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High Spectral Resolution Infrared Radiance Modeling Using Optimal Spectral Sampling (OSS) Method

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Parameterization of radiative transfer equation is necessary for operational remote sensing

- A class of techniques widely used in space-based remote sensing based on McMillin and Fleming (1975) parameterizes the "effective layer optical depth" for molecule *m* with profile-dependent predictors

$$\ln\left(\frac{\bar{\tau}^m(p_l)}{\bar{\tau}^m(p_{l-1})}\right) = \sum_{i=1}^{N} a_{il} X_{il}^m$$

$$\bar{\tau}^m(p_l) = \int_{\Delta\nu} \phi_\nu \tau_\nu^m(p_l) d\nu$$

$$X_{il}^m\left(\theta_{scan}, \{(p_i, T_i, q_i^m), i = 1,..,l\}\right)$$

  - Very efficient for radiance calculations, and the accuracy is generally better than the sensor noise level
- Among the shortcomings of this method:
  - Not practical for use with changing observer altitude (e.g., airborne remote sensing)
  - Not amenable to multiple scattering atmospheres (e.g., cloud ice water path retrieval from sub-millimeter measurements)
  - Inefficient computation of Jacobians
  - Accuracy depends on choice of predictors
    - Generally determined by trial and error and depend on the type of application (viewing geometry, spectral band)
  - Not directly applicable to *sinc* function

OSS technique addresses the need for algorithm speed, accuracy and flexibility

- Model must be applicable to a wide-range of remote sensing platforms
  - Downlooking (satellite sensors)
  - Uplooking (ground-based sensors)
  - Aircraft or balloon (up or down looking with variable altitude range)
  - Limb and line-of-sight
- Ideal model has consistent physics throughout
  - Microwave to visible
  - Narrow-band and wide band applications
- Both accuracy and speed are important
  - Trade-off between accuracy and speed depending on the specifics of the problem at hand
    - Sensor noise level
    - Science-grade versus operational code
- Algorithm capable of calculating Jacobians necessary for inversion
  - Able to consider any number of “fixed” or “variable” molecular species and geophysical parameters

OSS technique derived from ESFT and *k*-distribution methods

Assumption breaks down for single absorber in the presence of lines of different strengths or non-regularly spaced lines

No satisfactory treatment of overlapping absorbers when relative abundance of individual species changes with altitude

- The exponential sum fitting (ESFT) and *k*-distribution methods approximate band transmittances in homogenous atmospheres as,

$$\bar{\tau}\ (u) = \sum_{i=1}^{N} w_i e^{-k_i u}$$

- Weights w_i can be interpreted in terms of the probability distribution of the absorption coefficient over the spectral interval

$$w_i = \Delta g_i = \int_{k'_{i-1}}^{k'_i} p(k)\,dk \qquad (k'_{i-1} < k'_i)$$

and k_i is a representative *k*-value for the interval $[k'_{i-1}, k'_i]$

- Extension of this *k*-distribution method to non-homogeneous atmospheres is based on observation that minima and maxima of absorption in different layers coincide spectrally
- Correlated-*k* method vertically integrates RT equation by assuming a correspondence between *k*'s in *g*-space in different layers, i.e. minimal impact on results of re-arranging k_ν by ascending order in individual layers

OSS selects the frequencies and absorption coefficients relevant to the calculation of radiance

- Proper treatment of overlapping absorbers requires accurate characterization of the multivariate probability distribution of absorption coefficients for all layers and molecules

- High dimensionality of the problem makes it impractical to attempt to solve directly for the *k* 's without appropriate constraints

- OSS solution
  - Reduce the problem to a one-dimensional frequency search
  - Require that the *k* 's correspond to actual values of absorption coefficient for all molecules and layers at the selected frequencies
  - Patent pending

OSS parameters generated from monochromatic calculations

Weights computed by linear regression for each trial combination of frequencies

- Parameter generation starts from a set of uniformly spaced monochromatic transmittances (or radiances)
  - Compute with a line-by-line model (e.g. LBLRTM)
  - Use a globally representative ensemble (*S*) of atmospheres
- Search for the smallest subset of frequencies (nodes) and associated weights for which the error is less than a prescribed tolerance for all levels

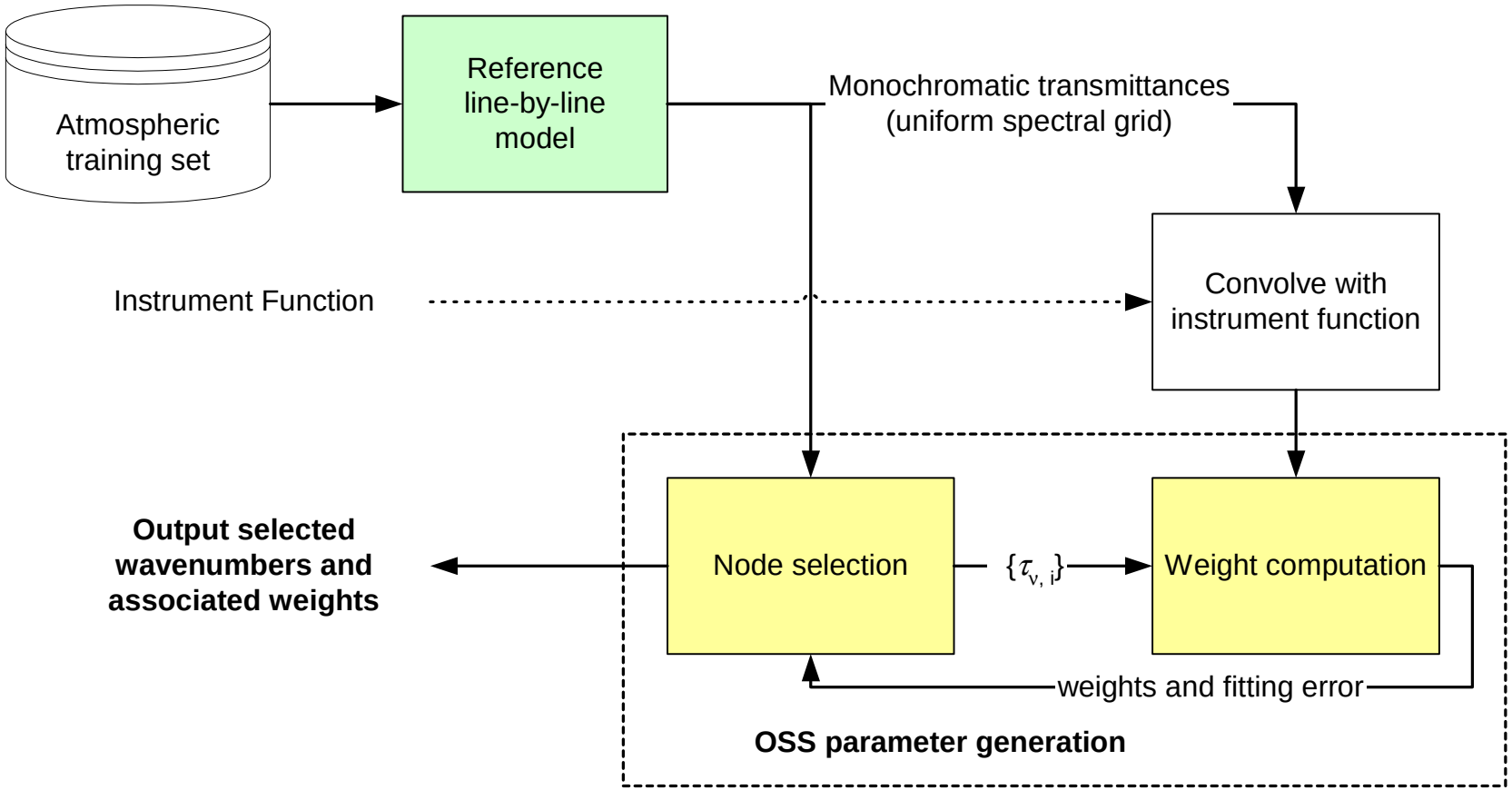
$$\left\{ \left(\nu_i , w_i \right) \;\; i = 1,.., N \right\}$$

$$\varepsilon_N = \sum_s \left(\bar{\tau}^s \left(p_l \right) - \sum_{i=1}^{N} w_i \tau_{\nu_i}^s \left(p_l \right) \right)^2$$

Radiative transfer accuracy and computation time requirements must be considered when selecting error threshold

(search method described below)

Flow diagram for OSS parameter generation



Model "training" done in terms of radiance and includes appropriate scene variability

Line-by-line calculation has largest impact on computation time requirements, not the search time

- Set of training scenes includes appropriate variability
  - Viewing angle
  - Surface emissivity and reflectivity
  - Observer altitude
  - Solar angles
- Fit is done in radiances (or brightness temperatures), which is equivalent to weighting the transmittances at each level by the channel weighting function

$$\varepsilon_N = \sum_s \left[r^s - \sum_{i=1}^{N} w_i r_{v_i}^s \right]^2$$

Scene stratification generally reduces the size of the OSS parameter file

- Scene stratification ensures model accuracy (threshold *rms*) is maintained for a larger set of conditions
  - "Global" ensemble includes all viewing angles, a wide range of atmospheric profiles, and the full range of surface emissivity
  - Stratified selection can be done for a subset of conditions (e.g. one view angle)

