

Error correlations and hyperspectral sounders

Fiona Smith, Bureau of Meteorology



Thank you to my co-authors and contributors

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- JMA Toshiyuki Ishibashi, Kozo Okamoto
- NRL Bill Campbell
- Met Office Chawn Harlow, Ed Pavelin, Fabien Carminati, Jemima Tabeart*
- ECMWF Niels Bormann, Marco Matricardi, Kirsti Salonen, Alan Geer, Reima Eresmaa*
- ECCC Sylvain Heilliette
- Meteo-France Nadia Fourrié, Vincent Guidard
- DWD Silke May, Olaf Stiller
- Old-KIAPS Hyong-Wook Chun
- EUMETSAT Tim Hultberg
- NCEP Kristin Bathmann

... and their colleagues who contributed too!

... and others whose work I am presenting without having asked (Pete Weston and Chris Burrows!)

* now moved on to pastures new

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Overview

- Quick look at current status
 - A look at the error correlations used
 - Impact of introducing correlated errors
- The main part of the talk
 - Methods used for estimation of error correlations
 - Justification for shrinkage and variance inflation
- Where is the research headed?
 - Reconstructed radiances
 - Situation-dependent errors
- Bonus slides for later
 - Alternative approach physical error model more work needed?
 - How to estimate errors for channel selection purposes where Desroziers assumptions fail



Status of use of error correlations for hyperspectral sounders



Operational error covariances

- What do the correlations look like?
 - Consistent between centres?
 - Consistent between instruments?
- What does the consistency (or lack of) tell us about the sources of correlation
- Mostly IASI and CrIS as the main instruments in use
 - Also AIRS, HIRAS, IKFS-2, GIIRS



All the following slides show correlation matrices

(Centres all use different channel selections)

IASI on the left

CrIS on the right



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Meteo-France

0.6 0.8 1.0 0.2 0.4 0.6 0.0 0.8 0.4 0.2 1.0 Т L I. 120 100 80 **IASI** channels 60 40 Nater vapour emperature 20 ace Ozone 0 0 20 40 60 80 100 120



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Ishibashi, T., 2020: DOI: 10.1175/MWR-D-19-0269.1





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Summary of centre comparison

- Diagnosed correlation structures for IASI and CrIS have a lot in common regardless of which model is used.
- Correlations are stronger in surface channels, and stronger again between water vapour channels
- Difference in behaviour of the ozone channels between the Météo-France and ECMWF models?
- The IASI observation error is diagonally dominant for the temperature sounding channels
- CrIS temperature sounding channel errors are more correlated than IASI
 - Instrument noise is lower; other sources of error with higher levels of correlation dominate
- CrIS shows more correlation between adjacent channels
 - Collard* channel selection for IASI avoided spectrally adjacent channels to reduce correlation

*Collard AD. 2007. Selection of IASI channels for use in numerical weather prediction. Q. J. R. Meteorol. Soc. 133: 1977–1991



Meteo-France vs ECMWF Ozone

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Comparisons of different sounders

- Different sounders have quite different diagnosed correlations
- Points to different sources of error dominating for each instrument
- All instruments show strong correlations for water vapour channels
- Strength of correlation for temperature sounding channels tends to be inversely related to the measurement error variance

Error correlation matrices for hyperspectral IR instruments



EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS



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CrIS FSR vs HIRAS – Full spectrum Bands 1&2 Fabien Carminati – Met Office





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Different instrument noise -> different correlations in diagnosed matrices

The standard deviation of O-B for the 15 micron CO₂ band is dominated by measurement error





Impact of introducing correlated errors



JMA results Ishibashi, T., 2020: DOI: 10.1175/MWR-D-19-0269.1

Forecast RMSE improvement rate (%) for temperature in global average.





NWP errors were significantly reduced by error covariance matrix improvement of

- Introducing Inter-channel error correlations of all radiances
- Refined observation error variances of all observations
 Refined background error variances

Impact at ECMWF when observation error covariance was first introduced for IASI





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NRL – Impact of correlated error for IASI + ATMS Right columns include Desroziers-derived error variances

Impact: SH, Temp (%)

mpact: SH, Vec-Wind (%)

Impact: SH, Geo-Pot H. (%

2 3 lead time (days)

NH



Campbell et al., 2017 https://doi.org/10.1175/MWR-D-16-0240.1



Met Office implementation of correlated error for IASI

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Summary of impact

Basically, all centres have reported positive impact from introduction of correlated errors for hyperspectral sounders...

