Detection and Characterization of Chemical Vapor Fugitive Emissions from Hyperspectral Infrared Imagery by Nonlinear Optimal Estimation

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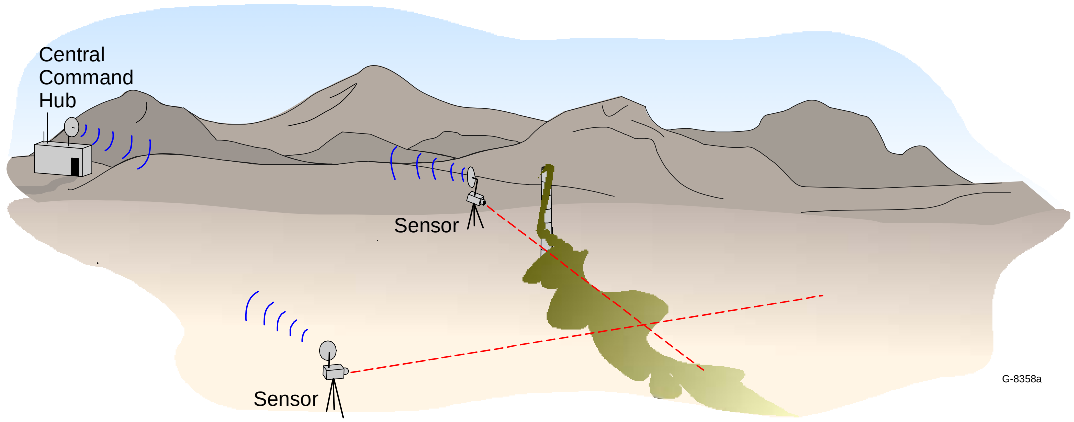
Agenda

- ***Introduction***

- **Nonlinear estimation**
  - Algorithm formulation
  - Test data
  - Results

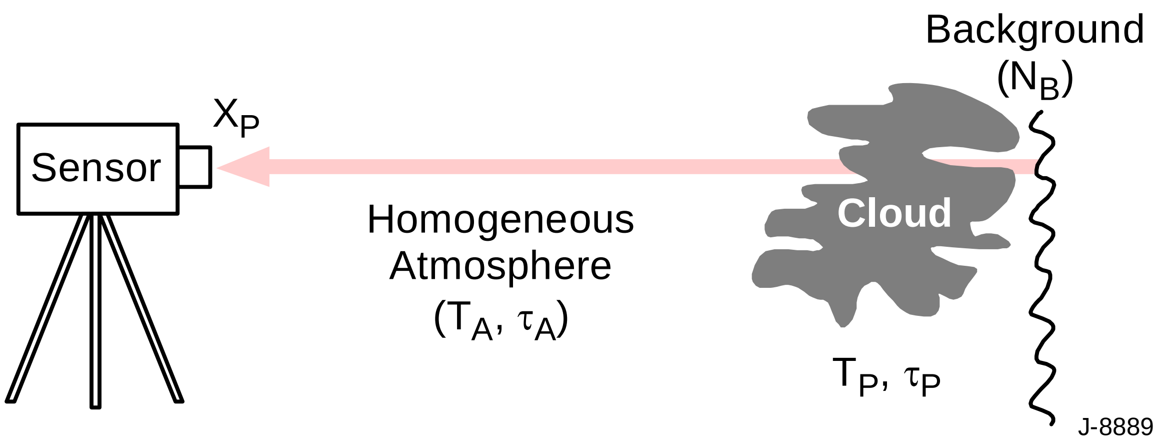
- **Conclusions**

Algorithm Development: Overview



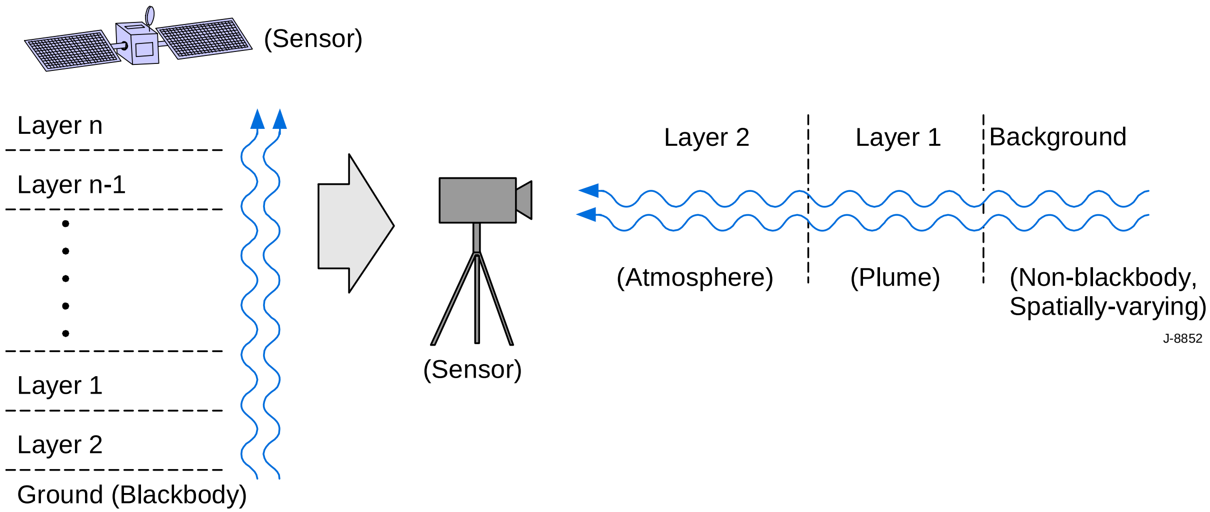
- **Objectives**
  - Improve pixel-level detection: Reduce probability of false alarm for given P_d
  - Address optically-thick plumes: Improve accuracy of estimated path integrated concentration (column density, CL)
  - Compatible with real-time processing
- **Limitations of current practice**
  - Matched-filter-based detection presumes optically-thin plume
  - Other approaches require prior measurements of background – not compatible with on-the-move detection
- ***Payoff: Improve detection immediately following large-scale release, low-lying plumes; improve mass estimate***

Problem Formulation



- **Ensemble of measured spectra**
- **Measured spectra are nonlinear functions of atmospheric temperature, constituent profiles, background characteristics, etc.**
- **Desire inverse solution to radiative transfer equation (RTE)**
- **Inverse solution is mathematically ill-posed – no unique solution for R_n**

Relation to Atmospheric Profile Retrieval



- **Stratified atmosphere model**
- **Profile retrieval**
  - Many stratifications
  - Simple background
  - Apply constraints to layer-to-layer variation
- **Plume detection**
  - Simple atmosphere
  - Complicated background
  - Apply constraints to background characterization

Simplified Radiative Transfer Model

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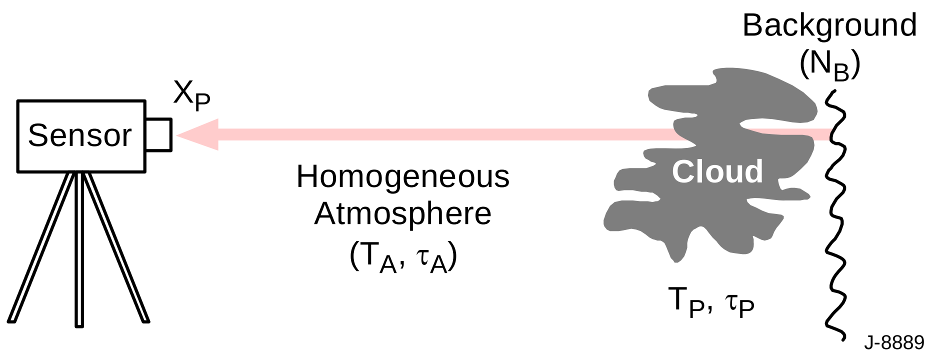

$$x_p = x_0 + (1-\tau_p)\cdot\left[(L_a - x_0) + \tau_a \cdot (L_p - L_a)\right]$$

	Linear (approx.)	Non-Linear (exact)
Plume transmission (τ_p)	**1-αs**	***exp(-αs)***
Radiance contrast (L_a-x_0)	$\propto \Delta T_{eff}$	***any***
Plume temperature (T_p)	**$T_p = T_a$**	**$T_p = T_a$**
Atmospheric scattering	**No**	**No**

- **Simplifying assumptions:**
  - Homogeneous atmosphere between sensor and vapor cloud
  - Cloud is at air temperature
- **Compare performance of non-linear (exact) RT model with linearized approximation**

Adaptive InfraRed Imaging Spectroradiometer (AIRIS)

