Can singular vectors reliably describe the distribution of forecast errors?

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Background and question

- singular vectors have been and are still being used as a method to generate initial perturbations for ensemble prediction (ECMWF, Météo-France, JMA)
- representing ensemble initial perturbations by distribution in space of leading singular vectors involves a number of approximations/assumptions
  - replace true analysis error covariance matrix by simple estimate (initial time metric)
  - rank-reduction of the analysis error covariance matrix
  - setting of the variance in the space of the singular vectors
  - approximation of the non-linear model by a tangent-linear model
  - ...
- how do these approximations/assumptions impact the ability to make *reliable* predictions of the pdf of forecast errors?

Outline

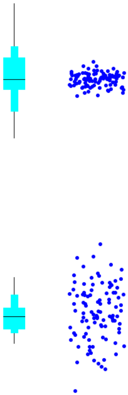
- Ensemble forecasts and reliability
- Singular vectors, linear/non-linear fc error covariance predictions
- A diagnostic to assess reliability in the context of singular vectors
- All uncertainties represented by initial SVs
  - Rank-reduction, amplitude and reliability
  - The tangent-linear approximation
- The operational configuration of the ECMWF ENS
- Summary

Reliability and sharpness

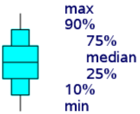
unreliable

broad

sharp

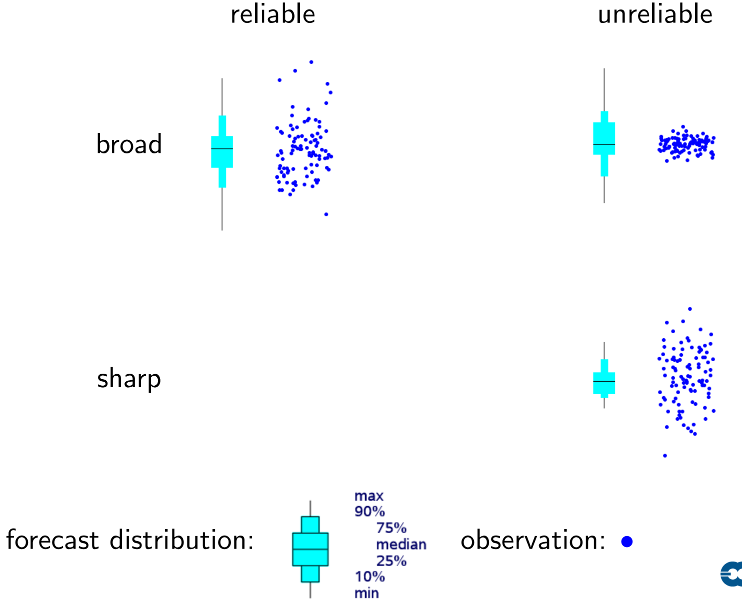


forecast distribution:

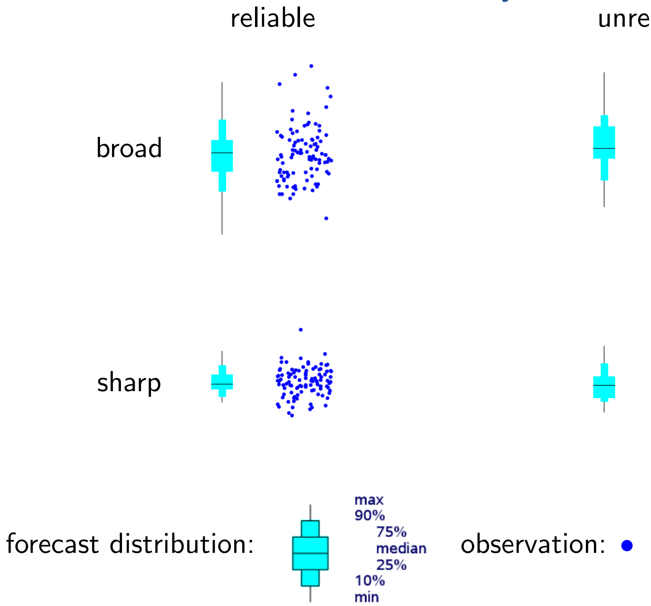


observation: ●

Reliability and sharpness

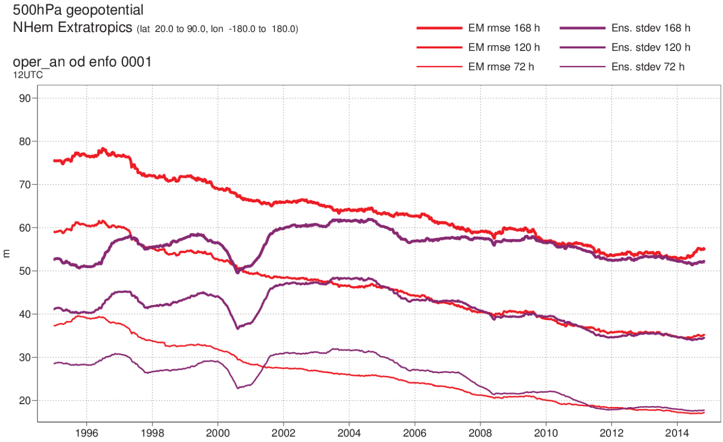


Reliability and sharpness



Evolution of overall ENS reliability

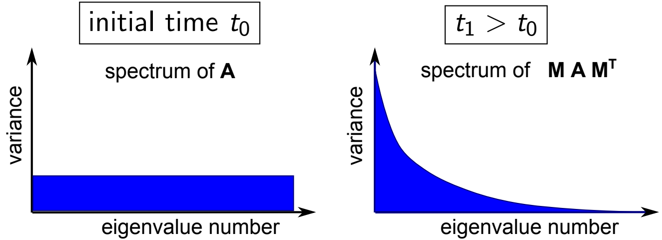
Z500 N-Hem: ensemble stdev versus ens. mean rmse