... but definitely a need to tune those inflation factors!



Covariance estimation



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Process of covariance estimation

- How do centres estimate their covariance matrices?
- What do the observation error variances look like?
- The fudge factor a.k.a. error variance inflation

Error covariance for first 120 AIRS channels from 324 channel subset. From Collard et al., 2010 <u>https://rmets.onlinelibrary.wiley.com/doi/full/10.1002/qj.701</u>





Method for estimation of error covariances

- Every centre who replied uses a matrix derived using the Desroziers* method for operational covariance estimation.
- Every centre performs operations to improve the condition number of the resultant matrix
- Every centre inflates the observation error variance

* Desroziers G, Berre L, Chapnik B, Poli P. 2005. Diagnosis of observation, background and analysis-error statistics in observation space. Q. J. R.Meteorol. Soc. 131: 3385–3396.



Methods differ in the details but generally similar

- Start with an initial estimate of errors
 - Diagonal
 - Hollingsworth-Lönnberg
 - Desroziers from 1D-Var
 - Possibly multiply by a scaling factor
- Output diagnostics to allow estimation of covariances using Desroziers method
- Symmetrise Desroziers matrix
 - Covariance or correlation
- Inflate error variance
 - Spectrally variant or invariant multiplicative factor
 - Additive factor (see next step)
- Manipulate covariance matrix to improve conditioning
 - Adjust smallest eigenvalues to reduce spread ("shrink" matrix)



Observation error variances

- Initial estimated errors from Desroziers are usually much smaller than previously used uncorrelated error variances
- Often lie somewhere between the observed SD(O-B) and instrument noise (right)
- Can occasionally be "too small" – below NEDT
- Iterating Desroziers technique can have varying success

Plot from Coopmann et al., 2020: https://doi.org/10.5194/amt-13-2659-2020





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Operational obs error estimation methods

Centre	Shrinkage Method	Inflation	Condition number	
Met Office + UM Partners	Add constant to all eigenvalues	Effectively: IASI T ~1.5, W.V. ~1.1	IASI 67	
NRL	Add constant to all eigenvalues	IASI: T 1.65, WV 1.9	IASI 169	
ECMWF	Increase small eigenvalues	IASI: 1.75 CrIS: 2.75	IASI 131 CrIS 4075	
Meteo-France		IASI: 2.0		
NCEP	Increase small eigenvalues to condition number IASI: 200 CrIS: 125	T 1.6, WV 1.3, Window 1.8*	IASI 93 CrIS 53	
DWD	Increase small eigenvalues	IASI: 1.75		
JMA		1.7**		
ECCC	Ensure positive definite	1.6		

* NCEP find that stricter cloud detection is necessary to get good results with correlated error covariances ** JMA justify their inflation with a corresponding deflation of background error by the equivalent factor (1/1.7)



Environment Canada - diagnosed errors for IASI







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Fabien Carminati – experiments with CrIS FSR conditioning





CrIS FSR

N320L70 UM, N108/N216L70 hybrid 4DVar, coupled hybrid N216L70 44m/9h ensemble forecasts September 2020 configuration

Verification against EC analyses.

Period of study so far: 14 days (18/09-01/10 2020).

3 different inflations:

- R1000 (left)
 - \circ condition number = 1000
 - \circ inflation = diagonal +
 - ~0.028
- R250 (middle) •
 - condition number = 250 0
 - inflation= diagonal +
 - ~0.113
 - R100 (right)

•

- \circ condition number = 100
- inflation = diagonal + 0 ~0.28

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Justification for shrinkage and error inflation



What did contributors say?

