Aspects of the Ensemble Kalman Filter

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Abstract

he Ense le Kal an Fl er EnKF s a da a ass l a on e hod de s gned o prov de es a es of he s a e of a sys e y lend ng nfor a on fro a odel of he sys e w h o serva ons a n a ns an ense le of s a e es a es fro wh ch a s ngle es s a e es a e and an assess en of es a on error ay e cal c l a ed Co pared o ore es a l shed e h ods o ers advan ages of red ced co p a onal cos e er hand ng of non near y and grea er ease of ple en a on

h s d sser a on s ar s y rev ew ng d eren for l a ons of he EnKF cover ng s ochas c and se de er n s c var an s wo for l a ons are sel ec ed for ple en a on and he adap a on of her algor h s for e er n er cal ehav o r s descr ed Nex as a s jec for exper en s a s ple echan cal sys e s descr ed ha s of n eres o e eordolog s s as an ll s ra on of he prol e of n a sa on Exper en al res l s are presen ed ha show so e nexpec ed fea res of he ple en ed l ers nd d ng ense les a s cs ha are ncons s en w h he ac al error Ex pl ana ons of hese fea res are prov ded and po n o a po en al aw n he general fra ewor for se de er n s c for l a ons of he EnKF af fec ng so e no al s ch for l a ons h s aw appears o have een overl oo ed n he l era re

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C EAKF perfec oserva ons N ense le s a s cs

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List of Symbols

Latin

$\mathbf{A}$	Ensemble adjustment matrix in EAKF
a (superscript)	Analysis value
e (subscript)	Ensemble value
$\mathbf{F}$	Orthogonal matrix
f	Frequency
f (superscript)	Forecast value
$\mathbf{G}$	Diagonal matrix of square roots of eigenvalues
g	Acceleration due to gravity
H	Nonlinear observation operator [illegible]
$\mathbf{H}$	Linear observation operator (tangent linear model) [illegible]

m	Dimension of observation space; mass of bob of swinging spring
N	Ensemble size
n	Dimension of state space
$\mathbf{P}$	State error covariance matrix
p	Number of nonzero singular values in SVD generalised to moment m
$\mathbf{Q}$	Model noise covariance matrix
$\mathbf{R}$	Observation noise covariance matrix
r	Radial polar coordinate
r'	Radial displacement of swinging spring relative to equilibrium length
$\mathbf{S}$	Ensemble version of innovations covariance matrix
T	Period of oscillation
$\mathbf{T}$	Positive multiplier in deterministic formulations of EnKF
t (superscript)	True value at time
t	Discrete v a l e
p	l s o s R

θ	Angular polar coordinate
$\mathbf{\Lambda}$	Diagonal matrix of eigenvalues
$\mathbf{\Sigma}$	Matrix of singular values in SVD
ω	Angular frequency

Miscellaneous

Some of the vector operators below may be applied to scalars and matrices as well.

$\mathbf{1}_N$	$N \times N$ matrix in which every element is $1/N$
$\mathbf{z}$	Population mean of $\mathbf{z}$
$\mathbf{z}$	Version of $\mathbf{z}$ in augmented state space, $\mathbf{z}$ scaled by inverse square root of covariance matrix, Fourier transform of $\mathbf{z}$
$\overline{\mathbf{z}}$	Ensemble mean of $\mathbf{z}$
$\mathbf{Z}'$	Perturbation matrix of ensemble matrix $\mathbf{Z}$
$\widetilde{\mathbf{z}}$	Analogue in EAKF of $\mathbf{z}$ or $\widehat{\mathbf{z}}$ in ETKF

List of Abbreviations

EAKF	Ensemble Adjustment Kalman Filter
EKF	Extended Kalman Filter
EnKF	Ensemble Kalman Filter
ETKF	Ensemble Transform Kalman Filter
KF	Kalman Filter
NWP	Numerical Weather Prediction
SVD	Singular Value Decomposition

Chapter 1

Introduction

1.1 Background

Data assimilation addresses the problem of incorporating observations into a model of some system. For example, the system could be the atmosphere of the Earth, the model could be a weather forecasting model, and the observations could be measurements made by surface stations, radiosondes, weather radars, and satellites. In this case the problem is to combine the state of the atmosphere as predicted by an earlier forecast with recent observational data to produce an updated estimate of the state of the atmosphere (known as the analysis) that can be used as the starting point for a new forecast. For a detailed overview of data assimilation in a meteorological context, see Kalnay ( ) or Bowman et al ( ).

The data assimilation techniques of 3D-Var and 4D-Var are currently popular at national meteorology centres. These are variational techniques that use numerical methods to minimise a cost function that is a weighted measure of the distances from the analysis to the forecast and the observations. The weightings in the cost function are intended to reflect the relative uncertainties in different components of the forecast and observations. The resulting analysis thus represents a combination of the information sources of forecast and observation, with greater weight being given to more certain information. The difference between 3D-Var and 4D-Var is that 4D-Var treats

so small that it is statistically unrepresentative when the extra work needed to maintain an ensemble of state estimates is more than offset by the work saved through not maintaining a separate covariance matrix. The EnKF also does not use tangent linear operators, which eases implementation and may lead to a better handling of nonlinearity.

The EnKF was originally presented in Evensen. An important subsequent development was the recognition by Burgers **et al** and independently by Houtekamer and Mitchell of the need to use an ensemble of pseudo random observation perturbations to obtain the right statistics from the analysis ensemble. Deterministic methods for forming an analysis ensemble with the right statistics have also been presented. The former approach to the EnKF is comprehensively reviewed in Evensen, whilst variants of the latter approach are placed in a uniform framework by Tippett **et al**. These variants include the Ensemble Transform Kalman Filter (ETKF) of Bishop **et al** and the Ensemble Adjustment Kalman Filter (EAKF) of Anderson.

1.2 Goals

The goals of this dissertation are to review the principal formulations of the EnKF, to select one or more formulations for implementation and to implement them, to perform experiments with the implemented filters using a simple mechanical system (see below) as a test case and searching for interesting phenomena, and to interpret the experimental results and draw any important conclusions.

The mechanical system to be used as a test case in the experiments is the two-dimensional swinging spring. This simple system is of interest to meteorologists because it possesses interacting motions with two distinct timescales analogous to the Rossby and gravity waves of the atmosphere. It may be used as an illustration of the problem of initialisation (see Chapter).

