PCA based information content studies from high spectral resolution infrared observations

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Questions we are trying to answer

- What is the impact of PCA on hyperspectral IR data?
  - Estimation of the Information Loss
  - Noise reduction
- What do the Principal Components represent?
  - Statistical meaning
  - Physical meaning
- What are the benefits and risks in applying PCA to hyperspectral IR data for noise filtering?
  - How should it be applied?
  - When should it be applied?

Outline

- PCA used to Filter out random component of instrument Noise (PNF)
  - Theory
- Application of PNF to simulated data
  - Aircraft FTS data
- Application of PNF to real data
  - Airborne FTS and Spaceborne Grating observations
- Conclusions

Noise Filter Problem

$$L_{obs}(\nu)=L_{atm}(\nu)+\eta(\nu)$$

Find F such that: $L_{est}(\nu)=F(L_{obs}(\nu))$

With minimal Estimation Errors: $EE(\nu)=L_{est}(\nu)-L_{atm}(\nu)$

MMSE

If $S=cov(\eta)$ and $R=cov(L_{atm})$ are known,
the optimal linear filter in the least square sense is
$F=R(R+S)^{-1}$

PCA

$L_{est}(\nu)=P(L_{obs}(\nu))$

Useful Quantities

Estimation Error (EE): difference between noise free and filtered signals

Atmospheric Information Loss (AIL): difference between noise free signal before and after filtering

Reconstructed Noise (RN): noise signal after filtering

Reconstruction Residuals (RR): difference between observed signal before and after filtering

PCA Noise Filter: Implementation Strategy

- Normalize each spectrum L_{obs} by estimated Noise Equivalent Radiance
- Derive the Principal Components from observations (Eigenfunctions of Covariance Matrix of dependent L_{obs})
- Project each L_{obs} onto PCs
- Estimate noise normalized signal (L_{est}) by retaining only N_t PCs
- Remove normalization

Noise Reduction Factor (NRF)

After Noise Normalization data: $\sigma_i=1 \ \forall\ i$

Original space: $\Phi^2= \Sigma\ \sigma_j^{\ 2}=N$ $j=1,\ldots,N$

Reduced space: $\Gamma^2= \Sigma\ \sigma_j^{\ 2}=N_t$ $j=1,\ldots,N_t$

Noise Reduction Factor (NRF)

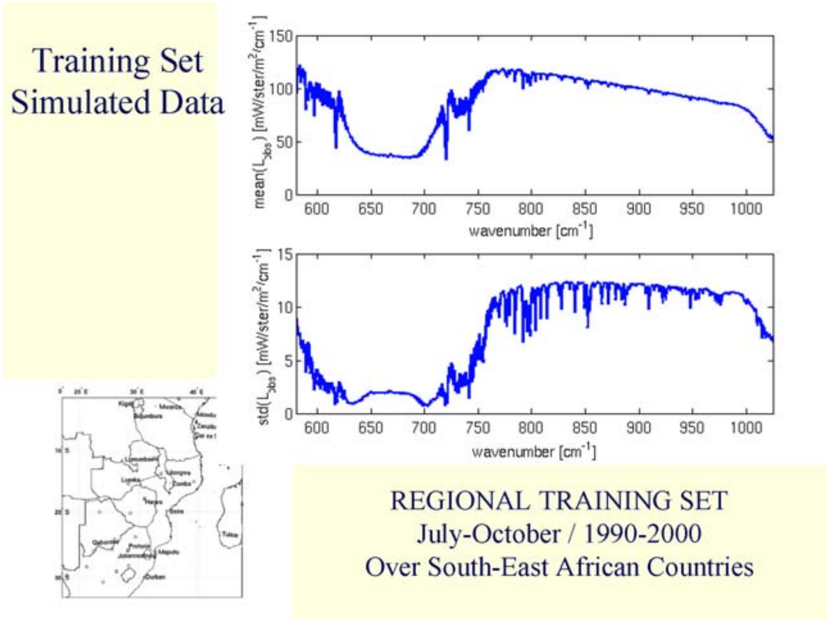
$NRF=sqrt(\Phi^2/\ \Gamma^2)=sqrt(N/N_t)$

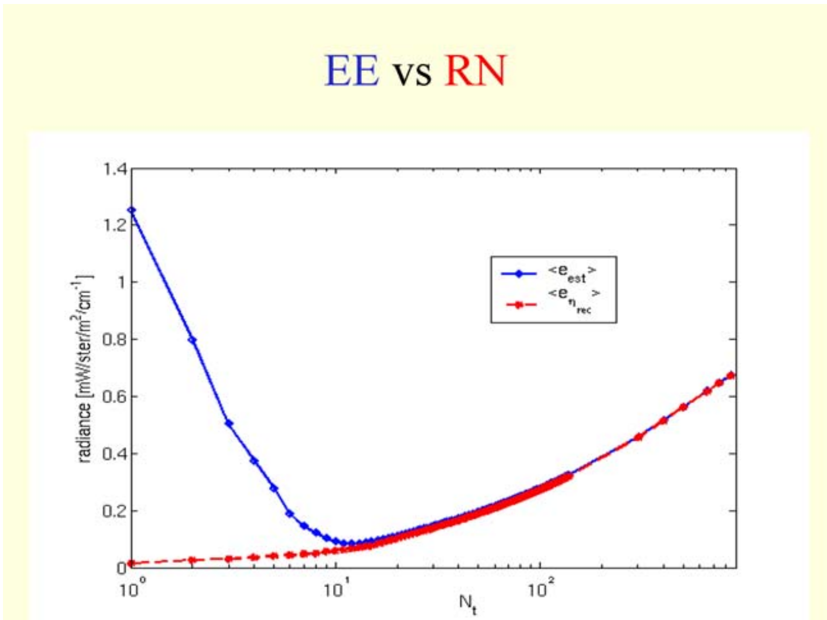
PNF on Simulated Data

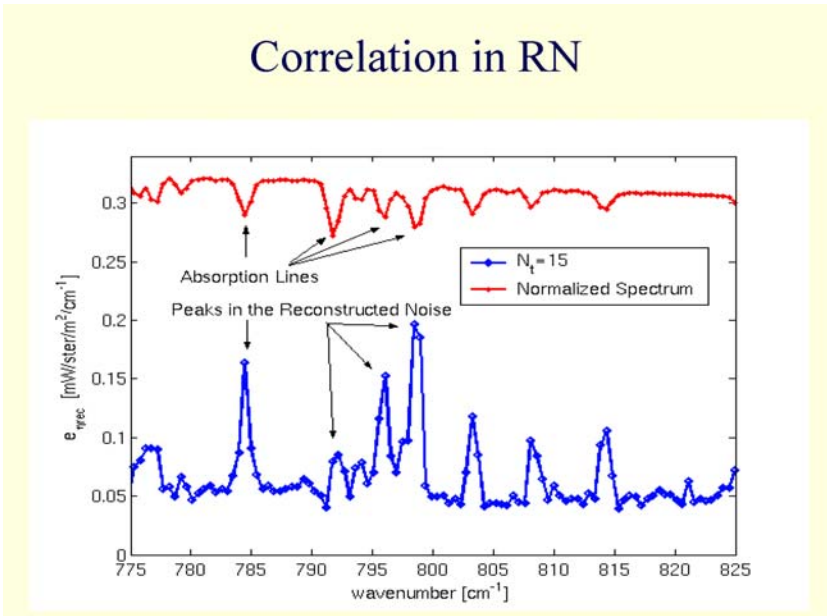
- Quantification of:
  - Atmospheric Information Loss (AIL)
  - Reconstructed instrument Noise (RN)
- Comparison between:
  - Accuracy of PNF (PCA Noise Filter)
  - Accuracy of MMSE (Minimum Mean Square Error from Estimation Theory)
- Verification importance of:
  - Noise normalization
  - Importance of large training sets

