



1                   **Precision Annealing Monte Carlo Methods**  
2                   **for Statistical Data Assimilation: Metropolis-Hastings**  
3                   **Procedures**

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## 17 1 Abstract

18 Statistical Data Assimilation (SDA) is the transfer of information from field or lab-  
19 oratory observations to a user selected model of the dynamical system producing  
20 those observations. The data is noisy and the model has errors; the informa-  
21 tion transfer addresses properties of the conditional probability distribution of the  
22 states of the model conditioned on the observations. The quantities of interest  
23 in SDA are the conditional expected values of functions of the model state, and  
24 these require the approximate evaluation of high dimensional integrals. We in-  
25 troduce a conditional probability distribution and use the Laplace method with  
26 annealing to identify the maxima of the conditional probability distribution. The  
27 annealing method slowly increases the precision term of the model as it enters the  
28 Laplace method. In this paper, we extend the idea of precision annealing (PA) to  
29 Monte Carlo calculations of conditional expected values using Metropolis-Hastings  
30 methods.

## 31 2 Introduction

32 We begin with a description of a framework within which we will discuss transfer  
33 of information from data to a model of the processes producing the data.

34 Within an observation window in time,  $[t_0 \leq t \leq t_F]$ , we make a set of measure-  
35 ments at times  $t = \{\tau_1, \tau_2, \dots, \tau_k, \tau_F\}$ ;  $t_0 \leq \tau_k \leq t_F$ . At each of these measurement  
36 times, we observe  $L$  quantities  $\mathbf{y}(\tau_k) = \{y_1(\tau_k), y_2(\tau_k), \dots, y_L(\tau_k)\}$ . The number  $L$   
37 of observations at each measurement time  $\tau_k$  is typically less, often much less, than  
38 the number of degrees of freedom  $D$  in the model of the observed system;  $D \gg L$ .

39 The quantitative characterization of the dynamical processes is through a  
40 model we choose. It describes the interactions among the states of the observed  
41 system. From the data  $\{\mathbf{y}(\tau_k)\}$  we want to estimate the *unmeasured states* of the  
42 model as a function of time as well as estimate any time independent physical  
43 parameters in the model. At the end of the observation window  $t = t_F$ , we use the  
44 estimated values of all model states and parameters to predict the model response  
45 to new forcing of the system for  $t \geq t_F$ . The predictions are used to validate the  
46 model (or not) as well as the estimation procedure.

47 The  $D$ -dimensional state of the model we call  $x_a(t)$ ;  $a = 1, 2, \dots, D \geq L$ . These  
48 are selected by the user to describe the dynamical behavior of the observations  
49 through a set of differential equations in continuous time

$$\frac{dx_a(t)}{dt} = F_a(\mathbf{x}(t), \mathbf{p}), \quad (1)$$

50 Equivalently, in discrete time  $t_n = t_0 + n\Delta t$ ;  $n = 0, 1, \dots, N$ ;  $t_N = t_F$ , the



51 dynamics is written as

$$x_a(t_{n+1}) = f_a(\mathbf{x}(t_n), \mathbf{p}) \text{ or } x_a(n+1) = f_a(\mathbf{x}(n), \mathbf{p}), \quad (2)$$

52 where  $\mathbf{p}$  is a set of parameters, fixed in time, associated with the model.  $\mathbf{f}(\mathbf{x}(n), \mathbf{p})$   
 53 is related to  $\mathbf{F}(\mathbf{x}(t), \mathbf{p})$  through the choice the user makes for solving the continuous  
 54 time flow for  $\mathbf{x}(t)$  through a numerical solution method of choice (Press et al. 2007).

55 To make the discussion here a bit more compact, we will work henceforth  
 56 in discrete time  $t_n = t_0 + n\Delta t$ ;  $n = 0, 1, \dots, N$ ;  $t_N = t_F$ , and we will choose the  
 57 observation times  $\tau_k$  to be multiples of  $\Delta t$  as well:  $\tau_k = t_0 + k[n\tau] \Delta t$ ;  $k = 1, 2, \dots, F$ .

58 As we proceed from the initiation of observations at  $t_0$ , we must use our model  
 59 equations to move the state variables  $\mathbf{x}(t_0) = \mathbf{x}(0)$ , Eq. (2), from  $t_0$  to  $\tau_1 = t_0 +$   
 60  $1[n\tau] \Delta t$  where the first measurement is made. Then we use the model dynamics  
 61 again to move along to  $\tau_2 = t_0 + 2[n\tau] \Delta t$ , where the second measurement is made,  
 62 and so forth until we reach the time of the last measurement  $t = \tau_F = t_0 + F[n\tau] \Delta t$   
 63 and finally move the model from  $\mathbf{x}(\tau_F)$  to  $\mathbf{x}(t_F)$ .

64 We collect the  $\mathbf{x}(t_n)$  for all  $n$  into the **path** of the state of the model through  
 65  $D$ -dimensional space:  $\mathbf{X} = \{\mathbf{x}(0), \mathbf{x}(1), \dots, \mathbf{x}(n), \dots, \mathbf{x}(N) = \mathbf{x}(F)\}$ . The dimension  
 66 of the path is  $(N+1)D + N_p$ , where  $N_p$  is the number of parameters  $\mathbf{p}$  in our  
 67 model. In  $\mathbf{X}$  we do not explicitly show the fixed parameters  $\mathbf{p}$ . This notation is  
 68 illustrated in Fig. (1).

69 We now have two of the three required ingredients to effect our transfer of the  
 70 information in the collection of all measurements  $\mathbf{Y} = \{\mathbf{y}(\tau_1), \mathbf{y}(\tau_2), \dots, \mathbf{y}(\tau_F)\}$   
 71 to the model  $\mathbf{f}(\mathbf{x}(n), \mathbf{p})$  along the path  $\mathbf{X}$  through the observation window  $[t_0, t_F]$ :

- 72 • (1) our noisy data  $\mathbf{Y}$  and
- 73 • (2) a model of the processes producing the  $\mathbf{Y}$ . This model is devised by  
 74 our experience and knowledge of those processes. The notation and a visual  
 75 presentation of this is found in Fig. (1).

76 The **third** ingredient is comprised of methods to generate the transfer from  
 77  $\mathbf{Y}$  to properties of the model. This will command our attention throughout this  
 78 paper.

79 If the transfer methods are successful and, according to some metric of success,  
 80 we arrange matters so that at the measurement times  $\tau_k$ , the  $L$  model variables  
 81  $\mathbf{x}(t)$  associated with  $\mathbf{y}(\tau_k)$  are such that  $x_l(\tau_k) \approx y_l(\tau_k)$ ;  $l = 1, 2, \dots, L$ , we are *not*  
 82 finished. We have then only demonstrated that the model is consistent with the  
 83 known data  $\mathbf{Y}$ . We must further use the model, completed by the estimates of  
 84 the  $\mathbf{p}$  and the state of the model at  $t_F$ ,  $\mathbf{x}(t_F)$ , to predict forward for  $t > t_F$ , and  
 85 we should succeed in comparison with measurements for  $\mathbf{y}(\tau_r)$  for  $\tau_r > t_F$ . As the  
 86 measure of success for predictions, we may use the same metric as utilized in the

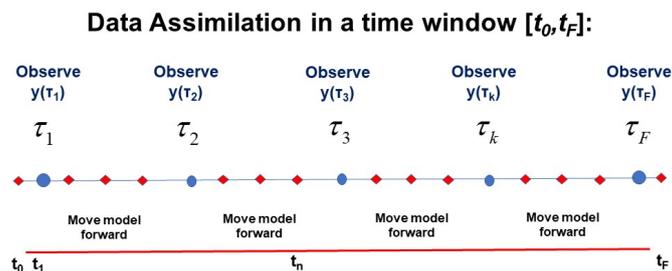


Figure 1: A visual representation of the time window  $t_0 \leq t \leq t_F$  during which  $L$ -dimensional observations  $\mathbf{y}(\tau_k)$  are performed at observation times  $t = \tau_k$ ;  $k = 1, \dots, F$ ;  $t_0 \leq \tau_k \leq t_F$ . We also show times at which the  $D$ -dimensional model developed by the user  $\mathbf{x}(n+1) = \mathbf{f}(\mathbf{x}(n), \mathbf{p})$  is used to move forward from time  $n$  to time  $n+1$ :  $t_n = t_0 + n\Delta t$ ;  $n = 0, 1, \dots, N$ ;  $t_F = t_N$ .  $D \geq L$ .



