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Identification of possible improvement in Low and Midlatitude Sea Surface Temperature Retrievals

Visiting Scientist Report

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1. Executive Summary

Priorities for sea surface temperature (SST) algorithm development relative to OSI-SAF state-of-the-art were reviewed. In conclusion, the improvement of optimal estimation SST (OE SST) is seen as offering the most important potential gains. Three areas are most relevant: better estimation of the error covariance matrices for OE SST; extension of the retrieval state vector to include desert dust; and bias-aware techniques to improve bias correction. The prerequisites for the first topic are in largely place, and thus a small study on that topic is proposed for this year, 2018. The prerequisites for the second will require more time and preparation, and thus could be addressed during 2019. The third area is most logically addressed after upgrades to the OE SST scheme, and is thus an concept for future work.

1.1.1. Applicable Documents

[1] Desroziers, G, L Berre, B Chapnik and P Poli
Diagnosis of observation, background and analysis-error statistics in observation space
doi: 10.1256/qj.05.108, 2005

1.1.2. Disclaimer

1. Analysis of Potential Activities and Benefits

Activity	Potential benefits	Prepara-tory effort	Potential VS effort	Priority
Radiance bias correction by bias-aware methods	Decrease/break the current feedback between OSI-SAF bias correction and biases in OSTIA. This is important, but desert-dust related biases are probably of more immediate concern.	Significant	>1 month	Medium
Reducing calibration biases in Metop AVHRR using FIDUCEO results	Calibration biases of a few tenths of kelvin (related to errors in internal calibration target temperature under particular conditions) could be corrected, improving SST	Minor	1 week	Medium
Expand optimal estimation (OE) SST state vector to include desert dust	Thought to be the most likely successful approach to reducing dust-related SST biases, replacing the “Saharan Dust Index” methods that correct some problems but also introduce artefacts, and which are less general, maintainable and adaptable to sensors with additional relevant channels.	Significant	1 month	High
Improved smooth-atmosphere OE SST techniques	Current techniques could be better optimised in terms of the assumptions about scales and interaction with cloud detection, but no urgent need to improve is apparent	Intermediate	Not estimated	Low
Desroziers-method estimation of OE SST error covariance matrices	OE SST is currently undertaken with error covariance matrix assumptions based on heuristics and expert assumptions. Incorrect specification causes the “optimal” retrievals in fact to be sub-optimal, and this could be significantly improved.	Significant	1 or 2 weeks	High
Revisit prior, linearization and iteration assumptions	OE linearizes a particular prior and in the current implementation, a single iteration is performed. Review and optimisation of these assumptions may be possible informed by the new ERA5 re-analysis, including lessons on prior error covariance from the ensemble.	Significant	Not estimated	Low
Cloud detection improvements	Isolated residual-cloud related biases continue to require improvement, but logically this should be revisited better after expanding the state vector and work on radiance bias correction.	Significant	Not estimated	Low

2. Proposed VS Study on Error Covariance Specification

2.1. Objective and rationale

Optimal estimation makes optimal use of observations to infer the retrieved state under certain conditions. One condition is that error covariances are appropriately specified. There are three relevant error covariance matrices:

- $\boldsymbol{S}_a$, which characterises the uncertainty in the prior (and linearization) state assumed for the OE.
- $\boldsymbol{S}_y$, which characterises the observation (brightness temperature, BT) uncertainty
- $\boldsymbol{S}_F$, which characterises the uncertainty in the fast forward model process assuming a correct state specification

There is partial information and understanding of each of these terms, which has been used to create the matrices currently used in OE SST retrieval (e.g., in the SEVIRI processing). However,

- it is likely that the matrices could be made more realistic
- we know the matrices should not necessarily be constant, but do not know how better to parameterise them

The objective of the proposed study is to adapt Desroziers methods from data assimilation to the OE SST cases, and derive new estimates of $\boldsymbol{S}_a$ and $\boldsymbol{S}_\epsilon = \boldsymbol{S}_y + \boldsymbol{S}_F$. (These methods cannot disentangle $\boldsymbol{S}_y$ from $\boldsymbol{S}_F$, but improved OE only requires better knowledge of their sum.) The new estimates should be tested to verify the expected improvement in SST.

The objective is to address one of SEVIRI within the VS frame, with the possibility to follow up with the Metop-B AVHRR based on the outcomes.

$\boldsymbol{S}_a$ is NWP-dependent, in principle, and for SEVIRI it will be re-analysis data. $\boldsymbol{S}_\epsilon$ should be explicable from understanding of the instruments and expectations of the RTTOV performance.

