Predicting forecast uncertainty with singular vectors and ensemble-derived analysis error covariances

Mark Buehner

Meteorological Service of Canada Dorval, Quebec

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Introduction

- several applications require accurate prediction of forecast uncertainty or its origins: ensemble prediction, observation targeting, data assimilation, data QC
- singular vectors (SVs) identify the most unstable subspace of the (linearized) forecast model according to specified norms at initial and optimization times
- current applications (ECMWF, NRL) use SVs with total energy (TE) norms for ensemble prediction and observation targeting
- if initial-time norm is inverse analysis error covariances, SVs optimally describe forecast uncertainty at optimization-time (if model error negligible, TL error growth)
- EnKF provides estimate of flow-dependent analysis error covariances via Monte Carlo simulation to model effect of all error sources in forecast-analysis cycle
- <u>goal</u>: evaluate use of these flow-dependent or (more easily obtained) stationary analysis error cov from ensemble approaches to define initial-time norm for SVs

Outline

- SV theory and calculation
- approaches for estimating analysis error cov with:
 - 1. EnKF (flow-dependent)
 - 2. perturbed 3d-var (stationary)
- impact of covariance norms on structure of SVs (vs TE)
- impact of norms on distribution of sensitive regions (targeting application)
- in context of ensemble prediction (fraction of explained NH fcterr), compare:
 - 1. SVs
 - 2. EnKF members
 - 3. random perturbations
- conclusions and future directions

SV Theory and Calculation

• given an analysis, find perturbation \mathbf{x}_0 that maximizes ratio:

$$rac{\mathbf{x}_t^T \mathbf{W}_t \mathbf{x}_t}{\mathbf{x}_0^T \mathbf{W}_0 \mathbf{x}_0}$$
, where $\mathbf{x}_t = \mathbf{M} \mathbf{x}_0$

- reformulate in terms of control variable γ , where $\mathbf{x}_0 = \mathbf{W}_0^{-1/2} \gamma$
- results in eigenvalue problem: $\mathbf{W}_0^{-T/2} \mathbf{M}^T \mathbf{W}_t \mathbf{M} \mathbf{W}_0^{-1/2} \gamma_k = \sigma_k^2 \gamma_k$
- W_t : final-time norm typically TE, restricted to geographical region of interest
- W_0 : initial-time norm commonly TE (TESV), but...
- when $\mathbf{W}_0 = \mathbf{P}_a^{-1}$, the final-time SVs are the leading eigenvectors of $\mathbf{MP}_a \mathbf{M}^T$ (predictability error \equiv forecast error for perfect model)

Experimental Setup

 like 4d-var, transfer data between 3d-var software (Lanczos solver and norms) and GEM (TLM and ADJ):



- TLM and ADJ at 120x60x28L with simplified linear physics package
- final time norm is TE north of 30°N, 48 hr optimization time interval
- SVs computed each day, 1-14 Dec, 2003
- different initial time (global) norms used :
 - total energy (as commonly used at several NWP centres)
 - inverse analysis error covariances (stationary and flow-dependent)

Approaches for Sampling Analysis Error

Kalman Filter equations: $\mathbf{P}_a = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{P}_f, \quad \mathbf{P}_f = \mathbf{M}\mathbf{P}_a\mathbf{M}^T + \mathbf{Q}$

- not feasible for realistic model, only valid for linear model, little knowledge of ${\bf Q}$
- approx with Monte Carlo simulation approaches (perturb uncertain quantities):

EnKF: different ensemble of 128 error samples every 6h

- analysis uses perturbed observations and flow-dependent ensemble covariances
- model error: random perturbations with similar cov as ${f B}$ in oper. 3d-var
- for SV norm: deviations of analyses from ensemble mean: flow-dependent \mathbf{P}_a

Perturbed 3d-var: single ensemble of 138 error samples from 4 week period

- analysis uses perturbed observations and 3d-var (ECMWF; EPS at CMC)
- $\bullet\,$ model error: random perturbations from adaptively scaled ${\bf B}\,$
- for SV norm: differences between analyses from perturbed and unperturbed exp'ts: stationary \mathbf{P}_a



Geostrophic Balance in Perturbed 3d-var Covariances



- ratio of unbalanced T to total T variance
- in operational BG covariances T almost completely balanced with winds
- less mass/wind balance in perturbed 3d-var (and EnKF) BG covariances
- analysis error even less balanced than background error

Std Dev of (a) Ψ at 250hPa and (b) T at 500hPa

BG error cov from perturbed 3d-var (138 error samples from 4 week period)



Analysis error cov from perturbed 3d-var (138 error samples from 4 week period)



Std Dev of (a) Ψ at 250hPa and (b) T at 500hPa (2)

