Non-smooth optimization in the 1D-Var data assimilation of all-sky infrared satellite observations

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Abstract

We test the ability of non-smooth optimization algorithms to improve the variational data assimilation of all-sky infrared satellite observations from the Atmospheric Infrared Sounder (AIRS). Such observations are challenging to assimilate because of the sharp transition between clear to cloudy conditions in the observation operator. Using empirically derived background and observation error covariance matrices, we test the relative performance of several large-scale optimization algorithms, including the non-smooth LMBM method of Karmitsa etȧl, to run identical and non-identical observing system simulation experiments (OSSEs) with the RTTOV and CRTM radiative transfer models. We conclude that non-smooth optimization offers significant promise for the assimilation of all-sky infrared radiances.

Keywords: reduced order model, principal component analysis, proper orthogonal decomposition, error covariance matrix

1. Introduction

The problem of clear-sky data assimilation using infrared satellites is well understood (e.g. [8], [5]), and while several studies have addressed cloud-fraction data assimilation, the full all-sky infrared data assimilation problem is currently a topic of intense research, especially at cloud-resolving scales.

At such scales, the presence of clouds introduces strong non-linearities in the observation (forward) operator with respect to the cloud micro-physical control variables between cloudy and clear-sky radiances due to the sharp transitions from clear skies to clouds within the atmosphere. This high degree of non-linearity ([14]) in the cost function may become an issue for any optimization algorithm being employed in a variational assimilation system. A highly non-linear or discontinuous cost function may lead to a poor solution or even a divergence of the minimization algorithm ([10]). Different methods are used to try to work around these non-linear and discontinuous issues including smoothing and regularization (e.g. [2], [13]); however, these resolutions are often ad-hoc and it is not clear that these remedies can be applied in more general settings. In addition, it is not known how these workarounds impact the final data assimilation solution. Many issues in this area still remain unresolved. For example, while in one recent study which contained cloud information in the initial condition, the data assimilation converged and improved the cloud information based on all-sky infrared radiances ([29]), in another study, where a cloud was not present in the initial condition, data assimilation with a traditional 4D-Var method for the infrared all-sky problem fails to reconstruct the desired cloud ([23]). We will survey these problems and offer a new solution that treats the non-linearities and non-discontinuities directly. through the use of a penalized 1D-Var with non-smooth optimization. State of the art non-smooth optimization algorithms may be beneficial in handling the sharp transitions between clear and cloudy conditions. Steward et al 2012 showed the potential for non-smooth optimization algorithms in similar circumstances.

In Bauer et al. ([2]) and Geer et al. ([9]), some interesting statistics are given. While satellite observations provide 90-95% of the data that is assimilated, over 75% of these observations must be discarded due to cloud contamination and unknown surface emissivities. While all-sky microwave data is currently used around the world in operational centers, all-sky infrared data is still being investigated. While many cloudy-infrared products are already available ([14]), these products focus primarily on single-layer retrieval products from the infrared data such as cloud-top pressure and temperature, which introduce a source of error ([23]). This work examines assimilating all-sky infrared radiances directly through the use of a parameterized multiple-scattering radiative transfer model. The potential benefits of this approach are many, and include improving initial conditions of the optical depth and hydrometeor species and concentration of the cloudy column under investigation. When used in conjunction with microwave information, in particular, this method may greatly enhance cloud information in the initial conditions ([1]).

Another challenge in assimilating these observations is the development of realistic background and observation error covariance representations. Using sample statistics from training data from the WRF atmospheric model, we give realistic approximations to the background and observation error covariance matrices. We use the Singular Value Decomposition of these matrices to obtain a reduced-order basis that accounts for 99% of the variance with only 200 principal components. In addition, by neglecting small-scale components of the error covariance matrices, we effectively regularize the variational problem.