2.2. Tasks and methods

2.2.1. Preparatory tasks prior to VS

To ensure the efficiency of the VS period, datasets suitable for the work will be prepared in advance.

- Identify and prepare/consolidate a match-up database extractions for the study for SEVIRI. it will need to have the following properties to facilitate calculation of Desroziers-like diagnostics:
  - Sampling at least two annual cycles
    - One to be used as 'train' and the other as 'test'
  - Sample size adequate for purpose, but not larger than necessary
    - Probably 200,000 matches per year is about right
    - Quality level 4 and 5, 50:50 day and night, avoiding high SDI
    - Evenly spread by geographical location and day of year – i.e., thinned out where matching rates tend to be high

- Containing all the necessary fields: SST in situ, prior SST (x_a), prior TCWV (w_a), SST retrieved ($\hat{x}$), SST retrieved ($\hat{w}$), RTTOV-12[1] forward model outputs ($\boldsymbol{F}(\boldsymbol{x}_a), \frac{dF(x_a)}{dx}, \frac{dF(x_a)}{dw}$) all available channels, SST correction, observed BTs, BT adjustment, SDI and any SDI correction applied, QL and any relevant proximity to cloud indicators, time, latitude, longitude, satellite zenith angle, match ID
- For each match ID put the corresponding a-priori pressure, temperature, and humidity profiles and surface parameters into an RTTOV input profile file :
  - Test that running these inputs reproduce $\boldsymbol{F}(\boldsymbol{x}_a)$ etc
  - Then run $\boldsymbol{F}(\hat{\boldsymbol{x}}), \frac{dF(\hat{x})}{dx}, \frac{dF(\hat{x})}{dw}$ and append to match-up records
  - Preserve instructions/script for the RTTOV run for further use during VS
- Provide the error covariances assumed for the retrieval originally

- Arrange with RTTOV team to get the RTTOV-minus-LBL residuals as data for the target sensors from the simulations used to determine clear-sky RTTOV coefficients. This will enable calculation of an initial estimate of $\boldsymbol{S}_F$ for comparison with later results, and it may be that this estimate forms the basis for constraining/parameterising the observation error covariance matrix.

2.2.2. VS tasks and methods

The task overall is to apply the insight from Desroziers et al (2005) that analysis increments in a data assimilation system can be combined in particular ways to produce matrices that should (for a well-balanced system) match the error covariance matrices of the system. Since the equations of DA and OE are analogous in form, these diagnostics can be applied in OE also. If disagreement is (as expected) found, then iterative application of diagnostic-based estimates can be applied until there is convergence on results that are assumed to be more representative of the true error covariances. In addition, various considerations can be applied as checks on the new estimates:

1. there should be consistency in observation error covariance for day and night, except to the degree that diurnal variability could explain ;
2. the observation error covariance should be broadly explicable in magnitude and structure as “RTTOV error + noise”;
3. the prior error covariance should be reasonable compared to what we think we know about NWP TCWV and SST uncertainty;
4. in validation, we should find that retrieved-minus-reference SST statistics improve (or at least do not degrade) and that the dispersion is consistent with the OE-generated retrieval error plus our understanding of in situ and matching errors.
5. The distribution of retrieval chi-square should be close to the theoretical distribution.

Assuming all looks appropriate, it may be possible to produce error covariance estimates banded by auxiliary variables such as TCWV or latitude that may be more locally appropriate. If coherent tendencies are found, a parameterisation of the error covariances giving smooth behaviour can be proposed. This sort of analysis is extensive in DA, but appears not to have been undertaken/published previously to improve OE remote sensing, therefore the aim is to make the VS report in the form of a draft journal paper.

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[1] Using RTTOV 12 means re-simulation of BTs, but seems to be worthwhile to make the study results more resilient to the coming upgrade from 11 to 12.