1.3 Principal Results

he E KF and EAKF are sel ec ed for pl e en a on n Chap er s fo nd o advan ageo s o refor l a e he raw al gor h s rev ewed n Chap er o g ve al gor h s ha are anal y cal l y eq val en n er cal l y e er ehaved

Exper en s w h he E KF and he sw ng ng spr ng n Chap er show a col l apse n he n er of d s nc ense le e ers af er ass l a ng each o serva on h s col l apse s expl a ned n ec on and po n s o a l ed sef l ness of he E KF for l ow d ens onal sys e s s ch as he sw ng ng spr ng al ho gh he h gh d ens onal sys e s yp cal of N P are na ec ed

he os por an res l of he d sser a on s ha here s a po en al aw n he general fra ewor for se de er n s c for l a ons of he EnKF as presen ed n ppe **et al** h s aw ay l ead so e for l a ons of he EnKF o prod ce anal ys s ense les w h s a s cs ha are ncons s en w h he ac al error eng o h ased ean end ng o e n he wrong pl ace and overcon den n Chap er as a s jec for exper en s he wo d ens ona sw ng ng spr ng s n rod ced h s s p e echan ca sys e s of n eres o e eord og s s as an ll s ra on of he pro e of n a sa on he chap er d sc sses he concep of n a sa on and s por ance for N P

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Chap er prov des exp ana ons of he fea res o served n Chap er he exp ana on of he ncons s en s a s cs po n s o a po en a aw n he genera fra ewor for se de er n s c for l a ons of he EnKF a ec ng so e no a l s ch for l a ons he E KF s a ec ed a l eas n so e c rc s ances he EAKF s no h s aw appears o have een over oo ed n he l era re

he d sser a on cond des n Chap er w h a rev ew of he preced ng chap ers and so e s gges ons for f r her wor

We shall denote the dimension of the state space of the system by n and vectors in this space by $\mathbf{x}$, usually with various arguments, subscripts and superscripts. In particular the true state of the system at time t will be denoted by $\mathbf{x}^t(t)$ and the forecast and analysis at this time by $\mathbf{x}^f(t)$ and $\mathbf{x}^a(t)$ respectively. We shall denote the dimension of observation space by m and the observation vector at time t by $\mathbf{y}$.

o pro nence n aerospace app ca ons and are pop l ar for ses s ch as rac ng a r orne o jec s w h radar For hese app ca o error covar ance a r x a e t_{-1} forward o e t s ng he eq a ons

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$$\mathbf{P}(t \quad \mathbf{MP}(t_{-1}\ \mathbf{M}^T \quad \mathbf{Q}.$$

he analys s s ep a e t s ar s y cal c l a ng he Kal an ga n a r x

$$\mathbf{K}(t \quad \mathbf{P}(t \ \mathbf{H}^T(\mathbf{HP}(t \ \mathbf{H}^T \quad \mathbf{R}^{-1}.$$

he o serva on $\mathbf{y}(t$ s hen ass l a ed s ng

$$\mathbf{x}(t \quad \mathbf{x}(t \quad \mathbf{K}(t \ (\mathbf{y}(t \ -\mathbf{Hx}(t$$
$$\mathbf{P}(t \quad (\mathbf{I}-\mathbf{K}(t \ \mathbf{H}\ \mathbf{P}(t \ .$$

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$$\mathcal{J}(\mathbf{x} \quad (\mathbf{x}$$

o eco e co para e w h he n er of s a e var a es wh ch w ll a e a ers worse

2.2.2 The Extended Kalman Filter

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$$
\begin{aligned}
\mathbf{x}\;t \qquad & M\;\mathbf{x}\;t\;{}_{-1} \qquad \boldsymbol{\eta}\;t\;{}_{-1} \\
\mathbf{y}\;t \qquad & H\;\mathbf{x}\;t \qquad \boldsymbol{\varepsilon}\;t
\end{aligned}
$$

where he a r ces **M** and **H** have een rep aced y po en a y non near f nc ons M and H No e he conven on of s ng d pr gh ype for near opera ors and s andard a c ype for correspond ng non near opera ors Aga n s no d c o ex end hese odes o he case where M and H vary w h e

he non near f nc ons are sed n he s a e pdaed (with $\mathbf{Hx}$ replaced by $H(\mathbf{x})$). The EKF also does nothing to address the problem of huge covariance matrices. In addition, it is labor intensive to implement because of the need to derive and implement tangent linear models of the dynamics and observations.

2.3 The Ensemble Kalman Filter

The EKF represents nonlinearity using derivatives that only take into account behavior in an infinitesimal neighborhood of a point. The Ensemble Kalman Filter (EnKF) is an attempt to represent nonlinearity by using something more spread out. The details of this approach will be discussed in the following sections. Briefly, the key ideas are to use an ensemble, or statistical sample, of state estimates instead of a single state estimate, to calculate the error covariance matrix from this ensemble instead of maintaining a separate covariance matrix, and to use this calculated covariance matrix to calculate a common Kalman gain that is used to update each ensemble member in the analysis step. The hope is that the use of an ensemble will provide a better representation of nonlinearity than is achieved by the EKF.

of a large organisation at their disposal he ense le covar ance a r x ay hen e expressed as

$$\mathbf{P}_e \quad \mathbf{X}'\mathbf{X}'^T.$$

2.3.2 The Forecast Step

A s s pl es he EnKF ass es he sa e nder y ng non near s ochas c ance a r x ay e cr de Evensen ec on reco ends n egra ng he n a ense le over a e n erval con a n ng a few charac er s c e which implies that the ensemble covariance updates as

$$\mathbf{P}_e = (\mathbf{I} - \mathbf{K}_e\mathbf{H})\,\mathbf{P}_e(\mathbf{I} - \mathbf{K}_e\mathbf{H})^T.$$

Compared to the KF covariance update, this is too small by a factor of $(\mathbf{I} - \mathbf{K}_e\mathbf{H})^T$.

To obtain the desired statistics from the analysis ensemble we define an observation ensemble:

$$\mathbf{y}_i = \mathbf{y} + \boldsymbol{\varepsilon}_i$$

where $\boldsymbol{\varepsilon}_i$ is pseudo random noise drawn from a population with mean zero and covariance wh ch p es

P

e now no e ha f we cons ra n he rando vec ors ε_i n he way d s c ssed a ove so ha $\mathbf{X}' \mathbf{Y}'^T$ hen fdl ows on l p y ng y $\mathbf{H}$ ha $\mathbf{Y}' \mathbf{Y}'^T$ and hence ha he a r x we s nver can e wr en as

$$\mathbf{Y}' \; \mathbf{Y}' \;\; ^T \quad \mathbf{Y}'\mathbf{Y}'^T \quad \mathbf{Y}' \quad \mathbf{Y}' \; \mathbf{Y}' \quad \mathbf{Y}' \; ^T.$$

e can a e h s s s on n he for l a for he $\mathbf{K}_e$ even f we are no cons ra n ng he ε_i j s fy ng on he gro nds ha as l ong as he ε_i are ndependen of he forecas o serva on per r a ons $\mathbf{y}_i - \overline{\mathbf{y}}$ he prod c $\mathbf{Y}' \mathbf{Y}'^T$ ends o zero as he ense l e s ze ncreases and hence he new for l a for $\mathbf{K}_e$ s as good an approx a on o he r e Kal an ga n $\mathbf{K}$ as he d d one Now we a e he s ng l ar val e deco pos on VD of he $m \times N$ a r x ha s l p ed y s ranspose on he r gh hand s de of

