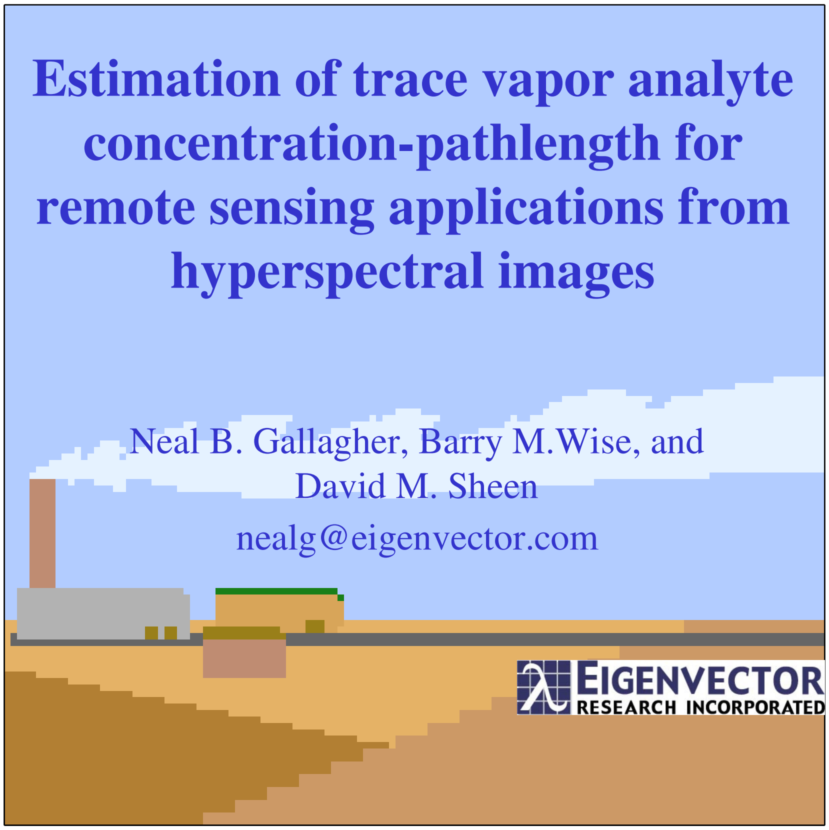

Estimation of trace vapor analyte concentration-pathlength for remote sensing applications from hyperspectral images

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Outline

- Remote sensing objective
- IR-SAGE (Synthetic Scene Generator)
  - Radiance model
  - Noise model
- Quantification
- Results
- Conclusions
- Future work

Objective

- 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

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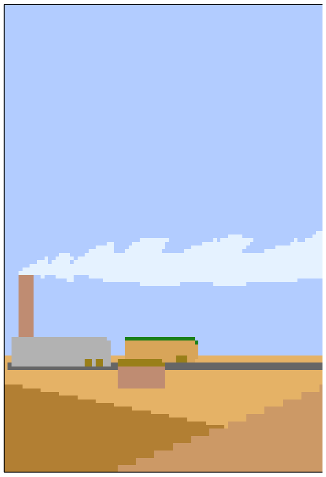
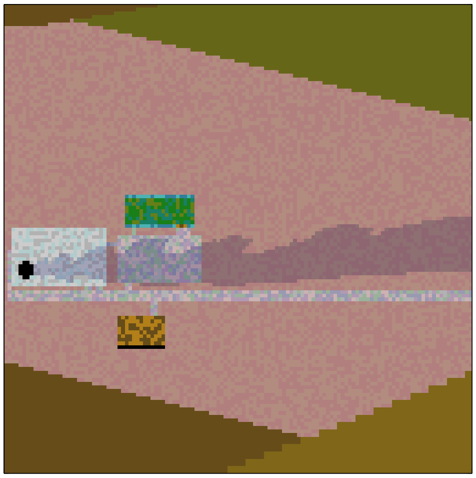
Scenarios

side-looking



down-looking



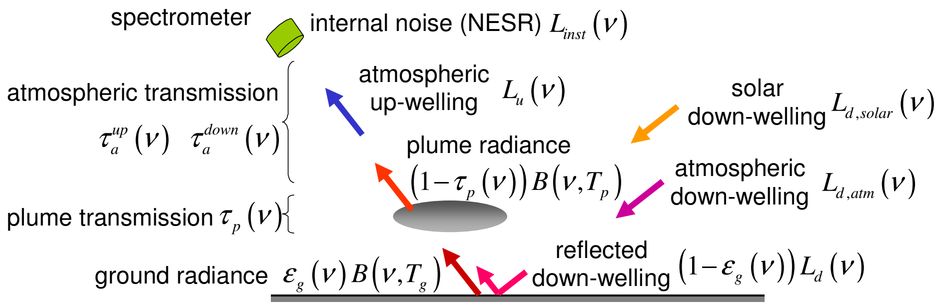
IR-SAGE

- Hyperspectral images are rarely well-characterized
  - plume location, contents, and concentration-pathlength are *unknown*
  - background, atmospheric variability, ground temperature, and plume temperature are *unknown*
- IR-SAGE: InfraRed - Systems Analysis in General Environments
  - flexible synthetic scene generator (in MATLAB)
  - *everything is known*
  - can be used to test detection, classification, and quantification algorithms