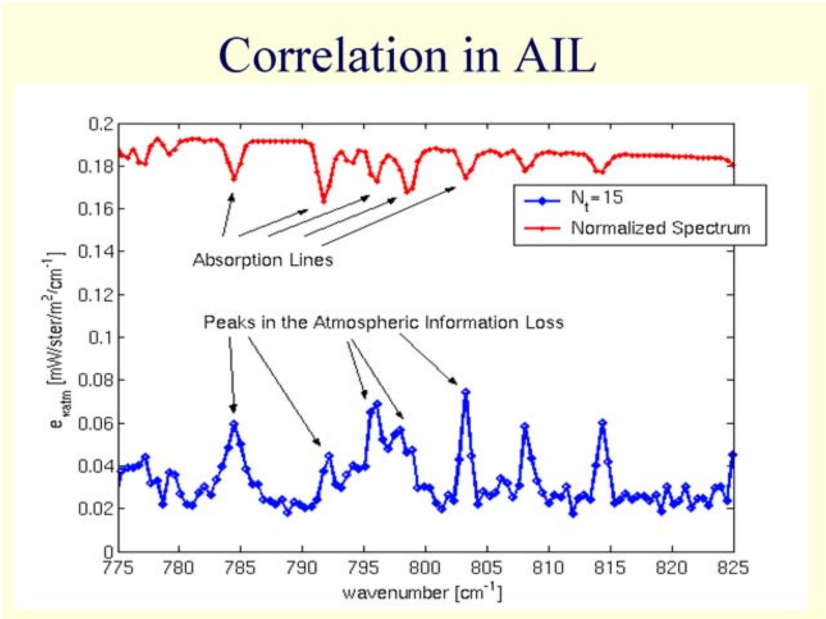
Training Set

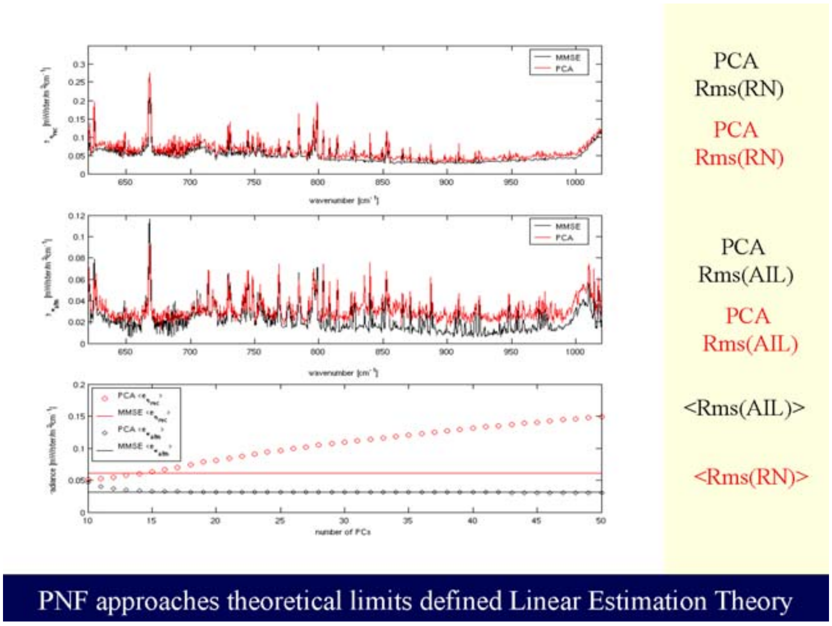
- 10000 raob profiles collected over South Africa (REGIONAL or Local DATASET)
- Clear Sky radiances only, simulated with LBLRTM 8.1 and convoluted at Scanning-HIS resolution (.5 cm^{-1})
- Noise RMS estimated from observed instrument noise (Scanning-HIS, 7 Sep 2000)

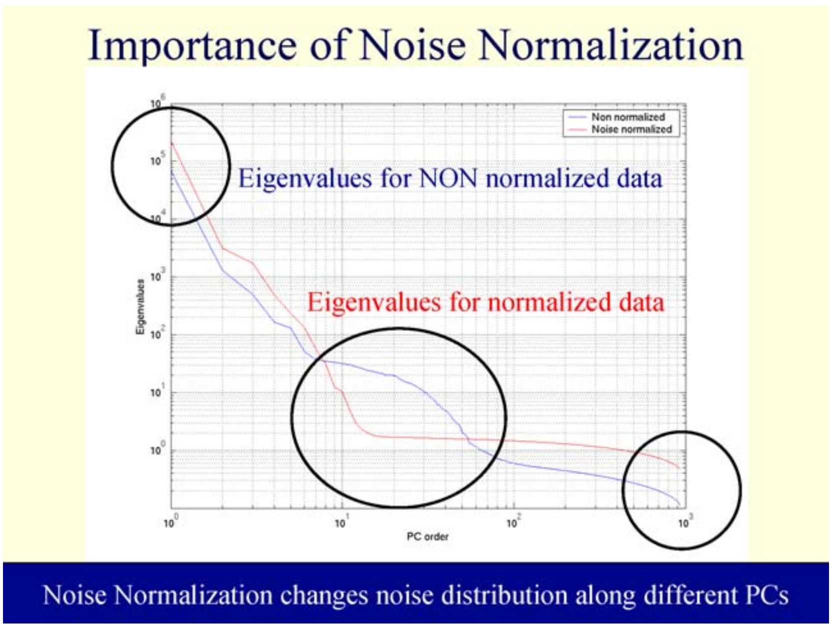

Training Set
Simulated Data
REGIONAL TRAINING SET
July-October / 1990-2000
Over South-East African Countries
wavenumber [cm^{-1}]

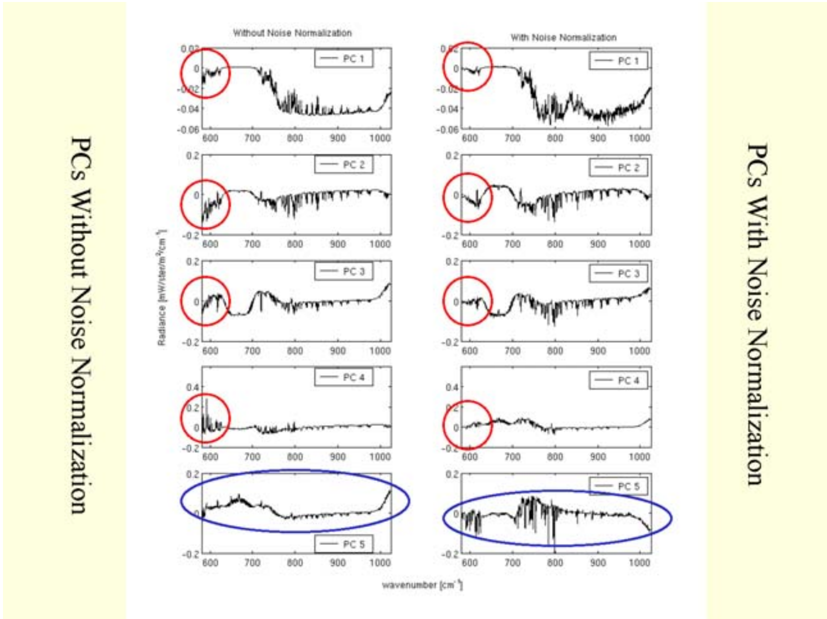

EE vs RN
radiance [mW/ster/m^2/cm^{-1}]
N_t
$<e_{est}>$
$<e_{\eta_{rec}}>$

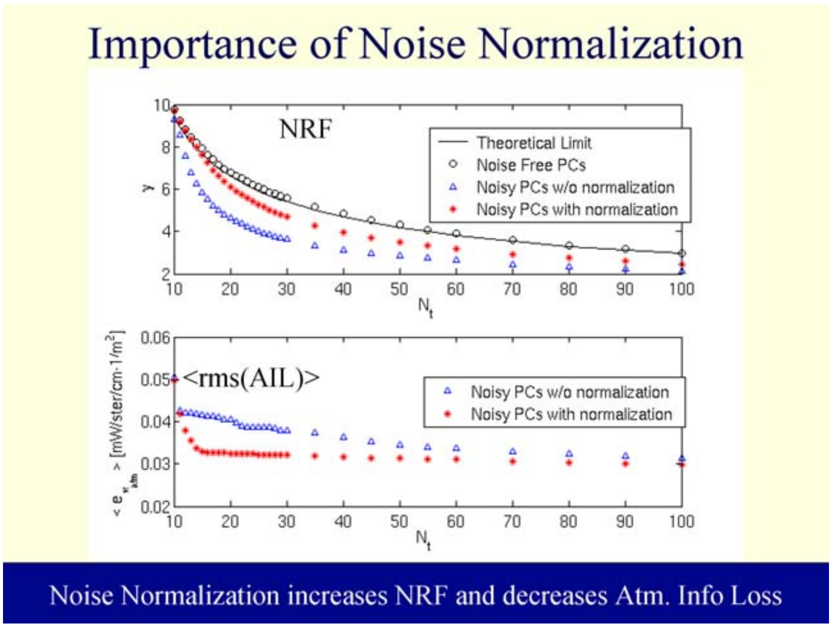

Correlation in RN
Absorption Lines
Peaks in the Reconstructed Noise
N_t=15
Normalized Spectrum
$e_{\eta rec}$ [mW/ster/m^2/cm^{-1}]
wavenumber [cm^{-1}]

