Polarimetric aerosol remote sensing using neural networks

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SRON

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SPEX: Spectropolarimeter for planetary exploration

- Innovative measurement concept: spectral modulation
- Linear polarization parameters encoded in radiance spectrum by passive optical components

$$I(\lambda) = \frac{I_0(\lambda)}{2} \left[1 \pm P(\lambda) \cos\left(\frac{2\pi\delta(\lambda)}{\lambda} + 2\phi(\lambda)\right) \right]$$



Ground based SPEX instruments

- Two SPEX exemplars developed so far
 - 1. Prototype operated by SRON, developed for space applications and currently operated from ground
 - 2. Instrument operated by RIVM/Leiden University, dedicated to ground-based observations
- Wavelength ranges: 370-850 nm for SPEX prototype, 360-900 for RIVM SPEX





Spectropolarimetric aerosol retrievals at SRON

- Retrieval scheme developed during the last decade
- Variational retrieval based on Phillips-Tikhonov regularization

 $\hat{\mathbf{x}} = \arg\min\{[\mathbf{y} - \mathbf{F}(\mathbf{x}, \mathbf{b})]^T \mathbf{S}_{\epsilon}^{-1} [\mathbf{y} - \mathbf{F}(\mathbf{x}, \mathbf{b})] + \gamma (\mathbf{x} - \mathbf{x}_a)^T \mathbf{H} (\mathbf{x} - \mathbf{x}_a)\}$

- Extensively applied to POLDER measurements (presentations by O. Hasekamp and A. Stap during this meeting)
- Retrieval concept extended to ground based observations (SPEX)



Retrieval concept: some details

• Iterative cost function minimization (Gauss-Newton)

$$J(\mathbf{x}) = [\mathbf{y} - \mathbf{F}(\mathbf{x})]^T \mathbf{S}_{\epsilon}^{-1} [\mathbf{y} - \mathbf{F}(\mathbf{x})] + \gamma (\mathbf{x} - \mathbf{x}_a)^T \mathbf{H} (\mathbf{x} - \mathbf{x}_a)$$

$$\mathbf{F}(\mathbf{x}_{i+1}) \approx \mathbf{F}(\mathbf{x}_i) + \mathbf{K}_i (\mathbf{x}_{i+1} - \mathbf{x}_i)$$

$$\mathbf{K}_i = \mathbf{F}'(\mathbf{x}_i)$$

$$\mathbf{x}_{i+1} = (\mathbf{K}_i^T \mathbf{S}_{\epsilon}^{-1} \mathbf{K}_i + \gamma \mathbf{H})^{-1} [\mathbf{K}_i^T \mathbf{S}_{\epsilon}^{-1} (\mathbf{y} - \mathbf{F}(\mathbf{x}_i) + \mathbf{K}_i \mathbf{x}_i) + \gamma \mathbf{H} \mathbf{x}_a]$$

- Regularization parameter $\boldsymbol{\gamma}$ heuristically adjusted at each iteration
- First guess provided by look-up table and also used as a priori (\mathbf{x}_a)



LUT first guess generation

- LUT consists of about 600 aerosol models
- Each model defined by
 - Effective radius (r_{eff})
 - Effective variance (v_{eff})
 - Complex refractive index (m)
 - Fraction of spherical particles (f_{spher}) for fine and coarse mode
- First guess generation process
 - 1. Find model that best matches observations
 - 2. Iteratively update fine and coarse mode AOT for the chosen model using the LUT as simplified radiative transfer model



Looking for a better first guess

- Limitations of LUTs
 - Need for crude interpolations affects first guess quality
 - Need to read in LUT makes retrieval code less efficient
- First guess quality important for successful aerosol retrievals
- Idea to overcome LUTs: use neural networks
 - Fast computations
 - Do not require large memory allocation (after training)
 - Already proven good stand-alone retrieval algorithms
 - Might provide high quality first guesses for variational retrievals as well



NNs in one slide (ambitious goal)

Feedforward NN input-output function

$$y_k^{(0)} = x_k \qquad k = 1, \dots, N_{in}$$

$$y_k^{(l+1)} = \varphi^{(l+1)} \left(\sum_{j=1}^{N_l} w_{jk}^{(l)} y_j^{(l)} + b_k^{(l)} \right)$$

$$k = 1, \dots, N_{l+1}, \ l = 0, \dots, N_L - 1$$



- x_k input vector, N_L number of layers, $\varphi^{(l+1)}$ nonlinear function for $l = 0, ..., N_L 2$, either linear or nonlinear for $l = N_L 1$
- Goal: adjust {w_{jk}^(l), b_k^(l)} based on a training set Θ = {(x_p, t_p)}, so as to obtain approximately correct outputs even for x∉Θ



Neural network design

- Observation vector: log-reflectance and degree of linear polarization at 3 wavelengths, 6 VZA, rel. azimuth angle of 180°
- Auxiliary variables: SZA, surface pressure
- Output vector: 8 retrieved aerosol parameters + surf. albedo at 870 nm
- 7.7 X 10⁵ input-output pairs used to train the NN
- Random Gaussian noise added to input vector
 - Log-reflectance noise std: 0.02
 - DLP noise std: 0.005
 - SZA uncertainty: 0.25°
 - Surf. pressure uncertainty: 5 hPa
- Radiometric measurements compressed via linear PCA