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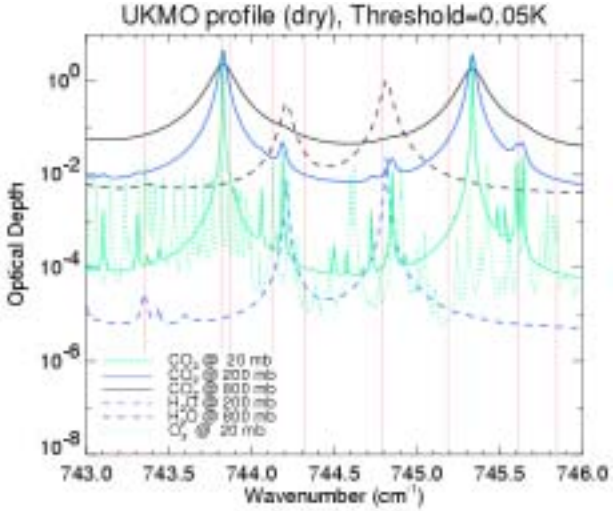
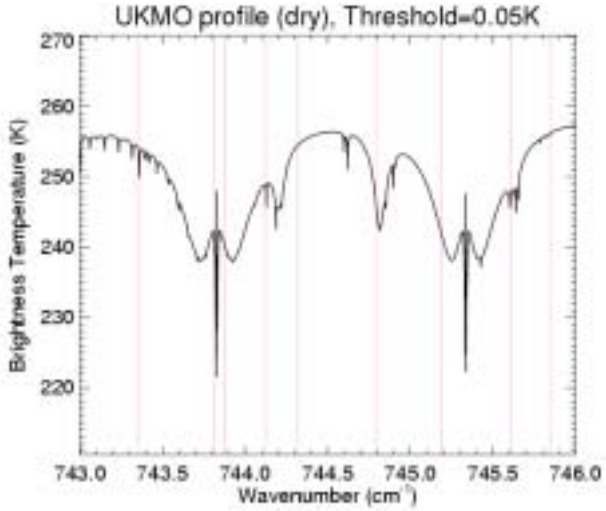
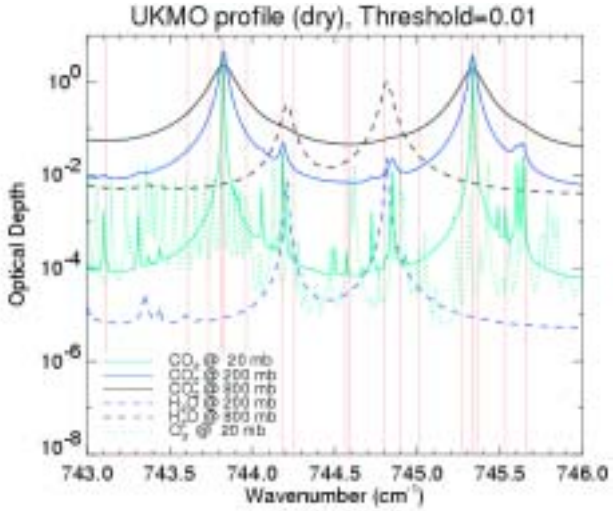
Example of OSS selection shows exploitation of redundant information

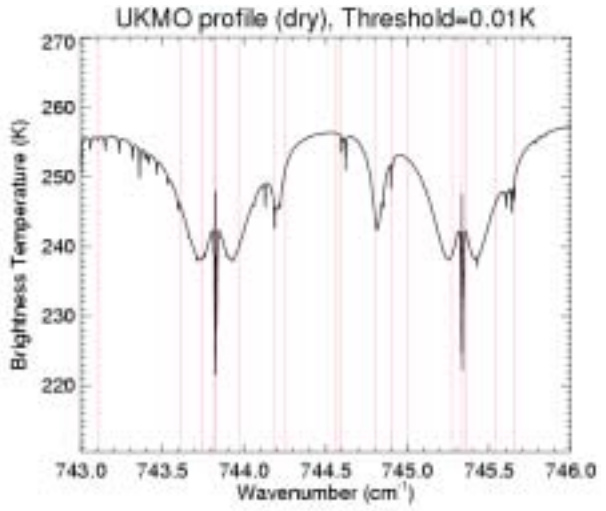
Smaller threshold results in larger number of selected points

Redundant spectral information utilized only to the extent needed to meet threshold requirement









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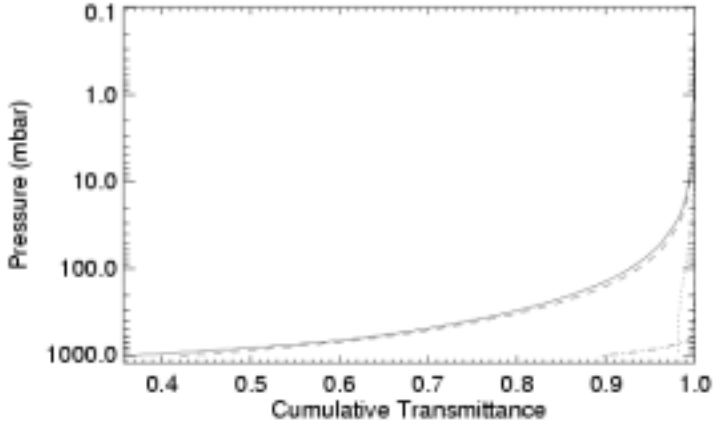
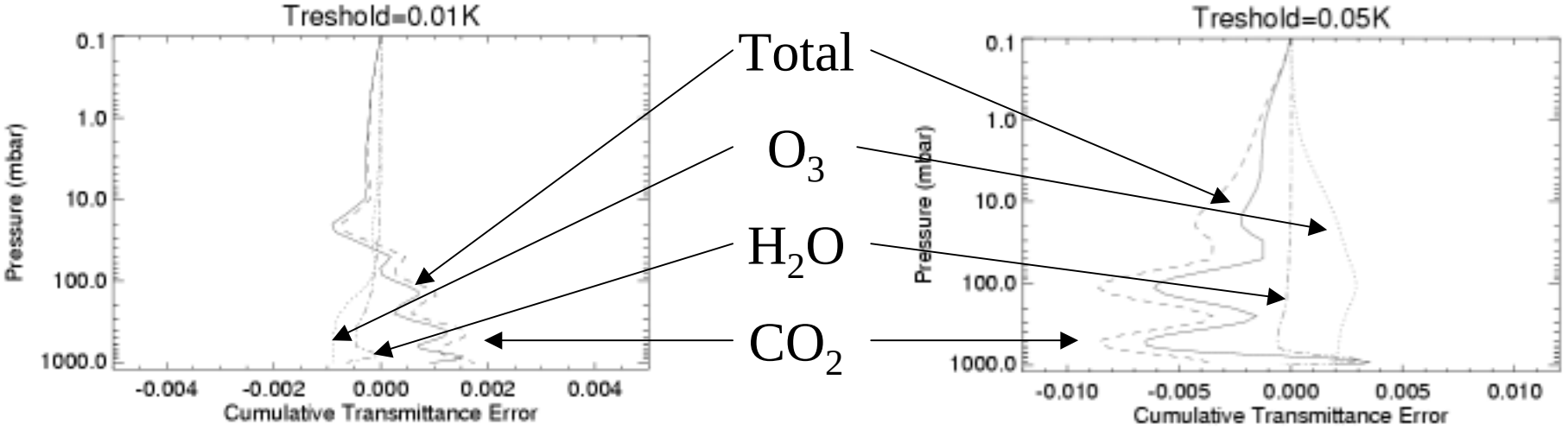
Species transmittance accuracy contributes only a small part of the overall radiance error





