

Atmospheric Retrieval Methods Projects

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Atmospheric Retrieval Methods

Projects: Definitions

- Retrieval characterisation:

$$\hat{\mathbf{x}} = \mathbf{R}(\mathbf{y}, \hat{\mathbf{b}}, \mathbf{x}_a, \mathbf{c}) \quad \mathbf{y} = \mathbf{F}(\mathbf{x}, \mathbf{b}) + \mathbf{e} = \mathbf{F}(\mathbf{x}_a, \mathbf{b}) + \mathbf{K}_x(\mathbf{x} - \mathbf{x}_a) + \mathbf{e}$$

$$\hat{\mathbf{x}} = \mathbf{x}_a + \mathbf{A}(\mathbf{x} - \mathbf{x}_a) + \mathbf{G}_y \mathbf{e}_y \quad \hat{\mathbf{x}} - \mathbf{x} = (\mathbf{A} - \mathbf{I})(\mathbf{x} - \mathbf{x}_a) + \mathbf{G}_y \mathbf{e}_y$$

$$\mathbf{A} = \mathbf{G}_y \mathbf{K}_x = \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{x}} \quad \mathbf{K}_x = \frac{\partial \mathbf{F}}{\partial \mathbf{x}} \quad \mathbf{G} = \frac{\partial \mathbf{R}}{\partial \mathbf{y}}$$

- MAP solution to a nearly-linear problem for Gaussian pdf's

$$\hat{\mathbf{x}} = \mathbf{x}_a + (\mathbf{K}^T \mathbf{S}_e^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1} \mathbf{K}^T \mathbf{S}_e^{-1} (\mathbf{y} - \mathbf{F}(\mathbf{x}_a))$$

$$\mathbf{G}_y = (\mathbf{K}^T \mathbf{S}_e^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1} \mathbf{K}^T \mathbf{S}_e^{-1} \quad \mathbf{A} = \mathbf{G}_y \mathbf{K} = (\mathbf{K}^T \mathbf{S}_e^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1} \mathbf{K}^T \mathbf{S}_e^{-1} \mathbf{K}$$

- Retrieval noise covariance $\mathbf{S}_n = \mathbf{G}_y \mathbf{S}_e \mathbf{G}_y^T = (\mathbf{K}^T \mathbf{S}_e^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1} \mathbf{K}^T \mathbf{S}_e^{-1} \mathbf{K} (\mathbf{K}^T \mathbf{S}_e^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1}$
- Smoothing error covariance $\mathbf{S}_s = (\mathbf{A} - \mathbf{I}) \mathbf{S}_a (\mathbf{A} - \mathbf{I})^T = (\mathbf{K}^T \mathbf{S}_e^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1} \mathbf{S}_a^{-1} (\mathbf{K}^T \mathbf{S}_e^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1}$
- Retrieval total covariance $\hat{\mathbf{S}} = \mathbf{S}_s + \mathbf{S}_n = (\mathbf{K}^T \mathbf{S}_e^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1}$



Atmospheric Retrieval Methods Projects: Definitions

- Entropy of a multivariate Gaussian distribution

$$S[P(\mathbf{y})] \propto \frac{1}{2} \ln |\mathbf{S}_y| = \frac{1}{2} \ln |\mathbf{K}\mathbf{S}_a\mathbf{K}^T + \mathbf{S}_e|$$

