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Nonlinear Data Assimilation by Deep Learning Embedded in an Ensemble Kalman Filter

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Abstract

Recent progress in the particle filter has made it possible to use it for nonlinear or non-Gaussian data assimilation in high-dimensional systems, but a relatively large ensemble is still needed to outperform the ensemble Kalman filter (EnKF) in terms of accuracy. An alternative ensemble data assimilation method based on deep learning is presented, in which deep neural networks are locally embedded in the EnKF. This method is named the deep learning-ensemble Kalman filter (DL-EnKF). The DL-EnKF analysis ensemble is generated from the DL-EnKF analysis and the EnKF analysis deviation ensemble. The performance of the DL-EnKF is investigated through data assimilation experiments in both perfect and imperfect model scenarios using three versions of the Lorenz 96 model and a deterministic EnKF with an ensemble size of 10. Nonlinearity in data assimilation is controlled by changing the time interval between observations. Results demonstrate that despite such a small ensemble the DL-EnKF is superior to the EnKF in terms of accuracy in strongly nonlinear regimes and that the DL-EnKF analysis is more accurate than the output of deep learning due to positive feedback in assimilation cycles. Even if the target of training is an EnKF analysis with a large ensemble or a simulation by an imperfect model, the improvement introduced by the DL-EnKF is not very different from the case where the target of training is the true state.

1. Introduction

Data assimilation in nonlinear or non-Gaussian systems has been a challenge in meteorology and other geosciences (Bocquet et al., 2010). For instance, it is well known that cumulus convection exhibits strong non-Gaussianity in data assimilation (e.g., Kondo and Miyoshi, 2019; Kawabata and Ueno, 2020). The ensemble Kalman filter (EnKF) is formulated under the Gaussian assumption and is close to optimal in weakly nonlinear regimes, but it does not work well if nonlinearity is strong.   On the other hand, the particle filter (PF) does not need the Gaussian assumption, but the weight degeneracy had been preventing the use of the PF for high-dimensional data assimilation (Snyder et al., 2008; van Leeuwen 2009). However, this limitation is disappearing due to recent developments in the PF, including the use of localization and hybrids with the EnKF (Farchi and Bosquet, 2018; van Leeuwen et al., 2019). Despite this progress, a relatively large ensemble is still needed for the PF to outperform the EnKF (e.g., Penny and Miyoshi, 2016).   This may be plausible since non-Gaussian data assimilation needs some information on higher-order moments of probability density functions (PDFs). As for the 4-dimensional variational method (4D-Var), Tsuyuki (2014) showed that the 4D-Var with a conventional cost function implicitly used a non-Gaussian prior PDF that evolved according to the Liouville equation (Ehrendorfer, 1994) if a certain condition was satisfied, and that the difficulty caused by multiple minima could be alleviated by combining with the EnKF. The iterative ensemble Kalman filter/smoother (IEnKF/IEnKS) have been shown to be the missing link between the PF and the EnKF and

3

73 4D-Var, and can work very well with mild nonlinearity and generate a much better analysis

74 than the above data assimilation methods (Sakov et al., 2012; Bocquet and Sakov, 2013,

75 2014; Bocquet, 2016). However, the IEnKF/IEnKS need much larger computational cost due

76 to the iterative application of the EnKF/EnKS and the use of a long assimilation window.

77 Recent developments in machine learning, in particular in deep learning (Le cum et al.,

78 2015), have demonstrated impressive skills in various fields. Data-driven modeling,

79 including data-driven parametrizations, based on machine learning has been extensively

80 explored for improving simulations and predictions of nonlinear dynamical systems. Dueben

81 and Bauer (2018) discussed the question of whether models that were based on deep

82 learning and trained on atmospheric data could compete with weather and climate models

83 that were based on physical principles. Reichstein et al. (2019) advocated a hybrid modeling

84 approach in which physical process models were coupled with machine learning to further

85 improve understanding and predictive ability in earth system science. Abarbanel et al. (2018)

86 and Geer (2020) showed an equivalence in formulation between data assimilation and deep

87 learning. Lists of literature of recent studies are available in Reichstein et al. (2019) and

88 Chattopadhyay et al. (2020), for instance. Quite recently the combination of data assimilation

89 and machine learning has been explored to address sparse and noisy observations in data-

90 driven modeling (Brajard et al., 2020a; Bocquet et al., 2020; Tomizawa and Sawada, 2020;

91 Gottwald and Reich, 2021; Wikner et al., 2021), data-driven parametrizations (Brajard et al.,

92 2020b), and model error correction (Farchi et al., 2021).

93 Research on the application of deep learning to data assimilation itself has also started. Arcucci et al. (2021) proposed a method for integrating variational data assimilation with deep learning, in which a recurrent neural network is trained on the state of a dynamical model and the result of data assimilation. Silva et al. (2021) proposed the use of a generative adversarial network to make prediction and to assimilate observations by using a low-dimensional space for the spatial distribution of the simulated state. However, it is difficult to directly apply those methods to data assimilation in high-dimensional systems such as atmospheric models for numerical weather prediction.

101 In this study, we present an ensemble data assimilation method combining the EnKF and deep learning as an alternative to the PF for high-dimensional systems. The additional computational cost to assimilate observations is a very small fraction of that of the EnKF. Since a deep neural network (DNN) can learn a data assimilation method for a specific dynamical system and a specific observing system by training, we could expect this method to work with a relatively small ensemble size even in strongly nonlinear regimes. However, data assimilation in meteorology is generally a large-scale problem, and the background error covariance and the distribution of radar and satellite data change with the analysis time. The EnKF, as well as the PF and 4D-Var, can properly deal with this nonstationarity in data assimilation. On the other hand, deep learning is based on the minimization of the sum of errors over many samples. In addition, it would be difficult to provide sufficient information on the forecast error covariance to a DNN, because the feasible size of a DNN is limited,

113   where we define the size of a DNN as the total number of weights including bias parameters

114   to be optimized by training. If the output of a DNN is not well optimized for each analysis

115   time, the analysis accuracy may deteriorate in assimilation cycles. However, since the EnKF

116   does not work very well in strongly nonlinear regimes, we could expect data assimilation by

117   deep learning to outperform the EnKF in such regimes.

118   The purpose of this study is to propose a nonlinear data assimilation method based on

119   deep learning that is locally embedded in an EnKF and to investigate its performance

120   through data assimilation experiments in both perfect and imperfect model scenarios using

121   toy models. By applying deep learning in combination with an EnKF, we can reduce the size

122   of a DNN and address the nonstationarity in data assimilation. This method is named the

123   deep learning-ensemble Kalman filter (DL-EnKF).

124   The remainder of this paper is organized as follows. Section 2 introduces the method of

125   DL-EnKF. Section3 describes the design of experiments in both perfect and imperfect model

126   scenarios. Section 4 presents the results of these experiments. Summary and discussion

127   are mentioned in Section 5.

128

129   **2. Method**

130   Since data assimilation is generally a large-scale problem, it is desirable to keep the

131   size of a DNN as small as possible. For instance, the size of a feedforward neural network

132   with m layers with n nodes per layer is about $n^2(m\text{-}1)$ and a greater number of samples

133   would be required for training. If we directly apply deep learning to data assimilation, the

134   number of input nodes is at least the sum of the number of observations and the degrees of

135   freedom of a numerical model, and the number of output nodes is the degrees of freedom

136   of the model, while the number of nodes of a hidden layer is usually required to be larger

137   than the number of input or output nodes. For high-dimensional systems such as

138   atmospheric models, the size of a DNN would become too large to be stored in the memory

139   of a computer and to prepare sufficient training samples. To apply deep learning to data

140   assimilation for atmospheric models, we need to introduce a localization procedure and to

141   train a DNN to have some versatility so that it is applicable to each grid point in a certain

142   range of geographical areas.

143   Figure 1a shows the workflow of the DL-EnKF, in which deep learning is locally   Fig. 1

144   embedded in an EnKF. The "EnKF" box in this figure represents the analysis step of the

145   EnKF, and "Deep Learning" box consists of an ensemble of several DNNs. The inputs of

146   DNNs to create the DL-EnKF analysis at a grid point are the EnKF analysis, forecast,

147   observations, availability of observations in binary, and pseudo-observations that

148   supplement missing observations. The EnKF analysis and forecast are the ensemble means

149   of each ensemble. We do not explicitly use the information contained in the forecast

150   ensemble other than the ensemble mean to reduce the size of DNNs. Since observational

151   data for which the DNN has input nodes may be sometimes missing, it is necessary to

152   provide the information on the availability of observations to DNNs. The pseudo-

153   observations are prepared by using the EnKF analysis and the observation operators of the

154   missing observations. Those input data are extracted from a small domain centered at the

155   analysis grid point. The radius of this domain is hereafter referred to as the input radius, and

156   it is assumed that this value is smaller than the covariance localization radius of the EnKF.

157   According to Hsieh and Tang (1998), the DL-EnKF analysis is the average of outputs from

158   the ensemble of DNNs. The individual outputs from DNNs would be scattered in phase

159   space due to multiple minima of a loss function of deep learning, and we would likely obtain

160   a better DL-EnKF analysis by averaging those individual outputs.

161   The analysis ensemble $\{x_m^a\}_{m=1}^M$, where M is the ensemble size, is created by

162   modifying the EnKF analysis ensemble $\{x_{\mathrm{EnKF},\,m}^a\}_{m=1}^M$ such that its ensemble mean is equal

163   to the DL-EnKF analysis $x_{\mathrm{DL-EnKF}}^a$ as follows:

164   $$x_m^a = x_{\mathrm{DL-EnKF}}^a + \alpha\big(x_{\mathrm{EnKF},\,m}^a - x_{\mathrm{EnKF}}^a\big), \tag{1}$$

165   where x_{EnKF}^a is the EnKF analysis and α is a parameter for adjusting the spread of the

166   analysis ensemble. If adaptive covariance inflation is used in the EnKF, we can set α to 1

167   since the effect of tuning α is almost canceled by this procedure. However, if we conduct

168   ensemble forecasts using the analysis ensemble, we may need to adjust the value of α.

169   The members of the analysis ensemble thus generated are evolved by the time integration

170   of a numerical model to prepare the forecast ensemble for the next analysis time.

171   For the training of a DNN, we use the EnKF analysis and forecast provided by an EnKF

172   run as shown in Fig. 1b. The weights including bias parameters are optimized by reducing

173   a loss function that measures a difference between the output of the DNN and the target of

174   training. We prepare several DNNs by randomly initializing the weights before the training.