87 observation window. In the prediction window no further information from the  
 88 observations is passed to the model.

89 As a small aside, the same overall setup applies to supervised machine learning  
 90 networks (Abarbanel, Rozdeba, and Shirman 2018) where the observation window  
 91 is called the training set; the prediction window is called the test set, and prediction  
 92 is called generalization.

## 93 2.1 The Data are Noisy; the Model has Errors

94 Inevitably, the data we collect is noisy, and with equal assurance the model we  
 95 select to describe the production of those data has errors. This means we must,  
 96 at the outset, address a conditional probability distribution  $P(\mathbf{X}|\mathbf{Y})$  as our goal  
 97 in the data assimilation transfer from  $\mathbf{Y}$  to the model. In Abarbanel 2013, we  
 98 describe how to use the Markov nature of the model dynamics  $\mathbf{x}(n) \rightarrow \mathbf{x}(n+1) =$   
 99  $\mathbf{f}(\mathbf{x}(n), \mathbf{p})$  and the definition of conditional probabilities to derive the recursion  
 100 relation connecting observations and dynamics at times  $t_{n+1}$  and  $t_n$ :

$$\begin{aligned}
 P(\mathbf{X}(n+1)|\mathbf{Y}(n+1)) &= \frac{P(\mathbf{y}(n+1), \mathbf{x}(n+1), \mathbf{X}(n)|\mathbf{Y}(n))}{P(\mathbf{y}(n+1)|\mathbf{Y}(n)) P(\mathbf{x}(n+1), \mathbf{X}(n+1)|\mathbf{Y}(n))} \bullet \\
 &= \frac{P(\mathbf{x}(n+1)|\mathbf{x}(n)) P(\mathbf{X}(n)|\mathbf{Y}(n))}{\exp[CMI(\mathbf{y}(n+1), \mathbf{x}(n+1), \mathbf{X}(n)|\mathbf{Y}(n))]} \bullet \\
 &= \frac{P(\mathbf{y}(n+1)|\mathbf{x}(n+1), \mathbf{X}(n), \mathbf{Y}(n))}{P(\mathbf{y}(n+1)|\mathbf{Y}(n))} \bullet \\
 &= \frac{P(\mathbf{x}(n+1)|\mathbf{x}(n)) P(\mathbf{X}(n)|\mathbf{Y}(n))}{P(\mathbf{y}(n+1)|\mathbf{Y}(n))}, \quad (3)
 \end{aligned}$$

101 where we have identified  $CMI(a, b|c) = \log[\frac{P(a,b|c)}{P(a|c)P(b|c)}]$ . This is Shannon's con-  
 102 ditional mutual information (Fano 1961) telling us how many bits (for  $\log_2$ ) we  
 103 know about  $a$  when observing  $b$  conditioned on  $c$ . For us  $a = \{\mathbf{y}(n+1)\}$ ,  $b =$   
 104  $\{\mathbf{x}(n+1), \mathbf{X}(n+1)\}$ ,  $c = \{\mathbf{Y}(n)\}$ .

105 Using this recursion relation to move backwards from the end of the observation  
 106 window from  $t_F = t_0 + N\Delta t$  through the measurements at times  $\tau_k$  to the start of  
 107 the window at  $t_0$ , we may write, up to factors independent of  $\mathbf{X}$

$$P(\mathbf{X}|\mathbf{Y}) = \left\{ \prod_{k=1}^F P(\mathbf{y}(\tau_k)|\mathbf{X}(\tau_k), \mathbf{Y}(k-1)) \prod_{n=0}^{F-1} P(\mathbf{x}(n+1)|\mathbf{x}(n)) \right\} P(\mathbf{x}(0)). \quad (4)$$

108 If we now write  $P(\mathbf{X}|\mathbf{Y}) \propto \exp[-A(\mathbf{X})]$ .  $A(\mathbf{X})$ , the negative of the log likelihood,  
 109 we call the action. Conditional expected values for functions  $G(\mathbf{X})$  along the path  
 110  $\mathbf{X}$  are defined by

$$E[G(\mathbf{X})|\mathbf{Y}] = \langle G(\mathbf{X}) \rangle = \frac{\int d\mathbf{X} G(\mathbf{X}) e^{-A(\mathbf{X})}}{\int d\mathbf{X} e^{-A(\mathbf{X})}}, \quad (5)$$



111  $d\mathbf{X} = \prod_{n=0}^N d^D \mathbf{x}(n)$ , and all factors in the action independent of  $\mathbf{X}$  cancel out  
 112 here. The action takes the convenient expression

$$A(\mathbf{X}) = - \sum_{k=1}^F \left\{ \log[P(\mathbf{y}(\tau_k)|\mathbf{X}(\tau_k), \mathbf{Y}(k-1))] - \sum_{n=0}^N \log[P(\mathbf{x}(n+1)|\mathbf{x}(n))] \right\} - \log[P(\mathbf{x}(0))], \quad (6)$$

113 which is the sum of the terms which modify the conditional probability distribution  
 114 when an observation is made at  $t = \tau_k$  and the sum of the stochastic version of  
 115  $\mathbf{x}(n) \rightarrow \mathbf{x}(n+1) - \mathbf{f}(\mathbf{x}(n), \mathbf{p})$  and finally the distribution when the observation  
 116 window opens at  $t_0$ .

117 What quantities  $G(\mathbf{X})$  are of interest? One natural one is the path of model  
 118 states and parameters  $G(\mathbf{X}) = \mathbf{X}_\mu; \mu = \{a, n\}; a = 1, 2, \dots, D; n = 0, 1, 2, \dots, N$   
 119 itself; another is the covariance around that mean  $\langle \mathbf{X}_\mu \rangle = \bar{\mathbf{X}}_\mu : \langle (\mathbf{X}_\mu - \bar{\mathbf{X}}_\mu)(\mathbf{X}_\nu - \bar{\mathbf{X}}_\nu) \rangle$ .  
 120 Other moments are of interest, of course. If one has an anticipated form for  
 121 the distribution at large  $\mathbf{X}$ , then  $G(\mathbf{X})$  may be chosen as a parametrized version  
 122 of that form and those parameters determined near the maximum of  $P(\mathbf{X}|\mathbf{Y})$ .

123 The action simplifies to what we call the ‘standard model’ of data assimilation  
 124 when (1) observations  $\mathbf{y}$  are related to their model counterparts via Gaussian  
 125 noise with zero mean and diagonal precision matrix  $\mathbf{R}_m$ , and (2) model errors are  
 126 associated with Gaussian errors of mean zero and diagonal precision matrix  $\mathbf{R}_f$ :

$$A(\mathbf{X}) = \sum_{k=1}^F \sum_{l=1}^L \frac{R_m}{2} (x_l(\tau_k) - y_l(\tau_k))^2 + \sum_{n=0}^{N-1} \sum_{a=1}^D \frac{R_f(a)}{2} (x_a(n+1) - f_a(\mathbf{x}(n), \mathbf{p}))^2. \quad (7)$$

127 If we have knowledge of the distribution  $P(\mathbf{x}(0))$  at  $t_0$  we may add it to this action,  
 128 Eq. (6). If we have no knowledge of  $P(\mathbf{x}(0))$ , we may take its distribution to be  
 129 uniform over the dynamic range of the model variables, then it, as here, is absent,  
 130 canceling numerator and denominator in Eq. (5).