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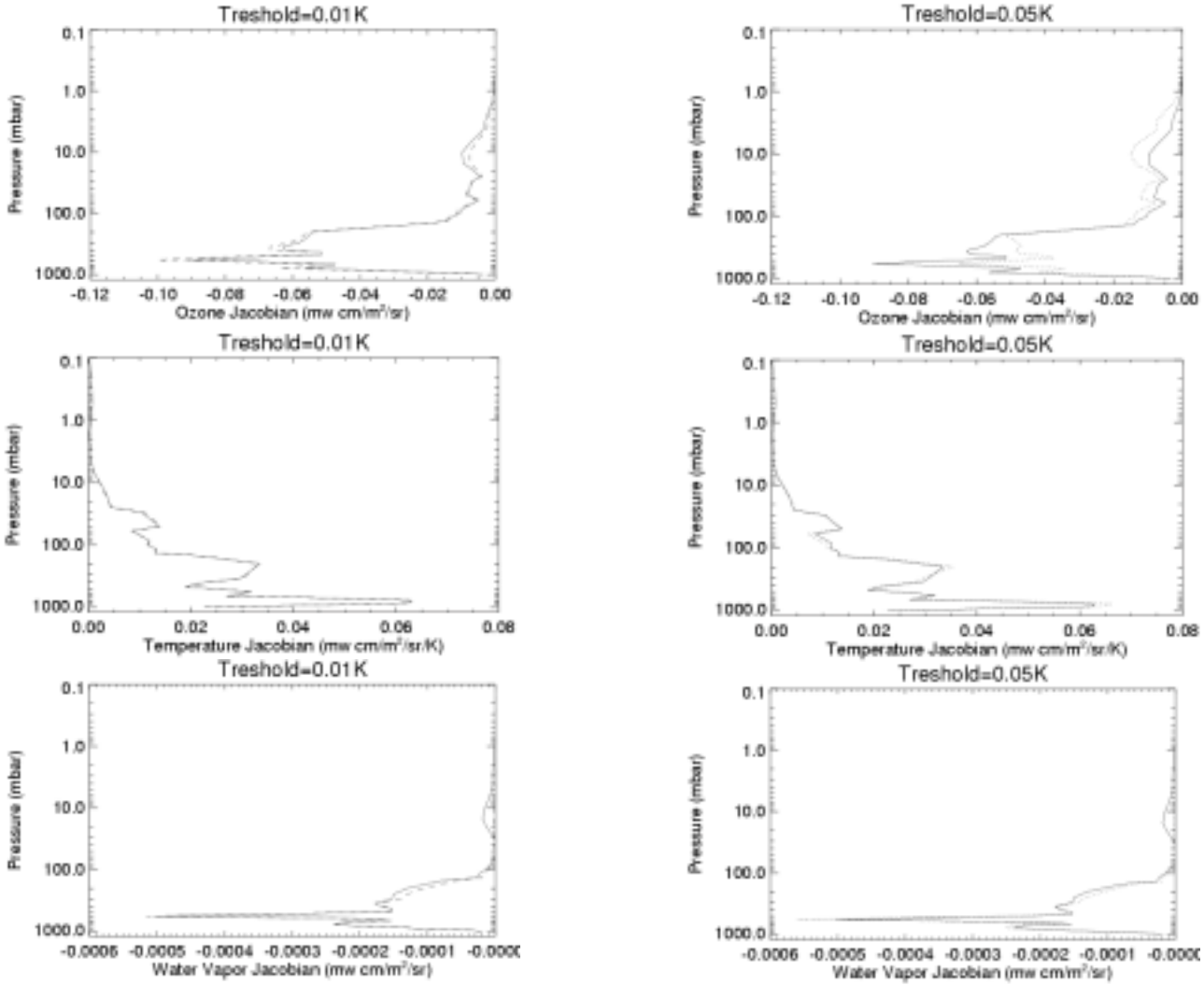
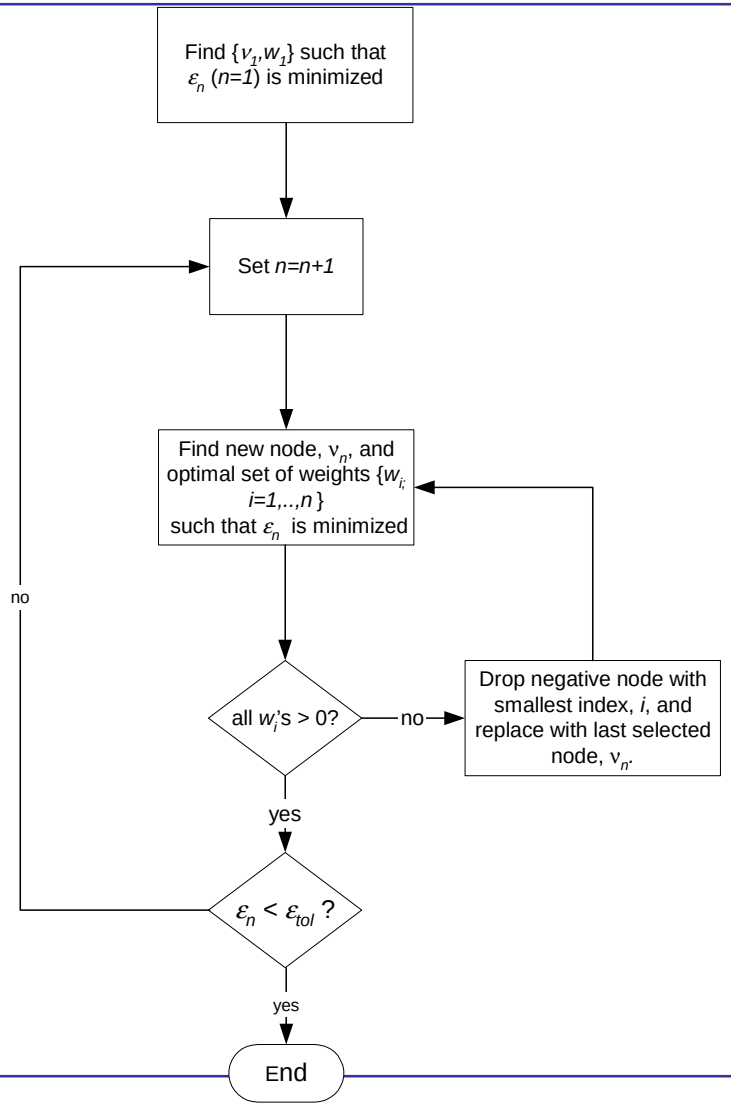
Examination of Jacobians illustrates the technique works well for both the forward and inverse problem



Automated process for sequential search based on Wiscombe and Evans (1977)

- The procedure consists of starting with *N*=1 and searching for the spectral location that produces the smallest error among the *M* possible locations
- Once ν_1 and its associated weight have been determined, the fitting error is compared to the prescribed tolerance
  - If $\varepsilon_1 < \varepsilon_{tol}$ the procedure stops. Otherwise, *N* is incremented by one and the search for ν_2 proceeds in the same fashion
  - Weights are reevaluated for each trial combination of nodes
- Weights are constrained (sum is 1.0 and all weights positive)
  - Pairs of nodes with almost identical absorption characteristics results in ill-conditioned solution (large negative weights)
    - Occurs most often with large number of nodes (search is on the wrong "path")
    - Negative node eliminated and search restarted using remaining weights



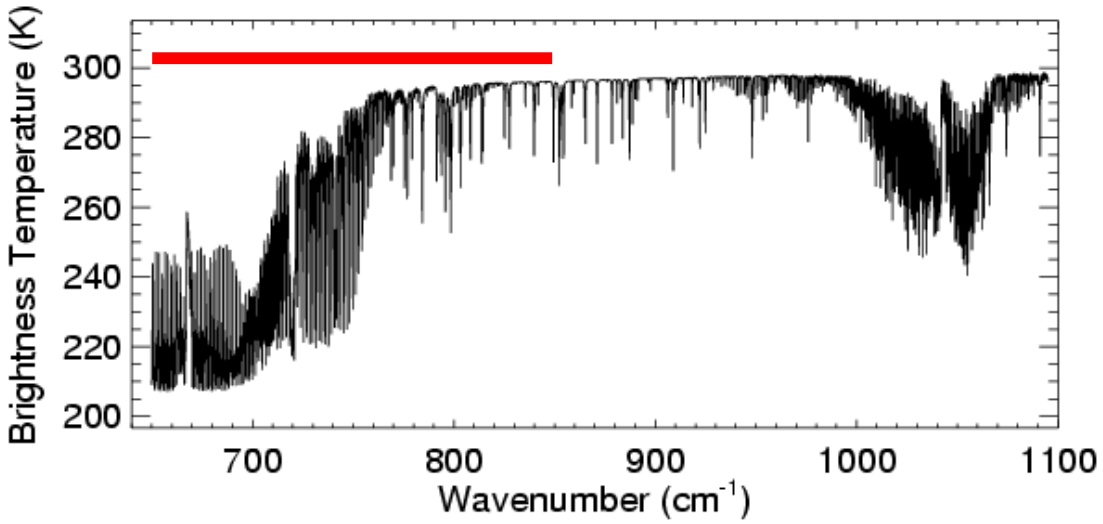
Monte-Carlo search has advantages over other search techniques

With any method it is best to start training on a small interval and increase progressively until sensor resolution is achieved

- Random search can be slow due to non-unique solution
  - Many combinations of nodes produce similar performance
  - Computational issues dominate with moderate number of candidates
    - 100 points at 0.0001 cm^{-1} implies 0.01 cm^{-1} channel
- Sequential search approach is faster than random search
  - Non-optimal when number of nodes approaches or exceeds 10
  - Not applicable to non-positive instrument functions (e.g., non-apodized interferometer ILS)
- Monte-Carlo approach replaces a selected node by one randomly chosen from remaining candidates
  - Acceptance depends on difference in *rms* errors
  - Number of replacements is restricted
    - Pre-defined based on based on selected nodes and total available
    - Acceptance test adjusted if acceptance rate is low

Use a subset of the sounding bands to examine OSS node selection properties

- Spectral region: 650-850 cm^{-1} (CO_2 band)
- Variable species: water vapor and ozone
- Surface emissivity set to unity
- Training set: AIRS/UMBC 48 profile set
- 5 scan angles with corresponding secant = 0, 0.5, 1, 1.5 and 2
- Reference line-by line model: LBLRTM