175   One of the reasons for including the EnKF analysis in the inputs of DNNs is that this

176   analysis at a grid point contains some information on the forecast, observations, and

177   forecast error covariance in a domain within the covariance localization radius, so that we

178   can reduce the input radius of DNNs and implicitly utilize some information of the forecast

179   error covariance. In addition, even if DNNs cannot deal with some observational data

180   because the input nodes for these observations are absent, they are assimilated by the

181   EnKF part of DL-EnKF and their information is partly provided to the deep learning part

182   through the EnKF analysis.

183   We can prepare pseudo-observations by other methods. However, it is easily shown by

184   the sequential assimilation method (e.g., Houtekamer and Mitchell, 2001) that if observation

185   errors are independent of each other the additional assimilation of pseudo-observations

186   does not change the EnKF analysis. Therefore, it can be considered that the pseudo-

187   observations thus created are assimilated in the EnKF part of DL-EnKF along with the real

188   observations, and that the same observations including the pseudo-observations are

189   provided to the deep learning part. In this sense, the method adopted in this study may be

190   a natural choice, although it may not be optimal and spurious correlations and biases will be

191   generated. We could expect that DNNs will learn to properly deal with this problem by

192   training.

193   Lawson and Hansen (2004) showed that an analysis ensemble generated by a

194   deterministic EnKF tends to retain multi-modality that may appear in a forecast ensemble,

195   while this is not the case for a stochastic EnKF. Therefore, a stochastic EnKF is better than

196   a deterministic EnKF for generating an analysis ensemble of the DL-EnKF. However, it is

197   well known that if the ensemble size is relatively small, a stochastic EnKF is inferior in terms

198   of the accuracy of the ensemble mean due to random perturbations that are added to

199   observations (e.g., Sakov and Oke, 2008; Bowler et al., 2013), so that we adopt a

200   deterministic EnKF for the EnKF part in the present paper.

201

202   **3. Design of experiments**

203   *3.1. Outline*

204   The performance of the DL-EnKF is investigated through both perfect and imperfect

205   model experiments using three versions of the 40-variable Lorenz 96 models (Lorenz, 1996)

206   and the serial ensemble square root filter (EnSRF; Whitaker and Hamill, 2002), which is one

207   of the deterministic EnKFs. The ensemble size of the serial EnSRF is set to 10, because we

208   are interested in the performance of the DL-EnKF with a relatively small ensemble. In this

209   and the next sections, the EnKF means the serial EnSRF unless otherwise stated. The

210   purpose of the perfect model experiments is to clarify the basic performance of the DL-EnKF,

211   while that of the imperfect model experiments is to gain insight into the performance of the

212   DL-EnKF when applied to data assimilation in the real atmosphere.

213   The experiments consist of two phases: the training phase of DNNs and the test phase

214   using data assimilation experiments. In the training phase, we run the models and the EnKF

215   to prepare training and validation datasets, which are used to train DNNs and to verify the

216   accuracy of the output of DNNs, respectively. The length of period and time interval of these

217   datasets are 1 000 and 1, respectively. This large time interval is taken to ensure that each

218   data is almost independent of each other. In the test phase, we run the models to prepare a

219   test dataset for the data assimilation experiments. The length of period of this dataset is also

220   1 000. The accuracy of the DL-EnKF analysis is compared with the deep learning and EnKF

221   analyses to evaluate the performance of the DL-EnKF. The workflow to create the deep

222   learning analysis is the same as that of the DL-EnKF analysis except for the absence of

223   feedback from the deep learning part to the EnKF part (Fig. 2). The analysis accuracy is | Fig. 2

224   evaluated by the RMSE that is the square root of the squared error averaged over the grid

225   points and the period of the test dataset at a time interval of 1.

226   In the perfect model experiments, we use the original 40-variable Lorenz 96 model and

227   conduct two types of experiments, Exp-PA and Exp-PB, in which the targets of training are

228   different. The target in Exp-PA is the true state generated by the model, while the target in

229   Exp-PB is an analysis by the stochastic EnKF (Evensen, 1994; Burgers et al., 1998) with an

230   ensemble size of 1 000. This analysis is hereafter referred to as the EnKF1000 analysis.

231   Although this ensemble size may be unrealistic for the 40-variable model, the purpose of

232   Exp-PB is to examine the performance of the DL-EnKF when an analysis with a high

233 accuracy is used as a target.

234   In the imperfect model experiments, the two-scale Lorenz 96 model with 40 large-scale

235 variables and 400 small-scale variables is used as a substitute of the real atmosphere, while

236 a parameterized Lorenz 96 model with a parameterization of large-scale forcing by small-

237 scale variables is used as a substitute of a numerical model of the real atmosphere. We

238 conduct two types of experiments, Exp-IA and Exp-IB. In Exp-IA, we train DNNs using the

239 simulation data generated by the parameterized model, and conduct the data assimilation

240 experiment using observations generated by the two-scale model. The idea behind Exp-IA

241 is that if a dynamical system and a observing system that are used for the taining of a DNN

242 resemble the real-world systems, we could expect that a data assimilation method the DNN

243 has learned by training also works in the real-world applications. In Exp-IB, the two-scale

244 Lorenz 96 model is used for the training and data assimilation experiments in a perfect model

245 scenario for comparison to Exp-IA.

246   Table 1 summarizes the models used in the training and test phases of the experiments. | Table 1 |

247 The following subsections describe further details of the experimental design.

248

249 *3.2. Models*

250   The governing equations of the Lorenz 96 model for the perfect model experiments are

251 $$\frac{dX_k}{dt} = -X_{k-1}(X_{k-2} - X_{k+1}) - X_k + F,$$ (2)

252 for $k = 1, \cdots, K$, satisfying periodic boundary conditions: $X_{-1} = X_{K-1}$, $X_0 = X_K$, and $X_1 =$

12

253   X_{K+1}. The number of variables K and the forcing parameter F are set to 40 and 8,

254   respectively. Note that since the number of positive Lyapunov exponents of the model is 13

255   for those parameter values (Lorenz and Emanuel, 1998), the ensemble size of 10 is not very

256   small. The leading Lyapunov exponent corresponds to a doubling time of 0.42 (Lorenz and

257   Emanuel, 1998). When the nonlinearity in data assimilation is controlled by changing the

258   time interval between observations as in the present study, this value can be used as a

259   reference for estimating the degree of nonlinearity. The fourth-order Runge-Kutta scheme is

260   adopted for the time integration of the model with a time step 0.01.

261   The governing equations of the two-scale Lorenz 96 model for the imperfect model

262   experiments are

263
$$\frac{dX_k}{dt} = -X_{k-1}(X_{k-2} - X_{k+1}) - X_k + F - \frac{hc}{b}\sum_{j=1}^{J} Y_{j,k}, \tag{3}$$

264
$$\frac{dY_{j,k}}{dt} = -cbY_{j+1,k}(Y_{j+2,k} - Y_{j-1,k}) - cY_{j,k} + \frac{hc}{b}X_k, \tag{4}$$

265   for $k = 1, \cdots, K$ and $j = 1, \cdots, J$, where $\{X_k\}$ are large-scale variables and $\{Y_{j,k}\}$ are small-

266   scale variables, satisfying periodic boundary conditions: $X_{-1} = X_{K-1}$, $X_0 = X_K$, $X_1 = X_{K+1}$,

267     $Y_{0,1} = Y_{J,K}$, $Y_{J+1,K} = Y_{1,1}$, and $Y_{J+2,K} = Y_{2,1}$. To make Eq. (4) meaningful, we further define

268     $Y_{0,k} = Y_{J,k-1}$, $Y_{J+1,k} = Y_{1,k+1}$, and $Y_{J+2,k} = Y_{2,k+1}$. Large- and small-scale variables interact

269   with each other through the last terms on the right-hand side of Eqs. (3) and (4). We set the

270   parameters as follows: $K = 40$, $J = 10$, $F = 10$, $h = 1$, $c = 10$, and $b = 10$. These values

271   are the same as the ones used by Lorenz (1996) except for K. Note that the forcing

272   parameter F is larger than in the perfect model experiments. The fourth-order Runge-Kutta

273   scheme is adopted for the time integration of the model with a time step 0.005.

274   We also need the parameterized Lorenz 96 model in the imperfect model experiments.

275   Although advanced parametrization methods such as stochastic parametrization (e.g., Wilks,

276   2005) and machine learning-based parametrization (e.g., Schneider et al., 2017) are

277   available, a simple function fitting is adopted in the present study; the last term on the right-

278   hand side of Eq. (3) is approximated by a linear function of X_k. The reason we adopt such

279   a simple approach is that we intend to demonstrate that even an unsophisticated imperfect

280   model works well for the training of a DNN. Then the governing equations of the

281   parameterized Lorenz 96 model are

282    $$\frac{dX_k}{dt} = -X_{k-1}(X_{k-2} - X_{k+1}) - X_k + F + (a_1 X_k + a_0), \tag{5}$$

283   for $k = 1, \cdots, K$, satisfying periodic boundary conditions: $X_{-1} = X_{K-1}$, $X_0 = X_K$, and $X_1 =$

284   X_{K+1}. The number of variables K and the forcing parameter F were set to 40 and 10,

285   respectively, to be consistent with the two-scale Lorenz 96 model. The constants a_1 and

286   a_0 are to be determined by the function fitting. The fourth-order Runge-Kutta scheme is

287   adopted for the time integration of the model with a time step 0.01.

288   The three models are integrated from $t = 0$ to $t = 2\,050$ for preparing the training and

289   validation datasets. The initial condition at each grid point is F plus an independent random

290   number drawn from the normal distribution with the mean 0 and the variance 1, except that

291   the small-scale variables of the two-scale Lorenz 96 model are set to 0 at the initial time.

292   The data from $t = 51$ to $t = 1\,050$ are used for preparing the training dataset, and those

293   from $t = 1\,051$ to $t = 2\,050$ for the validation dataset. The other time integration of the

294   models from $t = 0$ to $t = 1\,050$ with initial conditions generated by using another random

295   number sequence is conducted for preparing the test dataset, and the state variables from

296      $t = 51$ to $t = 1\,050$ are used as the true state (target) for computing the analysis error.

297

298   *3.3. Observations*

299   Observations are generated by adding random errors to the results of the time

300   integration of the models. The observation errors are independent random draws from the

301   normal distribution with the mean 0 and the variance 1, so that the standard deviation of

302   observation errors is 1. Observations used in the imperfect experiments are of large-scale

303   variables of the two-scale Lorenz 96 model except for the training phase of Exp-IA, in which

304   observations are prepared by the parameterized Lorenz 96 model.

