Application of Singular Value Decomposition to High Spectral Resolution Measurements

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What is this about?

- A spectrum has several thousand elements
- But only a few degrees of freedom for signal (d_s)
- Plus a lot of degrees of freedom for noise (d_n)
- We should be able to represent the useful signal in terms of a few coefficients
- This can be done using singular vectors of a large ensemble of actual spectra

Acknowledgement

- This will be an ill-digested description of a technique I've picked up from the AIRS community
- They are using it to
  - Reduce noise in spectral data
  - Improve the efficiency of retrieval
  - Extract small signals from spectra
  - Data compression

Some Basic Philosophy

- A measurement $\mathbf{y}$ is some known function $\mathbf{f}(\mathbf{x})$ of a 'state' $\mathbf{x}$, plus measurement error $\boldsymbol{\epsilon}$
- $\mathbf{x}$ includes *all* unknown quantities that affect the measurement
- A retrieval $\mathbf{r}(\mathbf{y})$ is some way of finding a state $\mathbf{x}_r$ such that $\mathbf{f}(\mathbf{x}_r)$ is consistent with $\mathbf{y}$
- This leads to a transfer function $\mathbf{x}_r=\mathbf{t}(\mathbf{x})=\mathbf{r}(\mathbf{f}(\mathbf{x})+\boldsymbol{\epsilon})$

Continued…

- $\mathbf{x}_r = \mathbf{t}(\mathbf{x})$ can be linearised to relate the true state to the retrieval:

$$\mathbf{x}_r = \mathbf{x}_a + \mathbf{A}(\mathbf{x} - \mathbf{x}_a) + \mathbf{G}\epsilon$$

- Knowledge of $\mathbf{A}$ and $\mathbf{S}_\epsilon$ evaluated at $\mathbf{x}_a$ fully characterises the retrieval
- Errors are correlated
- We can us SVD to find orthogonal functions of the state that have uncorrelated errors
- But that isn't what I want to talk about today…

What is the best estimate of a spectrum given a measurement?

- This is related to
  - Image enhancement
  - Cleaning up noisy sound recordings

- Forward model is

$$\mathbf{y}_m = \mathbf{x} + \epsilon$$

$\mathbf{x}$ is true spectrum, $\mathbf{y}_m$ is measurement, ϵ is noise

- Minimum variance estimate of $\mathbf{x}$ is

$$\mathbf{x}_r = \mathbf{x}_a + \mathbf{S}_a(\mathbf{S}_a+\mathbf{S}_\epsilon)^{-1}(\mathbf{y}_m-\mathbf{x}_a)$$

Continued…

- If we have a large sample of spectra:
  - Expect that $\mathbf{x}_a = \langle \mathbf{x} + \epsilon \rangle = \langle \mathbf{y}_m \rangle$
  - Can estimate $\mathbf{S}_a + \mathbf{S}_\epsilon$ from statistics of $\mathbf{y}_m$
  - Should have a good idea of $\mathbf{S}_\epsilon$
- But $\mathbf{S}_a(\mathbf{S}_a + \mathbf{S}_\epsilon)^{-1}$ will be a large matrix, and $\mathbf{S}_a$ found from $\mathbf{S}_a + \mathbf{S}_\epsilon$ and $\mathbf{S}_\epsilon$ is likely to be ill-conditioned
- $\mathbf{S}_a$ is likely to have a 'small' number of eigenvalues greater than noise

Singular Vectors
(or Principal Components)

- Let the ensemble of spectra be columns of a matrix **Y**

- Represent **Y** as its singular vector decomposition:

$$\mathbf{Y} = \mathbf{U}\Lambda\mathbf{V}^T$$

where Λ is diagonal, $\mathbf{U}^T\mathbf{U}=\mathbf{I}$ and $\mathbf{V}^T\mathbf{V}=\mathbf{I}$

- The j'th individual spectrum $\mathbf{y}_j$ is then

$$\mathbf{y}_j = \Sigma_i \, \boldsymbol{u}_i \lambda_i v_{ij}^T$$

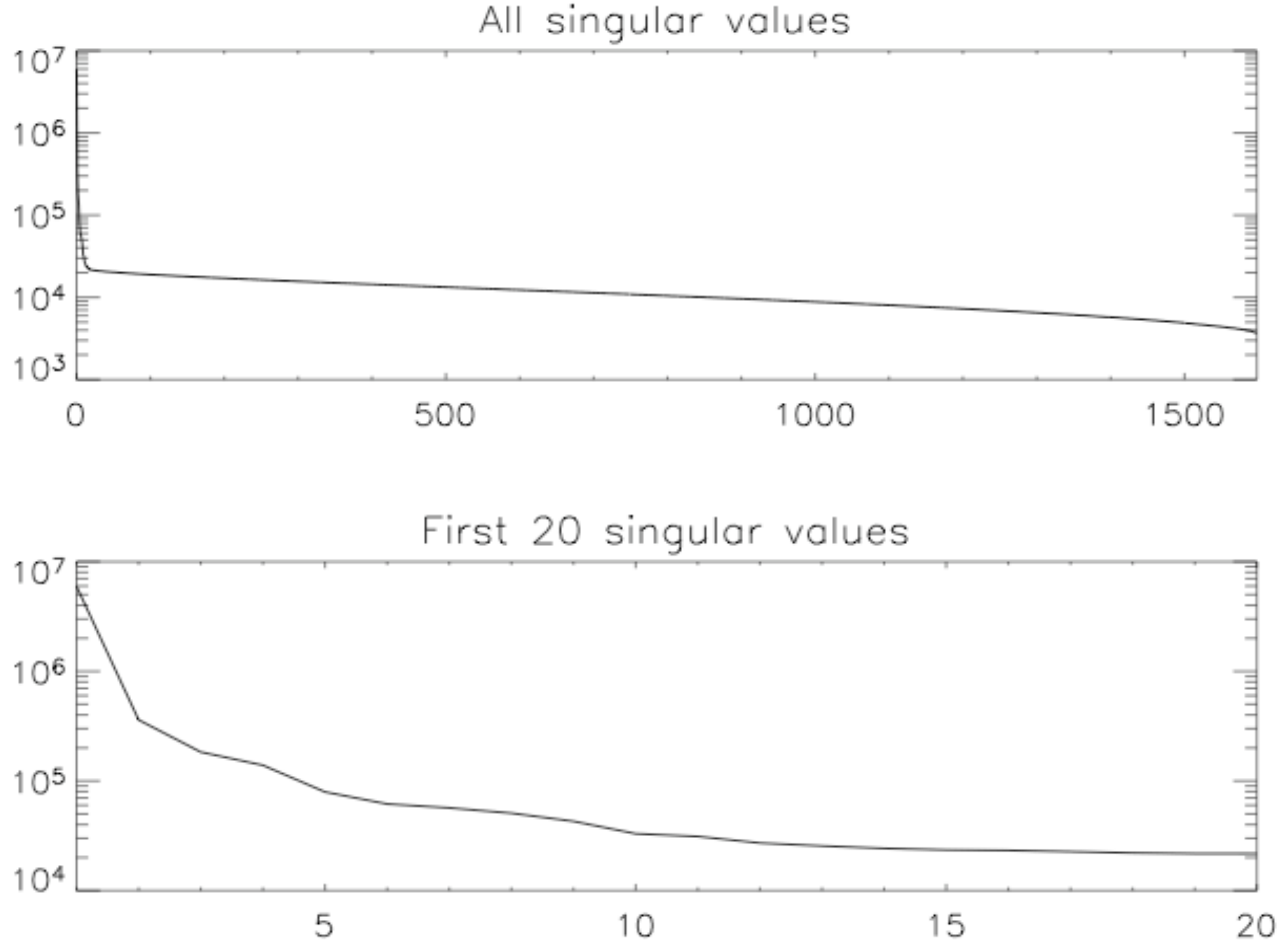
- The spectrum is represented as a sum of columns $\boldsymbol{u}_i$ of **U**, with coefficients $\lambda_i v_{ij}^T$.