## 131 2.2 The Goal of SDA

132 Our challenge is to perform integrals such as Eq. (5). One should anticipate  
 133 that the dominant contribution to the expected value comes from the maxima of  
 134  $P(\mathbf{X}|\mathbf{Y})$  or, equivalently the minima of  $A(\mathbf{X})$ .

135 We note, as before, that when  $\mathbf{f}(\mathbf{x}(n), \mathbf{p})$  is nonlinear in  $\mathbf{X}$ , as it always is in  
 136 interesting examples, the expected value integral Eq. (5) is not Gaussian. So,  
 137 some thinking is in order before approximating this high dimensional integral. We  
 138 turn to that now. After consideration of methods to do the integral, we will return  
 139 to an example taken from an instructional model often used in the geosciences.



140 Two generally useful methods available for evaluating this kind of high-dimensional  
141 integral are Laplace’s method (Laplace 1774; Laplace 1986) and Monte Carlo tech-  
142 niques (Press et al. 2007; Kostuk et al. 2012; Neal 2011). The Laplace methods,  
143 including the idea of precision annealing for the model error term are discussed in  
144 Quinn 2010; Ye 2016; Ye, Rey, et al. 2015; Ye, Kadakia, et al. 2015.

145 The drawbacks of using Laplace methods, including precision annealing meth-  
146 ods, include the need for evaluating very high dimensional derivatives of  $A(\mathbf{X})$   
147 with respect to  $\mathbf{X}$  and using them in the nonlinear optimization algorithms se-  
148 lected. Further, when successful in identifying the path yielding the smallest value  
149 of  $A(\mathbf{X})$ , thus the potentially dominant contribution to Eq. (5), we do not sample  
150 the desired conditional probability distribution away from its maximum. Evalu-  
151 ating corrections to the leading Laplace contributions is familiar as perturbation  
152 theory in statistical physics. The convergence of such perturbation methods can  
153 depend sensitively on the functional form of the action in  $\mathbf{X}$ .

154 We now turn to extending the annealing techniques that explore the variation  
155 of  $\langle G(\mathbf{X}) \rangle$  in the magnitude of the precision matrix  $\mathbf{R}_f$  for the model error from  
156 Laplace’s method to Monte Carlo methods for approximating the path integral for  
157  $\langle G(\mathbf{X}) \rangle$ .

### 158 3 Precision Annealing Monte Carlo Methods

159 Monte Carlo methods for the approximate evaluation of quantities such as  $\langle G(\mathbf{X}) \rangle$   
160 via Eq. (5) have been intensively explored and utilized for decades (Metropolis  
161 et al. 1953; Hastings 1970; Neal 2011).

162 Standard MC calculations, following many years of developments from Metropo-  
163 lis et al. 1953; Hastings 1970, seek to estimate the conditional probability distribu-  
164 tion  $P(\mathbf{X}|\mathbf{Y})$  by starting somewhere in **path** space  $\mathbf{X}[\text{init}]$ , making moves in path  
165 space from this initial path and accepting and rejecting proposed moves according  
166 to a criterion based on detailed balance.

167 The folklore about these calculations is that one can begin more-or-less any-  
168 where in path space and after a large enough number of steps leading to rejected  
169 paths and accepted paths proceeding from  $\mathbf{X}[\text{init}]$ , one will arrive at a good ex-  
170 pected value in Eq. (5). Indeed the error is order the inverse square root of  
171 the number of accepted paths with the numerator essentially the variance in the  
172 function  $G(\mathbf{X})$  whose expected value one wishes to estimate.

173 In practice, if one can choose  $\mathbf{X}[\text{init}]$  ‘close’ to the maximum of  $P(\mathbf{X}|\mathbf{Y})$  the  
174 more efficient the procedure is expected to be; namely high accuracy may be  
175 achieved with fewer steps. Of course, if we knew where the maximum of  $P(\mathbf{X}|\mathbf{Y})$   
176 were located (Shirman 2018), we’d start there and sample, through proposals for  
177 acceptable paths, a sufficient neighborhood of that minimum action path to arrive



178 at a good estimation of  $\langle G(\mathbf{X}) \rangle$ . It is not hard to see that as we do **not** know  
 179 the global minimum of the action, there is a lot of room for algorithms that make  
 180 good proposals for new acceptable paths and clever choices for  $\mathbf{X}[\text{init}]$ .

181 Our idea in this paper is to follow the suggestions of Quinn 2010; Ye 2016; Ye,  
 182 Rey, et al. 2015; Ye, Kadakia, et al. 2015 about how we can ‘anneal’ the precision  
 183 of the model error term of the action starting with  $R_f = 0$ , at which the global  
 184 minimum of the standard model action is clear. From there, we slowly increase  $R_f$   
 185 until it is very large and imposes the underlying dynamical model more and more  
 186 precisely. This method was developed in the context of Laplace approximations  
 187 to the expected value integrals (Quinn 2010; Ye 2016; Ye, Rey, et al. 2015; Ye,  
 188 Kadakia, et al. 2015) and has been extensively tested in several areas of application  
 189 of SDA.

### 190 **3.1 $R_f = 0$ ; Choosing Initial Paths $\mathbf{X}^q[\text{init}]$ ; $q = 1, 2, \dots, N_I$** 191 **for the PAMC Procedure**

192 Our strategy in this paper is to vary the ‘hyperparameter’  $R_f$  that sets the scale  
 193 for the precision of the model error term in Eq. (7). When  $R_f \rightarrow \infty$  the model is  
 194 very precise and deterministic.

195 In our precision annealing strategy, we start at the other end of the scale where  
 196  $R_f = 0$ . At this value the model error term is absent, and the ‘standard’ model  
 197 action is quadratic in the measured variables  $x_l(n)$ . At  $R_f = 0$  the action is a  
 198 minimum when we select  $x_l(\tau_k = t_0 + k[n\tau]\Delta t) = y_l(\tau_k)$ ;  $l = 1, 2, \dots, L$ . This is the  
 199 global minimum of the action at  $R_f = 0$ , and it is quite degenerate as the action  
 200 does not depend on the unmeasured model state variables or the parameters in  
 201 the model.

202 The path of the model state (not showing the  $N_p$  fixed parameters  $\mathbf{p}$ ) is com-  
 203 prised of

$$\mathbf{X} = \{x_1(0), x_2(0), \dots, x_D(0), x_1(1), x_2(1), \dots, x_D(1), \dots, x_1(N), x_2(N), \dots, x_D(N)\}. \quad (8)$$

204 In our  $N_I$  initial paths for the Monte Carlo search,  $\mathbf{X}^q[\text{init}]$ , we always choose  
 205  $x_l(\tau_k = t_0 + [n\tau k]\Delta t) = y_l(\tau_k)$ ;  $l = 1, 2, \dots, L$ , and we wish to select the other  
 206 components of  $\mathbf{X}[\text{init}]$  in a manner that is ‘close’ to a minimum action path. We  
 207 select  $q = 1, 2, \dots, N_I$  initial paths  $\mathbf{X}^q[\text{init}]$  so we will be tracking an *ensemble* of  
 208 paths using various Monte Carlo protocols.

209 To complete our choice of initial paths, we now split the state variables  $x_a(n)$   
 210 into those observed  $a = 1, 2, \dots, L$  and those unobserved  $a > L$ . The latter we  
 211 call the ‘rest’ and write them as  $x_R(n)$ ;  $R = L + 1, L + 2, \dots, D$ . The dynamical  
 212 equations (in discrete time) can now be written

$$x_l(n + 1) = f_l(x_l(n), x_R(n)) \quad x_R(n + 1) = f_R(x_l(n), x_R(n)). \quad (9)$$



213 Starting with any initial condition  $\{x_l^q(0), x_R^q(0)\}$  we generate solutions to these  
 214 dynamical equations by using Eq. (9). We proceed by choosing  $q = 1, 2, \dots, N_I$   
 215 initial conditions  $\{x_l^q(0), x_R^q(0)\}$  from a uniform distribution over the ranges of  
 216  $\{x_l(0), x_R(0)\}$  which we can infer from the data and from forward integration  
 217 of the model. Using the  $N_I \{x_l^q(0), x_R^q(0)\}$  we generate  $N_I$  paths. However, we  
 218 substitute for  $x_l(t_0 + k[n\tau])$ , **whenever** it occurs in the equations Eq. (9), the  
 219 observed value  $y_l(\tau_k = t_0 + k[n\tau]\Delta t) = x_l(t_0 + k[n\tau])$ .