Radiance Model

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

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



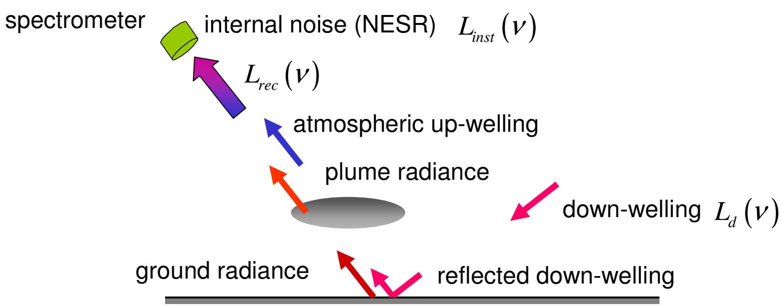
Noise Model

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

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

multiple sources:

fore optics, cold shield, cold filter, spectrometer body, ...



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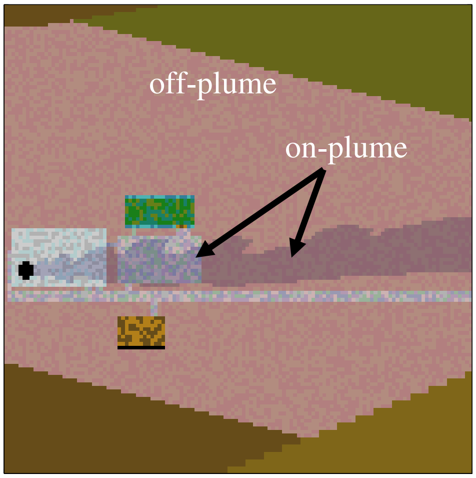
Quantification: Setup



ples for down-
ıg scenarios

be used for side-, up-

ssumed that:

know where the
me is (detection), and

know what is in the
me (classification)

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Quantification: Setup

- Rearrange radiance equations for plume transmittance and substitute

$$\tau_p(\nu) = e^{-\mathbf{cS}^T(\upsilon)} \approx 1 - \mathbf{cS}^T(\upsilon)$$

- result is

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

- where L_{bkg} is what an on-plume pixel would look like in the absence of plume (i.e. it should look like an off-plume pixel)

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Quantification: Setup

1) Approx. L_u, τ_a^{up}, and L_{bkg} with respective means from the off-plume $\bar{L}_u$, $\bar{\tau}_a^{up}$, and $\bar{L}_{bkg}$

2) Assume T_p is known

- previous work assumed that we know

T_p, T_g, $\bar{\tau}_a^{up}$ and $\bar{L}_{bkg}$ (and possibly ε_g or $\bar{\varepsilon}_g$)

3) Multiply each spectra by the denominator term

$d(\upsilon) = \bar{\tau}_a^{up}B(T_p) + \bar{L}_u - \bar{L}_{bkg}$ to yield

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

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Quantification: ELS

1) Extended Least Squares (ELS)

- assume that L_{bkg} lies in the sub-space spanned by the off-plume pixels $L_{off}(\upsilon) = \mathbf{TP}_{bkg}^{T}(\upsilon) + \mathbf{E}(\upsilon)$

2) Extended mixture model

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

- which can be solved for $[\mathbf{c} \quad \mathbf{t}]$ using least squares

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

- estimates tend to be ~biased so what else can be done?

Quantification: ELSI

- In ELS, estimates of $\hat{\mathbf{t}}_i$ are often of little interest
- In this case, it provides an estimate of L_{bkg} behind the plume!
  - The equation is non-linear in the background radiance

i) re-estimate the denominator term

$$d_i(\upsilon) = \bar{\tau}_a^{up} B\left(T_p\right) + \bar{L}_u - \hat{\mathbf{t}}_i \mathbf{P}_{bkg}^{T}(\upsilon)$$

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

$$[\mathbf{c} \quad \mathbf{t}_{i+1}]\left[\tilde{\mathbf{S}}_i \quad \mathbf{P}_{bkg}\right]^{T} = \mathbf{L}_{on}$$

Quantification: GLSI

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

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

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

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

- The GLS weighting, after the last ELSI iteration, resulted in ~good estimates for broad-featured

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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

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_2$0, 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}