In this paper we compare the relative performance of four state-of-the-art optimization methods: the Limited-Memory Broyden-Fletcher-Goldberg-Shanno (L-BFGS, citations) Quasi-Newton method; the Limited-Memory Bundle Method (LMBM, citations) non-smooth optimization method; and the conjugate gradient methods of Hager and Zhang (CG-Descent, citations) and Andrei (DESCON, citations).

We test our method on all-sky conditions: a clear column, retrievals of which have been used in operational assimilation for many years (add e.g. citation); optically thin overcast settings (with cirrus, stratus, and cumulus clouds); and optically thick convective clouds (cumulonimbus with and without precipitation). We show how this method behaves in all of these situations starting from a near-clear sky (i.e. no cloud background information) and has good potential to retrieve cloud-top properties.

We consider synthetic data from the Atmospheric Infrared Sounder (AIRS) satellite with the Weather Research and Forecasting numerical weather prediction model. We use the ECWMF RTTOV fast radiative transfer model (citation) and Joint Center for Satellite Data Assimilation Community Radiative Transfer Model (CRTM, citation). We use these two for identical and non-identical twin OSSE experiments.

1.1. Survey

Bayler et al. (2000, [3]) used a successive correction algorithm for cloud initialization using infrared GOES sounder data with an 80 km resolution, Kessler microphysics (cloud, rain, and water vapor species) and a Kuo cumulus parameterization scheme. Janiskova et al. (2002, [12]) made preliminary investigations of the 1D-Var data assimilation of temperature, humidity, and pressure as proxies for the development of stratiform clouds. Most importantly for this work, careful development of the linearization of the observation operator and cloud parameterization was described. This work used M1QN3, an implementation of the limited- memory BFGS algorithm. The use of cloud microphysical variables as control variables was discussed, but it was decided that directly including these variables would be too difficult due to the need for statistics of background errors and performance considerations. Finally, the authors noted a difficulty in triggering new clouds when the atmospheric state was far from the conditions of cloud formation. McNally (2002, [18]) measured the cloud-modified, adjoint-derived sensitivity of the ECMWF model error to clouds, and found that there was a high degree of correlation between areas of baroclinic instability (which contributes to model error) and clouds. He also concluded that the use of hyper-spectral cloudy IR radiances could have a large impact on improving model error, although a great deal of effort would be needed to address various issues. The issues he noted include specifying background error statistics, optimally selecting which channels to use, and the large sensitivity of the observation to errors in cloud cover fraction. Szyndel et al. (2004, [26]) examined 1D-Var assimilation of cloud data using a simplistic single-layer cloud model with an ensemble of related synthetic satellite observations. Their control variables consisted of an atmospheric profile without clouds, effective cloud amount and cloud-top pressure of their single layer cloud using 4–6 infrared channels. They used the minimum-residual method as a background first guess for their 1D-Var approach. The effective cloud amount and cloud-top pressure were "clamped" to between 0.01 and 1.0, respectively. As detailed below, this clamping can cause issues for the convergence of the algorithm, which indeed Szyndel et al. acknowledged. They used a Gauss-Newton method and the Levenberg-Marquardt method for least-squares fitting, both of which require storage on the order of N^2, where N is the number of control variables. Since the only control variables used in their study were cloud-top pressure and effective cloud amount, this is not an issue. In this work, where the cloud variables are considered at each cloud-level, such optimization methods become computationally infeasible, and the limited-memory approaches detailed above become vital to success.

Chevallier et al. (2004, [4]) investigated the issue of 4D-Var of cloud-affected AIRS and MVIRI infrared radiances using control variables of temperature, humidity, ozone, surface temperature and pressure. Like Janiskova et al. (2002, [12]), the decision was made not to include cloud variables as control variables due to the difficulty of specifying background errors and concerns about the non-linearity of the observation operator. The observation operator was kept simple "so that thresholds and strong nonlinearities do not make the 4D-Var minimization stop before reaching the absolute minimum of the cost function." This statement alludes to the fact that discontinuities and highly non-linear observation operators can cause the algorithms to terminate in their line searches, especially if they are not set in the context of non-smooth optimization. In a similar study, Tompkins and Janiskova (2004, [27]) describe a variational model that determines cloud cover from infrared observations based on parameterizations and statistical properties.

