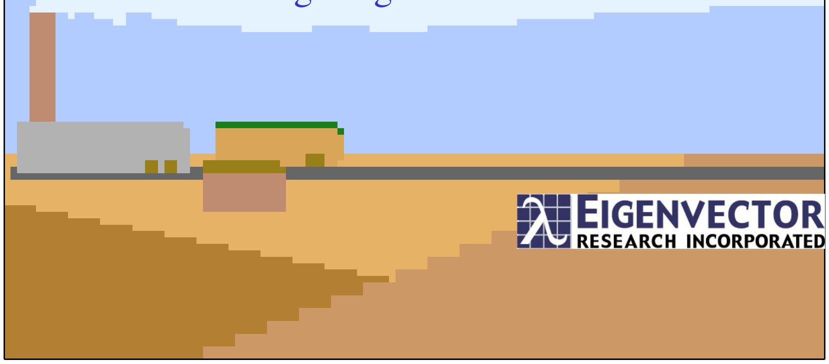
Estimation of trace vapor concentration-pathlength in plumes for remote sensing applications from hyperspectral images

Neal B. Gallagher, David M. Sheen, Jeremy M. Shaver, Barry M.Wise, and John F. Shultz
nealg@eigenvector.com



Objective and Outline

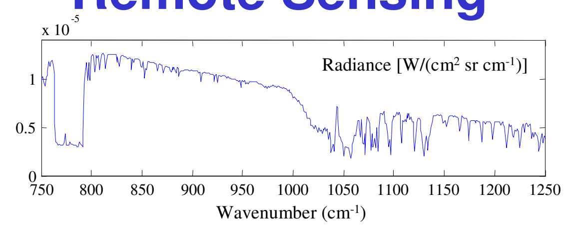
- Objective
  - Show that end members extracted from the off-plume can be used as a basis for the quantification of plume analytes
    - Allows non-negativity constraints to be employed
  - Show how mismatch between the plume temperature and estimator spectra affect the quantification error
- Remote sensing problem
- IR-SAGE (Synthetic Scene Generator)
- Quantification Algorithm
- End-Member Extraction
- Results
- Conclusions

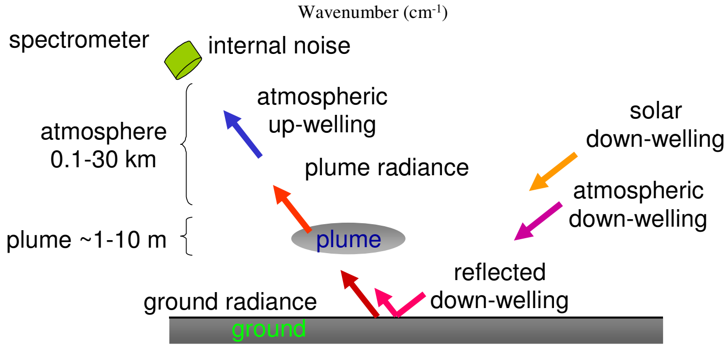
Remote Sensing Problem

- Remote sensing for chemical analytes can be split into 3 tasks:
  - Detection (where is the plume?),
  - Classification (what is in the plume?), and
  - Quantification (how much is in the plume?).
- Interest is in quantification
  - quantification is limited to concentration-pathlength since the actual pathlength is usually unknown

EIGENVECTOR RESEARCH INCORPORATED

Remote Sensing





EIGENVECTOR RESEARCH INCORPORATED

Problem with Measured Data

- Hyperspectral images are rarely well-characterized
- There are a large number of factors influencing the measured radiance
  - plume location, contents, quantities, temperature,
  - atmosphere down- and up-welling radiance, and transmittance,
  - ground emissivity and temperature ...
- are *unknown*
- so how to judge performance of algorithms?

EIGENVECTOR RESEARCH INCORPORATED

Synthetic Data

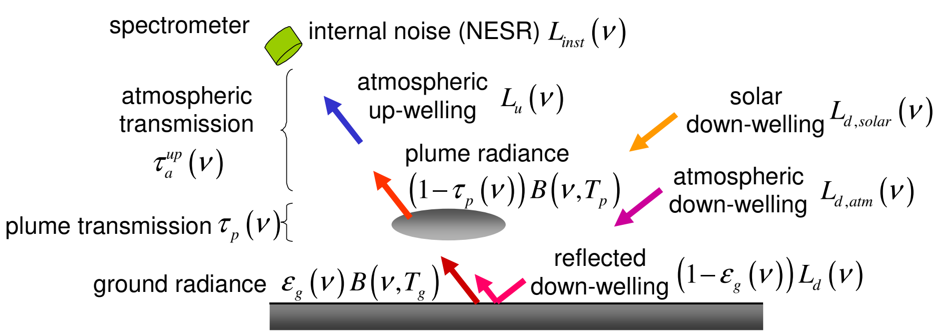
- IR-SAGE: InfraRed - Systems Analysis in General Environments
  - flexible synthetic scene generator (in MATLAB)
    - combines physical models and measured spectra
  - *everything is known*
  - can be used to test detection, classification, and quantification algorithms