220 This generates  $q = 1, 2, \dots, N_I$  initial paths  $\mathbf{X}^q[\text{init}]$ , one from each selection  
 221 of  $\{x_l^q(0), x_R^q(0)\}$ , everyone of which has zero standard action. Each of these  
 222 paths corresponds to an initial action at the global minimum for  $R_f = 0$ , namely  
 223  $A(\mathbf{X}^q[\text{init}]) = 0$ .

### 224 3.2 Precision Annealing Procedure

225 We next move from  $R_f = 0 \rightarrow R_{f0} > 0$  and using the  $N_I \mathbf{X}^q[\text{init}]$  paths, perform  
 226 an MCMC procedure.

227 Our first procedure is to use a fixed number of iterations of Metropolis-Hastings  
 228 (M-H) proposals/acceptance steps comprised of a fixed number of “burn-in” steps  
 229 followed by a fixed number of iteration steps. The M-H step size is changed as we  
 230 go along to assure a good acceptance rate.

231 At the termination of the M-H steps, we will have  $j = 1, 2, \dots, N_A(q, 0)$  accepted  
 232 paths  $\mathbf{X}_j^q[\text{init}]$  for each of the  $q = 1, 2, \dots, N_I$  initial paths. We use these  $N_A(q, 0)$   
 233 accepted paths to estimate  $N_I$  expected paths  $\bar{\mathbf{X}}^q[0]$  using

$$\bar{\mathbf{X}}^q[0] = \frac{1}{N_A(q, 0)} \sum_{j=1}^{N_A(q, 0)} \mathbf{X}_j^q[\text{init}]. \quad (10)$$

234 These  $N_I$  paths,  $\bar{\mathbf{X}}^q[0]$ , evaluated at  $R_f = R_{f0}\alpha^0$  are set aside and retained for use  
 235 as initial paths for the next step in the PA procedure. This completes the first  
 236 step of the PAMC process;  $R_f = R_{f0}\alpha^0$  at this step.

237 The PA strategy is exposed now: at  $R_f = 0$  choose a dynamically selected set  
 238 of  $N_I$  initial paths  $\mathbf{X}^q[\text{init}]$ . All these paths have zero action. Then raise the value  
 239 of  $R_f$  to a small positive number  $R_f \rightarrow R_{f0} > 0$ , thus introducing the model error  
 240 into the action, but keeping  $R_f$  quite small, and at this value of  $R_f$  use the  $N_I$   
 241 paths  $\mathbf{X}^q[\text{init}]$  in the selected M-H procedure resulting in a set of paths ‘near’ the  
 242  $\mathbf{X}^q[\text{init}]$  as  $R_f$  is small. The resulting  $N_I$  paths at this small value of  $R_f$  are then  
 243 used as initial paths when we raise  $R_f \rightarrow R_{f0}\alpha$ . This sequential use of accepted  
 244 paths from the previous value of  $R_f$  comprises the precision annealing approach.  
 245 Now we describe this in a bit more detail.

246 As the second step in PAMC we move  $R_f$  from  $R_{f0} \rightarrow R_{f0}\alpha^1$  with  $\alpha > 1$ . At  
 247 this increased value of  $R_f$  we use the same MCMC procedure but now starting at



248 the  $\bar{\mathbf{X}}^q[0]$  as  $N_I$  initial paths. This results in  $j = 1, 2, \dots, N_A(q, 1)$  accepted paths  
 249  $\bar{\mathbf{X}}_j^q[0]$  for each  $q$ . Again we form  $N_I$  expected paths using

$$\bar{\mathbf{X}}^q[1] = \frac{1}{N_A(q, 1)} \sum_{j=1}^{N_A(q, 1)} \bar{\mathbf{X}}_j^q[0]. \quad (11)$$

250 This completes the second step of the PAMC process;  $R_f = R_{f0}\alpha^1$  at this step.  
 251 Next we move  $R_f$  from  $R_{f0}\alpha^1 \rightarrow R_{f0}\alpha^2$  with  $\alpha > 1$ . At this increased value of  
 252  $R_f$  we use the same MCMC procedure but now starting at the  $\bar{\mathbf{X}}^q[1]$  as  $N_I$  initial  
 253 paths. This results in  $j = 1, 2, \dots, N_A(q, 2)$  accepted paths  $\bar{\mathbf{X}}_j^q[1]$  for each  $q$ . Again  
 254 we form  $N_I$  expected paths

$$\bar{\mathbf{X}}^q[2] = \frac{1}{N_A(q, 2)} \sum_{j=1}^{N_A(q, 2)} \bar{\mathbf{X}}_j^q[1]. \quad (12)$$

255 This completes the third step of the PAMC process;  $R_f = R_{f0}\alpha^2$  at this step.  
 256 Continue on in this manner increasing the value of  $R_f$  from  $R_f = R_{f0}\alpha^{\beta-1}$  to  
 257  $R_f = R_{f0}\alpha^\beta$ . At this new value of  $R_f$  we use the same MCMC procedure but now  
 258 starting at the  $\bar{\mathbf{X}}^q[\beta-1]$  as  $N_I$  initial paths. This results in  $j = 1, 2, \dots, N_A(q, \beta)$   
 259 accepted paths  $\bar{\mathbf{X}}_j^q[\beta]$  for each  $q$ . Form the  $N_I$  expected paths

$$\bar{\mathbf{X}}^q[\beta] = \frac{1}{N_A(q, \beta)} \sum_{j=1}^{N_A(q, \beta)} \bar{\mathbf{X}}_j^q[\beta-1]. \quad (13)$$

260 This completes the  $\beta^{th}$  step of the PAMC process;  $R_f = R_{f0}\alpha^\beta$  at this step.  
 261 This ‘stepping in  $\beta$ ’ continues until  $\beta$  is ‘large enough’; we will discuss a criterion  
 262 for that shortly. At this value of ‘large enough’  $\beta$ , we will have performed the  
 263 MCMC procedure one last time (at  $R_f = R_{f0}\alpha^\beta$ ) to collect, for each  $q$ ,  $N_A(q, \beta)$   
 264 accepted paths  $\bar{\mathbf{X}}[\beta]_j$ ;  $j = 1, 2, \dots, N_A(q, \beta)$ .  
 265 Finally, we estimate  $\langle G(\mathbf{X}) \rangle$  as the average (expected value) over the  $N_I$  paths  
 266 reached at  $R_f = R_{f0}\alpha^\beta$

$$\langle G(\mathbf{X}) \rangle = \frac{1}{N_I} \sum_{q=1}^{N_I} G(\bar{\mathbf{X}}^q[\beta]), \quad (14)$$

267 and this completes our PA Monte Carlo procedure. Note that at each increment  
 268 of  $\beta$  we use as initial paths the  $N_I$  expected paths from the previous  $\beta$ .  
 269 We evaluate the action on each of the  $N_I$  paths at each value of  $R_f$  and plot  
 270  $A(\mathbf{X}^q)$  versus  $\log[R_f/R_{f0}]$ . In such an ‘action level’ plot, as the precision of the



271 model is increased, if the model is consistent with the data and the number of  
 272 observed measurements,  $L$ , at each  $\tau_k$  is large enough, the action level plot values  
 273 will become independent of  $R_f$  and one will stand out as lower than the rest. The  
 274 path corresponding to that lowest action level will dominate the expected value  
 275 integral of interest.