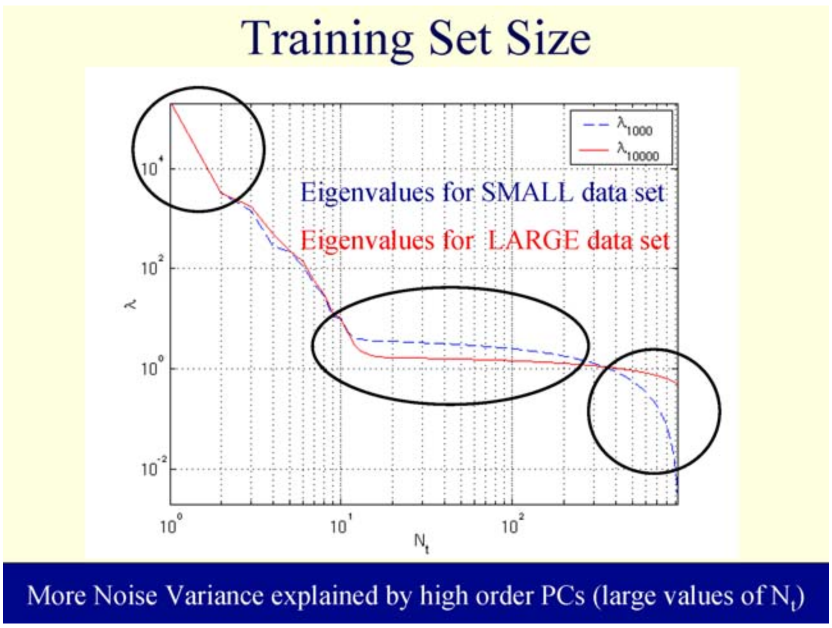

Correlation in AIL
Absorption Lines
Peaks in the Atmospheric Information Loss
N_t=15
Normalized Spectrum
e_νatm [mW/ster/m²/cm⁻¹]
wavenumber [cm⁻¹]


PCA
Rms(RN)
PCA
Rms(RN)
PCA
Rms(AIL)
PCA
Rms(AIL)
<Rms(AIL)>
<Rms(RN)>
MMSE
PCA
number of PCs
PNF approaches theoretical limits defined Linear Estimation Theory

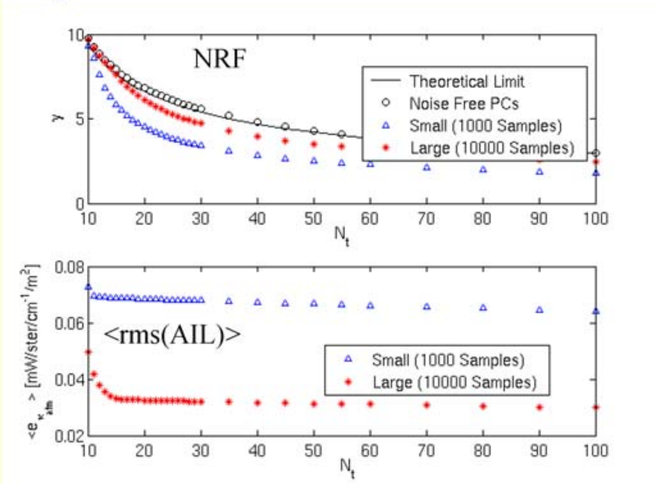

Importance of Noise Normalization
Non normalized
Noise normalized
Eigenvalues for NON normalized data
Eigenvalues for normalized data
Eigenvalues
PC order
Noise Normalization changes noise distribution along different PCs


PCs Without Noise Normalization
Without Noise Normalization
With Noise Normalization
PC 1
PC 2
PC 3
PC 4
PC 5
Radiance [mW/ster/m²/cm⁻¹]
wavenumber [cm⁻¹]
PCs With Noise Normalization


Importance of Noise Normalization
NRF
Theoretical Limit
Noise Free PCs
Noisy PCs w/o normalization
Noisy PCs with normalization
γ
N_t
<rms(AIL)>
Noisy PCs w/o normalization
Noisy PCs with normalization
< e_{v_atm} > [mW/ster/cm-1/m²]
N_t
Noise Normalization increases NRF and decreases Atm. Info Loss


Training Set Size
λ_1000
λ_10000
Eigenvalues for SMALL data set
Eigenvalues for LARGE data set
λ
N_t
More Noise Variance explained by high order PCs (large values of N_t)

Importance of Noise Normalization



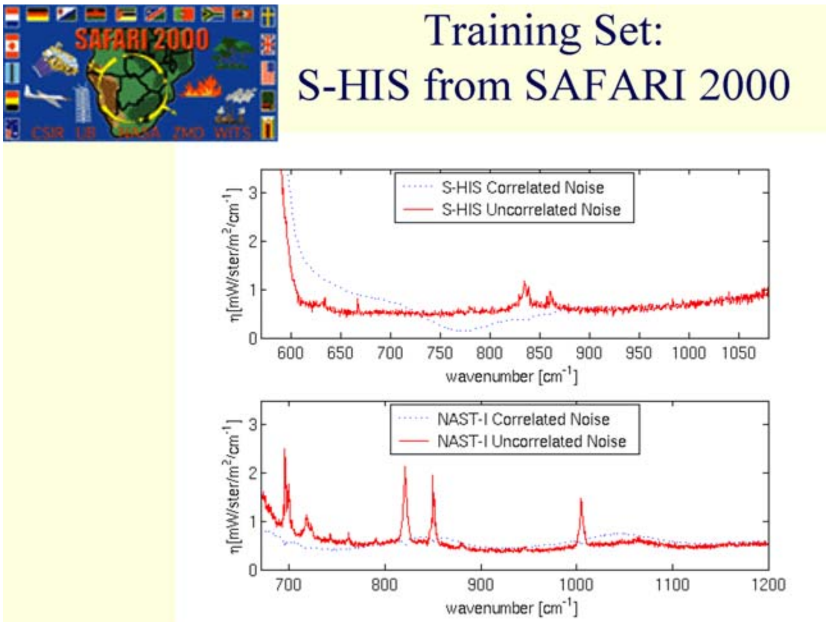
Large Training Sets* increase NRF and decrease Atm. Info Loss

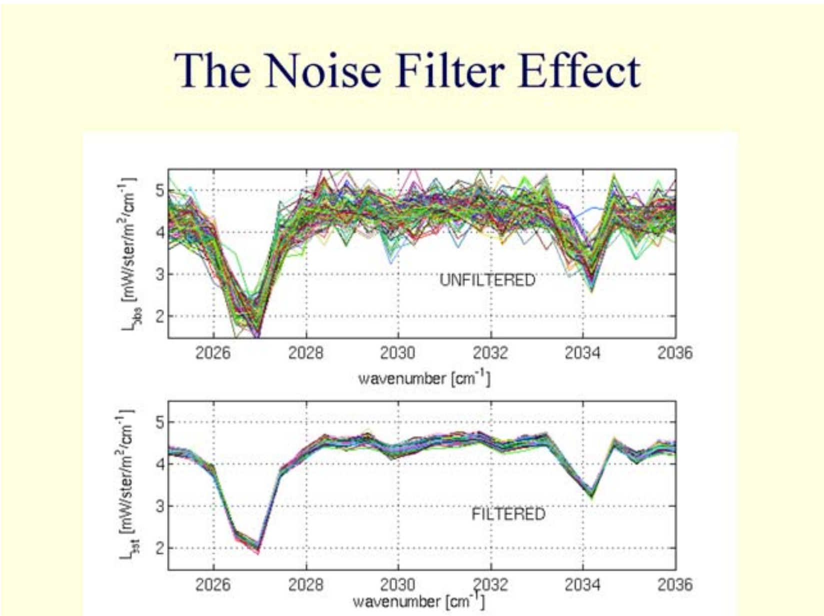
Conclusions on PNF impact on Simulated Data