305   Nonlinearity in data assimilation is controlled by changing the time interval between

306   observations Δt. All experiments are performed for three values of Δt: 0.05, 0.20, and 0.50.

307   The case of $\Delta t = 0.05$ corresponds to a weakly nonlinear case, and that of $\Delta t = 0.50$

308   corresponds to a strongly nonlinear one. Note that the latter value is close to the doubling

309   time 0.42 mentioned in Subsection 3.2, and that Penny and Miyoshi (2016) used $\Delta t = 0.50$

310   for their experiments of a local PF. All observations are prepared such that observations at

311   the same analysis time are the same regardless of the time interval between observations.

312   For the spatial distribution of observations, two cases are examined. In one case,

313   observations are available at all grid points, and the number of observations is always 40.

314   In other words, observations are available at each grid point with a probability of 1. In the

315   other case, observations are available at each grid point with a probability of 1/2. It is

316   assumed that events that an observation exists are independent of each other in space and

317   time so that the spatial distribution of observations randomly changes at every observation

318   time. The average number of observations is 20, and the standard deviation of the number

319   of observations is $\sqrt{40 \cdot (1/2)^2} \approx 3.16$. Hence, the number of pseudo-observations used by

320   deep learning is about the same as that of observations. The probability of observations is

321   hereafter denoted by p.

322

323   *3.4. Data assimilation by EnKF*

324   Covariance localization and covariance inflation are needed to optimize the performance

325   of the EnKF. The correlation function defined by Eq. (4.10) of Gaspari and Cohn (1999) is

326   taken for covariance localization. The parameter c in this equation is regarded as the

327   localization radius r_L (unit: grid intervals) in the present study, at which radius the

328   correlation coefficient decreases to 5/24. An adaptive inflation method proposed by Li et al.

329   (2009) is used for multiplicative covariance inflation. This method is based on the innovation

330   statistics by Desroziers et al. (2005). Li et al. (2009) imposed lower and upper limits in the

331   "observed" inflation factor $\tilde{\Delta}^o$ before applying a smoothing procedure: $0.9 \leq \tilde{\Delta}^o \leq 1.2$. Since

332   we conduct data assimilation over a much wider range of the time interval between

16

333 observations Δt, we optimize the upper limit of $\tilde{\Delta}^o$ for each set of parameters (r_L, Δt, p)

334 leaving the lower limit at 0.9. The candidates of the upper limit are 1.2, 1.3, 1.4, 1.5, 2.0, 3.0,

335 5.0, and no limit. In addition, although Li et al. (2009) set the error growth parameter κ to

336 1.03, we adopt a larger value κ = 1.1 because this value leads to a better analysis in the

337 present study. A set of values of r_L and the upper limit of $\tilde{\Delta}^o$ with the best analysis accuracy

338 is hereafter referred to as the optimal parameters. We determine the optimal parameters for

339 each pair of (Δt, p) in Exp-PA and Exp-IA by data assimilation experiments using the target

340 and observations in each training dataset. The optimal parameters thus determined are also

341 used in Exp-PB and Exp-IB, respectively, unless otherwise stated.

342   In Exp-PB, the target of training is the EnKF1000 analysis that is yielded by the

343 stochastic EnKF with an ensemble size of 1 000, as mentioned in Subsection 3.1. The

344 reason we adopt the stochastic EnKF is that when an ensemble size is very large the

345 accuracy of the serial EnSRF tends to deteriorate and to become less accurate than the

346 stochastic EnKF. We can avoid this problem with the serial EnSRF by applying the mean-

347 preserving random rotation of an analysis ensemble (Sakov and Oke, 2008), but an

348 additional computational cost is very large for the random rotation of a 1000-member

349 ensemble. Figure 3 compares the analysis accuracy of the two EnKFs for ensemble sizes | Fig. 3 |

350 of 10 (in cold colors) and 1 000 (in warm colors), plotting the RMSEs averaged over the

351 period from $t = 51$ to $t = 1050$. This result is obtained by using the target and observations

352 in the training datasets of Exp-PA. The localization radius and the upper limit of $\tilde{\Delta}^o$ are

17

353   optimized in the case of the ensemble size 10, while no covariance localization is applied

354   and the upper limits of $\tilde{\Delta}^o$ is set to 1.2 in the case of the ensemble size 1 000. It is found

355   from Fig. 3 that in the latter case the RMSE of the stochastic EnKF is smaller than that of

356   the serial EnSRF for all values of the time interval between observations Δt and probability

357   of observations p. Note that the serial EnSRF with an ensemble size 10 outperforms the

358   serial EnSRF with an ensemble size 1 000 in the three cases: $(\Delta t,\; p) = (0.05, 1),\; (0.05, 1/2),$

359   and $(0.20, 1)$.

360   In Exp-IB, the two-scale Lorenz 96 model is used to assimilate observations of large-

361   scale variables. As noted by Tsuyuki (2019), when the ensemble size is relatively small,

362   forecast correlations between large- and small-scale variables are not reliable. Hence, these

363   forecast correlations are neglected in the EnKF, and the analysis ensemble of small-scale

364   variables is left unchanged from the forecast ensemble at each analysis time.

365

366   *3.5. Deep learning*

367   A simple feedforward neural network with the same number of nodes for all hidden layers

368   is adopted for the deep learning part of the DL-EnKF. As we assume that the input radius of

369   DNNs is relatively small, a convolutional neural network would not be needed. We could use

370   a recurrent neural network instead of the feedforward neural network to utilize the

371   information obtained by the previous processing in deep learning, but it is not adopted in the

372   present study for simplicity.

373   The inputs of a DNN are the EnKF analysis using the optimal parameters, forecast,

374   observations, availability of observations, and pseudo-observations in a small domain

375   centered on an analysis grid point within the input radius r_I (unit: grid intervals). The

376   availability of observation at a grid point is set to 1 if the observation is available and set to

377   -1 if not available. The DNN assumes that observations are always available at all grid points,

378   and we supplement missing observations with pseudo-observations. Since the availability

379   of observations is not necessary in the case of $p = 1$, the input layer of the DNN has $3(2r_I +$

380     $1)$ nodes for $p = 1$, and $4(2r_I + 1)$ nodes for $p = 1/2$. The number of hidden layers is set

381   to 5 or 10 and the number of nodes per hidden layer is optimized as will be mentioned later.

382   Since the balance of analysis (Kalnay, 2003) is not a serious issue in Lorenz 96 models, we

383   let the output of the DNN be the analysis value at the analysis grid point only. For Exp-IB in

384   which the two-scale Lorenz 96 model is used in the EnKF part of DL-EnKF, the input and

385   output of the DNN are of large-scale variables only.

386   Table 2 summarizes the architecture and training of the DNN. All input and output data | Table 2 |

387   except for the availability of observations are normalized by using the mean and standard

388   deviation of the target state in the training dataset of Exp-PA for the perfect model

389   experiments and of Exp-IB for the imperfect model experiments. Since the statistical

390   behavior of the models does not depend on the location of a grid point, the data at all grid

391   points are used to prepare the training and validation datasets. Hence, the number of

392   samples of each dataset is $40 \times 1\,000 = 40\,000$. The training dataset is split into small

19

393   batches called mini-batches that are used to compute the loss function and update the

394   weights of the DNN. Learning rate decay is adopted in the training to avoid the situation in

395   which the DNN converges towards minima in a noisy manner and ends up oscillating far

396   away from actual minima. The number of epochs is the number of times each element in the

397   training dataset is used by the DNN for optimizing the weights. For most of the cases,

398   iterations almost converge within 10 epochs. We use PyTorch (Paszke et al., 2019) as the

399   deep learning software.

400   To determine the optimal number of nodes per hidden layer, we train two DNNs with 5

401   and 10 hidden layers by changing the number of nodes using the training and validation

402   datasets of Exp-PA. Figure 4 plots the RMSEs of the two DNNs against the input radius r_I Fig. 4

403   for the case of $\Delta t = 0.50$ and $p = 1$. The RMSEs are computed by using the validation

404   datasets. For the DNN with 10 hidden layers and 5 nodes per hidden layer, the training fails

405   for six values of the input radius, so that the RMSE of this case is not plotted in Fig. 4b.

406   Since the RMSE is not very different between 5 and 10 hidden layers, we adopt the DNN

407   with 5 hidden layers. It is found from Fig. 4 that when the input radius and number of nodes

408   are large to some extent, the RMSE tends to increase due to the generalization error of deep

409   learning. Since the DNN with 20 nodes per hidden layer has the smallest RMSE for most of

410   the input radii, we set the optimal number of nodes to 20 for the case of $\Delta t = 0.50$ and $p =$

411   1.

412   The optimal numbers of nodes of the DNN with 5 hidden layers are summarized in Fig.   Fig. 5

413   5 by blue bars for $p = 1$ and by cyan bars for $p = 1/2$. They tend to increase as the time

414   interval between observations increases because the estimation of state variables becomes

415   more difficult as nonlinearity increases. Although this result is obtained for Exp-PA, those

416   number of nodes are used in all experiments. We also compute the optimal numbers of

417   nodes for the case where the EnKF analysis is not included in the inputs of the DNN. The

418   RMSEs for this case are plotted in Fig. 5 by red bars for $p = 1$ and by orange bars for $p =$

419   $1/2$. It is found that the inclusion of the EnKF analysis tends to reduce the optimal number

420   of nodes. This is probably because the EnKF analysis plays the role of a first guess and

421   makes it easier to estimate state variables.

422   The appendix discusses the impacts of the increase in the ensemble size of EnKF and

423   the sample size for training on the accuracy of output of a DNN. The result of experiments

424   shows that when the ensemble size of EnKF is increased to 40 the improvement by deep

425   learning is considerably reduced, and that we need to increase the sample size much larger

426   to obtain a larger improvement.

427

428   *3.6 Data assimilation by DL-EnKF*

429   In the data assimilation experiments with the DL-EnKF, the EnKF part of DL-EnKF

430   adopts the optimal parameters, and the DL-EnKF analysis is the average of outputs of 5 or

431   10 DNNs. Since the adaptive covariance inflation is used in the EnKF part, the parameter

432   α in Eq. (1) is set to 1. In the test phase of Exp-IB, the deep learning part receives only

433 large-scale variables from the EnKF part and generates the DL-EnKF analysis of large-scale

434 variables. The analysis ensemble of large-scale variables is modified by using this analysis,

435 while the analysis ensemble of small-scale variables is left unchanged from the one

436 generated by the EnKF part. The RMSEs of the DL-EnKF, deep learning, and EnKF analysis

437 in Exp-IB are computed by using large-scale variables only.