- Because $\mathbf{U}^T\mathbf{U}=\mathbf{I}$, we can compute $\lambda_i v_{ij}^T$ for any spectrum as $\mathbf{U}^T\mathbf{y}_j$.

Example from TES

- Run 2147, Sept 20-21 2004
- A set of nadir spectra
- First 100 observations of the day
- Each of 16 pixels, 1600 spectra in total
- Filter 1B2, 923 to 1160 cm^{-1}

Singular Values



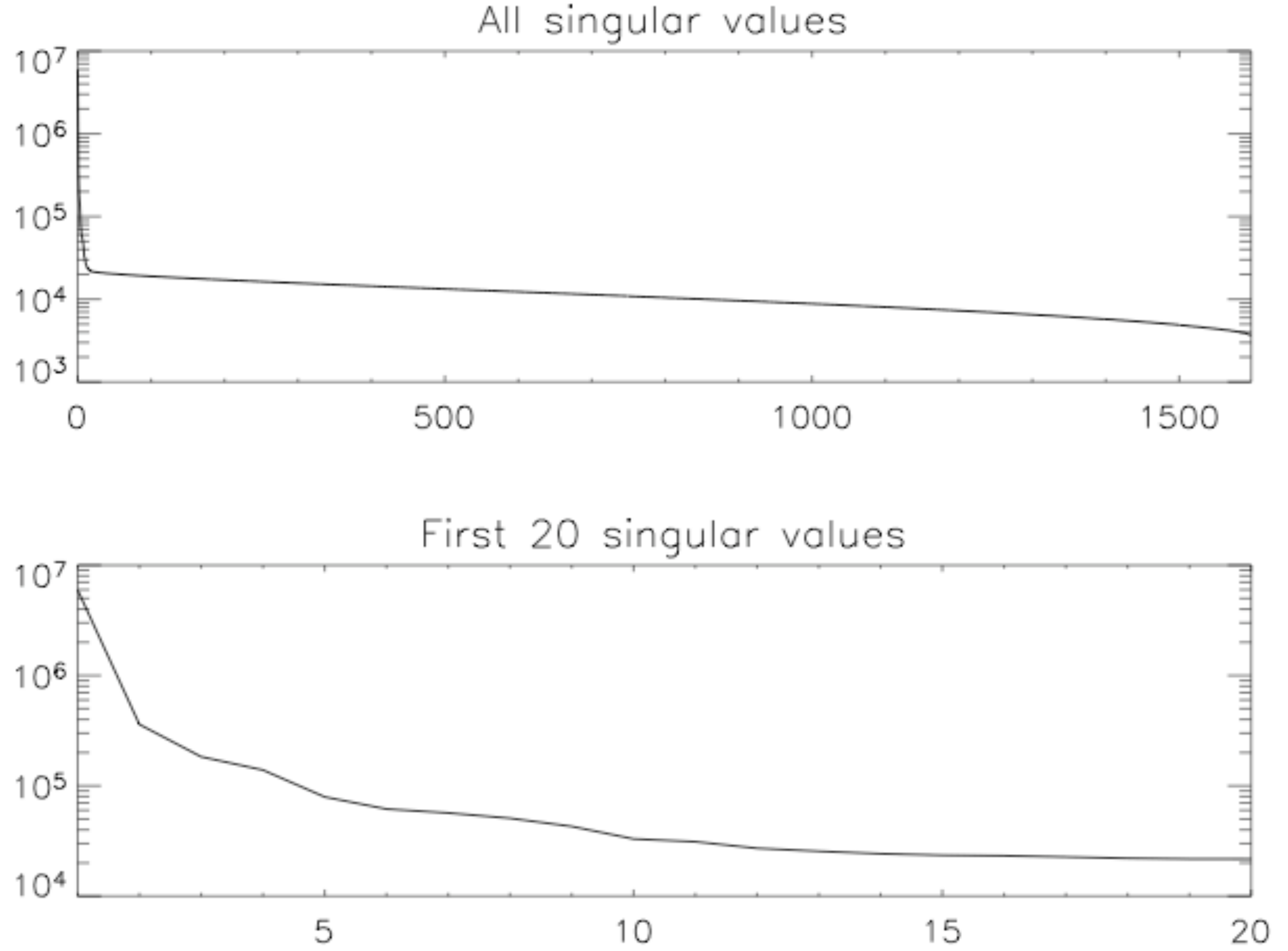
What do we expect?

- Singular vectors are the same as eigenvectors of $\mathbf{YY}^T$, singular values are the square roots of its eigenvalues
- $\mathbf{YY}^T$ is the covariance matrix of the spectra
- In the linear case with independent constant noise, this would be

$$\mathbf{S}_y = \mathbf{KS}_a\mathbf{K}^T + \sigma_\epsilon^2 \mathbf{I}$$

- $\mathbf{KS}_a\mathbf{K}^T$ has rank $\leq n$, $\mathbf{I}$ is of dimension $m \gg n$
- Eigenvalues of $\mathbf{S}_y$ are $\lambda_i^2 + \sigma_\epsilon^2$ where λ_i^2 are the eigenvalues of $\mathbf{KS}_a\mathbf{K}^T$