- Varied statements regarding justification for shrinkage and error inflation
- Most view the process pragmatically
 - A process that must be done to make 4D-Var work effectively
 - Reduce iterations
 - Improve forecast benefit
- Some feel the justification is physical
 - Accounting for errors that are not diagnosed properly by the Desroziers method
 - E.g. quality control problems
 - More on this from Alan Geer's talk on all-sky assimilation
- Some mathematical justification
 - Large body of work on covariance estimation especially in biostatistics and finance


Mathematical Justification for Shrinkage

- The estimation of error covariances is inherently "overdispersed"
 - The largest eigenvalues are over-estimated, and the smallest ones are underestimated
 - Covariance matrices perform better if they are "shrunk" i.e. all eigenvalues are brought towards the mean
- Effron and Morris (1977): <u>https://statweb.stanford.edu/~ckirby/brad/other/Article1977.pdf</u>
- Daniels and Kass (2001): <u>https://onlinelibrary.wiley.com/doi/abs/10.1111/j.0006-341X.2001.01173.x</u>



Stein's Paradox in Statistics

The best guess about the future is usually obtained by computing the average of past events. Stein's paradox defines circumstances in which there are estimators better than the arithmetic average

by Bradley Efron and Carl Morris

Sometimes a mathematical result is strikingly contrary to generally held belief even though an obviously valid proof is given. Charles Stein of Stanford University discovered such a paradox in statistics in 1955. His result undermined a century and a half of work on estimation theory. going back to Karl Friedrich Gauss and Adrien Marie Legendre. After a long period of resistance to Stein's ideas, punctuated by frequent and sometimes angry debate, the sense of paradox has diminished and Stein's ideas are being incorporated into applied and theoretical statistics.

jor-league players as they were recorded after their first 45 times at bat in the 1970 season. These were all the players who happened to have batted exactly 45 times the day the data were tabulated. A batting average is defined, of course, simply as the number of hits divided by the number of times at bat; it is always a number between 0 and 1. We shall denote each such average by the letter y.

The first step in applying Stein's method is to determine the average of the averages. Obviously this grand average, which we give the symbol \overline{y} , must also lie between 0 and 1. The essential procfactor c is .212. Substituting these values in the equation, we find that for each player z equals .265 + .212(\overline{y} - .265). Because c is about .2, each average will shrink about 80 percent of the distance to the grand average, and the total spread of the averages will be reduced about 80 percent.

As an example consider the late Roberto Clemente, who was the leading batter in the major leagues when our statistics were compiled. For Clemente y is equal to .400, and z can be determined by evaluating the expression z = .265 + .212(.400 - .265). The re-



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Steinian Shrinkage



JAMES-STEIN ESTIMATORS for the 18 baseball players were calculated by "shrinking" the individual batting averages toward the overall "average of the averages." In this case the grand average is .265 and each of the averages is shrunk about 80 percent of the distance to this value. Thus the theorem on which Stein's method is based asserts that the true batting abilities are more tightly clustered than the preliminary batting averages would seem to suggest they are.



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JOURNAL ARTICLE Shrinkage Estimators for Covariance Matrices

Michael J. Daniels and Robert E. Kass

Biometrics

Vol. 57, No. 4 (Dec., 2001), pp. 1173-1184 (12 pages) Published By: International Biometric Society

https://www.jstor.org/stable/3068250

Cite this Item

We consider here two general shrinkage approaches to estimating the covariance matrix and regression coefficients. The first involves shrinking the eigenvalues of the unstructured ML or REML estimator. The second involves shrinking an unstructured estimator toward a structured estimator. For both cases, the data determine the amount of shrinkage. These estimators are consistent and give consistent and asymptotically efficient estimates for regression coefficients. Simulations show the improved operating characteristics of the shrinkage estimators of the covariance matrix and the regression coefficients in finite samples. The final estimator chosen includes a combination of both shrinkage approaches, i.e., shrinking the eigenvalues and then shrinking toward structure.



Which method is more justifiable?

- Some like the idea that increasing smallest eigenvalues is essentially Ky Fan p-k norm covariance adjustment
 - Tanaka and Nakata (2013) https://link.springer.com/article/10.1007/s11590-013-0632-7
 - "Positive definite matrix approximation with a condition number constraint is an optimization problem to find the nearest positive definite matrix whose condition number is smaller than a given constant."
- Adding a constant to the eigenvalues is effectively Steinian shrinkage
 - Ledoit and Wolf (2004) <u>https://www.sciencedirect.com/science/article/pii/\$0047259X03000964?via%3Dihub</u>
 - "This paper introduces an estimator that is both well-conditioned and more accurate than the sample covariance matrix asymptotically. This estimator is distribution-free and has a simple explicit formula that is easy to compute and interpret. It is the asymptotically optimal convex linear combination of the sample covariance matrix with the identity matrix."