438

439 **4. Results**

440 *4.1 perfect model experiments*

441 The first issue to be clarified is whether deep learning can outperform the EnKF in terms

442 of analysis accuracy. The EnKF is close to optimal in weakly nonlinear regimes, and the

443 deep learning part of DL-EnKF does not explicitly utilize the forecast error covariance. Figure | Fig. 6 |

444 6a compares the analysis accuracy between deep learning and the EnKF in Exp-PA for all

445 values of Δt and p, in which the RMSEs are plotted against the RMSE of EnKF for the

446 input radius of 2 grid intervals. The dots indicate the RMSEs of a single DNN, and the short

447 horizontal bars indicate the RMSE of the average of outputs from 5 DNNs. It is found from

448 this figure that all RMSEs of deep learning analysis are the same for each case and that

449 deep learning outperforms the EnKF when $\Delta t = 0.50$. Note that since the EnKF analysis is

450 included in the inputs of DNNs, the accuracy of deep learning analysis does not become

451 worse than that of the EnKF analysis if sufficient training samples are available.

452 The second issue is whether the accuracy of the DL-EnKF analysis is better than that

22

of the EnKF and deep learning analyses. As mentioned in the introduction, the analysis by deep learning is based on the minimization of the sum of errors over many samples and not optimized for each analysis time. Hence, the analysis accuracy may deteriorate during assimilation cycles by the DL-EnKF. Figure 6b compares the analysis accuracy between the DL-EnKF and EnKF for Exp-PA. The dots indicate the RMSEs of DL-EnKF when the output of a single DNN is used as the DL-EnKF analysis, and the horizontal bars indicate the ones when the average of outputs from 5 DNNs is used as the DL-EnKF analysis. It is found that when $\Delta t = 0.05$ the RMSEs of DL-EnKF based on a single DNN are scattered and larger than that of EnKF. In other words, the accuracy of the deep learning analysis shown in Fig. 6a is not maintained during assimilation cycles in a weakly nonlinear case. Taking the average over 5 DNNs does not improve the accuracy very well. When $\Delta t = 0.20$ and 0.50, on the other hand, the RMSEs of DL-EnKF based on a single DNN become almost the same for each case and taking the average over 5 DNNs slightly improves the accuracy in the case of $\Delta t = 0.50$. In addition, a comparison of Fig. 6a and 6b shows that the RMSE of DL-EnKF is smaller than that of deep learning when $\Delta t = 0.50$ due to positive feedback in assimilation cycles.

We conduct additional experiments in which the ensemble size of DNNs is increased to 10 in Exp-PA. The initial conditions of weights used for the training are different from the ones used in the case of 5 DNNs. Results are presented in Figs. 6c and 6d, and the former figure looks the same as Fig. 6a. The benefit of taking the average over 10 DNNs for the

473   DL-EnKF is evident when $\Delta t = 0.05$, although its analysis accuracy is still lower than that of

474   EnKF. When $\Delta t = 0.20$ and $\Delta t = 0.50$, the RMSEs of DL-EnKF are almost the same as in

475   the case of 5 DNNs. This suggests that an ensemble size of 5 is sufficient except for a

476   weakly nonlinear case. Then, all the results shown below are based on the average of

477   outputs from 5 DNNs, because our interest is primarily in the performance of the DL-EnKF

478   in strongly nonlinear regimes.

479   Figure 7 compares the time sequences of RMSEs of the EnKF (red line) and the DL- | Fig. 7 |

480   EnKF (green line) in the case of $p = 1$. When $\Delta t = 0.05$ (Fig. 7a), the DL-EnKF is

481   outperformed by the EnKF during the whole period. When $\Delta t = 0.20$ (Fig. 7b), the analysis

482   accuracy of the two methods is close; the correlation coefficient between the two RMSEs

483   computed for the period from $t = 51$ to $t = 1\,050$ is 0.761. When $\Delta t = 0.50$ (Fig. 7c), the

484   EnKF sometimes exhibits a significant deterioration of accuracy, but the DL-EnKF does not

485   show such a tendency. This result demonstrates an excellent performance of the DL-EnKF

486   in strongly nonlinear regimes.

487   The third issue is whether the optimal input radius of deep learning is smaller than the

488   optimal localization radius of the EnKF. Figure 8 plots the RMSEs of EnKF (orange lines), | Fig. 8 |

489   deep learning (green lines), and DL-EnKF (blue lines) analysis against the input radius for

490   all cases of Exp-PA (solid lines) and Exp-PB (broken lines). The RMSE of EnKF in Exp-PB

491   is the same as the one in Exp-PA. An orange broken line indicates the RMSE of the

492   EnKF1000 analysis that is used for the training in Exp-PB. The optimal localization radius is

24

493   plotted by a red arrow, except for the case of $(\Delta t,\ p) = (0.05, 1/2)$ where the optimal

494   localization radius is 11 grid intervals. The RMSEs of EnKF and deep learning overlap in

495   Figs. 8a and 8b, and the RMSEs except for the EnKF1000 analysis almost overlap in Figs.

496   8c and 8d.

497   When $\Delta t = 0.05$ (Figs. 8a and 8b), the DL-EnKF is outperformed by the EnKF.

498   Reflecting that an ensemble of 5 DNNs is not sufficient (see Fig. 5b), the graphs of the DL-

499   EnKF are not smooth due to large sampling errors. When $\Delta t = 0.20$ (Fig. 8c and 8d) the

500   two data assimilation methods exhibit almost the same accuracy while when $\Delta t = 0.50$

501   (Figs. 8e and 8f) the DL-EnKF outperforms the EnKF irrespective of the input radius. The

502   accuracy of the DL-EnKF analysis is higher than that of the deep learning analysis for the

503   latter case due to positive feedback in assimilation cycles. We can conclude that the input

504   radius of 2 grid intervals is sufficient to attain the best accuracy of the DL-EnKF analysis.

505   This value is smaller than the optimal localization radii for both $p = 1$ and $p = 1/2$. Even if

506   the input radius is further increased, the accuracy of the DL-EnKF and deep learning

507   analysis remains almost the same, although slight degradations are seen due to the

508   generalization error of deep learning. This small sensitivity of RMSEs on the input radius

509   indicates that the information at distant grid points contributes little to the DL-EnKF analysis

510   even within the localization radius of the EnKF. The inclusion of the EnKF analysis in the

511   inputs of DNNs also contributes to this insensitivity.

512   Another point to be noted in Figs. 8e and 8f is that even if DNNs are trained on the

513   EnKF1000 analysis, the accuracy of the DL-EnKF analysis is not very different from the one

514   trained on the true state. Given the large errors of the EnKF1000 analysis shown in Figs. 8e

515   and 8f, this result may look surprising. That is probably because this analysis well represents

516   the basic dynamics of the Lorenz 96 model despite the large errors. If the difference in the

517   ensemble size between the DL-EnKF and the target analysis is decreased, the accuracy of

518   the DL-EnKF analysis in Exp-PB is more deteriorated. For instance, according to an

519   additional experiment in which the ensemble size of the DL-EnKF is set to 40 for the case

520   of $\Delta t = 0.50$ and $p = 1$ (see the appendix), the RMSEs of the EnKF analysis and DL-EnKF

521   analyses in Exp-PA and Exp-PB are 0.682, 0.617, and 0.638, respectively, for the input

522   radius of 2 grid intervals. The corresponding values for the ensemble size of 10 are 0.798,

523   0.675, and 0.689 (see Fig. 8e), so that the deterioration of accuracy in Exp-PB is still not

524   very large.

525   Finally, we examine the impact of including the EnKF analysis in the inputs of DNNs on

526   the accuracy of the deep learning analysis using the test datasets of Exp-PA. Figure 9 plots   Fig. 9

527   the RMSE of deep learning in which the EnKF analysis is not included (cyan line) and the

528   one in which the EnKF analysis is included (green line) against the input radius. The green

529   lines are the same as in Fig. 8, and the two RMSEs overlap in Fig. 9f. For comparison, the

530   RMSE of EnKF of which localization radius is not optimized is also plotted by an orange line

531   against the localization radius with the upper limit of $\tilde{\Delta}^o$ optimized for each localization

532   radius. Note that the RMSE of EnKF does not always attain the minimum at the optimal

26

533 localization radius indicated by a red arrow, because the values of the optimal parameters

534 are determined by using the training datasets.

535 We can see from Fig. 9 that the accuracy of the deep learning analysis is improved by

536 including the EnKF analysis in the inputs of DNNs except for Fig. 9f, in which the EnKF

537 analysis is too inaccurate to be useful. It is also found in Figs. 9c and 9e for $p = 1$ that this

538 procedure reduces the dependence of the analysis accuracy on the input radius. This is

539 because the EnKF analysis contains some information on the forecast ensemble and

540 observations in a domain within the localization radius. Such a reduction in the dependence

541 brought about by including the EnKF analysis is not clearly seen in Figs. 9d and 9f for $p =$

542 1/2, since deep learning partly utilizes the EnKF analysis through pseudo-observations.

543

544 *4.2 Imperfect model experiments*

545 The parametrization procedure for the parameterized Lorenz 96 model is described in

546 Subsection 3.2. Figure 10 is the scatter plot between the large-scale variables and the Fig. 10

547 forcing. The initial condition is the same as that used for preparing the training dataset of

548 Exp-IB. The number of samples is 40 000 and the result of linear function fitting is plotted by

549 a straight line. The values of constants in Eq. (5) are $a_1 = -0.320$ and $a_0 = -0.165$. Since

550 the slope of this line is negative, the forcing acts on large-scale variables as negative

551 feedback. Figure 11 compares the Hovmöller diagrams of the Lorenz 96 model, Fig. 11

552 parameterized Lorenz 96 model, and large-scale variables of the two-scale Lorenz 96 model.

553 The initial condition is the same as that used in Fig. 10. Note that the forcing parameter F

554 is larger than in the perfect model experiments. A comparison of the three panels in Fig. 11

555 shows that the parameterization works well, although the parametrized Lorenz 96 model

556 evolves a little more regularly than the two-scale Lorenz 96 model. Stochastic

557 parameterizations could remedy this defect (Wilks, 2005).