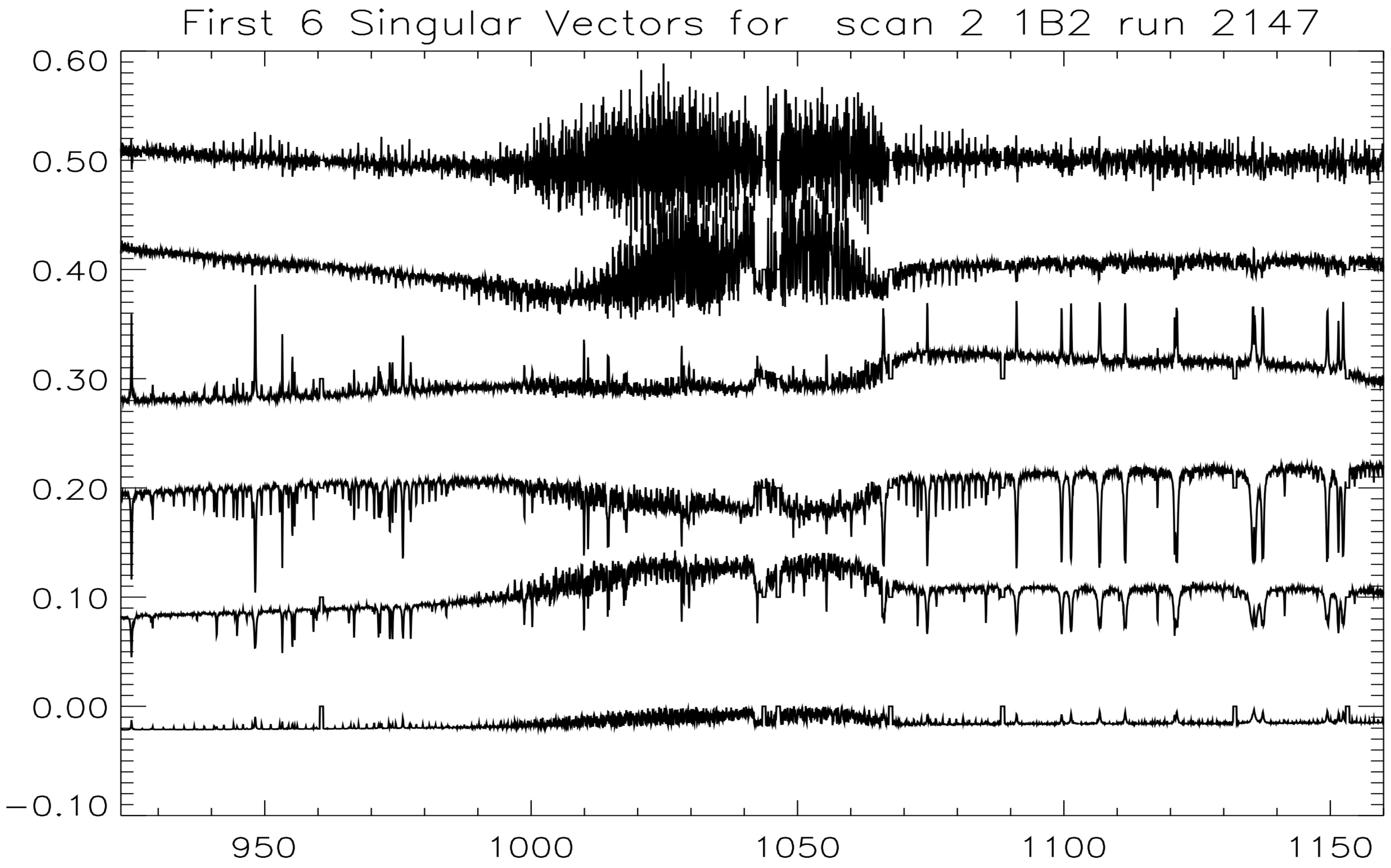
Singular Values



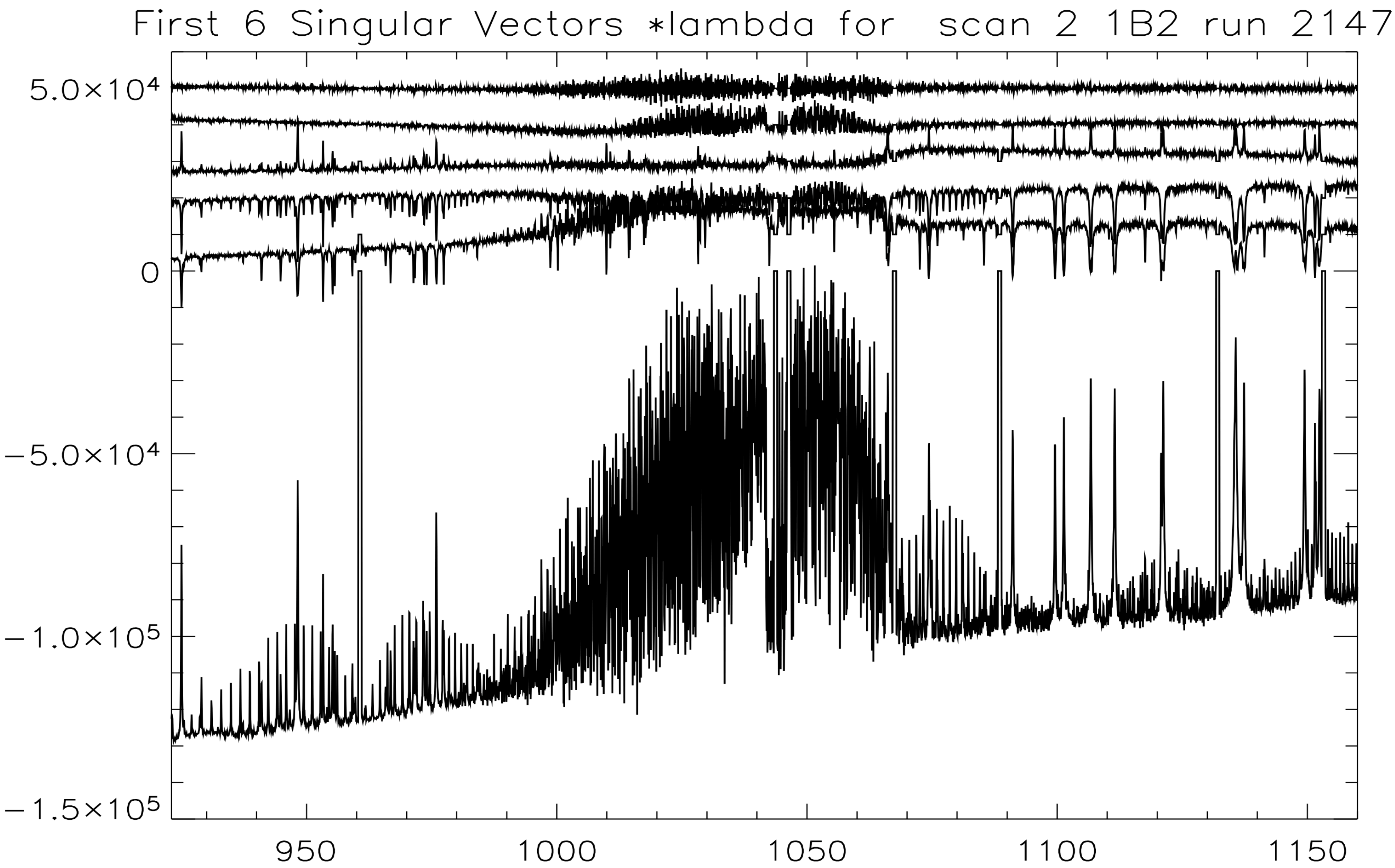
Reconstructing Spectra

- We can drop terms with $\lambda_i \ll \sigma_\epsilon$ without significant loss
  - they correspond to noise only
  - Better, multiply retained terms by something like $\lambda_i^2 / (\sigma_\epsilon^2 + \lambda_i^2)$
- So spectra can be reconstructed from the first few coefficients.
- The noise can be reconstructed from the rest…
- Reconstructed spectra have much reduced noise