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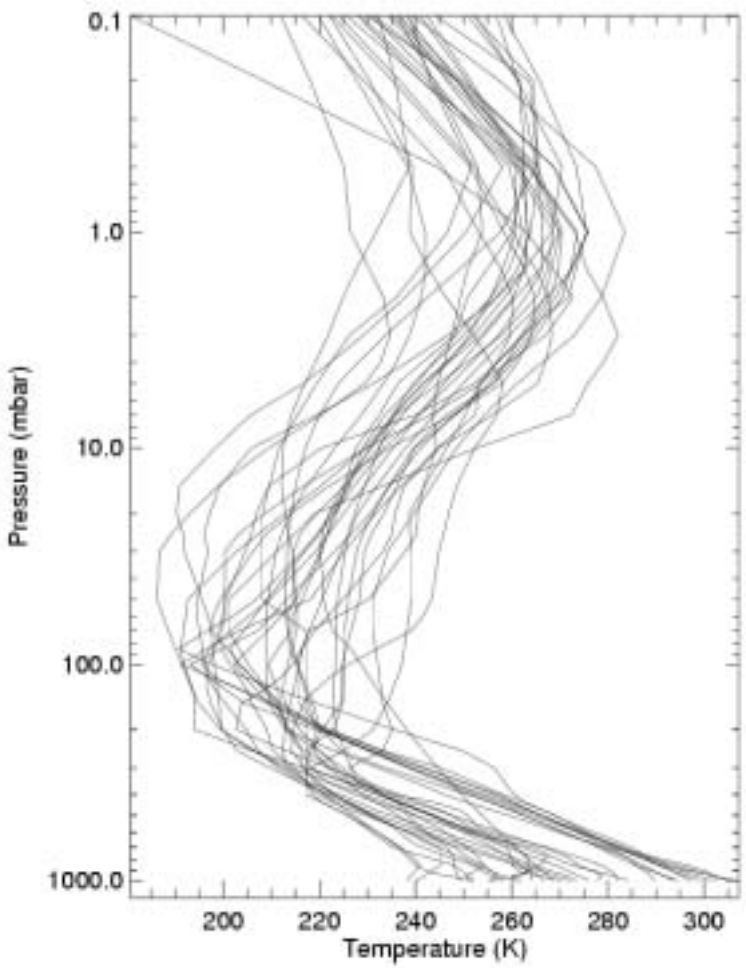
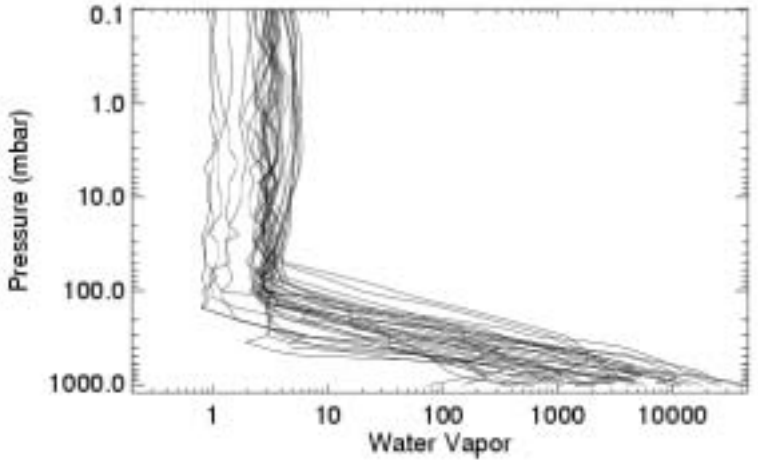
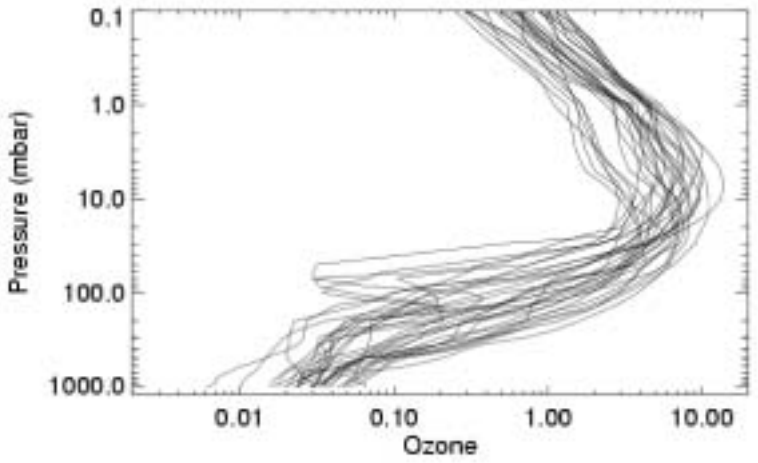
Training profiles provided by UMBC (AIRS profile set)

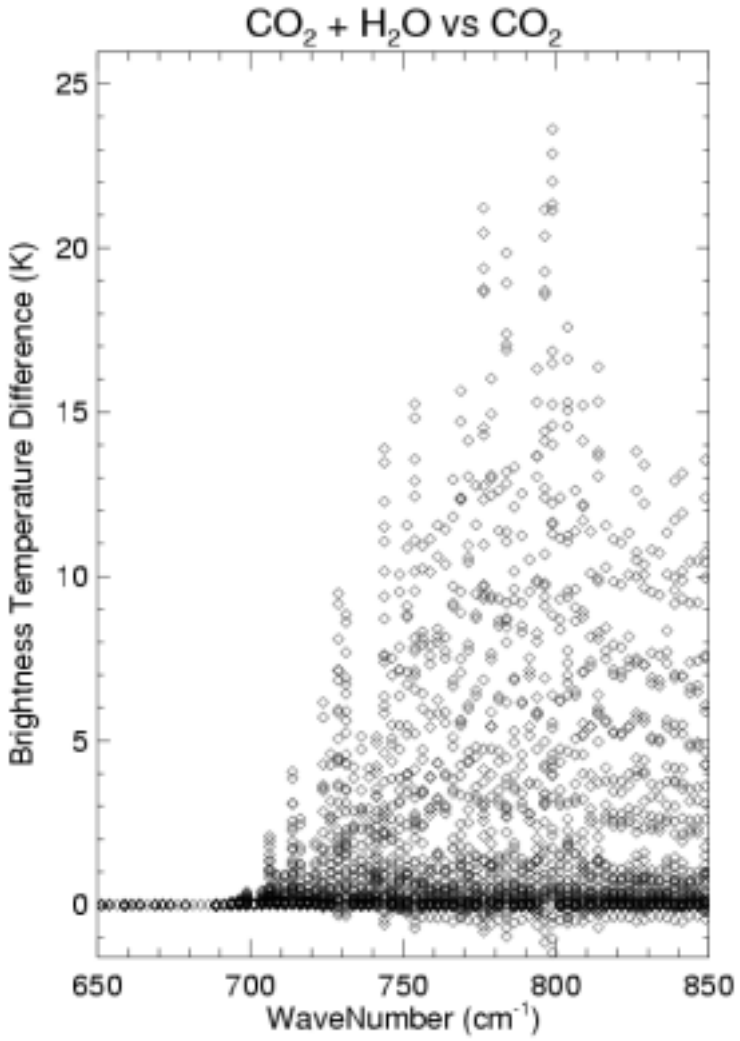


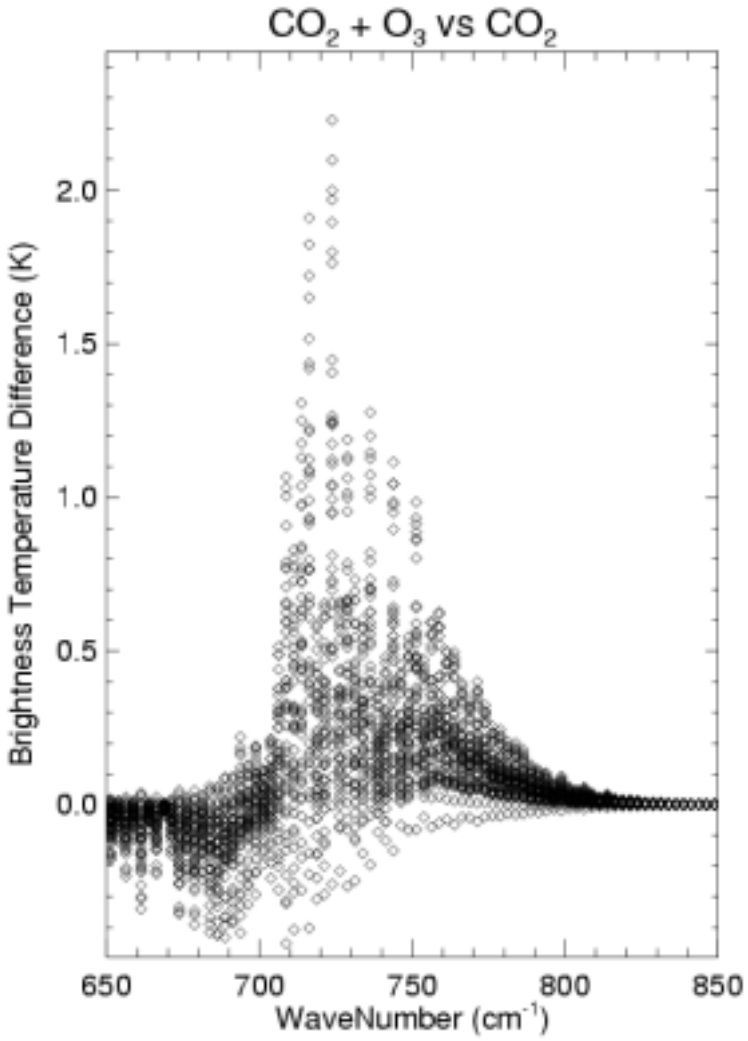




Examination of brightness temperature differences illustrates impact of H_2O and O_3 in the CO_2 band