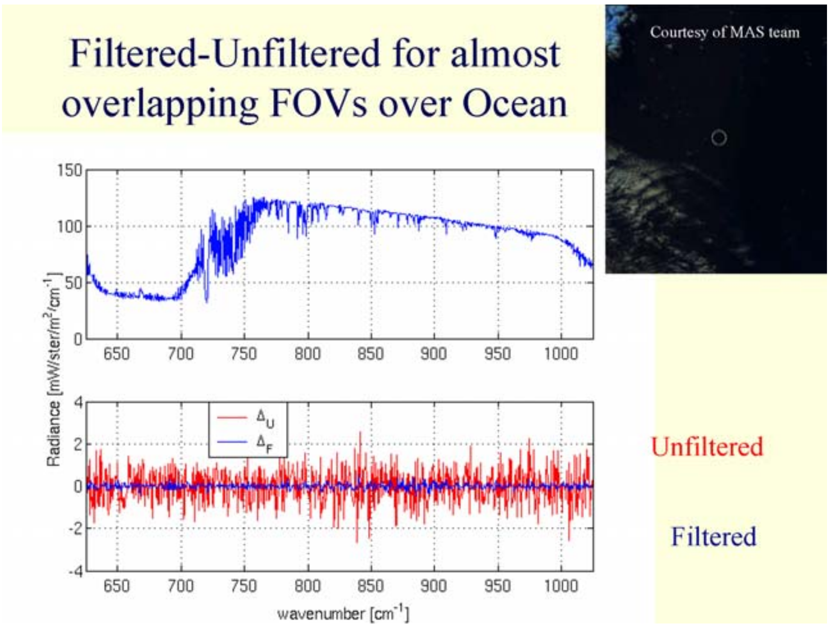
- In RMS sense PNF approaches optimal values defined by Linear Estimation Theory for both AIL and RN
- RMS of AIL and RN are about 7 times* smaller that RMS of Original Noise
- Noise normalization and Large Training Sets improve filter efficiency and accuracy

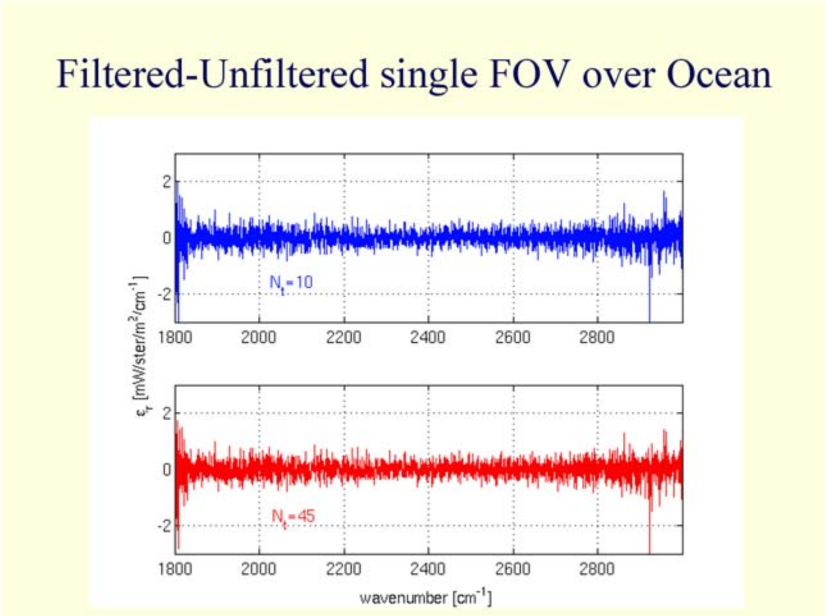
* This Value depends on the specific instrument used

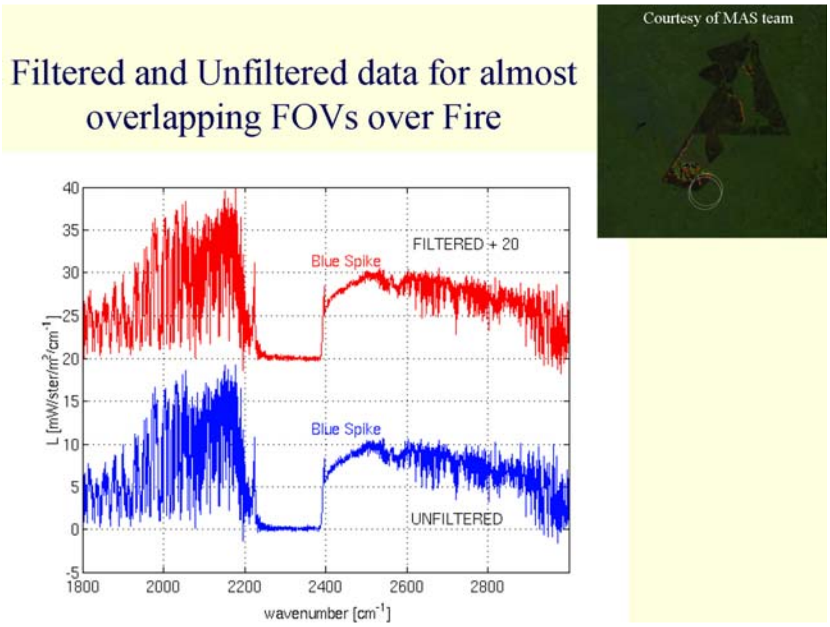
- ER-2 (cruise altitude: 20 km), its instruments are above 94% of the earth's atmosphere
  - NAST-I (FTS, 3.7-16 microns @ .25 cm^{-1})
  - S-HIS (FTS, 3.3-18 microns @ .5 cm^{-1})
- AQUA (Orbit altitude 705 km)
  - AIRS (Grating, 3.7-15.4 microns, resolving power 1200)

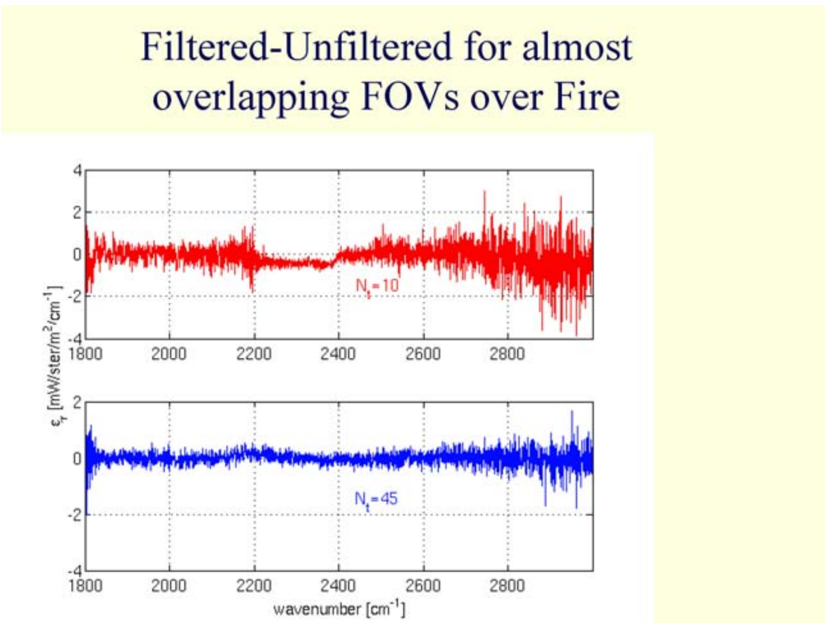

SAFARI 2000
Training Set:
S-HIS from SAFARI 2000
S-HIS Correlated Noise
S-HIS Uncorrelated Noise
η[mW/ster/m²/cm⁻¹]
wavenumber [cm⁻¹]
NAST-I Correlated Noise
NAST-I Uncorrelated Noise
η[mW/ster/m²/cm⁻¹]
wavenumber [cm⁻¹]