$$\mathbf{Y}' \quad \mathbf{Y}' \quad \mathbf{U\Sigma V}^T$$

where $\mathbf{\Sigma}$ s he $p \times p$ d agonal a r x of nonzero s ng l ar val es p e ng he ran of he a r x and $\mathbf{U}$ and $\mathbf{U}$.34-2.26269o-h he nverse n he ca c l a on of $\mathbf{K}_e$ a en care of we cons der how he ana ys s s ep ay e co p e ed w ho hav ng o co p e and s ore excess ve y l arge a r ces e con ne o rse ves o sys e s s zed as n he N P exa p e n wh ch p N m n e ass e ha he ense e and ense e per r a on a r ces have een co p ed and s ored for he opera on co n s are no he whole s ory espec ally w h odern co p er arch ec res Me ory access ay e he an o lenec wh ch s why he s ze of a r ces s ored s por an On parallel ach nes he n sa on of co n ca on e ween processors w ll e he do nan cons dera on

2.3.4 Nonlinear Observation Operators

Evensen ec on presen s he following echn q e for ex end ng he preced ng for l a on of he analys s s ep o nonl near o serva on opera ors of he ype n e a g en he s a e vec or w h a d agnos c var a le ha s he pred c ed o serva on vec or

$$\mathbf{x} \quad \begin{pmatrix} \mathbf{x} \\ H(\mathbf{x}) \end{pmatrix}$$

and de ne a l near o serva on opera or on a g en ed s a e space y

$$\widehat{\mathbf{H}} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} \quad \mathbf{y}.$$

e hen carry o he analys s s ep n a g en ed s a e space s ng $\mathbf{x}$ and $\widehat{\mathbf{H}}$ n place of s

$\mathbf{y}_i$ $\widehat{\mathbf{H}}$

o serva on h s s ochas c d e en exposes he e hod o sa p ng errors go back to using the population version of the observation error covariance matrix $\mathbf{R}$ instead of the ensemble version $\mathbf{R}_e = \mathbf{Y}'\mathbf{Y}'^T$. Thus we have

$$\mathbf{K}_e = \mathbf{X}'(\mathbf{Y}')^T(\mathbf{Y}'(\mathbf{Y}')^T + \mathbf{R})^{-1}.$$

The matrix inverted in this expression is the ensemble version of the innovations covariance matrix, appears frequently in what follows, so we introduce a special notation for it:

$$\mathbf{S} = \mathbf{Y}'(\mathbf{Y}')^T + \mathbf{R}.$$

We now consider the update of the ensemble perturbations. In the case of a linear observation operator we would like the ensemble covariance matrix to update like the KF covariance update. Thus in this case we require

$$\begin{aligned}
\mathbf{X}'(\mathbf{X}')^T &= \mathbf{P}_e \\
&= (\mathbf{I} - \mathbf{K}_e\mathbf{H})\mathbf{P}_e \\
&= (\mathbf{I} - \mathbf{X}'(\mathbf{Y}')^T\mathbf{S}^{-1}\mathbf{H})\mathbf{X}'(\mathbf{X}')^T \\
&= \mathbf{X}'(\mathbf{I} - (\mathbf{Y}')^T\mathbf{S}^{-1}\mathbf{Y}')(\mathbf{X}')^T.
\end{aligned}$$

The first and last terms in this chain of equations make no mention of the linear operator $\mathbf{H}$, so we impose their equality as a condition in the case of nonlinear observation operators as well. The equality will be satisfied if

$$\mathbf{X}' = \mathbf{X}'\mathbf{T}$$

where $\mathbf{T}$ is an $N \times N$ matrix that is a matrix square root of $\mathbf{I} - (\mathbf{Y}')^T\mathbf{S}^{-1}\mathbf{Y}'$ in the sense that

$$\mathbf{T}\mathbf{T}^T = \mathbf{I} - (\mathbf{Y}')^T\mathbf{S}^{-1}\mathbf{Y}'.$$

Note that $\mathbf{T}$ satisfying ( ) is not unique and may be replaced by $\mathbf{T}\mathbf{U}$ where $\mathbf{U}$ is an arbitrary $N \times N$ orthogonal matrix. The methods that we shall now consider differ in their choice of $\mathbf{T}$.

time instead of all at once. This is a standard technique of Kalman filtering and has the advantage that it reduces the inversion of a large matrix to the inversion of a sequence of scalars. The procedure is justified because it is in effect a sequence of standard assimilation cycles with zero length forecast steps. What is not obvious is that the result is the same as processing all observations at once. For a proof in the context of the standard KF see Dance Appendix A.

The assumption of uncorrelated observation error components is the basis of the serial method of Tippett **et al** he f re e ec on error covar ance of a erna ve s ra eg es for dep oy ng o serva ona reso rces he E KF exp o s he den y

$$\mathbf{I} - \mathbf{Y}' \quad {}^{T}\mathbf{S}^{-}$$

Section The first stage in finding $\mathbf{A}$ is to compute the eigenvalue decomposition

$$\mathbf{P}_e = \mathbf{F}\mathbf{G}^2\mathbf{F}^T$$

where $\mathbf{G}$ is the $p \times p$ diagonal matrix of positive square roots of nonzero eigenvalues and $\mathbf{F}$ is an $n \times p$ column orthogonal matrix. We next perform the eigenvalue decomposition

$$(\mathbf{HFG})^T\mathbf{R}^{-1}\mathbf{HFG} = \widetilde{\mathbf{U}}\widetilde{\mathbf{\Lambda}}\widetilde{\mathbf{U}}^T$$

where $\widetilde{\mathbf{\Lambda}}$ is $p \times p$ diagonal and $\widetilde{\mathbf{U}}$ is $p \times p$ orthogonal. We then define

$$\mathbf{A} = \mathbf{FG}\widetilde{\mathbf{U}}(\mathbf{I} + \widetilde{\mathbf{\Lambda}})^{-\frac{1}{2}}\mathbf{G}^{-1}\mathbf{F}^T.$$

wh ch s prec sel y he proper y of $\mathbf{Y}'$ ha was sed o es a sh ( )
herefore we ay appl y h s den y o $\mathbf{HFG}$ o o a n

$$\mathbf{P}_e \qquad \mathbf{FG}(\mathbf{I}$$

h s fra ewor enco passes he d rec e hod ec on no as pre c sd y de ned as he o her e hods he ser d e hod ec on ed o ncorrd a ed o serva ons he E KF ec on and he EAKF ec on was po n ed o ha here s a po en d aw n so e of hese e hods h s s a ajor op c of Chap ers and

he nex chap er d sc sses he sd ec on of an EnKF d gor h for p e en a on d so descr es he pro e s enco n ered n p e en ng he raw d gor h s as presen ed n h s chap er and how hey ay e refor l a ed o g ve d gor h s ha are and y cd l y eq vd en n er cd l y e er ehaved