Linear model and low rank representation of initial uncertainties

error covariances at

full rank



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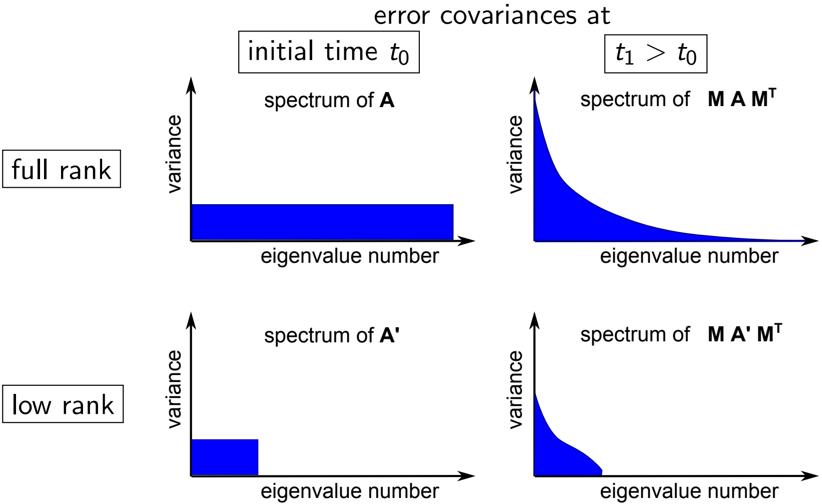

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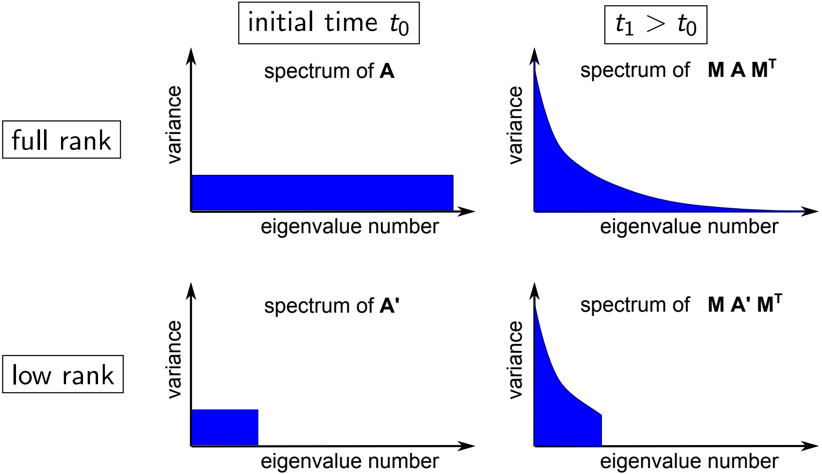


Linear and nonlinear forecast error covariance estimates

The linear estimate, as assumed in SV approach

$$\mathbf{M}\mathbf{A}'\mathbf{M}^{\mathrm{T}}$$

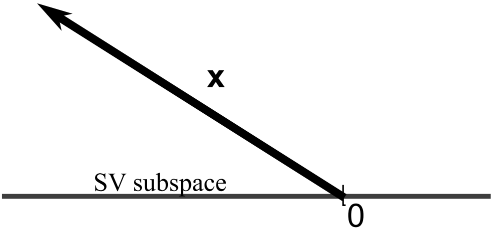
The non-linear estimate as used in practice with ensembles (N members)

$$(N-1)^{-1}\sum_{k=1}^{N}\left[\mathcal{M}(\mathbf{x}_k)-\overline{\mathcal{M}(\mathbf{x}_\cdot)}\right]\left[\mathcal{M}(\mathbf{x}_k)-\overline{\mathcal{M}(\mathbf{x}_\cdot)}\right]^{\mathrm{T}}$$

- the two estimates will differ unless nonlinear model $\mathcal{M}$ and TL model $\mathbf{M}$ are identical
- focus on the nonlinear estimate (will return to linear estimate later)

Is ensemble variance in SV subspaces matching actual error variances?

verification of forecast valid at t_1 and initialized at t_0 using SVs that grow from t_0 to t_1.



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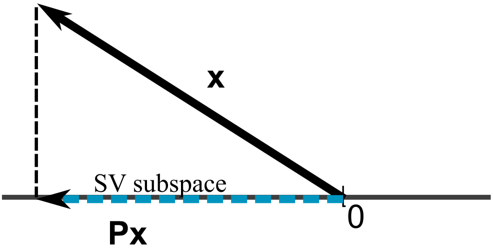

- define operator **P** that projects on the subspace spanned by the evolved SVs (valid at t_1).
- **x**: error of ensemble mean or one of the perturbations about ensemble mean
- compute variance of error and ensemble variance

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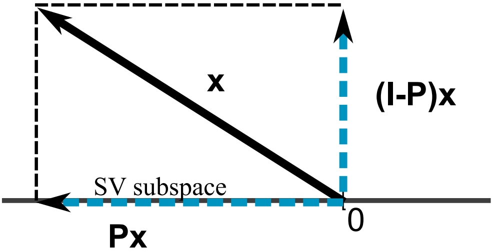

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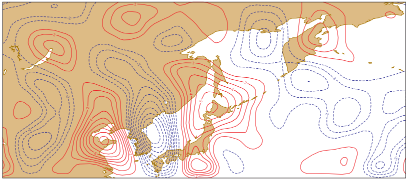
Projection example