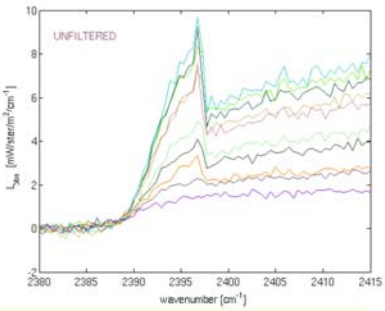

The Noise Filter Effect
L_obs [mW/ster/m²/cm⁻¹]
UNFILTERED
wavenumber [cm⁻¹]
L_est [mW/ster/m²/cm⁻¹]
FILTERED
wavenumber [cm⁻¹]


Filtered-Unfiltered for almost overlapping FOVs over Ocean
Courtesy of MAS team
Radiance [mW/ster/m²/cm⁻¹]
Δ_U
Δ_F
wavenumber [cm⁻¹]
Unfiltered
Filtered


Filtered-Unfiltered single FOV over Ocean
N_t=10
N_t=45
ε_r [mW/ster/m²/cm⁻¹]
wavenumber [cm⁻¹]

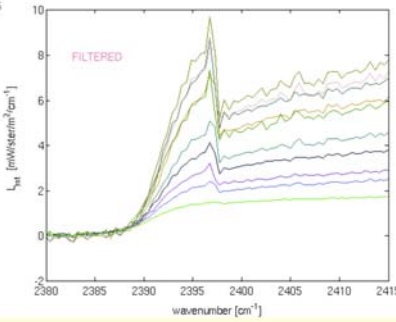

Filtered and Unfiltered data for almost overlapping FOVs over Fire
Courtesy of MAS team
FILTERED + 20
Blue Spike
Blue Spike
UNFILTERED
L [mW/ster/m²/cm⁻¹]
wavenumber [cm⁻¹]

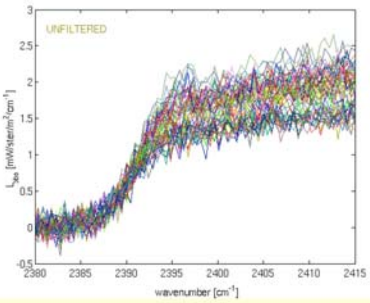

Filtered-Unfiltered for almost overlapping FOVs over Fire
N_t=10
N_t=45
ε_r [mW/ster/m²/cm⁻¹]
wavenumber [cm⁻¹]