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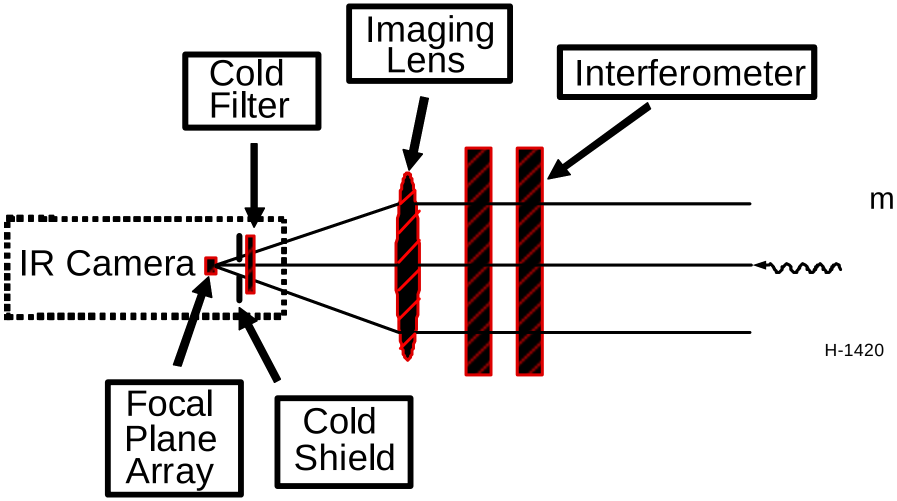

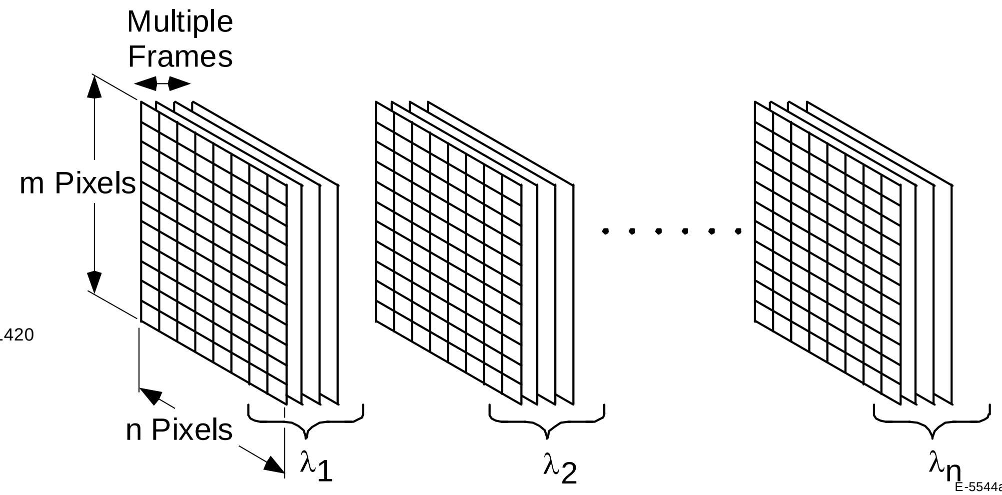

- **Imaging Fabry-Perot spectrometer**
  - Mirror spacing ~ λ
  - Staring IR FPA
  - Band sequential data acquisition
  - Co-registration of narrowband images
  - Tune time ~ 2 ms
- **Selective sampling of wavelengths**
  - Acquire imagery only at wavelengths which facilitate target ID
  - Minimize data volume
- **Wide field-of-view, wide spectral coverage**

TEP Detection: Shortcoming of Thin Plume Approximation

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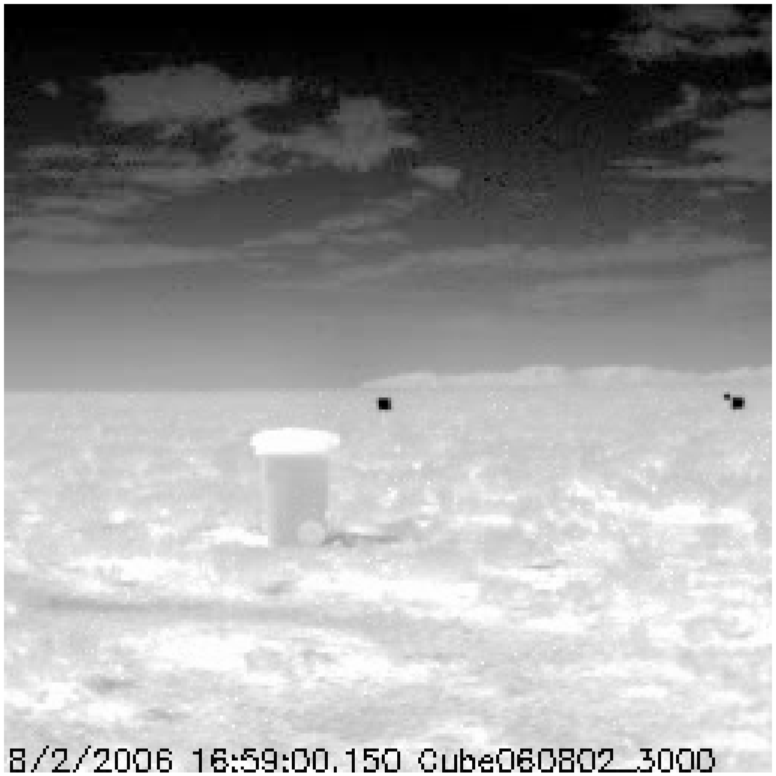

- **Triethyl phosphate (TEP) release**
- **Post-processing:**
  - Non-linear estimator in IDL
  - False alarm mitigation: 4 of 8 spatial filter
  - Bad pixels substituted
- **Detection key:**
  - TEP only
  - Yellow: OD ~ 0
  - Red: OD $\geq$ 1

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- ***Nonlinear estimation***
  - *Algorithm formulation*
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Optimal Estimation: Bayesian Approach

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- **Bayesian posterior pdf for model parameter values:**

$$\boxed{p(\theta|\tilde{x}) = \frac{p(\tilde{x}|\theta)p(\theta)}{p(\tilde{x})}}$$

- **Maximum likelihood parameter values maximize posterior:**

$$\begin{aligned}\hat{\theta} &= \arg\max\{p(\theta|\tilde{x})\} \\ &= \arg\min\{-\ln p(\theta|\tilde{x})\}\end{aligned}$$

- **Multi-variate normal pdf for deviation between model and measurement:**

$$-\ln p(\tilde{x}|\theta) = \tfrac{1}{2}[\tilde{x} - f(\theta)]^T D^{-1}[\tilde{x} - f(\theta)] + c_{x|\theta}$$

$$D = diag\{[\sigma_1^2, \sigma_2^2, \ldots, \sigma_k^2]\}$$

- **Prior pdf for model parameter values**

$$-\ln p(\theta) = \tfrac{1}{2}[\theta - \theta_a]^T R[\theta - \theta_a] + c_\theta$$

Optimal Estimation: Signal Model

- **Signal model:**

$$\underbrace{f(\theta)}_{\text{calculated spectrum}} = \underbrace{\tau_e}_{\text{calculated plume trans.}} \circ \underbrace{x_0}_{\text{estimated "baseline"}} + [1-\tau_e] \circ \underbrace{L_a}_{\text{Blackbody at } T_{atm}}$$

- **Plume transmission:**

$$\tau_e = \exp[-\underbrace{\alpha}_{\text{peak OD}} \underbrace{s}_{\text{reference spectrum}}]$$

- **Infrared background:**
  - Linear mixing model
  - Probabilistic Principal Components
  - Robust estimate of sample covariance (Huber-type M-estimator)

$$\boxed{x_0 = \mu + B\beta}$$

- **Model parameters:**
  - α: Plume OD
  - T_a: Plume/air temperature
  - β: Parameters which account for bkgd. radiance given bkgd. model

$$\boxed{\theta = [\alpha, T_a, \beta]}$$

Minimize Cost Function

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- **Maximum likelihood parameter values minimize cost function**
- **Multivariate normal pdfs result in "quadratic" cost function**

$$C = \left[\tilde{x} - f(\theta)\right]^T D^{-1}\left[\tilde{x} - f(\theta)\right] + \left[\theta - \theta_a\right]^T R_\theta \left[\theta - \theta_a\right]$$

deviation between measured and model spectra

deviation of parameters from nominal values

  - Quadratic formulation: $C = r^T r$
  - Prior applied to background coefficients only: $\boxed{\left[\theta - \theta_a\right]^T R_\theta \left[\theta - \theta_a\right] = \beta^T \beta}$
  - Residuals vector: $r \equiv \left[D^{-1/2}\left[\tilde{x} - f(\theta)\right]; \beta\right]$

- **Determine maximum likelihood parameter values by nonlinear estimation**
  - Approach not limited to quadratic cost function
  - Quadratic cost function amenable to computationally-efficient solution

Nonlinear Optimization Algorithms

- **Iterative determination of parameters, e.g., Newton's Method:**

cost function

$$\boldsymbol{\theta}_{i+1} = \boldsymbol{\theta}_i - \mathbf{H}_i^{-1} \left(\nabla C \right)_i$$