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Effect of Steinian shrinkage on correlation structure

Weston et al., 2014 https://rmets.onlinelibrary.wiley.com/doi/epdf/10.1002/qj.2306

Observation error standard deviation Before and after reconditioning / shrinkage

Correlation Before reconditioning / shrinkage Correlation After reconditioning / shrinkage





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Which method is better? Jemima Tabeart – Poster!

• Both methods strictly increase standard deviations, inflation results in a bigger increase than changing only the smallest eigenvalues

Inflating all eigenvalues (ridge regression) strictly decreases the absolute value of off-diagonal correlations

"Changes to the analysis of data assimilation problems due to the application of reconditioning methods are likely to be highly system-dependent"





Covariance? Correlation? Inverse Covariance?

- Does it matter whether the shrinkage operation is done on the covariance or the correlation matrix?
 - Plenty of centres shrink the covariance and then inflate the diagonal as well
- Small eigenvalues matter because error covariances are used in their inverted form (R⁻¹ appears in the cost function, not R)
 - 1/ very small number = very big number
 - Think of the small eigenvalues as a mode with a very small error it's "well measured"...
 except that as it goes towards zero, you would say there is no information about it at all.
 - This is very confusing!
 - Is it better to shrink the inverse matrix?



Physical Justification for error inflation

- Most (published) thoughts on this from ECMWF
- Eresmaa et al. 2017
 - It is not fully understood why a scaling factor is needed, nor why it should be higher for CrIS than for IASI. It is our guess that the scaling compensates for sub-optimalities associated with various simplifications needed for practical reasons. These might include ignoring horizontal and temporal error correlation altogether, lack of situation dependency, mis-specification in background-error covariance, and correlation between observation and background errors. Furthermore, our interpretation is that such sub-optimalities are amplified in the case of CrIS, because the uncorrelated observation-error contribution (i.e. instrument noise) is relatively small in the overall error budget.
 - <u>https://rmets.onlinelibrary.wiley.com/doi/full/10.1002/qj.3171</u>



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- Alan Geer in context of all-sky assimilation:
 - Can get equivalent clear-sky error covariance to Desroziers*1.75 by just taking covariance of O-B departures (for water vapour channels at least)
 - Representivity error also dominates in clear sky, driven by inability of model to correctly represent inertia-gravity waves
 - Trailing eigenvectors amplify small inter-channel differences
 - If resulting from biases, these will be incorrectly amplified and generate increments that oscillate in the vertical
 - Even without bias, can amplify signals that map onto vertical temperature oscillations (gravity waves) that DA cannot properly handle



What's the difficulty with the trailing eigenvectors? Alan Geer





Amplification of oscillations in Jo



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Reconstructed Radiances

Splitting the spectrum in two (in two ways) Tim Hultberg



Only the noise orthogonal to the signal space is removed. There is no noise reduction within the signal space!



So now that I use reconstructed radiances instead of the original, I must charge my observation error covariance accordingly, right?

No! The role of the observation error covariance matrix is to assign a scalar penalty for differences between the observation vector and a forward model simulation. If we remove the orthogonal complement of the signal space from the observation vector, there is no reason to increase the penalty for deviations along these directions – in fact doing so may be harmful because it could amplify the effect of any forward model errors orthogonal to the signal space.



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Effect of PC compression on measurement error inter-channel correlations



My view: you have considerably more latitude to play games with error covariances for stand alone retrievals.

The error covariances that are used/required for NWP contain contributions from many sources of error.

At the moment, the most pragmatic way to model these is via diagnostic methods – it doesn't really matter in that case whether the correlations are from your PC compression or another source, as long as you capture them all. Failure to do so can result in undesirable oscillatory behaviour.



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Reconstructed radiance Desroziers diagnosed errors Marco Matricardi

Error correlation is diagnosed in PC space (400 PCs) then converted. The PC matrix is wellconditioned. RR matrix conditioning is improved and variances are inflated empirically with different factors for different regions





Compare with raw radiance diagnosed errors





DWD IASI correlation matrices





Situation dependent error covariances

NCEP Surface-type dependent obs errors

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Kristen Bathmann https://rmets.onlinelibrary.wiley.com/doi/10.1002/qj.3925



Error correlation matrix for IASI-A over land. Anticorrelations are between certain surface channels, and ozone channels and some surface channels sensitive to quartz, a feature not well modelled. The affected surface channels have large, negative bias over



NCEP Surface-dependent observation errors



The new observation errors compared to the orginal errors from a diagonal R matrix. These are after reconditioning and variance inflation. The six channels that have been assigned very large error over land are sensitive to quartz and have large, negative bias over deserts.



