi_t^{M_i}),
$$

\[8\]
Figure 3: Illustration of the convexity of the relative entropy $P$ used to obtain estimates on the performance of the Multi Model Ensembles (MME) for improving imperfect statistical predictions of the truth dynamics with probability density function $\pi_t$. The schematic geometry for fixed time is sketched in two distinct cases depending on the class of available imperfect models $\mathcal{M}$ with the best model $m_*$. In both cases the predictive skill of the single model $m_\diamond$ can be improved via MME containing imperfect models $m_\diamond$ and $m_1$. However, in b) the information barrier of MME at time $t$ (gray shaded) is the same as that of the single model predictions and equal to $P(\pi_t, \pi_{m_*}^t)$, while in a) the information barrier of MME $\{m_\diamond, m_1\}$ at $t$ (magenta shaded) is reduced to $P(\pi_t, \pi_{m_\diamond}^t + \pi_{m_1}^t) < P(\pi_t, \pi_{m_*}^t)$.

Note also that the model error of MME cannot exceed the worst model in the ensemble.

where now $\pi_t^l$ is the practically measurable, least-biased density (see, e.g., [49, 43, 52, 10]) associated with the marginal truth dynamics which maximizes the Shannon’s entropy given $l$ moment constraints at time $t$ (see [57, 49] and (11) below); this fact is particularly useful when considering the improvement of the forced response prediction from equilibrium $\pi_{eq}$, since in such a case the least-biased densities, $\pi_{eq}^l$, in (10) can be directly estimated based on the fluctuation-dissipation theorem (see Appendix D and [49, 2, 44, 26, 27, 52, 42]) and the model densities, $\pi_{m_1}^{\mathcal{M}_1}$, are known.

### 3.1.1 Sufficient condition for prediction improvement via MME exploiting the least-biased density representation

It turns out that a significant insight can be gained by representing the condition (10) through the least-biased densities of the imperfect models in MME (1); the least-biased density $\pi_t^l$ of the true density $\pi$ given a set of $L$ statistical constraints is a member of the exponential family of densities which maximizes
the Shannon entropy $S = - \int \pi^i \ln \pi^i$ subject to (e.g., [49, 57])

$$\int \pi^i(u)E_i(u)du = \int \pi(u)E_i(u)du, \quad i = 1, \ldots, L,$$

where $E_i$ are some functionals on the space of the resolved variables $u$; here we assume these functionals to be $i$-th tensor power of $u$, i.e., $E_i(u) = u^\otimes i$, so that their expectations yield the components of the first $L$ statistical moments of $\pi$ about the origin. Consequently, the least-biased densities of the truth and of the imperfect models are given by (e.g., [49, 1, 57, 51])

$$a) \quad \pi^{i^1}_t = C^{-1}_t \exp \left(- \sum_{i=1}^{l_1} \theta_i(t)E_i(u) \right), \quad b) \quad \pi^{M,12}_t = (C^M_t)^{-1} \exp \left(- \sum_{i=1}^{l_2} \theta^M_i(t)E_i(u) \right),$$

where the normalization factors $C_t$ and $C^M_t$ are chosen so that $\int \pi^{i^1}_t du = \int \pi^{M,12}_t du = 1$. We denote the expected values of the functionals $E_i$ in (11) with respect to $\pi^{i^1}_t$ as $\bar{E}_t$ and with respect to $\pi^{M,12}_t$ as $\bar{E}^M_t$; it is convenient to write these expectations in the vector form as

$$a) \quad \bar{E} = \left( \bar{E}_1, \ldots, \bar{E}_{L_1} \right)^T, \quad b) \quad \bar{E}^M = \left( \bar{E}^M_1, \ldots, \bar{E}^M_{L_2} \right)^T;$$

note that $\theta_t = \theta(\bar{E}_t)$ and $\theta^M_t = \theta^M(\bar{E}^M_t)$ in (11) so that the normalization factors in the least-biased densities are functions of the time-dependent statistical moments, i.e, $C_t = C(\bar{E}_t)$ and $C^M_t = C^M(\bar{E}^M_t)$.

Based on the least-biased representations (11) of the truth and model probability densities, the sufficient condition (10) for improvement of imperfect predictions via the MME approach can be written in a form which is particularly suited for further approximations (see Appendix A for a simple proof):

**FACT 4.** The sufficient condition (10) for improvement of the forced response prediction via MME can be expressed in terms of the least-biased densities (11) as

$$\mathcal{A}_\alpha \left( \pi^{i^1}_t, \left\{ \pi^{M,12}_t/\pi^{i^1}_t \right\} \right) + \mathcal{B}_\alpha \left( \left\{ \bar{E}^M_t \right\} \right) + \mathcal{C}_\alpha \left( \bar{E}_t, \left\{ \bar{E}^M_t \right\} \right) > 0,$$

where

$$\mathcal{A} = \int du \pi^{i^1}_t(u) M(u), \quad M(u) = \sum_{i\neq j} \beta_i \left[ \log \frac{\pi^{M,12}_t(u)}{\pi^{i^1}_t(u)} - \log \frac{\pi^{M,12}_t(u)}{\pi^{i^1}_t(u)} \right],$$

is non-zero only when some of the model densities are not in the least-biased form, i.e., $\pi^{M,12}_t \neq \pi^{i^1}_t$ for some $i$, and

$$\mathcal{B}_\alpha = \sum_{i\neq j} \beta_i \left[ \log C^{M,12}_t \left( \bar{E}^M_t \right) - \log C^{M,12}_t \left( \bar{E}^M_t \right) \right], \quad \mathcal{C}_\alpha = \sum_{i\neq j} \beta_i \left[ \theta^{M} - \theta^{i^1}_t, \bar{E}_t \right],$$

where the weights $\beta_i$ are defined in (9) and the vectors of the Lagrange multipliers are given by

$$\theta = \left( \theta_1, \ldots, \theta_{L_1} \right)^T, \quad \theta^M = \left( \theta_1, \ldots, \theta_{L_2}, 0, \ldots, 0 \right)^T, \quad \text{if } L_1 \geq L_2,$$

$$\left( \theta_1, \ldots, \theta_{L_2} \right)^T, \quad \text{if } L_1 < L_2.$$

**Remarks:**

- The second term, $\mathcal{B}_\alpha$, in (13) is independent of the truth density and involves only the model densities, $\pi^{M}_t$, in MME.
- The last term, $\mathcal{C}_\alpha$, in (13) depends linearly on the expectations, $\bar{E}_t$, with respect to the least-biased truth density $\pi^{i^1}_t$; these can be estimated from the ‘fluctuation-dissipation’ formulas when considering the skill improvement of the forced response predictions, as discussed below in §3.2 and Appendix D.
- The expected value in $\mathcal{A}_\alpha$ can be evaluated as long the least-biased approximation, $\pi^{i^1}_t$, of the truth $\pi_t$ is known. Moreover, if the MME contains only least-biased models $\mathcal{A}_\alpha = 0$.

We will exploit the consequences of the above result extensively in the following sections; the main advantage of the above ‘least-biased’ representation of the condition (10) lies in the fact that it depends explicitly and linearly on the statistical moments $\bar{E}_t$ of the truth which are, in principle, amenable to approximations and estimates through the fluctuation-dissipation formulas when considering the forced response prediction (see [49, 2, 44, 26, 27, 51, 43, 52, 42], as well as §3.2 and Appendix D).
3.1.2 Formal guidelines for constructing MME with superior predictive skill relative to the single model predictions

The formula in (10) or its alternative, ‘least-biased’ density representation (13) provide sufficient conditions for the MME with density $\pi_t^{\text{MME}}$ in (1) to have an improved predictive skill relative to the single model $\pi_t^{M_0}$. However, the following issues need to be addressed in this framework in order to allow for practical applications:

- the conditions (10) or (13) can be used to assess the skill improvement for a given MME but do not provide direct guidelines for constructing MME,
- evaluating (10) or (13) requires the knowledge of the $L$-measurement time-dependent estimates of the marginal truth density $\hat{\pi}_t$.

Here, we consider a perturbative approach aimed at elucidating the sufficient conditions (10) or (13) for skill improvement through MME relative to the single ‘reference’ model $M_0$. First, we consider this issue in terms of arbitrary model densities $\pi_t^M$. While this representation provides a simple form of the condition (10), the perturbations of the probability densities representing the evolution away from the initial conditions are difficult to interpret or approximate. Thus, we subsequently consider the same problem starting from the least-biased density representation in (13) which is linear in the statistical moments of the truth (see FACT 5). While this representation is not always possible [57, 6], except in the Gaussian setting, its advantage lies in the fact that the changes in the statistical moments can be estimated more easily, especially when considering the forced response prediction of the equilibrium dynamics subjected to small external perturbations (see [51, 43, 52], §3.2, §3.3.2 and Appendix D).

Consider a Multi Model Ensemble with mixture density $\pi_t^{\text{MME}}$ in (1) created by perturbing a single model density $\pi_t^{M_0}$ so that

$$\pi_t^M(u) = \pi_t^{M_0}(u) + \epsilon \hat{\pi}_t^M(u), \quad \epsilon \ll 1, \quad \int \pi_t^M(u) du = 0,$$

for each ensemble member $M_i \in \mathcal{M}$; existence of such perturbations which are non-singular (smooth at $\epsilon = 0$) was shown to exist under minimal assumptions in [30]. Now, we rewrite the relative entropy $\mathcal{P}(\pi_t^M, \pi_t^M)$ in (10) as

$$\mathcal{P}(\pi_t^M, \pi_t^M) = \mathcal{P}(\pi_t^M, \pi_t^{M_0} + \epsilon \hat{\pi}_t^M) = \mathcal{P}(\pi_t^M, \pi_t^{M_0}) - \epsilon \int du \frac{\pi_t^M}{\pi_t^{M_0}} \hat{\pi}_t^M + \mathcal{O}(\epsilon^2),$$

which, when combined with (10), yields the sufficient condition for prediction improvement through MME in the following form

$$\epsilon \sum_{i \neq \phi} \beta_i \int du \frac{\pi_t^M}{\pi_t^{M_i}} \hat{\pi}_t^{M_i} + \mathcal{O}(\epsilon^2) > 0, \quad (15)$$

with the weights $\beta_i$ are defined in (9); the interested reader should consult [43, 52, 47] for a related perturbative treatment of the predictive skill in the single imperfect model configuration. It is worth stressing that the least-biased estimate of the truth, $\pi_t^M$ given by (11a), can be realistically estimated only on the attractor which is exploited when assessing the MME prediction improvement for the forced response (see §3.2, §3.3.2 and Appendix D).

A more practical version of the condition in (15) can be obtained by considering the condition (13) for improving the imperfect predictions via the MME approach in the least-biased density representation. Assuming that the ensemble members are obtained from small perturbations of a single model $M_0$, the evolution of the statistical moments $E_t^M$ for the ensemble members can be written as

a) $E_t^{M_i, \epsilon} = E_t^{M_0} + \epsilon E_t^M$, b) $\theta_t^{M_i, \epsilon} = \theta_t^{M_0} + \epsilon \hat{\theta}_t^M(E_t^M) + \mathcal{O}(\epsilon^2)$, \quad $\epsilon \ll 1$, \quad (16)

where

$$\hat{\theta}_t^M = \left( E_t^{M_0} \cdot \nabla \theta_t^{M_1}_{|\epsilon=0}, E_t^{M_0} \cdot \nabla \theta_t^{M_2}_{|\epsilon=0}, \ldots, E_t^{M_0} \cdot \nabla \theta_t^{M_i}_{|\epsilon=0} \right)^T.$$

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The asymptotic expansions in (16) can be combined with the condition (13) to yield the following:

**FACT 5.** Assume the Multi Model Ensemble is generated by perturbing a single model $M_0$ so that the statistical moments $E_i^{M_0}$ and the coefficients $\theta_i^{M_0}$ in the least-biased model densities $\pi_t^{M_0,i}$ are given by (16). In such a framework the sufficient condition (13) for improvement of the imperfect predictions via the MME approach can be expressed as

$$A_\alpha \left( \pi_t^{M_0,i}, \{ \pi_t^{M_0,i+2}/\pi_t^{M_0,i} \} \right) + \epsilon \bar{G}_\alpha \left( E_i, \{ E_i^{M_0} \} \right) + O(\epsilon^2) > 0,$$

(17)

where $A_\alpha$ is given by (14) and

$$\bar{G}_\alpha = \sum_{i \neq 0} \beta_i \left[ \left( \theta_i^{M_0} \left( E_i^{M_0} \right) - \theta_i^{M_0} \left( E_i^{M_0} \right) \right) \cdot \left( E_i - \bar{E}_i^{M_0} \right) \right],$$

with the weights $\beta_i$ defined in (9).

**Remarks:**
- The perturbations $\theta_i^{M_0}$ can be computed directly from the imperfect models $M_i$ in MME.
- The condition in (17) for improving the imperfect predictions through perturbing the reference model $M_0$ simplifies further for Gaussian mixture MME discussed in §3.3.

### 3.1.3 Predictive skill of MME in the context of initial value problem

Here, we represent the general condition (10) for improving imperfect predictions via the MME approach in the formulation suitable for various time-asymptotic estimates of the prediction skill in the context of the initial value problem. We approach this issue in two alternative and complementary representations, similar to the discussion in §3.1.2. First, we rewrite the condition (10) as a sum of two distinct terms involving (i) only the initial conditions of the truth density, and (ii) terms corresponding to the evolution from the initial density distribution; both the initial value problem prediction and the forced response prediction from equilibrium can be cast in such a form, as discussed in the next section. While this formulation provides a simple and intuitive representation of the general condition (10), the evolution of the probability densities away from the initial conditions cannot be easily estimated in practice from measurements even in the time-asymptotic limits. On the other hand, the representation (13) of the condition (10) in terms of least-biased densities (11), which is discussed subsequently, provides a formulation which is amenable to practical approximations especially when considering the forced response predictions. In the following sections we combine the time-asymptotic approximations obtained from the representation discussed below with the perturbative approach from §3.1.2 which is useful for obtaining asymptotic approximations.

Consider the evolution of a mixture density, $\pi_t^{MME}$, in (1) associated with a Multi Model Ensemble (MME) containing imperfect models $M_i$ from some class $\mathcal{M}$ which evolve from the initial statistical conditions represented by $\pi_0(u)$ for the truth and by $\pi_0^{M}(u)$. The time-dependent density of the truth can be written in the form

$$\pi_t(u) = \pi_0(u) + \delta \bar{\pi}_t(u), \quad \bar{\pi}_t(u) = 0, \quad \int \bar{\pi}_t(u) du = 0,$$

(18)

which separates the initial conditions from the subsequent evolution of the marginal probability density for the resolved dynamics; the parameter $\delta$ in (18) is arbitrary at this stage but it plays the role of an ‘order’ parameter in the time-asymptotic considerations discussed later in §3.3.

The formulation in (18) allows for the following representation of the sufficient condition (10) for improving predictive skill via MME approach:

**FACT 6.** Given the decomposition (18) of the truth density, the sufficient condition (10) for prediction improvement through MME is linear in the perturbation $\bar{\pi}_t^{M}(u)$ and can be written as

$$\tilde{A}_\alpha \left( \pi_0^{M}, \{ \pi_t^{M} \} \right) + \int du \bar{\pi}_t^{M} \tilde{G}_\alpha \left( \{ \pi_t^{M} \} \right) > 0,$$

(19)
where
\[ \tilde{\mathcal{A}}_\alpha = \sum_{i \neq 0} \beta_i \left[  \mathcal{P}(\pi_i^M, \pi_i^M) - \mathcal{P}(\pi_0^M, \pi_i^M) \right], \quad \tilde{\mathcal{R}}_\alpha = \sum_{i \neq 0} \beta_i \ln \frac{\pi_i^M}{\pi_t^C}, \]
with the weights \( \beta_i \) defined in (9). Similar to (15) in the previous section, the least-biased estimate of the truth, \( \pi_t^1 \), can be realistically estimated only for perturbations from equilibrium which is exploited when assessing the MME prediction improvement for the forced response (see §3.3.2 and Appendix D).

Consider now the condition (13) for improving the imperfect predictions via the MME approach for forced response prediction in the least-biased density representation which is more amenable to practical estimates. We denote the evolution of the statistical moments \( \bar{E}_t \) of the truth from some initial values in the following form
\[ E_t = E_0 + \delta E_t, \quad \delta E_0 = 0, \]
which leads to the following:

**FACT 7.** The sufficient condition (13) for improvement of the imperfect predictions via the MME approach can be expressed in terms of the least-biased approximations of the true density evolving from the initial density characterized by \( E_0, \theta_0 \) as
\[ \mathcal{A}_\alpha \left( \pi_i^1, \{ \pi_i^{M1,2} / \pi_i^M \} \right) + \tilde{\mathcal{R}}_\alpha \left( \{ E_t^M \}; E_0 \right) + \tilde{\mathcal{G}}_\alpha \left( \{ E_t^M \}, \delta E_t \right) > 0, \quad (20) \]
where \( \mathcal{A}_\alpha \) is defined in (14) and
\[ \tilde{\mathcal{A}}_\alpha = \sum_{i \neq 0} \beta_i \left[ \mathcal{P}(\pi_i^M, \pi_i^M) - \mathcal{P}(\pi_0^M, \pi_i^M) \right], \quad \tilde{\mathcal{G}}_\alpha = \sum_{i \neq 0} \beta_i \left[ (\theta_t^M(\bar{E}_t^M) - \theta_t^M(E_t^M)) \cdot \delta E_t \right], \]
where the weights \( \beta_i \) are defined in (9) and the initial least-biased density of the truth is given by \( \pi_0^M(u) = C_0^{-1} \exp(-\theta_0 \cdot E(u)) \).

**Remarks:**
- The evolution of \( E_t^M \) and \( \theta_t^M \) can be computed directly from the imperfect model.
- The expected changes, \( \delta \bar{E}_t \), in the truth statistics can be estimated only when considering the forced response prediction to perturbations of the attractor dynamics based on the correlations on the unperturbed attractor using the fluctuation-dissipation formulas, as discussed in [51, 43, 52] and in Appendix D.