- Information content

$$H_m = S[P(\mathbf{y})] - S[P(\mathbf{y} | \mathbf{x})] = \frac{1}{2} \ln |\mathbf{S}_e^{-1}(\mathbf{K}\mathbf{S}_a\mathbf{K}^T + \mathbf{S}_e)| = \frac{1}{2} \ln |\mathbf{S}_e^{-1/2}\mathbf{K}\mathbf{S}_a\mathbf{K}^T\mathbf{S}_e^{-1/2} + \mathbf{I}| = \frac{1}{2} \ln |\tilde{\mathbf{K}}\tilde{\mathbf{K}}^T + \mathbf{I}|$$

$$\tilde{\mathbf{K}} = \mathbf{S}_e^{-1/2}\mathbf{K}\mathbf{S}_a^{-1/2} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^T$$

$$H_m = \sum_i \frac{1}{2} \ln(1 + I_i^2) = -\frac{1}{2} \ln |\mathbf{I} - \mathbf{A}|$$

$$(H_m)_i = \frac{1}{2} \ln(1 + I_i^2)$$



Atmospheric Retrieval Methods

Projects: Definitions

- The most probable state consistent with a measurement with m degrees of freedom and Gaussian pdf's is found minimising

$$c^2(\mathbf{x}) = (\mathbf{x} - \mathbf{x}_a)^T \mathbf{S}_a^{-1} (\mathbf{x} - \mathbf{x}_a) + \mathbf{e}^T \mathbf{S}_e^{-1} \mathbf{e} \quad \mathbf{e} = \mathbf{y} - \mathbf{F}(\mathbf{x}, \mathbf{b})$$

$$E\{\min(c^2(\mathbf{x}))\} = E\{c^2(\hat{\mathbf{x}})\} = E\{(\hat{\mathbf{x}} - \mathbf{x}_a)^T \mathbf{S}_a^{-1} (\hat{\mathbf{x}} - \mathbf{x}_a) + \hat{\mathbf{e}}^T \mathbf{S}_e^{-1} \hat{\mathbf{e}}\} = m$$

- Degrees of freedom for signal

$$d_s = E\{(\hat{\mathbf{x}} - \mathbf{x}_a)^T \mathbf{S}_a^{-1} (\hat{\mathbf{x}} - \mathbf{x}_a)\} = \text{tr}([\tilde{\mathbf{K}}^T \tilde{\mathbf{K}} + \mathbf{I}]^{-1} \tilde{\mathbf{K}}^T \tilde{\mathbf{K}}) = \text{tr}(\mathbf{A}) = \sum_i I_i^2 / (1 + I_i^2)$$

$$(d_s)_i = I_i^2 / (1 + I_i^2)$$



Atmospheric Retrieval Methods Projects: Example

- SCIA

idl

@diag

case description file? o3_CH_0.2

case file read

wf file read

noise file read

Sa file read

% Compiled module: CHOLESKY_INVERSE.

covariances inverted

KT#Sel #K computed

Shat done

Shat vectors

G done

Sn done



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Atmospheric Retrieval Methods