48-hour ens. mean error: 200–500 hPa meridional wind

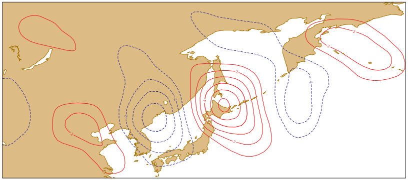
full error

error ensemble mean



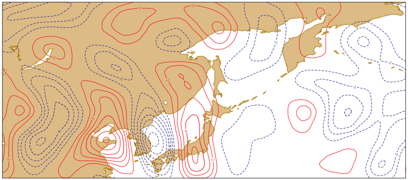
subspace of leading SVs

error ensemble mean



orthogonal complement

error ensemble mean

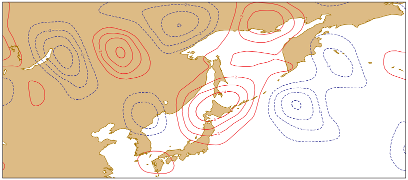


Projection example

48-hour perturbation member 2: 200–500 hPa meridional wind

full perturbation

perturbation member 2



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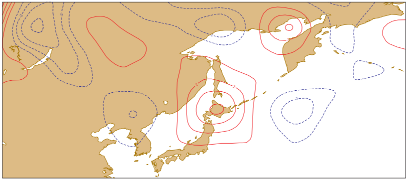

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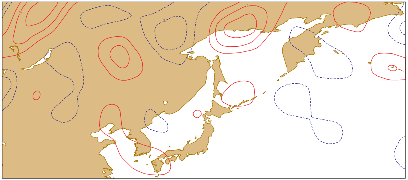

Variances in subspace S

Ensemble variances and mean squared errors computed with

$$\|\mathbf{x}\|^2 = \mathbf{x}^{\mathrm{T}}\,\mathbf{E}_1\mathbf{x} \tag{1}$$

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Compare ensemble variance in subspace V_{ens} with mean squared error of ensemble mean ("error variance") V_{err}:

$$V_{\mathrm{ens}}[S] = \left\langle \frac{1}{M}\sum_{k=1}^{M} \left\| \mathbf{P}_S \mathbf{L}_D \left(\mathbf{x}_k - \bar{\mathbf{x}}\right) \right\|^2 \right\rangle \tag{2}$$

$$V_{\mathrm{err}}[S] = \left\langle \left\| \mathbf{P}_S \mathbf{L}_D \left(\bar{\mathbf{x}} - \mathbf{y}\right) \right\|^2 \right\rangle \tag{3}$$

- M members $\mathbf{x}_k$, ens. mean $\bar{\mathbf{x}}$ and analysis $\mathbf{y}$
- subdomain D and localization operator $\mathbf{L}_D$
- subspace S and orthogonal projection $\mathbf{P}_S$ into S
- sample mean $\langle \quad \rangle$

ECMWF

Singular vectors

The initial SVs $\mathbf{v}_j$ and singular values $\sigma_j$are solutions of

$$\mathbf{M}^{\mathrm{T}}\mathbf{L}_D^{\mathrm{T}}\mathbf{E}_1\mathbf{L}_D\mathbf{M}\mathbf{v}_j = \sigma_j^2\mathbf{E}_0\mathbf{v}_j \tag{4}$$

- $\mathbf{M}$ propagator from t_0 to t_1
- $\mathbf{E}_0$, $\mathbf{E}_1$ symm. pos. def. matrix; initial and final metric
- $\mathbf{E}_0^{-1}$ and $\mathbf{M}\mathbf{E}_0^{-1}\mathbf{M}^{\mathrm{T}}$ are the analysis error and forecast error covariance matrices assumed in SV computation

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Define subspace basis vectors and projections with evolved, localized and normalized SVs:

$$\mathbf{w}_j = \sigma_j^{-1}\mathbf{L}_D\mathbf{M}\mathbf{v}_i \quad \text{which are the leading eigenvectors of} \tag{5}$$

$$\mathbf{C}_1 = \mathbf{E}_1^{1/2}\mathbf{L}_D\ \mathbf{M}\mathbf{E}_0^{-1}\mathbf{M}^{\mathrm{T}}\ \mathbf{L}_D^{\mathrm{T}}\mathbf{E}_1^{1/2}$$

The projection operator

For a singular vector subspace

$$S(\mathcal{J}) = \operatorname{span}\{\mathbf{w}_j \mid j \in \mathcal{J}\}$$

the orthogonal projection of a vector $\mathbf{x}$ into S is given by

$$\mathbf{P}_{S(\mathcal{J})}\mathbf{x} = \sum_{j \in \mathcal{J}} \mathbf{w}_j \underbrace{\mathbf{w}_j^{\mathrm{T}} \mathbf{E}_1 \mathbf{x}}_{\equiv \alpha_j(\mathbf{x})}$$

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The squared norm of the projection in S can be expressed as

$$\left\|\mathbf{P}_{S(\mathcal{J})}\,\mathbf{x}\right\|^2 = \sum_{j\in\mathcal{J}} \sum_{k\in\mathcal{J}} \alpha_j(\mathbf{x})\alpha_k(\mathbf{x})\mathbf{w}_j^{\mathrm{T}} \mathbf{E}_1 \mathbf{w}_k = \sum_{j\in\mathcal{J}} \alpha_j^2(\mathbf{x})$$

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Variances are additive for mutually orthogonal subspaces

$$V\left[S_1 + \cdots + S_K\right] = \sum_{j=1}^{K} V\left[S_j\right]$$

$$V\left[\text{full space}\right] = V\left[S\right] + V\left[\text{orth. compl. of } S\right]$$

Spaces

space	notation
$\mathcal{J} = \{1, 2, \ldots, 10\}$	SV1–10
$\mathcal{J} = \{1, 2, \ldots, 50\}$	SV1–50
$\mathcal{J} = \{96, 97, \ldots, 100\}$	SV96–100
$\mathcal{J} = \{101, 102, \ldots, N\}$	C(SV1–100)
	orthogonal complement of SV1–100

N is the dimension of the SV state space.