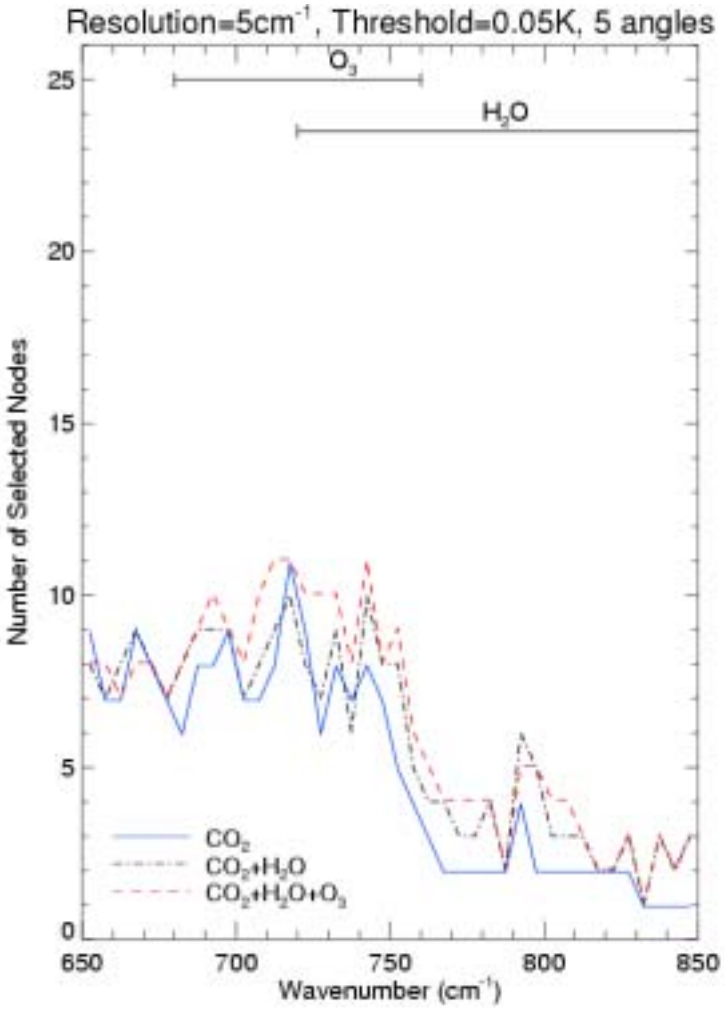
Expect more selection nodes in regions where there are overlapping gases

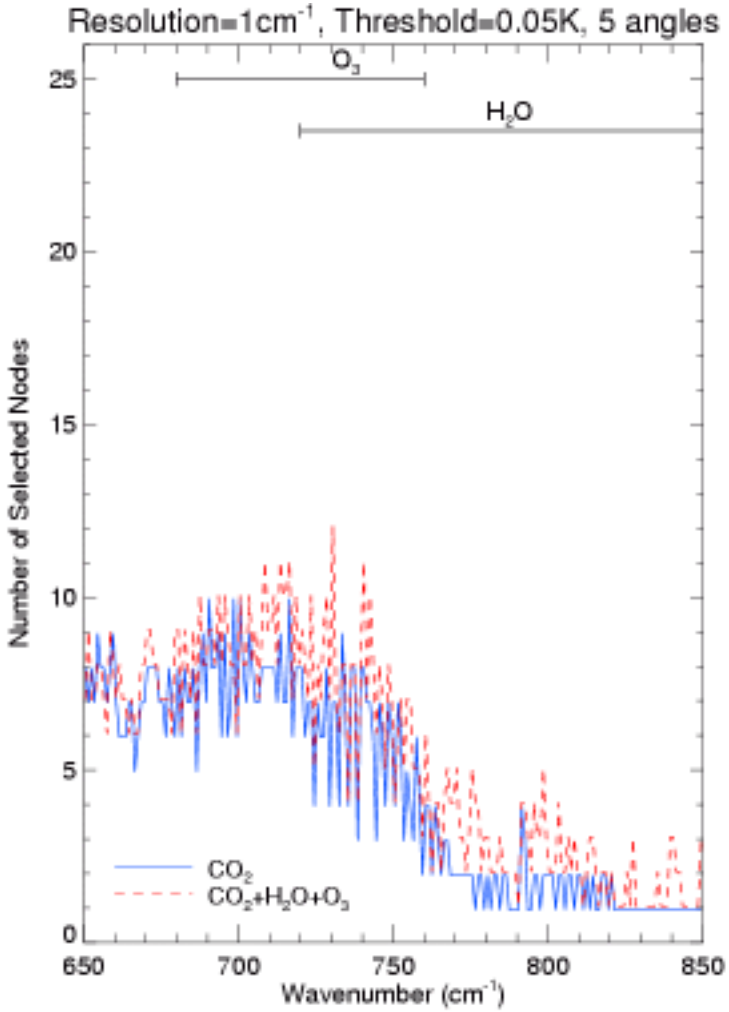




Number of selected nodes varies depending on number of atmospheric gases considered

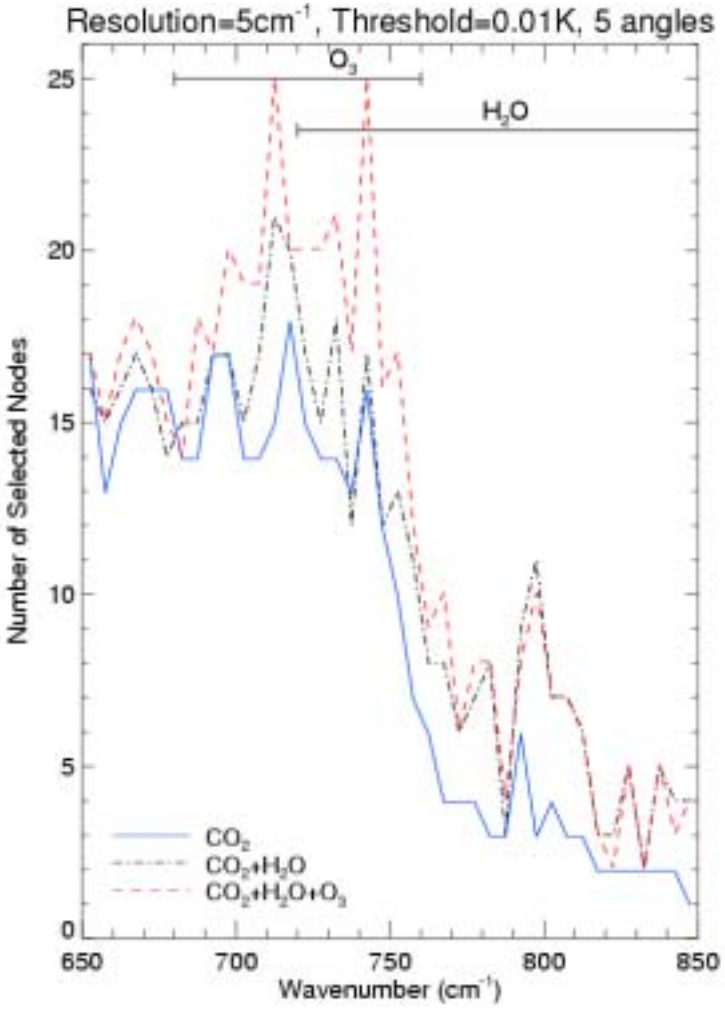
Spectral resolution has minimal impact on number of nodes