EIGENVECTOR RESEARCH INCORPORATED

Radiance Model

$$L_{off}(\upsilon) = \left\{ \varepsilon_g(\upsilon)B(\upsilon,T_g) + (1-\varepsilon_g(\upsilon))L_d(\upsilon) \right\} \tau_a^{up}(\upsilon) + L_u(\upsilon)$$

$$L_{on}(\upsilon) = \left[\left\{ \varepsilon_g(\upsilon)B(\upsilon,T_g) + (1-\varepsilon_g(\upsilon))L_d(\upsilon) \right\} \tau_p(\upsilon) + \left(1-\tau_p(\upsilon)\right) B(\upsilon,T_p) \right] \tau_a^{up}(\upsilon) + L_u(\upsilon)$$



EIGENVECTOR RESEARCH INCORPORATED

How to Quantify?

- Lot’s of parameters, so ...
  - split the problem into parts, and assume some parameters are known
    - (future work)
    - assume plume location is known (detection)
    - assume plume analytes are known (classification)
- Assume that on-plume pixel “looks like” an off-plume pixel if there were no plume
  - on-plume “background” lies in subspace spanning off-plume pixels

EIGENVECTOR RESEARCH INCORPORATED

Rearrange Radiance Model for τ_p

as $\tau_p \to 1$ (no plume), $L_{on}(\upsilon) \to L_{off}(\upsilon) \equiv L_{bkg}(\upsilon)$

$$\tau_p = e^{-\mathbf{cS}^T} = \frac{L_{on}(\upsilon) - L_u(\upsilon) - \tau_a^{up} B(\upsilon, T_p)}{L_{bkg}(\upsilon) - L_u(\upsilon) - \tau_a^{up} B(\upsilon, T_p)}$$

EIGENVECTOR RESEARCH INCORPORATED

Assumptions

- Assumed we know: $\bar{L}_{u,off}$, $\bar{\tau}_{a,off}^{up}$, T_p
- Don't require knowledge of: T_g and ε_g
- Taylor Series, substitute known parameters

$$\mathbf{cS}^T(\upsilon) = \frac{L_{on}}{d(\upsilon)} - \frac{L_{bkg}}{d(\upsilon)} \qquad d(\upsilon) = \bar{L}_u + \bar{\tau}_a^{up} B\left(T_p\right) - \bar{L}_{bkg}$$

$$\mathbf{c}\tilde{\mathbf{S}}^T(\upsilon) = L_{on} - L_{bkg}$$

EIGENVECTOR RESEARCH INCORPORATED

Quantification: ELS

- Extended mixture model (extended least squares) which can be solved for $[\mathbf{c} \quad \mathbf{t}]$ using least squares

$$\mathbf{l}_{on} = [\mathbf{c} \quad \mathbf{t}]\left[\tilde{\mathbf{S}} \quad \mathbf{P}_{bkg}\right]^T$$

- End-member extraction for background basis

$$\mathbf{l}_{on} = \left[\mathbf{c} \quad \mathbf{c}_{bkg}\right]\left[\tilde{\mathbf{S}} \quad \mathbf{S}_{bkg}\right]^T$$

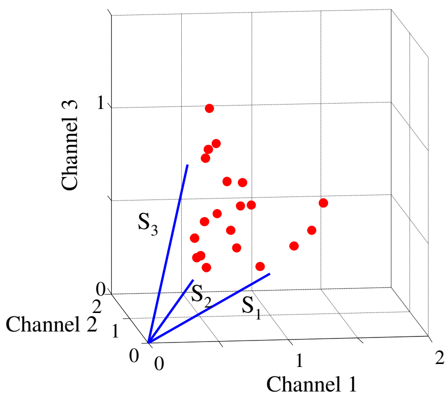
  - can apply non-negativity constraints