### 3.2 Initial value problem vs forced response

As already mentioned, the framework introduced in §3.1 applies to both (i) improving imperfect predictions from given non-equilibrium statistical initial conditions of the truth, and (ii) to improving predictions the response of the truth equilibrium dynamics due to external perturbations. However, apart from the differences in the statistical initial conditions, an important feature distinguishing predictions associated with the initial value problem from the forced response prediction, is that in the latter case the evolution of the truth statistics from equilibrium in response to small external perturbations can be estimated via the fluctuation-dissipation formulas (e.g., [49, 46]). This allows for practical assessment of the predictive skill improvement for the forced response via MME through the general conditions (10), (13) or their subsidiaries discussed in §3.1.2 and §3.1.3; we clarify these differences below and provide further details on the use of the fluctuation-dissipation theory in this context in Appendix D.

Recall first the evolution of the truth density from given initial statistical conditions at \( t = 0 \) can be written in the form (18). Adopting the same decomposition for the imperfect model densities, \( \pi_t^M = \).
\( \pi_0 + \delta \pi^M_{t} \), allows for the mixture density \( \pi^\text{MME}_t \) in (1) associated with the Multi Model Ensemble (MME) to be written as

\[
\pi^\text{MME}_t = \sum_i \alpha_i \pi^0_{t,i} + \sum_i \alpha_i \delta \tilde{\pi}^M_{t,i}, \quad \tilde{\pi}^M_{t} = 0, \quad \int \tilde{\pi}^M_t(u)du = 0, \quad \sum_i \alpha_i = 1,
\]

where the first term represents the initial mixture density on the resolved subspace and the second term in (21) represents the evolution of the mixture density from the initial condition. Similar decomposition can be adopted for the evolution of the statistical moments (12) of the truth density and the imperfect model densities

\[
\bar{E}_t = \bar{E}_0 + \delta \bar{E}_t, \quad \bar{E}^M_t = \bar{E}^0_t + \delta \bar{E}^M_t, \quad \bar{E}_0 = 0.
\]

The similarities and differences between the initial value problem and the forced response prediction can be summarized as follows:

- For the initial value problem, the initial marginal densities for the resolved dynamics, \( \pi_0 \) and \( \pi^M_{t,i} \), or their initial statistics \( \bar{E}_0 \) and \( \bar{E}^M_t \) correspond to any smooth probability densities. However, in the case of the forced response prediction the statistical initial conditions are restricted to the respective equilibrium states, i.e., \( \pi_0 = \pi^\text{eq} \) and \( \pi^M_{0,i} = \pi^{M,\text{eq}}_{i} \), and \( \bar{E}_0 = \bar{E}^\text{eq} \) and \( \bar{E}^M_t = \bar{E}^{M,\text{eq}}_t \).

- The fundamental difference between the initial value problem discussed in §3.1.3 and the forced response prediction lies in the existence of the decomposition (18) and (22). In particular,
  - The marginal probability density associated with the evolution of a non-degenerate truth in the initial value problem can always be written in the form (18) and (22). However, the time-dependent terms in (18) and (22) are generally small only for sufficiently short times.
  - In the case of estimating the truth response to external perturbations, the decompositions (18) and (22) apply to non-degenerate hypoelliptic noise (see [30] and Appendix D). For sufficiently small external perturbations the time-dependent perturbations with \( \delta \ll 1 \) in (18) and (22) can remain small for all time and the evolution of the perturbed statistics (22) can be estimated via the fluctuation-dissipation formulas, see Appendix D.

### 3.3 Improving imperfect predictions via MME in the Gaussian framework

The analysis presented in §3.1-3.2 becomes particularly revealing in the Gaussian framework, i.e., when \( L_1 = L_2 = 2 \) in (13), due to the existence of the analytical formula for the relative entropy between two Gaussian densities (e.g., [49]). In such a case the probability density, \( \pi^\text{MME}_t \), in (1) of the Multi Model Ensemble is a Gaussian mixture and the error, \( \delta \pi^M_t \) in the conditions (13), (17), and (20), due to the least-biased approximation vanishes identically. In order to achieve the maximum simplification of the problem while retaining the crucial features of the framework, we assume here that the reduced-order models on the subspace of the resolved variables \( u \in \mathbb{R}^K \) for predicting the marginal statistics \( \pi_t \) of the resolved truth dynamics are given by the three-parameter family of Gaussian Ito SDE’s (e.g., [60]) given by

\[
du^M = \left(-G^M u^M + f^M(t)\right)dt + \sigma^M(t)dW(t),
\]

where \( G^M, \sigma^M \) are diagonal matrices with \( G^M, \sigma^M > 0 \), \( W(t) \) is a vector-valued Wiener process with independent components, and the mean dynamics and its covariance are given by the well-known formulas

\[
\mu^M_t = E \pi^M_t[u] = e^{-\Gamma^M(t-t_0)}u_0 + \int_{t_0}^{t} e^{-\Gamma^M(t-s)}f^M(s)ds,
\]

\[
R^M_t = E \pi^M_t[u \otimes u] - \mu^M_t \otimes \mu^M_t = e^{-\Gamma^M(t-t_0)}R_0 e^{-\Gamma^M(t-t_0)} + \int_{t_0}^{t} e^{\Gamma^M(s-t)}Q e^{\Gamma^M(s-t)}ds,
\]

where \( Q = \sigma^M \otimes (\sigma^M)^T \). Consequently, the MME density, \( \pi^\text{MME}_t \), in (1) is a linear superposition of Gaussian densities with the statistics evolving according to (24)-(25).
3.3.1 Improving predictions via MME in the initial value problem context

In this section we derive guidelines for constructing ensembles of imperfect models with improved predictive skill relative to any single imperfect model; as already mentioned, these considerations simplify significantly in the Gaussian framework due to the existence of analytical formula for the relative entropy between two Gaussian densities which simplifies the MME skill improvement condition (10). Here, we derive the guidelines for predictive skill improvement via MME in the context of initial value problem with the initial conditions away from the truth equilibrium statistics; a related information-theoretic framework for improving imperfect single-model predictions was discussed in [43, 52, 47, 10, 50]. Discussion of the conditions for improvement of predictive skill of the forced response via MME of the truth dynamics perturbed from equilibrium is presented in §3.3.2.

We set $\mu_0$ and $R_0$ as the initial mean and covariance of the truth, and $\mu_0^{\delta}$ and $R_0^{\delta}$ are the initial mean and covariance of the model. We write the truth mean and covariance as

$\mu_t = \mu_0 + \delta \mu_t, \quad \mu_0 = 0, \quad R_t = R_0 + \delta R_t, \quad R_0 = 0,$

and the mean and covariance of the imperfect Gaussian models (23) as

$\mu_t^{\delta} = \mu_0^{\delta} + \delta \mu_t^{\delta}, \quad \mu_0^{\delta} = 0, \quad R_t^{\delta} = R_0^{\delta} + \delta R_t^{\delta}, \quad R_0^{\delta} = 0,$

where $\delta$ is an ordering parameter utilized below in some short-time symptomatic expansions. Note that in contrast to the general considerations in §3.1, we use here centered statistical moments. The general condition (13) for improving MME predictions, which holds at any time $t$ and $\delta$ in (26)-(27), can be easily rewritten in terms of the centered moments in the Gaussian framework, as discussed in Appendix A. Here, we highlight a simpler and more revealing version of this condition which is valid only at sufficiently short times; this asymptotic short-time constraint arises from the technical requirement that the time-dependent terms in the statistical moments (26) and (27) be small. For arbitrary statistical initial conditions this constraint implies $t \ll 1$, as may be seen by rewriting (24)-(25) in the from compatible with (27); formally the ‘smallness’ of $\mu_t$, $\mu_t^{\delta}$ and of $R_t$, $R_t^{\delta}$ required in the asymptotic expansions is achieved by assuming $\delta \ll 1$ in (26) and (27). The above assumptions lead to the following simple and revealing result (see Appendix A for a simple proof and generalizations):

FACT 8. Consider the initial value problem and imperfect statistical predictions with Gaussian models $\mu_t$ in (23) with correct initial statistical conditions, i.e., $\mu_0^{\delta} = \mu_0$, $R_0^{\delta} = R_0$. The condition for improvement of imperfect predictions in the initial value problem at short times $t \ll 1$ via Gaussian mixture MME is

$\delta^2 \left\{ D_t(\{\tilde{\mu}_t - \mu_t^{\delta}\}) + E(\{\tilde{R}_t^{\delta}\}) - \text{tr}[\tilde{R}_t F(\{\tilde{R}_t^{\delta}\})] \right\} + O(\delta^3) > 0,$

(28)

where

$D_t = \frac{1}{2} \sum_{i \neq \phi} \beta_i \left[ (\tilde{\mu}_t - \mu_t^{\phi})^T (R_0)^{-1} (\tilde{\mu}_t - \mu_t^{\phi}) - (\tilde{\mu}_t - \mu_t^{\phi})^T (R_0)^{-1} (\tilde{\mu}_t - \mu_t^{\phi}) \right],

E_t = \frac{1}{2} \sum_{i \neq \phi} \beta_i \text{tr} \left( (\tilde{R}_t^{\phi})^{-1} (R_0)^{-1} \right) \text{tr} \left( (\tilde{R}_t^{\phi} + \tilde{R}_t^{\phi}) (R_0)^{-1} \right),

F_t = \frac{1}{2} \sum_{i \neq \phi} \beta_i \text{tr} \left( \tilde{R}_t (R_0)^{-1} (\tilde{R}_t^{\phi} - \tilde{R}_t^{\phi}) (R_0)^{-1} \right),

with the weights $\beta_i$ defined in (9).

Remarks:

- Underdamped MME helps improve the short-time skill of imperfect predictions ($E_t > 0$) but it is not sufficient to guarantee the skill improvement. The interplay between the truth and model response in $D_t$ and the truth and model response in the variance in $F_t$ are both important.
- When the truth response in the variance $\delta R_t$ is sufficiently negative the short term prediction skill is not improved through the underdamped MME.
• Even if the short-time condition (28) is satisfied, the medium-range predictive skill of MME might not beat the single model (see §5 for examples).

The insight gained from the ‘short-time’ asymptotic condition in (28) will be used when interpreting the numerical results in §5.

3.3.2 Improving forced response predictions via MME

In this section we consider the essential features of a Multi Model Ensemble which provide improvement of statistical predictions of the response of the truth dynamics to small external perturbations of its equilibrium state; the information-theoretic framework for improving the response of imperfect single-model predictions was discussed in [52, 47, 10, 50] As in the previous section, we consider imperfect equilibrium state; the information-theoretic framework for improving the response of imperfect single-

Consider the time-dependent truth marginal density $\pi^\delta_t$ on the subspace of resolved variables $u \in \mathbb{R}^K$ which arises in response to small external perturbations of the truth equilibrium dynamics with equilibrium marginal density $\pi_{eq}$ so that

$$\pi^\delta_t = \pi_{eq} + \delta \tilde{\pi}_t, \quad \delta \ll 1, \quad \tilde{\pi}_0 = 0, \quad \int \tilde{\pi}_t(u)du = 0.$$  \hfill (29)

We assume the perturbation in (29) is be non-singular so that $\pi^\delta_t$ is smooth at $\delta = 0$ which holds under minimal assumptions outlined in [30]. Moreover, we assume that the perturbed second-order marginal statistics decomposes as

$$\mu^\delta_t = \mu_{eq} + \delta \tilde{\mu}_t, \quad R^\delta_t = R_{eq} + \delta \tilde{R}_t, \quad \delta \ll 1,$$  \hfill (30)

where $\mu_{eq}$ and $R_{eq}$ are the equilibrium marginal mean and covariance of the truth on the subspace of the resolved variables $u$, the time-dependent perturbations $\tilde{\mu}_t, \tilde{R}_t$ of the statistical moments and, consequently, the least-biased perturbed truth density, $\pi^{\delta,\mu}_{eq}$, can be estimated via the fluctuation-dissipation theorem (see, e.g., [49, 38, 2, 44, 27, 52, 42]) and Appendix D).

As in the general case outlined in §3.1.3, the MME density $\pi^\text{MME}_t$ is assumed to have the form as in (21) but the simplification arises due to the Gaussian nature of the models in the ensemble, i.e.,

$$\pi^{\text{MME}}_t = N(\mu^M_t, \tilde{\rho}_t^M, \delta_t^M, \rho^M_{\mu^M_t})$$  \hfill (31)

where $\mu^M_t = \mu_{eq} + \delta \tilde{\mu}_t$, $\tilde{\rho}_t^M = R_{eq} + \delta \tilde{R}_t$, $\delta \ll 1$.

Note that, in general, $\pi^{M\mu}_{eq} \neq \pi_{eq}$ so that the imperfect model equilibrium densities do not necessarily coincide with the marginal equilibrium density of the truth. Moreover, the perturbations of the equilibrium statistics (31) of the imperfect models do not have to be small since they can be computed from the models; however, this assumption simplifies the asymptotic analysis. For a Gaussian mixture MME with tuned equilibrium statistics, $\mu^{\text{MME}}_{eq} = \mu_{eq}$, $R^{\text{MME}}_{eq} = R_{eq}$, it can be easily shown (see Appendix A) that a condition equivalent to that in (28) holds for sufficiently small perturbations. Moreover, we also have the following important and simple result (see Appendix A for a more general version):

**FACT 9.** Consider the forced response prediction via Gaussian mixture MME containing imperfect Gaussian models (23) with correct equilibrium mean and covariance, i.e., $\mu^{\text{MME}}_{eq} = \mu_{eq}$ and $R^{\text{MME}}_{eq} = R_{eq}$. The sufficient condition for improvement predictions of the truth response to the small external forcing perturbations via MME is independent of the truth covariance response, $\tilde{R}_t$, and it is given by

$$D_t(\{\dot{\mu}_i - \dot{\mu}^{\text{MME}}_t\}) > 0.$$  \hfill (32)
where $\tilde{\mu}_t$ is the perturbation of the true mean, $\tilde{\mu}_t^{Mi}$ and $\tilde{R}_t^{Mi}$ are perturbations of the model means and covariances, and

$$D_t = \frac{1}{2} \sum_{i \neq o} \beta_i \left[ (\tilde{\mu}_t - \tilde{\mu}_t^{o})^T R_{eq}^{-1}(\tilde{\mu}_t - \tilde{\mu}_t^{o}) - (\tilde{\mu}_t - \tilde{\mu}_t^{Mi})^T R_{eq}^{-1}(\tilde{\mu}_t - \tilde{\mu}_t^{Mi}) \right],$$

with the weights $\beta_i$ defined in (9).

**Remarks:**

- In a more general setting (see Appendix A), where only the equilibrium means are tuned, $\mu_{eq}^{Mi} = \mu_{eq}$ but $R_{eq}^{Mi} \neq R_{eq}$, the interplay between the truth and model response in both the mean and covariance are important (see also [51, 43, 52] for the related analysis in the single-model configuration). Under-damped MME helps improve the short-time imperfect predictions of the forced response predictions but it is not sufficient to guarantee the skill improvement.

- In §4.4 we show, based on a very simple but revealing example involving Gaussian dynamics, that the prediction of forced response at large times $t \to \infty$ is improved for overdamped MMEs (i.e., such that the correlation times in the imperfect models $\tau^{Mi}$ satisfy $\tau^{Mi} = \tau^{trth} > \tau^{Mi}$ with $\tau^{trth}$ the correct correlation time of the resolved equilibrium dynamics). At the same time, the issue of reducing the information barrier (see FACT 2 in §3) in the MME prediction is much more subtle; this simple example illustrates the general case discussed in §3 (see §§3 and figure 3).

The insight gained from the above asymptotic condition in (32) and its generalizations presented in Appendix A will be used when interpreting the numerical results in §5.

### 4 Setup for studying the performance of MME skill using exactly solvable test models

The goal of any reduced-order prediction technique, including MME prediction, is to achieve statistically accurate estimates of the evolution of the truth on the resolved subspace of variables. In general, the marginal equilibrium statistics of the resolved dynamics can be reproduced by many different imperfect models (e.g., [50]). Moreover, tuning the marginal equilibrium statistics of imperfect models does not necessarily reduce the error in the transient dynamics and statistics of the models (e.g., [43, 52, 10, 50]).

In order to elucidate these issues further in the context of MME prediction, we exploit two classes of exactly solvable stochastic test models which are used to generate the ‘truth’ dynamics in the subsequent analysis of imperfect prediction skill improvement which merges the information-theoretic estimates derived in §3 with simple numerical simulations in §5.

The first class of test models, described in §4.1, is given by two-dimensional linear Gaussian models [56, 48, 50] which couple linearly the ‘resolved’ and ‘unresolved’ dynamics; these models are very useful for identifying the essential features of MME that lead to the reduction of uncertainty in imperfect predictions in the typical case when the reduced-order models neglect the effects of the ‘unresolved’ dynamics on the ‘resolved’ dynamics. Moreover, these revealing models represent the simplest non-trivial examples of dynamics where the effects of the unresolved processes may lead to information barriers to improving the predictive skill of imperfect models (see [48, 43, 52, 50]); we discuss this issue in detail in §4.4 and later in §5.2 in the context of MME predictions of the forced response.

The nonlinear, non-Gaussian test models outlined in §4.2 and introduced in [20] allow for incorporating a wealth of important effects due to the unresolved turbulent processes on the resolved dynamics; these include the intermittent energy bursts due to nonlinear interactions with the unresolved scales and forcing fluctuations at large scales. Another important feature of these non-Gaussian models which is not explored here stems from the fact one could consider various existing closures for the statistics of these non-Gaussian systems [10] and consider the effects of these closures on the predictive skill in the MME setting relative to the single model prediction.

For both classes of the test models the Multi Model Ensembles used for predicting the marginal statistics of the ‘resolved’ truth dynamics consist of reduced-order linear Gaussian models which, in this case,
are one-dimensional and were described in §3.3; the important issue of tuning the marginal equilibrium statistics for these models is described in §4.3. The prediction skill improvement through the MME approach relative to the single model predictions is analyzed in various dynamical configurations in §5 based on the information-theoretic framework developed in §3 and numerical experiments.