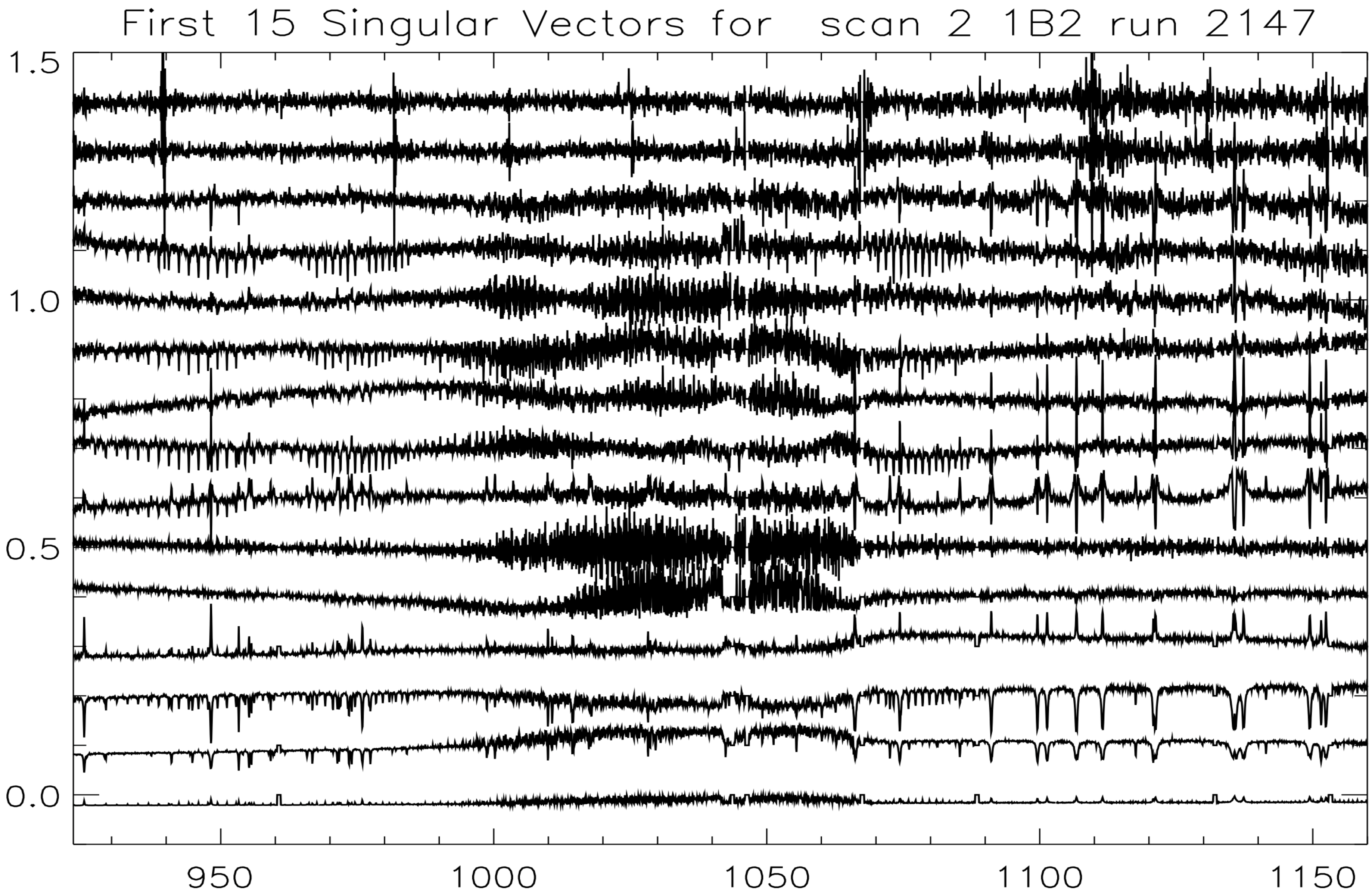
Singular Vectors



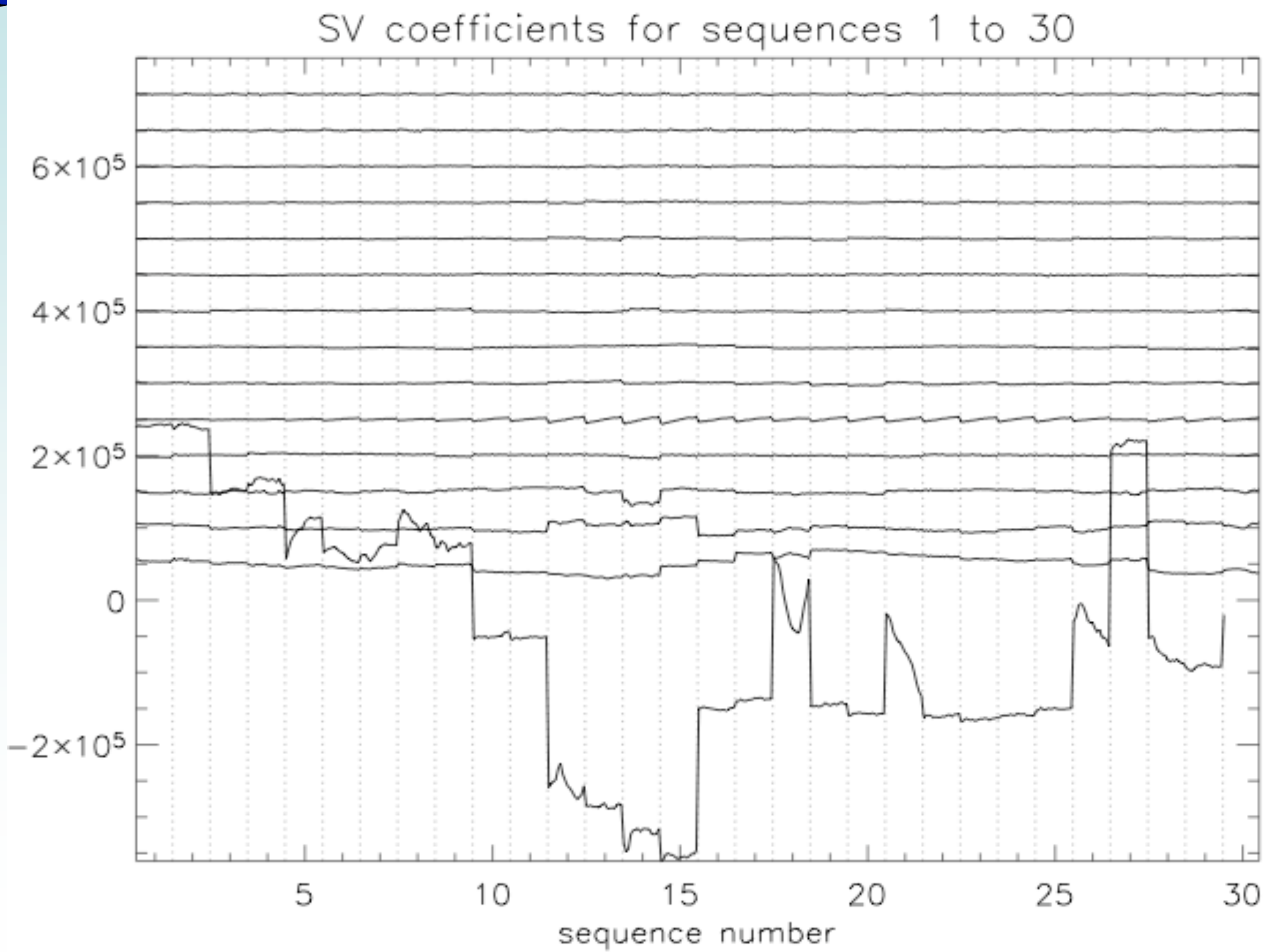
Singular vectors * Lambda



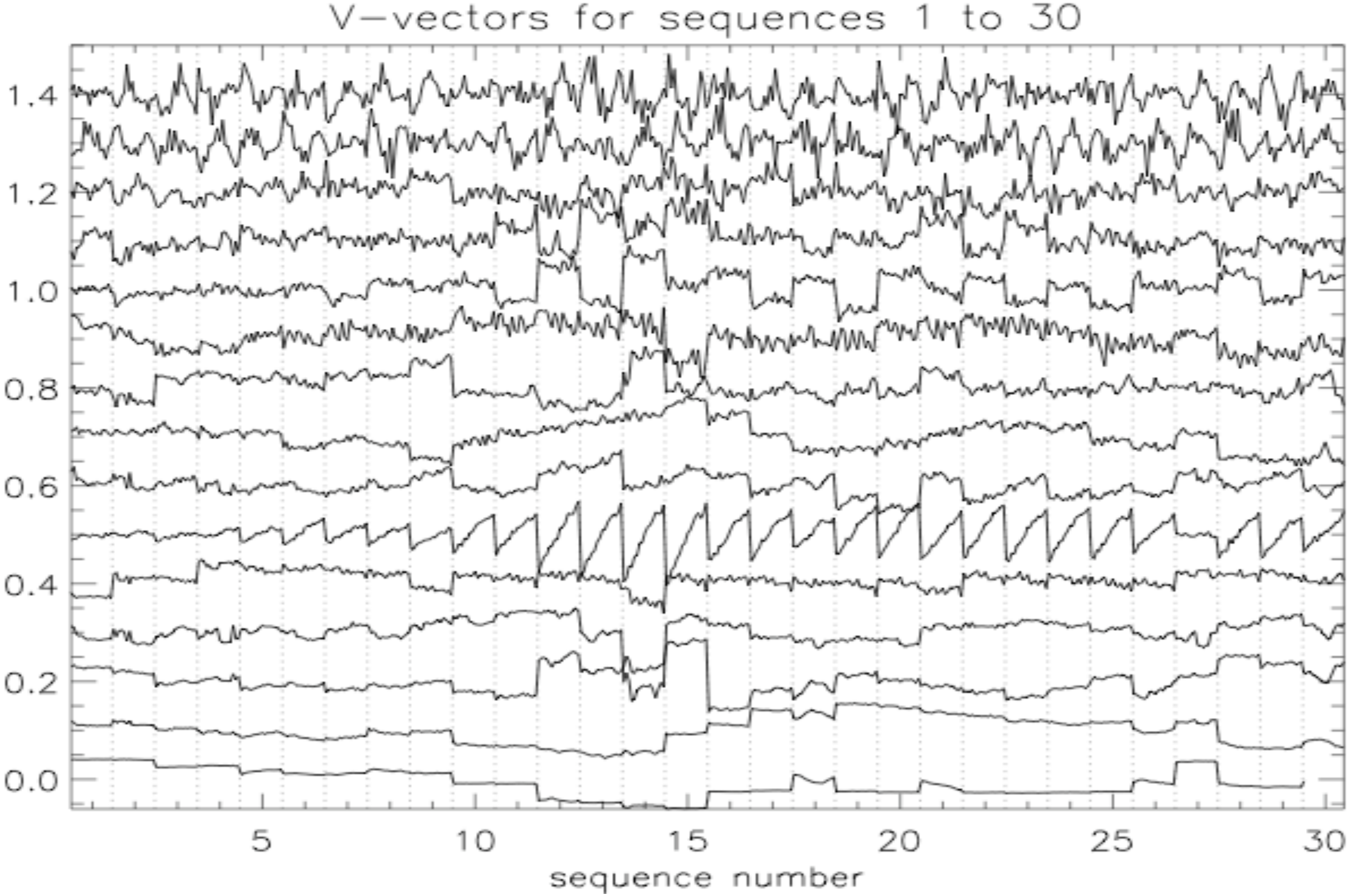
Singular Vectors



Coefficients for first 30*16 spectra



V-vectors



V–vectors for sequences 1 to 30
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
5
10
15
20
25
30
sequence number

Features

- Most of variation is in the first singular vector. First six are:

  5.96×10^6 3.6×10^5 1.83×10^5 1.39×10^4 7.93×10^4 6.16×10^4

- Data spikes - identified

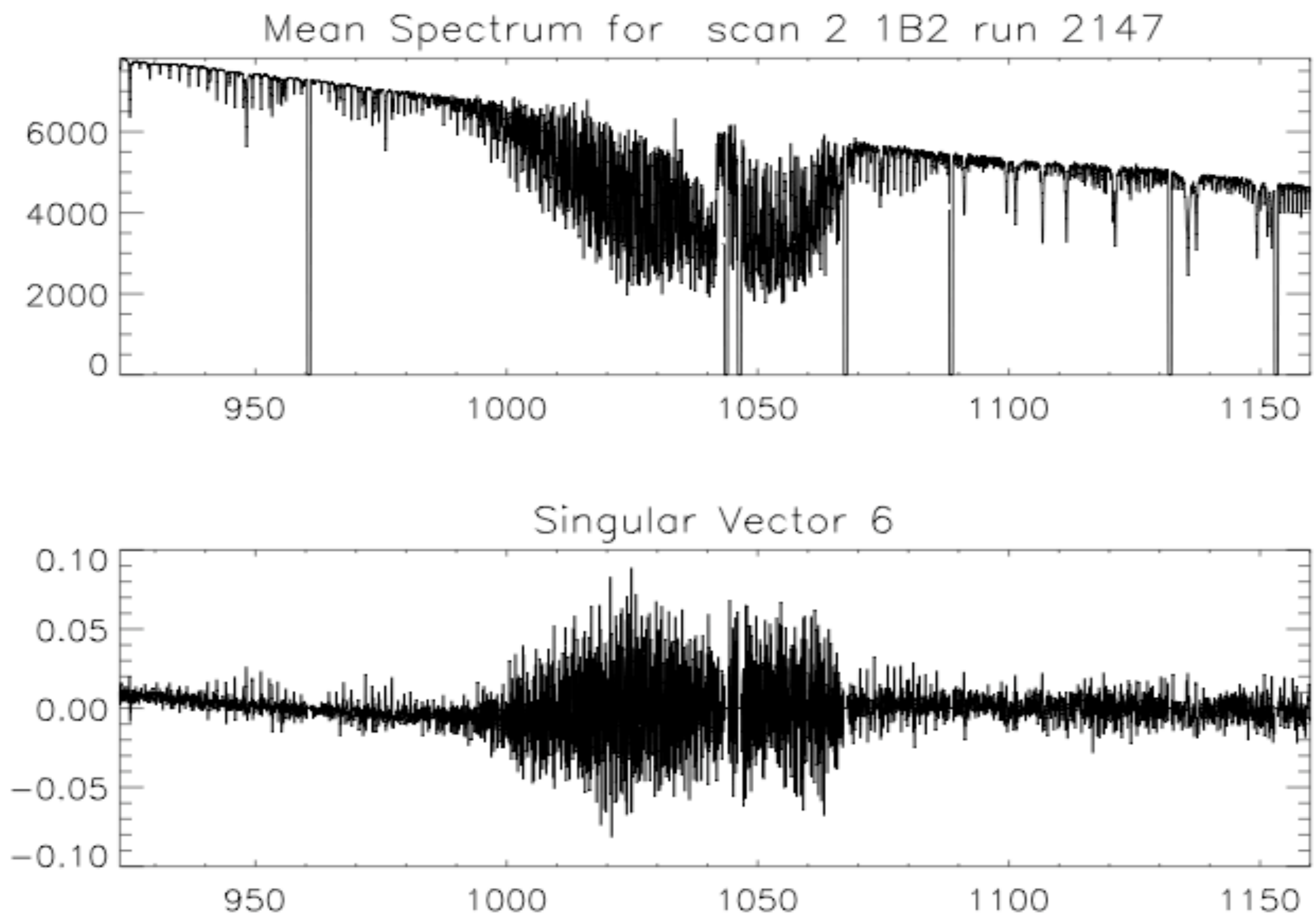
- Data spikes - unidentified

- Pixel-dependent variation in the spectra

Singular Vector 6

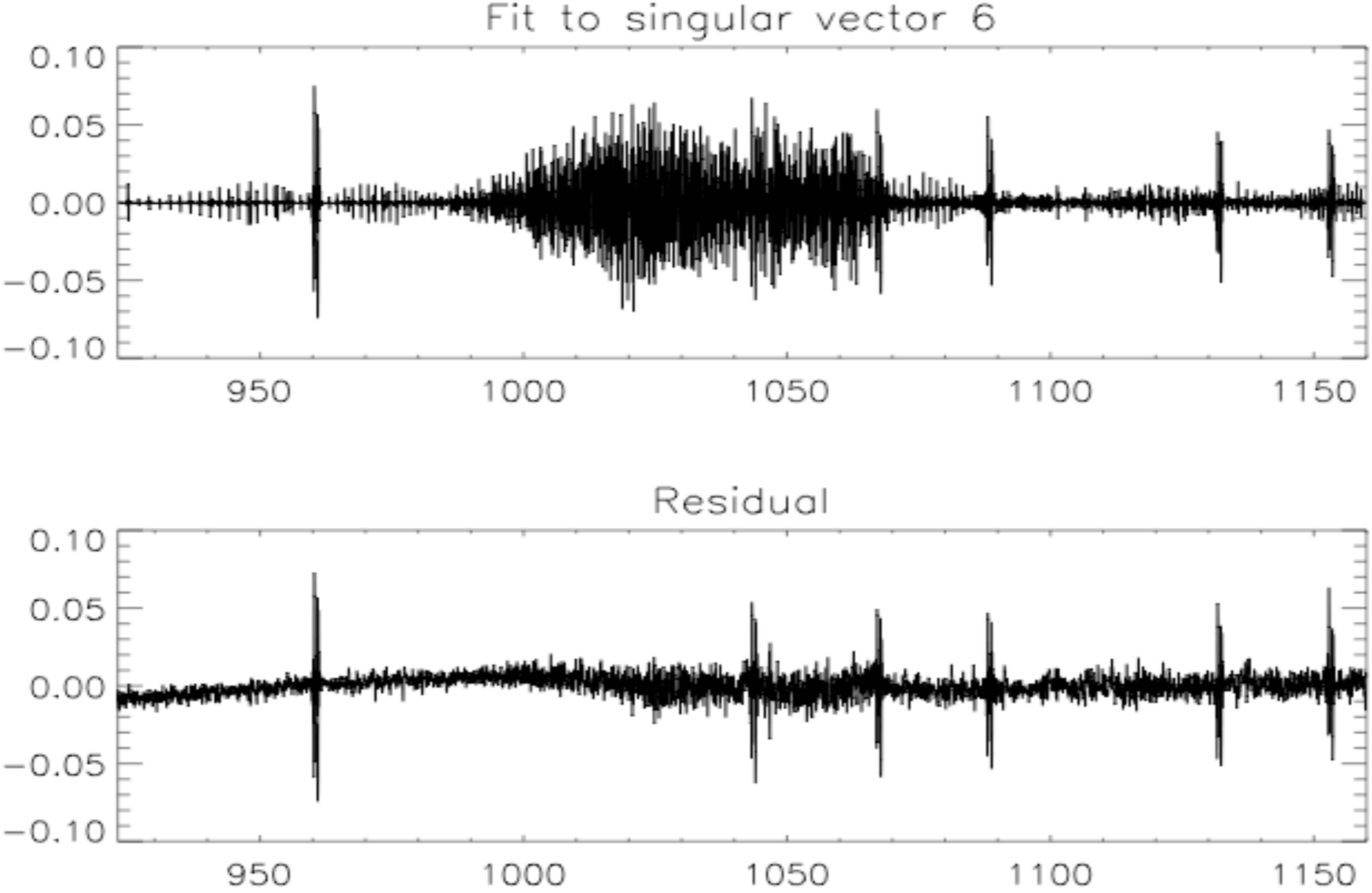
- Systematic variation across the detector array
- Must be an artifact
- Suggests systematic error in ILS
- How is it related to mean spectrum?
- Least squares fit to find function that when convolved with mean spectrum gives SV6

SV6

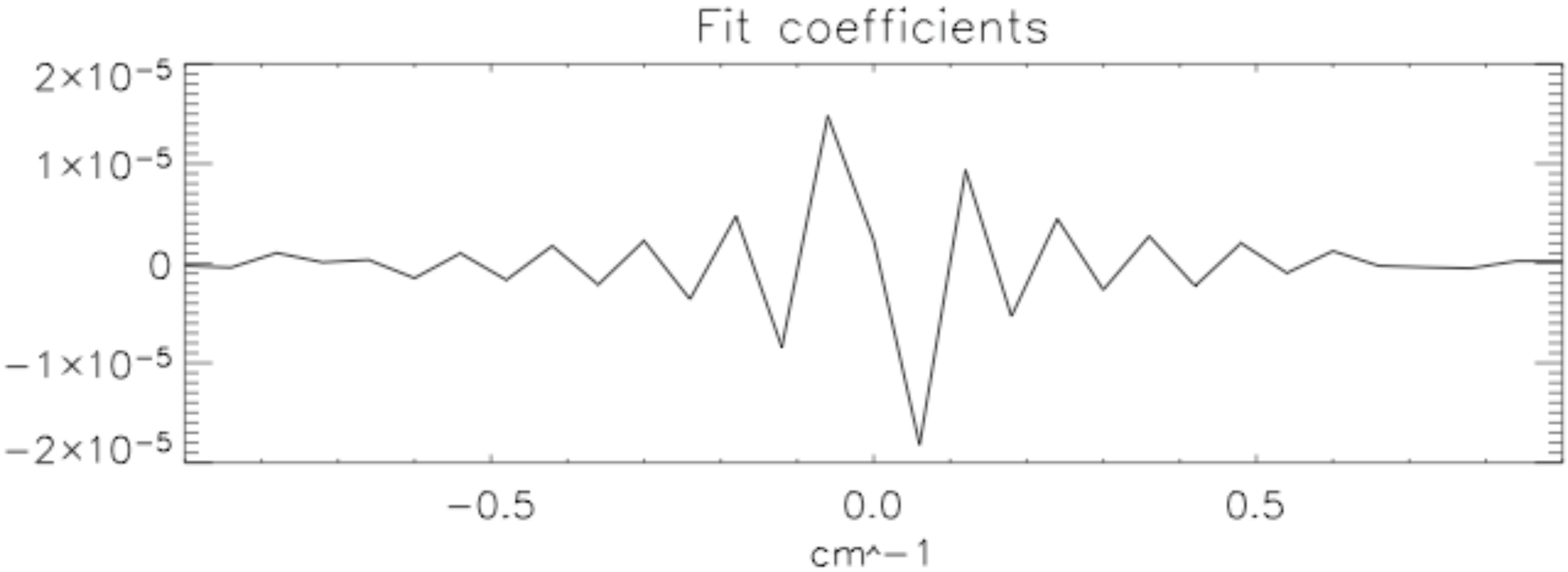


Mean Spectrum for scan 2 1B2 run 2147
6000
4000
2000
0
950
1000
1050
1100
1150
Singular Vector 6
0.10
0.05
0.00
−0.05
−0.10
950
1000
1050
1100
1150