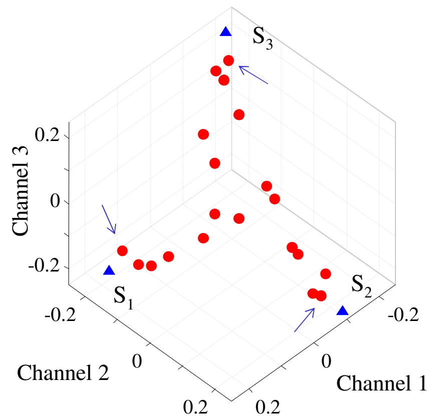
End-Member Extraction

- Initial solution: extremes of mean centered 1-norm
- ALS with non-negativity constraints
- Sequential for “smaller” factors
  - extracted 14 to 53 factors
- Provides a basis on which non-negativity constraints can be used in quantification

$$\mathbf{L}_{off} = \mathbf{c}_{bkg}\mathbf{S}_{bkg}^T + \mathbf{E}$$

End-Member Extraction





Quantification: GLSI

- ELSI predictions were good for narrow-featured spectra but not as good for broad-featured spectra

$$\mathbf{c}\tilde{\mathbf{S}}_i^T(\upsilon) = \left[L_{on}(\upsilon) - \bar{L}_{off}(\upsilon)\right] - \left[L_{off}(\upsilon) - \bar{L}_{off}(\upsilon)\right]$$

$$\mathbf{W} = \left[\mathbf{L}_{off} - \bar{\mathbf{L}}_{off}\right]$$

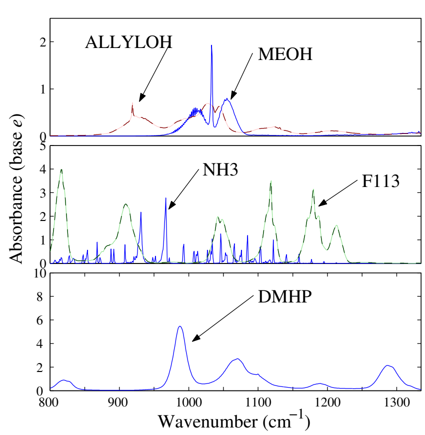
$$\hat{\mathbf{c}} = \left(\mathbf{l}_{on} - \bar{\mathbf{L}}_{off}\right)\mathbf{W}^{-1}\left[\tilde{\mathbf{S}} \quad \mathbf{S}_{bkg}\right]\left(\left[\tilde{\mathbf{S}} \quad \mathbf{S}_{bkg}\right]^T \mathbf{W}^{-1}\left[\tilde{\mathbf{S}} \quad \mathbf{S}_{bkg}\right]\right)^{-1}$$

- GLS, after the last ELSI iteration, resulted in better estimates for broad-featured

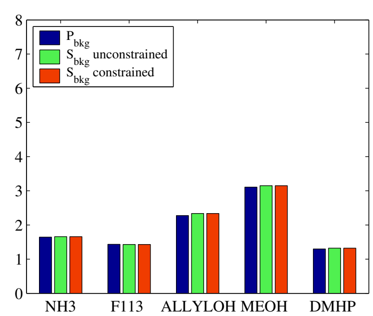
Algorithm Testing

- Image 128x128 x 536 (800 to 1335 cm^{-1})
  - 1, 2, 4, 8, 128 different background materials ε_g
  - temperature variability, T_p-T_g (12 to 32 K)
  - plume 16x128 pixels
    - plume spectra at 298 K, estimator at 298 K: matched
    - plume spectra at T_p, estimator at 298 K: unmatched
  - 5 analytes in the plume, 9 to 26 ppm·m
  - atmospheric variability
  - 0.112 cm^{-1} res, 0.06 cm^{-1} spacing, convoluted to 1 cm^{-1}

Unconstrained vs. Constrained

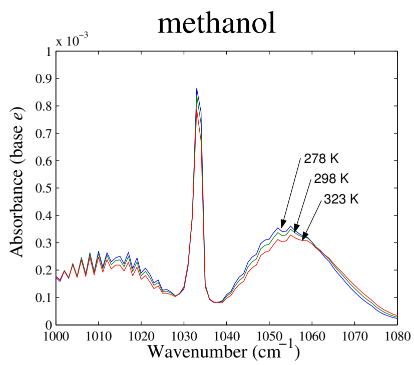


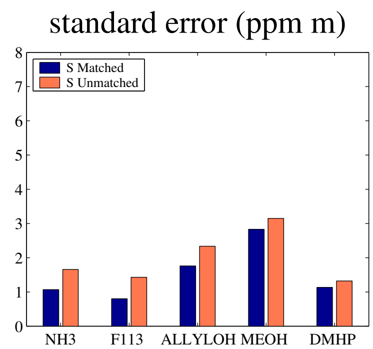
standard error (ppm m)