558   Figure 12 plots the RMSEs of EnKF (orange lines), deep learning (green lines), and DL-   Fig. 12

559 EnKF (blue lines) analysis against the input radius for all cases of Exp-IA (solid lines) and

560 Exp-IB (broken lines). Note that Exp-IA is conducted in an imperfect model scenario, while

561 Exp-IB is conducted in a perfect model scenario for comparison. Unlike Fig. 8, an orange

562 broken line indicates the RMSE of EnKF using the two-scale Lorenz 96 model. The optimal

563 localization radius of the EnKF is indicated by a red arrow. The RMSEs of EnKF and deep

564 learning for each case overlap in Figs. 12a-12d. It is found that the RMSE of EnKF using

565 the two-scale Lorenz 96 model is smaller than the one using the parameterized Lorenz 96

566 model. We can confirm that the basic performance of the DL-EnKF is the same as in the

567 perfect model experiments; the DL-EnKF is inferior to the EnKF in a weakly nonlinear case

568 (Figs. 12a and 12b), while the opposite is true in a strongly nonlinear case (Figs. 12e and

569 12f), in which the optimum input radius is smaller than the optimum localization length. A

570 difference from the perfect model experiments is that when $\Delta t = 0.20$ (Figs. 12c and 12d),

571 the accuracy of the DL-EnKF analysis is a little worse than that of the EnKF analysis for $p =$

572 1 and a little better for small values of the input radius for $p = 1/2$.

<div align="center">28</div>

573　　　　An important point to be noted in Figs. 12e and 12f is that even if DNNs are trained on

574　　the training dataset prepared by the parameterized Lorenz 96 model, the improvement in

575　　analysis accuracy introduced by the DL-EnKF is not very different from the case where the

576　　training dataset is prepared by the two-scale Lorenz 96 model. The former model is run in

577　　the data assimilation experiments in the test phase of Exp-IA without any trouble, implying

578　　that this model well represents the basic dynamics of large-scale variables of the two-scale

579　　Lorenz 96 model. When we use the Lorenz 96 model with $F = 10$, of which evolution is

580　　shown in Fig.11a, in the above data assimilation experiments, we often experience failures.

581

582　**5. Summary and discussion**

583　　　　An ensemble data assimilation method based on deep learning was presented, in which

584　　an ensemble of DNNs was locally embedded in an EnKF. This method was named the DL-

585　　EnKF. The inputs of a DNN were the EnKF analysis, forecast, observations, availability of

586　　observations, and pseudo-observations in a small domain centered on an analysis grid point.

587　　Missing observations were supplemented with the pseudo-observations created from the

588　　EnKF analysis. The DL-EnKF analysis was the average of outputs from an ensemble of

589　　DNNs. The DL-EnKF analysis ensemble was generated from the DL-EnKF analysis and the

590　　EnKF analysis deviation ensemble. The members of the DL-EnKF analysis ensemble thus

591　　generated were evolved by the time integration of a numerical model to prepare the forecast

592　　ensemble for the next analysis time.

The performance of the DL-EnKF was investigated through data assimilation experiments in both perfect and imperfect model scenarios using three versions of the Lorenz 96 model and the serial EnSRF with an ensemble size of 10. The target of training in the perfect model experiments was the true state generated by the Lorenz 96 model or the EnKF1000 analysis generated by the stochastic EnKF with an ensemble size of 1000. In the imperfect model experiments, the true state and observations were provided by the two-scale Lorenz 96 model, while the training dataset was prepared by using the parameterized Lorenz 96 model. Nonlinearity in data assimilation was controlled by changing the time interval between observations.

The DL-EnKF was outperformed by the serial EnSRF in a weakly nonlinear case, but it was superior to the serial EnSRF in terms of analysis accuracy in a strongly nonlinear case despite such a small ensemble size. The DL-EnKF analysis was more accurate than the output of deep learning due to positive feedback in assimilation cycles in the latter case. Even if the target of training was the EnKF1000 analysis or the simulation by the parametrized Lorenz 96 model, the improvement introduced by the DL-EnKF was not very different from the case where the target of training was the true state. The inclusion of EnKF analysis in the inputs of DNNs not only improved the accuracy of the deep learning analysis but also reduced the optimal number of nodes per hidden layer and the dependence of the accuracy on the input radius.

Although the above results were obtained from experiments using toy models, they

suggest that the DL-EnKF may be a promising methods for data assimilation in strongly

nonlinear regimes. The DL-EnKF works with a relatively small ensemble size compared to

the PF, and we can prepare a training dataset for deep learning from simulation data by a

numerical model used in data assimilation. Observational data and EnKF analysis data

generated with a large ensemble could be used for this purpose, but a huge computational

cost may be needed to obtain sufficient samples and a period when observations are

available is limited.

The DL-EnKF may be suitable for data assimilation in cloudy or convective regions in

the atmosphere to assimilate radar and satellite observations. We need to extend the inputs

and output of DNNs in the vertical to assimilate satellite radiance data, since they are

nonlocal observations. As for radial wind data by a Doppler radar, the direction and distance

of a radar site differ depending on a grid point. However, if the radar site position relative to

the grid point is included in the inputs of a DNN, we can train the DNN collectively regardless

of the grid point as in the present study.

There are a couple of issues to be addressed before applying the DL-EnKF to data

assimilation in the atmosphere. In the data assimilation experiments using Lorenz 96 models,

the analysis value at a single grid point is sufficient for the output of a DNN, but we need to

take the balance of analysis into account for atmospheric data assimilation. One of the

methods for ensuring the balance is to extend the output of a DNN to include analysis values

at surrounding grid points. Then the target of training consists of the target state in a small

633   domain centered on an analysis grid point. Since the target state is usually well balanced,

634   the DNN could learn the balance. Adding a penalty term for suppressing imbalance to a loss

635   function of the DNN may help enhance the balance. In addition, taking a weighting average

636   of the outputs in adjacent domains may be effective in improving analysis accuracy.

637   This study demonstrates that the DL-EnKF is inferior to the EnKF in a weakly nonlinear

638   case. It is found that an increase in the ensemble size of DNNs can mitigate this problem,

639   but it would be difficult to increase the ensemble size sufficiently, given the computational

640   cost needed for the training of DNNs. We may need a criterion for replacing the EnKF

641   analysis with the corresponding DL-EnKF analysis in DL-EnKF assimilation cycles. An

642   advanced DNN such as a recurrent neural network would be useful for improving the

643   performance of DL-EnKF in weakly nonlinear regimes as well as in strongly nonlinear ones.

644

645   **Data Availability Statement**

646   The Python programs used for Exp-PA in this study are available on J-STAGE Data.

647

653 Fugaku (Large Ensemble Atmospheric and Environmental Prediction for Disaster

654 Prevention and Mitigation; hp200128, hp210166), and by the Japan Society for the

655 Promotion of Science through KAKENHI (Study on Uncertainty of Cumulonimbus Initiation

656 and Development Using Particle Filter; JP17H02962).

657

658 **Appendix**

659   In this study, we perform the experiments using the serial EnSRF with 10 members and

660 the 40 000 training samples. It may be of interest to examine how the accuracy of output of

661 a DNN changes when the ensemble size and the sample size are increased. This appendix

662 presents some results of additional experiments in which the ensemble size of EnKF is set

663 to 10 and 40 and the sample size is set to 40 000, 160 000 and 640 000. These experiments

664 correspond to Exp-PA for $\Delta t = 0.50$. The ensemble size of 40 is the same as the degrees

665 of freedom of the Lorenz 96 model and, according to Fig. 5 of Penny and Miyoshi (2016),

666 an EnKF still outperforms a local PF with this ensemble size. The periods of time integration

667 of the model for preparing the training and validation datasets are 2 050, 8 050, and 32 050

668 with the first periods of 50 in length are discarded.

669   Figure A1 shows the optimum numbers of nodes per hidden layer of a DNN, obtained | Fig. A1 |

670 by using the validation datasets. The maximum number of nodes is limited to 100. Although

671 we choose the number of nodes that performs the best for the various input radius, the

672 determination of the optimal number becomes difficult with the increase of the sample size.

33

When the number of training samples is increased, the generalization error of deep learning

tends to reduce and, therefore, the optimal number of nodes per hidden layer tends to

increase.

Figure A2 compares RMSE between the serial EnSRF and the output of a DNN obtained [Fig. A2]

by using the test datasets of Exp-PA. Note that they are not the average over 5 DNNs, so

that the RMSEs shown by green lines in Figs. A2a and A2b are different from those in Figs.

8e and 8f, respectively. The optimal localization radius of the serial EnSRF in Fig. A2c is 12

grid intervals. It is found from this figure that the improvement by deep learning is

considerably reduced for the ensemble size of 40. When the sample size is increased, the

RMSE of the output of a DNN is reduced, but we need much more training samples to obtain

a large improvement.

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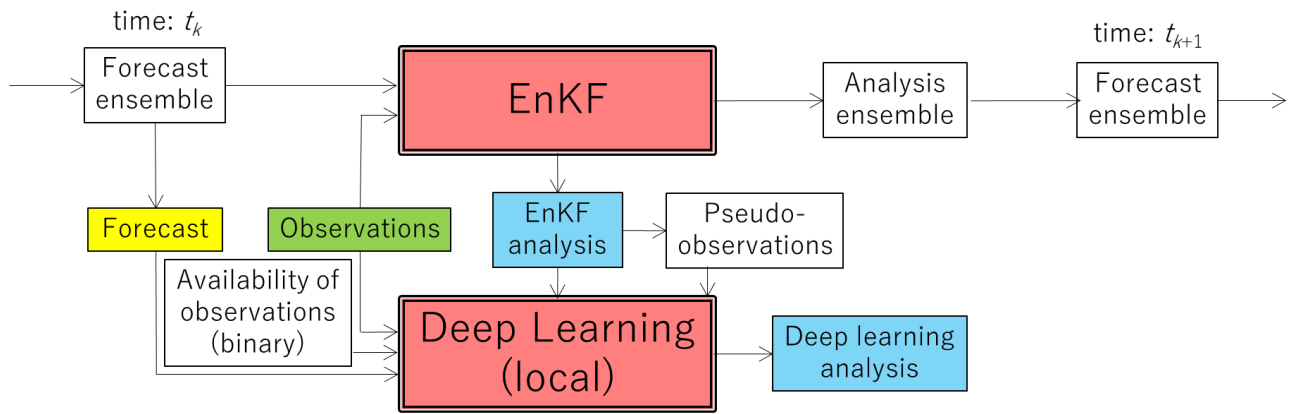
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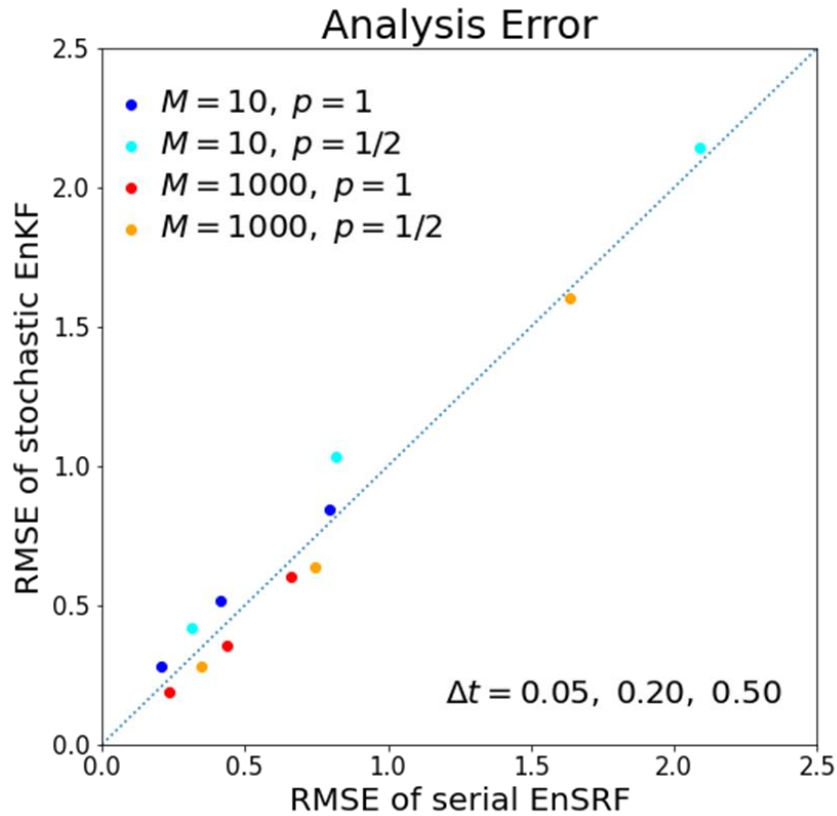Fig. 1   (a) Workflow of DL-EnKF and (b) workflow to train a DNN for DL-EnKF. See text