Model parameters

iteration no. Hessian matrix gradient vector

- **Gauss-Newton algorithm**
  - Appoximate Hessian matrix: $\mathbf{H} \approx 2\mathbf{J}^T\mathbf{J}$
  - Parameter update equation: $\boxed{\boldsymbol{\theta}_{i+1} = \boldsymbol{\theta}_i - \left(\mathbf{J}_i^T \mathbf{J}_i \right)^{-1} \mathbf{J}_i^T \mathbf{r}_i}$
  - Initial guess at θ from linear model

- **Levenberg-Marquardt algorithm also applicable**

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- ***Nonlinear estimation***
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- **Next generation algorithm(s)**

Test Regions

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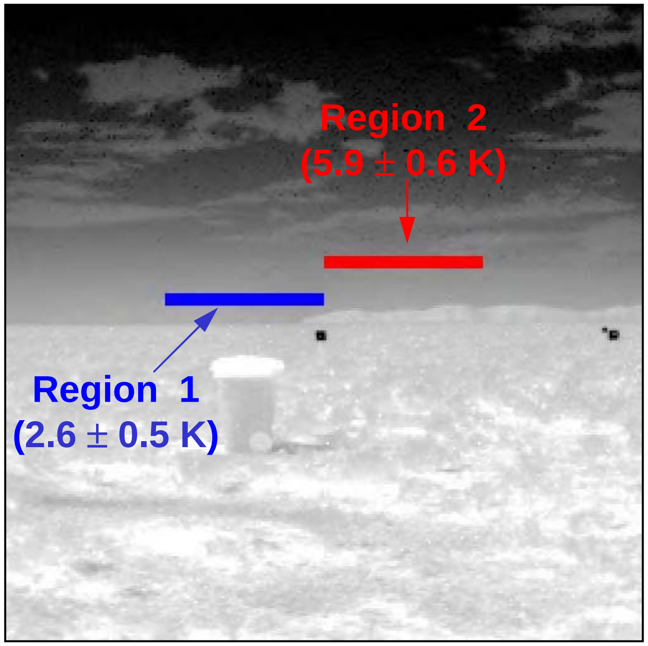
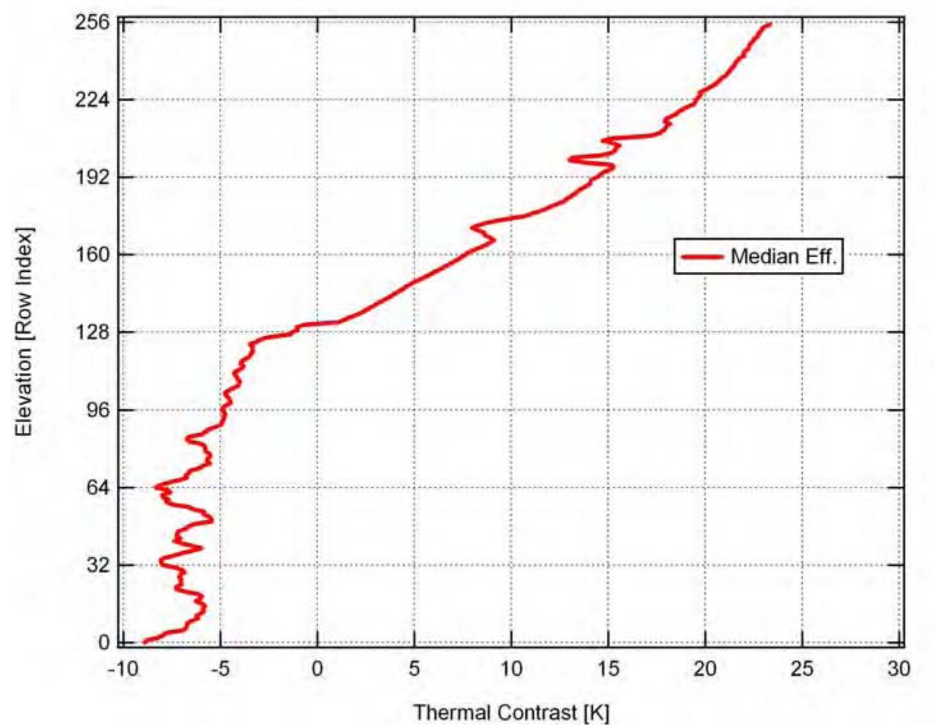


AIRIS-WAD datacube: 256 x 256 pixels



- **Plume-free data augmented with synthetic plumes:**
  - 64 x 5 pixels
  - Max OD from 0 to 3.0 (base e)
  - T(plume) = T(air) = 25.0 deg C
- **Thermal contrast**
  - ~0 K along horizon
  - Monotonic increase with elev. angle
- **Test both favorable and unfavorable regions**

Simulation: Synthetic R-134a Plumes

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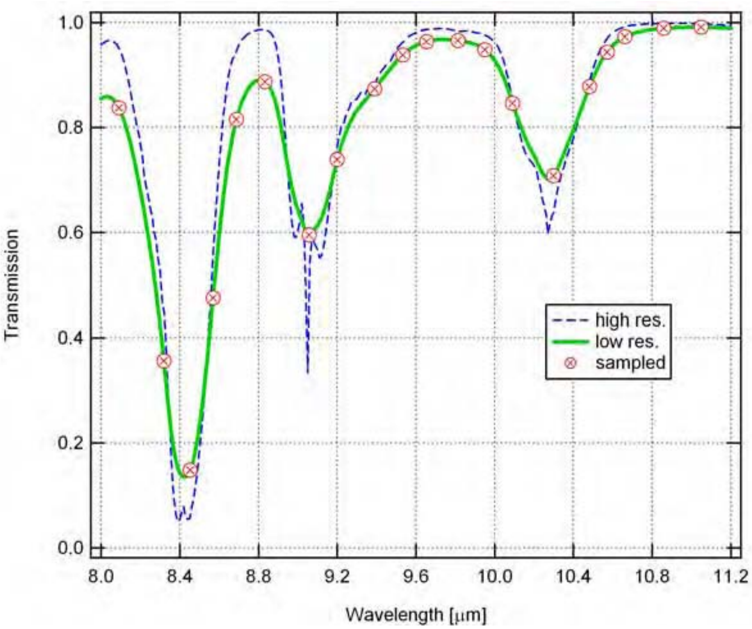
- **Effective plume transmission:**
  - Reference spectrum from PNNL library

$$\tau(\lambda) = \exp[-CL \cdot \sigma(\lambda)]$$

  - Specify column density
  - Beer's Law + instrument resolution function



$$\bar{\tau}_p(\lambda_s) = \int \tau(\lambda) \cdot g(\lambda, \lambda_s) \cdot d\lambda$$

- **Data augmentation:**
  - Partition measurement into estimated signal, noise
  - Modify signal w/plume signature
  - Add back estimated noise

$$x_p = \hat{x}_0 + [1 - \tau_p] \circ [L_a - \hat{x}_0] + \hat{e}$$

Performance Metric: ROC Curves

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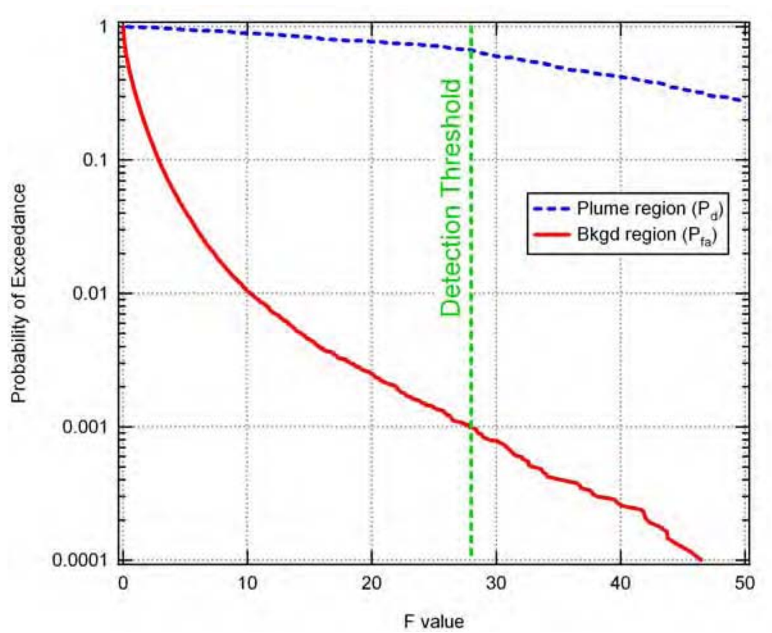