4.1 The two-dimensional linear Gaussian system

In this linear Gaussian system the ‘resolved’ dynamics $u(t)$ is linearly coupled to the ‘unresolved’ dynamics $v(t)$ according to (see [56, 48, 50])

$$
\frac{d}{dt} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} L & 0 \\ F(t) & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} dt + \begin{pmatrix} 0 \\ \sigma \end{pmatrix} dW(t). \tag{33}
$$

The matrix $L$ in the system (33) and its eigenvalues $\lambda_{1,2}$ are

$$
L = \begin{pmatrix} a & 1 \\ q & A \end{pmatrix}, \quad \lambda_{1,2} = \frac{1}{2} \left( a + A \pm \sqrt{(a - A)^2 + 4q} \right), \tag{34}
$$

where $a$ is the damping in the resolved dynamics $u(t)$, $q$ is the damping in the unresolved dynamics $v(t)$, and $A$ the coupling parameter between the unresolved and resolved dynamics. We assume that the deterministic forcing $F(t)$ acts only in the resolved subspace $x$, and the stochastic noise with amplitude $\sigma$ generated by the scalar Wiener process $W(t)$ affects directly only the unresolved dynamics of $v(t)$. Since the system (33) is linear with additive noise, it can be easily shown that for constant forcing $F$ it has a Gaussian invariant measure provided that

$$
a + A = \lambda_1 + \lambda_2 < 0, \quad aA - q = \lambda_1 \lambda_2 > 0, \tag{35}
$$

so that the stable equilibrium mean of (33) is given by $\mathbf{\mu} = (\mu^u, \mu^v)$ where

$$
\mu^u_{eq} = -\frac{AF}{aA - q}, \quad \mu^v_{eq} = \frac{qF}{aA - q}, \tag{36}
$$

and the equilibrium covariance in (33) is

$$
R_{eq} \equiv \begin{pmatrix} 1 & -a \\ -a & aA - q + a^2 \end{pmatrix} \frac{\sigma^2}{2(a + A)(q - aA)}. \tag{37}
$$

The autocovariance at equilibrium, $C_{eq}(\tau) = \langle x(t + \tau) \otimes x^T(t) \rangle_{att}$, depends only on the lag $\tau$ and it is given by

$$
C_{eq}(\tau) = \lim_{t_0 \to -\infty} C(\tau, t, t_0) = \Sigma e^{Lt_\tau}, \tag{38}
$$

Extensions to the nonautonomous case with time-periodic forcing are trivially accomplished provided that the stability conditions (35) are satisfied so that there exists a time-periodic Gaussian measure on the attractor (defined in the nonautonomous sense; see, e.g., [46, 5]) with the time-periodic mean, $\mathbf{\mu}_{att}(t) \equiv \lim_{t_0 \to -\infty} \mathbf{\mu}(t, t_0)$, and autocovariance (38).

Despite the simplicity of the system (33), the transient dynamics in systems with identical equilibrium can be quite different depending on the coefficients $\{a, q, A, \sigma\}$. In fact, there exist three distinct regimes of transient dynamics in (33) with stable Gaussian system equilibrium; these regimes are [50]:

**Transient dynamics with purely real eigenvalues $\lambda_{1,2}$:**

- *Normal mean dynamics:* In this regime the two eigenvectors of the system matrix $\hat{L}$ with purely real eigenvalues $\lambda_{1,2}$ are nearly orthogonal. Provided that $\Lambda \equiv \lambda_1/\lambda_2 \neq 1$, this configuration occurs for

$$
a \approx \frac{1}{2} \left( (\Lambda + 1)\lambda_1 \pm \sqrt{(\Lambda + 1)^2\lambda_1^2 - 4(1 + \Lambda\lambda^2)} \right). \tag{39}
$$
• Non-normal mean dynamics: For large eigenvalue ratio $\Lambda \gg 1$ and weak damping, $a \ll \Lambda$, in the resolved dynamics the angle between the eigenvectors is sensitive to variations of $a$ but only one of the eigenvectors significantly changes its orientation. For $\Lambda \sim 1$ corresponding to $(a - A)^2 + 4q \approx 0$, the eigenvectors are nearly collinear and the direction of both eigenvectors depends strongly on the damping $a$ in the resolved dynamics.

**Transient dynamics with complex-conjugate eigenvalues $\lambda_{1,2}$:**

• Mean dynamics with complex-conjugate eigenvalues. This configuration occurs for $(a - A)^2 + 4q < 0$ when the complex conjugate eigenvalues satisfy the stability condition (35).

The marginal equilibrium statistics of the resolved variable $u(t)$ in (33) can be reproduced by many different imperfect models; this can be achieved, in particular, by appropriately tuning the simple models (23), as shown in §4.3. Of course, tuning the marginal equilibrium statistics of imperfect models does not fix the transient dynamics/statistics; for example, one might attempt to use the same imperfect model (23) with tuned equilibrium to predict the initial value problem for $u(t)$ in (33) with either normal dynamics or with non-normal dynamics characterized by a high sensitivity to model parameters and to the statistical initial conditions. Thus, the interesting and important practical question concerns the issue of predicting the resolved marginal dynamics $u(t)$ of the truth using ensembles of imperfect models which do not account for the effects of the unresolved processes on the resolved dynamics. These are exactly the issues considered in §3 and they will be clarified further using numerical tests in §5.

### 4.2 The nonlinear non-Gaussian model

The non-Gaussian dynamics of the second test model is given by the following nonlinear stochastic stochastic system (see [20, 7, 10, 9, 50])

$$
\begin{align*}
(a) \quad du(t) &= \left[(-\gamma(t) + i\omega)u(t) + F(t)\right]dt + \sigma_u dW_u(t), \\
(b) \quad d\gamma(t) &= -d_\gamma(\gamma(t) - \hat{\gamma})dt + \sigma_\gamma dW_\gamma(t),
\end{align*}
$$

(39)

where $W_u$ is a complex Wiener processes with independent components and $W_\gamma$ is a real Wiener process. The nonlinear system (39), introduced first in a more general form in [20] for filtering multiscale turbulent signals with hidden instabilities, has a number of attractive properties as a test model in our analysis of the skill of MME prediction exploiting reduced-order models. Firstly, it has a surprisingly rich dynamics mimicking signals in various regimes of the turbulent spectrum, including regimes with intermittently positive finite-time Lyapunov exponents [7, 10, 9]. Secondly, exact path-wise solutions and exact second-order statistics of this non-Gaussian system can be obtained analytically, as discussed in [20].

As in the previous test model (33), we consider $u(t)$ in (39) to be the ‘resolved’ variable which is nonlinearly coupled with the ‘unresolved’ variable $\gamma(t)$ which induces damping fluctuations in the resolved dynamics; this nonlinear coupling between the resolved and unresolved dynamics is capable of generating a highly non-Gaussian dynamics which proved valuable in a number of earlier considerations concerned with uncertainty quantification and filtering of turbulent dynamical systems [55, 7, 10, 9, 50]. In section 5 we will consider statistical predictions of $u(t)$ in (39) using the Gaussian mixture MME consisting of reduced-order Gaussian models (23) in various dynamical regimes of (39) determined by the parameters of the hidden, unresolved dynamics of $\gamma(t)$.

Three out of five parameters in the system (39) control the physically relevant dynamical regimes of (39) with stable mean dynamics [7] which occurs when [7]

$$
\chi = -\hat{\gamma} + \frac{\sigma_\gamma^2}{2d_\gamma^2} < 0,
$$

(40)

with $\hat{\gamma}$ the mean damping in $u(t)$, and $d_\gamma$, $\sigma_\gamma$ denoting the damping and noise variance in the hidden dynamics of damping fluctuations $\gamma(t)$ in (39b); the regimes examined later in §5 are (see also [7]).
(I) *Regime of plentiful, short-lasting transient instabilities in the resolved component* \(u(t)\) *with fat-tailed marginal equilibrium PDF*; it occurs for \(\sigma_\gamma, d_\gamma \gg 1\), \(\sigma_\gamma/d_\gamma \sim \mathcal{O}(1)\) and \(\gamma\) sufficiently large so that \(\chi < 0\). In this ‘inertial range’ regime the damping fluctuations \(\gamma(t)\) decorrelate rapidly and the correlation time of \(u(t)\) given approximately by \(1/\gamma\) (see [7]).

(II) *Regime of intermittent large-amplitude bursts of instability in* \(u(t)\) *with fat-tailed marginal equilibrium PDF*; it occurs for small \(\sigma_\gamma, d_\gamma\), with \(\sigma_\gamma/d_\gamma \sim \mathcal{O}(1)\) and \(\gamma\) sufficiently large so that \(\chi < 0\). In this ‘dissipation range’ regime the correlation time of the damping fluctuations \(\gamma(t)\) is long compared to (I) but the correlation time of \(u(t)\) can vary widely, as in regime (I).

(III) *‘Laminar’ regime with nearly Gaussian equilibrium PDF* which occurs for \(\dot{\gamma}^2 \gg \sigma_\gamma^2/2d_\gamma\) and \(\chi < 0\). Here, the transient instabilities in \(u(t)\) occur very rarely.

The equilibrium probability densities in the above regimes can be made skewed by retaining a non-zero deterministic forcing \(F\) in (39a). In §5 various numerical tests employing the Gaussian mixture MME for predicting the resolved dynamics \(u(t)\) of the non-Gaussian model (39) confirm the estimates obtained from the general information-theoretic framework of §3 and provide insight into additional subtleties associated with MME prediction.

### 4.3 Tuning the reduced-order models in the Multi Model Ensemble

For simplicity in exposition we restrict the considerations of improving imperfect predictions via the MME approach to the case when the densities, \(\pi_{mme}^j\) in (1), are given by Gaussian mixtures with reduced-order, imperfect models given by (23). In this section we show that the equilibrium statistics of the reduced-order models for the resolved dynamics \(u(t)\) can be easily tuned to mimic the true equilibrium second-order statistics on the resolved variables; in fact, there exists a one-parameter family of such imperfect models with correct marginal equilibrium statistics (see [50]). Thus, it is possible to create a Multi Model Ensemble containing different imperfect models which all have correct marginal equilibrium statistics. However, it is important to stress that the models in MME do not necessarily have to have correct equilibrium statistics for improved prediction skill, as already indicated in the general analysis presented in §3.

We assume that the marginal equilibrium mean and covariance, \(\langle u \rangle_{eq}, \text{Var}_{eq}[u]\), of the resolved truth dynamics can be estimated accurately from measurements. The following result (see [50]) provides the basis for tuning the marginal equilibrium statistics of the imperfect models in MME:

**Proposition 1** Consider the linear Gaussian Mean Stochastic Models (23) with constant forcing and coefficients \(\{\gamma^M, \sigma^M, F^M\}\). Provided that \(\gamma^M > 0\), the equilibrium statistics of (23) is controlled by two parameters

\[
\left\{ \mu^M_{eq} = \frac{F^M}{\gamma^M}, \quad R^M_{eq} = \frac{(\sigma^M)^2}{2\gamma^M} \right\},
\]

which correspond, respectively, to the model mean and variance. If the truth dynamics is given by (33), the models (23) have correct marginal equilibrium statistics for the resolved variable \(u\) when

\[
(\sigma^M)^2 = -\gamma^M \frac{\sigma^2}{(a+A)(aA-q)}, \quad F^M = -\gamma^M \frac{AF}{aA-q},
\]

where \(a, A, q, \sigma\) are the coefficients of the system (33) with constant forcing \(F\). If the truth dynamics is given by (39), then the models (23) have correct marginal equilibrium statistics for the resolved variable \(u\) when

\[
(\sigma^M)^2 = -2\gamma^M \text{Var}_{eq}[u], \quad F^M = -\gamma^M \langle u \rangle_{eq},
\]

where \(\langle u \rangle_{eq}\) and \(\text{Var}_{eq}[u]\) denote the marginal equilibrium mean and variance of the truth dynamics of \(u(t)\). Since there are three coefficients in the system (23) with constant forcing and two constraints, there is a one-parameter family of reduced-order models (23) with correct marginal equilibrium statistics of the resolved dynamics \(u\).

**Remarks:**
• It is possible to create a Multi Model Ensemble containing imperfect models with correct marginal equilibrium statistics but different characteristics of the transient dynamics,

• The models in MME do not necessarily have to have correct equilibrium statistics for improved prediction skill, as already indicated in the general analysis presented in §3.

In general, the Mean Stochastic Models in (23) cannot reproduce the marginal two-point equilibrium statistics of the true resolved dynamics (see [50] for details). However, there exists a linear Gaussian model (23) with the correct decorrelation time, $\tau^m = \tau^{truth}$, where

$$\tau^m \equiv R_{eq}^m \int_0^\infty \langle u^m(t)u^m(t+\tau) \rangle d\tau, \quad \tau^{truth} \equiv \text{Var}_{eq}[u] \int_0^\infty \langle u(t)u(t+\tau) \rangle d\tau. \quad (44)$$

Apart from estimating the mean and covariance components for the resolved variables from real measurements, the correlation time from the measurements is the next easiest quantity to estimate from the measurements. Therefore, in the analysis of §4.4 and §5 we will assume that the single reference model, denoted by $m_0$ in the general considerations of §3, is given by the model with correct correlation time for the resolved dynamics.

4.4 Information barriers in MME prediction

Here, we consider a simple example of predicting the infinite-time response of a Gaussian truth dynamics to forcing perturbations in order to show explicitly that the MME prediction improvement depends on the properties of the unresolved truth dynamics. The example discussed below represents the simplest non-trivial configuration capable of illustrating these effects, and it augments the previous considerations discussed in [43, 48, 50] in the context of single model predictions. In particular, we show that even if the prediction skill improvement is achieved via the MME approach, the information barrier (see §3.1 and FACT 2) in the MME prediction may or may not be reduced relative to the single model prediction depending on the characteristics of the unresolved truth dynamics and the structure of MME; a sketch of these two scenarios was shown earlier in figure 3 of §3, as a similar situation can in the context of the initial value problem (e.g., figure 1 of §2).

Consider the predictions of the forced response of the truth dynamics to forcing perturbations in the simple configuration when the truth is given by the model of (33) discussed in §4.1; the imperfect models for the resolved dynamics $u$ are given by the linear Gaussian models (23) with correct marginal equilibrium statistics on the resolved subspace $u$ so that

$$\mu_{eq,u} = \mu_{eq}^m, \quad \text{and} \quad \text{Var}_{eq}[u^m] = \text{Var}_{eq}[u] \equiv E, \quad (45)$$

where $\mu_{eq,u}, \mu_{eq}^m$ are the equilibrium means of the truth (33) and of the model (23) for the resolved dynamics

$$\mu_{eq,u} = -\frac{AF}{aA - q}, \quad \mu_{eq}^m = \frac{F^m}{\gamma^m}, \quad (46)$$

and the corresponding variances given by

$$\text{Var}_{eq}[u] = \frac{\sigma^2}{2(a + A)(aA - q)}, \quad \text{Var}_{eq}[u^m] = \frac{(\sigma^m)^2}{2\gamma^m}. \quad (47)$$

We assume that the truth dynamics in (33) with parameters $(a, q, A, \sigma)$ and constant forcing $F$ satisfies the stability conditions (35) so that the stable Gaussian equilibrium exists and that the perturbed statistics is given by (31), as in §3.3.2.

As shown in [43, 48] in such a case no imperfect model in the class (23) with stable equilibrium (i.e., $\gamma^m > 0$ in (23)) can match the sensitivity of the truth dynamics to the forcing perturbations. This is easy to see by considering the asymptotic, infinite-time response of the truth dynamics (33) to forcing perturbations from equilibrium; the forcing perturbations are represented by replacing $F$ in (33)
by $F + \delta F$ while the same experiment in the imperfect models for (23) involves replacing $F^m$ by $F^m + \delta F$. Since the considered models are linear and Gaussian, the only change in the expected response to forcing perturbations is through the change in mean

$$ a) \quad \delta \mu_a = -\frac{A}{aA - q} \delta F, \quad b) \quad \delta \mu^\ast = \frac{1}{\gamma^m} \delta F, $$

while the variance of $u$ and $u^\ast$ for the perfect and imperfect models in (47) remain unchanged with the value $E$ as in (45). In such a case the model error for the infinite response via the relative entropy (2) becomes

$$ \mathcal{P}(\pi^\delta, \pi^m_\infty) = \frac{1}{2E} \left( \frac{A}{aA - q} + \frac{1}{\gamma^m} \right)^2 |\delta F|^2, $$

which can be easily derived using the formula for the relative entropy between two Gaussian densities (see (49) in Appendix A).

For the truth dynamics (33) with stable equilibrium (so that (35) holds) there exist two distinct configurations for single model prediction which depend on the sign of the coupling parameter $A$ in (33) between the resolved and unresolved dynamics:

(i) For $A < 0$, there exists an imperfect model (23) with $\gamma^m = -(aA - q)/A > 0$ and correct infinite time-response to the forcing perturbations so that $\mathcal{P}(\pi^\delta, \pi^m_\infty) = 0$ and the correlation time is

$$ \tau^\text{opt} = 1/\gamma^m = A/(q - aA); $$

note the imperfect model (23) with $\tau^\text{opt}$ does not have to have correct finite-time response which can be easily seen [?] using the standard ‘fluctuation-dissipation’ formulas for the response in the mean of (23), see also figure (12) in §5.2.

(ii) For $A > 0$ there is an intrinsic barrier to sensitivity improvement for the MSM models (23) given by

$$ \mathcal{P}(\pi^\delta, \pi^m_\infty) = \frac{1}{2E} \left( \frac{A}{aA - q} \right)^2 |\delta F|^2 $$

which is achieved only when $\gamma^m \to \infty$. This information barrier can only be overcome by enlarging the class of models beyond (23) by introducing more degrees of freedom in the model.

The existence of two possible scenarios (i), (ii) in single model predictions in this simple example provides important insight into the MME prediction improvement and reduction of information barriers. Note first that the condition (32) for the improvement of the forced response prediction via the MME approach discussed in §3.3.2 becomes in this case

$$ \frac{|\delta F|^2}{2E} \sum_{i \neq 0} \beta_i \left[ \left( \frac{A}{aA - q} + \frac{1}{\gamma^m} \right)^2 - \left( \frac{A}{aA - q} + \frac{1}{\gamma^m} \right)^2 \right] > 0. $$

The above condition for improving the forced response in the Gaussian framework leads to two distinct cases which are related to the cases (i)-(ii) above (see also figure 3):

- No information barrier in the single model prediction ($A < 0$ in the unresolved part of the truth (33)

  - If $M_0 \neq M_*$ with optimal damping $\gamma^m_*$ in the imperfect model (23), the MME approach can improve the infinite time forced response prediction based on (52), see also figure 12. In particular the MME skill is improved for any overdamped MME with $\gamma^m_* \geq \gamma^m$, see also figure 11. The above conclusion holds for any imperfect model (23) and, in particular, for the MSM with the correct correlation time $\tau^m = \tau^\text{opt}$ in (50) which can be tuned based on the measurements of the resolved equilibrium dynamics of the truth.