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Meteo-France – model configuration dependent errors





Met Office All-sky error characterisation Ed Pavelin

Desroziers-diagnosed correlations corresponding to scenes broadly classified as clear sky, moderately cloudy and very cloudy (based on the the cloud radiative effect in one window channel), diagnosed from all-sky 1D-Var retrievals.

Correlations increase as a function of "cloudiness", presumably in response to increasing forward model error (also probably a contribution from inaccuracies in the B-matrix).

It is likely that it will be necessary to find ways of representing cloud-dependent observation error correlations in all-sky assimilation, instead of just varying the observation errors as we do currently.





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ECMWF All-sky error characterisation Kirsti Salonen

Alternative approach to classifying error, this time by cloud height.

See Kirsi's poster



0.4

0.3

0.2

0.1

-0.1

662





- Everyone estimates full error covariance in brightness temperatures not radiances
- Measurement errors for interferometers (CrIS, IASI) are constant with respect to scene temperature in radiance space
 - Should we do something about that?
 - Has anyone tried to assimilate radiances? Would it make a difference?



Summary



- Most centres are using correlated errors for hyperspectral sounders in operations
- Everyone uses Desroziers!
- Everyone does some manipulation to the output
- Justifications for this manipulation vary
- Results are surprisingly consistent between centres
- Not much research into improving these error estimates has happened
- Some moves towards scene-dependent errors
 - Surface differentiation
 - Cloud effects
- Reconstructed radiances have different error properties, but essentially the same methods can be used



Physical Modelling of error terms





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Physical model

Desroziers



Physical model error components H-W Chun

Imperfect cloud detection

Forward model error includes regression error and fast vs LBL errors

Representativeness error















Observation errors for channel selection


Observation errors for channel selection

- Desroziers assumes that you are assimilating the channels for which error covariances are estimated
- What do you do if you want to do a channel selection? You need observation errors for the full spectrum
 - Use the Hollingsworth-Lönnberg¹ method
 - Use O-B only; assumes zero separation between observations
 - Use a 1D-Var and use "Obs minus Retrieval" to provide the "Obs minus Analysis" statistics
 - Different behaviour using 1D-Var (Stewart et al, 2013)²

¹Hollingsworth A, Lönnberg P. 1986. The statistical structure of short-range forecast errors as determined from radiosonde data. Part 1: The wind field. Tellus 38A: 111–136.

²Stewart, L.M., Dance, S.L., Nichols, N.K., Eyre, J.R. and Cameron, J. (2014), Estimating interchannel observation-error correlations for IASI radiance data in the Met Office system⁺. Q.J.R. Meteorol. Soc., 140: 1236-1244. doi:10.1002/qj.2211



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Estimation of CrIS FSR observation error covariance from 1D-Var Fabien Carminati

Correlation matrix





1o standard deviation in the C-B





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Observation error covariance matrix



Causing a drift of diag(R) to unreliable values when iterating on Desroziers diagnostic.

Successive iterations of Desroziers *increases* the estimate of observation error towards the clearly erroneous values in the window region



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Improving quality control essentially solves this problem

With improved QC ... but it keeps increasing with the iterations!





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Desroziers estimation of IASI errors from 1D-Var Chawn Harlow



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First and Second Desroziers Iterations – IASI from 1D-Var

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Choice of resolution is important (Weston et al., 2014)

Correlation matrix of the difference in diagnostic IASI error covariance matrices from 4D-Var output run at N216 and N48 resolutions





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4D-Var vs 1D-Var – how much is background error? Stewart, 2013 <u>https://rmets.onlinelibrary.wiley.com/doi/full/10.1002/gj.2211</u>

0.75

0.5

0.25

-0.25

-0.5

-0.75

0





1D-Var Desroziers

4D-Var Desroziers



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4D-Var vs 1D-Var – WV channels only

-0.25

-0.5

Stewart, 2013 https://rmets.onlinelibrary.wiley.com/doi/full/10.1002/qj.2211





1D-Var Desroziers

4D-Var Desroziers