Vukicevic (2004, [28]) investigated assimilating visible and infrared measurements for mesoscale cloud-state estimation using a 4D-Var algorithm with the RAMS model with explicit microphysics and an explicit visible and infrared radiative transfer observation operator. Vukicevic included model error, and found that she was able to achieve some improvement in cloud cover when compared to the background state; however, not much improvement was seen when the background state was clear. Greenwald (2004, [10]) studied the adjoint sensitivity of three infrared channels and found that these channels are sensitive to microphysical parameters. Wei et al. (2004, [30]) studied the AIRS channels and found the same. Vukicevic (2006, [29]) found that increasing the number of channels and frequency of observation had a clear impact on improving the assimilation results, that infrared could not trigger clouds, and that a simple linear model error approach was insufficient for controlling the error in boundary conditions.

Li et al. (2005, [15]) treat the 1D-Var problem with full microphysical particles including particle size and radiative transfer for AIRS data. Similar studies on the benefits of assimilating hyperspectral infrared channels were conducted by Smith et al. (2005, [24]) and Zhou et al. (2005, [32], 2007, [33]). [25].

Errico et al. (2007, [6]) reports on the outcome of a 2005 international workshop where the issues in assimilating cloudy satellite transfer was discussed. A variety of issues were identified that needed to be improved including: issues with the observations (including improving utilization of millimeter data); issues regarding models (including improved microphysical schemes, especially with ice); issues with radiative transfer (including quantifying satellite biases and standard deviations, using improved microphysical schemes); and issues with the data assimilation itself (including how to deal with highly non-linear and non-smooth processes, moving beyond perfect model assumptions, and improving uncertainty quantification). Errico et al. emphasizes the interdisciplinary nature of this problem.

Lopez (2007, [17]) reviews the issues facing the variational assimilation of cloud and precipitation radiance data from the perspective of the models. Based on time-scale arguments, he concludes that it is sufficient to assimilate humidity values as a proxy for cloud microphysics when the clouds are precipitating or convective, but for cirrus clouds the microphysical variables are needed. Lopez stresses the difficulties in dealing with a highly nonlinear observation operator. Lopez says that "improved linearity is usually achieved either by using smooth functions to describe each physical process or by artificially reducing or neglecting the perturbations of problematic quantities involved in the parameterization." This work treats the non-linearities directly.

Weisz et al. (2007, [31]) demonstrate a model for determining cloud-top pressure for AIRS data based on training of a global data model. They use an eigenvalue regression to determine regression coefficients for either water or ice clouds. Li and Liu (2009, [16]) used this model and showed improved tracking of a hurricane using AIRS infrared data assimilation with the WRF/DART testbed, which uses an Ensemble Adjustment Kalman Filter.

Heilliette and Garand (2007, [11]) describe a method for assimilating infrared radiances using a highly simplified cloud model with four parameters: single layer cloud height, 15 μm effective emissivity, and effective particle size of water and ice. Scattering was not considered as they used the RTTOV-8 model. They used a 1D-Var formulation for full columns of water vapor and temperature in addition to the four cloud parameters mentioned above. They considered that these four cloud parameters were independent and thus had a diagonal term in the background error covariance matrix B, and assimilated synthetic radiances corresponding to 100 channels of AIRS. Starting from a first guess for cloud parameters based on the CO_2 slicing method, they found that they were able to reduce the variance of these variables and have a significant impact on the retrieved values. Pavelin et al. (2008, [21]) performed a similar study and found that while they achieved positive results for temperature and humidity, their cloudy parameters showed less accuracy when multiple channels were used, attributed in part to the lack of multiple scattering.