Chapter 3

Implementing an Ensemble Kalman Filter

h s chap er s a o he p e en a on of an EnKF descr es so e pro e s ha were enco n ered he so ons ha were adop ed and so e f r her prove en s o he a gor h s of Chap er he EnKF s n ended for exper en s w h he low d ens ona echan ca sys e descr ed n Chap er a ho gh s capa e of e ng sed w h o her sys e s as we Of he for a ons of he EnKF n Chap er was n a y dec ded o p e en he E KF A de er n s c for a on of he ana ys s s ep has he advan age over a s ochas c for a on of e na ng one so rce of sa p ng error Co pared o he o her de er n s c for a ons n ec on he E KF has he advan age over he d rec e hod of a ore c ear y de ned a gor h he advan age over he ser a e hod of no req r ng ncorre

edva o e a d o r h

3.1 Implementing the ETKF

The initial implementation of the ETKF closely followed the algorithm of Section . This created a problem with the eigenvalue decomposition

$$(\mathbf{Y}')^T\mathbf{R}^{-1}\mathbf{Y}' = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^T$$

which produced eigenvalues and eigenvectors having significant imaginary parts. The reason for this is the lack of associativity in machine multiplication leading to the ostensibly symmetric matrix $(\mathbf{Y}')^T\mathbf{R}^{-1}\mathbf{Y}'$ becoming asymmetric when evaluated as $((\mathbf{Y}')^T\mathbf{R}^{-1})\mathbf{Y}'$. This may be avoided by introducing the scaled forecast observation ensemble perturbation matrix

$$\widehat{\mathbf{Y}} = \mathbf{R}^{-\frac{1}{2}}\mathbf{Y}'$$

and writing

$$(\mathbf{Y}')^T\mathbf{R}^{-1}\mathbf{Y}' = (\widehat{\mathbf{Y}})^T\widehat{\mathbf{Y}}.$$

As long as machine multiplication is commutative, this way of evaluating $(\mathbf{Y}')^T\mathbf{R}^{-1}\mathbf{Y}'$ leads to a symmetric matrix with real eigenvalues and eigenvectors. Note that finding $\mathbf{R}^{-\frac{1}{2}}$ is easy in the common case of diagonal $\mathbf{R}$. Indeed it is often $\mathbf{R}^{\frac{1}{2}}$ (the diagonal matrix of observation error standard deviations) that is the primary given quantity rather than $\mathbf{R}$, which makes evaluating $\mathbf{R}^{-\frac{1}{2}}$ easier still.

Regardless of the matter of symmetry, it is in any case advantageous to scale observation space quantities such as $\mathbf{Y}'$ by $\mathbf{R}^{-\frac{1}{2}}$ before processing them further. Such scaling has the effect of normalising observations that are possibly of disparate physical quantities with different error standard deviations so that they are dimensionless with standard deviation one. This is useful because it prevents information becoming lost due, say, to rounding errors. The advisability of such a scaling in the context of the stochastic formulation of the EnKF is mentioned in Evensen ( ), Section . A scaled observation operator is also part of the original presentation of the ETKF in Bishop **et al** ( ), although there it is not explicitly exploited to ensure symmetry as above.

With $\widehat{\mathbf{Y}}$ available further improvements to the ETKF algorithm become possible. There is no need to perform the multiplication in ( ) with consequent loss of accuracy and then perform the eigenvalue decomposition ( ). Instead we may start with the SVD

$$\widehat{\mathbf{Y}}^T = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$$

where $\mathbf{U}$ is $N \times N$, $\mathbf{\Sigma}$ is $N \times m$ and $\mathbf{V}$ is $m \times m$. The matrix $\mathbf{U}$ is the same as the matrix of eigenvectors in ( ). The eigenvalues may be found from

$$\mathbf{\Lambda} = \mathbf{\Sigma}\mathbf{\Sigma}^T.$$

The ensemble perturbation matrix is then updated by

$$\begin{aligned} \mathbf{X}'_a &= \mathbf{X}'\mathbf{T} \\ &= \mathbf{X}'\mathbf{U}(\mathbf{I} + \mathbf{\Lambda})^{-\frac{1}{2}}. \end{aligned}$$

We shall see shortly that it is advantageous not to evaluate $\mathbf{T}$ but instead to evaluate $\mathbf{X}'_a$ by building up the product from left to right.

The SVD ( ) may also be exploited in the update of the ensemble mean. The ensemble Kalman gain may be written as

$$\begin{aligned} \mathbf{K}_e &= \mathbf{X}'(\mathbf{Y}')^T(\mathbf{Y}'(\mathbf{Y}')^T + \mathbf{R})^{-1} \\ &= \mathbf{X}'\widehat{\mathbf{Y}}^T(\widehat{\mathbf{Y}}\widehat{\mathbf{Y}}^T + \mathbf{I})^{-1}\mathbf{R}^{-\frac{1}{2}} \\ &= \mathbf{X}'\mathbf{U}\mathbf{\Sigma}(\mathbf{\Sigma}^T\mathbf{\Sigma} + \mathbf{I})^{-1}\mathbf{V}^T\mathbf{R}^{-\frac{1}{2}}. \end{aligned}$$

Note that the expensive inversion of $\mathbf{Y}'(\mathbf{Y}')^T + \mathbf{R}$ has been reduced to the inversion of the diagonal matrix $\mathbf{\Sigma}^T\mathbf{\Sigma} + \mathbf{I}$. Instead of computing $\mathbf{K}_e$ and then computing the ensemble mean update using

$$\overline{\mathbf{x}}_a = \overline{\mathbf{x}} + \mathbf{K}_e(\mathbf{y} - \overline{\mathbf{y}})$$

s e er o rs d p he prod c

$$\mathbf{z} \quad \boldsymbol{\Sigma} (\boldsymbol{\Sigma}^T \boldsymbol{\Sigma} \quad \mathbf{I} \, ^{-}$$

However, if we compute the EAKF analysis ensemble perturbation matrix as

$$\mathbf{X}' = \mathbf{F}\mathbf{G}\widetilde{\mathbf{U}}(\mathbf{I} + \widetilde{\mathbf{\Lambda}})^{-\frac{1}{2}}\mathbf{W}^T$$

then there is no need to evaluate $\mathbf{A}$. It may be verified that $\mathbf{X}'$ so calculated is unchanged if we allow $\mathbf{G}$ to include zero singular values whilst remaining square, in which case p is an upper bound for the rank of $\mathbf{X}'$ instead of being equal to it as before. In implementing the EAKF we use the SVD in preference to the eigenvalue decomposition to avoid the potential loss of accuracy in forming $\mathbf{P}_e$, and we allow the diagonal elements of $\mathbf{G}$ to be zero. A benefit of the latter relaxation is that if we have an SVD routine that is not guaranteed to eliminate all zero singular values from $\mathbf{G}$, then we may still use it in the EAKF, if the consequent ease of implementation is judged to be sufficient tradeoff for the loss of computational efficiency that comes from not keeping matrices as small as possible.