SV6

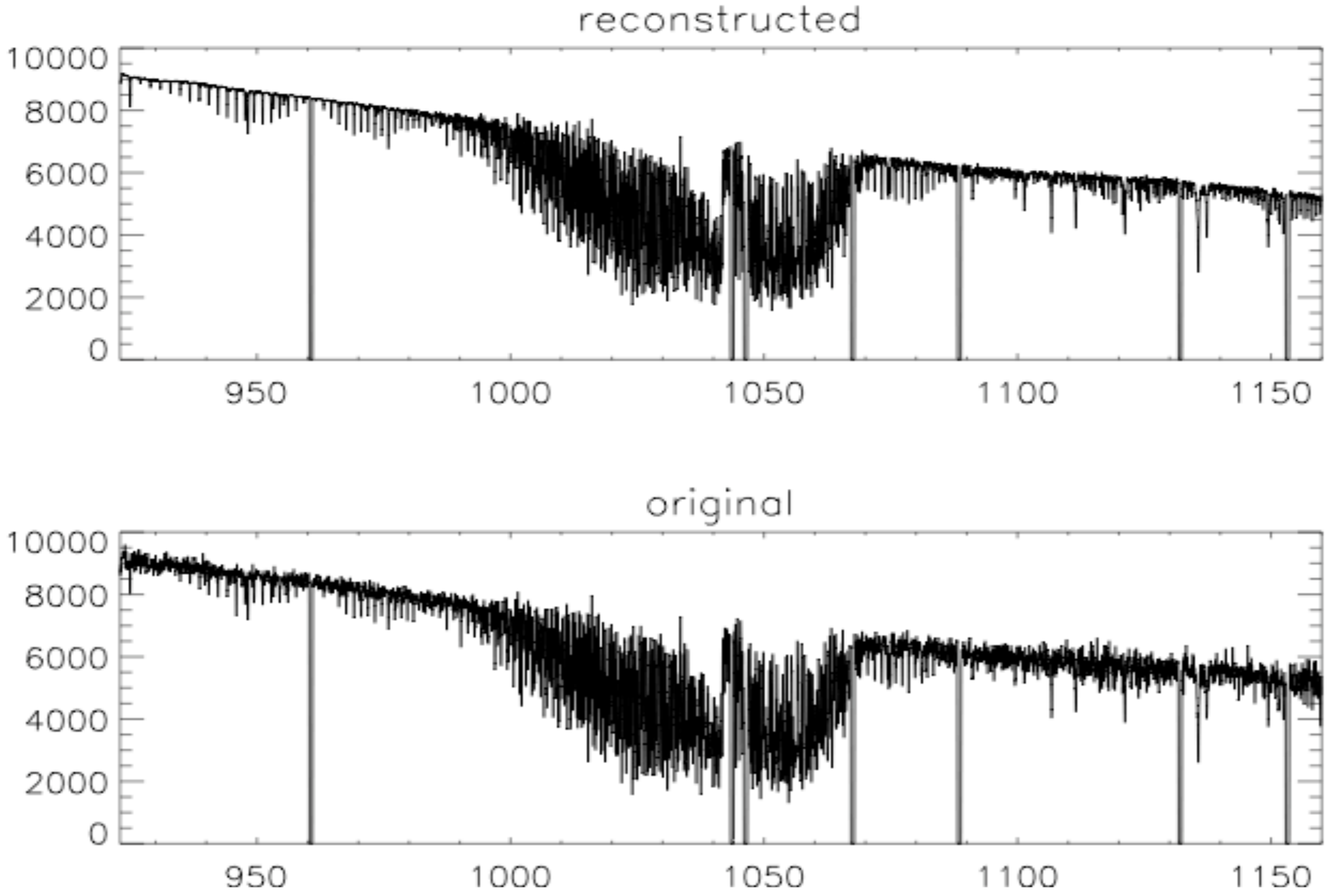

Fit to singular vector 6
0.10
0.05
0.00
−0.05
−0.10
950
1000
1050
1100
1150
Residual
0.10
0.05
0.00
−0.05
−0.10
950
1000
1050
1100
1150

SV6

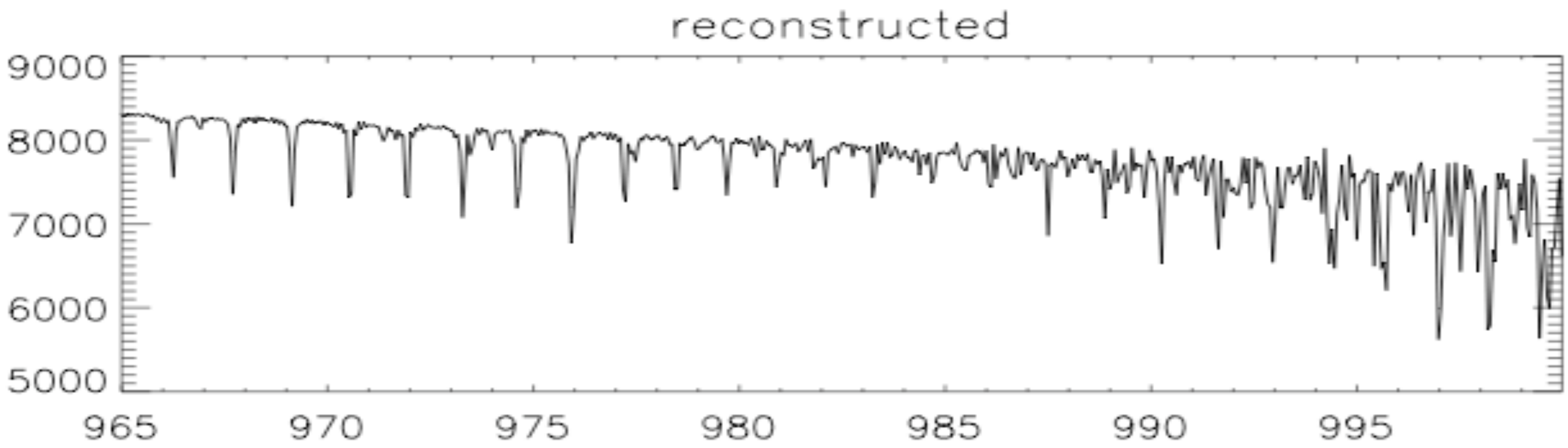


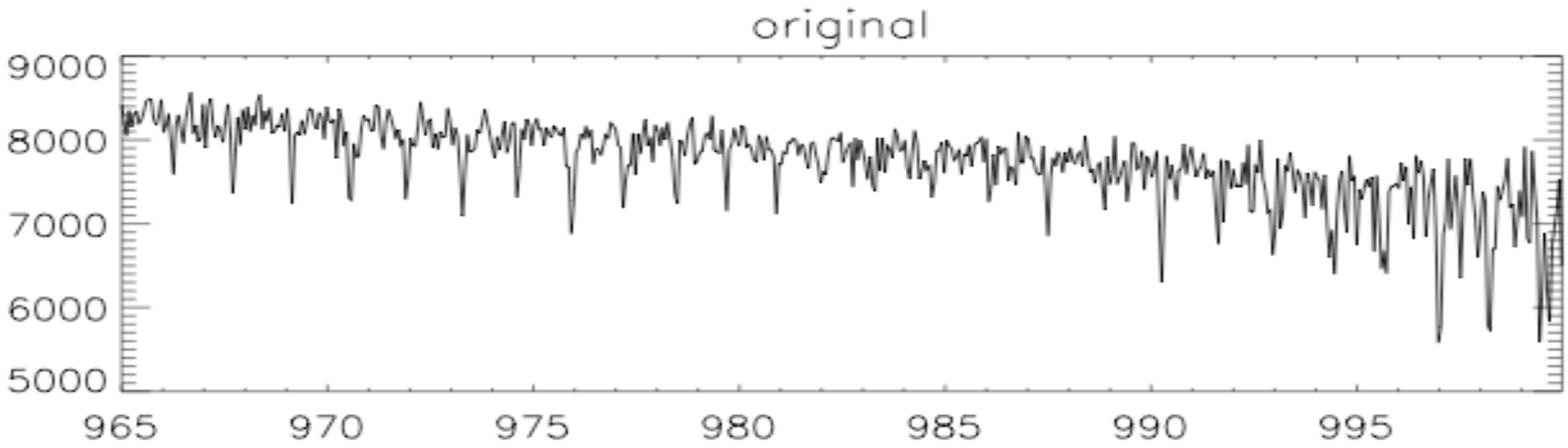
- Suggests the derivative of the ILS

Example spectrum reconstructed from 20 vectors



Example spectrum reconstructed from 20 vectors





What use is it?