  If, additionally, $M_* \notin M_0$, the information barrier in MME can be reduced relative to the single model prediction (see also figure 3a).
– If $m_0 = m_*$ with optimal damping $\gamma^{m_*}$ in the imperfect model (23) given in (i), the MME approach does not improve the infinite-time forced response prediction based on (52), see also figure 12. The information barrier in MME cannot be reduced relative to the single model prediction.

- Information barrier in the single model prediction ($A > 0$ in the unresolved part of the truth (33))
  - The infinite-time forced response prediction is improved (at least) for any overdamped MME. The information barrier in MME prediction cannot be reduced relative to the single model prediction; this situation is depicted schematically in figure 3b. Recall that the model error of the optimal-weight MME, which corresponds to the information barrier of the class of models $\mathcal{M}$, coincides in such a case with the single optimal model $m_*$ (see figures 11-12 and figure 2c for analogous situation in the context initial value problem).

Further study of this revealing example of the forced response MME skill in the finite-time case is presented in §5.2.

5 Tests of the theory for MME prediction

In this final section we use exactly solvable Gaussian and non-Gaussian test models introduced in §4 in order to illustrate the general information-theoretic estimates derived in §3 for skill improvement in imperfect predictions via MME approach. Two such examples were already shown in figures 1-2 and discussed in §2 in order to motivate the need for the analytical estimates. Moreover, we validate and extend the asymptotic results of §3.3.1 and §3.3.2 involving short-times or small perturbations. The numerical examples studied below highlight the differences between the structure of Multi Model Ensembles providing skill improvement for short and medium range predictions.

The following discussion is divided into two parts: First, in §5.1 we discuss various examples of initial value problem prediction in the context of MME. Section §5.2 contains examples of improving the forced response prediction via the MME approach. The truth dynamics in all the tests is generated using the two exactly solvable models introduced in §4. For the sake of simplicity, and in order to make a connection with the analytical results of §3, the imperfect models in MME are all Gaussian and given by the Mean Stochastic Models (33) introduced in §3.3. In an attempt to adhere to realistic constraints, we assume that a collection of MSMs (33) is available with various correlation times/dampings, and that the MME optimization is carried out only through adjusting the time-independent weights in the ensemble. In this context the optimal-weight MME represents the ‘golden standard’ and the practically important question concerns the skill differences between the optimal weight and equal weight MME, and their performance relative to the single model; here the single model is usually taken to be the one with correct correlation time/damping.

Apart from validating the analytical estimates of §3, particular emphasis in this section is on the following themes:

- How significant are the differences in skill between the optimal-weight and equal weight MME’s?
- Are MME’s with good short prediction skill likely to have good medium range prediction skill?
- Given a collection of reduced-order models which are either underdamped or overdamped relative to the truth marginal dynamics, how does the structure of optimal-weight MME change depending on the prediction horizon? In particular:
  - When considering short and medium range predictions, is it always better to tune the individual models in MME for correct equilibrium statistics or is it better to constrain only the equilibrium statistics of MME?

The above themes appear recurrently throughout the remaining sections.
5.1 Tests of MME prediction skill in the context of initial value problem

We begin the analysis by considering the simplest possible configuration in which both the truth dynamics and the imperfect models in the Multi Model Ensemble are Gaussian. The truth dynamics is given by the two-dimensional Gaussian model outlined in §4.1 where the resolved dynamics is linearly coupled to the unresolved dynamics. The scalar imperfect Gaussian models for the resolved dynamics do not account for the unresolved processes which, in general, leads to model errors and associated information barriers to prediction improvement, as shown in [48, 43, 50] for single model prediction and §4.4 for MME prediction. One example involving this simple configuration was already shown in figure 1 of §2. Below, we expand the relevant analysis in order to provide a more complete picture of MME prediction improvement in this simplest possible non-trivial configuration.

In the second part of this section we discuss the essential ingredients necessary for improving predictions of non-Gaussian truth dynamics via the MME approach. To this end we employ the exactly solvable test model outlined in §4.2 for the truth dynamics and consider various aspects of predictive skill improvement via the MME approach; one example exploiting this configuration was already shown in figure 2 of §2. This non-Gaussian case where the resolved dynamics is nonlinearly coupled with the unresolved dynamics provides a very useful test bed for validating the analytical estimates derived §3 and it allows for considering the effects of some additional important details which are present in the analytical estimates but are not easily discernible in the analytical expressions of §3.

**Simple framework with Gaussian truth & Gaussian mixture MME**

In this case the truth dynamics is given by the two dimensional Gaussian model (33) and the MME density, $\pi^\text{MME}_t$, is a Gaussian mixture involving the imperfect model densities, $\pi^\text{m}_i$, associated with the one-parameter class $\mathcal{M}$ linear Gaussian Mean Stochastic models (33) with correct initial conditions and correct marginal equilibrium statistics for the resolved dynamics, i.e.,

$$
\mathcal{M} := \left\{ \pi^\text{M}_t(u) = N(\mu(t), R(t)) : \lim_{t \to \infty} P(\pi_t, \pi^\text{m}_i) = 0, \quad \pi^\text{m}_i(u) = N(\mu_0, R_0) \right\},
$$

where $P$ is the relative entropy in (2). Given the constraints on the initial conditions and the equilibrium distribution in the models (23) in the family $\mathcal{M}$, there is one free parameter left in the models (23) which we choose to the correlation time $\tau^\text{M}_i = 1/\gamma^\text{M}_i$. Therefore, the MME densities (1) can be written in this case as

$$
\pi^\text{MME} _t; \alpha, [\tau](u) = \sum_{i=1}^I \alpha_i \pi^\text{m}_i, \tau(u), \quad \alpha_i \geq 0, \quad \sum \alpha_i = 1,
$$

so that the time-dependent MME density, $\pi^\text{MME} _t; \alpha, [\tau](u)$, in (54) is parameterized by the weights vector $\alpha \equiv [\alpha_1, \ldots, \alpha_I]$ and the distribution of the correlation times denoted by $[\tau]$; here, we assume that $[\tau]$ is given by a vector of correlation times evenly distributed between $\tau_{\text{min}}$ and $\tau_{\text{max}}$

$$
[\tau] = \left\{ \tau_{\text{min}}, \tau_{\text{min}} + \Delta \tau, \ldots, \tau_{\text{min}} + (n-1)\Delta \tau, \tau_{\text{max}} \right\}, \quad \Delta \tau = (\tau_{\text{max}} - \tau_{\text{min}})/n,
$$

and that $\tau_{\text{trth}} \in [\tau]$ with $\tau_{\text{trth}}$ denoting the correct correlation time of the marginal dynamics $u(t)$ in (39). We adopt the following terminology for the structure of MME:

- **Balanced MME** is given by imperfect models (23) with correlation times $\tau^\text{M} = 1/\gamma^\text{M} \\{\tau^\text{M}_i\}_{i \in I} < \tau_{\text{trth}} < \{\tau^\text{M}_j\}_{j \in J}$. \#I = \#J and correct marginal equilibrium statistics for the resolved dynamics,
- **Underdamped MME** is given by imperfect models (23) with correlation times $\tau^\text{M}_i \geq \tau_{\text{trth}}$ and correct marginal equilibrium statistics for the resolved dynamics,
- **Overdamped MME** is given by imperfect models (23) with correlation times $\tau^\text{M}_i \leq \tau_{\text{trth}}$ and correct marginal equilibrium statistics for the resolved dynamics.
Figures 4, 5 illustrate two common features associated with the dependence of MME prediction skill on the structure of the imperfect model ensemble; the skill (i.e., statistical accuracy) of the imperfect predictions is assessed using two information measures exploiting the relative entropy (2): (i) the model error

\[ E_m^t = P(\pi_t(u), \pi_{t}^m(u)), \quad E_{\text{MME}}^t = P(\pi_t(u), \pi_{t}^{\text{MME}}(u)), \]

and (ii) the internal prediction skill

\[ I_t^u = P(\pi_t(u), \pi_{\text{eq}}(u)), \quad I_{t}^M = P(\pi_t(u), \pi_{t}^M(u)), \quad I_{t}^{\text{MME}} = P(\pi_t(u), \pi_{t}^{\text{MME}}(u)), \]

where the respective superscripts stand for either the information measures based on the single model \( M \) or the MME. The MME is a Gaussian mixture of MSMs (23) with different correlation times \( \tau_m \) and the optimal-weight MME is obtained by minimizing the relative entropy between the MME statistics and the marginal truth density.

Figure 4 shows the dependence of the prediction skill on the structure of MME (i.e., balanced, underdamped or overdamped) for the initial value problem for estimating the resolved dynamics \( u \) in the Gaussian truth (33) with hidden dynamics and perfect initial conditions in MME; the ensemble of initial conditions for the unresolved variable \( v \) in (33) is drawn from the equilibrium distribution \( v_0 \sim N(\langle v \rangle_{\text{eq}}, \text{Var}_{\text{eq}}[v]) \). While an improvement of predictive skill can be achieved for the underdamped MME, even for the equal-weight MME, there is no gain in prediction skill for the overdamped MME; for the balanced MME the predictive skill can be improved for the optimal-weight MME which requires good estimates of the truth dynamics and is generally unrealistic in practice. Note that in this Gaussian truth case the optimal-weight MME is a single Gaussian model; this is a common situation for Gaussian truth dynamics, especially for small initial covariance, but it is certainly not the possibility (see, for example, figures 5, 12).

Figure 5 shows an example of dependence of imperfect prediction skill on the spread of the statistical initial conditions in the initial value problem for the resolved dynamics \( u \) in the Gaussian truth (33) with hidden dynamics and perfect initial conditions in MME; in all cases shown the balanced MME is used which does not have improved skill for the equal-weight MME, as in figure 4. The interesting transition concerns the structure of the optimal-weight MME: for sufficiently small initial uncertainty in the statistical initial conditions the optimal MME is underdamped, while the overdamped MME becomes optimal for the distribution of initial conditions approaching the equilibrium distribution. This trend in the structure of MME with improved prediction skill is also reflected in the equal-weight MME when estimating the forced response (see figures 11-12), and it is in full agreement with FACT 9 of §3.3.2 and the discussion in §4.4.

Below we summarize the most important points illustrated in figures 4, 5:

- The equal-weights MME tends to outperform the single model predictions with correct correlation time \( \tau_{\text{truth}} \) provided that the MME is either underdamped or balanced (see (56) and figures 4, 5). The equal-weights MME containing overdamped MSMs tends to have a worse prediction skill than the single model predictions; see also Fact 8 of §3.3.1.

- Weight optimization in MME provides a significant prediction skill improvement for underdamped and balanced MME (see figures 1, 4, 5); however, this type of optimization is impractical since it requires good estimates of the truth dynamics.

- For a given spread \( \tau \) (55) of correlation times in MME with correct equilibrium and correct statistical initial conditions the prediction skill is not very sensitive to the number members in the MME. Optimizing the correlation times is impractical but improves the prediction skill; the improvement is more pronounced for increasing size of MME (not shown).

**Simple framework with non-Gaussian truth & Gaussian mixture MME**

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Here, we present numerical examples of the improvement of skill in imperfect predictions of non-Gaussian dynamics in the context of the initial value problem; the theoretical considerations associated with this configuration were presented in §3 and in particular in §3.1.3 and §3.3.1. We consider a configuration where the non-Gaussian truth dynamics is given by the exactly solvable model (39) with hidden dynamics that induces fluctuations in the effective damping in the resolved dynamics; this revealing test model was used previously in the context of uncertainty quantification in single model predictions in [10, 9, 50, 6]. As in the Gaussian case discussed above, the imperfect models in MME are in the class $M$ (53) of linear Gaussian Mean Stochastic models (23) so that the MME density $\pi_{t,\alpha,\gamma}^{MME}$ in (54) is given by the Gaussian mixture in (54) which is parameterized by the weights vector $\alpha$ and the distribution $[\gamma]$ in (55) of correlation times in the imperfect models (23). With the perfect model given by the non-Gaussian system with hidden dynamics described in §4.2 and the imperfect models given by the MSMs we have a potential for an intrinsic information barrier.

The results for this configuration are shown in the figures 6-10 for perfect statistical initial conditions and correct marginal equilibrium statistics in all models of MME. Similar to the Gaussian case discussed above, the skill of the imperfect statistical estimates is quantified using two information measures based on the relative entropy (2): the model error given by (57) and the internal prediction skill defined in (58). The single model prediction skill (green) is shown for the model $m_0$ with correct correlation time $\tau_{\text{trt}}$ of the resolved equilibrium dynamics $u(t)$. The optimal-weight Gaussian mixture of MSMs (23) with different correlation times $\tau_M$ is obtained by minimizing the relative entropy between the MME statistics and the marginal truth density, as in (7); recall that the optimal-weight MME corresponds to the information barrier in the MME predictions and it is useful for gauging the skill of equal-weight MME.

We focus on two extremes for the equal-weight MME:

- **Best equal-weight MME** corresponds to the ensemble with density $\pi_{t,\alpha,\gamma}^{MME}$ in (54) with $\alpha = 1/M$ and the smallest prediction error (57) within the examined spread $[\gamma] = [0 \enspace 11]$ of correlation times $\tau_M$ of the models in MME.

- **Worst equal-weight MME** corresponds to the ensemble with density $\pi_{t,\alpha,\gamma}^{MME}$ in (54) with with $\alpha = 1/M$ and the largest prediction error (57) within the examined spread $[\gamma] = [0 \enspace 11]$ of correlation times $\tau_M$ of the models in MME.

Figures 6-8 illustrate the dependence of the predictive skill of Gaussian mixture MME (54) as a function of increasing variance $\text{Var}(u)$ of the initial statistical conditions for the resolved variable $\pi_0(u)$ in the non-Gaussian truth dynamics (39). Three distinct cases for the truth dynamics are considered. In figure 6 the marginal equilibrium statistics of the truth is symmetric but non-Gaussian (see regime II in §4.2 and [7]) and the initial statistical conditions for the unresolved dynamics are in the stable dynamical regime of (39), i.e. $\pi_0(\gamma) = N(\alpha(\gamma)|_{eq}, \beta\text{Var}_{eq}[\gamma]), \alpha > 0, \beta \ll 1$. In figure 7 the initial statistical conditions for the unresolved dynamics are in the unstable dynamical regime of (39), i.e. $\pi_0(\gamma) = N(-\alpha(\gamma)|_{eq}, \beta\text{Var}_{eq}[\gamma]), \alpha > 0, \beta \ll 1$, and the initial stage of the truth evolution is characterized by a rapid transient dynamics. Finally, in figure 8 the marginal equilibrium statistics of the resolved dynamics $u$ in the truth is skewed (fat tailed with positive skewness) and the statistical initial conditions for the unresolved variable $\gamma$ coincide with the marginal equilibrium distribution. The prediction skill of the equal-weight MME is shown for the spread $[\gamma]$ in (55) with the best ‘all-time’ skill (solid blue) and for the spread $[\gamma]$ with the worst ‘all-time’ skill (dotted blue) within the maximum spread of $[\gamma]_{max} = 10 \tau_{\text{trt}}$, these two curves help judge the sensitivity of the equal weight MME to the spread of the correlation times in the ensemble which is further discussed in the subsequent figures.

Figures 9 and 10 show the optimal spread $[\gamma]$ in (55) of correlation times $\tau_M$ in the Gaussian mixture MME (54) grows with the uncertainty, $\text{Var}(u_0)$, of the initial condition in the resolved dynamics. Figure 9 shows the optimal spread for both the equal-weight and the optimal-weight MME with best ‘all-time’ prediction skill, while figure 10 shows analogous results for the two types of MME with best short-time prediction skill; in both figures the results are shown as a function of the the uncertainty, $\text{Var}(u_0)$, of the initial condition for the resolved dynamics in (39).

Based on the examples illustrated in figures 6-10, we recapitulate the general features of MME prediction as follows:
• For symmetric marginal attractor density $\pi_{eq}(u)$ of the truth the following facts are important:
  
  − MME prediction skill tends to be superior to that of the single model with correct correlation time $\tau_{trth}$ for the resolved dynamics except when $\pi_0(\gamma)$ is in unstable regime of the truth dynamics in (39).

  − The following trends in the structure of MME (cf (56)) are observed depending on the characteristics of the ensemble of initial conditions for the unresolved dynamics:
    
    * For the statistical initial conditions of the unresolved dynamics $\gamma$ in the stable regime of (39), i.e., $\pi_0(\gamma) = \mathcal{N}(\langle \gamma \rangle_{eq}, Var_{eq}[\gamma])$, $\alpha > 0, \beta \ll 1$, the optimal-weight MME (7) consists mostly of underdamped models relative to the single model $m_0$ with correct correlation time $\tau_{\text{MME}} = \tau_{trth}$ (figure 6).
    
    * For the statistical of initial conditions of $\gamma$ in (39) drawn from the equilibrium distribution, $\pi_0(\gamma) = \mathcal{N}(\langle \gamma \rangle_{eq}, Var_{eq}[\gamma])$, the optimal-weight MME (7) consists mostly of underdamped models (not shown).

  * For the statistical of initial conditions of $\gamma$ in the unstable regime of the truth dynamics (39), i.e., $\pi_0(\gamma) = \mathcal{N}(\langle \gamma \rangle_{eq}, Var_{eq}[\gamma])$, $\alpha > 0, \beta \ll 1$, the optimal-weight MME (7) consists mostly of overdamped models (figure 7).

  − The spread $[\tau]$ in (55) of correlation times $\tau^{\text{eq}}$ in the best ‘all-time’ equal-weight MME ($T \rightarrow \infty$ in (4)) shadows the spread of correlation times in the optimal-weight MME (see figure 9). The optimal spread $[\tau]$ in the Gaussian mixture MME (54) grows with the uncertainty, $Var_0[u]$, of the initial condition in the resolved dynamics (figure 9).