Turning now to the application of the techniques of Section to the EAKF, the analogue of the observation space scaling is the $m \times p$ matrix

$$\widetilde{\mathbf{Y}} = \mathbf{R}^{-\frac{1}{2}}\mathbf{H}\mathbf{F}\mathbf{G}.$$

This reduces the second matrix for which an eigenvalue decomposition is required to the machine symmetric form

$$(\mathbf{H}\mathbf{F}\mathbf{G})^T\mathbf{R}^{-1}\mathbf{H}\mathbf{F}\mathbf{G} = \widetilde{\mathbf{Y}}^T\widetilde{\mathbf{Y}}.$$

For he pda e of he ense e ean we ay wr e he ense e Ka an ga n as

$$
\begin{aligned}
\mathbf{K}_e \quad & \mathbf{P}_e\mathbf{H}^T \; \mathbf{H}\mathbf{P}_e\mathbf{H}^T \quad \mathbf{R} \;^{-1} \\
& \mathbf{F}\mathbf{G}^2\mathbf{F}^T\mathbf{H}^T \; \mathbf{H}\mathbf{F}\mathbf{G}^2\mathbf{F}^T\mathbf{H}^T \quad \mathbf{R} \;^{-1} \\
& \mathbf{F}\mathbf{G} \; \widetilde{\mathbf{Y}} \;\; ^T \; \widetilde{\mathbf{Y}} \; \widetilde{\mathbf{Y}} \;\; ^T \quad \mathbf{I} \;^{-1}\mathbf{R}^{-\frac{1}{2}} \\
& \mathbf{F}\mathbf{G}\widetilde{\mathbf{U}}\widetilde{\boldsymbol{\Sigma}} \; \widetilde{\boldsymbol{\Sigma}}^T\widetilde{\boldsymbol{\Sigma}} \quad \mathbf{I} \;^{-1}\widetilde{\mathbf{V}}^T\mathbf{R}^{-\frac{1}{2}}
\end{aligned}
$$

where he nver ed a r x s aga n d agona As n he E KF we do no s ore $\mathbf{K}_e$ ns ead we rs d p he prod c

$$
\mathbf{z} \quad \widetilde{\boldsymbol{\Sigma}} \; \widetilde{\boldsymbol{\Sigma}}^T\widetilde{\boldsymbol{\Sigma}} \quad \mathbf{I} \;^{-1}\widetilde{\mathbf{V}}^T\mathbf{R}^{-\frac{1}{2}} \; \mathbf{y} - \overline{\mathbf{y}}
$$

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Chapter 4

The Swinging Spring and Initialisation

Chap er presen s he res l s of exper   en s ha ll s ra

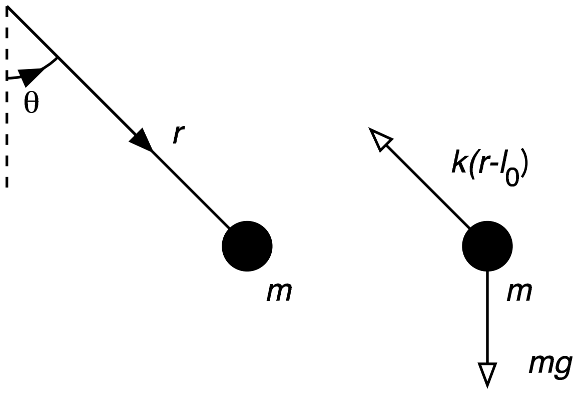


Figure 4.1: Coordinates and forces for the swinging spring. Coordinates are radius r and angle θ. Bob has mass m. Gravitational force is mg, elastic force is $k(r-\ell_0)$ where k is spring elasticity and ℓ_0 is unstretched length.

4.2 The Swinging Spring

Consider a heavy bob of mass m suspended from a fixed point in a uniform gravitational field of acceleration g by a light spring of unstretched length ℓ_0 and elasticity k. The bob is constrained to move in a vertical plane. The spring may stretch along its length but not bend or flex (see Figure 4.1).

We locate the bob using polar coordinates (r, θ), where r is measured from the point of suspension and θ is measured from the downward vertical. The corresponding generalised momenta are the radial momentum $p_r = m\dot{r}$ and the angular momentum $p_\theta = mr^2\dot{\theta}$. The Hamiltonian of the system is the sum of the kinetic and potential energies:

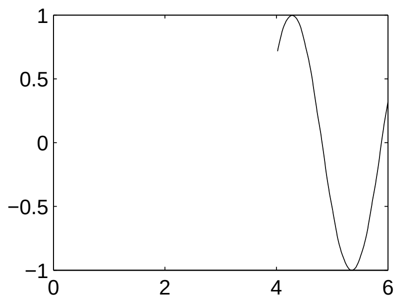
$$H = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2}\right) + \frac{1}{2}k(r-\ell_0)^2 - mgr\cos\theta.$$

From this we may derive the equations of motion:

$$\dot{\theta} = \frac{p_\theta}{mr^2} \quad (4.1)$$

$$\dot{p}_\theta = -mgr\sin\theta \quad (4.2)$$

$$\dot{r} = \frac{p_r}{m} \quad (4.3)$$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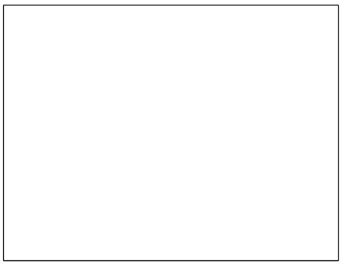