Unfiltered data for 10 FOVs over Fire

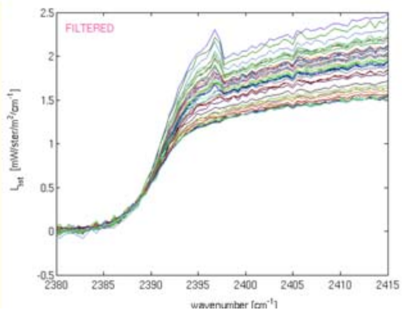
Filtered data for 10 FOVs over Fire





Unfiltered data for 10 FOVs after Fire

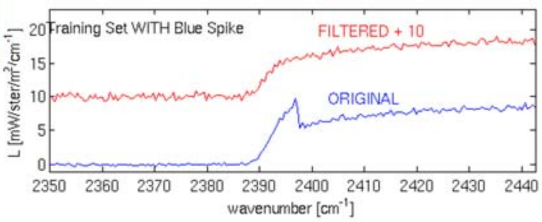
Filtered data for 10 FOVs after Fire

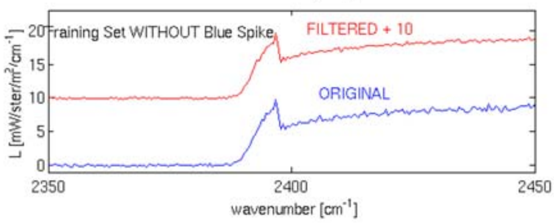


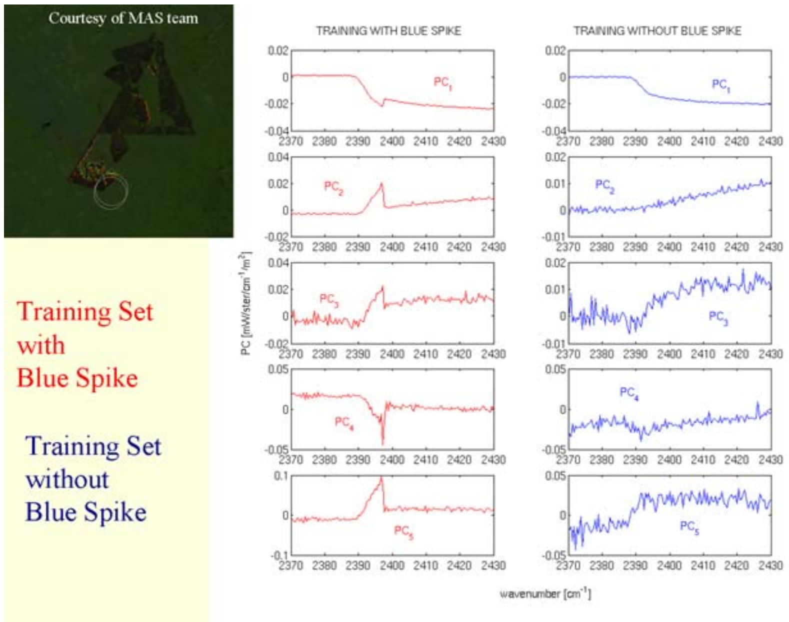
Importance Dependent Training

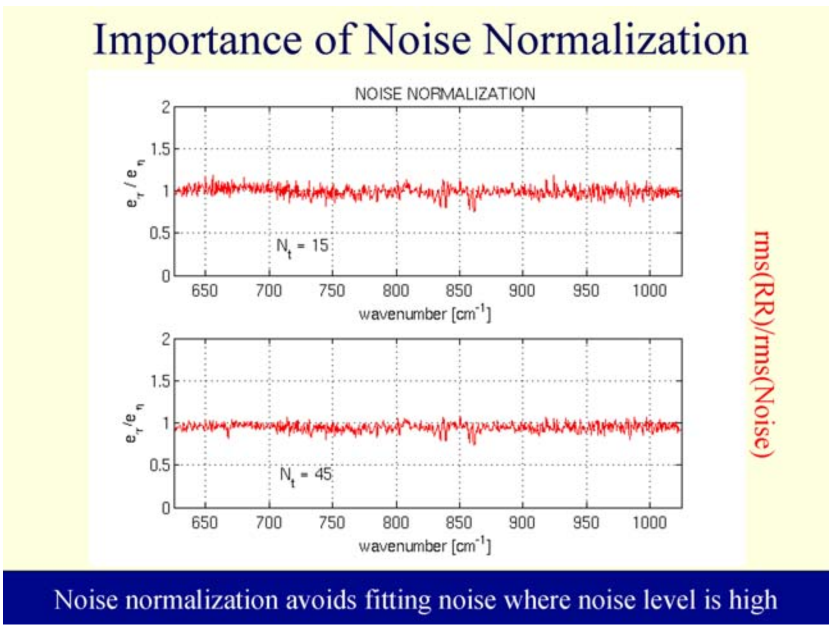
Poorly Estimated

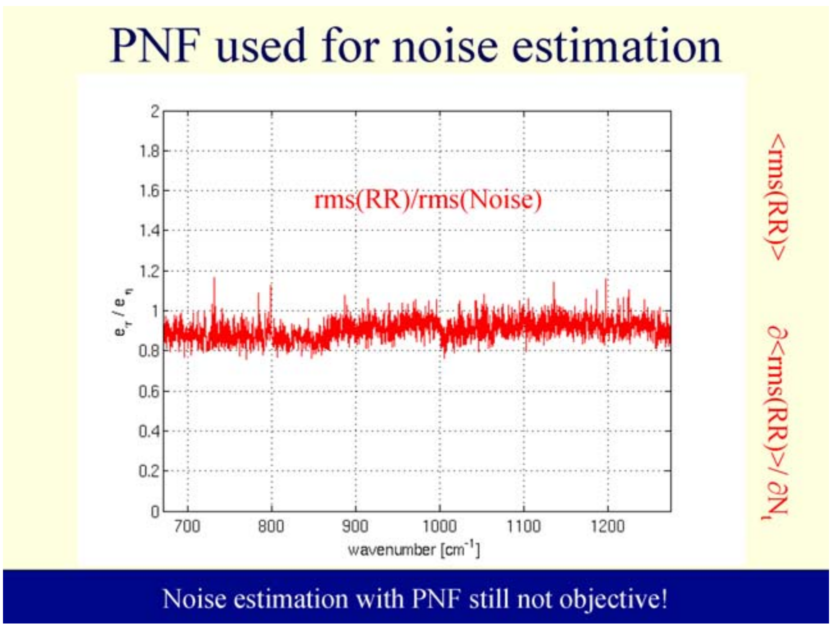
Properly Estimated

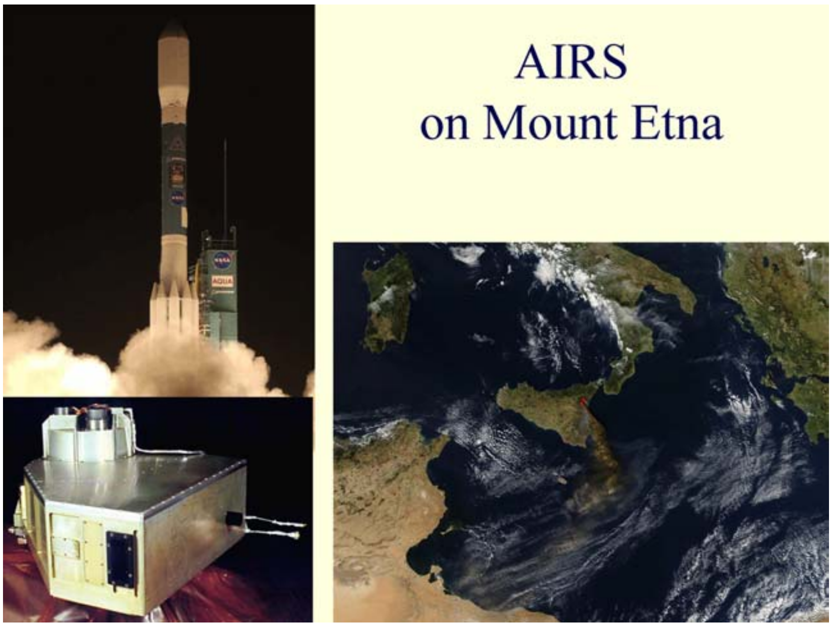


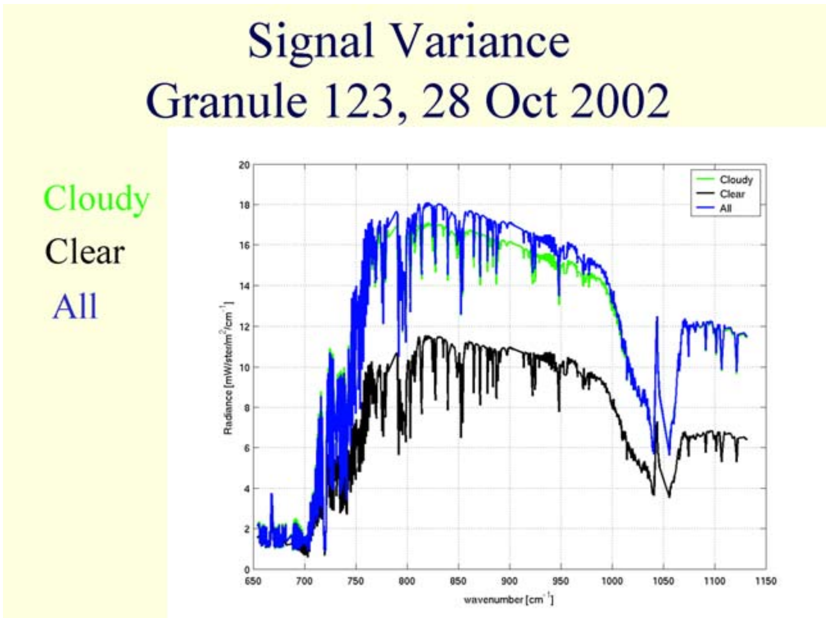


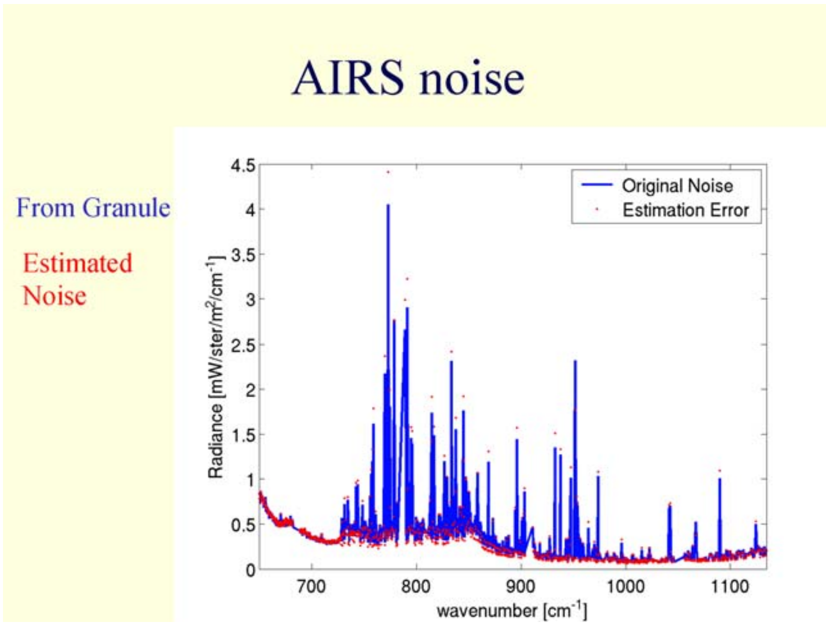

Courtesy of MAS team
Training Set with Blue Spike
Training Set without Blue Spike
TRAINING WITH BLUE SPIKE
TRAINING WITHOUT BLUE SPIKE
PC [mW/ster/cm-1/m2]
wavenumber [cm-1]

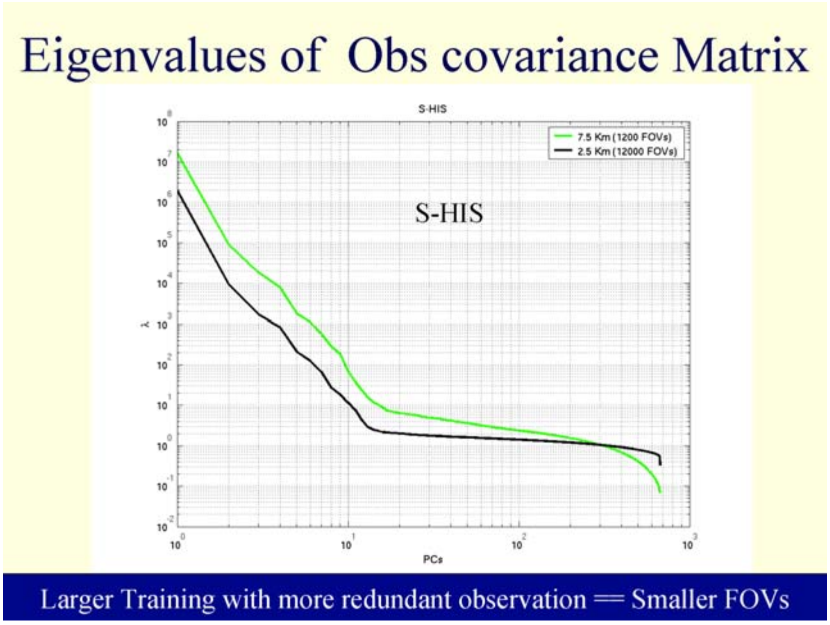

Importance of Noise Normalization
NOISE NORMALIZATION
e_r / e_n
N_t = 15
N_t = 45
wavenumber [cm-1]
rms(RR)/rms(Noise)
Noise normalization avoids fitting noise where noise level is high