BG error cov from EnKF (128 error samples valid 2003121212)



Analysis error cov from EnKF (128 error samples valid 2003121212)



Estimation of Error Correlations

- cannot accurately estimate full correlation matrix (rank O(10⁶)) from small number of samples (O(10²))
- therefore must impose constraints on structure of correlations (extra information)
- operational BG error correlations assume homogeneity/isotropy
- alternatively, we can spatially localize horizontal and vertical correlations (currently done in EnKF analysis and in experimental 3d-var)
- demonstrate by plotting BG error covariances of U @ 250 hPa with wind and GZ (next slide)

Estimation of Error Correlations (2)

Original sample estimate of correlations:

Homogeneous/isotropic correlations:

Spatially localized correlations:



Impact of Initial-time Norm on SV structure

Leading total energy SV on 2003121600

initial time:



final time:

Impact of Initial-time Norm on SV structure (2)

Leading analysis error covariance SV on 2003121600 (perturbed 3d-var, homogeneous/isotropic correlations)

initial time:



final time:

Impact of Initial-time Norm on SV structure (3)

Leading analysis error covariance SV on 2003121600 (perturbed 3d-var, localized correlations)



Impact of Initial-time Norm on SV structure (4)

Vertically integrated power spectra for 20 SVs on 2003121600 with initial-time norm:



Impact of Initial-time Norm on SV structure (5)

Partition of energy for 20 SVs on 2003121600 with initial-time norm:



Impact of Initial-time Norm on Observation Targeting

Initial-time vertically integrated total energy, growth factor weighted average of 20 SVs with initial-time norms on 2003121600:

- (a) total energy
- (b) analysis error cov (perturbed 3d-var, homogeneous/isotropic correlations)
- (c) analysis error cov (perturbed 3d-var, localized correlations)



Type of map used to select locations for adaptive observation deployments (e.g. dropsondes)

Impact of Initial-time Norm on Observation Targeting (2)

NH FctErr and its projection onto 20 SVs at optimization time (2003121800)



Impact of Initial-time Norm on Observation Targeting (3)

Pseudo-Inverse of FctErr projection onto 20 SVs - like KAE (linear combination of initial-time SVs on 2003121600)



Impact of Initial-time Norm on Predicting FctErr

- total energy growth factor of leading SV ($\sqrt{TE_{48}/TE_0}$)
 - TESV: initial SV norm is total energy
 - <u>PERT-HI</u>: initial SV norm from perturbed 3d-var analysis error cov with homogeneous/isotropic corr
 - <u>PERT-LOC</u>: initial SV norm from perturbed 3d-var analysis error cov with localized corr
 - <u>ENKF-LOC</u>: initial SV norm from flow-dependent EnKF analysis error cov with localized cor



• fraction of 48-hour NH forecast error energy explained by 20 SVs and total fcterr



EnKF Members vs Random Pert. for Predicting FctErr

- total energy growth factor of one ensemble member ($\sqrt{TE_{48}/TE_0}$)
 - <u>ENKF-20,-128</u>: 48h TLM forecasts initialized with 20 or 128 members from analysis ensembles
 - Pa-RAND-20,-128: 48h TLM forecasts initialized with 20 or 128 random perturbations drawn from Gaussian distribution with perturbed 3d-var analysis error cov (homogeneous/isotropic corr)
 - <u>ENKF-NOLOC</u>: 20 SVs from non-localized EnKF P_a (orthogonal linear combinations of EnKF members)



• fraction of 48-hour NH forecast error energy explained and total fcterr



Conclusions

- 1. large impact on spatial and multi-variate structure of initial-time SVs and location of most sensitive regions from using analysis error covariance norms, and
- 2. for the case examined, SVs using stationary P_a^{-1} norm better predict sensitive region than TESV (i.e. more consistent with pseudo-inverse of fcterr)
- 3. using different SV norms results in small impact on final-time SVs and on ability to explain 48-hour forecast error
- 4. EnKF analysis ensemble members and random pertubations from stationary analysis error distribution explain similar fraction of 48-hour forecast error
- 5. 20 ensemble members (or random perturbations) explain about half the amount of forecast error as 20 SVs, but 128 members explain about 50%-100% more

Future Directions

- apply standard ensemble prediction diagnostics to evaluate SVs, EnKF and random perturbations (diagnostics that account for spread)
- perform longer ensemble predictions with nonlinear model
- explore sensitivity to ensemble size for SVs, EnKF and random perturbations (determine relative cost of each approach for equivalent quality)
- explore application of SVs to observation targeting (A. Zadra) and application of analysis error covariance norms to Key Error Analysis (S. Laroche)

The End