

Atmos. Meas. Tech. Discuss., referee comment RC2  
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## Comment on amt-2021-122

Anonymous Referee #2

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Referee comment on "A minimum curvature algorithm for tomographic reconstruction of atmospheric chemicals based on optical remote sensing" by Sheng Li and Ke Du, Atmos. Meas. Tech. Discuss., <https://doi.org/10.5194/amt-2021-122-RC2>, 2021

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### GENERAL COMMENTS

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The paper describes a minimum curvature based regularization scheme for deriving 2-D trace gas concentrations from optical remote sensing and tomography. The chosen regularization scheme is sensible and the method seems to be an improvement over the state of the art in the field.

The topic fits the journal.

The textual description is severely lacking and a rewrite to better guide the reader through the numerous methods is necessary. The description of the compared methods is severely lacking mathematical rigour and precise definitions causing the research to be not replicable in its current state.

I believe that the paper can only be published after a major revision and restructuring. See below for some general guidelines and a number of specific issues.

## MAJOR COMMENTS

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### Precise Mathematical description

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The problem requires a much more precise mathematical introduction with clear definitions of employed terms. The paper gives a wide overview over several methods from literature and introduces many of these and related terms without clear definitions. At least those discussed later should be introduced well enough to follow the paper without further referencing.

The continuous and discrete view of the problem needs to be separated and the relationship clarified (see specific comments). Very often it is useful to specify the formulas for the continuous case and then "simply" discretize the resulting integrals and derivatives. In this case one achieves results that are less dependent on the chosen discretization/gridding. This is particularly true as the sampling distance is (wrongly) used in the regularization strength instead of the integrals itself.

### Motivation for minimum curvature

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This chosen regularization is criticized for producing oversmoothed results. The major question is, what kind of regularization term would best describe the a priori information. The Laplacian is an obvious choice due to its relationship with the Poisson-Equation. If diffusion is the major process than a norm related to an exponential covariance would be very useful (see "Inverse Problem Theory" by Tarantola); also here, the Laplacian pops up at least for the 3-D exponential covariance. It would be interesting to motivate the choice of regularization form the underlying physics.

There is also a host of literature with respect to regularization for optical remote sensing methods from nadir and limb sounding satellites. It would be very interesting to put this method into this context and/or discuss the statistical angle.

Diagnosis

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Due to the choice of a grid with more unknowns than measurements, diagnostics become more important. This can be done in a simple fashion with "resolution" measures. Rodgers' "Inverse Methods for Atmospheric Sounding" shows in great detail what kind of diagnostic quantities are relevant (resolution, measurement contribution, smoothing error, uncertainties...)

SPECIFIC COMMENTS

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line 35

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"which can detect a large area in situ and provide near real-time information"  
Maybe cover? Also "in situ" may be an unconventional use for a remote sensing instrument, depending on the community.

line 43

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To be precise both an infinite number of beams and beams of infinite length are required. One typically assumes a zero signal outside the reconstruction domain, which, for your problem, is a very reasonable assumption and at least alleviates the latter condition. How does the finite number of beams affect the solution?

line 44

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"Series-expansion-based methods". Unclear what is meant here. Cite needed.

The explanation sounds like a simple discretization, transforming the "continuous problem" of finding a function over  $L^2$  to a discrete problem of identifying a number of samples.

line 48

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Also medical reconstruction techniques employ discrete samples and basis functions.

With many more samples, obviously.

line 49

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I do not understand the difference between a pixel based approach and a basis function based. A pixel is a basis function with rectangular, non-overlapping support.

line 51

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"best" in what sense?

line 52

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Typically a basis is a basis of a (vector) space. Which space is spanned here?

Is the full space spanned or only a subspace thereof?

line 53

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What parameters? Typically one derives pre-factors of normed basis functions.

line 54

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What equations? Why are those equations non-linear? Typically this problem would be linear even for non-trivial basis functions.

line 55

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Best in what sense?

line 56

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Too general. Fits to nearly any problem. What error function based on which criteria?

line 58

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Define ill-posed. Define very large (millions?).

line 61

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Many classes of non-linear problem can be solved efficiently by deterministic methods. Particularly convex optimization problems such as this.

line 65

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Exploiting previous (a priori) knowledge of a problem is almost always key in inverse problems. Doesn't dispersion/diffusion suggest a Laplacian as

regularizing term? Is there a physical relationship between the dispersion processes and the minimum curvature?

line 69

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This is the first time NNLS is mentioned in the main text and a cite should be placed here with more detail. The EPA cite does not detail the NNLS algorithm.

line 74

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If the number of unknowns is smaller than the number of measurements, such a problem may still be solved by using pseudo-inverses and or regularization techniques, which are computationally cheap.

line 88

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"But the theory basis of the LTD algorithm was not clearly given". By whom?