  − The spread $[\tau]$ in (55) of correlation times in the best ‘short-time’ equal-weight MME ($T \ll \tau_{trth}$ in (4)) is similar to that of the spread $[\tau]$ in the optimal-weight MME (7). The optimal spread $[\tau]$ in the Gaussian mixture MME (54) has a maximum for intermediate values of the uncertainty, $Var_0[u]$, of the initial condition in the resolved dynamics (figure 10).

  − The following trends in the structure of ‘all-time’ optimized MME (see (4)) are observed for varying uncertainty $Var[u_0]$ in the initial condition $\pi_0(u)$ for the resolved dynamics in the truth (39); see insets in figures 6-8:
    
    * For underdamped and balanced MME – from single model with largest possible $\tau^{m_0}$ for uncertainty $Var_{0}[u]$ approaching the equilibrium variance $Var_{eq}[u]$, to MME with bi-modal weight distribution for intermediate $Var_{0}[u]$, to two-model MME for deterministic initial conditions.

    * For overdamped MME – from single model for $Var_{0}[u] \sim Var_{eq}[u]$ with smallest possible $\tau^{m_0}$ to MME unimodal weight distribution for decreasing uncertainty $Var_{0}[u]$.

• For skewed marginal attractor density $\pi_{eq}(u)$ of the truth the following points are worth noting:

  − Prediction skill of equal-weight underdamped MME (see (56)) is good for sufficiently small uncertainty in the initial statistical conditions.

  − Prediction skill of equal-weight balanced MME (see (56)) is poor and comparable to that of the single model $m_0$ with correct correlation time $\tau_{trth}$. The imperfect prediction skill of the marginal truth dynamics with skewed equilibrium PDF improves for MME containing imperfect models with different equilibrium densities (not shown).

  − The optimal spread $[\tau]$ in (55) of correlation times $\tau^{m_0}$ in the Gaussian mixture MME is largely independent of the uncertainty, $Var_{0}[u]$, of the initial condition in the resolved dynamics.

• The above features are largely independent of the number of models in MME (not shown).
5.2 MME prediction of forced response

As discussed in §3, the sufficient condition for improving imperfect estimates of forced response of the truth dynamics to external perturbations can be obtained from the general condition (10); the simplified but revealing case in the Gaussian framework was discussed in §3.3. Moreover, the simplest non-trivial analytical example was discussed in §4.4. In this section we augment the analytical considerations of §3.3, and the asymptotic infinite-time results derived in §4.4, with simple numerical tests of the forced response estimation at finite times through a Gaussian mixture MME. We utilize the same setup as at the beginning of §5.1 where the truth dynamics is Gaussian and given by the model (33) with hidden dynamics that induces fluctuations in the resolved dynamics. The imperfect models in MME are in the class $M$ (53) of linear Gaussian Mean Stochastic models (23) so that the MME density $\pi^{\text{MME}}_{\tau,\alpha,\tau}$ is given by the Gaussian mixture in (54) which is parameterized by the weights vector $\alpha$ and the distribution $[\tau]$ (55) of correlation times in the imperfect models (23). As we will point out below, the qualitative understanding of the results below can be obtained with the help of the schematic figure 3 discussed in §3.

Figures 11 and 12 show two examples of imperfect prediction skill for the forced response of the resolved dynamics $u$ in the Gaussian model (33) with hidden/unresolved dynamics; the two cases correspond to the imperfect predictions with information barrier and without information barrier in the same class of imperfect models which were discussed in §4.4 for the infinite-time case. Similar to the initial value problem discussed in §5.1, the skill of the imperfect statistical estimates is quantified using two information measures based on the relative entropy (2): the model error given by (57) and the internal prediction skill defined in (58). The optimal-weight Gaussian mixture of MSMs (23) with different correlation times $\tau^{m}$ is obtained by minimizing the relative entropy between the MME statistics and the marginal truth density, as in (7). In contrast to the initial value problem, the initial statistical conditions coincide with the resolved equilibrium dynamics. The imperfect models in MME are in the class $M$ of imperfect Gaussian models (23); these simulations represent finite-time analogues of the infinite-time case discussed in §3.3. Moreover, the simplest non-trivial small perturbations $\delta F$ (see Appendix D and [49, 38, 2, 44, 27, 52, 42] for additional information).

Figure 11 shows the skill of imperfect predictions of the forced response of the truth dynamics $u$ in the Gaussian model (33) to small forcing perturbations when there is no ‘infinite-time’ information barrier (see §4.4) in the class $M$ (53) of the imperfect Gaussian models (23); these simulations represent finite-time analogues of the infinite-time configuration discussed in §4.4 for the three different structures of MME (see (56)). Here, the MME is created relative to the single model $M_{0}$ which is taken to be the one with correct correlation time, $\tau^{m_{0}} = \tau^{\text{truth}}$. As predicted in §4.4 based on the sufficient condition (52), the predictive skill of equal-weight MME is improved relative to the single model $M_{0}$ for any overdamped MME relative to $M_{0}$; additionally the equal-weight balanced MME also provides an improved skill of the forced response prediction. Recall that, based on the sufficient condition (32) in FACT 9 of §3.3.2, the improved predictive skill for the forced response is independent of the truth response in the covariance and depends on the difference of the responses in the mean.

Figure 12 shows the skill of imperfect predictions of the forced response of the truth dynamics $u$ in the Gaussian model (33) to small forcing perturbations when there is no ‘infinite-time’ information barrier (see §4.4) in the class $M$ (53) of imperfect Gaussian models (23). In this case we compare the predictive skill of two special single models with the three different types of MME defined in (56). The first single model $M_{0}$ has the correct correlation time $\tau^{\text{truth}}$ for the resolved equilibrium dynamics $u$; the correlation time $\tau^{\text{opt}}$ in the second single model $M_{0}$ guarantees its perfect infinite-time forced response, i.e. $\tau^{\text{opt}}$ is given by (50). The balanced, underdamped and overdamped MME defined in (56) are constructed relative to the model $M_{0}$ with correct correlation
time for the resolved unperturbed equilibrium dynamics. Similar to the case with information barrier in figure 11, the equal-weight overdamped or balanced MME provides improved prediction skill of the forced response. Moreover, the information barrier in the overdamped or balanced MME is significantly reduced through the MME approach provided that $m_* \notin \mathcal{M}$; in these cases the optimal-weight MME representing the information barrier of MME (see FACT 2 in §3) picks up the imperfect model with correlation time closest to $\tau^\text{opt}$ and the second time scale helps improve the short-time prediction skill (see generalized version of FACT 9 in Appendix A).

Below we summarize the most important points illustrated in figures 11 and 12:

- In contrast to the initial value problem, the equal-weights overdamped or balanced MME (see (56)) tends to outperform the single model predictions with correct correlation time $\tau^\text{truth}$ (figures 11 and 12). The equal-weights MME containing underdamped MSMs tends to have a worse prediction skill than the single model predictions; see also Fact 9 of §3.3.2 for the infinite-time case.

- When the model $m_*$ with perfect infinite-time forced response (see (50)) belongs to the class $\mathcal{M}$ of imperfect models only the short-time forced response prediction can be improved via the MME approach.

- Weight optimization in MME provides a significant prediction skill improvement for MME (see figures 1, 4, 5) over the equal-weight MME. While this type of optimization is impractical and it requires good estimates of the truth dynamics, it helps reveal the information barriers in the MME prediction; recall that the optimal-weight MME represents the information barrier for MME prediction with imperfect models in a given class $\mathcal{M}$ (see FACT 2 of §3 and figure 3). The following cases are worth noting:

  - **No information barrier in single model prediction** ($A < 0$ in the unresolved part of the truth (33))
    * If $m_0 \neq m_*$ with optimal damping $\gamma^m_*$ in the imperfect model (23), the MME approach can improve the infinite-time forced response prediction based on (52), see also figure 12. In particular the MME skill is improved for any overdamped MME with $\gamma^m_1 \geq \gamma^m_2$, see also figure 11. The above conclusion holds for any imperfect model (23) and, in particular, for the MSM with the correct correlation time $\tau^m_0 = \tau^\text{opt}$ in (50) which can be tuned based on the measurements of the resolved equilibrium dynamics of the truth.
    If, additionally, $m_* \notin \mathcal{M}$, the information barrier in MME can be reduced relative to the single model prediction (see also figure 3a).
    * If $m_0 = m_*$ with optimal damping $\gamma^m_*$ in the imperfect model (23) given in (i), the MME approach does not improve the infinite-time forced response prediction based on (52), see also figure 12. The information barrier in MME cannot be reduced relative to the single model prediction.

  - **Information barrier in the single model prediction** ($A > 0$ in the unresolved part of the truth (33))
    * The infinite-time forced response prediction is improved (at least) for any overdamped MME. The information barrier in MME prediction cannot be reduced relative to the single model prediction; this situation is depicted schematically in figure 3b. Recall that the model error of the optimal-weight MME, which corresponds to the information barrier of the class of models $\mathcal{M}$, coincides in such a case with the single optimal model $m_*$ (see figures 11-12 and figure 2c for analogous situation in the context initial value problem).

- Increasing the spread $[\tau]$ (55) of correlation times in overdamped MME with correct equilibrium and correct statistical initial conditions improves the MME prediction skill of the forced response.

- In a more general setting (see Appendix A), where only the equilibrium means are tuned, $\mu^m_0 = \mu_0$ but $R^m_0 \neq R_0$, the interplay between the truth and model response in both the mean and covariance are important. Underdamped MME helps improve the short-time imperfect predictions of the forced response predictions but it is not sufficient to guarantee the skill improvement. (Note also that in the bottom inset of figure 12 the presence of the second time scale closer to $\tau^\text{truth}$ makes the optimal-weight MME ‘less overdamped’ and improves the short range prediction skill.)
Figure 4: Prediction skill of 9-member MME for the initial value problem for the resolved dynamics $u$ in the Gaussian truth (33) with hidden dynamics and perfect initial conditions in MME for different classes of imperfect model ensembles: (top) balanced MME ($\{\tau^i\}_{i \in I} < \tau_{\text{trth}} < \{\tau^j\}_{j \in J}$, $|I| = |J|$), (middle) underdamped MME ($\tau^i \geq \tau_{\text{trth}}$), (bottom) overdamped MME ($\tau^i \leq \tau_{\text{trth}}$); the ensemble of initial conditions for the unresolved variable $v$ in (33) is drawn from the equilibrium $v_0 \sim \mathcal{N}(\langle v \rangle_{\text{eq}}, \text{Var}_{\text{eq}}[v])$. The MME is a Gaussian mixture of MSMs (23) with the spread of corecorrelation times $[\tau] = 0.5\tau_{\text{trth}}$ (see (55)); the optimal-weight MME is obtained by minimizing the relative entropy $\mathcal{P}(\pi(u), \pi_{\text{MME}}(u))$ between the MME statistics and the truth marginal density of associated with the resolved dynamics $u(t)$ in (33).

Truth parameters in (33): $A = -0.5, a = -5.5, \lambda_{1,2} = -1, -5; \sigma = 0.77, F_0 = 1, E = 0.01, \langle u \rangle_{\text{eq}} = 0.1, \langle v \rangle_{\text{eq}} = 1.35$.

Initial conditions (both truth and MME): $\langle u \rangle_0 = 1.05\langle u \rangle_{\text{eq}}, \langle v \rangle_0 = 1.1\langle v \rangle_{\text{eq}}, R_0 = 0.2R_{\text{eq}}$. 

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**Figure 5:** Prediction skill of 9-member MME for the initial value problem for the resolved dynamics $u$ in the Gaussian truth (33) with hidden dynamics and **perfect initial conditions** in MME for balanced MME (see (56)) and different initial covariances $R_0$; the ensemble of initial conditions for the unresolved variable $v$ in (33) is drawn from the unperturbed equilibrium $\gamma_0 \sim \mathcal{N}(v_{eq}, \text{Var}_{eq}[v])$. The MME is a Gaussian mixture of MSMs (23) with the spread of correlation times $[\tau] = 0.5 \tau_{trth}$ (see (55)); the optimal weight MME is obtained by minimizing the relative entropy $\mathcal{H}(\pi^t(u), \pi^{\text{MME}}(u))$ between the MME statistics and the truth marginal density of associated with the resolved dynamics $u(t)$ in (33).

Truth parameters in (33): $A = -0.5, a = -5.5, \Lambda_{1,2} = -1, -5; \sigma : 0.77, F_0 : 1, E = 0.01, \langle u \rangle_{eq} = 0.1, \langle v \rangle_{eq} = 1.35$.

Initial conditions (both truth and MME):
Mean: $\langle u \rangle_0 = 1.1 \langle u \rangle_{eq}, \langle v \rangle_0 = 1.05 \langle v \rangle_{eq}$.
Covariance - (top) $R_0 = 0.05 R_{eq}$; (middle) $R_0 = 0.5 R_{eq}$; (bottom) $R_0 = 0.9 R_{eq}$.
Figure 6: Prediction skill of 17-model MME for the initial value problem for the resolved dynamics $u$ in SPEKF (39) with with perfect statistical initial conditions in MME for different uncertainties $\text{Var}[u]$: the ensemble of initial conditions of the unresolved variable $\gamma$ in SPEKF is in the stable regime $\gamma_0 \sim \mathcal{N}(1.8\langle \gamma \rangle_{eq}, 0.2\text{Var}_{eq}[\gamma])$. The MME is a Gaussian mixture of MSMs (23) with correlation times $\tau_{ui}$ sampled symmetrically around the correct correlation time $\tau_{corr}^{true}$ (i.e., balanced MME in (56)) with the spread $[\tau]$ in $\pi_{true}[\tau]$ defined in (55); the optimal-weight MME (magenta) is obtained by minimizing the relative entropy $\mathcal{D}(\pi_{true}(u), \pi_{MME}(u))$ between the statistics of MME and the marginal statistics of the resolved truth dynamics $u(t)$ in (39). Truth parameters: $\gamma = 1.5, d_v = 2, \sigma_x = 2, \sigma_u = 0.5, F = 0$.

**Initial conditions** (both truth and MME):

- (top) $\text{Var}[u] = 0.01\text{Var}_{eq}[u]$, $\langle u \rangle_0 = 0.4\langle u \rangle_{eq}$, $\langle \gamma \rangle_0 = 1.2\langle \gamma \rangle_{eq}$, $\text{Var}[\gamma] = 0.2\text{Var}_{eq}[\gamma]$.
- (middle) $\text{Var}[u] = 0.25\text{Var}_{eq}[u]$, $\langle u \rangle_0 = 0.4\langle u \rangle_{eq}$, $\langle \gamma \rangle_0 = 1.2\langle \gamma \rangle_{eq}$, $\text{Var}[\gamma] = 0.2\text{Var}_{eq}[\gamma]$.
- (bottom) $\text{Var}[u] = 0.95\text{Var}_{eq}[u]$, $\langle u \rangle_0 = 0.4\langle u \rangle_{eq}$, $\langle \gamma \rangle_0 = 1.2\langle \gamma \rangle_{eq}$, $\text{Var}[\gamma] = 0.2\text{Var}_{eq}[\gamma]$.
Figure 7: Prediction skill of 17-model MME for the initial value problem for the resolved dynamics $u$ in SPEKF (39) with with perfect statistical initial conditions in MME for different uncertainties $\text{Var}[u]$; the ensemble of initial conditions of the unresolved variable $\gamma$ in SPEKF is in the unstable regime $\gamma_0 \sim \mathcal{N}(-1.2\gamma_{eq}, 0.2\text{Var}_{eq}[\gamma])$. The MME is a Gaussian mixture of MSMs (23) with correlation times $\tau^{MMS}$ sampled symmetrically around the correct correlation time $\tau^{\text{trth}}$ (i.e., balanced MME in (56)) with the spread $[\tau]$ in $\tilde{t}_{\text{corr}}^{\text{MME}}[\gamma]$ defined in (55); the optimal-weight MME (magenta) is obtained by minimizing the relative entropy $\mathbb{P}(\pi^M(u), \pi^{\text{MME}}(u))$ between the statistics of MME and the marginal statistics of the resolved truth dynamics $u(t)$ in (39). Truth parameters in (39): $\hat{\gamma} = 1.5, d_\gamma = 2, \sigma_\gamma = 2, \sigma_u = 0.5, F = 0$.

Initial conditions (both truth and MME):

(top) $\text{Var}[u] = 0.01\text{Var}_{eq}[u], \quad \langle u \rangle_0 = 0.4\langle u \rangle_{eq}, \quad \langle \gamma \rangle_0 = -1.2\langle \gamma \rangle_{eq}, \quad \text{Var}[\gamma] = 0.2\text{Var}_{eq}[\gamma]$.

(middle) $\text{Var}[u] = 0.1\text{Var}_{eq}[u], \quad \langle u \rangle_0 = 0.4\langle u \rangle_{eq}, \quad \langle \gamma \rangle_0 = -1.2\langle \gamma \rangle_{eq}, \quad \text{Var}[\gamma] = 0.2\text{Var}_{eq}[\gamma]$.

(bottom) $\text{Var}[u] = 0.95\text{Var}_{eq}[u], \quad \langle u \rangle_0 = 0.4\langle u \rangle_{eq}, \quad \langle \gamma \rangle_0 = -1.2\langle \gamma \rangle_{eq}, \quad \text{Var}[\gamma] = 0.2\text{Var}_{eq}[\gamma]$.
Skewed non-Gaussian truth, IVP with perfect stat. ini. cond. in stable regime

![Model Error](image1)

![Internal prediction skill](image2)

![Model Error](image3)

![Internal prediction skill](image4)

![Model Error](image5)

![Internal prediction skill](image6)

Figure 8: Prediction skill of 17-model MME for the initial value problem for the resolved dynamics $u$ in SPEKF (39) with perfect statistical initial conditions in MME for different uncertainties $\text{Var}_0[u]$; the ensemble of initial conditions of the unresolved variable $\gamma$ in SPEKF is drawn from the equilibrium distribution $\gamma_0 \sim \mathcal{N}(\gamma_{eq}, \text{Var}_{eq}[\gamma])$. The MME is a Gaussian mixture of MSMs (23) with correlation times $\tau_{\text{trth}}$ sampled symmetrically around the correct correlation time $\tau_{\text{trth}}$ (i.e., balanced MME in (56)) with the spread $[\tau]$ in $\tau_{\text{trth}}$ defined in (55); the optimal-weight MME (magenta) is obtained by minimizing the relative entropy $\mathcal{P}(\sigma(u), \sigma_{\text{MME}}(u))$ between the statistics of MME and the marginal statistics of the resolved truth dynamics $u(t)$ in (39). Truth parameters in (39): $\gamma = 1.5, d_\gamma = 10, \sigma_\gamma = 2, \sigma_u = 2, F = 1$.