276 We will see this happen in the example discussed in the next section. It also  
 277 happens in the Laplace approximation to finding the largest values of  $P(\mathbf{X}|\mathbf{Y})$   
 278 (Quinn 2010; Ye 2016; Ye, Rey, et al. 2015; Ye, Kadakia, et al. 2015). The interpre-  
 279 tation of this transition is that the number of directions in model state space that  
 280 are explored by the  $L$ , independent measurements at each  $\tau_k$ ,  $y_l(\tau_k)$ ;  $l = 1, 2, \dots, L$   
 281 reveal, and through the estimation procedure (PAMC), ‘cure’ the intrinsic local  
 282 unstable directions in the nonlinear model  $\mathbf{x}(n+1) = \mathbf{f}(\mathbf{x}(n), \mathbf{p})$ . This happens  
 283 with higher precision as  $R_f$  becomes larger and larger.

## 284 4 Example of PAMC Calculations

285 We explore the instructional model from Lorenz 2006, widely used in numerical  
 286 weather prediction analyses, as a test bed for methods of data assimilation. This  
 287 model has a  $D$ -dimensional state variable  $\mathbf{x}(t) = \{x_1(t), x_2(t), \dots, x_D(t)\}$  satisfying

$$\frac{dx_a(t)}{dt} = x_{a-1}(t)[x_{a+1} - x_{a-2}(t)] - x_a(t) + \nu \quad a = 1, 2, \dots, D, \quad (15)$$

288 in which  $x_{-1}(t) = x_{D-1}(t)$ ,  $x_0(t) = x_D(t)$ , and  $x_1(t) = x_{D+1}(t)$ .  $\nu$  is a constant  
 289 forcing term; the solutions of these equations for  $D \geq 4$  are chaotic when  $\nu \approx 8.0$  or  
 290 more. We will report on calculations with  $D = 5$  and with  $D = 20$  with  $\nu = 8.17$ .

291 Our numerical calculations are ‘twin experiments’ in which for a selected  $D$  we  
 292 choose  $\mathbf{x}(t_0) = \mathbf{x}(0)$  and using a time step  $\Delta t = 0.025$  generate solutions  $\mathbf{x}(t)$  over  
 293 an observation window  $[t_0, t_F] : t_0 \leq t \leq t_0 + N\Delta t = t_F$ . To each  $x_a(t)$  we add  
 294 Gaussian noise with mean zero and variance  $\sigma^2$ , these now comprise our library  
 295 of ‘observed data,’  $y_a(t) = x_a(t) + \sigma N(0, 1)$ . We then select  $L \leq D$  of these noisy  
 296 data, and form the action

$$A(\mathbf{X}) = \sum_{n=0}^N \sum_{l=1}^L \frac{R_m(n)}{2} (y_l(n) - x_l(n))^2 + \frac{R_f}{2} \sum_{n=0}^{N-1} \sum_{a=1}^D [x_a(n+1) - f_a(\mathbf{x}(n))]^2, \quad (16)$$

297 and  $R_m(n)$  is nonzero only when there is a measurement at  $t_n$ , and at each of these  
 298 times  $L$  quantities are observed. The first term on the right in Eq. (16) is the  
 299 measurement error, and the second, the model error.

300 Our calculations were performed with the choices:  $D = 20$ ,  $\alpha = 1.4$ ,  $R_{f0} = 1.0$ ,  
 301  $R_m = 1.0$ ,  $N_I = 50$ ,  $\Delta t = 0.025$ , and various choices of  $L$  from 5 to 12.



302 In Fig. (2) we display the action levels as a function of  $\beta$  at  $L = 5$ . We  
303 can see that PAMC identifies many action levels, corresponding to many peaks in  
304 the conditional probability distribution  $P(\mathbf{X}|\mathbf{Y}) \propto \exp[-A(\mathbf{X})]$ , Eq. (16). From  
305  $\beta \approx 30$  we see one level moving away from the collection of larger action levels  
306 as  $\beta$  increases. However, no action level has become essentially independent of  
307  $R_f$  suggesting that the accuracy with which the model is enforced remains too  
308 small. We expect that as the number of measurements at each  $\tau_k$  is increased  
309 more information about the phase space instabilities will be passed from the data  
310 to the model and that the structure of the action level plot will change.

311 In Fig. (3) we now display the action levels and its components, the measure-  
312 ment errors and the model errors, when  $L = 12$ . Here the behavior of the action  
313 levels is quite different. The model error decreases over a large range of  $R_f$  until  
314 the numerical stability of the evaluation of this term is reduced as small errors in  
315  $\mathbf{x}(n+1) - \mathbf{f}(\mathbf{x}(n), \mathbf{p})$  are magnified by large values of  $R_f$ . As this result appears,  
316 the action for each of the  $N_I$  paths at each  $\beta$  levels off, becoming essentially inde-  
317 pendent of  $R_f$ , and matches the measurement error, as it must do for consistency  
318 (Quinn 2010; Ye 2016; Ye, Rey, et al. 2015; Ye, Kadakia, et al. 2015).

319 The PAMC procedure, as does the Laplace approximation version of precision  
320 annealing (Quinn 2010; Ye 2016; Ye, Rey, et al. 2015; Ye, Kadakia, et al. 2015),  
321 permits the estimation of the parameter  $\nu$  at each value of  $\beta$ . In Fig. (4) we display  
322 all  $N_I = 50$  estimated values of  $\nu$  at each value of  $\beta$ . As PAMC is an ensemble  
323 method sampling in the neighborhood of a peak (or peaks) of the conditional  
324 probability distribution, we do not arrive at a single value for  $\nu$ . Taking the  $N_I$   
325 values of  $\nu(\beta)$  and evaluating the means and standard deviation at each  $\beta$ , we show  
326 the result in Fig. (5) in which it is clear that the estimated value of  $\nu$  becomes  
327 essentially independent of  $\beta$  for  $\beta \approx 40$  and larger.

328 Until this point we have examined outcomes of the PAMC estimation proce-  
329 dure. All of the state variables, **measured** and **unmeasured**, as well as the  
330 forcing parameter were reported over the observation window  $[0 \leq t \leq 5.0]$ . In a  
331 ‘twin experiment’ as here, we have generated the data by solving a known dynam-  
332 ical equation and adding noise to the output of the  $D = 20$  times series with a  
333 known value of  $\nu$ . The point of a twin experiment is to test the method of transfer  
334 of information in SDA. As we have  $D - L$  **unobserved** state variables at each  $L$ ,  
335 and an **unobserved** parameter  $\nu$ , the only tool to determine how well the estima-  
336 tion procedure has done in its task is to predict for  $t > 5$  into a prediction window  
337 where no information from observations is passed back from the model. We now  
338 examine how well the estimation has been performed by predicting both an ob-  
339 served and an unobserved time series among the  $D$  available. We already see from  
340 Fig. (5) that the input value of  $\nu = 8.17$  has accurately been estimated; the ap-  
341 parent bias in this parameter estimation has also been seen in earlier Monte Carlo