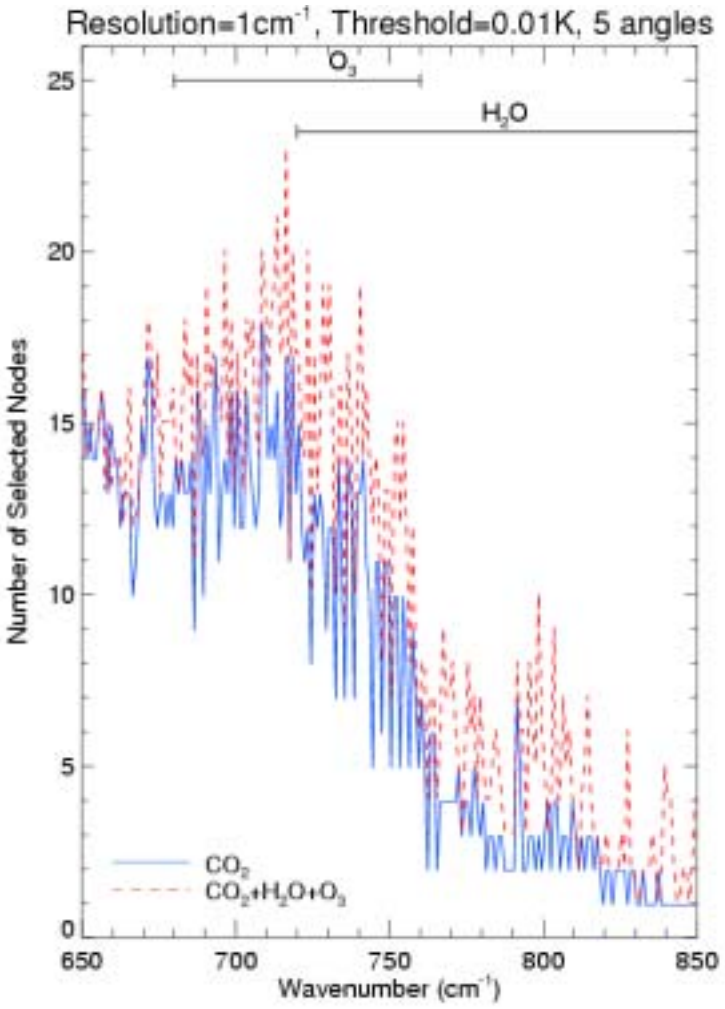




Number of selected nodes increases as accuracy threshold decreases

Larger increase in number of points where gases overlap





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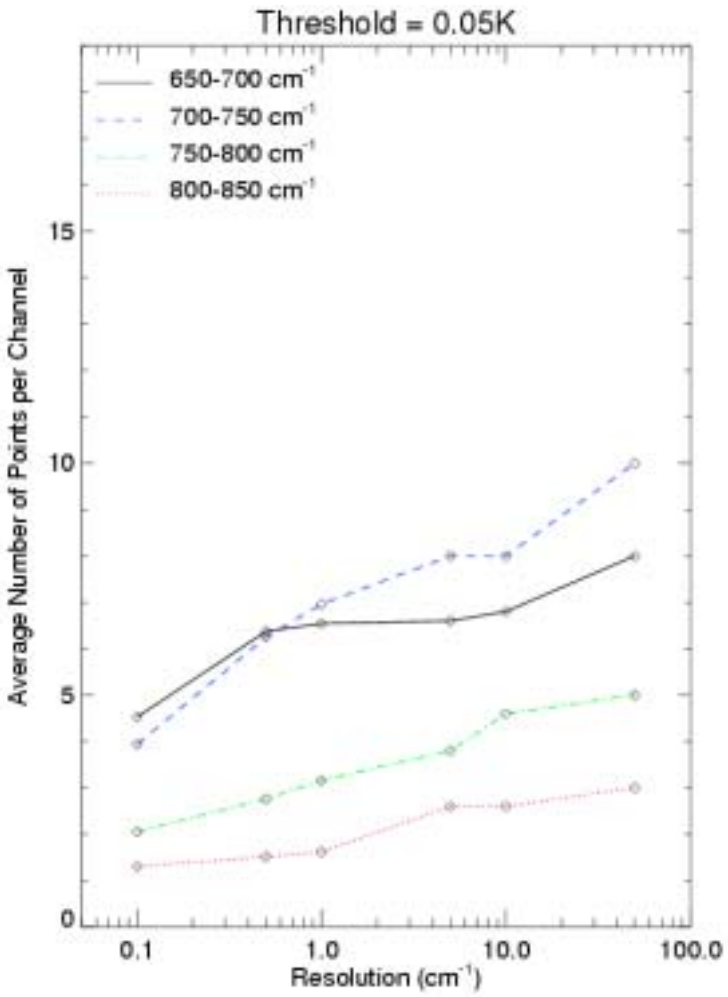
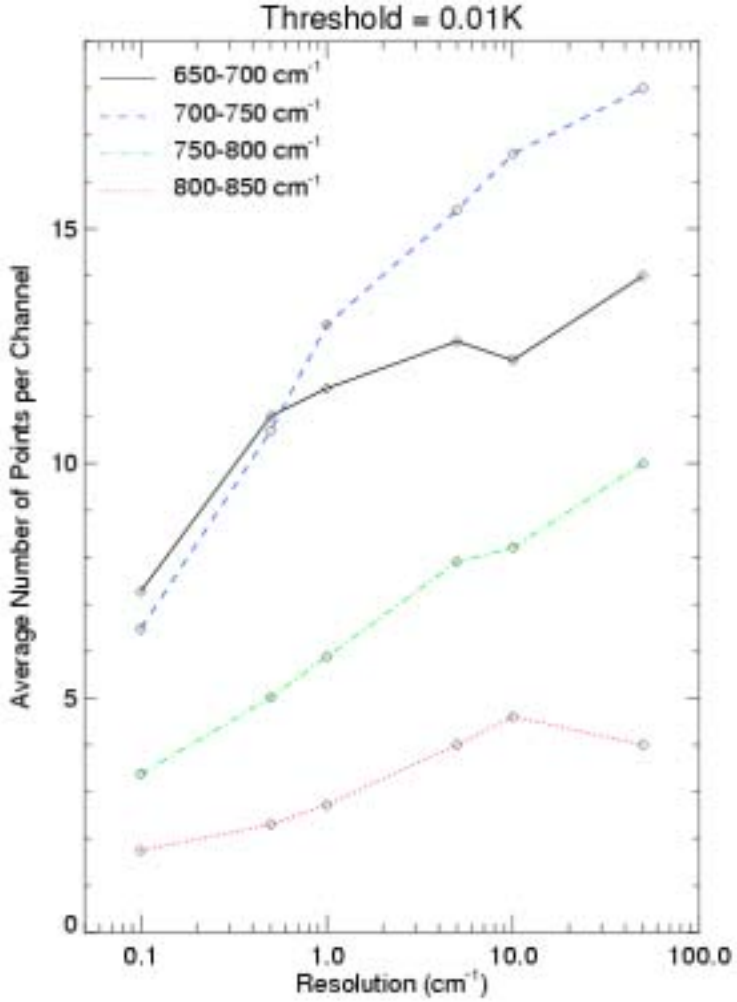
Number of selected nodes depends on accuracy, resolution, and spectrum complexity

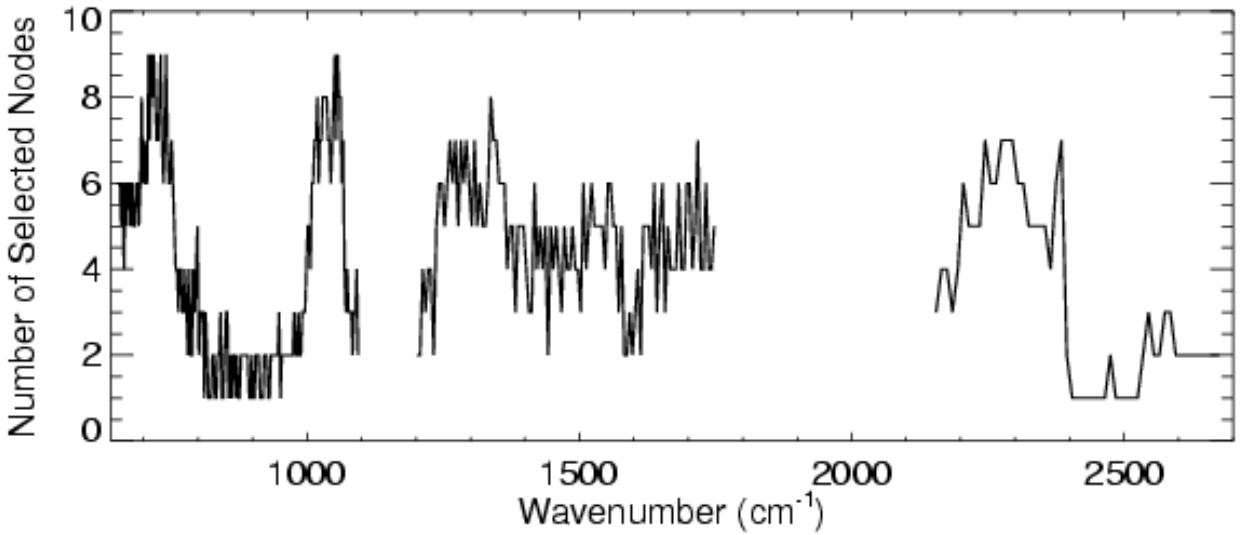
N^3 points required for gases with totally independent contributions (27 for three gases)





OSS has been applied to an “boxcar” instrument

- Three spectral bands: 600-1100 cm^{-1}, 1200-1750 cm^{-1} and 2150-2700 cm^{-1}
- Boxcar instrument function
  - Width: 1.25 cm^{-1}, 2.5 cm^{-1} and 5 cm^{-1}
- Selection accuracy of 0.05K in brightness temperature
- Nadir only

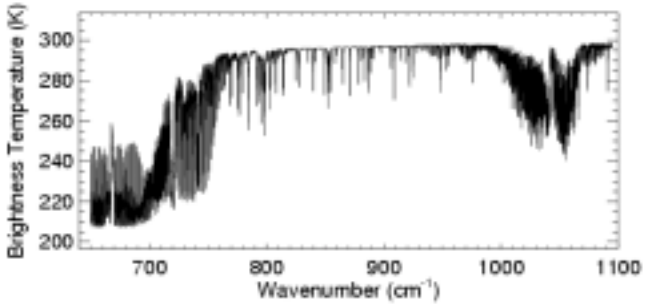


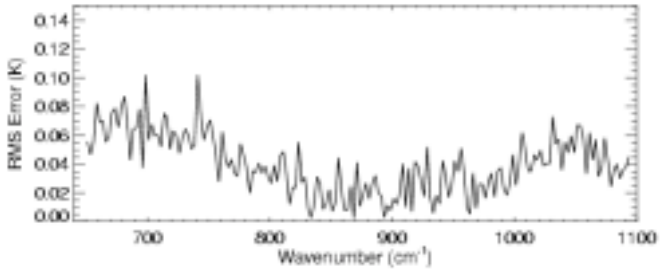
Model accuracy is very good when compared with independent set of profiles