Initial conditions (both truth and MME):

(top) $\text{Var}_0[u] = 0.01 \text{Var}_{eq}[u]$, $\langle u \rangle_0 = 0.1 \langle u \rangle_{eq}$, $\langle \gamma \rangle_0 = \langle \gamma \rangle_{eq}$, $\text{Var}_0[\gamma] = \text{Var}_{eq}[\gamma]$.

(middle) $\text{Var}_0[u] = 0.5 \text{Var}_{eq}[u]$, $\langle u \rangle_0 = 0.1 \langle u \rangle_{eq}$, $\langle \gamma \rangle_0 = \langle \gamma \rangle_{eq}$, $\text{Var}_0[\gamma] = \text{Var}_{eq}[\gamma]$.

(bottom) $\text{Var}_0[u] = 0.95 \text{Var}_{eq}[u]$, $\langle u \rangle_0 = 0.1 \langle u \rangle_{eq}$, $\langle \gamma \rangle_0 = \langle \gamma \rangle_{eq}$, $\text{Var}_0[\gamma] = \text{Var}_{eq}[\gamma]$. 

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Symmetric non-Gaussian truth attractor density $\pi_{eq}(u)$

Skewed truth attractor density $\pi_{eq}(u)$

Figure 9: Model error (57) and spread $[\tau]$ (55) of correlation times in “all-time” optimal Gaussian mixture MME with density $\pi_{\text{sum}}^{\alpha}[\tau]$ as a function of the uncertainty $\text{Var}[u_0]$ in the initial condition for the resolved dynamics in the SPEKF system (39). Balanced MME (56) is used with correlation times $\tau^{\text{sym}}$ symmetrically distributed around the true correlation time; $\tau^{\text{true}} \approx 0.5$; blue/circle curves correspond to the equal-weight MME with the smalls error for given $\text{Var}[u_0]$; magenta/star curves correspond to optimal-weight MME which is obtained via relative entropy minimazation for all time (i.e., $T \rightarrow \infty$ in (4)) by tuning the weights $\alpha$ of the ensemble members. The structure of the optimal-weight MME (7) is indicated in the respective insets. Three ensembles of initial conditions for the unresolved variable $\gamma$ in the truth (39) are used:

(a) $\gamma_0$ is in the stable regime $\langle \gamma \rangle_0 = 1.2 \langle \gamma \rangle_{eq}, \text{Var}[\gamma] = 0.2 \text{Var}_{eq}[\gamma]$;
(b) $\gamma_0$ has climatological distribution $\langle \gamma \rangle_0 = \langle \gamma \rangle_{eq}, \text{Var}[\gamma] = \text{Var}_{eq}[\gamma]$;
(c) $\gamma_0$ is in the unstable regime $\langle \gamma \rangle_0 = -1.2 \langle \gamma \rangle_{eq}, \text{Var}[\gamma] = 0.2 \text{Var}_{eq}[\gamma]$.

Truth parameters in (39): $\hat{\gamma} = 1.5, \sigma_\gamma = 2, \sigma_u = 0.5$, (top) $F = 0$, (bottom) $F = 1$. 

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Figure 10: Model error (57) and spread $[\tau]$ (55) of correlation times in “short-time” optimal Gaussian mixture MME with density $\pi_{\text{eq}}(u)$ as a function of the uncertainty $\text{Var}[u_0]$ in the initial condition for the resolved dynamics in the SPEKF system (39). Balanced MME (56) is used with correlation times $\tau_{\text{eq}}$ symmetrically distributed around the true correlation time; $\tau_{\text{tr}} \approx 0.5$; blue/circle curves correspond to the equal-weight MME with the smallest error for given $\text{Var}[u_0]$; magenta/star curves correspond to optimal-weight MME which is obtained via relative entropy minimization for short-times (i.e., $T = 0.2\tau_{\text{tr}}$ in (4)) by tuning the weights $\alpha$ of the ensemble members. Three ensembles of initial conditions for the unresolved variable $\gamma$ in the truth (39) are used: (a) $\gamma_0$ is in the stable regime $\langle \gamma \rangle = 1.8\langle \gamma \rangle_{\text{eq}}, \text{Var}[\gamma] = 0.2\text{Var}_{\text{eq}}[\gamma]$, (b) $\gamma_0$ has climatological distribution $\langle \gamma \rangle = \langle \gamma_{\text{att}} \rangle, \text{Var}[\gamma_0] = \text{Var}[\gamma_{\text{att}}]$, (c) $\gamma_0$ is in the unstable regime $\langle \gamma \rangle = -0.8\langle \gamma \rangle_{\text{eq}}, \text{Var}[\gamma_0] = 0.2\text{Var}_{\text{eq}}[\gamma]$.

The optimal-weight MME for the initial (c) consists of overdamped imperfect models, while the MME in (a) and (b) consists mostly of underdamped imperfect models.

Truth parameters: $\tilde{\gamma} = 1.5, d = 2, \sigma = 2, \sigma_\alpha = 0.5$, (top) $F = 0$, (bottom) $F = 1$. 

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Forced response prediction, Gaussian truth with information barrier, perfect stat. ini. cond.

Figure 11: Skill of 9-member MME for predicting the forced response (see §4.4) of the resolved dynamics $u$ in the Gaussian truth (33) with hidden dynamics and perfect initial conditions in MME for different classes of imperfect model ensembles: (top) balanced MME ($\{\tau_{\text{m}}^i\}_{i \in I} < \tau_{\text{thr}}$, $\#I = \#J$), (middle) underdamped MME ($\tau_{\text{m}}^i \geq \tau_{\text{thr}}$), (bottom) overdamped MME ($\tau_{\text{m}}^i \leq \tau_{\text{thr}}$); the ensemble of initial conditions for the unresolved variable $v$ in (33) is drawn from the unperturbed equilibrium $\gamma_0 \sim N(\langle v \rangle_{\text{eq}}, \text{Var}_{\text{eq}} [v])$. The MME is a Gaussian mixture of MSMs (23) with the spread of correlation times $\tau_{\text{m}}^i = 0.8 \tau_{\text{thr}}$ (see (55)); the optimal weight MME is obtained by minimizing the relative entropy $\mathcal{P}(\pi^t(u), \pi_{\text{MME}}^t(u))$ between the MME statistics and the least-biased truth density.

Truth parameters in (33): $A = 0.5, \alpha = -5.5, \lambda_{1,2} = -1, -4, \sigma : 0.63, F_0 : -0.8, E = 0.01, \langle u \rangle_{\text{eq}} = 0.1, \langle v \rangle_{\text{eq}} = 1.35$.

Forcing (both truth and MME):
$F(t) = F_0$ for $t \leq 0$, $F(t) = F_0(1 + 0.05t)$ for $0 < t \leq 1$, $F(t) = F_0(1 + 0.05)$ for $t > 1$.  

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Forced response prediction, Gaussian truth without information barrier, perfect stat. ini. cond.

Figure 12: Skill of 9-member MME for predicting the forced response (see §4.4) of the resolved dynamics $u$ in the Gaussian truth (33) with hidden dynamics and perfect initial conditions in MME for different classes of imperfect model ensembles: (top) balanced MME $\{x^{\text{bal}}_j\}_{j \leq t} < \tau^{\text{truth}} < \{x^{\text{im}}_j\}_{j \leq t}$. #I = #J. (middle) underdamped MME $u^{\text{im}} \geq \tau^{\text{truth}}$. (bottom) overdamped MME $u^{\text{im}} \leq \tau^{\text{truth}}$; the ensemble of initial conditions for the unresolved variable $v$ in (33) is drawn from the unperturbed equilibrium $\gamma_0 \sim N(\langle v \rangle_{eq}, \text{Var}_{eq}[v])$. The MME is a Gaussian mixture of MSMs (23) with the spread of MME weights $\lambda_j = \#\text{MME weights}$.

Truth parameters in (33): $A = -5.5, a = -5.5, \lambda_{1,2} = -1, -10; \sigma : 1.48, F_0 : 0.18, E = 0.01, \langle u \rangle_{eq} = 0.1, \langle v \rangle_{eq} = 0.37$. Forcing (both truth and MME): $F(t) = F_0$ for $t \leq 0, F(t) = F_0(1 + 0.05t)$ for $0 < t \leq 1, F(t) = F_0(1 + 0.05)$ for $t > 1$. 

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6 Conclusions

In this work we developed a mathematical framework, rooted in information theory, for a systematic assessment of the predictive skill of Multi Model Ensemble (MME) prediction which is aimed at improving the accuracy of imperfect predictions through combining a collection of forecasts obtained from different models with model error. Predicting complex high-dimensional turbulent systems based on imperfect models and sparse observations of some coarse-grained system variables is a notoriously difficult problem which is, nevertheless, essential in many applied sciences (e.g., [16, 63, 12, 59, 14, 18, 33]). Despite the increasingly common use of the MME approach in such applications, especially in the climate and atmospheric sciences (e.g., [62, 69, 15, 73, 74, 70, 71]), the mathematical framework justifying this technique was lacking. Consequently, many heuristic procedures developed in the context of MME predictions in the hope of mitigating model error lack systematic guidelines for constructing model ensembles with improved predictive skill. For example, it is generally not obvious which imperfect models to include in the ensemble forecast and what weights to assign to the individual models in MME.

Here, we focused on uncertainty quantification and systematic understanding of the benefits and limitations associated with the MME approach, as well as on the development of practical guidelines and design principles for constructing model ensembles with improved predictive skill. The statistical prediction framework can be utilized in two different contexts: First, when dealing with deterministic imperfect models, one can consider a time-dependent probability density function (PDF) constructed by initializing the model from a given PDF of initial conditions. Second, the statistical prediction framework arises naturally when using stochastic reduced-order models in imperfect predictions of the resolved truth dynamics. The main issues discussed in the context of MME predictions were the following:

(I) The advantages/disadvantages of the MME framework relative to using a single model predictions with an ensemble of initial conditions. In particular,

- Derivation of the sufficient condition guaranteeing improvement of the skill (statistical accuracy) of MME predictions relative to the single model predictions (see (10) and §3).

(II) Sensitivity of the MME skill to the unresolved truth dynamics, and guidelines for constructing MME for best prediction skill at short, medium and long time ranges (see §3, §5 and Appendices B, C).

We showed that a particularly useful insight into this problem could be achieved within the stochastic-statistical framework which exploits tools from information theory and is capable of addressing the issue of statistical fidelity of imperfect predictions of the truth dynamics in a systematic fashion. The use of information theory and the fluctuation-dissipation theorem in the context of improving imperfect predictions in the presence of model error has been extensively studied before in the ‘single model’ setup (see, for example, [35, 45, 36, 51, 43, 52, 22, 10, 50]); here we extended this approach to the Multi Model Ensemble case which provides a concise and much needed mathematical framework for assessing the predictive skill improvement through the MME approach. Based on the information-theoretic considerations, we derived a simple condition (10) which guarantees predictive skill improvement of statistical predictions within the MME framework; this sufficient condition stems from the convexity of relative entropy (2) which was used as a measure of the lack of information in the imperfect models relative to the resolved characteristics of the truth dynamics. We showed that the sufficient condition (10) for MME skill improvement can be practically implemented for improving imperfect prediction of the forced response of the truth equilibrium dynamics to external perturbations with the help of linear response theory and the ‘fluctuation-dissipation’ approach for forced dissipative systems (see, e.g., [49, 38, 2, 44, 27, 52, 42])). When considering the initial value problem the practical implementation of the condition for skill improvement through MME is more involved but techniques similar to those discussed in [23, 24, 25] could be used to effectively assess the skill of a given ensemble of imperfect models. Moreover, the information-theoretic approach advocated here allows to understand why some MME configurations which lead to predictive skill improvement over a single model do not reduce the overall information barrier to prediction improvement within a given family of models; this was illustrated further in §4.4 using a simple but revealing example in the context of forced response predictions. A set of particularly useful results was derived and discussed in §3.3 in the Gaussian framework which utilizes Gaussian models in the Multi Model Ensembles; this approach provides useful
intuition and guidelines in more complex cases in the general results of §3. The general theoretical results were validated and illustrated in §5 which combines the analytical estimates of §3 with simple numerical tests based on statistically exactly solvable Gaussian and non-Gaussian test models described in §4.

Although we focused on mitigating model error through the Multi Model Ensemble forecasting, the ultimate goal in imperfect reduced-order prediction should involve a synergistic approach that combines MME forecasting, data assimilation [19, 54, 8, 11], and improving individual models through various stochastic superparameterization [28, 53], and reduced subspace closure techniques [66, 67, 65]. The natural and important extension of this work involves combining the MME framework for improving imperfect predictions with MME approach to data assimilation/filtering in high-dimensional turbulent systems [54] based on imperfect models and sparse observations of some coarse-grained system variables. Such a combined framework, blending the MME approach to data assimilation and imperfect forecasts, should provide a valuable tool for improving real-time predictions in complex partially observed dynamical systems.

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A Some simple proofs of general facts from §3

Here, we complement the discussion of §3 by providing simple proofs of the facts established in that section.

Proof of the sufficient condition in (8): The proof relies on the convexity properties of the relative entropy (e.g., [13, 49]), which leads to the following upper bound on the lack of information in the MME mixture density $\pi^{\text{MME}}_t$ (1) and the marginal truth density $\pi_t$

$$
P(\pi_t, \pi^{\text{MME}}_t) = P(\pi_t, \sum_i \alpha_i \pi^M_i) \leq \sum_i \alpha_i P(\pi_t, \pi^M_i) = \sum_{i \neq \diamond} \alpha_i P(\pi_t, \pi^M_i) + \alpha_{\diamond} P(\pi_t, \pi^M_{\diamond}). \quad (60)
$$

Rearranging the terms in (60) leads to the sufficient condition (8) for improving predictions via MME relative to the predictions of the single model $\pi^M_{\diamond}$. The important observation leading to the practically implementable form (10) of the condition in (8) is associated with the general fact [49] that, given the least-biased density $\pi^L_t$ of the truth based on measured $L$ moment constraints, the relative entropy $P(\pi_t, \pi^M_t)$ can be written as

$$
P(\pi_t, \pi^M_t) = P(\pi_t, \pi^L_t) + P(\pi^L_t, \pi^M_t), \quad (61)
$$

where the first term, representing the intrinsic information barrier between the truth density and its least-biased approximation, is independent of the model density $\pi^M_t$; consequently the first term in (61) drops out after substitution into (8), leading to the practical representation (10).

Proof of FACT 4: The proof of this fact is straightforward and follows by direct calculation but consists of two steps:

1) We start by rewriting the condition (10) in terms of the least-biased of the truth $\pi_t$ and $\pi^{M_0}_t$ defined in (11) densities which leads to

$$
P(\pi^L_t, \pi^{M_0}_{M_0}) > \sum_{i \neq \diamond} \beta_i \int \pi^L_t \left[ \log \frac{\pi^{M_1}_{L_2}}{\pi^M_{L_1}} - \log \frac{\pi^{M_0}_{M_0}}{\pi^{M_0}_{M_0}} \right], \quad (62)
$$
where the last term represents expected value, with respect to \( \pi_t^{M,i} \), of the discrepancy between the imperfect model densities and their least-biased approximations; note that this last term vanishes identically when the MME contains only least biased models, i.e., \( \pi_t^{M,i} = \pi_t^M \).

2) Next, we notice that the relative entropy between two least biased densities \( \pi_t^{L} \) and \( \pi_t^{M,L} \) is given by

\[
\mathcal{P}(\pi_t^{L}, \pi_t^{M,L}) = \log C_t^M + \theta_t^M \cdot \bar{E}_t - \left( \log C_t + \theta_t \cdot \bar{E}_t \right) = \log \frac{C_t^M}{C_t^L} + (\theta_t^M - \theta_t) \cdot \bar{E}_t, \tag{63}
\]

where \( \bar{E}_t \) is the vector of expectations of the functionals \( E_i \) defined in (12) with respect to the truth marginal density \( \pi_t \), and the Lagrange multipliers in (11), \( \theta_t = \theta(\bar{E}_t) \), \( \theta_t^M = \theta^M(\bar{E}_t^M) \), are defined as

\[
\theta_t = \left\{ (\theta_1(t), \ldots, \theta_{l_2}(t)) \right\}^T, \quad \theta_t^M = \left\{ (\theta_1(t), \ldots, \theta_{l_2}(t), 0, \ldots, 0_{l_2}) \right\}^T, \quad \text{if } L_1 \geq L_2,
\]

\[
\theta_t = \left\{ (\theta_1(t), \ldots, \theta_{l_2}(t)) \right\}^T, \quad \text{if } L_1 < L_2.
\]

while the normalization constants in the least biased densities are \( C_t = C(\bar{E}_t) \), \( C_t^M = C^M(\bar{E}_t^M) \).

The expression for the relative entropy in (63) is straightforward to derive and it follows from substituting (11) into the general definition of the relative entropy in (2) which leads to

\[
\mathcal{P}(\pi_t^{L}, \pi_t^{M,L}) = \log \frac{C_t^M}{C_t^L} + \sum_i (\theta_t^M(t) - \theta_t(t)) \int \pi_t^{L}(u) E_i(u) du = \log \frac{C_t^M}{C_t^L} + (\theta_t^M - \theta_t) \cdot \bar{E}_t, \tag{64}
\]

where \( \bar{L} = \max\{L_1, L_2\} \).