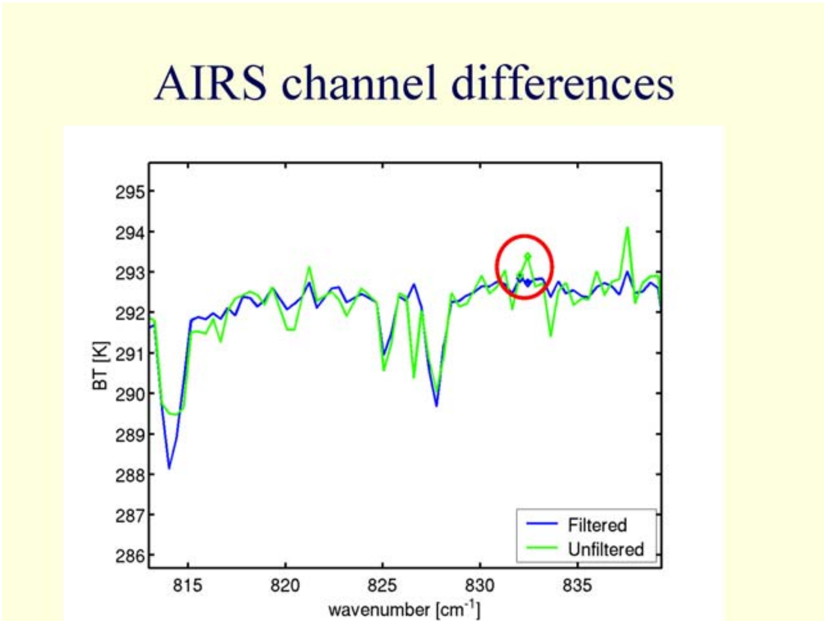

PNF used for noise estimation
rms(RR)/rms(Noise)
e_r / e_n
wavenumber [cm-1]
<rms(RR)>
∂<rms(RR)>/∂N_t
Noise estimation with PNF still not objective!

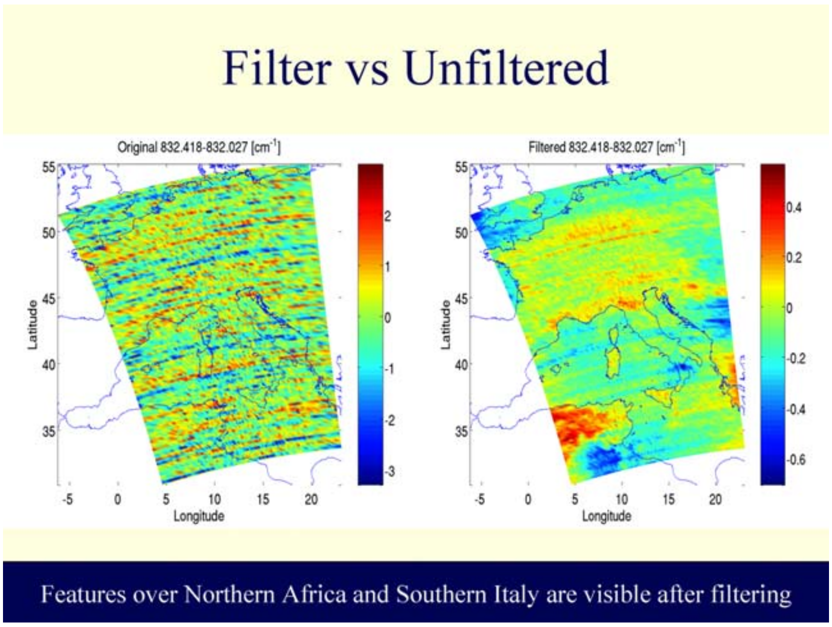

AIRS
on Mount Etna

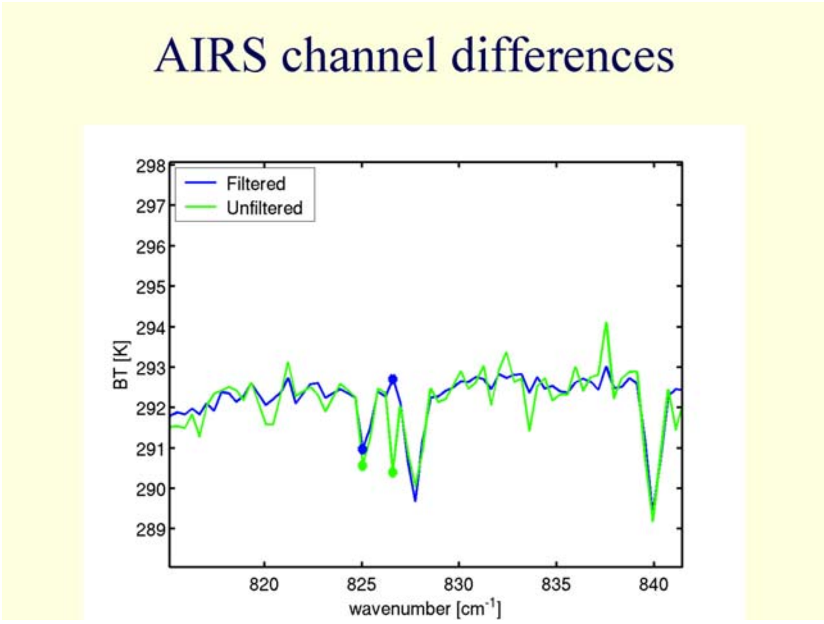

Signal Variance
Granule 123, 28 Oct 2002
Cloudy
Clear
All
Cloudy
Clear
All
Radiance [mW/ster/m^2/cm^{-1}]
wavenumber [cm^{-1}]

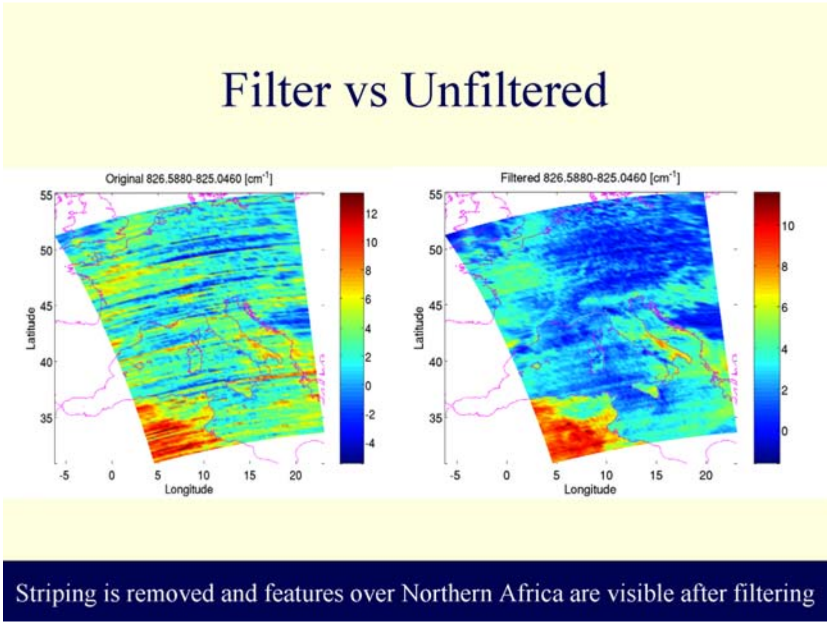

AIRS noise
From Granule
Estimated Noise
Original Noise
Estimation Error
Radiance [mW/ster/m^2/cm^{-1}]
wavenumber [cm^{-1}]