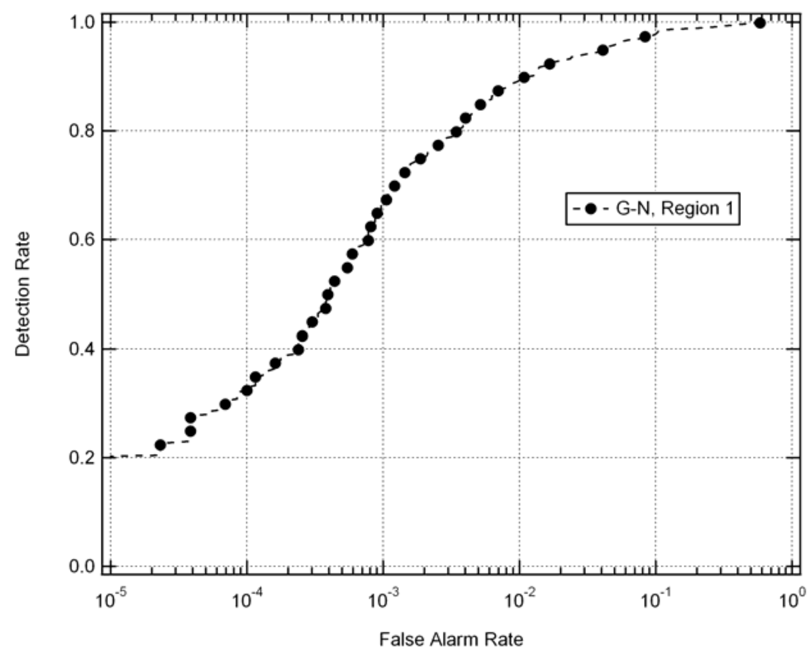

- **Binary decision hypotheses**
  - H_0 ("plume absent") and H_1 ("plume present")
  - pdfs for detection statistic: $p(F \mid H_i)$
- **ROC curve is $P_d(F_{th})$ vs $P_{fa}(F_{th})$**
  - P_d from plume-augmented region
  - P_{fa} from rest of scene
- **ROC "surface": $P_d(\alpha; F_{th})$**

$$P_{fa}(F_{th}) = \int_{F_{th}}^{\infty} p(F \mid H_0) d\eta$$

$$P_d(F_{th}) = \int_{F_{th}}^{\infty} p(F \mid H_1) d\eta$$

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Performance Comparison with Matched Filter

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- **Objective: Compare nonlinear estimation with matched filter estimation**
  - Detection statistics
  - Column density/optical density
- **Detection with nonlinear estimator: F test**

$$F(\tilde{x}) = (k-1)\cdot\left[\frac{C(\tilde{x},\hat{\theta}_0)}{C(\tilde{x},\hat{\theta})} - 1\right]$$

- **Analogous metric for clutter-matched filter: Adaptive Cosine Estimator (ACE)**

$$D_{MF}(\tilde{x}) = \frac{\left(s'^T\,\hat{\Sigma}^{-1}[\tilde{x}-\mu]\right)^2}{\left(s'^T\,\hat{\Sigma}^{-1}s'\right)\left([\tilde{x}-\mu]^T\,\hat{\Sigma}^{-1}[\tilde{x}-\mu]\right)}$$

$$F_{MF} = (k-1)\frac{D_{MF}}{1-D_{MF}}$$

- **Matched-filter optical density estimate:**

$$\hat{\alpha}_{MF} = \frac{s'^T\,\hat{\Sigma}^{-1}(\tilde{x}-\mu)}{s'^T\,\hat{\Sigma}^{-1}s'}\cdot\frac{\Delta T_0}{\Delta T_{eff}}$$

- ***Expect near identical results for optically-thin plumes***

R-134a Detection: Optically-Thin Plume, OD=0.1

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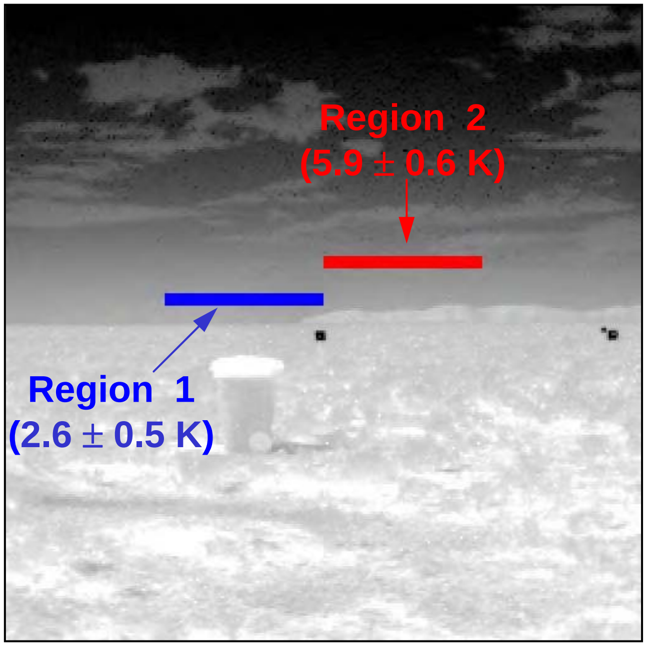
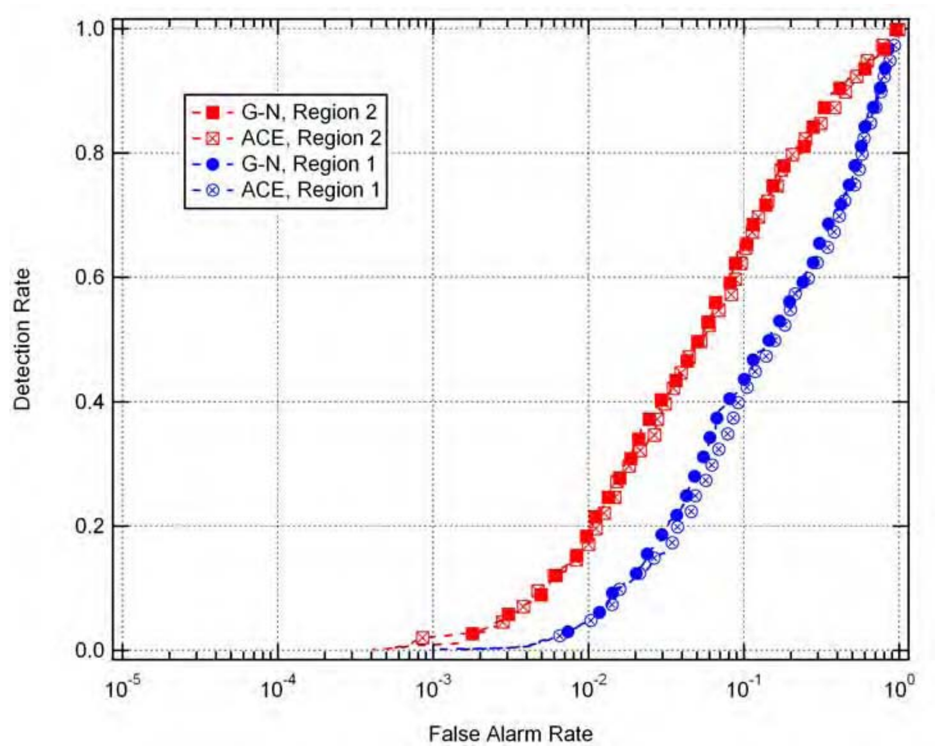


AIRIS-WAD datacube: 256 x 256 pixels



- **Plume column density = 82 mg/m^2 (20 ppmv-m)**
- **Detection statistics not favorable in either Region**
- **ACE and Gauss-Newton ROC curves are nearly identical**
  - 20 bands in test datacube
  - OD=0 reference spectrum