for details.
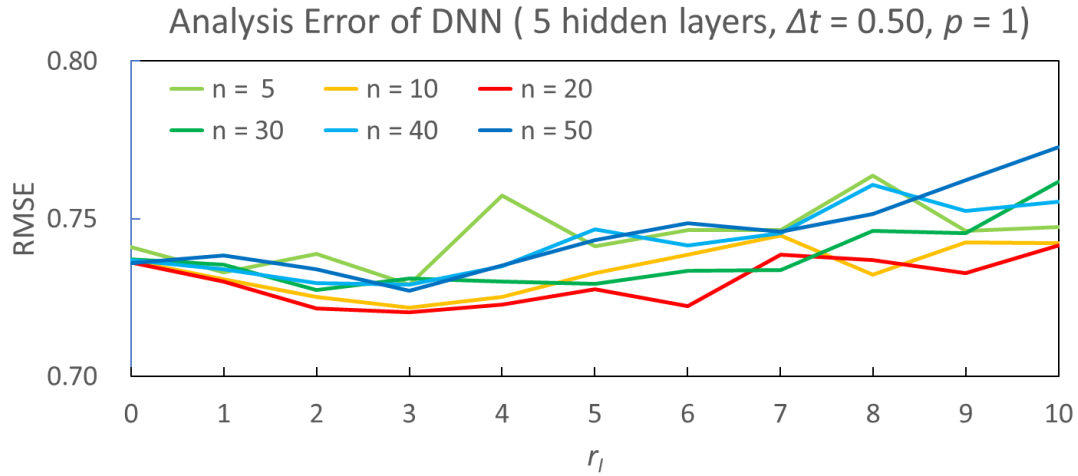
819
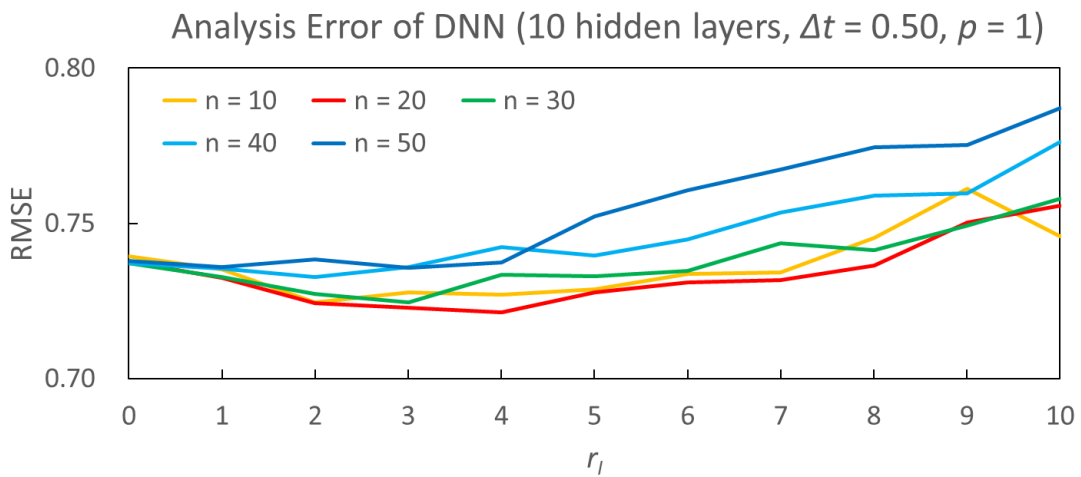
Fig. 2   Workflow to generate deep learning analysis.

821

Fig. 3   Comparison of RMSEs between the serial EnSRF (abscissa) and stochastic EnKF

(ordinate) for the training dataset of Exp-PA. Dots in cold colors are for an ensemble size

10 and dots in warm colors are for an ensemble size 1 000. Dots in dark colors are for

the probability of observations 1 and dots in light colors are for the probability of

observations 1/2. The three dots in the same color correspond to the observation time

intervals 0.05, 0.20, and 0.50 from left to right.

828
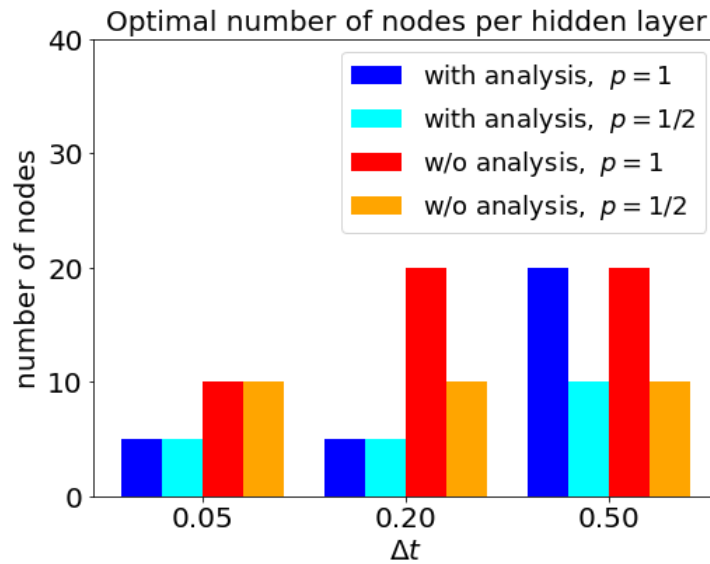
Fig. 4   Comparison of RMSEs of a single DNN with 5 (light green), 10 (orange), 20 (red),

30 (green), 40 (cyan), and 50 (blue) nodes per hidden layer for the validation dataset of

Exp-PA. The RMSEs are plotted against the input radius. The number of hidden layers is

(a) 5 and (b) 10. The observation time interval is 0.50 and the probability of observations
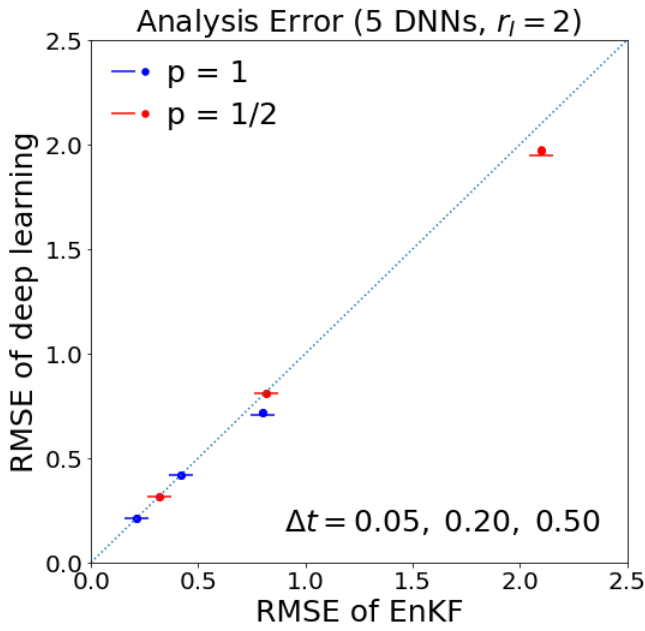
is 1.

834

835   Fig. 5   The optimal number of nodes per hidden layer of a DNN with 5 hidden layers. The

836   abscissa is the observation time interval. Blue and cyan bars are for the case of including

837   EnKF analysis in input for the probability of observations 1 and 1/2, respectively. Red and

838   orange bars are for the case of not including EnKF analysis in input for the probability of

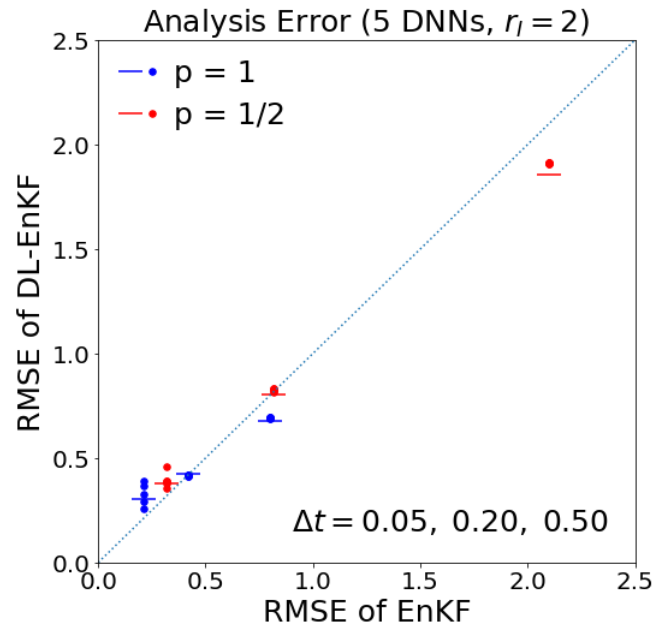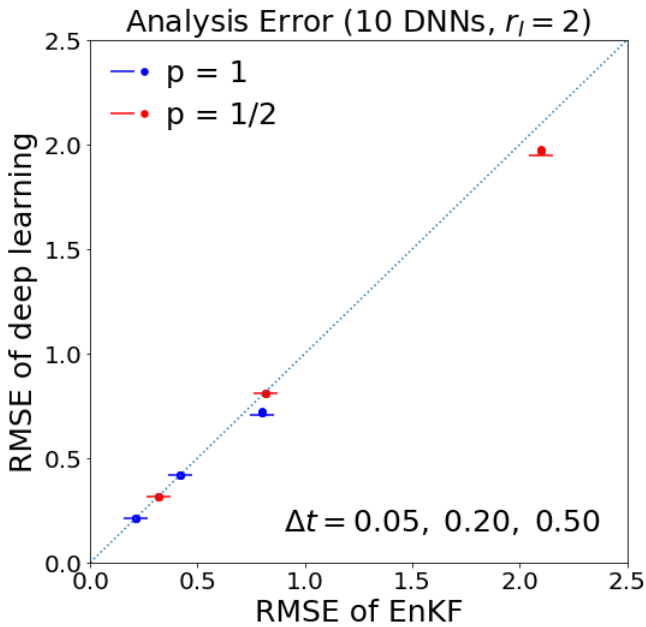839   observations 1 and 1/2, respectively.