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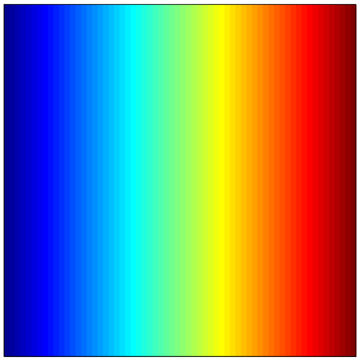
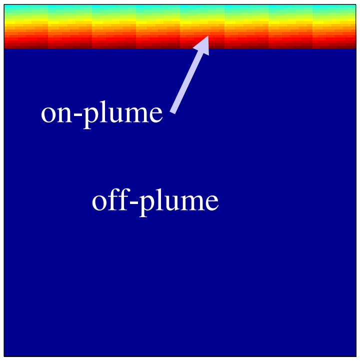
"Mathematical Construct"

background



plume



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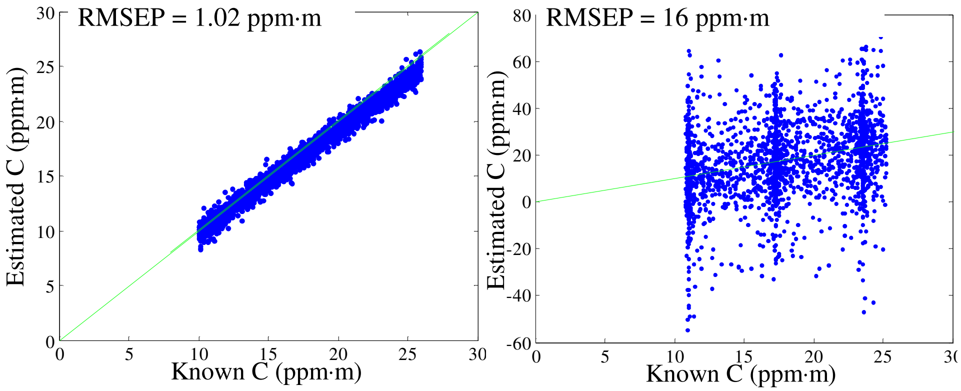
Results: 4 Dissimilar Analytes

Plume: NH3, N-Butanol, F113, CH4
Background: 128 ε_g



Predictions for NH3

RMSEP = 1.02 ppm·m

Predictions for NBUTANOL

RMSEP = 16 ppm·m

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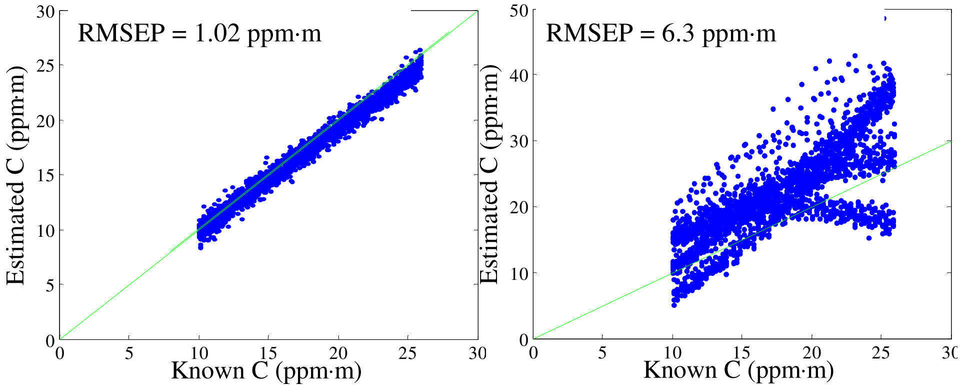
Results: 4 Dissimilar Analytes

Plume: NH3, N-Butanol, F113, CH4



Predictions for NH3 - GLSI

RMSEP = 1.02 ppm·m

Predictions for NH3 - SOA

RMSEP = 6.3 ppm·m

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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

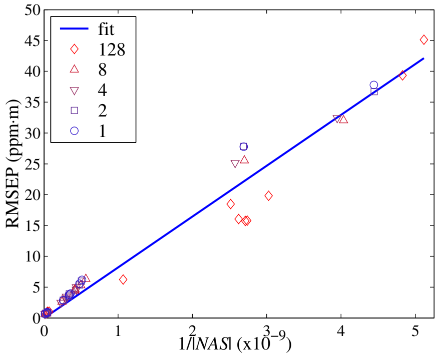
Results: Num. of Backgrounds

- 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

Estimation vs. NAS

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



Conclusions

- IR-SAGE synthetic hyperspectral images
  - highly flexible code
  - testing and comparing algorithms
- Iterative quantification uses ELS and GLS
  - removes many of the biases in the SOA and
  - with fewer required assumptions
- Quantification strongly dependent on NAS
  - scenario specific (background, atms variability, temperatures)

Future Work

- develop detection (plume location) algorithms
- develop classification (plume analyte identification) algorithms
- obtain estimates of off-plume $\bar{L}_u$, $\bar{\tau}_a^{up}$, and T_p

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