A global-local hybrid approach to retain new signals in hyperspectral PC products

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• **Strategies for retaining new signal:**
  1. Retain the original (raw) spectra for outliers (i.e. spectra for which signal orthogonal to the PC signal space can be detected)
  2. Compute local PCs for each granule/PDU/dwell/…
  3. Take a hybrid approach. First compute PC scores based on global PCs, then do local PC compression of the residuals

• **Why local eigenvectors are “evil”**

• **A hybrid approach (global PCs complemented with local PCs when needed to retain new signal)**

• **How do we know when it is needed? (outlier detection)**

• **[if time is left] Aging of current IASI eigenvectors**
Overview of the hybrid approach

PC compression performed with eigenvectors based on a big global set of past observations works excellent.

Only in very rare situations new spectral features orthogonal to the previously observed directions occur, which can not be represented well (but are flagged).

Using eigenvectors based on the local set of current observations being compressed would solve this issue, but retain more noise and less atmospheric signal.

Instead we can supplement the global eigenvectors with a few local eigenvectors, when needed to represent new signals.
Noise or signal – what do we want to keep?

A naïve approach: select number of PCs based on residual RMS

Residual RMS: \( \sqrt{\frac{1}{m} \sum_{i=1}^{m} r_i^2} \) with \( r = N^{-\frac{1}{2}}(y - \hat{y}) \) (the reconstruction residual)

Eigenvalues of observations and synthetic noise

More noise in leading eigenvectors when the size of the training set is smaller
Equal number of PCs for local and global. Which retains most atmospheric signal?

\[
\begin{align*}
P_G(I-A_L)C_L(I-A_L)^T P_G^T & \quad \text{Thrown away by local, retained by global} \\
P_L(I-A_G)C_L(I-A_G)^T P_L^T & \quad \text{Thrown away by global, retained by local} \\
A_G(I-A_L)C_L(I-A_L)^T A_G^T & \\
A_L(I-A_G)C_L(I-A_G)^T A_L^T
\end{align*}
\]

Local PCs throw away more signal and keep more noise.
Calbuco eruption 2015.04.22

Evidence of new signal (not captured in the operational eigenvectors)
Effect of Hybrid PCs, 4 consecutive PDUs

Volcanic eruption, Calbuco (Chile), 23 April 2015

- on EV global training set itself
- on the granule with global EV
- on the granule with global + 1 hybrid EV

Residual rms (noise-normalised)

First hybrid EV

SO$_2$ signal
Effect of Hybrid PCs, 4 consecutive PDUs

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6.3295, 3.2251

First hybrid EV
Effect of Hybrid PCs, 4 consecutive PDUs

Volcanic eruption, Calbuco (Chile), 23 April 2015

SO$_2$ signal

- on EV global training set itself
- on the granule with global EV
- on the granule with global + 1 hybrid EV

Residual rms (noise-normalised)

First hybrid EV
Noise normalised residual RMS for 89 outliers

Base eigenvectors
1 hybrid + base eigenvectors
2 hybrid + base eigenvectors
Thresholding the reconstruction score for outlier classification

Reconstruction score (RMS of noise normalised residual)

$$\sqrt{\frac{1}{m} \sum_{i=1}^{m} r_i^2} \quad \text{where} \quad r = N^{-1}(y - \hat{y})$$

The noise and therefore the expected value of the residual RMS depends on the radiancesum (increase of photonic noise) and the detector.

This must be taken into account to get a sensitive detection of outliers.

Classified as outlier if:

$$\text{ReconstructionScore} > \text{Threshold}[\text{detector}] + \text{slope} \times \text{RadianceSum}$$

Scatter plots of residual RMS vs. radiancesum (Band 2)
Evolution of normalised residual standard deviation (Band 1)

When the noise increase, so does the variance of the residuals ➔ Outliers threshold should be dynamic
Band 1 normalised residual RMS
Band 1 “outliers”
Band 2 normalised residual RMS
Band 2 “outliers”
Band 3 normalised residual RMS
Band 3 "outliers"
Square root of the 3 highest eigenvalues of the covariance matrix of noise normalised residuals
One possibility would be to:

For each granule (PDU, dwell,...), in addition to the **global PC scores** and associated **reconstruction scores** always to disseminate:

- **3 local eigenvectors** and the corresponding **local PC scores**
- The first 3 **local eigenvalues** and the **trace of the covariance of the residuals** (the sum of all local eigenvalues)
Conclusions

- Must use global eigenvectors for better separation of noise and signal

- A hybrid approach in which the global PC scores are supplemented with a few local PC scores can be used to retain new signal

- Monitoring of the ratio of the highest local eigenvalues to the trace of the local covariance matrix, can help deciding when it is time to update the global eigenvectors

- Looking forward to feedback on the approach, especially in view of MTG-IRS
SPARE SLIDES ➔
Mean of noise normalized residuals (first week of November 2017, both IASI-A and IASI-B)
Evolution of mean residual

Average normalised residual at 923 cm\(^{-1}\), IASI-A

- Eigenvectors from 20110102
- Eigenvectors from 2011 to 2016

Average normalised residual at 948 cm\(^{-1}\), IASI-A

- Eigenvectors from 20110102
- Eigenvectors from 2011 to 2016
PC compression

Raw radiance (minus background) = Reconstructed radiance (minus background) + Residual

Raw radiance (minus background) = Reconstructed radiance + Residual
Reconstruction score

Reconstruction score (RMS of noise normalised residual)

\[ \sqrt{\frac{1}{m} \sum_{i=1}^{m} r_i^2} \quad \text{where} \quad r = N^{-1}(y - \bar{y}) \quad (\text{the reconstruction residual}) \]

Used to detect outliers (spectra which do not reconstruct well)
How about local eigenvectors?

Naively one might think that computing eigenvectors for each individual granule (local in time and space) would result in the need of less PC scores and therefore a higher compression ratio. I will try to explain why this is not the case.

• Lets say there is a PC capturing SO2 signal. If there is no SO2 in the local granule, you do not need to disseminate the corresponding score. True, but for most of the PCs we have reduced variance within a local granule, not zero variance.

• The PCs are orthogonal directions. There is no way to join two PCs into a single one.

• The data volume of the (quantised) PC scores depends on their variability. Reduced local variability gives smaller PC score products also for global PCs. The number of PC scores alone does not determine the data volume to be disseminated.