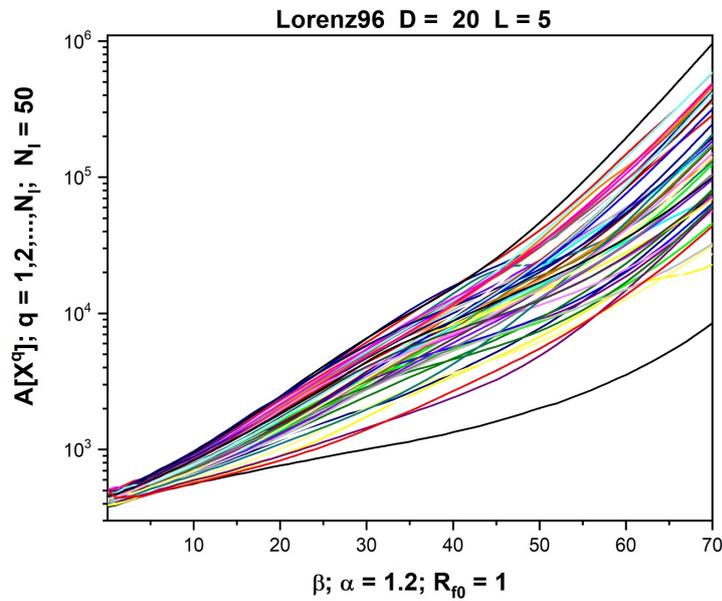


Figure 2: The values of the actions Eq. (16) for the  $D = 20$  dimensional Lorenz96 model when  $L = 5$  of the dynamical variables  $\mathbf{x}(t)$  are observed. The actions are evaluated as a function of  $\beta = \log_\alpha[R_f/R_{f0}]$  where  $\alpha = 1.4$  and  $R_{f0} = 1.0$ . We perform the Precision Annealing Monte Carlo (PAMC) calculation starting with  $N_I$  initial paths at each  $R_f$ . We used  $N_I = 50$  in these calculations. Displayed here are  $N_I$  action values at each  $R_f$  (or  $\beta$ ). These actions are evaluated along the expected path resulting from the accepted paths generated during the Metropolis-Hastings procedures from each of the  $N_I$  initial paths.

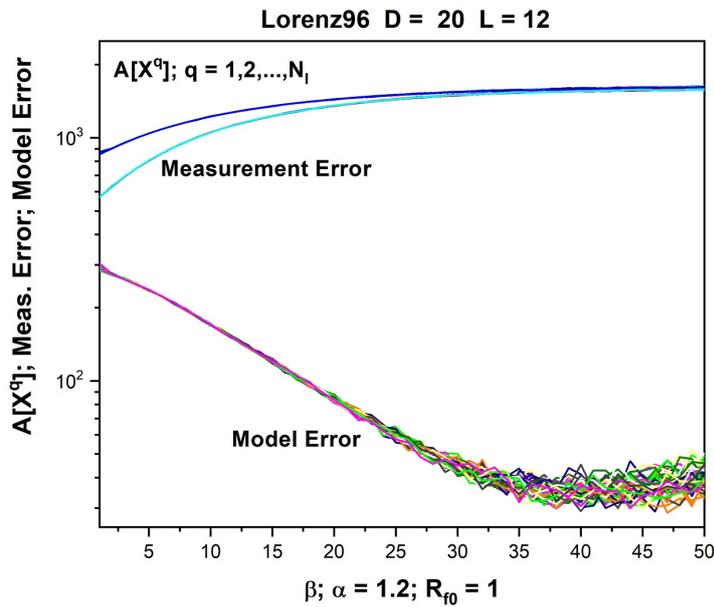


Figure 3: The values of the actions Eq. (16), the measurement error, and the model error for the  $D = 20$  dimensional Lorenz96 model when  $L = 12$  of the dynamical variables  $\mathbf{x}(t)$  are observed; the observed variables are  $[x_1(t), x_2(t), x_4(t), x_6(t), x_7(t), x_9(t), x_{11}(t), x_{12}(t), x_{14}(t), x_{16}(t), x_{17}(t), x_{19}(t)]$ . The actions, the measurement error, and the model error are evaluated as a function of  $\beta = \log_\alpha[R_f/R_{f0}]$  where  $\alpha = 1.4$  and  $R_{f0} = 1.0$ . We perform the Precision Annealing Monte Carlo (PAMC) calculation starting with  $N_I$  initial paths at each  $R_f$ . We used  $N_I = 50$  in these calculations; on display here are  $N_I$  action, measurement error, and model error values at each  $R_f$  (or  $\beta$ ). These are evaluated along the expected path resulting from the accepted paths generated during the Metropolis-Hastings procedures from each of the  $N_I$  initial paths. In this case, when  $L = 12$ , the model error becomes much smaller than the measurement error as  $\beta$  is increased. This leads the action to become effectively equal to the action itself and essentially independent of  $R_f$ . We have seen this before in the precision annealing variational principle calculations (Quinn 2010; Ye 2016; Ye, Rey, et al. 2015; Ye, Kadakia, et al. 2015).

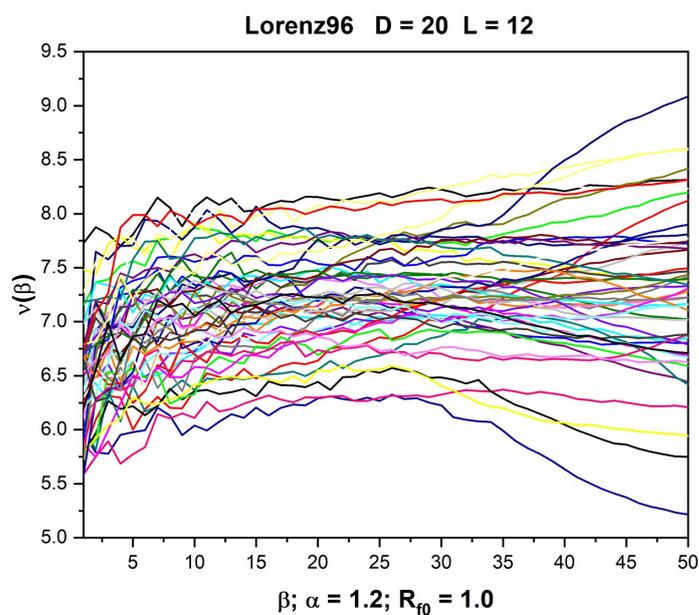


Figure 4: The values of the Lorenz96 model forcing parameter  $\nu$  at each value of  $\beta$  for each of the  $N_I$  paths associated with the  $N_I$  Metropolis-Hastings procedures from each of the  $N_I$  initial paths.

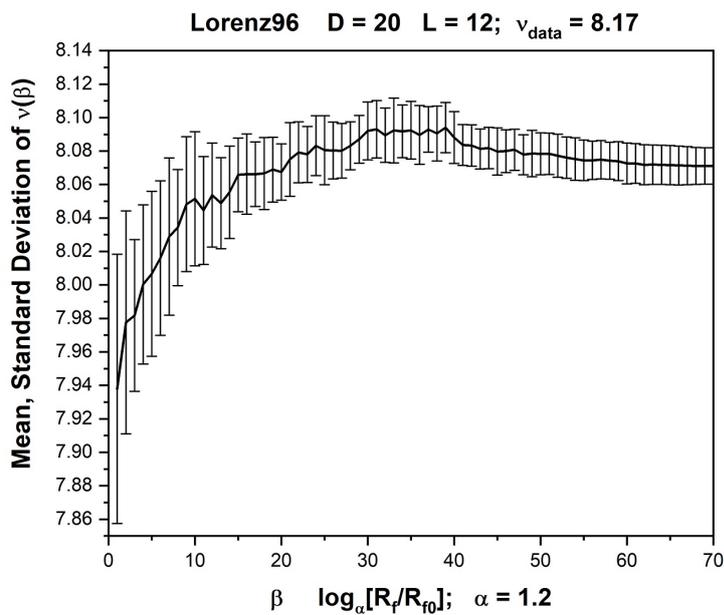


Figure 5: The estimated parameter in the Lorenz96,  $D = 20$  data when  $L = 12$ . The mean and standard deviation of  $\nu$  at each  $\beta$  is shown.



342 twin experiment Kostuk et al. 2012; Kostuk 2012, and its origins are discussed  
343 there.