R-134a Detection: Optically-Thin Plume, OD=0.3

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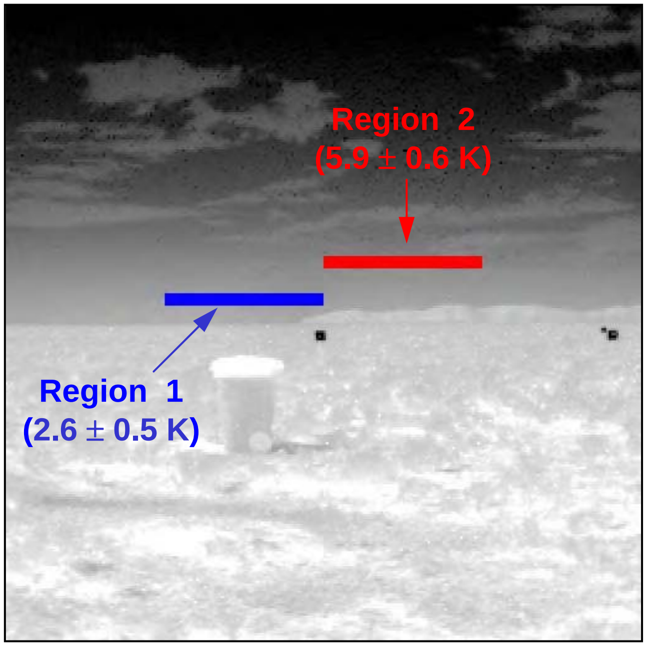
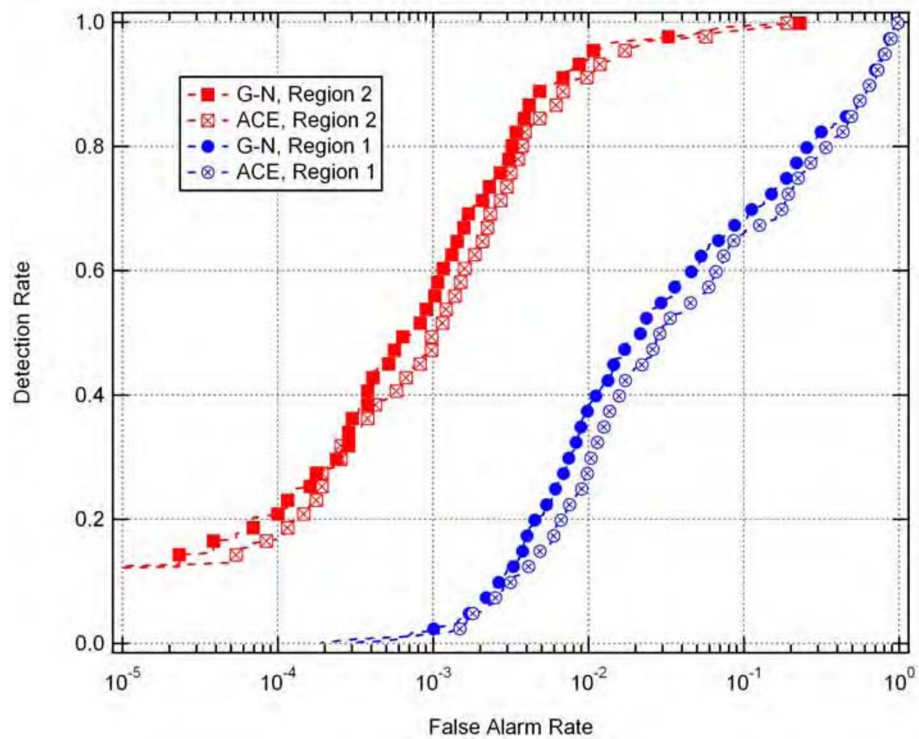
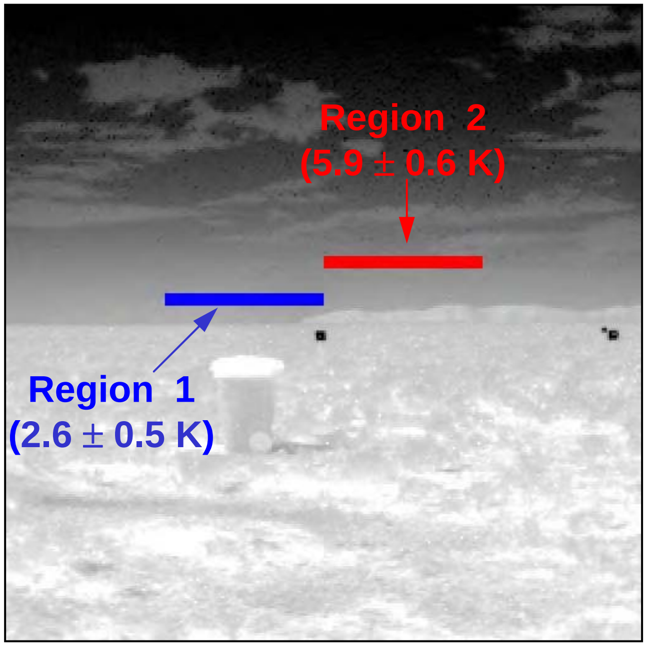


AIRIS-WAD datacube: 256 x 256 pixels

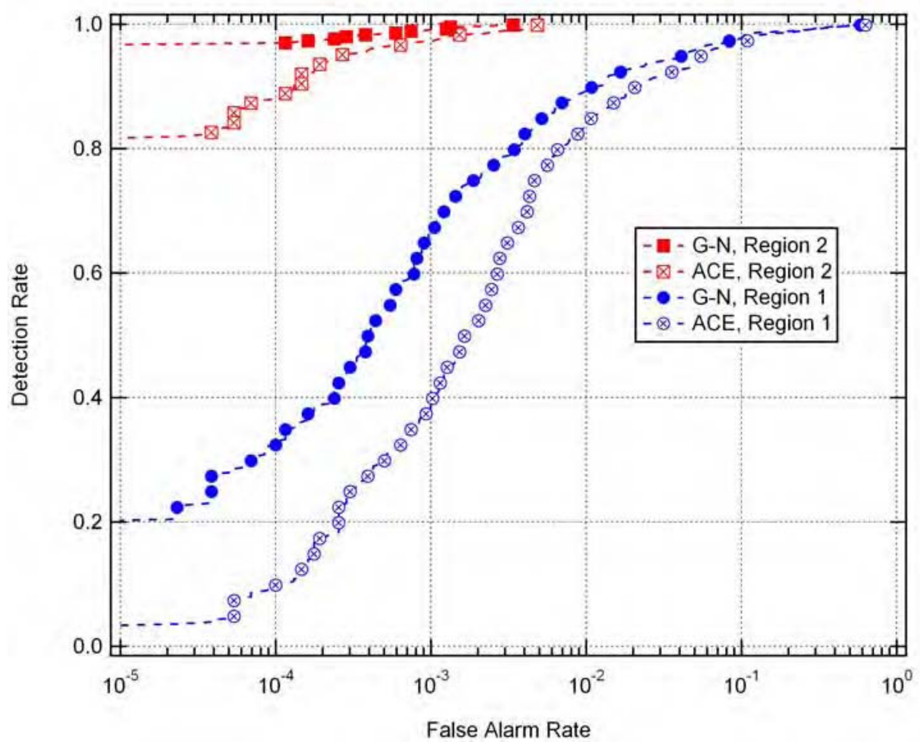


- **Plume column density = 246 mg/m^2 (59 ppmv-m)**
- **Detection statistics not favorable in Region 1, marginal in Region 2**
  - Lower thermal contrast
  - ~2 orders of magnitude reduction in P_{fa} from Region 1 to Region 2
- **ACE and Gauss-Newton ROC curves are nearly identical**

R-134a Detection: Optically-Thick Plume, OD=1.0



AIRIS-WAD datacube: 256 x 256 pixels



- **Plume column density = 822 mg/m² (197 ppmv-m)**
- **Detection statistics favorable in Region 2, marginal in Region 1**
  - >2 orders of magnitude reduction in P_{fa} from Region 1 to Region 2
- **Gauss-Newton produces significantly more favorable ROC curves than ACE**
  - Factor of ~2 improvement in Region 1 (P_{fa} for fixed P_d)
  - Multiple orders of magnitude improvement in Region 2