The condition in (13) is obtained by combining (62) with (63). □

**Proof of FACT 5:** The condition in (17) for improvement of the prediction skill via MME obtained by perturbing single model predictions can be obtained in the least-biased density representation as follows: Consider the condition (13) in the case when the ensemble members \( m_i \in \mathcal{M} \) are obtained from the single model \( m_o \in \mathcal{M} \) through perturbing some parameters of the single model; we assume that the statistics of the model depends smoothly on these parameters and that the perturbations are non-singular (which required minimal assumptions [30] of hypoelliptic noise in the truth dynamics) so that the evolution of the statistical moments \( \bar{E}_t^{M,i} \) for the ensemble members can be written as

\[
a) \quad \bar{E}_t^{M,i} = \bar{E}_t^{M_0} + \epsilon \bar{E}_t^{M}, \quad \epsilon \ll 1, \tag{65}
\]

\[
b) \quad \theta_t^{M,i} = \theta_t^{M_0} + \epsilon \theta_t^{M_1} (\bar{E}_t^{M_1}) + \mathcal{O}(\epsilon^2), \tag{66}
\]

\[
c) \quad C_t^{M,i} = C_t^{M_0} (1 - \epsilon \theta_t^{M_1} \cdot \bar{E}_t^{M_0}) + \mathcal{O}(\epsilon^2), \tag{67}
\]

where

\[
\theta_t^{M_1} = \left( \bar{E}_t^{M_0} \cdot \nabla \theta_{1|\epsilon=0}, \bar{E}_t^{M_0} \cdot \nabla \theta_{2|\epsilon=0}, \ldots, \bar{E}_t^{M_0} \cdot \nabla \theta_{l_2|\epsilon=0} \right)^T. \tag{68}
\]

The lack of information in the perturbed least-biased density, \( \pi_t^{M,i} \), of the imperfect model relative to the least-biased perturbation of the truth, \( \pi_t^{L} \), can be expressed through (65)-(68) in the following form

\[
\mathcal{P}(\pi_t^{L}, \pi_t^{M,L}) = \log \frac{C_t^{M,i}}{C_t} + (\theta_t^{M_1} - \theta_t) \cdot \bar{E}_t = \mathcal{P}(\pi_t^{L}, \pi_t^{M_0}) + \epsilon \theta_t^{M_1} (\bar{E}_t - \bar{E}_t^{M_0}) + \mathcal{O}(\epsilon^2), \tag{69}
\]

which is obtained by combining (65)-(67). Substituting (69) into the general condition (13) leads to the desired condition (17). □
The proof of the condition (19) follows by direct calculation. Consider the evolution of the truth probability density in the form (18). The relative entropy $\mathcal{P}(\pi_t, \pi_t^{M_i})$ can be written as

$$\mathcal{P}(\pi_t, \pi_t^{M_i}) = \mathcal{P}(\pi_0, \pi_0^{M_i}) + \int du \delta \hat{\pi} \log \frac{\pi_0}{\pi_0^{M_i}} + \int du \pi_t \left(1 + \delta \hat{\pi}_0 \right).$$  \hfill (70)

Substituting (70) into the general condition (13) leads to the desired condition (19). □

**Proof of FACT 7:** The condition in (20) for improvement of the prediction skill via MME in the context of initial value problem can be obtained as follows: Consider perturbations of the true expected values $\mathbf{E}_t$ of the functionals $E_i(u)$ with respect to the truth marginal density $\pi_t(u)$;

$$\mathbf{E}_t = \mathbf{E}_0 + \delta \mathbf{E}_t, \quad \theta_t = \tilde{\theta}_0 + \delta \tilde{\theta}_t(\mathbf{E}_t), \quad \mathbf{E}_t=0 = \tilde{\theta}_{t=0} = 0,$$

so that

$$C_t = C_0 \left(1 - \delta \tilde{\theta}_t \cdot \mathbf{E}_0\right) + \mathcal{O}(\delta^2).$$ \hfill (72)

The lack of information in (10) between the least-biased approximation of the truth $\pi_t^{b,1}$ and the imperfect model density $\pi_t^{b,1}$ can be written as

$$\mathcal{P}(\pi_t^{b,1}, \pi_t^{M_i}) = \mathcal{P}(\pi_0^{b,1}, \pi_0^{M_i}) + \int du \pi_t^{b,1} \log \frac{\pi_t^{M_i}}{\pi_t^{b,1}},$$ \hfill (73)

similarly to the result leading to (62). The lack of information in the perturbed least-biased density, $\pi_t^{M_i,b,1}$, of the imperfect model relative to the least-biased perturbation of the truth, $\pi_t^{b,1}$, can be expressed through (65)-(68) in the following form

$$\mathcal{P}(\pi_t^{b,1}, \pi_t^{M_i,b,1}) = \mathcal{P}(\pi_0^{b,1}, \pi_0^{M_i}) + \delta (\tilde{\theta}_0^{M_i} - \theta_0) \cdot \mathbf{E}_t + \log \left(1 - \delta \tilde{\theta}_t \cdot \mathbf{E}_0\right) + \delta \tilde{\theta}_t \delta \mathbf{E}_t \mathbf{E}_t,$$

where the last two terms in (74) are independent of the model $M_i$. Substituting (74) into the general condition (13) leads to the desired condition (20). □

**Proof of FACT 8:** The proof of the condition (28) is simple but tedious and follows from the short-time asymptotic expansion of the relative entropy between the Gaussian truth and the Gaussian models.

Consider the state vector $u \in \mathbb{R}^K$ for resolved dynamics and assume that short-times the statistics of the Gaussian truth density $\pi_t \equiv \mathcal{N}(\mu_t, R_t)$ and of the Gaussian model density $\pi_t^{M_i} \equiv \mathcal{N}(\mu_t^{M_i}, R_t^{M_i})$ are

$$\mu_t = \mu_0 + \delta \tilde{\mu}_t, \quad R_t = R_0 + \delta \tilde{R}_t, \quad \delta \ll 1,$$ \hfill (75)

and

$$\mu_t^{M_i} = \mu_0^{M_i} + \delta \tilde{\mu}_t^{M_i}, \quad R_t^{M_i} = R_0^{M_i} + \delta \tilde{R}_t^{M_i}, \quad \delta \ll 1.$$ \hfill (76)

Then, the relative entropy between the Gaussian truth density $\pi_t^{G}$ and a Gaussian model density $\pi_t^{M_i}$

$$\mathcal{P}(\pi_t^{G}, \pi_t^{M_i}) = \frac{1}{2} (\mu_t - \mu_t^{M_i})^T (R_t^{M_i})^{-1} (\mu_t - \mu_t^{M_i}) + \frac{1}{2} \text{tr} [R_t (R_t^{M_i})^{-1}] - \ln \det \left[R_t (R_t^{M_i})^{-1}\right] - K,$$ \hfill (77)

can be expressed as

$$\mathcal{P}(\pi_t^{G}, \pi_t^{M_i}) = \mathcal{P}(\pi_0^{G}, \pi_0^{M_i}) + \delta (X^\mu + X^R) + \delta^2 (Y^\mu + Y^{\mu,R} + Y^{R,R}) + \mathcal{O}(\delta^3),$$ \hfill (78)
where the respective coefficients in the above expansion are given by

\[
X^\mu = \frac{1}{2} \left[ (\bm{\mu}_0 - \bm{\mu}^{M_i}_0)^T (R_0^{M_i})^{-1} (\bar{\bm{\mu}}_t - \bar{\bm{\mu}}^{M_i}_t) + (\bar{\bm{\mu}}_t - \bar{\bm{\mu}}^{M_i}_t)^T (R_0^{M_i})^{-1} (\bm{\mu}_0 - \bm{\mu}^{M_i}_0) \right],
\]

\[
X^R = -\frac{1}{2} (\bm{\mu}_0 - \bm{\mu}^{M_i}_0)^T (R_0^{M_i})^{-1} \bar{R}_t^{M_i} (R_0^{M_i})^{-1} (\bm{\mu}_0 - \bm{\mu}^{M_i}_0)
+ \frac{1}{4} \text{tr} \left[ (I - R_0(R_0^{M_i})^{-1}) \bar{R}_t^{M_i} (R_0^{M_i})^{-1} \right]
+ \frac{1}{4} \text{tr} \left[ \bar{R}_t (R_0^{M_i})^{-1} \right],
\]

\[
Y^{\mu,\mu} = \frac{1}{2} (\bar{\bm{\mu}}_t - \bar{\bm{\mu}}^{M_i}_t)^T (R_0^{M_i})^{-1} (\bar{\bm{\mu}}_t - \bar{\bm{\mu}}^{M_i}_t),
\]

\[
Y^{\mu,R} = \frac{1}{2} \left[ (\bm{\mu}_0 - \bm{\mu}^{M_i}_0)^T (R_0^{M_i})^{-1} \bar{R}_t^{M_i} (R_0^{M_i})^{-1} (\bar{\bm{\mu}}_t - \bar{\bm{\mu}}^{M_i}_t)
+ (\bar{\bm{\mu}}_t - \bar{\bm{\mu}}^{M_i}_t)^T (R_0^{M_i})^{-1} \bar{R}_t^{M_i} (R_0^{M_i})^{-1} (\bm{\mu}_0 - \bm{\mu}^{M_i}_0) \right],
\]

\[
Y^{R,R} = \frac{1}{2} \left[ (\bm{\mu}_0 - \bm{\mu}^{M_i}_0)^T (R_0^{M_i})^{-1} \bar{R}_t^{M_i} (R_0^{M_i})^{-1} \bar{R}_t^{M_i} (R_0^{M_i})^{-1} (\bm{\mu}_0 - \bm{\mu}^{M_i}_0)
- \frac{1}{2} \text{tr} \left[ (I - R_0(R_0^{M_i})^{-1}) (\bar{R}_t^{M_i} (R_0^{M_i})^{-1})^2 \right]
- \frac{1}{2} \text{tr} \left[ \bar{R}_t (R_0^{M_i})^{-1} \bar{R}_t^{M_i} (R_0^{M_i})^{-1} \right]
+ \frac{1}{4} \left( \text{tr} \left[ \bar{R}_t (R_0^{M_i})^{-1} \right] \right)^2.
\]

For correct initial conditions, \( \mu_{0i}^{M_i} = \mu_0, \ \bar{R}_{0i}^{M_i} = R_0 \), the above formulas simplify to

\[
X^R = \frac{1}{7} \text{tr} \left[ \bar{R}_t (R_0)^{-1} \right],
\]

\[
Y^{\mu,\mu} = \frac{1}{2} (\bar{\bm{\mu}}_t - \bar{\bm{\mu}}^{M_i}_t)^T (R_0)^{-1} (\bar{\bm{\mu}}_t - \bar{\bm{\mu}}^{M_i}_t),
\]

\[
Y^{R,R} = \frac{1}{2} \left[ \text{tr} \left[ \bar{R}_t (R_0)^{-1} \bar{R}_t^{M_i} (R_0)^{-1} \right]
+ \frac{1}{4} \left( \text{tr} \left[ \bar{R}_t (R_0)^{-1} \right] \right)^2 \right],
\]

with the remaining coefficients identically zero. Substituting the relative entropy between \( \mathcal{P}(\pi_i^0, \pi_i^{M_i}) \) in the form (78) with the coefficients (79)-(81) into the general necessary condition (10) for improving the prediction via MME yields the condition (28). \( \Box \)

**Proof of FACT 9:** Here, we first prove a more general fact whose content reduces to that of FACT 9 in §3.3.2 under appropriate constraints.

Consider the forced response prediction via Gaussian mixture MME with correct second-order equilibrium statistics \( \mu_{eqi}^{M_i} = \mu_{eq}, \ \bar{R}_{eqi}^{M_i} = \bar{R}_{eq} \). The condition for improvement of forced response prediction at short times \( t \ll 1 \) via MME in the Gaussian framework is

\[
\delta^2 \left\{ D_t((\bar{\bm{\mu}}_t - \bar{\mu}^{M_i}_t)) + E_t((\bar{R}_t^{M_i})) - F_t(\bar{R}_t, \{\bar{R}_t^{M_i}\}) \right\} + \mathcal{O}(\delta^3) > 0,
\]

where

\[
D_t = \frac{1}{2} \sum_{i \neq \phi} \frac{\alpha_i}{1 - \alpha_\phi} \left[ (\bar{\bm{\mu}}_t - \bar{\mu}^{M_i}_t)^T (R_{eq})^{-1} (\bar{\bm{\mu}}_t - \bar{\mu}^{M_i}_t) - (\bar{\bm{\mu}}_t - \bar{\mu}^{M_i}_t)^T (R_{eq})^{-1} (\bar{\bm{\mu}}_t - \bar{\mu}^{M_i}_t) \right],
\]

\[
E_t = \frac{1}{2} \sum_{i \neq \phi} \frac{\alpha_i}{1 - \alpha_\phi} \text{tr} \left[ (\bar{R}_t^{M_i} - \bar{R}_t^{M_i})(R_{eq})^{-1} \right] \text{tr} \left[ (\bar{R}_t^{M_i} + \bar{R}_t^{M_i})(R_{eq})^{-1} \right],
\]

\[
F_t = \frac{1}{2} \sum_{i \neq \phi} \frac{\alpha_i}{1 - \alpha_\phi} \text{tr} \left[ \bar{R}_t (R_{eq})^{-1} (\bar{R}_t - \bar{R}_t^{M_i})(R_{eq})^{-1} \right].
\]

The proof of (82), and of the simplified result (32), is derived using the same short-time expansion of the relative entropy as in (78) but with different initial conditions, namely \( \mu_0 = \mu_{eq}, \ \bar{R}_0^{M_i} = \mu_{M_i}^{eq} \) and \( R_0 = R_{eq}, \ \bar{R}_0^{M_i} = \bar{R}_{eq}^{M_i} \) in (78). For tuned second-order statistics in all MME models, \( \mu_{eqi}^{M_i} = \mu_{eq} \) and \( \bar{R}_{eqi}^{M_i} = R_{eq} \), this
Then, the sufficient condition (10) for prediction improvement through MME has the following form:

\[ X^R = \frac{1}{2} \text{tr} \left[ \hat{R}_t(R_{eq})^{-1} \right], \]

\[ Y^{\mu,\mu} = \frac{1}{2} (\hat{\mu}_t - \hat{\mu}^{\mu}_t)^T (R_{eq})^{-1} (\hat{\mu}_t - \hat{\mu}^{\mu}_t), \]

\[ Y^{R,R} = -\frac{1}{2} \text{tr} \left[ \hat{R}_t(R_{eq})^{-1} \hat{R}^{\mu}_t(R_{eq})^{-1} \right] + \frac{1}{2} \left( \text{tr} \left[ \hat{R}^{\mu}_t(R_{eq})^{-1} \right] \right)^2, \]

with the remaining coefficients identically zero. We now use the expansion (78) for the relative entropies with the coefficients (83)-(85) in the general sufficient condition (10) for improving forced response prediction via Gaussian mixture MME at short times to obtain (82). Finally, Fact 9 of §3.3.2 is obtained by assuming that the response is due to the forcing perturbations so that \( \hat{R}^{\mu}_t = 0 \) for the Gaussian models and the coefficients \( X^R = 0 \) and \( Y^{R,R} = 0 \) so that only \( D_t \) remains non-zero and it is independent of the truth response in the covariance. □

B Further details of associated with the sufficient conditions for imperfect prediction improvement via MME

In §3.1.1 we discussed the sufficient condition (10) for improving imperfect predictions via MME in the least-biased density representation (13). Here, we represent the same condition in terms of general perturbations of probability densities which leads to some additional insight into the essential features of MME that leads to prediction improvement; in particular, it is shown at the end of this section that it is difficult to improve the short-term predictive skill via MME containing models with incorrect statistical initial conditions.

The formulation presented below relies on relatively weak assumptions that the truth and model densities can be written as

\[ \pi_t = \pi_t^0 + \delta \tilde{\pi}_t, \quad \pi_t^M = \pi_t^0 + \delta \tilde{\pi}_t^M, \quad \tilde{\pi}_0 = \tilde{\pi}_0^M = 0, \quad \int \tilde{\pi}_t^0 d\mu = \int \tilde{\pi}_t^M d\mu = 0, \]

The above decomposition is always possible for the non-singular initial value problem; in the case of the forced response prediction from equilibrium (i.e., when \( \pi_0^0 = \pi_0^M, \pi_0^M = \pi_0^M \)) such a decomposition exists for \( \delta \ll 1 \) under the minimal assumptions of hypoelliptic noise [30]. The possibility of estimating the evolution of statistical moments of the truth density \( \pi_t \) in the case of predicting the forced response within the framework of the fluctuation-dissipation theorem (FDT) makes this framework particularly important in this case; we discuss some aspects of FDT in Appendix D.

**FACT.** Assume the decomposition (86) of the truth and model densities exists as discussed above. Then, the sufficient condition (10) for prediction improvement through MME has the following form:

\[ \mathcal{A}_a \left( \pi_0^l, \{ \pi_0^M_l \} \right) + \delta \mathcal{B}_a \left( \pi_t^l, \{ \pi_t^M_l \} \right) + \delta^2 \mathcal{C}_a \left( \pi_t^l, \{ \pi_t^M_l \} \right) + \mathcal{O}(\delta^3) > 0, \]

where

\[ \mathcal{A}_a \left( \pi_0^l, \{ \pi_0^M_l \} \right) = \sum_{i \neq 0} \beta_i \left( \mathcal{P}(\pi_0^l, \pi_0^M) - \mathcal{P}(\pi_0^l, \pi_0^M) \right), \]

\[ \mathcal{B}_a \left( \pi_t^l, \{ \pi_t^M_l \} \right) = \sum_{i \neq 0} \beta_i \int d\mu \left( \pi_0^l \left[ \frac{\pi_t^M_l}{\pi_0^M} - \frac{\pi_t^M_l}{\pi_0^M} \right] + \tilde{\pi}_t^0 \log \frac{\pi_t^M_l}{\pi_0^M} \right), \]

\[ \mathcal{C}_a \left( \pi_t^l, \{ \pi_t^M_l \} \right) = \frac{1}{2} \sum_{i \neq 0} \beta_i \int d\mu \left( \pi_0^l \left[ \left( \frac{\pi_t^M_l}{\pi_0^M} \right)^2 - \frac{\pi_t^M_l}{\pi_0^M} \right] \right)^2 - 2 \tilde{\pi}_t^0 \left( \frac{\pi_t^M_l}{\pi_0^M} - \frac{\pi_t^M_l}{\pi_0^M} \right), \]
with the weights $\beta_i$ defined in (9). Note that the least-biased estimate of the marginal equilibrium density, $\pi_{\text{eq}}^i$ can be estimated from observations while the least biased estimate of the forced response $\tilde{\pi}_t^i$ in the condition (87) can be estimated via the use of the fluctuation-dissipation theorem, as shown below.