344 Fig. (6) shows the **observed** model variable  $x_2(t)$  for the Lorenz96 model  
345 with  $D = 20, L = 12$  and  $\Delta t = 0.025$ . The noisy data from solutions of the  
346 model equations from the ‘observed’ variables [1, 2, 4, 6, 7, 9, 11, 12, 14, 16, 17, 19].  
347 The estimation of  $x_2(t)$  during the observation window using PAMC to transfer  
348 information from the data to the model is shown in red, and the prediction using all  
349 the estimated states of the model,  $\mathbf{x}(t = 5)$ , and the estimated model parameter,  
350 is shown in green  $\mathbf{x}(t \geq 5)$ . Our knowledge of this dynamical system (Kostuk  
351 2012) indicates that the largest global Lyapunov exponent is approximately 1.2 in  
352 the time units indicated by  $\Delta t$ . The deviation of the predicted trajectory  $x_2(t)$   
353 from  $t \approx 6.0$  is consistent with the accuracy of the estimated state  $\mathbf{x}(t)$  and this  
354 Lyapunov exponent.

355 Fig. (7) shows the **unobserved** model variable  $x_{20}(t)$  for the Lorenz96 model  
356 with  $D = 20, L = 12$  and  $\Delta t = 0.025$ . The noisy data from solutions of the  
357 model equations from the ‘observed’ variables [1, 2, 4, 6, 7, 9, 11, 12, 14, 16, 17, 19].  
358 The estimation of  $x_{20}(t)$  during the observation window using PAMC to transfer  
359 information from the data to the model is shown in red, and the prediction using all  
360 the estimated states of the model,  $\mathbf{x}(t = 5)$ , and the estimated model parameter,  
361 is shown in blue  $\mathbf{x}(t \geq 5)$ . Our knowledge of this dynamical system (Kostuk  
362 2012) indicates that the largest global Lyapunov exponent is approximately 1.2 in  
363 the time units indicated by  $\Delta t$ . The deviation of the predicted trajectory  $x_{20}(t)$   
364 from  $t \approx 6.4$  is consistent with the accuracy of the estimated state  $\mathbf{x}(t)$  and this  
365 Lyapunov exponent.

## 366 5 Discussion and Summary

367 In statistical data assimilation, one transfers information from a set of noisy data  $\mathbf{Y}$   
368 to models of the observations. The models have errors and the probability  $P(\mathbf{X}|\mathbf{Y})$   
369 of the model states, conditioned on the data, plays a central role. From this  
370 conditional probability distribution, we want to approximate conditional expected  
371 values of functions  $G(\mathbf{X})$  on the model state

$$E[G(\mathbf{X})|\mathbf{Y}] = \int d\mathbf{X} P(\mathbf{X}|\mathbf{Y}) G(\mathbf{X}) = \frac{\int d\mathbf{X} \exp[-A(\mathbf{X})] G(\mathbf{X})}{\int d\mathbf{X} \exp[-A(\mathbf{X})]}, \quad (17)$$

372 where  $A(\mathbf{X}) \propto -\log[P(\mathbf{X}|\mathbf{Y})]$  is the ‘action’ associated with the information  
373 transfer process during an observation window in time, when the information trans-  
374 fer occurs. Observations of the dynamical system underlying the measurements  
375 may be sparse; the number of measurements one is able to accomplish at any mo-  
376 ment in time is typically small compared to the degrees of freedom in the model.

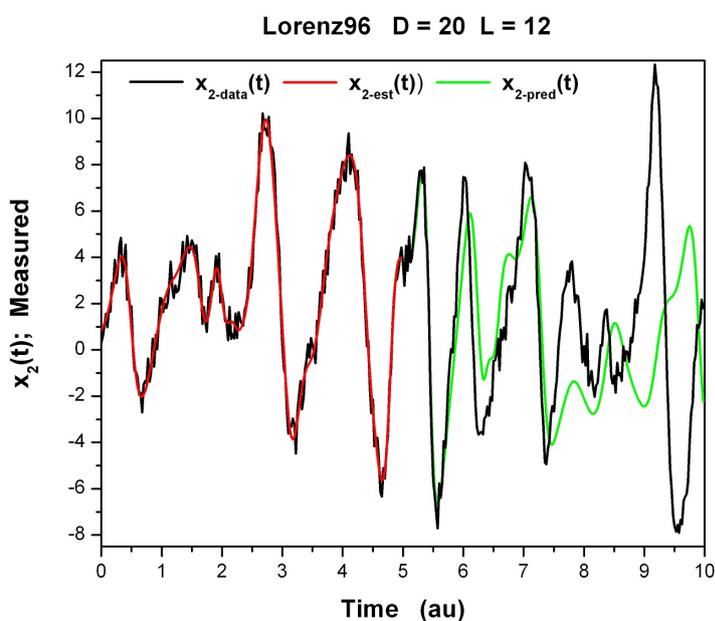


Figure 6: We display the **observed** dynamical variable  $x_2(t)$  for the time interval  $0 \leq t \leq 10.0$ . In black is the full set of data. In red is the estimated  $x_2(t)$  over the observation window  $0 \leq t \leq 5.0$ , and in green is the predicted  $x_2(t)$  over the prediction window  $5.0 < t \leq 10.0$ . The prediction uses the values of  $\mathbf{x}(t = 5.0)$  for the full estimated state at the end of the observation window as well as the parameter  $\nu$  estimated in the PAMC procedure. This calculation uses the Lorenz96 model with  $D = 20$  and  $L = 12$ .  $\Delta t = 0.025$ .

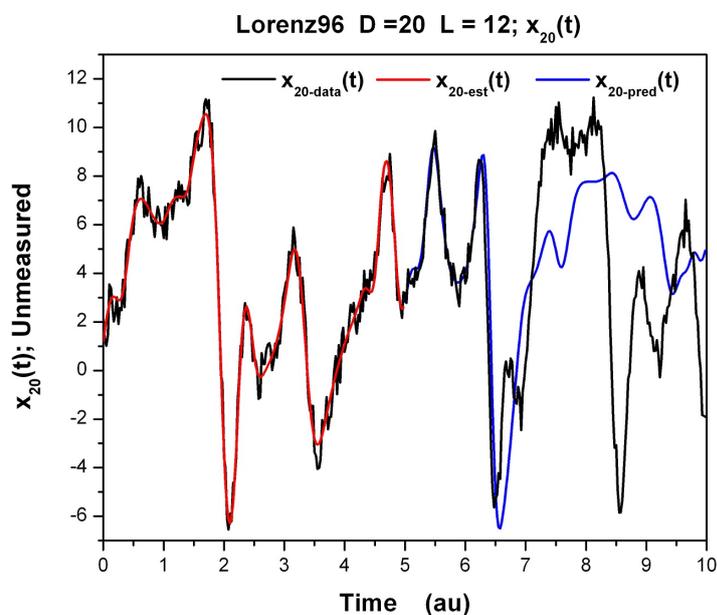


Figure 7: We display the **unobserved** dynamical variable  $x_{20}(t)$  for the time interval  $0 \leq t \leq 10.0$ . In black is the full set of data. In red is the estimated  $x_{20}(t)$  over the observation window  $0 \leq t \leq 5.0$ , and in blue is the predicted  $x_{20}(t)$  over the prediction window  $5.0 < t \leq 10.0$ . The prediction uses the values of  $\mathbf{x}(t = 5.0)$  for the full estimated state at the end of the observation window as well as the parameter  $\nu$  estimated in the PAMC procedure. This calculation uses the Lorenz96 model with  $D = 20$  and  $L = 12$ .  $\Delta t = 0.025$ .



377 However, one requires some approximate knowledge of the full state of the model  
378 at the final time-point of the observation window. This means one must estimate  
379 the **unmeasured** model state variables as well as any unknown time independent  
380 model parameters, then validate the model with predictions for times after the  
381 observation window.