Matched vs. Unmatched

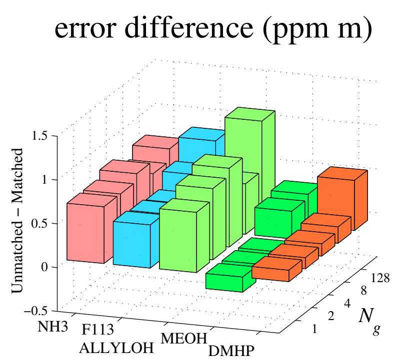
- temperature mismatch ⇒ higher estimation error





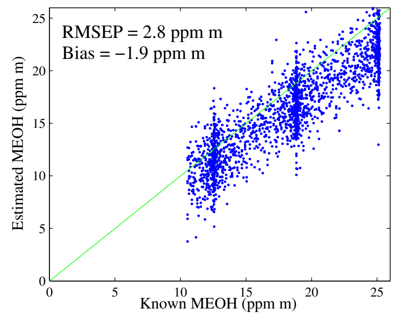
Unmatched - Matched

- Mismatch generally results in higher error



Model Bias

- Estimates of **c** tend to have a low bias due to model assumptions
  - Taylor series approx.
- Temperature mismatch can result in a high bias that partially offsets the model bias



EIGENVECTOR RESEARCH INCORPORATED

Conclusions

- End member extraction can be used to obtain a basis on which non-negativity constraints can be applied
- Temperature mismatch between the plume temperature and the spectrum used for estimation generally results in higher estimation error

EIGENVECTOR RESEARCH INCORPORATED

Acknowledgement

Funding for this work was provided by Pacific Northwest National Laboratory (PNNL), Richland, WA, USA, operated by Battelle for the U.S. Department of Energy. The work at PNNL was funded by the U. S. D.O.E. under Contract DE-AC06-76RL01830.

Extra Slides

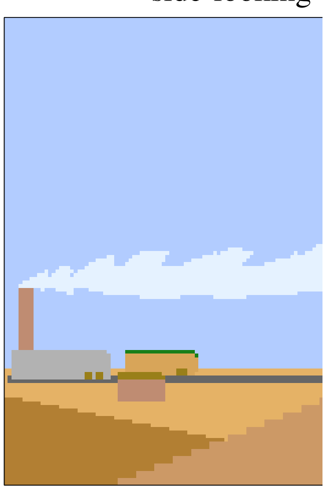
Summary of Assumptions

- plume location is known*
- plume analytes are known*
- for off-plume $\bar{L}_u$,** $\bar{\tau}_a^{up}$,* and $\bar{L}_{bkg}$* are known
- T_p is known*
- L_{bkg} lies in subspace spanned by off-plume $\mathbf{P}_{bkg}$

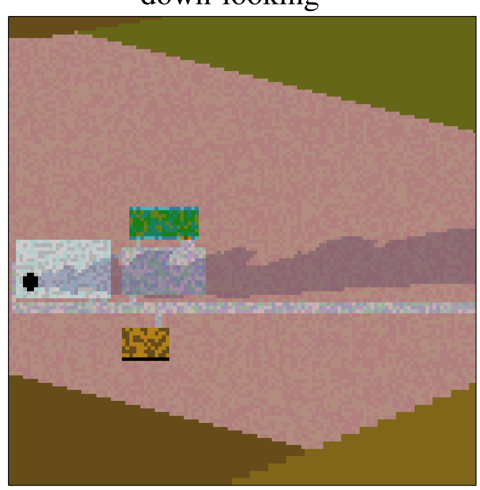
* same assumption as present state-of-the-art
** present state of the art assumes T_g is known