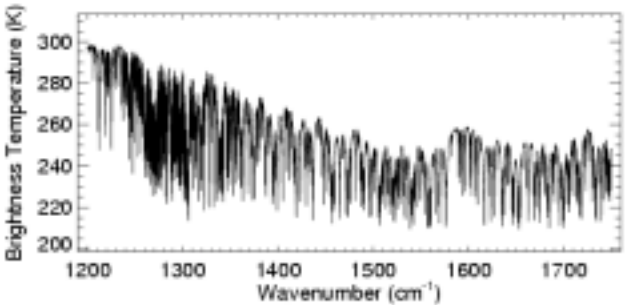
Train: UMBC

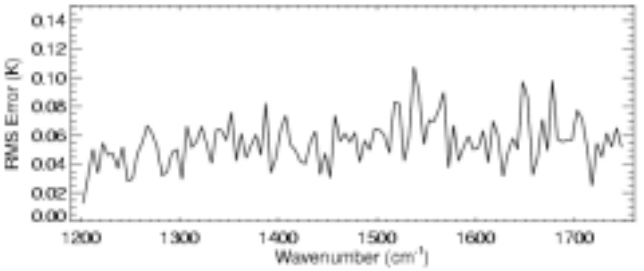
Validate: TIGR

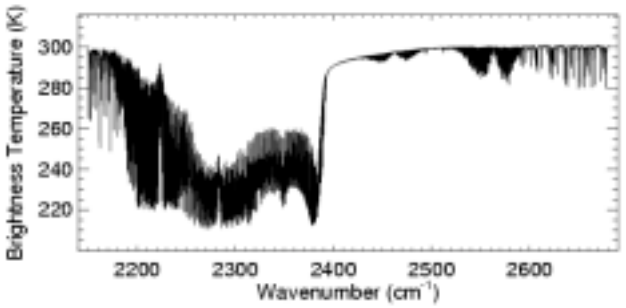
Errors are due ONLY to OSS sampling (no optical depth or radiative transfer errors)

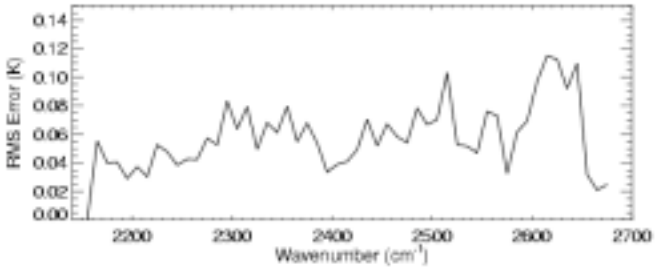












OSS-based radiative transfer model developed for sensor simulation and retrieval studies

Model used for retrieval algorithm development and to assess operational capabilities

- Radiative transfer is performed monochromatically from pre-computed absorption coefficients (at each selected node) for the fixed and variables constituents
- Gases are grouped into fixed (e.g. CO_2, CO and CFC's) and variable category (e.g. H_2O, O_3, CH_4, N_2O)
- Absorption coefficients are stored in each layer as a function of temperature
  - Absorption properties are linearly interpolated between temperature entries to preserve computational efficiency
- Water vapor requires special treatment for self-broadening effect
  - Total (self and foreign broadened) water vapor absorption coefficient (in cm^2/molecule) is stored as a function of both temperature and water vapor (takes into account self-broadening effects in the near wings; important for up-looking)
  - Approximately linear in specific humidity or partial pressure (i.e. two points are sufficient)

Main strength of the OSS approach is the analytical computation of the Jacobians

- For an average of 4.5 nodes/channel (0.05K accuracy), OSS model should be roughly two times slower than current fast models for AIRS
- Jacobian computation normally requires of the order of $(m+1)L^2$ operations for computation of transmittance and radiance derivatives (from $\partial\tau_l/\partial X_k$)

$$\partial R/\partial X_k = -\partial \mathrm{T}_{k+1}/\partial X_k\, \overline{B}_k + \sum_{l=k+1}^{L} \left(\partial \mathrm{T}_l/\partial X_k - \partial \mathrm{T}_{l+1}/\partial X_k\right)\overline{B}_l + \partial \mathrm{T}_L/\partial X_k\, \overline{B}_s$$

$$\partial \mathrm{T}_l/\partial X_k = \tau_l\, \partial \mathrm{T}_{l-1}/\partial X_k + \mathrm{T}_{l-1}\, \partial\tau_l/\partial X_k$$

- With monochromatic RT, Jacobian computation reduces to

$$\partial R/\partial X_k = \partial\tau_k/\partial X_k\, D_k$$

where $$D_k = \left(\overline{B}_k - \sum_{l=k+1}^{L} \left(\mathrm{T}_l - \mathrm{T}_{l+1}\right)\overline{B}_l - \mathrm{T}_L \overline{B}_s \right)$$

is independent of *X* and is derived in the process of adding layers successively during radiance computation

Minimal computational penalty for calculation of radiance derivatives

- Average number of operations per channel and per layer
  - No derivative case: optical depth and radiance calculation only
  - Temperature derivatives only: don't consider change of τ with T
  - Molecular derivatives and temperature derivatives
  - All derivatives, including temperature dependence of molecular absorption

Full calculation of derivatives only doubles the number of operations

	No Drv	Dr/Dt	Dr/Dq	Dr/Dt+
OD	33.42	33.42	33.42	47.89
RT	30.25	50.15	64.78	69.25
Total	**63.67**	**83.57**	**98.20**	**117.15**

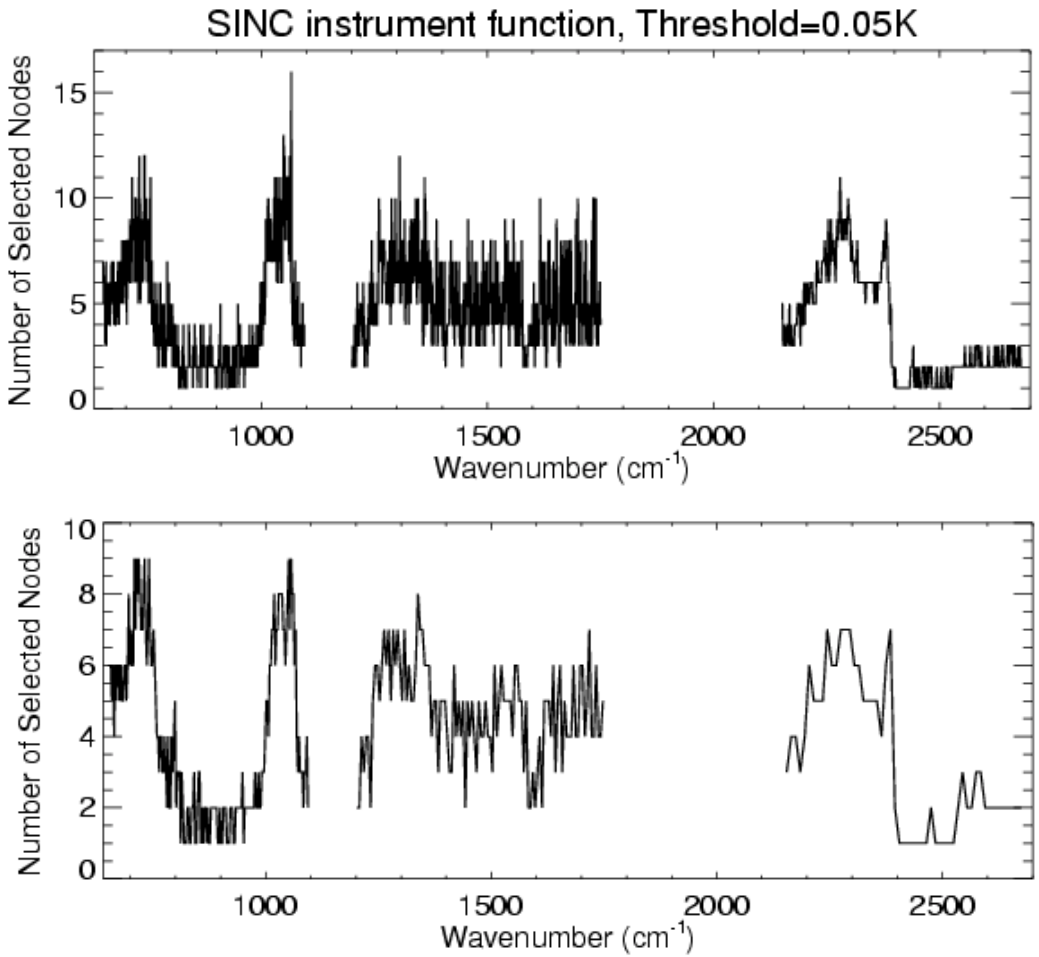
Direct application to Fourier interferometer (non-localized instrument function)

OSS model is directly applicable to non-apodized instrument functions

- Barnett (2000) and McMillin (2000) have devised approaches to extend application of narrow band models to *sinc* functions
- Extended instrument functions can present problems for model training
  - Instrument function is not positive, and negative weights cannot be used to indicate the presence of close pairs (or ill-conditioning)
    - Fix for OSS: use determinant control
  - Planck function and surface emissivity vary over the wavenumber span of the *sinc* function
    - Center frequency approximation used for localized instrument functions is non longer valid
    - Fix for OSS: use additional parameters for training
      - Accuracy may be enhanced by scene stratification
- Overlapping node points exploited in radiative transfer calculation
  - Using the same selection points for multiple channels reduces the overall number of radiative transfer calculations (application of channel weights requires minimal amount of computation time)
  - Duplication range of about 50% is typical

Number of selected nodes increases for non-localized instrument function (nadir-only case)

Must consider total number of independent points selected, not total number of selected nodes for each channel