For an isotropic distribution in the space of the initial SVs, the ensemble variance in the direction of j-th SV scales as

$$V_{\mathrm{ens}}(\mathrm{SV}\, j) \propto \sigma_j^2$$

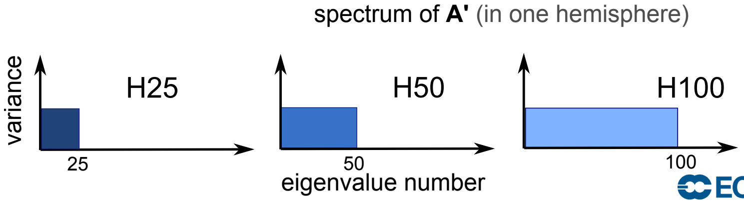
if perturbations are evolved with the TL-model.

Experiment setup

singular vectors

- TL159 singular vectors
- 48-hour opt. time; $\mathbf{E}_0$, $\mathbf{E}_1$ total energy
- moist processes represented in TL
- initial uncertainties represented by
    - leading 25 SVs in each hemisphere (H25)
    - leading 50 SVs in each hemisphere (H50)
    - leading 100 SVs in each hemisphere (H100)
- leading 100 SVs in each hem. used for the diagnostics

Assumed reduced rank analysis error covariance matrices

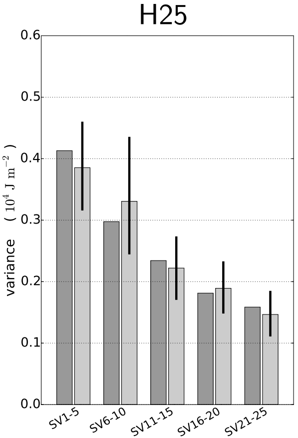


Experiment setup

ensemble forecasts

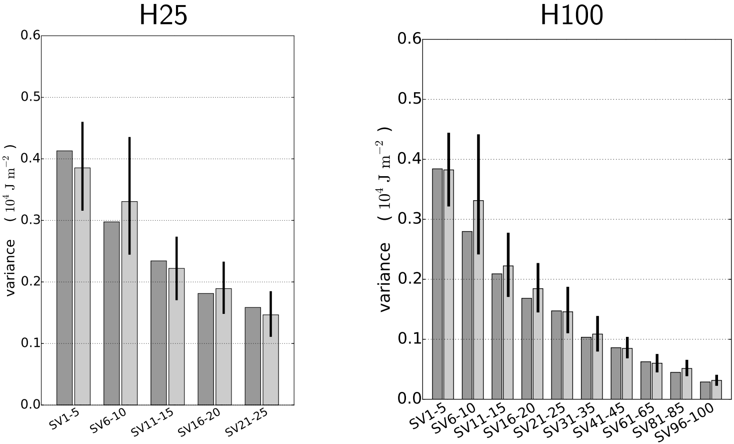
- T_L639 ensembles ($\Delta x = 32\,\mathrm{km}$)
- 50 members
- 20 start dates
- only initial uncertainties represented with SVs
- singular vectors sample isotropic Gaussian distribution in space spanned by initial singular vectors
- reliable variances can be obtained in a particular SV subspace by adjusting variance of initial perturbations
- for 3 experiments H25, H50, H100 variance of init. pertns. is set so that error variance matches ensemble variance in space SV1–25.

Variance “spectra”



dark grey: variance of nonlinear ens. perturbations projected into SV spaces
light grey: RMS of ensemble mean error projected into SV spaces
bars: 95% confidence interval of difference of ens. and err. variances

Variance "spectra"



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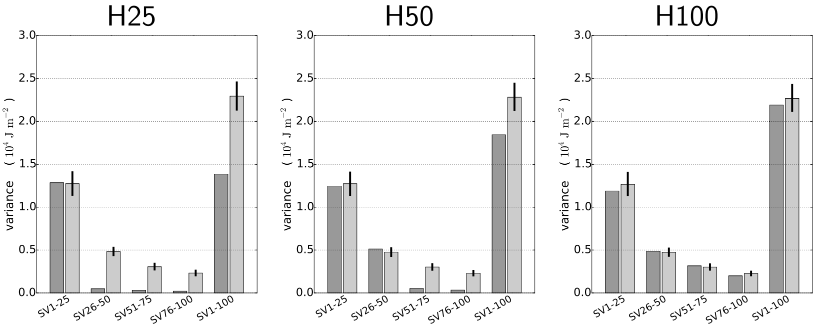
Different ranks of the assumed analysis error covariance



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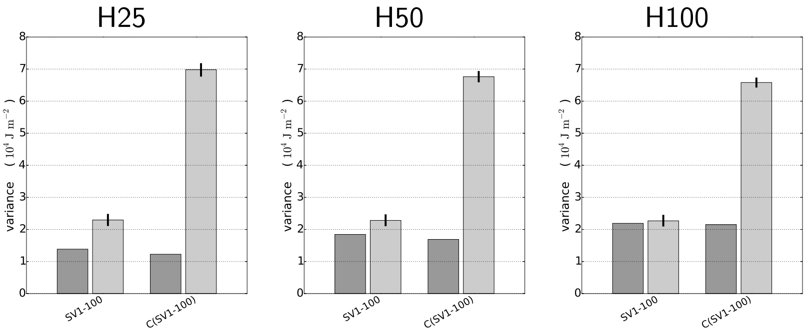
Orthogonal complement subspaces



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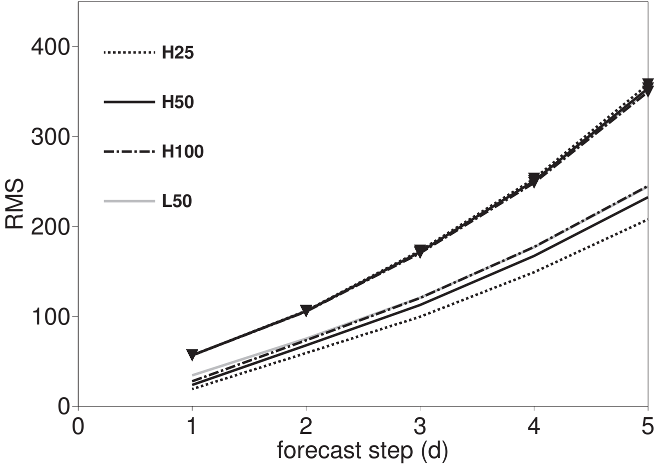
NH (20°N–90°N) spread and RMSE