382 In this paper we have addressed approximating such integrals using a precision  
383 annealing Monte Carlo method. In the context of a model  $\mathbf{x}(t_{n+1}) = \mathbf{f}(\mathbf{x}(t_n), \mathbf{p})$   
384 and observations  $y_l(\tau_k)$  at times  $t_0 \leq \tau_k \leq t_F$  (with  $t_F = t_0 + N\Delta t$ ), the action  
385 reflects Gaussian errors of the measurements and of the nonlinear model, given by

$$A(\mathbf{X}) = \sum_{n=0}^N \sum_{l=1}^L \frac{R_m(n)}{2} (y_l(n) - x_l(n))^2 + \frac{R_f}{2} \sum_{n=0}^{N-1} \sum_{a=1}^D [x_a(n+1) - f_a(\mathbf{x}(n))]^2, \quad (18)$$

386 where  $R_m(n)$  is nonzero only when there is a measurement at  $t_n$ . The precision of  
387 the model error is  $R_f$  and the annealing procedure is initiated at  $R_f$  very small,  
388 then continued to a very large  $R_f$ . The core idea is that when  $R_f$  is small, the  
389 global minimum of  $A(\mathbf{X})$  is easily identifiable where  $x_l(\tau_k) \approx y_l(\tau_k)$ . Increasing  $R_f$   
390 slowly allows one to track the global minimum as the nonlinearity in the action  
391 plays a more and more significant role.

392 The details of this PAMC procedure, implemented by a Metropolis-Hastings  
393 Monte Carlo method at each  $R_f$ , are given as a general outline. We then present  
394 results in detail for an instructional model - the Lorenz 1996 equations (Lorenz  
395 2006), widely used to explore geophysical SDA methods.

396 In addition to the PAMC method, we introduce an initialization method for  
397 selecting a starting point in **path** space  $\mathbf{X}$ . From this starting point, we begin  
398 to make proposals and accept new samples in order to evaluate the conditional  
399 probability distribution.

400 Our PAMC methods are clearly not restricted to the specific example we used  
401 to demonstrate its operation, nor is the use of a Metropolis-Hastings procedure  
402 required in its implementation. We will follow this paper with one describing the  
403 use of a Hamiltonian Monte Carlo (HMC) procedure (Duane et al. 1987; Neal  
404 2011; Betancourt 2018).

405 How is one to choose between the use of a precision annealing method for  
406 the Laplace approximation to expected value integrals and Monte Carlo methods  
407 (Metropolis-Hastings or HMC)? The key difference among the methods is that  
408 the Metropolis-Hastings Monte-Carlo does not require carrying along Jacobians or  
409 Hessians of the action  $A(\mathbf{X})$  and samples the conditional probability distribution  
410 with paths  $\mathbf{X}$  in model state space. The Laplace method requires solving for zeros  
411 of the Jacobian  $\partial A(\mathbf{X})/\partial \mathbf{X}$  and results in a single path in model state space at the  
412 overall minimum of the action. The HMC method is a hybrid of these in which  
413 requires a symplectic integrator of the ‘Hamiltonian’  $H(\mathbf{P}, \mathbf{X}) = \mathbf{P}^2/2M + A(\mathbf{X})$



414 and uses  $\partial A(\mathbf{X})/\partial \mathbf{X}$  to move about in ‘canonical’  $\{\mathbf{P}, \mathbf{X}\}$  space. Neither Monte  
415 Carlo method requires evaluating or storing higher derivatives of the action, and  
416 each samples the conditional probability distribution in path space, while the  
417 Laplace method does not. At this early stage of development of these methods,  
418 we do not have a firm recommendation as to which one to select in general. From  
419 the calculations on a high dimensional Lorenz96 model, it appears that on this  
420 test model, all approaches yield excellent results when enough measurements are  
421 made at each measurement time in an observation window.

## 422 **6 Code Availability**

423 All of the code needed to reproduce our results are available [here](#).



## References

- 424
- 425 Abarbanel, H. D. I. (2013). *Predicting the Future: Completing Models of Observed*  
426 *Complex Systems*. Springer.
- 427 Abarbanel, H. D. I., P. J. Rozdeba, and Sasha Shirman (2018). “Machine Learn-  
428 ing; Deepest Learning as Statistical Data Assimilation Problems”. In: *Neural*  
429 *Computation*.
- 430 Betancourt, Michael (2018). “The convergence of Markov chain Monte Carlo meth-  
431 ods: from the Metropolis method to Hamiltonian Monte Carlo”. In: *Annalen*  
432 *der Physik*, p. 1700214. DOI: [doi.org/10.1002/andp.201700214](https://doi.org/10.1002/andp.201700214).
- 433 Duane, Simon et al. (1987). “Hybrid Monte Carlo”. In: *Physics Letter B* 195.2,  
434 pp. 216–222. DOI: [doi.org/10.1016/0370-2693\(87\)91197-X](https://doi.org/10.1016/0370-2693(87)91197-X).
- 435 Fano, Robert M. (1961). *Transmission of Information; A Statistical Theory of*  
436 *Communication*. MIT Press.
- 437 Hastings, W. K. (1970). “Monte Carlo Sampling Methods Using Markov Chains  
438 and Their Applications”. In: *Biometrika* 57, pp. 97–109.
- 439 Kostuk, Mark (2012). “Synchronization and Statistical Methods for the Data As-  
440 similation of HVC Neuron Models”. PhD thesis. University of California San  
441 Diego. URL: <http://escholarship.org/uc/item/2fh4d086>.
- 442 Kostuk, Mark et al. (2012). “Dynamical estimation of neuron and network prop-  
443 erties II: path integral Monte Carlo methods”. In: *Biological Cybernetics* 106,  
444 pp. 155–167.
- 445 Laplace, P. S. (1774). “Memoir on the Probability of Causes of Events”. In:  
446 *Mathématique et de Physique, Tome Sixième*, pp. 621–656.
- 447 — (1986). “Memoir of the Probability of Causes of Events”. In: *Statistical Science*  
448 1 (3). Translation to English by S. M. Stigler., pp. 365–378.
- 449 Lorenz, Edward N (2006). “Predictability: A problem partly solved”. In: *Pre-*  
450 *dictability of weather and climate*. Ed. by Tim Palmer and Renate Hagedorn.  
451 Cambridge.
- 452 Metropolis, N. et al. (1953). “Equation of State Calculations by Fast Computing  
453 Machines”. In: *J. Chem. Phys.* 21, pp. 1087–1092. DOI: [10.1063/1.1699114](https://doi.org/10.1063/1.1699114).
- 454 Neal, Radford (2011). “MCMC Using Hamiltonian Dynamics”. In: *Handbook of*  
455 *Markov Chain Monte Carlo*. Ed. by Andrew Gelman, Galin Jones, and Xiao-Li  
456 Meng. Chapman and Hall; CRC Press. Chap. 5.
- 457 Press, W. H. et al. (2007). *Numerical Recipes: The Art of Scientific Computing,*  
458 *Third Edition*. Cambridge University Press.
- 459 Quinn, John C. (2010). “A path integral approach to data assimilation in stochastic  
460 nonlinear systems”. PhD thesis. University of California San Diego.
- 461 Shirman, Sasha (2018). “Strategic Monte Carlo and Variational Methods in Sta-  
462 tistical Data Assimilation for Nonlinear Dynamical Systems”. PhD thesis. Uni-  
463 versity of California San Diego.



- 464 Ye, Jingxin (2016). “Systematic Annealing Approach for Statistical Data Assimi-  
465 lation”. PhD thesis. University of California San Diego.
- 466 Ye, Jingxin, N. Kadakia, et al. (2015). “Improved variational methods in statistical  
467 data assimilation”. In: *Nonlinear Processes in Geophysics* 22.2, pp. 205–213.  
468 DOI: 10.5194/npg-22-205-2015. URL: [https://www.nonlin-processes-  
469 geophys.net/22/205/2015/](https://www.nonlin-processes-geophys.net/22/205/2015/).
- 470 Ye, Jingxin, Daniel Rey, et al. (2015). “Systematic Variational Method for Sta-  
471 tistical Nonlinear State and Parameter Estimation”. In: *Phys. Rev. E* 92 (5),  
472 p. 052901. DOI: 10.1103/PhysRevE.92.052901. URL: [https://link.aps.org/  
473 doi/10.1103/PhysRevE.92.052901](https://link.aps.org/doi/10.1103/PhysRevE.92.052901).