McNally (2009, [19]) describes a near-operational 4D-Var assimilation of infrared brightness temperature using an infrared radiative model based on simple brightness temperatures (i.e. a single-layer blackbody cloud with no multiple scattering). The background for this study was chosen using the minimum-residual method ([7]) using two channels. Only completely clear or overcast values were considered. i.e. no cloud fraction was chosen. By using the minimum residual method, no error covariances on the cloud-top were required, and only the cloud-top pressure was adjusted. This procedure showed slight positive impact on the RMS temperature and humidity. Pangaud et al. (2009, [20]) publish a similar study and show positive impact on geopotential up to 72 hours.

Seaman et al. (2010, [23]) use 4D-Var system to assimilate infrared radiances, and find that if no cloud is present in the initial condition, the analysis proceeds as if no cloud was present. In this dissertation we explain why this occurred and an easy remedy.

Zupanski et al. (2011, [34]) describe a system for assimilating synthetic GOES-R infrared data in cloudy conditions with the WRF model. This was a "non-identical twin" experiment as they used the RAMS model for creating their observations. Using a single channel of infrared data with a two-stream delta-Eddington radiative transfer model with a cloud optical property model, they examined the assimilation of a hurricane with potential temperature, specific humidity, and five hydrometeor classes as control variables, and experimented with leaving different hydrometeor classes out. They concluded that it is essential to use as many classes of hydrometeor as possible in order to obtain the maximum benefit of assimilating cloudy radiances, with the possible exception of rain or graupel. Polkinghorne and Vukicevic (2011, [22]) describe a 4D-Var system for the assimilation of GOES-8 infrared cloudy radiances. A cloud-mask is first used so that only the same cloud type is considered. They performed a wide variety of experiments including varying the assimilation window. They conclude that "while increasing the length of the assimilation window does not lead to a greater decrease in cost function, it does lead to a smoother dynamical response to the assimilation and a better forecast." That increasing the assimilation window does not decrease the cost function is somewhat apparent since the cost function is a non-decreasing function of assimilation window, i.e. the more non-exact observations considered, the greater the value of the cost function will be. They conclude that their main hindrance to achieving better errors was the cloud location problem, which may be fundamentally related to their cloud mask approach. It is probably better to solve the cloud location problem through an all-sky observation assimilation approach rather than determining an inaccurate cloud mask a priori; this is the approach is taken in this dissertation.

Finally, Bauer (2011, [1]) concludes with a survey of the all-sky and microwave and infrared schemes used operationally across the world. The focus is currently still on single-layer clouds for infrared data across the world, although research is being conducted into full gray cloud, multiple scattering infrared radiances. Most operational centers only assimilate fully clear or fully cloudy-skies, and effective cloud amount is not considered. Lavanant et al. (2011, [14]) discuss the cloud-derived products that are available for the Infrared Atmospheric Sounding Interferometer (IASI) satellite.

References

[1] P. Bauer, T. Auligne, W. Bell, A. Geer, V. Guidard, S. Heilliette, M. Kazumori, M.-J. Kim, E. H.-C. Liu, A. P. McNally, B. Macpherson, K. Okamoto, R. Renshaw, and L.-P. Riishojgaard. Satellite cloud and precipitation assimilation at operational NWP centres. *Quarterly Journal of the Royal Meteorological Society*, 137(661):1934–1951, October 2011.

[2] P. Bauer, A. J. Geer, P. Lopez, and D. Salmond. Direct 4D-Var assimilation of all-sky radiances. Part I: implementation. *Quarterly Journal of the Royal Meteorological Society*, 136(652):1868–1885, October 2010.

[3] G. M. Bayler, R. M. Aune, and W. H. Raymond. NWP cloud initialization using GOES sounder data and improved modeling of nonprecipitating clouds. *Monthly Weather Review*, 128:3911–3920, November 2000.

[4] F. Chevallier, P. Lopez, A. Tompkins, M. Janiskova, and E. Moreau. The capability of 4D-Var systems to assimilate cloud-affected satellite infrared radiances. *Q. J. R. Meteorol. Soc.*, 130:917–932, 2004.