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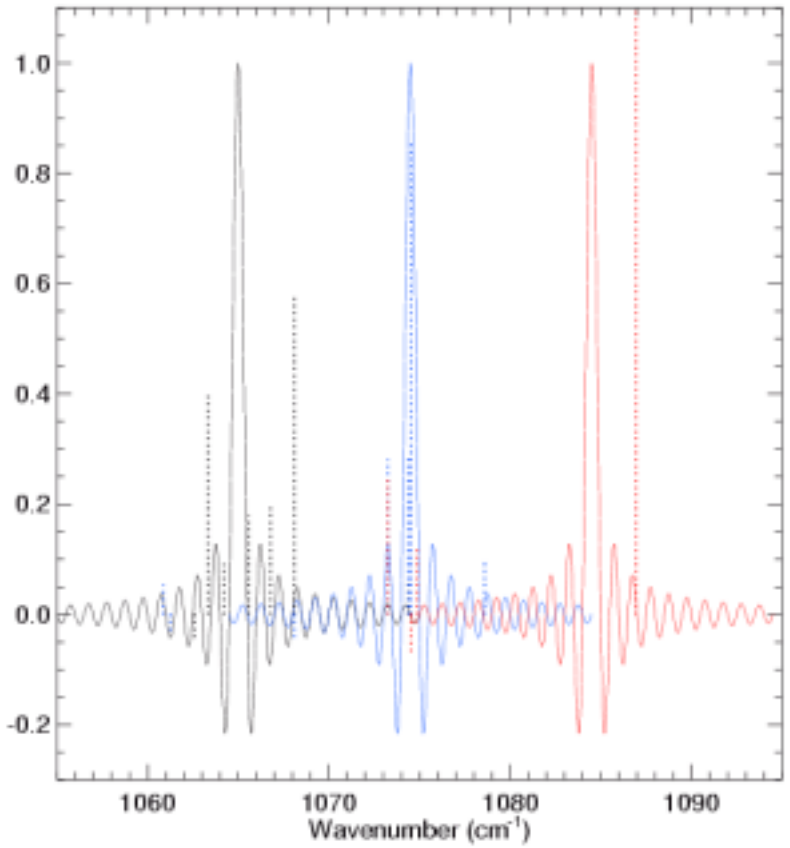
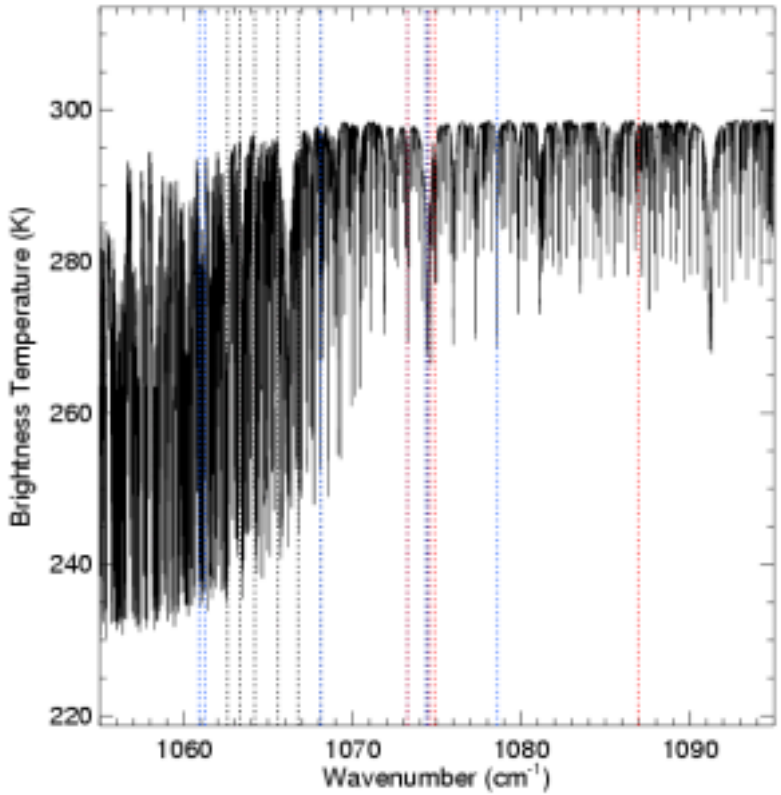
Examination of widely-spaced *sinc* functions illustrates redundant node selection



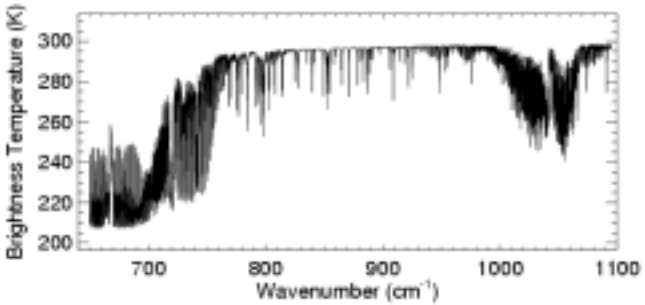


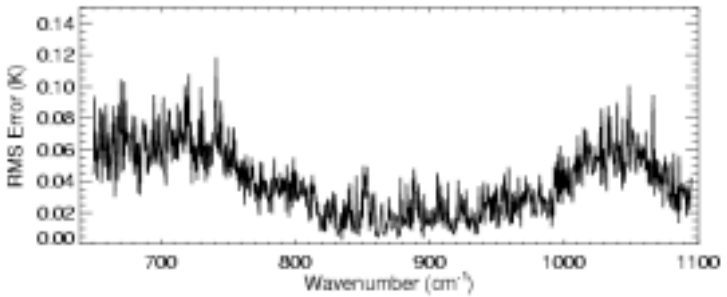
OSS selection performs very well for *sinc* function

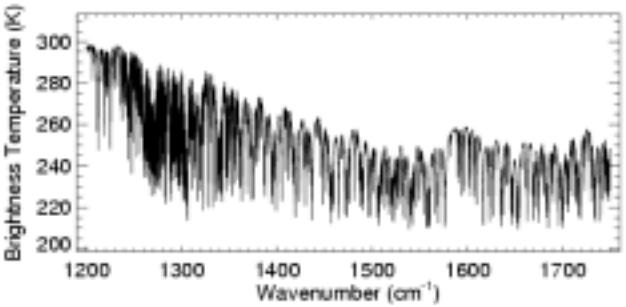
Train: UMBC

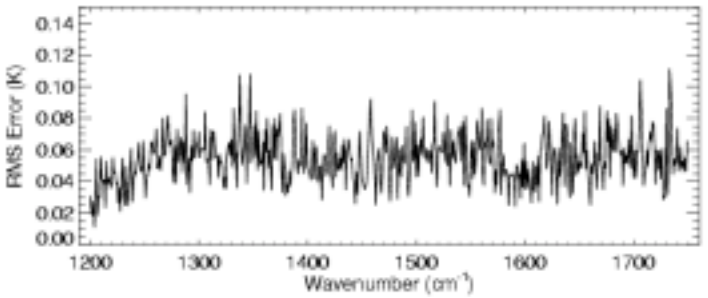
Validate: TIGR

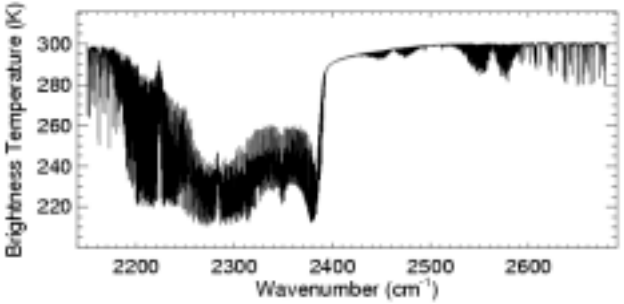
Errors are due ONLY to OSS sampling (no optical depth or radiative transfer errors)

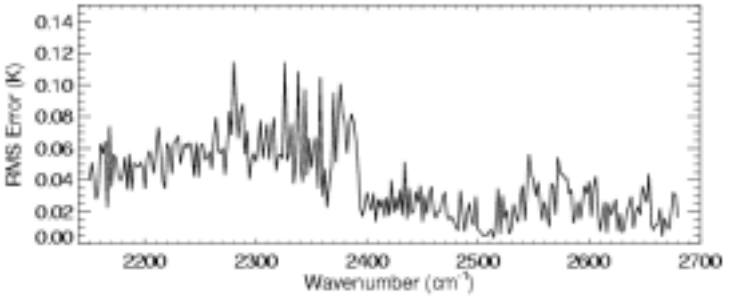












OSS technique addresses the need for algorithm speed, accuracy and flexibility

- OSS generation process is automated and unsupervised
  - No tuning needed; no check for instabilities; able to adapt quickly to changes in the instrument function or to update spectroscopy
- The method is robust with respect to training
  - Scene stratification improves performance over range of scene types
- Radiative transfer is monochromatic:
  - Accurate treatment of surface reflection
  - Amenable to multiple scattering applications
  - Flexible for use with varying observer levels or viewing geometries
- Model is both fast (especially when Jacobians are required) and accurate
  - Accuracy can be traded for speed depending on the sensor noise level and computational requirements of the problem
- On-going development at AER for range of applications
  - NPOESS CrIS (IR) and CMIS (microwave)
  - NAST-I (IR)
  - AIRS (IR)
  - Naval Post-Graduate School (microwave – visible)