500 hPa geopotential



Lines with symbols: RMSE of ensemble mean
Lines without symbols: Ensemble standard deviation

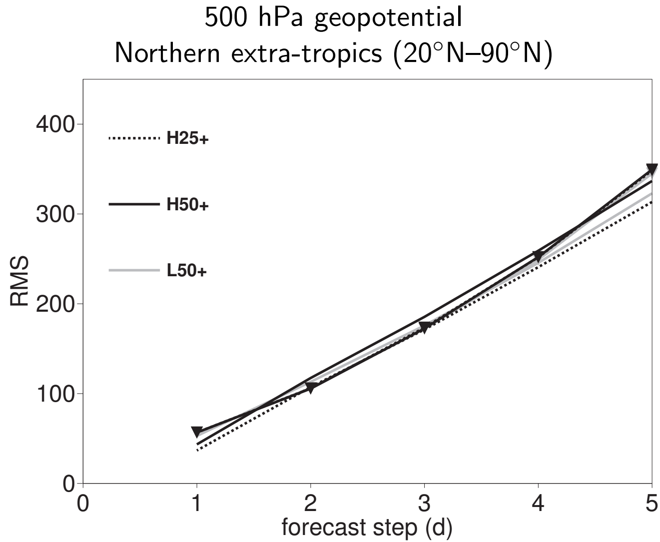
ECMWF

Scaling of analysis error standard deviation

- In past, the amplitude of the singular vector initial perturbations used to be adjusted so that the domain averaged ensemble variance matches the mean squared error (e.g. for Z500 in the extratropics).
- What are the implications? $\rightarrow$ additional experiments H25+ and H50+ with inflated initial perturbation amplitude
- The standard deviation of the initial singular vector perturbations is proportional to a scaling parameter γ

Exp.	N_{SV}	γ_{NH}	γ_{SH}
H25	25	0.0048	0.0051
H25+	25	0.0095	0.0092
H50	50	0.0048	0.0051
H50+	50	0.0091	0.0089
H100	100	0.0048	0.0051

Increased analysis error variances



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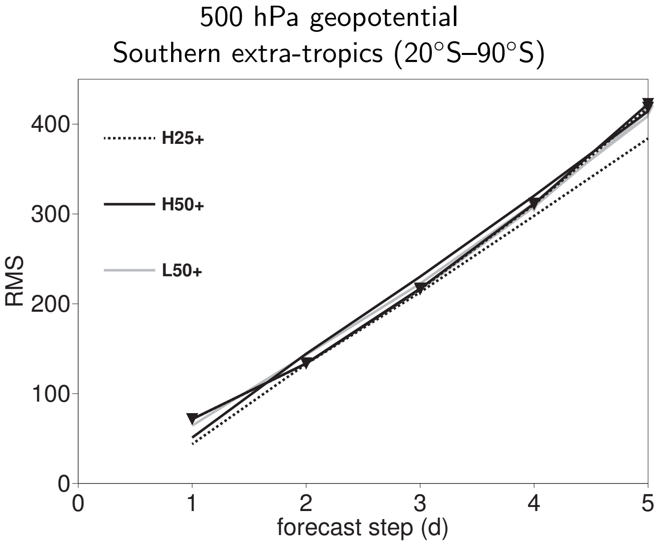
Increased analysis error variances



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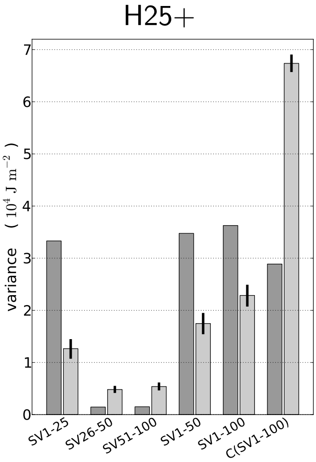
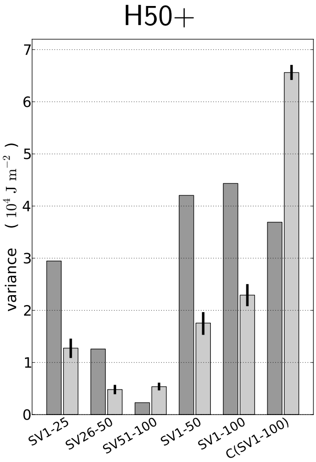
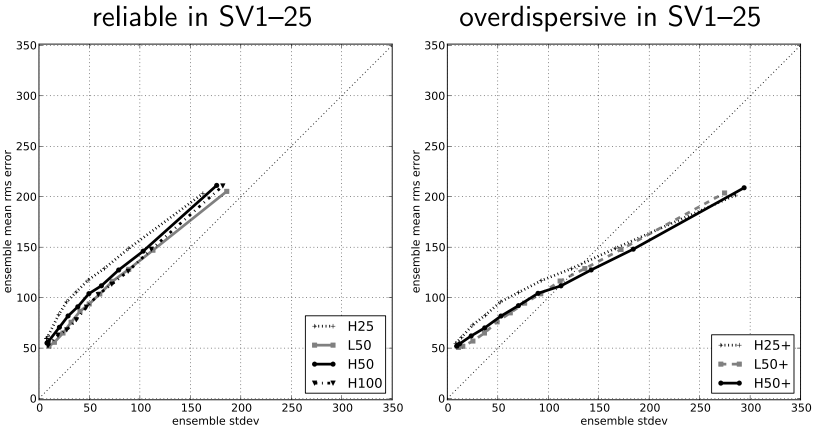
Forecast error variances

in experiments with increased analysis error variances





Local spread-reliability

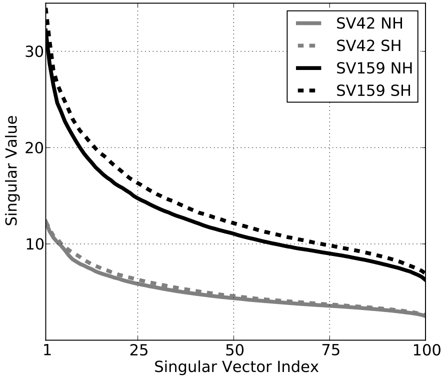


- ensemble mean error stratified by ensemble standard deviation in bins with similar spread
- 500 hPa geopotential (m^2s^{-2})
- 48-hour lead time