[5] F. Chevallier and J. F. Mahfouf. Evaluation of the Jacobians of infrared radiation models for variational data assimilation. *Journal of Applied Meteorology*, 40(8):1445–1461, August 2001.

[6] R. M. Errico, G. Ohring, P. Bauer, B. Ferrier, J. F. Mahfouf, J. Turk, and F. Z. Weng. Assimilation of satellite cloud and precipitation observations in numerical weather prediction models: Introduction to the JAS special collection. *Journal of the Atmospheric Sciences*, 64(11):3737–3741, November 2007.

[7] J. R. Eyre. Inversion of cloudy satellite sounding radiances by nonlinear optimal estimation. I: theory and simulation for TOVS. *Quarterly Journal of the Royal Meteorological Society*, 115(489):1001–1026, July 1989.

[8] J. R. Eyre, G. A. Kelly, A. P. McNally, E. Andersson, and A. Persson. Assimilation of TOVS radiance information through one-dimensional variational analysis. *Quarterly Journal of the Royal Meteorological Society*, 119(514):1427–1463, October 1993.

[9] A. J. Geer, P. Bauer, and P. Lopez. Direct 4D-Var assimilation of all-sky radiances. Part II: assessment. *Quarterly Journal of the Royal Meteorological Society*, 136(652):1886–1905, October 2010.

[10] T. J. Greenwald, T. Vukicevic, L. D. Grasso, and T. Vonder Haar. Adjoint sensitivity analysis of an observational operator for visible and infrared cloudy-sky radiance assimilation. *Quarterly Journal of the Royal Meteorological Society*, 130(597):685–705, January 2004.

[11] S. Heilliette and L. Garand. A practical approach for the assimilation of cloudy infrared radiances and its evaluation using AIRS simulated observations. *Atmosphere-Ocean*, 45(4):211–225, 2007.

[12] M. Janiskova, J. F. Mahfouf, and J. J. Morcrette. Preliminary studies on the variational assimilation of cloud-radiation observations. *Quarterly Journal of the Royal Meteorological Society*, 128(586):2713–2736, October 2002.

[13] M. Janiskova and J. J. Morcrette. Investigation of the sensitivity of the ECMWF radiation scheme to input parameters using the adjoint technique. *Quarterly Journal of the Royal Meteorological Society*, 131(609):1975–1995, 2005.

[14] L. Lavanant, N. Fourrie, A. Gambacorta, G. Grieco, S. Heilliette, F. I. Hilton, M. J. Kim, A. P McNally, H. Nishihata, E. G. Pavelin, and F. Rabier. Comparison of cloud products within IASI footprints for the assimilation of cloudy radiances. *Quarterly Journal of the Royal Meteorological Society*, 2011. In early view.

[15] J. Li, H.-L. Huang, C.-Y. Liu, P. Yang, T. J. Schmit, H.-L. Wei, E. Weisz, L. Guan, and W. P. Menzel. Retrieval of cloud microphysical properties from MODIS and AIRS. *Journal of Applied Meteorology*, 44(10):1526–1543, October 2005.

[16] J. Li and H. Liu. Improved hurricane track and intensity forecast using single field-of-view advanced IR sounding measurements. *Geophysical Research Letters*, 36:4 PP., June 2009.

[17] P. Lopez. Cloud and precipitation parameterizations in modeling and variational data assimilation: A review. *Journal of the Atmospheric Sciences*, 64(11):3766–3784, November 2007.

[18] A. P McNally. A note on the occurrence of cloud in meteorologically sensitive areas and the implications for advanced infrared sounders. *Quarterly Journal of the Royal Meteorological Society*, 128(585):2551–2556, October 2002.

[19] A. P McNally. The direct assimilation of cloud-affected satellite infrared radiances in the ECMWF 4D-Var. *Quarterly Journal of the Royal Meteorological Society*, 135(642):1214–1229, July 2009.