840

841   Fig. 6   Comparison of RMSEs between (a) EnKF (abscissa) and deep learning with 5

842   DNNs (ordinate), (b) EnKF and DL-EnKF with 5 DNNs, (c) EnKF and deep learning with

843   10 DNNs, and (d) EnKF and deep learning with 10 DNNs for Exp-PA. The probability of

844   observations 1 is in blue and 1/2 in red, and the input radius is 2 grid intervals. Dots

845   indicate RMSEs based on a single DNN, and short horizontal bars indicate RMSEs based

846   on an ensemble of DNNs. The three groups of dots and a horizontal bar in the same color

847   correspond to the observation time intervals 0.05, 0.20, and 0.50 from left to right.

848

849   Fig. 7   Time sequences of RMSEs of EnKF (red lines) and DL-EnKF (blue lines) for

850   observation time interval (a) 0.05, (b) 0.20, and (c) 0.50 for Exp-PA. The probability of

851   observations is 1 and the input radius is 2 grid intervals.

852

853   Fig. 8   Comparison of RMSEs of EnKF (orange lines), deep learning (green lines), and

854   DL-EnKF (blue lines) for Exp-PA (solid lines) and Exp-PB (broken lines). An orange

855   broken line indicates the RMSE of EnKF1000 analysis used for training in Exp-PB. The

856   RMSEs are plotted against the input radius, and a red arrow indicates the optimal

857   localization radius of EnKF. The observation time interval and the probability of

858   observations are (a) 0.05 and 1, (b) 0.05 and 1/2, (c) 0.20 and 1, (d) 0.20 and 1/2, (e)

859   0.50 and 1, and (f) 0.50 and 1/2, respectively.

860

861 Fig. 9   Comparison of RMSEs of EnKF (orange line), deep learning not including EnKF

862   analysis in input (cyan line), and deep learning including the EnKF analysis in input

863   (green line) for Exp-PA. The RMSE of EnKF is computed for each localization radius. The

864   abscissa is the input radius for deep learning and the localization radius for the EnKF. A

865   red arrow indicates the optimal localization radius. The observation time interval and the

866   probability of observations are (a) 0.05 and 1, (b) 0.05 and 1/2, (c) 0.20 and 1, (d) 0.20

867   and 1/2, (e) 0.50 and 1, (f) 0.50 and 1/2, respectively.

868

869 Fig. 10   Scatter plot between large-scale variables (abscissa) and large-scale forcing by

870   small-scale variables (ordinate) of the two-scale Lorenz 96 model. A solid line is the result

871   of linear function fitting.

872

873 Fig. 11   Hovmöller diagrams of (a) the Lorenz 96 model, (b) the parametrized Lorenz 96

874   model, and (c) large-scale variables of the two-scale Lorenz 96 model.

875

Fig. 12   Same as Fig. 8 except for Exp-IA (solid lines) and Exp-IB (broken lines) and that

an orange broken line indicates the RMSE of EnKF using the two-scale Lorenz 96 model.

878

Fig. A1   The optimal number of nodes per hidden layer of a DNN with 5 hidden layers for

the time interval between observations of 0.50. The abscissa is the number of samples.

Blue and cyan bars are for the EnKF ensemble size of 10 for the probability of

observations 1 and 1/2, respectively. Red and orange bars are for the EnKF ensemble

size of 40 for the probability of observations 1 and 1/2, respectively.

884

Fig. A2   Comparison of RMSE between EnKF (orange lines) and the output of a DNN with

the number of samples of 40 000 (green lines), 160 000 (blue), and 640 000 (cyan) for

the observation time interval of 0.50. The ensemble size of EnKF and the probability of

observations are (a) 10 and 1, (b) 10 and 1/2, (c) 40 and 1, (d) 40 and 1/2, respectively.

The RMSEs are plotted against the input radius, and a red arrow indicates the optimal

localization radius of EnKF.

891

892

893 (a)

894

895 (b)

896

897 Fig. 1   (a) Workflow of DL-EnKF and (b) workflow to train a DNN for DL-EnKF. See text

898   for details.

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905   Fig. 3   Comparison of RMSEs between the serial EnSRF (abscissa) and stochastic EnKF

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907   10 and dots in warm colors are for an ensemble size 1 000. Dots in dark colors are for

908   the probability of observations 1 and dots in light colors are for the probability of

909   observations 1/2. The three dots in the same color correspond to the observation time

910   intervals 0.05, 0.20, and 0.50 from left to right.

911

912 (a)

913 (b)

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918   (a) 5 and (b) 10. The observation time interval is 0.50 and the probability of observations

919   is 1.

920

Fig. 5   The optimal number of nodes per hidden layer of a DNN with 5 hidden layers. The abscissa is the observation time interval. Blue and cyan bars are for the case of including EnKF analysis in input for the probability of observations 1 and 1/2, respectively. Red and orange bars are for the case of not including EnKF analysis in input for the probability of observations 1 and 1/2, respectively.

Fig. 6 Comparison of RMSEs between (a) EnKF (abscissa) and deep learning with 5 DNNs (ordinate), (b) EnKF and DL-EnKF with 5 DNNs, (c) EnKF and deep learning with 10 DNNs, and (d) EnKF and deep learning with 10 DNNs for Exp-PA. The probability of observations 1 is in blue and 1/2 in red, and the input radius is 2 grid intervals. Dots indicate RMSEs based on a single DNN, and short horizontal bars indicate RMSEs based on an ensemble of DNNs. The three groups of dots and a horizontal bar in the same color correspond to the observation time intervals 0.05, 0.20, and 0.50 from left to right.

940　(a)

Analysis Error ($\Delta t = 0.05$, $p = 1$, $r_l = 2$)

941　(b)

Analysis Error ($\Delta t = 0.20$, $p = 1$, $r_l = 2$)

942　(c)

Analysis Error ($\Delta t = 0.50$, $p = 1$, $r_l = 2$)

943

944　Fig. 7　　Time sequences of RMSEs of EnKF (red lines) and DL-EnKF (blue lines) for

945　　　　observation time interval (a) 0.05, (b) 0.20, and (c) 0.50 for Exp-PA. The probability of

946　　　　observations is 1 and the input radius is 2 grid intervals.

947

Fig. 8   Comparison of RMSEs of EnKF (orange lines), deep learning (green lines), and DL-EnKF (blue lines) for Exp-PA (solid lines) and Exp-PB (broken lines). An orange broken line indicates the RMSE of EnKF1000 analysis used for training in Exp-PB. The RMSEs are plotted against the input radius, and a red arrow indicates the optimal localization radius of EnKF. The observation time interval and the probability of observations are (a) 0.05 and 1, (b) 0.05 and 1/2, (c) 0.20 and 1, (d) 0.20 and 1/2, (e) 0.50 and 1, and (f) 0.50 and 1/2, respectively.

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Fig. 10   Scatter plot between large-scale variables (abscissa) and large-scale forcing by small-scale variables (ordinate) of the two-scale Lorenz 96 model. A solid line is the result of linear function fitting.

(a)

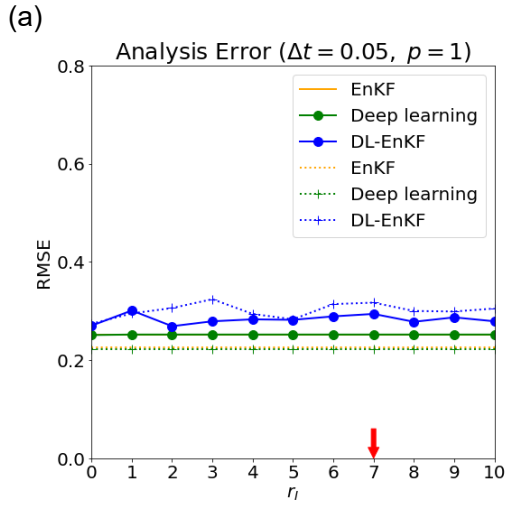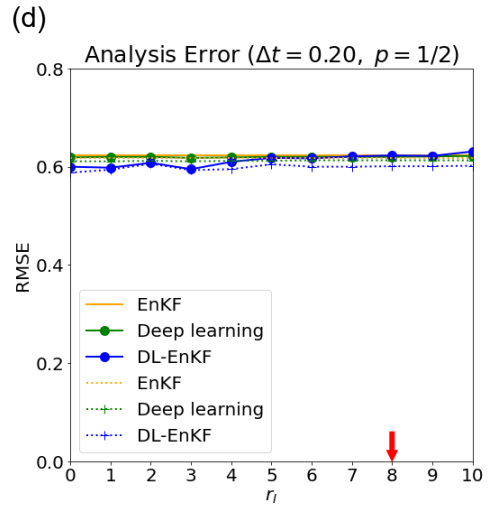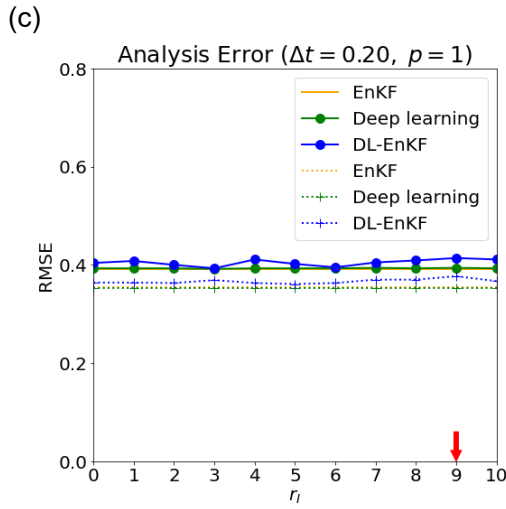Lorenz-96 model w/o parameterization