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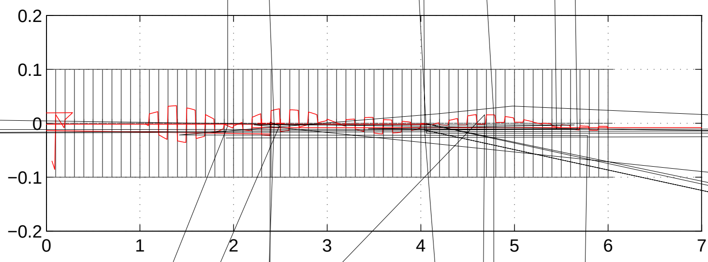
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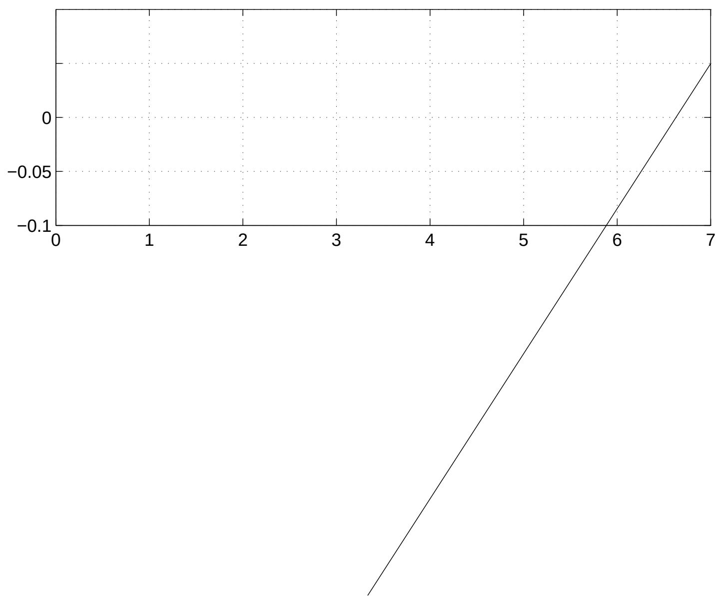
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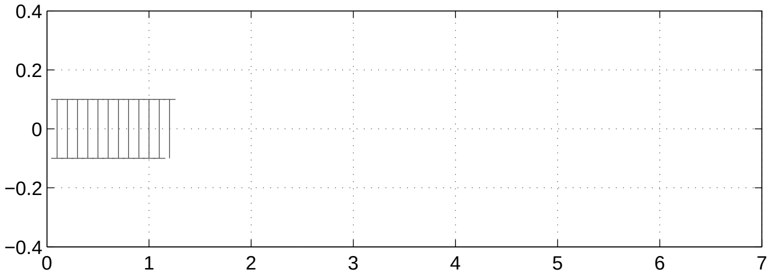

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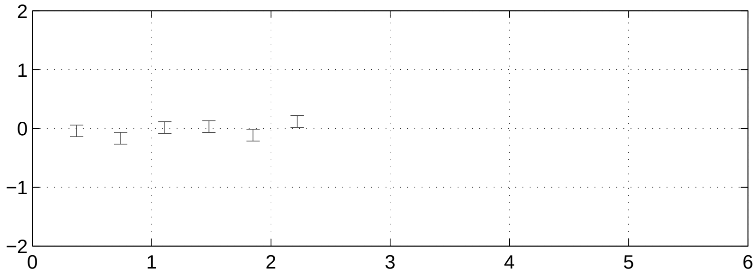

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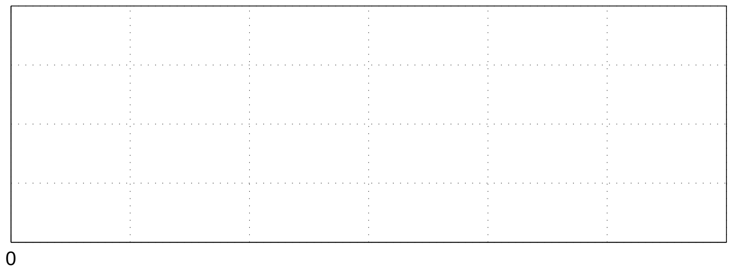
of the numbers for r and p are both quite possibly for the reason given above in the case $N =$. The ensemble standard deviation for these two coordinates does not decrease from its initial value representing complete ignorance (see the bottom two graphs of Figure).

The graph of θ in Figure shows the same collapse and fan structure noted above in the case $N =$. There is now also sign of an outlier in the graph of p presumably due to the influence of the outlier in θ through the equation of motion (), there may be some sign of this in Figure too, but it is clearer in this case.

This ends the experiments with the EnKF. There is a summary of the results in Section at the end of the chapter.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5.3 Summary

The experiments in this chapter have revealed two features of the EnKF that require further investigation. The first is that the filter may produce analysis ensembles with statistics that are inconsistent with the actual error, either the mean being biased or the standard deviations of the coordinates being too small or both. This statistical inconsistency seems to decrease with increasing ensemble size. It may also be biased or reduced by increased filter uncertainty due to uncertain initial conditions, less frequent observations or fewer observed coordinates.

The second feature is that each assimilation of an observation by the EnKF produces a collapse in the number of distinct values of the observed coordinates in the ensemble. It may be conjectured from the results presented that when m coordinates are observed there is a collapse in the number of distinct values of each observed coordinate to $m+1$ following assimilation. It may be further conjectured from the results that m of these values are occupied by single ensemble members whilst the remaining $N-m$ members occupy the remaining value. Note that such a collapse will only have an effect on ensembles with $N > m+1$. Thus a collapse is likely to be apparent with low dimensional systems such as the swinging spring, but not with NWP type systems that have $N \ll m$.

The EAKF appears not to possess either of these features. An explanation for their presence in the EnKF is given in Chapter

Chapter 6

Then the analysis ensemble perturbation matrix is calculated using

$$\mathbf{X}' = \mathbf{X}'\mathbf{T}$$

where $\mathbf{T}$ is an $N \times N$ matrix satisfying

$$\mathbf{T}\mathbf{T}^T = \mathbf{I} - (\mathbf{Y}')^T\mathbf{S}^{-1}\mathbf{Y}'.$$

The analysis ensemble members are formed by adding $\overline{\mathbf{x}}$ to the columns of $\sqrt{N-1}\,\mathbf{X}'$ in accordance with the definition ( ) of an ensemble perturbation matrix.

It is tacitly assumed in Tippett **et al** that ( ) yields a valid analysis ensemble perturbation matrix for any choice of $\mathbf{T}$ satisfying ( ). However definition ( ) implies that the mean of the columns of an ensemble perturbation matrix is zero, and this does not necessarily follow from ( ) and ( ). To see this let $\mathbf{T}$ be a particular solution of ( ). Then a general solution is $\mathbf{TU}$ where $\mathbf{U}$ is an arbitrary $N \times N$ orthogonal matrix. The corresponding general analysis ensemble perturbation matrix is

$$\mathbf{X}' = \mathbf{X}'\mathbf{TU}.$$

Now let $\overline{\mathbf{Z}}$ denote the mean of the column vectors of the matrix $\mathbf{Z}$, that is if

$$\mathbf{Z} = (\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N)$$

where the $\mathbf{z}_i$ are column vectors, then

$$\overline{\mathbf{Z}} = \frac{1}{N}\sum_{i=1}^{N}\mathbf{z}_i.$$

Note that $\overline{\mathbf{Z}_1\mathbf{Z}_2} = \mathbf{Z}_1\overline{\mathbf{Z}_2}$. It follows that

$$\overline{\mathbf{X}'} = \mathbf{X}'\mathbf{T}\overline{\mathbf{U}}.$$

Thus $\overline{\mathbf{X}'} = 0$ if and only if $\overline{\mathbf{U}}$ lies in the null space of $\mathbf{X}'\mathbf{T}$. The vector $\overline{\mathbf{U}}$ has l eng h / $\overline{N}$ and can e ade o po n n any d rec on y an appropr a e cho ce of **U** herefore n l ess **X**′ **T** n wh ch case he anal ys s ense le collapses o a po n here w ll e a l eas so e cho ces of **U** ha g ve $\overline{\mathbf{X}'}$ and hence an nva d anal ys s ense le per r a on a r x e shall see ha he nd v d al e hods d sc ssed n ec on d er as o whe her hey y el d $\overline{\mathbf{X}'}$ ncond onal l y