R-134a Detection: Optically-Thick Plume, OD=2.0

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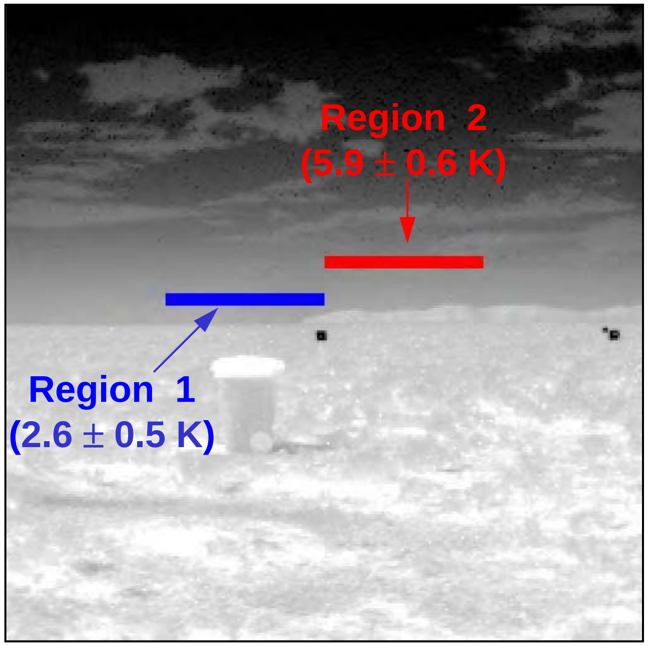
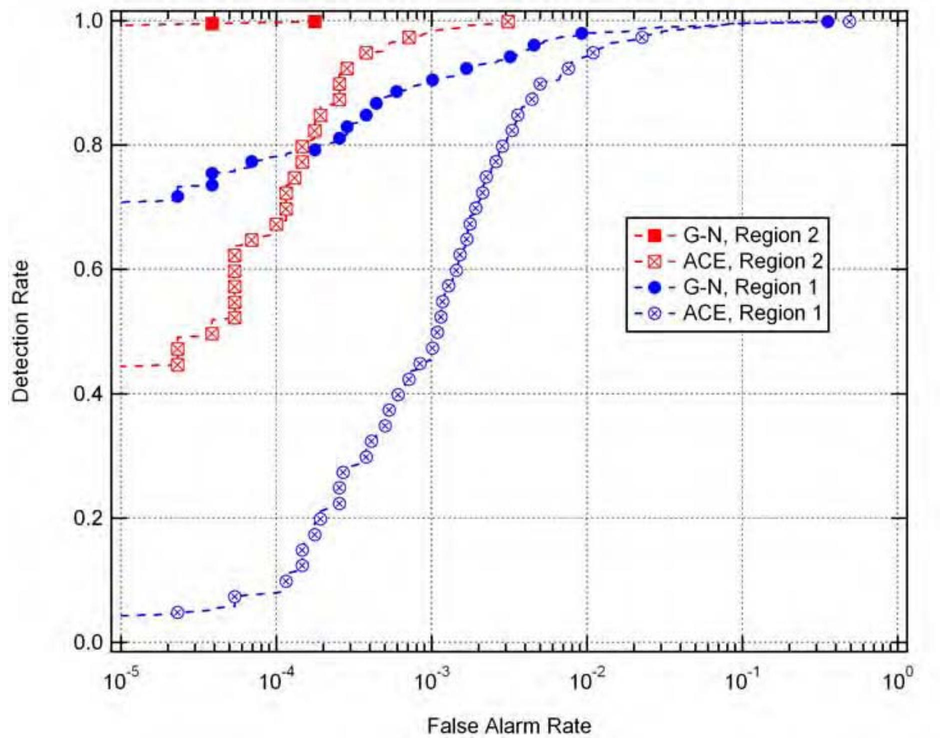
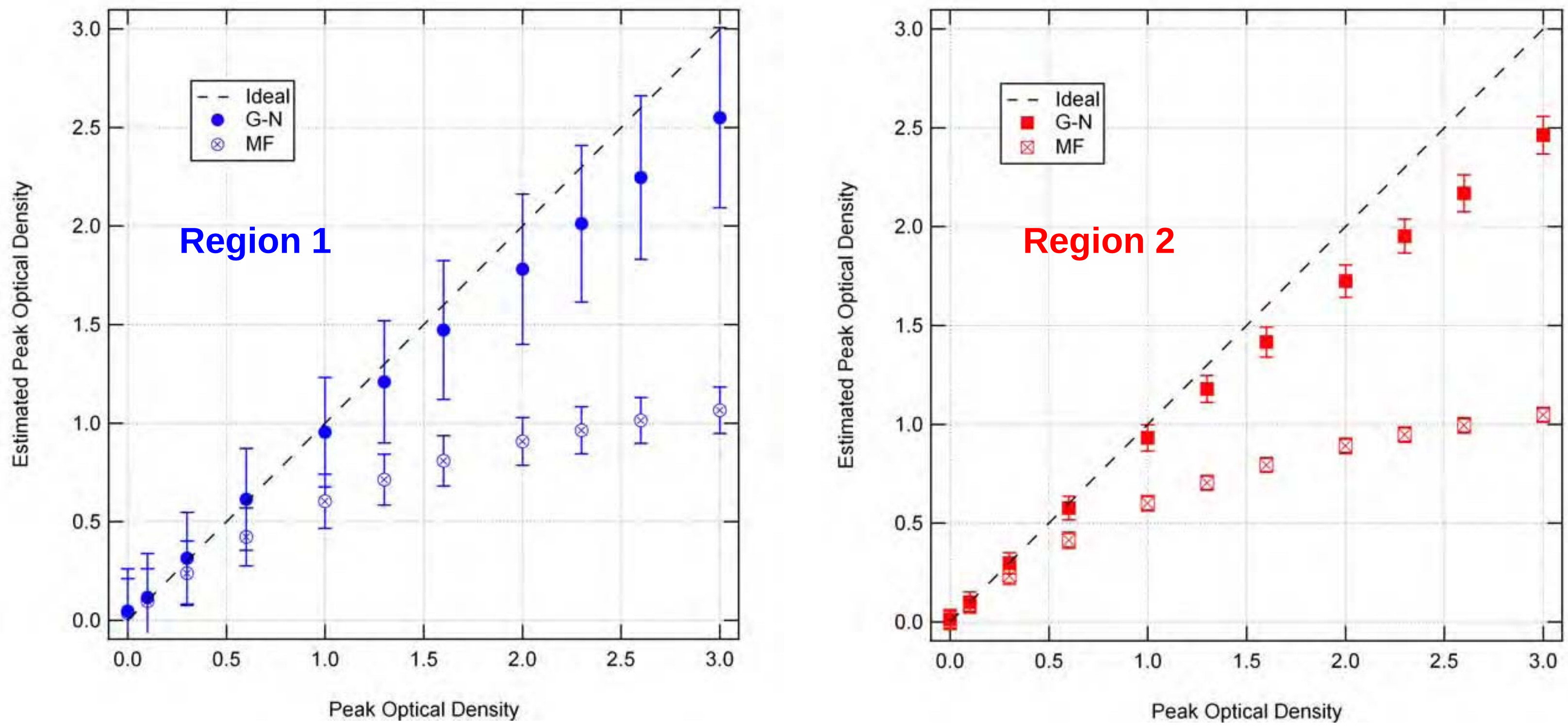


AIRIS-WAD datacube: 256 x 256 pixels



- **Plume column density = 1643 mg/m^2 (394 ppmv-m)**
- **Detection statistics favorable in both Regions**
- **Gauss-Newton produces significantly more favorable ROC curves than ACE**
  - >1 order of magnitude improvement in Region 1
  - Multiple orders of magnitude improvement in Region 2

Column Density Estimation



- **Increased thermal contrast reduces uncertainty, no effect overall accuracy**
- **Nonlinear estimation**
  - Accurately recovers embedded OD (CL)
  - Systematic deviation at OD>1 is instrument resolution effect
- **Matched Filter systematically underestimates CL**
- ***Nonlinear estimator always as good or better than MF***

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Algorithm Execution

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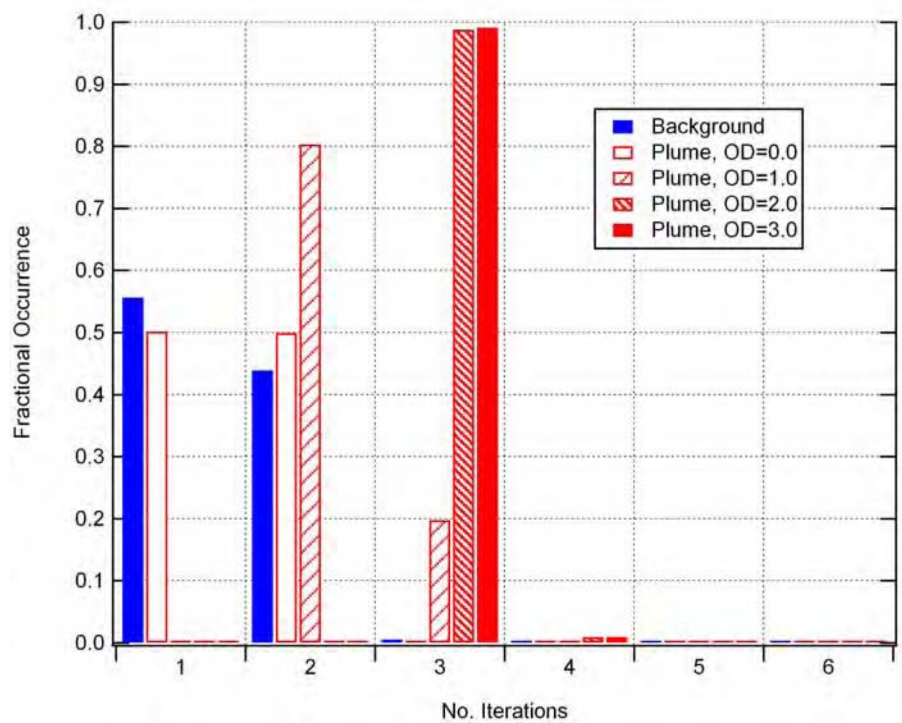
- **Gauss-Newton algorithm is iterative**
- **Termination criterion:**

$$0 < \left[1 - \frac{C_{i+1}}{C_i}\right] < \delta_{\max}$$

- **Initial guess is Iteration 0**
- **Typical results:**
  - 1-2 iterations for no plume (plume OD=0)
  - 3 iterations to converge for OD~2-3 TEP plume
- **Decreasing δ to 0.0001 increase no. iteration but no statistically-significant effect on CL**