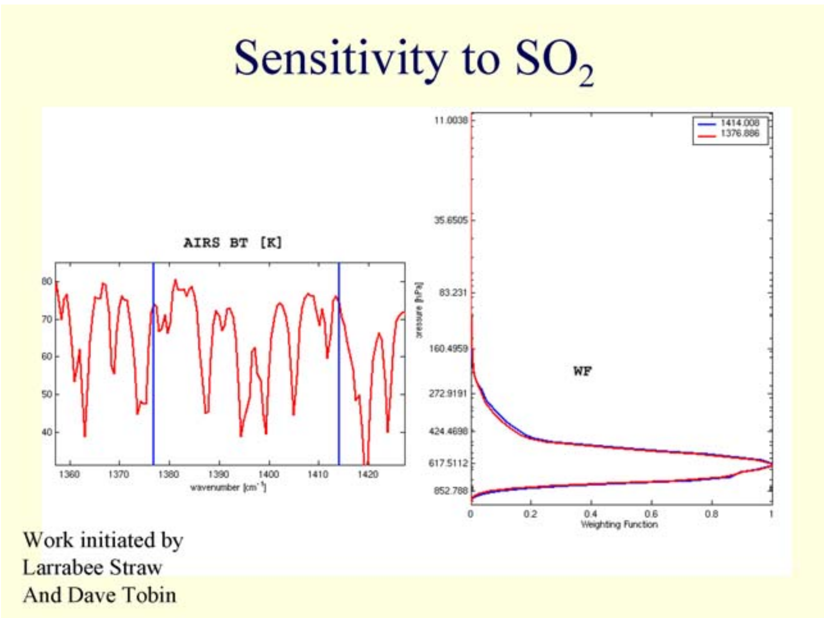

Eigenvalues of Obs covariance Matrix
S-HIS
7.5 Km (1200 FOVs)
2.5 Km (12000 FOVs)
S-HIS
λ
PCs
Larger Training with more redundant observation == Smaller FOVs

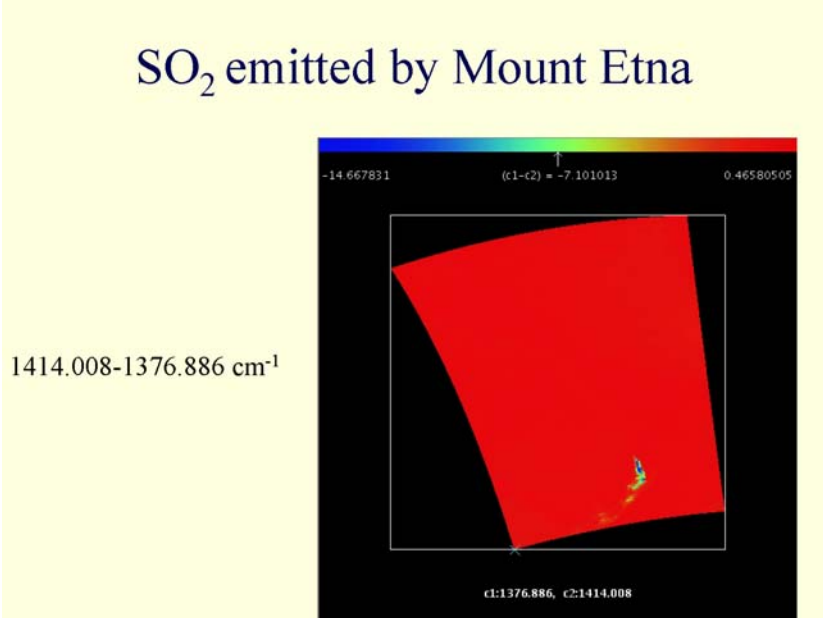

AIRS channel differences
BT [K]
wavenumber [cm^{-1}]
Filtered
Unfiltered

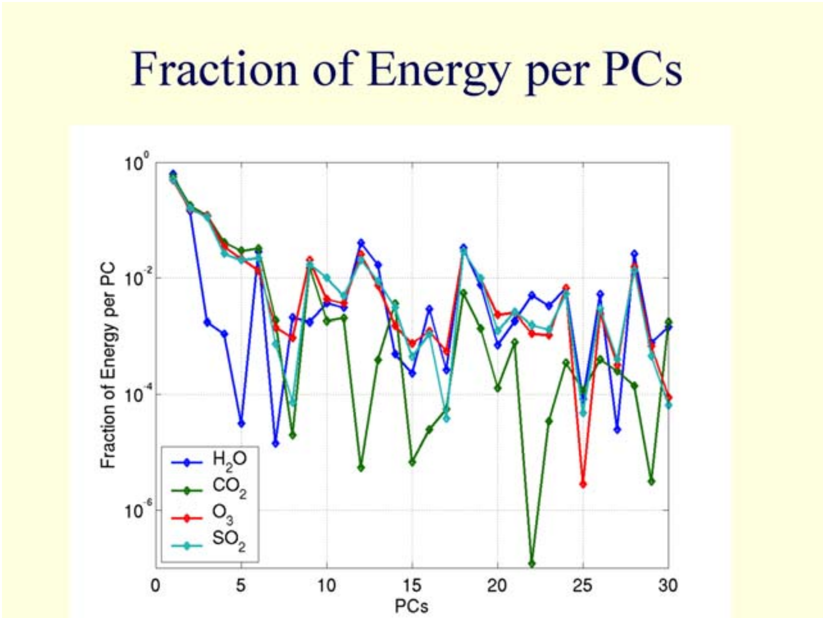

Filter vs Unfiltered
Original 832.418-832.027 [cm^{-1}]
Filtered 832.418-832.027 [cm^{-1}]
Latitude
Longitude
Features over Northern Africa and Southern Italy are visible after filtering

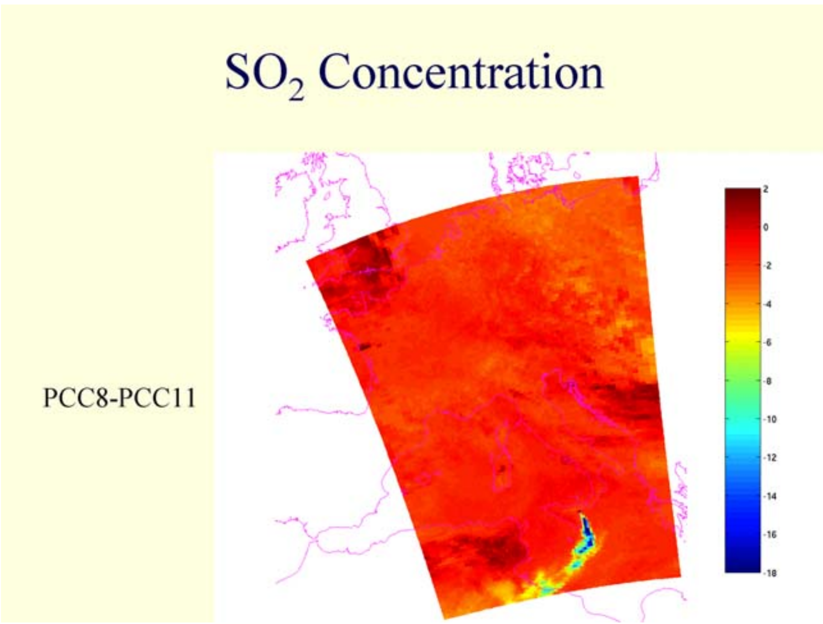

AIRS channel differences
Filtered
Unfiltered
BT [K]
wavenumber [cm^{-1}]
298
297
296
295
294
293
292
291
290
289
820
825
830
835
840


Filter vs Unfiltered
Original 826.5880-825.0460 [cm^{-1}]
Filtered 826.5880-825.0460 [cm^{-1}]
Latitude
Longitude
Striping is removed and features over Northern Africa are visible after filtering


Sensitivity to SO_2
AIRS BT [K]
wavenumber [cm^{-1}]
WF
1414.008
1376.886
Weighting Function
Work initiated by
Larrabee Straw
And Dave Tobin


SO2 emitted by Mount Etna
1414.008-1376.886 cm-1
-14.667831
(c1-c2) = -7.101013
0.46580505
c1:1376.886, c2:1414.008


Fraction of Energy per PCs
Fraction of Energy per PC
PCs
H2O
CO2
O3
SO2


SO2 Concentration
PCC8-PCC11

Conclusions

- PCA by taking advantage of redundancy reduces random component of Instrument noise (PNF)
- Both AIL and RN approach the optimal value defined by Linear Estimation Theory
- For simulated data (presented case) AIL and RN are 7 times smaller that original noise
- Both AIL and RN are correlated in wavenumber space
- Most difficult cases, observation highly deviant from mean, are properly treated if PCs are derived in Dependent Mode

Conclusions

- Noise normalization and large training set enhance accuracy and efficiency of PNF
- If not available, estimate of random component of instrument noise can be obtained by applying PCA to observations
- With real data (AIRS) achieved NR factor is between 4 and 5
- PNF is not quite ready to be used as Black Box, it requires tuning and monitoring of Reconstruction Residuals

Ongoing Work

- Characterization of AIL and RN spectral correlation
- Investigation of physical meaning of PCs