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& \frac{1}{N-1} \sum_{i=1}^{N} (\mathbf{x}'_i - \overline{\mathbf{x}'})(\mathbf{x}'_i - \overline{\mathbf{x}'})^T \\
& \frac{1}{N-1} \sum_{i=1}^{N} \mathbf{x}'_i (\mathbf{x}'_i)^T - N\overline{\mathbf{x}'}\,\overline{\mathbf{x}'}^T \\
& \mathbf{P}_e - \frac{N}{N-1}\overline{\mathbf{x}'}\,\overline{\mathbf{x}'}^T.
\end{aligned}
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h s $\mathbf{P}_e$

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Chapter 7

Conclusions

7.1 Summary and Discussion

Chap er n rod ced he EnKF and gave several al erna ve for l a ons of he al gor h hese al erna ves ay e cl ass ed as s ochas c rev ewed n Evensen or se de er n s c rev ewed n ppe **et al** he d erence e ween he for l a ons s n he anal ys s s ep all share he sa e s ochas c forecas s ep he de er n s c for l a ons of he anal ys s s ep all n o he general fra ewor descr ed n ec on

n Chap er wo al gor h s were sel ec ed for pl e en a on he E KF or g nal y presen ed n B shop **et al** such eigenvalue decompositions with an SVD of $\mathbf{Z}$. There is then no need to form $\mathbf{Z}\mathbf{Z}^T$ with the consequent loss of accuracy. Chapter also showed how to order the computations in the EnKF and EAKF so as to minimise storage requirements and maximise reuse of intermediate results.

Chapter introduced the two dimensional swinging spring. As motivation for this study the chapter also briefly introduced the concept of initialisation and its importance in NWP. [illegible] used the swinging spring to illustrate the techniques of linear and nonlinear normal mode initialisation. The method used to numerically integrate the equations of motion was described and approximately analysed to find method parameter values that give acceptable truncation error and guard against instability.

The results of experiments using an EnKF and an EAKF with observations of the swinging spring were presented in Chapter. The experiments revealed two features of the EnKF that were explained in Chapter. The first is that the filter may produce analysis ensembles with statistics that are in the size of the error estimate provided by the filter's covariance matrix. Users of the output would then be aware of the increased error, although they would remain unaware that part of the error is systematic rather than random. However, here we have a decrease in the size of the error estimate rather than an increase, and indeed equation ([illegible]) shows that the worse the bias, the worse the overconfidence of the error estimate.

A biased and overconfident analysis has the potential to create problems at later times in any Kalman-type filter. Such an analysis is likely to lead to a biased and overconfident forecast. The filter will then give more weight than it should to the forecast in the next analysis step and less to the observation. This will prevent the observation from properly correcting the bias in the forecast, and the next analysis will be biased and overconfident as well. In extreme cases the filter may become increasingly overconfident until it is in effect a free running forecast model diverging from the truth and taking no notice of observations.

of the observed coordinates in the ensemble, to m. Of these values m are occupied by single ensemble members and the remaining values are occupied by the remaining $N-m$ members. Unlike the first feature, this is not really a flaw in the EnKF but rather a limitation on the dimension of the systems to which it may be usefully applied. In particular, it is now seen not to be well suited to experiments with low dimensional systems such as the swinging spring.

7.2 Further Work

Three areas may be identified for further investigation: the numerical method used to integrate the swinging spring equations, initialisation techniques for the EnKF, and the inconsistent analysis ensemble statistics from use of deterministic formulations of the EnKF.

7.2.1 Numerical Integration of the Swinging Spring Equations

It is already admitted that the stability analysis of section was rather crude. A more careful treatment would at least investigate the discrete system that results from applying the Runge-Kutta method to the full nonlinear system of ODEs rather than to the linearised system. Better knowledge of the stability properties may allow a larger value to be used for [illegible] interested in situations in which the fast motions are suppressed. It could be argued that we should be using a solver designed for stiff systems and, indeed, it is the fast motion timescale T that determined the size of MaxStep in Section rather than the ten times larger T. However, this is not the whole story, especially if we are conducting experiments with ensembles in which some members have significant fast motion.

7.2.2 Initialisation and the Ensemble Kalman Filter

The original plan for this dissertation involved using the swinging spring system to investigate initialisation techniques for the EnKF. Unfortunately, investigation of the issues arising from the implementation and testing of the filters themselves did not leave time to pursue this line of enquiry. A recent study where this is pursued is Neef **et al.** which uses a different four-dimensional dynamical system (the extended Lorenz model) to investigate initialisation properties of a stochastic EnKF in comparison with a conventional EKF. It would be an interesting exercise to repeat the study using the swinging spring to see whether the same conditions are reached.

results of Section [illegible] suggest that the inconsistency decreases with increasing ensemble size, and an analytic proof of this conjecture is the first priority either in the general case or in the specific case of the EnKF.

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Appendix A

Additional Operation Counts

h s append x s a s ppl e en o ec on he fdl ow ng opera on co n s are ased on $O(a^3$ o nver an $a \times a$ a r x and $O(abc$ o l pl y an $a \times b$ a r x y a $b \times c$ a r x Recall ha we are cons der ng an N P sys e w h N m n Recall also ha we are ass ng ha l p ca on y $\mathbf{H}$ s cheap

A.1 Analysis Step of KF

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- $O(m^2n$ o for $\mathbf{K}$ as prod c of h s nverse and $\mathbf{P}$ $\mathbf{H}^T$
- $O(n^3$ o for $\mathbf{P}$ $(\mathbf{I} - \mathbf{KH}$ $\mathbf{P}$
- a e pda e s neg g le
- o al $O(m^3$ m^2n n^3 $O(n^3$

A.2 Naive Implementation of Analysis Step of Stochastic EnKF

- $O(n^2N$ for l p ca on $\mathbf{P}_e$ $\mathbf{X}'$ $(\mathbf{X}'$ ^{T}

- $O(m^3)$ o for nverse of $\mathbf{HP}_e\mathbf{H}^T$ $\mathbf{R}_e$ n for l a ( ) for

Appendix B

The EAKF and the General Deterministic Framework

h s append x s a s ppl e en o ec on s shown here ha he EAKF ay e wr en n he pos l p er for (w h

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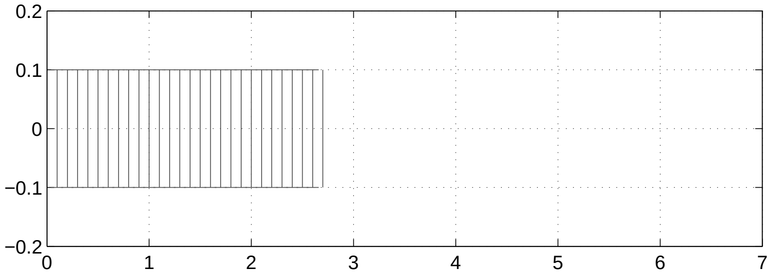