δ_{max} = 0.01

Summary and Conclusions

- **Developed nonlinear estimator for plume detection and characterization based on RTE**
  - Bayesian formulation
  - Statistical model for IR background
  - Gauss-Newton algorithm to estimate maximum *a posteriori* (MAP) values
- **Signal model developed for non-scattering atmosphere, single layer plume**
  - Easily modified to address more complicated atmospheres
- **Nonlinear estimation significantly outperforms matched-filter-based with optically-thick plumes**
  - "Orders of magnitude" improvement
  - NL estimator and matched filter produce equivalent results for optically-thin plumes
- **This work was performed under Contracts from the Defense Threat Reduction Agency (HDTRA01-07-C-0067) and US Army ECBC Aberdeen Proving Ground, MD (W911SR-06-C-0022). Any opinions, findings and conclusions or recommendations expressed in this material are those of the author and do not necessarily reflect the views of HDRA or the Army.**

Additional Material

Data Processing Chain

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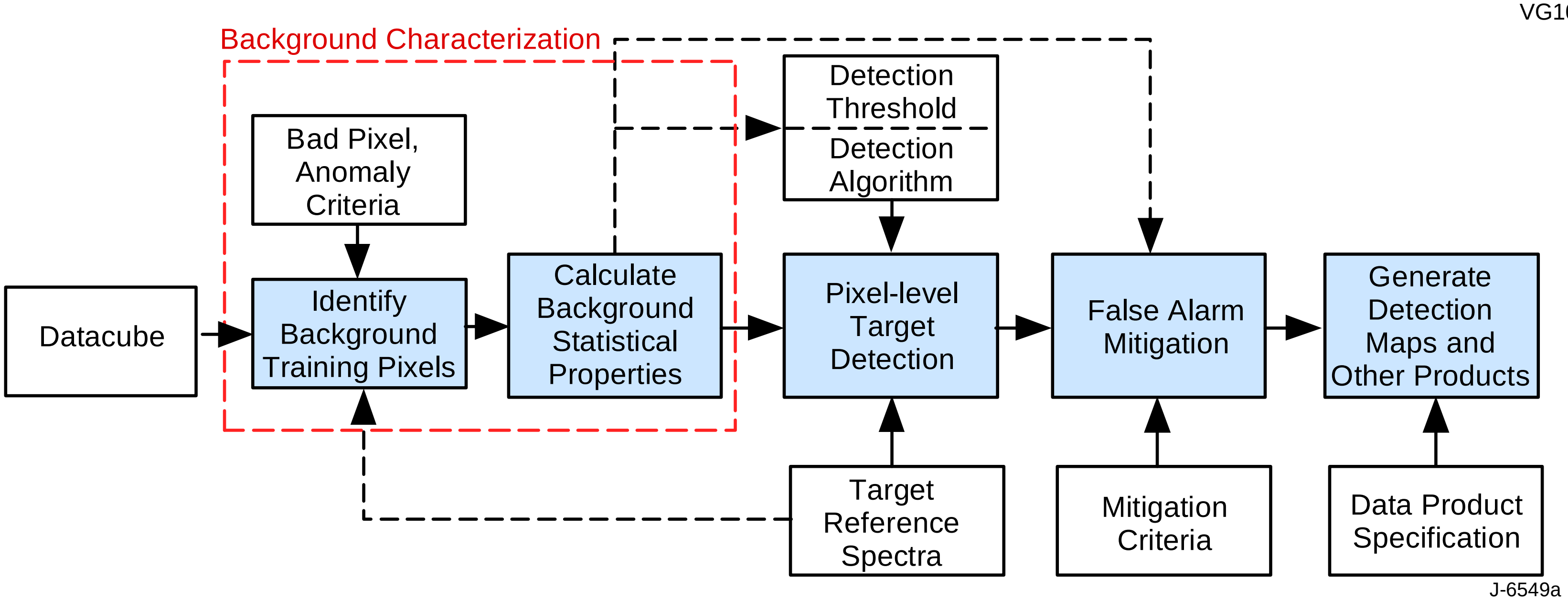

- **Focus is pixel-level target detection**
- **New background characterization approach facilitates improved pixel-level detection**
- **"A chain is only as strong as its weakest link."**
  - Provide higher quality input to False Alarm Mitigation block
  - False Alarm Mitigation is separate issue

Technical Approach

- **Adapt methodology used for atmospheric profile retrieval from space-based sensor data (e.g. AIRS, IASI, MODIS, TES)**
  - Parameterize Radiative Transfer Equation (RTE)
  - Apply Estimation Theory to determine max. likelihood parameter values
  - Exploit large data set: utilize ensemble statistics
- **Rationale:**
  - Physics-based model for observations
  - Statistically-justified constraints
  - Strong theoretical foundation (see, e.g., C.D.Rodgers, Inverse Methods for Atmospheric Sounding)
- **Benefits**
  - Adaptable framework
  - Immediate application to non-scattering atmosphere
  - Can modify RTE to address more complicated atmospheres

Linear Models

$$x_p = x_0 + \alpha' s'$$

$$x_0 = \mu + B\beta$$

"Structured background"

$$x_0 = \nu_b \sim N(\mu, \Sigma)$$

"Unstructured background"

- **"Structured Background"**
  - Values of β are unconstrained
  - Generalized Likelihood Ratio Test: $D_{GLRT}(x) = \dfrac{x^T P_B^{\perp} x}{x^T P_{SB}^{\perp} x}$ $\quad P_B^{\perp} = I - B\left(B^T B\right)^{-1} B^T$
  - Typical implementation: B = eigenvectors of sample covariance matrix
- **"Unstructured Background"**
  - ν_b is a random vector
  - Adaptive Cosine Estimator: $D_{ACE}(x) = \dfrac{\left[s'^T \Sigma^{-1} x\right]^2}{\left[s'^T \Sigma^{-1} s'\right]\left[x^T \Sigma^{-1} x\right]}$
- **Survey article: Manolakis, Marden, & Shaw, "Hyperspectral Image Processing for ATR Applications," *Lincoln Lab J.*, v.14 (2003)**

Pros and Cons of Linear Approximation

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- **Pro: Matrix multiplication results in fast computation**
  - All spectra in ensemble may be processed in parallel
  - Major computational expense is diagonalization of sample covariance matrix
  - *AIRIS-WAD: <150 ms to process 65536 twenty element spectra for four target signatures (using 2005 vintage technology)*

- **Pro: Detection statistics well-understood for Gaussian noise**

- **Con: Underlying physical assumptions not valid for detection scenarios of interest**
  - Mathematical model not matched to physics

$$\tau_p = \exp(-\alpha s) \approx \cancel{1 - \alpha s}$$

  - Linear approximation to Beer's Law can introduce significant error

Why Gauss-Newton Yields Better Results

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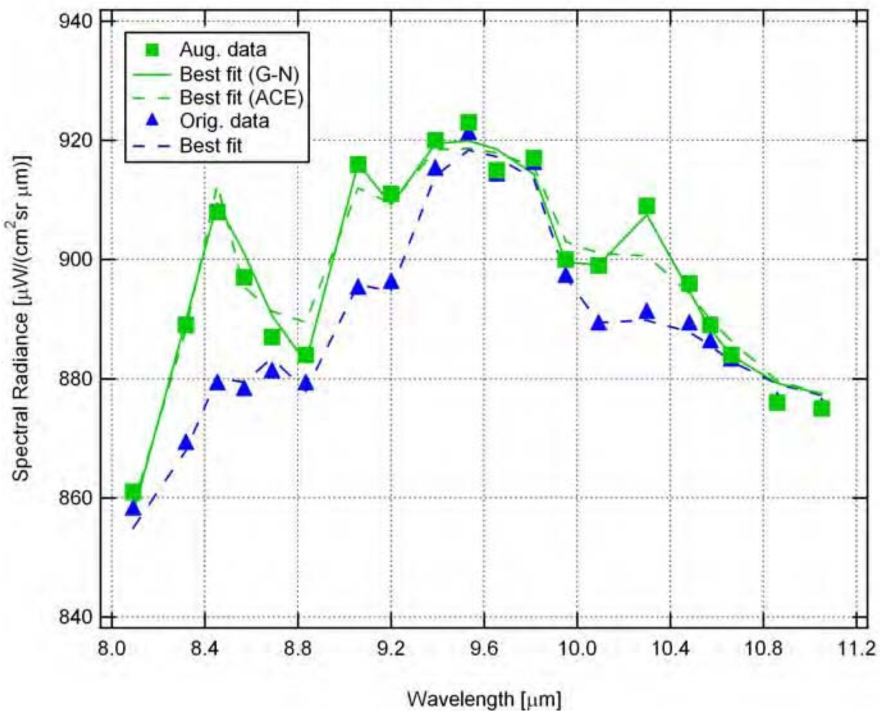
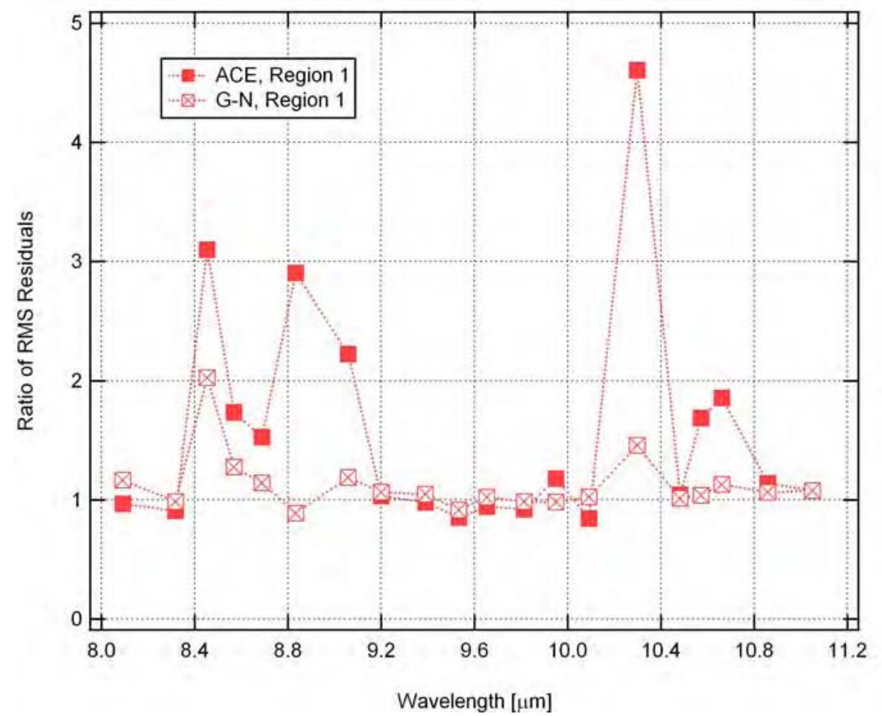