ECMWF

Two different SV configurations

- SV159: T_L159 resolution, moist physics included
- SV42: T42 resolution, dry physics (vertical mixing only)
- Ensemble experiment H50 uses leading 50 SV159 SVs
- Ensemble experiment L50 uses leading 50 SV42 SVs

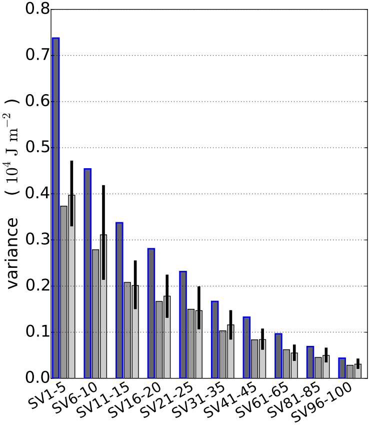


Linearisation errors

- RMS of linearisation error in subspace of SV42 SVs (1st row) and in subspace of SV159 SVs (2nd row)
- evaluated for finite amplitude perturbations of experiments L50 (1st column) and H50 (2nd column)
- quantified with $\mathbf{E}_1$ norm $\| \, . \, \|$
- normalized by RMS of linearly evolved initial perturbations

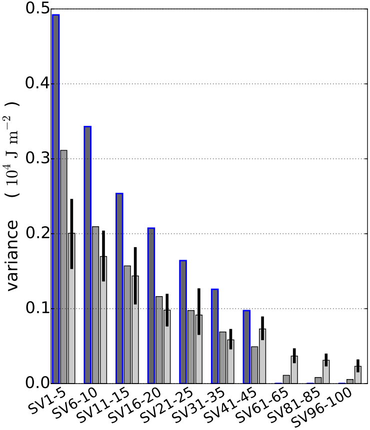
	Ensemble	
subspace	L50	H50
SV42	0.48	2.34
SV159	0.40	0.44

Linear (left/blue) versus nonlinear (middle) forecast error variance prediction



- Exp. H100
- Variances in subspaces of SV159

Linear (left/blue) versus nonlinear (middle) forecast error variance prediction



- Exp. L50
- Variances in subspaces of SV42

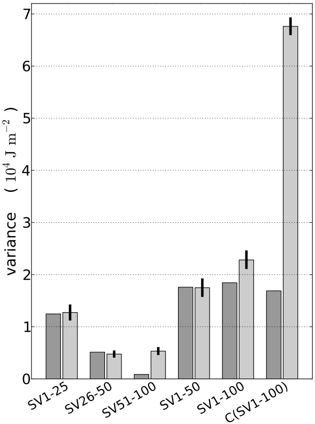
Improved reliability through use of a more accurate TL approximation?

Compare variances in subspaces of SV159 for experiments with initial perturbations based on

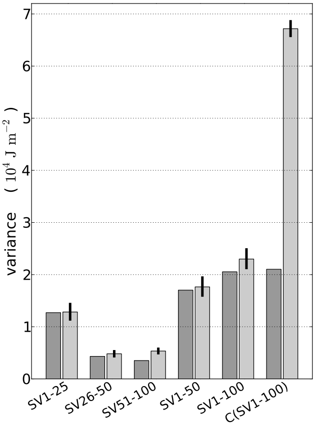
- SV42 (L50)
- SV159 (H50 and H100)

Variances in subspaces of SV159

H50 (SV159 init. pertns.)

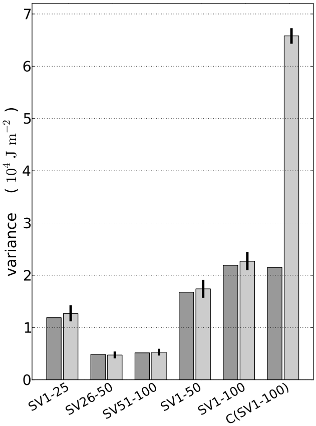


L50 (SV42 init. pertns.)

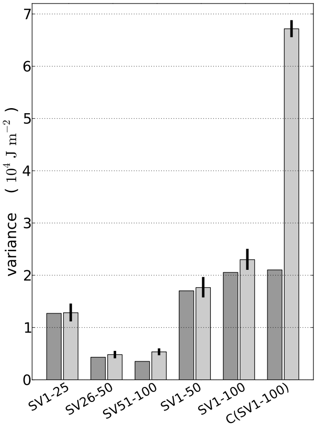


Variances in subspaces of SV159

H100 (SV159 init. pertns.)



L50 (SV42 init. pertns.)