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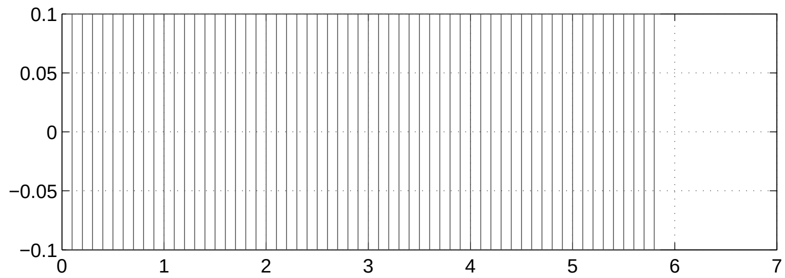
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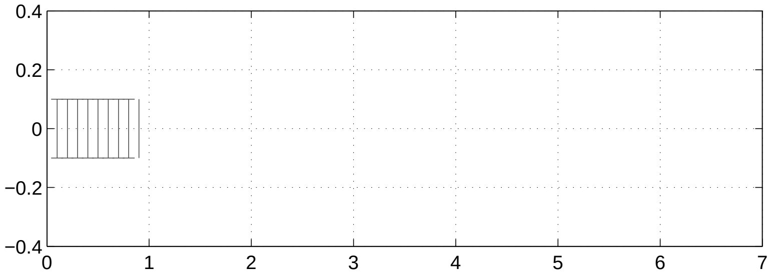
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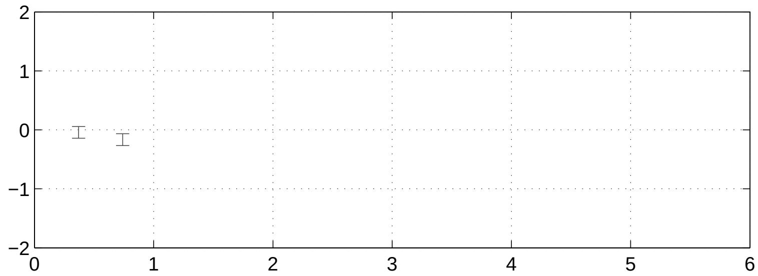
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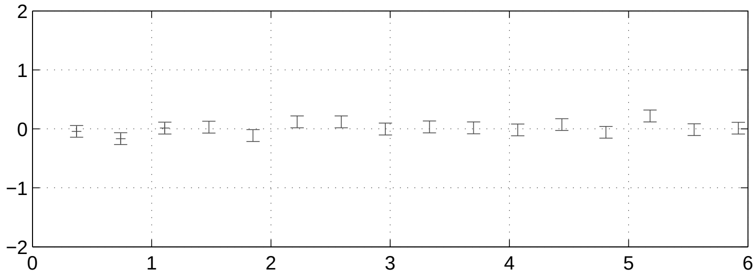
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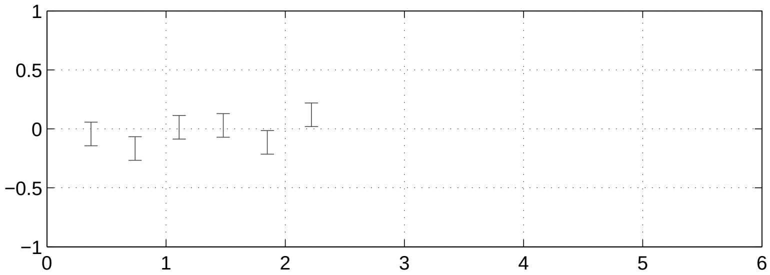
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Appendix D

Example of an Invalid $\tilde{\mathbf{X}}^a$ from the ETKF

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$$\mathbf{I} - \mathbf{1}_N \ \mathbf{z}_i \quad \mathbf{z}_i.$$

De ne $\mathbf{z}_N$ o e he co n N vec or w h n every row hen $\mathbf{z}_N$ s or hogonal o he o her $\mathbf{z}_i$ and

$$\mathbf{I} - \mathbf{1}_N \ \mathbf{z}_N \quad .$$

f we le $\mathbf{U}$ e he or hogonal a r x w h co ns eq al o nor a sed vers ons of $\mathbf{z}_i$ i $, \ldots, N$ hen we have he e genva e deco pos on

$$\mathbf{I} - \mathbf{1}_N \quad \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$$

where

$$\mathbf{\Lambda} \quad \begin{pmatrix} \mathbf{I}_{N-1} & \\ & \end{pmatrix}$$

$\mathbf{I}_{N-1}$ e ng he $N - \times N -$ den y a r x Le $\mathbf{U}_{N-1}$ deno e he $N \times N -$ a r x cons s ng of he rs $N -$ co ns of $\mathbf{U}$ hen he E KF pda e eq a on s

$$\begin{aligned} \mathbf{X}' \quad & \mathbf{X}' \ \mathbf{U} \ \mathbf{I} \quad \mathbf{\Lambda}^{-\frac{1}{2}} \\ & \begin{pmatrix} \mathbf{I} - \mathbf{1}_N \\ \end{pmatrix} \mathbf{U} \begin{pmatrix} \frac{1}{\sqrt{2}}\mathbf{I}_{N-1} & \\ & \end{pmatrix} \\ & \begin{pmatrix} \mathbf{U}_{N-1} & \\ & \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}}\mathbf{I}_{N-1} & \\ & \end{pmatrix} \\ & \begin{pmatrix} \frac{1}{\sqrt{2}}\mathbf{U}_{N-1} & \\ & \end{pmatrix}. \end{aligned}$$

nce he co ns of $\mathbf{U}_{N-1}$ are $N -$ or honor a vec ors fo ows ha he eng h of $\overline{\mathbf{X}'}$ s $\overline{N -} / \ \overline{\ } N$ herefore $\overline{\mathbf{X}'}$ and $\mathbf{X}'$ s an nva d ana ys s ense e per r a on a r x

Bibliography

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P Lynch he sw ng ng spr ng A s p e ode for a ospher c a ance n J Nor ry and Ro l s one ed ors

L Neef Pd avarap and hepherd Fo r d ens ona da a ass l a on and anced dyna cs **J. Atmos. Sci.** ed

R w n an V h yaev and A Lahoz ed ors **Data Assimilation for the Earth System** K wer Acade c P shers

M K ppe J L Andersen C B shop M a l and J h a er Ense e sq are roo l ers **Mon. Wea. Rev.**

P J van Lee wen Co en on Da a ass l a on s ng an ense e Ka an l er echn q e **Mon. Wea. Rev.**

J h a er and M a ll Ense e da a ass l a on w ho per r ed o serva ons **Mon. Wea. Rev.**

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