[20] Thomas Pangaud, Nadia Fourrie, Vincent Guidard, Mohamed Dahoui, and Florence Rabier. Assimilation of AIRS radiances affected by mid-to Low-Level clouds. *Monthly Weather Review*, 137(12):4276–4292, December 2009.

[21] E. G Pavelin, S. J English, and J. R Eyre. The assimilation of cloud-affected infrared satellite radiances for numerical weather prediction. *Quarterly Journal of the Royal Meteorological Society*, 134(632):737–749, April 2008.

[22] R. Polkinghorne and T. Vukicevic. Data assimilation of cloud-affected radiances in a cloud-resolving model. *Monthly Weather Review*, 139:755–773, March 2011.

[23] C. J. Seaman, M. Sengupta, and T. H. Vonder Haar. Mesoscale satellite data assimilation: impact of cloud-affected infrared observations on a cloud-free initial model state. *Tellus A*, 62(3):298–318, May 2010.

[24] W. L. Smith, D. K. Zhou, H. L. Huang, H. E. Revercomb, A. M. Larar, and C. Barnett. Ultra high spectral satellite remote sounding - results from aircraft and satellite measurements. In *14th International TOVS Study Conference, NASA, Beijing*, 2005.

[25] G. L. Stephens and C. D. Kummerow. The remote sensing of clouds and precipitation from space: A review. *Journal of the Atmospheric Sciences*, 64(11):3742–3765, November 2007.

[26] M. D. E Szyndel, A. D Collard, and J. R Eyre. A simulation study of 1D variational cloud retrieval with infrared satellite data from multiple fields of view. *Quarterly Journal of the Royal Meteorological Society*, 130(599):1489–1503, April 2004.

[27] A. M Tompkins and M. Janiskova. A cloud scheme for data assimilation: Description and initial tests. *Quarterly Journal of the Royal Meteorological Society*, 130(602):2495–2517, October 2004.

[28] T. Vukicevic, T. Greenwald, M. Zupanski, D. Zupanski, T. Vonder Haar, and A. S. Jones. Mesoscale cloud state estimation from visible and infrared satellite radiances. *Monthly Weather Review*, 132(12):3066–3077, December 2004.

[29] T. Vukicevic, M. Sengupta, A. S. Jones, and T. V Haar. Cloud-resolving satellite data assimilation: Information content of IR window observations and uncertainties in estimation. *Journal of the Atmospheric Sciences*, 63(3):901–919, 2006.

[30] H.-L. Wei, P. Yang, J. Li, B. A. Baum, H.-L. Huang, S. Platnick, Y.-X. Hu, and L. Strow. Retrieval of semitransparent ice cloud optical thickness from atmospheric infrared sounder (AIRS) measurements. *IEEE Transactions on Geoscience and Remote Sensing*, 42(10):2254– 2267, October 2004.

[31] E. Weisz, J. Li, J.-L. Li, D. K. Zhou, H.-L. Huang, M. D. Goldberg, and P. Yang. Cloudy sounding and cloud-top height retrieval from AIRS alone single field-of-view radiance measurements. *Geophysical Research Letters*, 34:5 PP., June 2007.

[32] D.-K. Zhou, W. L. Smith, X. Liu, A. M. Larar, H.-L. Huang, J. Li, M. J. McGill, and S. A. Mango. Thermodynamic and cloud parameters retrieval using infrared spectral data. *Geophys. Res. Lett*, 32(L15):805–1, 2005.

[33] D.-K. Zhou, W. L. Smith Sr, X. Liu, A. M. Larar, S. A. Mango, and H.-L. Huang. Physically retrieving cloud and thermodynamic parameters from

ultraspectral IR measurements. *Journal of the atmospheric sciences*, 64(3):969–982, 2007.

[34] D. Zupanski, M. Zupanski, L. D. Grasso, R. Brummer, I. Jankov, D. Lindsey, M. Sengupta, and M. Demaria. Assimilating synthetic GOES-R radiances in cloudy conditions using an ensemble-based method. *International Journal of Remote Sensing*, 32(24):9637–9659, 2011.