Scenarios

side-looking



down-looking

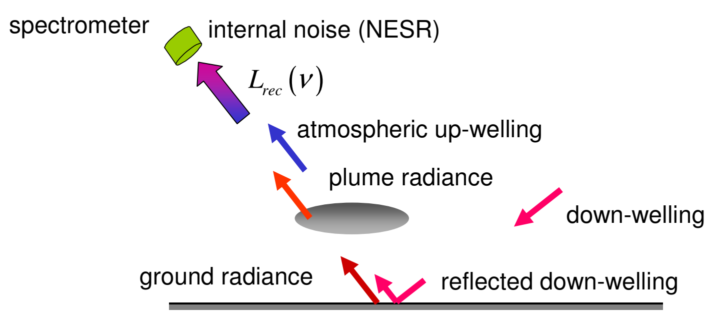


Noise Model

$$NESR(\upsilon) = {L_{rec}(\upsilon)}\Big/{SNR(\upsilon)}$$

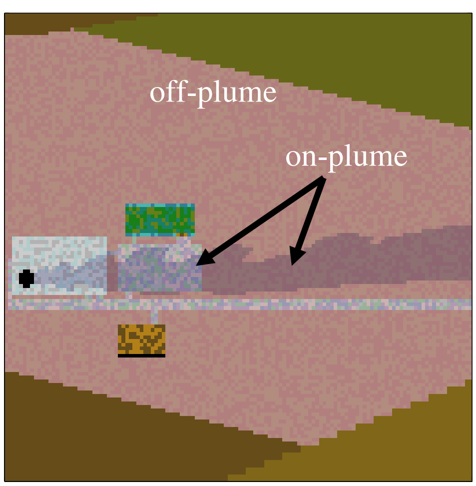
$$SNR(\upsilon) = \frac{\text{number of signal photo-electrons}}{(\text{total number of carriers from all sources})^{1/2}}$$

multiple sources:
fore optics, cold shield, cold filter, spectrometer body, electronics ...



EIGENVECTOR RESEARCH INCORPORATED

Quantification



ples for down-
ıg scenarios

be used for side-, up-

ne:

know where the
me is (detection), and

know what is in the
me (classification)

EIGENVECTOR RESEARCH INCORPORATED

Not all terms are known...

- Approximate $e^{-\mathbf{cS}^T} \approx 1 - \mathbf{cS}^T$
- isolate $\mathbf{cS}^T$
- and assume $L_u(\upsilon) \approx \bar{L}_{u,off}(\upsilon)$

  $\tau_a^{up}(\upsilon) \approx \bar{\tau}_{a,off}^{up}(\upsilon)$

  T_p known
- yielding

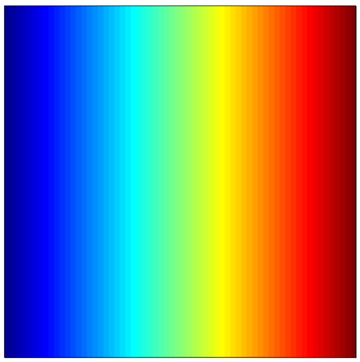
$$\mathbf{cS}^T(\upsilon) = \frac{L_{on} - L_{bkg}}{\bar{\tau}_{a,off}^{up} B(T_p) + \bar{L}_{u,off} - L_{bkg}}$$

Algorithm Testing

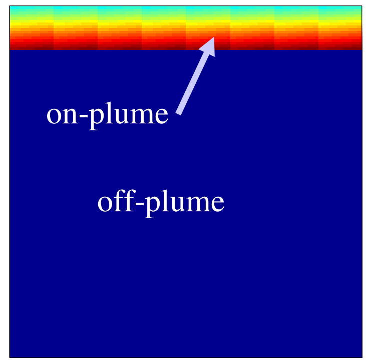
- Image 128x128 x 536 (800 to 1335 cm^{-1})
  - 1, 2, 4, 8, 128 different background materials ε_g
  - T_g (284 to 300 K), T_p-T_g (12 to 32 K)
- Plume 16x128 (9 to 26 ppm·m)
  - 1 to 4 analytes in the plume
- US 76 Standard Atms
  - 101 different FASCODE realizations
    - 1 % T and 3 % C variation w/in each layer
  - H_20, CO_2, O_3, N_2, CO, CH_4, O_2, and 25 others
- All spectra
  - 0.112 cm^{-1} res, 0.06 cm^{-1} spacing
  - convoluted to 1 cm^{-1}