Validation setup

- NN retrievals validated on 1.65 X 10⁵ independent simulations
- 3412 simulations used to compare variational retrieval schemes
 - Retrieval using the LUT as first guess
 - Retrieval using the NN as first guess
- Noise + random differences between non-retrieved quantities and assumed values ______ pseudo-operational scenario



Results on noisy simulated data

Fraction of successful retrievals ($\chi^2 < 2$): LUT 21.22%, NN 58.94%

Parameter	RMSE/MAE				
	fguess-LUT	fullretr-LUT	fguess-NN	fullretr-NN	
r _{eff} – fine	0.221/0.167	0.214/0.153	0.108/0.066	0.115/0.065	
Re(m) – fine	0.129/ <mark>0.107</mark>	0.115/0.092	0.064/ <mark>0.049</mark>	0.070/0.050	
Im(m) – fine	0.124/0.067	0.125/0.067	0.079/ <mark>0.034</mark>	0.081/0.035	
AOT – fine	0.723/ <mark>0.471</mark>	0.583/ <mark>0.357</mark>	0.279/ <mark>0.177</mark>	0.288/0.163	
r _{eff} – coarse	1.342/1.080	1.940/1.245	0.972/ <mark>0.753</mark>	1.145/ <mark>0.839</mark>	
Re(m) - coarse	0.092/0.075	0.098/ <mark>0.079</mark>	0.077/0.062	0.084/ <mark>0.066</mark>	
Im(m) – coarse	0.137/0.076	0.136/0.073	0.095/ <mark>0.049</mark>	0.099/ <mark>0.049</mark>	
AOT - coarse	0.844/0.549	0.909/ <mark>0.511</mark>	0.295/ <mark>0.193</mark>	0.348/0.185	



Results on noisy sim. data – successful retrievals

Fraction of successful retrievals ($\chi^2 < 2$): LUT 21.22%, NN 58.94%

Parameter	RMSE/MAE				
	fguess-LUT	fullretr-LUT	fguess-NN	fullretr-NN	
r _{eff} – fine	0.168/0.118	0.146/0.087	0.096/0.059	0.100/0.055	
Re(m) – fine	0.129/0.108	0.092/ <mark>0.069</mark>	0.059/ <mark>0.045</mark>	0.061/ <mark>0.044</mark>	
Im(m) – fine	0.099/ <mark>0.043</mark>	0.098/ <mark>0.042</mark>	0.071/0.031	0.073/0.032	
AOT – fine	0.451/0.262	0.192/ <mark>0.111</mark>	0.228/0.140	0.197/ <mark>0.104</mark>	
r _{eff} – coarse	1.300/1.048	2.225/1.322	0.944/ <mark>0.728</mark>	1.086/ <mark>0.807</mark>	
Re(m) - coarse	0.093/ <mark>0.076</mark>	0.099/ <mark>0.079</mark>	0.075/ <mark>0.061</mark>	0.084/ <mark>0.066</mark>	
Im(m) – coarse	0.139/ <mark>0.076</mark>	0.136/0.073	0.100/0.053	0.103/0.054	
AOT - coarse	0.394/ <mark>0.240</mark>	0.218/0.121	0.223/0.145	0.206/0.115	



Results – Fine mode AOT

Retrieved vs true AOT – Converging + non-converging retrievals





Results - Coarse mode AOT

Retrieved vs true AOT – Converging + non-converging retrievals



Results – Total AOT

Retrieved vs true AOT – Converging + non-converging retrievals



Application to RIVM SPEX measurements

- Ground-based RIVM-SPEX observations performed between 7 and 9 July 2013 at Cabauw (Netherlands)
- Intensity and degree of polarization in the principal plane at 441, 675 and 870 nm, used in the retrieval scheme
- Albedo at 870 nm fitted together with aerosol parameters





LUT vs NN first guess – SPEX retrievals

- 57 retrievals performed using LUT and NN first guess
- NN first guess yields more converging retrievals also with real measurements

N. data	LUT FG	NN FG	
$\chi^{2} < 1$	26 (45.6%)	36 (63.2%)	
χ ² < 2	36 (63.2%)	42 (73.7%)	
χ ² < 5	45 (78.9%)	49 (85.9%)	





SPEX vs AERONET : AOT and effective radius

LUT first guess

NN first guess





SPEX vs AERONET: refractive index

LUT first guess

NN first guess





Conclusions

Outline

- NNs seem a good replacement for LUTs in polarimetric aerosol retrieval schemes
- Evidence with simulated data seems confirmed by first (few) preliminary experiments with real observations
- More reliable conclusions to be drawn as soon as more SPEX measurements are available

Limitations and open challenges

- Reduced input flexibility (once trained for a set of wavelengths/angles, NN needs measurements at (or close to) those wavelengths/angles)
- Difficult extension to satellite geometry in case of multiangular observations (POLDER set of viewing angles is highly variable from pixel to pixel – difficult to define an uniform observation vector for training a NN)