The operational ECMWF ensemble

The full representation of uncertainties consists of

- SVs (T42 dry TL-model)
- EDA (TL399)
- representations of model uncertainties (SPPT, SKEB)

The operational ECMWF ensemble

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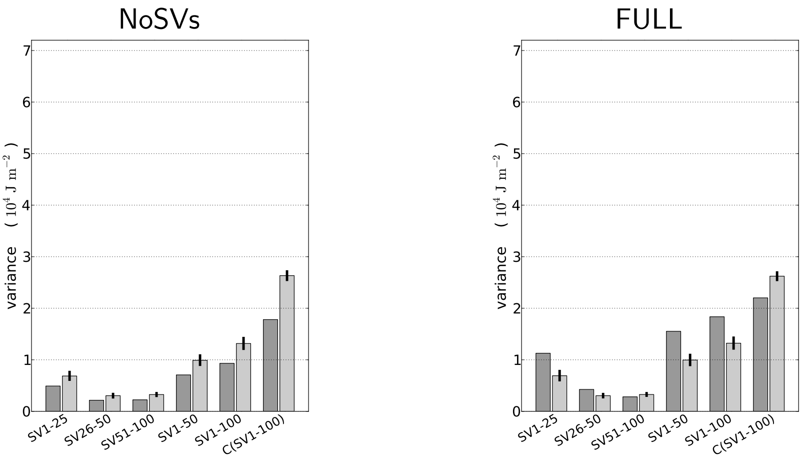
What happens to reliability of variances in SV subspaces if one suppresses SV initial perturbations in ensemble (FULL $\rightarrow$ NoSVs)?

Is there significant variance generated in the subspace of the leading SVs by the EDA initial perturbations and the representations of model uncertainties?

Impact of omitting singular vectors



Potential merit of modifying the SV configuration in the operational ENS

- T42 dry TL model $\longrightarrow$ TL95 moist TL model
- 50 $\longrightarrow$ 150 leading SVs

initial evaluation

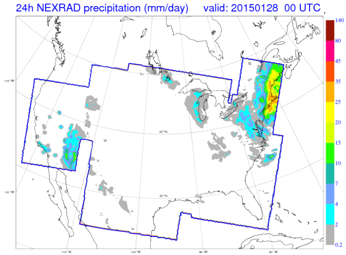
- A case study: US East Coast snow storm 27 January 2015
- Variances in SV subspaces (consistently evolved with same TL model: TL255 moist)

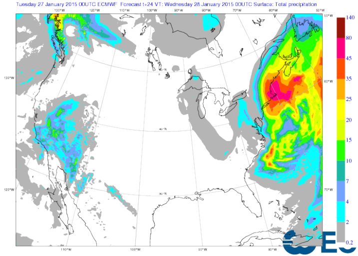
US East Coast blizzard

27/28 January 2015

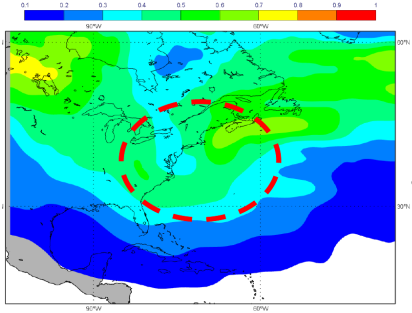
- worst affected areas were in a band from Long Island towards Boston and further north
- storm was expected to also hit New Jersey and New York City and strong actions were taken before the event
- NYC only got a little snow
- ECMWF model gave strong indication for severe snow over NYC

Acknowledgments: Linus Magnusson





Vertically integrated total energy of evolved SVs

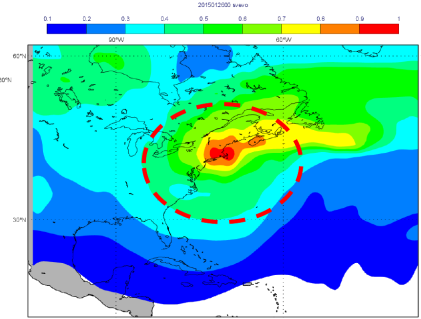


50 dry T42 evolved SVs

2015012600+48h

Normalised vertically integrated total energy: vte=vte/vte_max (global max)

150 moist TL95 evolved SVs



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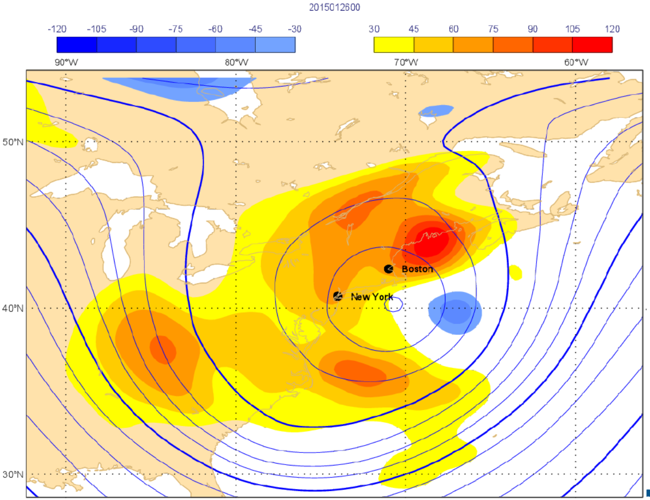
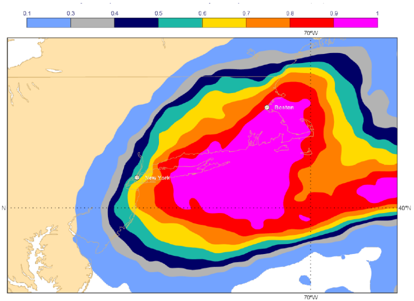
Change in ensemble spread (Z500)