The following particular cases of the condition (87) for improving the predictions via the MME approach are worth noting in this general representation:

- **Initial (statistical) conditions in all models of MME consistent with the initial conditions of the least-biased approximation of the truth;** i.e., $\pi^M_0 = \pi_0$. In such a case we have $A_0 = 0$, $B_0 = 0$ and the condition (87) for improvement of prediction via MME simplifies to

$$
\int du \frac{\left(\tilde{\pi}_t^i\right)^2}{\pi_0^i} < \sum_{i \neq \phi} \beta_i \int du \frac{\left(\tilde{\pi}_t^i - \tilde{\pi}_t^{M_i} + \tilde{\pi}_t^{M_i}\right)^2}{\pi_0^i}, \quad (91)
$$

In the case of forced response predictions, perturbation of the truth density $\tilde{\pi}_t^\alpha$ can be estimated from the statistics on the unperturbed equilibrium through the fluctuation-dissipation theorem, as shown below in Appendix D.

- **Multi Model Ensemble with attractor densities perturbed relative to the least-biased approximation;** i.e., $\pi^M_0 = \pi_0 + \epsilon \tilde{\pi}_t^{M_i}$, $\pi_t^{M_i} = \pi_0$. In such a case all terms in (87) are non-trivial but they simplify to

$$
A_\alpha\left(\pi_0^i, \{\pi_0^{M_i}\}\right) = -\sum_{i \neq \phi} \beta_i \int du \frac{\epsilon \tilde{\pi}_t^{M_i}}{\pi_0^i}, \quad (92)
$$

$$
B_\alpha\left(\pi_t^i, \{\pi_t^{M_i}\}\right) = \sum_{i \neq \phi} \beta_i \int du \frac{\epsilon \tilde{\pi}_t^{M_i}}{\pi_0^i} (\tilde{\pi}_t^i - \tilde{\pi}_t^{M_i}), \quad (93)
$$

$$
C_\alpha\left(\pi_t^i, \{\pi_t^{M_i}\}\right) = \sum_{i \neq \phi} \beta_i \int du \left(\frac{\tilde{\pi}_t^i}{\pi_0^i} (\tilde{\pi}_t^{M_i} - \tilde{\pi}_t^{M_i}) - \epsilon \frac{\tilde{\pi}_t^{M_i}}{\pi_0^i} \tilde{\pi}_t^{M_i}\right), \quad (94)
$$

with the weights $\beta_i$ defined in (9) so that the condition (87) simplifies, at the leading order in $\epsilon$, to

$$
\sum_{i \neq \phi} \beta_i \int du \frac{1}{\pi_0^i} \left(\tilde{\pi}_t^{M_i} (\tilde{\pi}_t^i - \tilde{\pi}_t^{M_i}) + \tilde{\pi}_t^{M_i} (\tilde{\pi}_t^{M_i} - \tilde{\pi}_t^{M_i}) - (\tilde{\pi}_t^{M_i})^2\right) > 0. \quad (95)
$$

Note that in this case it might be difficult to improve the forced response prediction at short times since at $t = 0$ the only non-zero term in the integrand of (95) is negative (i.e., $-(\tilde{\pi}_t^{M_i})^2 / \pi_0^i$).

C Further details on improving predictions via Gaussian mixture MME

The formulas (10) or (13) represent the sufficient condition for improving the imperfect predictions via the MME framework. Here, we derive guidelines for deriving ensembles of imperfect Gaussian models with improved predictive skill. Practical implementations of the the perturbative approach discussed below require approximations of the truth density perturbations;

Consider the MME to be the ensemble of gaussian models given by the MSM models

$$
\frac{du^M}{dt} = \left(-\gamma^M u^M + f^M\right)dt + \sigma^M dW(t). \quad (96)
$$

so that the Fokker-Planck operator associated with (96) becomes

$$
L_{FP}^M[\cdot] = -\partial_u \left[(-\gamma^M u + f^M) \cdot \right] + \frac{1}{2}(\sigma^M)^2 \partial_u^2 \left[\cdot\right]. \quad (97)
$$
It can be easily determined that for constant deterministic forcing $f$ the invariant measure is given by the Gaussian density with mean and variance

$$\langle u_{eq}^M \rangle = \frac{f^M}{\gamma^M}, \quad \text{Var}[u_{eq}^M] = \frac{(\sigma^M)^2}{2\gamma^M}. \quad (98)$$

We now have the following:

**FACT.** Consider the sufficient condition (10) for prediction improvement via MME constructed by perturbing the damping coefficients in a single Gaussian model $M_o$ given by (96) so that $\gamma^M_i = \gamma^{M_o} + \epsilon \gamma^M_i$, while retaining the correct equilibrium statistics; in such a case the condition (10) becomes

$$\varepsilon \left[ \mathcal{D}(\pi_t, \hat{\pi}^{M_o}_t)^{\pi^{M_o}_0} + \Delta \gamma^M \mathcal{F}(t, \pi_t, \hat{\pi}^{M_o}_t) \right] + \mathcal{O}(\varepsilon^2) > 0, \quad (99)$$

for prediction skill improvement pointwise-in time and

$$\varepsilon \left[ \mathcal{D}_T(\pi, \hat{\pi}^{M_o})^{\pi^{M_o}_0} + \Delta \gamma^M \mathcal{F}_T(\pi, \hat{\pi}^{M_o}) \right] + \mathcal{O}(\varepsilon^2) > 0, \quad (100)$$

for improved prediction over the time interval $T$ where $\Delta \gamma^M = (\gamma^{M_o})^{-1} \sum_{i \neq o} \beta_i \gamma^M_i$, and the functions $\mathcal{D}$, $\mathcal{F}$ of the truth density $\pi$ and the single model reference density $\pi^{M_o}$ are given by

$$\mathcal{D}(\pi_t, \hat{\pi}^{M_o}_t)^{\pi^{M_o}_0} = \int \mathcal{D}(\pi_t, \hat{\pi}^{M_o}_t)^{\pi^{M_o}_0} \pi_t \, d\pi_t \notag$$

$$\mathcal{F}(t, \pi_t, \hat{\pi}^{M_o}_t) = \int \mathcal{F}(t, \pi_t, \hat{\pi}^{M_o}_t) \pi_t \, d\pi_t \notag$$

the functions $\mathcal{D}_T$ and $\mathcal{F}_T$ in (100) are given by the respective time integrals of $\mathcal{D}$ and $\mathcal{F}$.

**Remarks:**

- For correct initial conditions in the Gaussian MME models, $\hat{\pi}_0^{M_i} = 0$, given $\mathcal{F}_T(\pi, \pi^{M_o})$ the predictive improvement via MME depends on the interplay between the ‘net’ damping perturbation $\Delta \gamma^M$ and $\mathcal{F}_T(\pi, \pi^{M_o})$. We have the following:
  - For $\mathcal{F}_T(\pi, \pi^{M_o}) < 0$ underdamped MME with $\Delta \gamma^M < 0$ provides improved prediction skill,
  - For $\mathcal{F}_T(\pi, \pi^{M_o}) > 0$ overdamped MME with $\Delta \gamma^M > 0$ provides improved prediction skill.

- In practical applications the functions $\mathcal{D}_T(\pi, \pi^{M_o})$ and $\mathcal{F}_T(\pi, \pi^{M_o})$ in (100) are not known since they involve the truth density $\pi_t$. The best one can hope for is the knowledge of the initial condition $\pi_0$ and the invariant measure $\pi_{eq}$. One possibility is to approximate $\mathcal{D}_T(\pi, \pi^{M_o})$ and $\mathcal{F}_T(\pi, \pi^{M_o})$ in (100) by expectations over appropriately constructed ensembles of time-dependent densities $\Pi_t$ such that $\Pi_0 = \pi_0$ and $\Pi_{eq} = \pi_{eq}$; this approach is discussed below after the derivation of the condition (99).

**Proof:** Given that there are three parameters in the class of models (96) and two constraints due to the requirement on the correct marginal equilibrium statistics, there exists a one-parameter family of models (96) with correct marginal equilibrium statistics; here we choose the free parameter to be the damping $\gamma^M_i$ so that the models in the MME perturbed relative to $M_o$ are given by

$$f^M_i = \left( 1 + \frac{\epsilon \gamma^M_i}{\gamma^{M_o}} \right) f^{M_o}, \quad (\sigma^M)^2 = \left( 1 + \frac{\epsilon \gamma^M_i}{\gamma^{M_o}} \right) (\sigma^{M_o})^2. \quad (103)$$

Assuming that the MME model densities are given by $\pi^{M_i, \epsilon} = \pi^{M_o} + \epsilon \pi^{M_i}$, it can be easily seen that the Fokker-Planck operator for the perturbed MME models is

$$\mathcal{L}^{M_i}_{FP} = \left( 1 + \frac{\epsilon \gamma^M_i}{\gamma^{M_o}} \right) \mathcal{L}^{M_o}_{FP}. \quad (104)$$
and the perturbations must satisfy, at the leading order in \( \epsilon \), the following linear inhomogeneous PDE

\[
\partial_t \tilde{n}_t^{M_1} = \left(1 + \frac{\epsilon^2 M_1}{\gamma M_0}\right) L_{pp}^{M_1} \tilde{n}_t^{M_1} + \frac{\epsilon^2 M_1}{\gamma M_0} L_{pp}^{M_1} \tilde{n}_t^{M_1}, \quad \int d\mathbf{\tilde{u}} \tilde{n}_t^{M_1} = 0, \tag{105}
\]

whose solutions may be formally written using the semi-group notation as

\[
\tilde{n}_t^{M_1} = e^{\left(1 + \frac{\epsilon^2 M_1}{\gamma M_0}\right) L_{pp}^{M_1} t} \tilde{n}_0^{M_1} + \frac{\epsilon^2 M_1}{\gamma M_0} \int_0^t dt' e^{(t-t')\left(1 + \frac{\epsilon^2 M_1}{\gamma M_0}\right) L_{pp}^{M_1}} \tilde{n}_t^{M_1} + \mathcal{O}\left(\frac{\epsilon^2 M_1}{\gamma M_0}\right)^2 \tag{106}
\]

Substitution of (106) into the condition (19) discussed in the main text leads to the result in (99); furthermore, the integration of (99) over a time interval \([0, T]\) yields (100). \(\square\)

Clearly, the main problem in practical applications is that \(\pi_t\) is unknown and the best one can hope for is the knowledge of the initial condition \(\pi_0\) and the invariant measure \(\pi_{eq}\); one possibility is to approximate \(\pi_t\) in (100) by some family of densities

\[
\mathcal{K} = \{\Pi^0_t(u); \quad \forall \theta \quad \Pi^0_t = \pi_0, \quad \Pi^0_{eq} = \pi_{eq}\} \tag{107}
\]

with some a priori constructed distribution, \(p(\theta)\), and use

\[
\mathcal{F}(\pi_{eq}) = \mathbb{E}^p[\mathcal{F}(\pi_{eq}, \pi_{eq})], \quad \mathcal{F}(t, \pi_t) = \mathbb{E}^p[\mathcal{F}(t, \Pi^0_t, \pi_{eq})], \tag{108}
\]

in (99) instead of the unknown \(\mathcal{D}(\pi_t, \pi_{eq})\) and \(\mathcal{F}(t, \pi_t, \pi_{eq})\). Similarly to the pointwise-in-time case, one could attempt to estimate the functions \(\mathcal{D}\) and \(\mathcal{F}\) in (100) via the expectation over some class \(\mathcal{K}\) in (107) of surrogate densities with respect to some physically justified prior \(p(\theta)\), leading to an approximate condition

\[
\in \left[\mathcal{F}(\pi_{eq}) \tilde{n}_0^{M_1} + \Delta \gamma^M \mathcal{F}(\pi_{eq}) + \mathcal{O}(\epsilon^2) > 0, \right] \tag{109}
\]

where \(\mathcal{F}(\pi_{eq}) = \mathbb{E}^p[\mathcal{F}(\Pi^0_t, \pi_{eq})], \quad \mathcal{F}(t, \pi_t) = \mathbb{E}^p[\mathcal{F}(t, \Pi^0_t, \pi_{eq})].\)

**Remark:** The accuracy of the approximate condition for improvement of statistical predictions via MME depends, of course, on the choice of the class of densities \(\mathcal{K}\) and the density \(p(\theta)\). Reliable choices of \(\mathcal{K}\) and \(p(\theta)\) still need to be investigated and the sensitivity to the associated uncertainties needs to be studied in order to assess the suitability of this method in practical applications; possible way forward can be achieved by exploiting the techniques developed in [23, 24, 25] for improving coarse-grained prediction skill.

\section*{D Forced response and FDT}

The attractive feature of the fluctuation-dissipation framework for forced dissipative systems is that it allows one to estimate the expected linear response of the system to small external perturbations by collecting lag-covariance statistics of the unperturbed equilibrium/attractor. Below we list the most important features of this framework (see [49, 47, 21] for details, and [26, 27] for applications of this framework to estimate the linear response in atmospheric general circulation models (AGCM)). The possibilities for the use of FDT estimates in evaluating the sufficient condition for improving the forced response prediction via the MME approach were discussed in §3.

Consider the dynamics of the process \(\mathbf{v}(t)\) satisfying the general Ito diffusion

\[
d\mathbf{v} = \mathbf{F}(\mathbf{v})dt + \sigma(\mathbf{v})d\mathbf{W}(t), \tag{110}
\]

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where $W(t)$ is a vector-valued Wiener process with independent components and the noise matrix $\sigma$, and $F(v)$ is some smooth nonlinear function of the state $v(t) = (u(t), v(t))$ where $u$ represents the vector of the resolved state variables and $v$ denotes the unresolved variables. Moreover, assume that $F$ and $\sigma$ are such that the standard existence and uniqueness solutions for the diffusion process in (110) hold.

We restrict attention to configurations with statistical equilibrium solutions so that there exists a time-independent probability density function $p_{eq}(v)$ such that $L_{FV} p_{eq}(v) = 0$, i.e., there exists an equilibrium solution of the Fokker-Planck equation associated with the Ito diffusion in (110) which is given by

$$p_e(v) = \text{solution of the Fokker-Planck equation associated with the Ito diffusion in (110)}$$

where $W$ is the resolved state variables and

$$W = \text{the unresolved state variables}$$

and the linear response operator in (119) is given by

$$\text{perturbations of the truth dynamics}$$

in (110) which leads to the perturbed density

$$\delta \tilde{p}_t = p_{eq} + \delta \tilde{p}_t, \quad \delta \ll 1, \quad \tilde{p}_{t=0} = 0, \quad \int \tilde{p}_t(v)dv = 0,$$

which are non-singular so that the decomposition in (113) is smooth at $\delta = 0$; this assumption holds under the minimal assumptions of hypoelliptic noise in (110), as shown in [30].

We consider perturbations of the invariant measure $p_{eq}$ which are induced by the time-dependent perturbations of the truth dynamics

$$\delta \tilde{F}(v, t) = \delta \tilde{F}(v) f(t),$$

which we assume to have the time-space separable form. The perturbation of the probability density, $\tilde{p}_t$, satisfies

$$\frac{\partial}{\partial t} \tilde{p}_t = L_{FV} \tilde{p}_t + f(t) L_{\delta} p_{eq} + O(\delta^2), \quad \delta \ll 1, \quad \tilde{p}_{t=0} = 0, \quad \int \tilde{p}_t(v)dv = 0,$$

so that the operator associated with the perturbations the equilibrium dynamics in (110) is given by

$$L_{\delta} p = -\nabla \cdot \left[ F(v) \right].$$

The formal solution of (115) can be written using the semi-group notation as

$$\tilde{p}_t = \int_0^t dt' f(t') e^{(t-t')L_{FV} L_{\delta} p_{eq}}.$$

Finally, we note that the marginal density of $p_t$ on the subspace of resolved variables $u$ is given by

$$\pi_t(u) = \int \tilde{p}_t(u, v)dv$$

with the marginal equilibrium density $\pi_{eq}(u) = \int p_{eq}(u, v)dv$ and the perturbation similarly represented by $\tilde{\pi}(u) = \int \tilde{p}_t(u, v)dv$.

Consider now the change at time $t$ in the expected value of any functional, $E(u)$, of the resolved variables, i.e.,

$$\delta E = \mathbb{E}^{\pi_t} [E(u)] - \mathbb{E}^{\pi_{eq}} [E(u)] = \int E(u) \tilde{\pi}_t(u) du.$$

Following the standard derivation of the linear response formula based on the fluctuation-dissipation arguments (e.g., [49]), one can express $\delta E$ via the statistics computed in the unperturbed equilibrium as

$$\delta E = \int_0^t dt' f(t') \int du E(u) e^{(t-t')L_{FV} L_{eq}(v)} = \int_0^t dt' R_E(t-t') f(t'),$$

where $f(t)$ is the time-dependent amplitude of the perturbation (114) of the equilibrium dynamics in (110) and the linear response operator in (119) is given by

$$R_E(t) = \mathbb{E}^{p_{eq}} [E(u(t + \tau)) B(v(\tau))].$$

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where

\[ B(v) = \frac{L_\delta p_{eq}(v)}{p_{eq}(v)}. \]  

(121)

The linear response operator \( R_F(t) \) is independent of \( \tau \) due to the assumed stationarity of the process \( v \) (see [47, 21] for formal generalizations of this framework to configurations with time-periodic attractors). The obvious difficulty with utilizing the formulas (119)-(121) is that the equilibrium measure \( p_{eq} \) is not known exactly (in particular on the unresolved subspace of variables \( v \)) and in any practical applications some approximations have to be utilized (see, e.g., [49, 27, 2, 3, 52, 42, 10]). The possibilities for the use of FDT estimates in evaluating the sufficient condition for improving the forced response prediction via the MME approach were discussed in §3.

References