(b)

Lorenz-96 model with parameterization

(c)

Two-scale Lorenz-96 model (large scale)

Fig. 11   Hovmöller diagrams of (a) the Lorenz 96 model, (b) the parametrized Lorenz 96

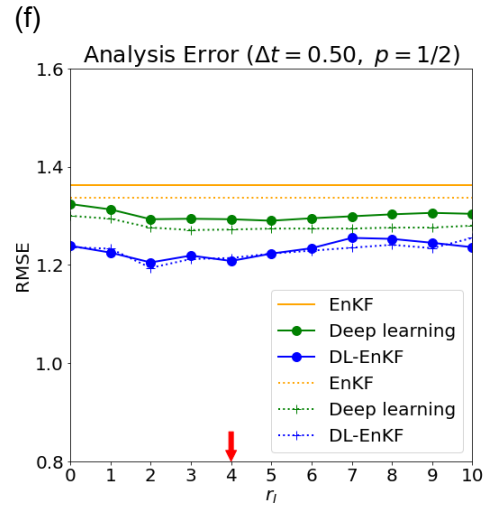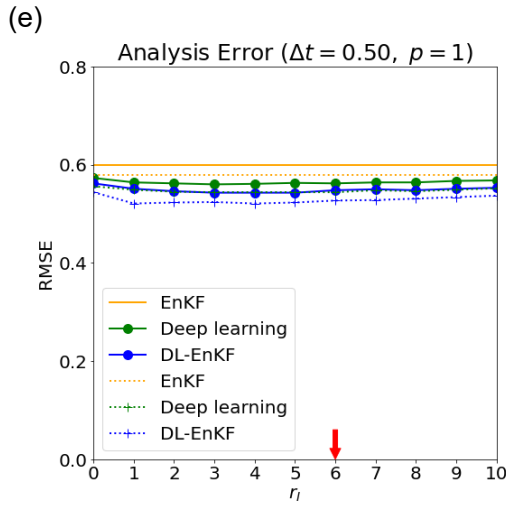model, and (c) large-scale variables of the two-scale Lorenz 96 model.

981

(a) Analysis Error ($\Delta t = 0.05$, $p = 1$)

(b) Analysis Error ($\Delta t = 0.05$, $p = 1/2$)

982

(c) Analysis Error ($\Delta t = 0.20$, $p = 1$)

(d) Analysis Error ($\Delta t = 0.20$, $p = 1/2$)

983

(e) Analysis Error ($\Delta t = 0.50$, $p = 1$)

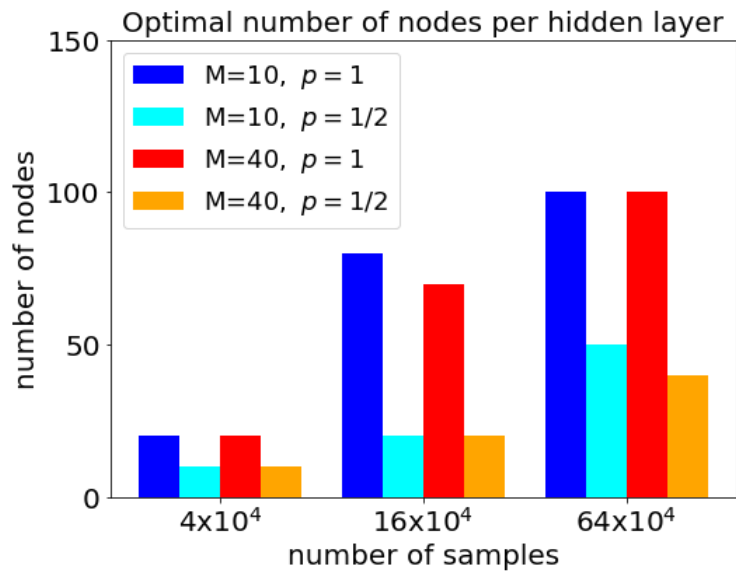(f) Analysis Error ($\Delta t = 0.50$, $p = 1/2$)

984

985   Fig. 12   Same as Fig. 8 except for Exp-IA (solid lines) and Exp-IB (broken lines) and that

986   an orange broken line indicates the RMSE of EnKF using the two-scale Lorenz 96 model.
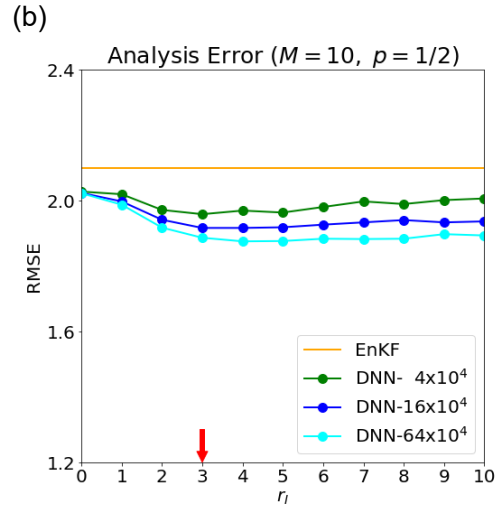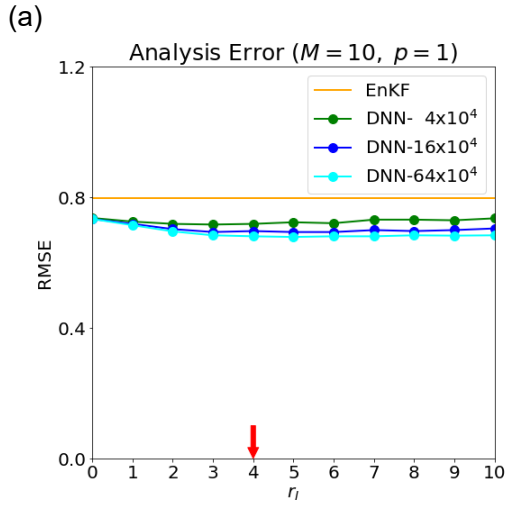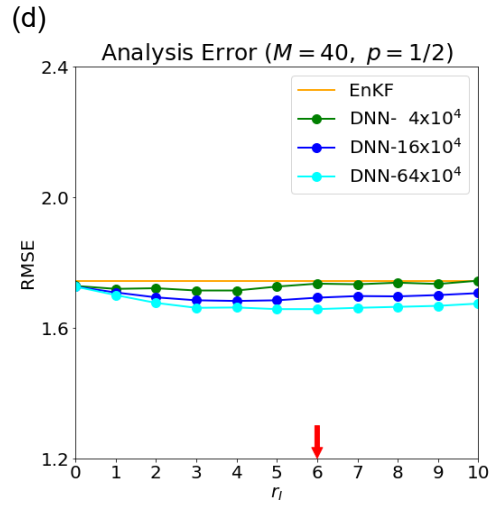
987

Optimal number of nodes per hidden layer

Legend:
- M=10, $p = 1$ (blue)
- M=10, $p = 1/2$ (cyan)
- M=40, $p = 1$ (red)
- M=40, $p = 1/2$ (orange)

y-axis: number of nodes

x-axis: number of samples (4×10^4, 16×10^4, 64×10^4)
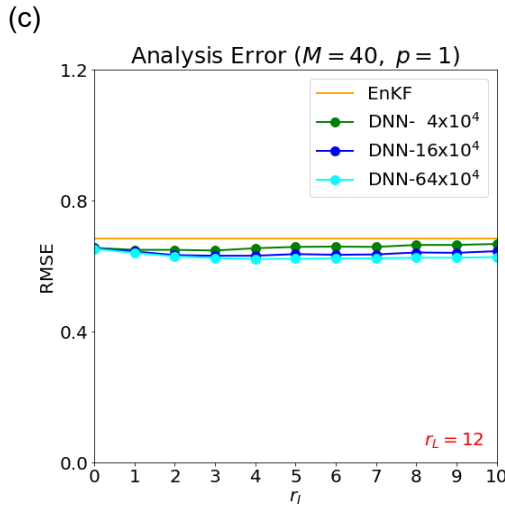
988

Fig. A1   The optimal number of nodes per hidden layer of a DNN with 5 hidden layers for the time interval between observations of 0.50. The abscissa is the number of samples. Blue and cyan bars are for the EnKF ensemble size of 10 for the probability of observations 1 and 1/2, respectively. Red and orange bars are for the EnKF ensemble size of 40 for the probability of observations 1 and 1/2, respectively.

995   (a)

996   (c)

997

998   Fig. A2   Comparison of RMSE between EnKF (orange lines) and the output of a DNN with

999   the number of samples of 40 000 (green lines), 160 000 (blue), and 640 000 (cyan) for

1000   the observation time interval of 0.50. The ensemble size of EnKF and the probability of

1001   observations are (a) 10 and 1, (b) 10 and 1/2, (c) 40 and 1, (d) 40 and 1/2, respectively.

1002   The RMSEs are plotted against the input radius, and a red arrow indicates the optimal

1003   localization radius of EnKF.

1004

List of Tables

Table 1　Models used in the training and test phases in the experiments.

(a) Perfect model experiments

	Exp-PA		Exp-PB	
	Training	Test	Training	Test
Target	L	L	Analysis	L
Observations	L	L	L	L
Forecast ensemble	L	L	L	L

L: Lorenz 96 model

(b) Imperfect model experiments

	Exp-IA		Exp-IB	
	Training	Test	Training	Test
Target	P	T	T	T
Observations	P	T	T	T
Forecast ensemble	P	P	T	T

P: parameterized Lorenz 96 model,　T: two-scale Lorenz 96 model

Table 2   Architecture and training of the feedforward neural network.

No. of nodes of input layer	$3(2r_I + 1)$ for $p = 1$
	$4(2r_I + 1)$ for $p = 1/2$
No. of hidden layers	5
No. of nodes per hidden layer	5, 10, or 20 (optimized)
No. of nodes of output layer	1
Activation function	ReLU
Loss function	Sum of squared error
Gradient descent method	Adam*
Learning rate	0.01 to 0.0001 (linear decay)
No. of samples	40 000
Mini-batch size	100
No. of epochs	100

*: Kingma and Ba (2014)