Spectrum augmented with OD=3.0 plume



Ratios of rms residuals in plume region, OD=3.0 to OD=0

- **Model is matched to the data**
- **Fit residuals are systematically larger with linear model**
  - Result of least-squares minimization
  - Location of largest residuals highly correlated with strongest R-134a absorption features

Adaptive Infrared Imaging Spectroradiometer – Wide Area Detector (AIRIS-WAD)

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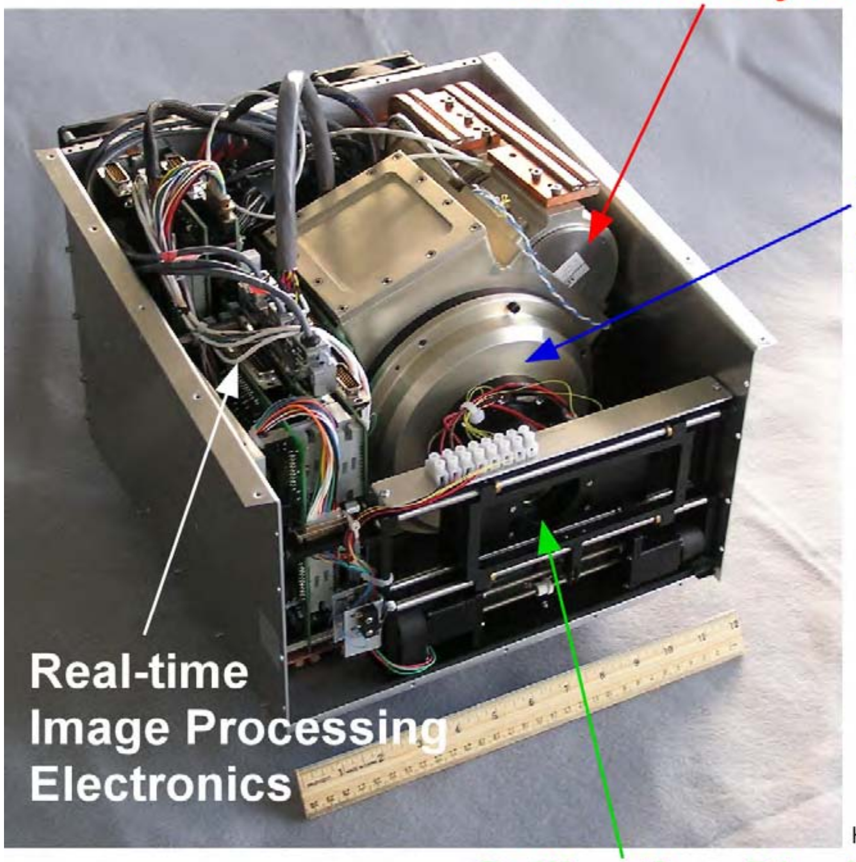
- **Optical:**
  - 256 x 256 pixels
  - 30 deg x 30 deg FOV
  - spectral coverage: 7.9 to 11.2 μm at ~0.1 μm resolution (~1% of λ)
- **Datacubes:**
  - 20 wavelengths
  - user selectable λ's, specified prior to mission
- ***Real-time datacube processing: up to 3 Hz***
- **Detection algorithm history:**
  - GLRT: Winter 2005-Spring 2006
  - ACE: since Spring 2006



Hyperspectral Background Model

Physical Sciences Inc.

VG10-076-33

- **Probabilistic Principal Components-based**
  - M.E.Tipping & C.M.Bishop, *J.R.Statist. Soc. B* (1999)
- **Linear mixing model**

$$x = \mu + B\beta$$

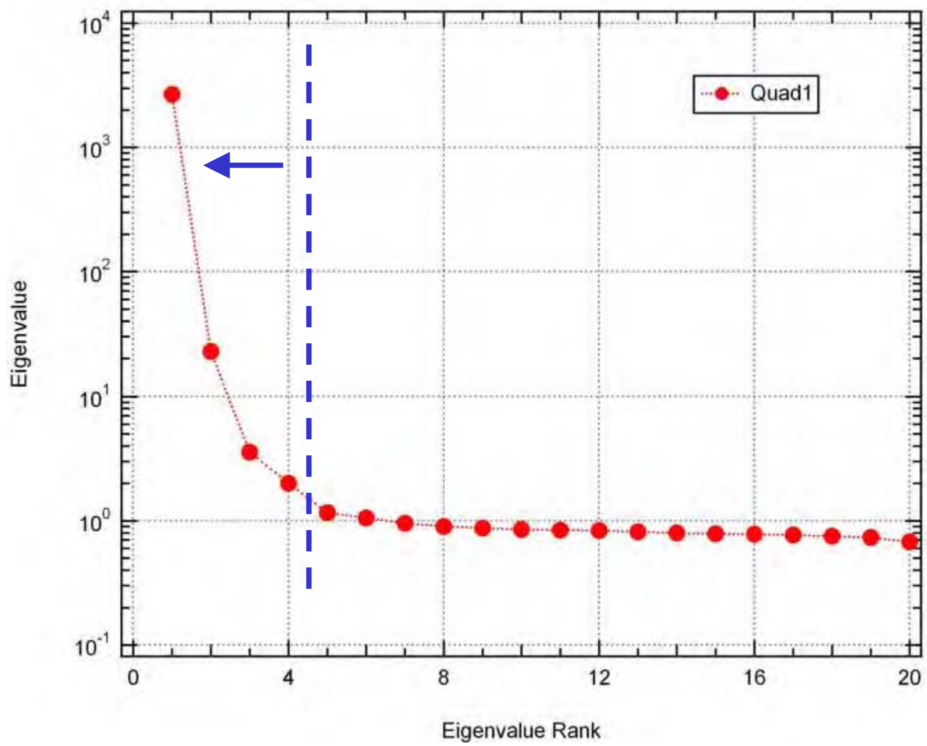
- **Eigenvalue-based covariance regularization**

$$\Sigma \approx \hat{\Sigma} = BB^T + \varepsilon D$$

$$\Sigma = D^{1/2}\left(U \Lambda U^T\right) D^{1/2}$$

$$B = D^{1/2} U_m \left(\Lambda_m - \varepsilon I_m\right)^{1/2}$$

- ***Σ = robust estimate of sample covariance: Huber-type M-estimator***



Gauss-Newton Algorithm

- **Follows from Newton's method – simplifying approximations**
- **Good for solving weakly nonlinear equations**
- **Hessian matrix:**

$$H_{jk} = 2\sum_{q=1}^{m}\left[\frac{\partial r_q}{\partial \theta_j}\frac{\partial r_q}{\partial \theta_k} + r_q\frac{\partial^2 r_q}{\partial \theta_j \partial \theta_k}\right]$$

$$\approx 2\sum_{q=1}^{m}\left[\frac{\partial r_q}{\partial \theta_j}\frac{\partial r_q}{\partial \theta_k}\right] = 2J^T J$$

$$J = \frac{\partial r}{\partial \theta}$$

Jacobian

- **Gradient:** $$\left[\nabla_\theta C\right]_j = \frac{\partial C}{\partial \theta_j} = 2\sum_{q=1}^{m}\left[r_q \frac{\partial r_q}{\partial \theta_j}\right]$$

$$\nabla_\theta C = 2J^T r$$

- **Parameter update equation:**

$$\boxed{\theta_{i+1} = \theta_i - \left(J_i^T J_i\right)^{-1} J_i^T r_i}$$

- **Initial guess at θ from linear model**