“Mathematical Construct”

background



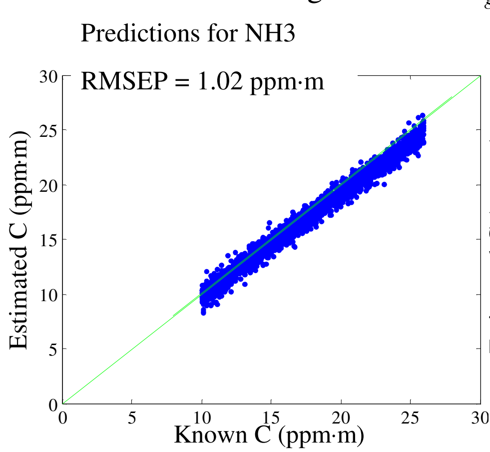
plume

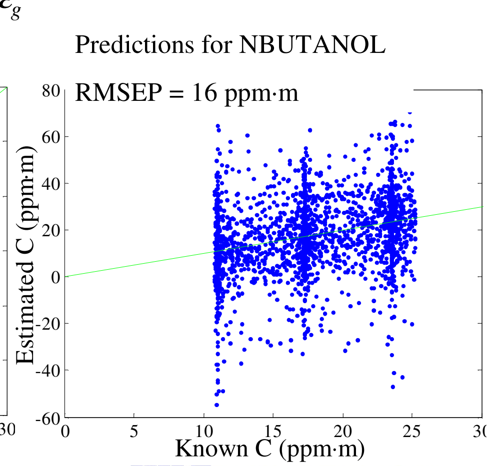


Results: 4 Dissimilar Analytes

Plume: NH_3, N-Butanol, F113, CH_4

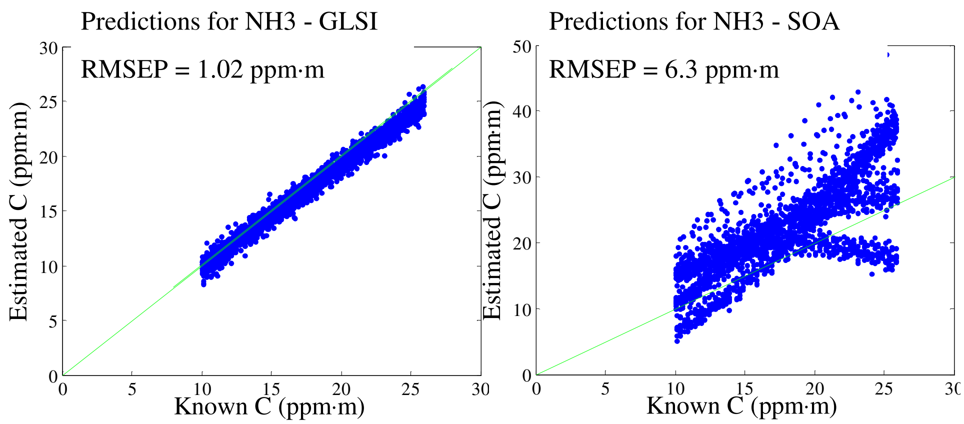
Background: 128 ε_g





Results: 4 Dissimilar Analytes

Plume: NH3, N-Butanol, F113, CH4



EIGENVECTOR RESEARCH INCORPORATED

Results: GLSI / SOA

- Compare GLSI to State-of-the-Art (SOA)
- For 4-analyte plume of dissimilar analytes

	RMSEP (ppm·m)	
Analyte	GLSI	SOA
NH3	1.0	6.3
NBUTANOL	16	69
CH4	39	49
F113	1.0	8.3

EIGENVECTOR RESEARCH INCORPORATED

Results: Num. of Backgrounds

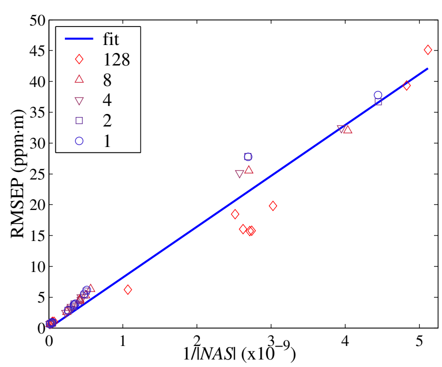
- Compare GLSI vs number of backgrounds
- For 4-analyte plume of dissimilar analytes

RMSEP (ppm·m)	Number of Backgrounds				
Analyte	128	8	4	2	1
NH3	1.0	0.85	0.85	0.93	0.94
NBUTANOL	16	4.7	3.4	3.9	3.9
CH4	39	32	32	36	38
F113	1.0	0.65	0.63	0.67	0.66

EIGENVECTOR RESEARCH INCORPORATED

Estimation vs. NAS

- Net Analyte Signal accounts for spectral modification and number of basis vectors in $\mathbf{P}_{bkg}$



EIGENVECTOR RESEARCH INCORPORATED