Projects: Example

Ss done

A done

entropy of Sa is 0.00000 bits

entropy of S_{hat} is -11.609530 bits

weighting fns scaled by root 1/Se

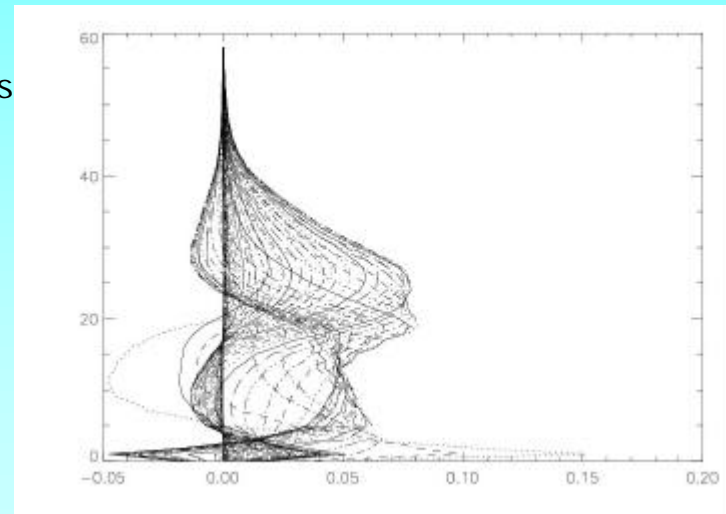
weighting fns scaled by root Sa

SVD of Ktilde

dfs: 2.1873260

info: 11.609530

zplot, A, xlabel

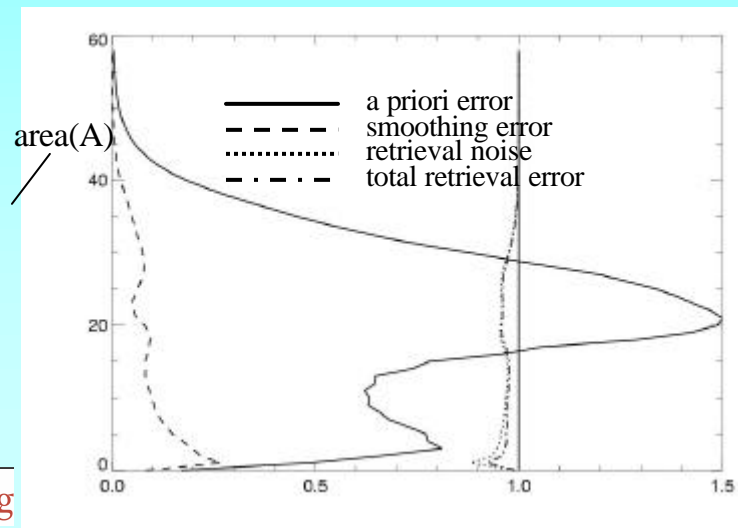


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Atmospheric Retrieval Methods Projects: Example

```
plot, sqrt(Sa[indgen(59), indgen(59)]), xlabel, xrange=[0,1.5]  
oplot, sqrt(Sn[indgen(59), indgen(59)]), xlabel, linestyle=2  
oplot, sqrt(Ss[indgen(59), indgen(59)]), xlabel, linestyle=1  
oplot, sqrt(Shat[indgen(59), indgen(59)]), xlabel, linestyle=3  
oplot, A#(fltarr(59)+1.), xlabel
```



Atmospheric Retrieval Methods

Projects: Example

@select

case description file? o3_CH_0.2

case file read

wf file read

noise file read

Sa file read

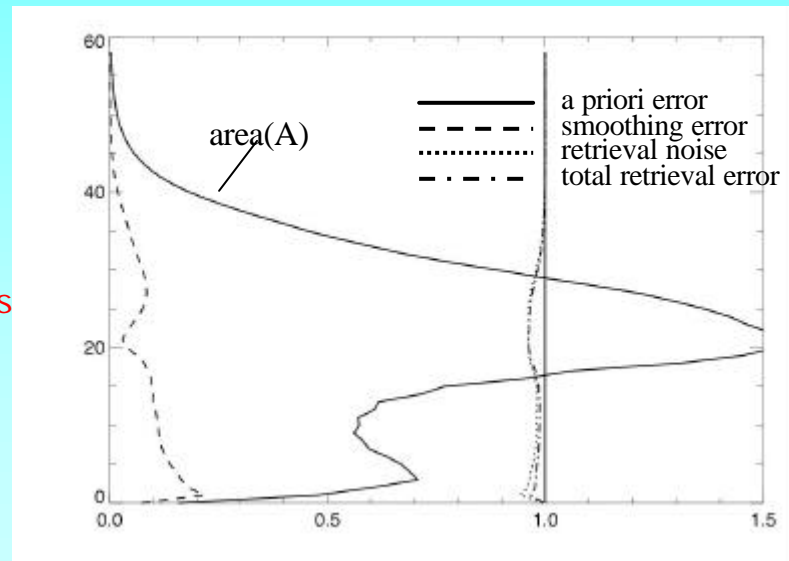
how many channels to select? 130

filename for output (n for none) ? tes

degrees of freedom: 130 (10%)

dfs: 1.5426242 (70.5%)

info: 9.4929594 (81.8%)



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