2015012600+48h z500hPa spread differences : 150 TL95 SVs – 50 T42 SVs



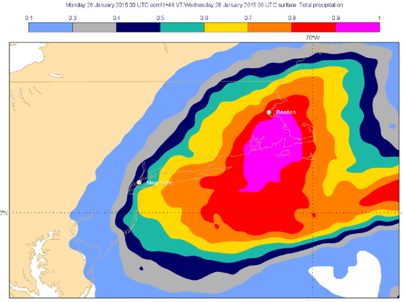
Probability of precipitation

2015012600 + 48h - Probability 24h acc precipitation > 30 mm



ENS with 50 dry T42 SVs

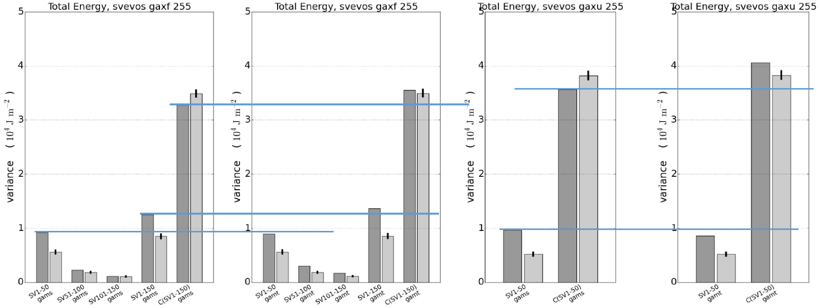
ENS with 150 moist TL95 SVs



Variances in SV subspaces

subspaces defined with

⟵ TL95 moist singular vectors ⟶ ⟵ T42 dry singular vectors ⟶



initial pertns.	T42 dry SVs	TL95 moist SVs	T42 dry SVs	TL95 moist SVs

- for diagnostic, all subspaces evolved with moist TL255 TL model
- 35 cases in boreal winter
- dark grey: ensemble variance, light grey: error variance

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Summary: rank reduction, amplitude

- An isotropic Gaussian distribution in the space of the leading singular vectors can
  - reliable represent forecast errors in the space spanned by the SVs used for the representation of initial uncertainties
  - not reliable represent forecast errors in the orthogonal complement of this space
- Inflating the singular vector perturbations in order reach reliable variances in full space leads to
  - pronounced overdispersion in space of leading SVs, i.e. lack of reliability
  - still not enough spread in the orthogonal complement
- Having used an initial time metric based on a simple approximation of the analysis error covariance matrix (total energy) did not hamper the reliability

Summary TL approximation

- Tangent-linear prediction of forecast error variances predicts systematically larger variances in subspaces of leading SVs than non-linear model
  - Reliable variance prediction with nonlinear model $\Rightarrow$ overdispersion with TL prediction
  - TL approximation errors lead to significant amount of variance leaking into orthogonal complement of leading SV subspace (may be beneficial for ensemble prediction)
- Initial perturbations based on SVs computed with less accurate TL model can generate about the right amount of overall variance in subspaces of SVs computed with a more accurate TL model (The two sets are not orthogonal.)
- However, SV159 SVs show more consistent reliability across spectrum of SVs while SV42 SVs exhibit overdispersion for leading 5–10 SVs while reliable for slower growing SVs

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Summary operational EPS configuration

- EDA initial perturbations and the model error representation generate a significant amount of ensemble spread in the space spanned by the leading 50 T42 extra-tropical SVs
- SVs are still justified to boost spread to the right level in subspace of leading SVs
- The diagnostic based on SVs can be used to decide when SV initial perturbations are inadequate
- Improving the operational ENS configuration may be possible through
  - further reduction in amplitude of SV perturbations
  - increasing the number of SVs used to define the initial perturbations
  - use of a more accurate TL approximation

see also Leutbecher and Lang (2014, QJ)

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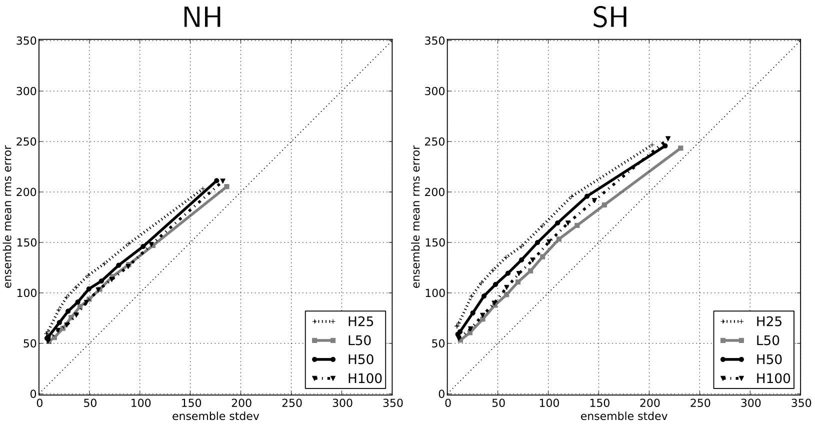
Discussion

As usual, more open questions than answers.

How would conclusions be affected by

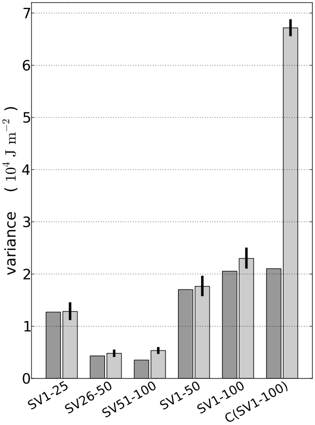
- bias: RMS error versus error variance
- analysis uncertainties
- domain size and number of SVs required to explain certain fraction of fc error variance
- initial time metric (proxy for $\mathbf{A}^{-1}$)
  - flow-dependent variations
  - fraction of fc error variance
- optimisation time
  - steepness of singular value spectrum
  - accuracy of TL approximation
- link to ensemble covariance EOF-based diagnostics

Local spread reliability again

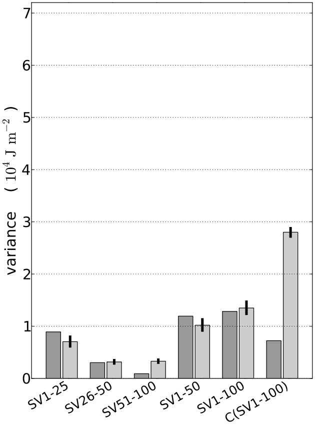


Using diagnostics for subspaces computed with different SV configurations

SV159 spaces



SV42 spaces



Experiment L50: Analysis error representation with SV42 SVs for both