The expected progression of tasks is:

- Calculate Desroziers diagnostics corresponding to $\boldsymbol{S}_a$ and $\boldsymbol{S}_\epsilon$ for the default OE configuration for
  - all night-time
  - all day-time
  - night-time banded by TCWV
  - night-time banded by latitude
  - night-time banded by view zenith angle
- Analyse the results, assessing the degree of consistency with assumed error covariance matrices, and the degree of consistency/trend of the diagnostics between day/night and bands of TCWV and latitude and view zenith
- Apply diagnosed/improved estimates of error covariances to a repeat retrieval, and assess whether match-up statistics for SST are improved and consistent with OE posterior error covariance. Iterate if beneficial.
- Devised parameterisation for improved $\boldsymbol{S}_a$ and $\boldsymbol{S}_\epsilon$ if found to be smoothly variable with respected to practical auxiliary variables

3. Outline of Study on Desert Dust in SST Retrieval

Currently, techniques to minimise SST biases related to atmospheric desert dust are based on "Saharan Dust Index" (SDI) techniques. These were devised at a time when RTTOV capability on aerosol was much less than in recent versions, which meant that desert dust could not then be directly included in a retrieval framework such as optimal estimation, or coefficient-based retrieval with a radiative transfer-based correction. SDI methods reduce biases, but are not sensitive to the specific atmospheric context and are prone to certain artefacts.

This proposed study is to address desert dust related biases better by

- taking advantage of RTTOV aerosol simulation capabilities
- taking advantage of the extended suite of infra-red channels on ABI/FCI/MetImage to better constrain the IR impacts of aerosol
- exploiting OE SST methods by incorporating desert dust parameters in the retrieved state vector along with SST and TCWV

This is a multi-faceted task that entails a series of steps, which it is recommended to work out in detail during 2018, with a view to VS and other effort on this problem during 2019.

Here, the outline of the research steps is given. Further preparatory investigations will be needed to form a detailed plan to address these.

- Confirm that one of the various options for configuring desert dust simulation in RTTOV can simulate IR desert dust impacts, with the following characteristics:
    - adequate correspondence of simulations to the modes of variability introduced by desert dust in multi-channel clear-sky observations
    - practicable specification of aerosol properties via summary (low-dimension) state vector variables (e.g., a "dust amount" variable, plus, perhaps, mean dust height[2])
    - adequate computational speed (probably cannot use too many scattering streams for speed reasons)

- Explore formulation of OE SST retrieval with dust, via a simulation study (linked to set up of RTTOV 12) with controlled observation errors and prescribed state variables, answering questions such as:
    - does, as expected, including desert dust in state vector enable the OE SST method to reduce dust-related biases relative to SDI methods?
    - what channels are effective in constraining the IR dust properties, including new channels on ABI/FCI/MetImage[3]?

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[2] One of the challenges of desert dust is that the relative VIS/NIR/TIR properties are variable depending on size distribution. It could be an advantage if we do not need VIS information: not only would an TIR-only method work day and night consistently, but it would allow the dust specification perhaps only to specify the coarse-mode abundance and not concern itself about the modes that affect visible AOD. In that context, something as simple as "log(amount) [TIR-relevant modes]" and "height" may be an adequate set of state variables.

[3] Preliminary thoughts on this. We know that the 10.5 – 12.5 μm channels, 8.7 μm and (at night) 3.9 μm are relevant from SDI experience. Considering the simulations results below for Himawari, the following observations can be made.

- does introducing desert dust necessitate more than one iteration of the OE – and if so, how many?
- how critical is the selection of dust radiative properties from the available models to the OE SST errors? Is an iteration across dust models essential?

- Survey the options for prior desert dust information. Options need to be operationally practical (timely and available) and their uncertainties need to be quantifiable. Possibilities include:
  - Build an appropriate desert dust climatological prior, specifically for the purpose, informed by the SEVIRI SDI reprocessed time series, the ULB IASI IR AOD product, simulations, etc.
  - Use desert dust amount forecasts, e.g., from the Copernicus Atmospheric Monitoring Service.
  - Don't require a prior: initialise dust amount from near-zero with large uncertainty and let the retrieval go in that direction if there is a dust signal (probably in an iterative retrieval)

- Devise and set up the appropriate match-up and imagery case-study datasets for detailed study, including desert dust profile information. Update the RTTOV simulation tools for routine dusty simulations.

- Test the OE SST method(s) determined from the simulation study on real match-up and imagery case-study data.

First, the 13.3 μm channel, which has only a low surface temperature sensitivity, has a significant Saharan dust sensitivity in this simulation, suggesting that this channel could help disentangle dust effects (disambiguating dust and surface temperature). Second, the 7.3 μm has almost no sensitivity to dust, despite that it is a lower-tropospheric water vapour channel and has a (dust-free) weighting function that peaks below the height of some dust (lowest 3 km of the troposphere). It is less clear, but possible, that this adds a useful constraint to the atmospheric state (disambiguating dust and water vapour to some degree).