- Singular vectors
  - To some extent they separate out different sources of variability
    - Atmospheric quantities
    - Artifacts in the data
- Reconstructed Spectra
  - Validation: you can see better what is going on
  - Identify artifacts
  - Retrieval from cleaner spectra
- Reconstructed Noise
  - Noise characteristics - spectrum, correlations, etc
  - Artifacts

Precautions

- Need a lot more spectra than I have used in this example
- If retrieving from reconstructed spectra, you need to pay attention to error analysis and correlations:
  - the error in the reconstructed spectrum is correlated in channel number

Rough Error Analysis

- Singular Vectors
  - Each vector is a combination of *n* (~1600) spectra
  - Each λ**u** will have noise ~$n^{-\frac{1}{2}}$ smaller
  - Reconstruction with *p* (~20) coefficients will have noise from this source ~$(p/n)^{\frac{1}{2}}$ smaller from this source.
  - White noise, but correlated between spectra
- Reconstruction coefficients
  - Each coefficient will have an error around $m^{-\frac{1}{2}}$ smaller than spectrum
  - Reconstruction will have noise ~$(p/m)^{\frac{1}{2}}$ smaller from this source.
  - A random combination of singular vectors, so correlated spectrally

Retrieval from Reconstructed Spectra

- The reconstructed spectrum has *p* (~20) degrees of freedom
- Its error covariance has rank *p*, and is singular
- A profile could in principle be retrieved from the *p* coefficients of the representation
  - if we had a forward model for the coefficients
- The obvious model, to apply the singular vectors to the complete simulated spectrum, would be very expensive

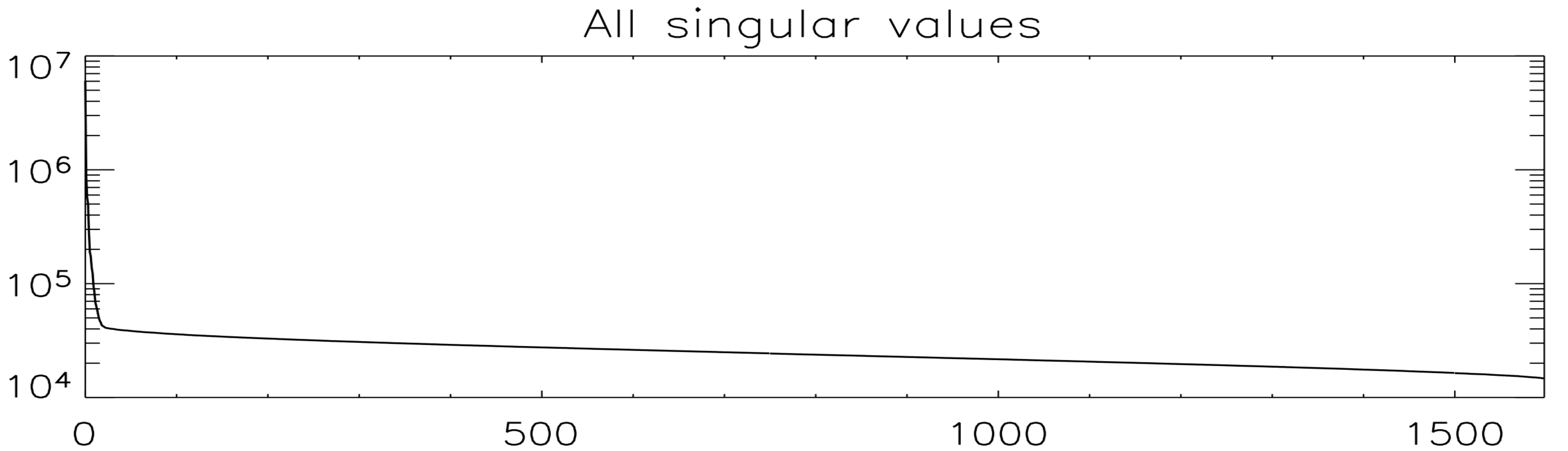
However…

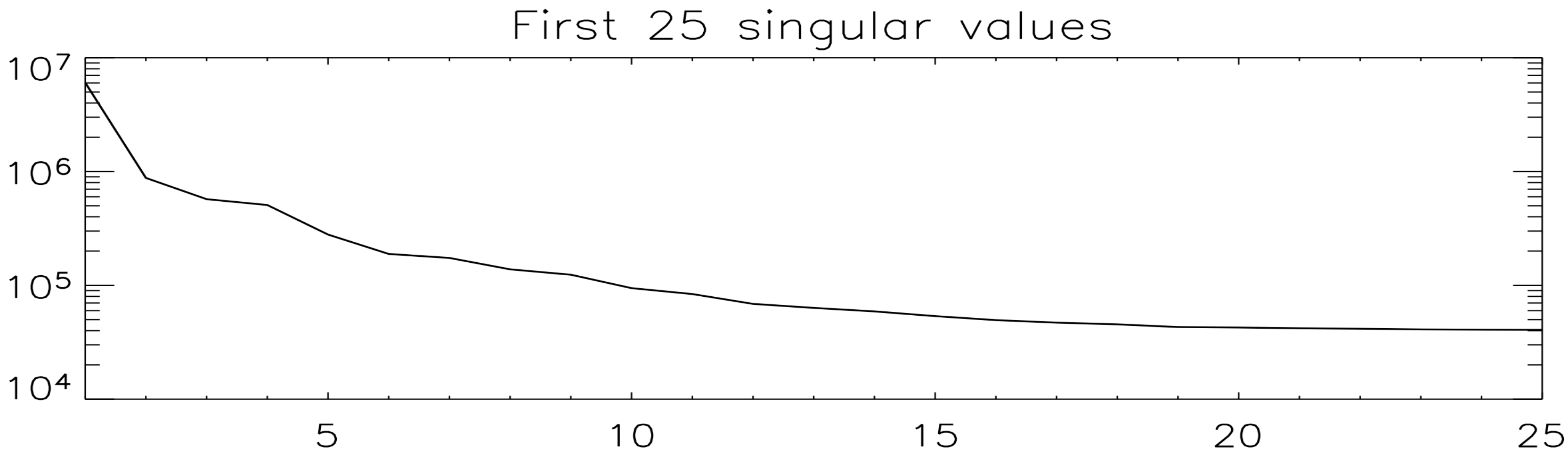
- The spectrum could in principle be re-reconstructed from just *p* spectral elements
- These *p* elements alone could be used to retrieve a profile
- An automated microwindow/channel selection process should stop finding more information after *p* elements have been selected.
- I havn't tried this yet…

Conclusion

This is a tool that I think is going to be very useful

Limb Spectra Singular Values





Limb Singular Vectors