This paper is so far not helping in this regard.

line 92

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What is regularization?

line 95

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Interpolation theory typically deals within interpolation of (mostly discrete) data. How does that relate to the problem at hand?

line 98

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"The solution to this problem is a set of spline functions." Please be precise about this. The algorithm derives, necessarily a vector. This vector can be interpreted in a various of ways. Of particular import is how it is interpreted by the "forward model", because that determines what is fit. This interpretation may differ from the interpretation for the regularisation term, but this introduces necessarily an error. One should be clear about that. Typically one sees the regularization term as an approximation: as the computation of derivatives by finite differences is inherently approximate. In the case that the gridding is very fine, the approximation error becomes small, and the point is moot, but this discussion is missing here. The discretization error has not been discussed and thus cannot be neglected. It is sensible to represent the 2-D field to be reconstructed here as a 2-D spline both in the forward model and the regularization term. This would remove approximation errors at the cost of a more complicated algorithms. Either way, the distinction and used assumptions must be made explicit and errors discussed.

line 102

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Maybe a bit more of the theory should be described to make this more obvious to the reader.

line 104

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Please properly and mathematically introduce the corresponding biharmonic equation and the smoothness seminorm.

line 106:

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Why does it half the number of equations?

line 107:

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If the number of \*grid points\* increases what does that mean for the amount of information contained in the results and to what degree are the resulting "pixels" correlated? I.e. how well is the result resolved?

line 137

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A very important interpretation of this approach is the statistical one (optimal estimation), where  $R^{TR}$  can be interpreted as precision matrix codifying a priori information about the given distribution (i.e. smoothness). Please discuss.

line 139

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In what sense is this an approximation? The given formula is discrete already, as such  $R_i$  is not a derivative, but a finite difference operator.

line 142

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The nomenclature is highly unusual. Typically derivatives are defined for continuous functions.  $c$  was so far a vector. This is an \*approximation\* of the third-order derivative of a function in  $y$ -direction by finite differences.

And even then, the division by the grid-distance is missing. In this form, the regularisation is grid-dependent and would change in strength for different grid sizes, which requires a re-tuning of regularisation strength for every change of



grid size. Please take the grid size into account.

line 148

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Why is the regularization parameter set to 1 over grid length? To compensate for the missing factor in  $R_3$ , the power three is missing. There is a host of literature discussing optimal choice of this parameter (L-curve, optimal estimation, etc.). Practically, it is a tuning parameter which often requires manual adjustments unless both measurements and a priori are very well understood.

line 148

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What is meant by "setting the derivative to zero"? Formula (3) minimizes the expression and thus allows for non-zero derivatives unless the factor  $\mu$  is chosen to be very large.

line 152

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$|c|$  is typically the absolute value of  $c$ . To describe more complicated regularization terms, one often uses a more general function  $\Phi(c)$  mapping  $\mathbb{R}^n$  to  $\mathbb{R}^+$  or a norm with a subscript like  $\|c\|_{\Phi}^2$ . Are you referring to Sobolev-Norms?

line 155

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The solution to the problem is a discrete vector  $c$ , whereby each element of  $c$  defines the concentration in one pixel (see (1)). A spline is something very

different, as it is a continuous. Your problem is set up to be non-continuous be definition. Please specify your model precisely and be careful with the distinction between the continuous and discrete view.

line 158

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c was defined as a vector, not as a continuous function.

line 159

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What items in which summation? There is an integral in (7).

line 160f:

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"This is how the LTD algorithm does to add additional(sic!) equations?" What does this mean?

line 161:

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Is such a complicated equation really more efficient computationally than two much simpler ones? What are the involved algorithmic complexities?

line 165:

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It is unclear why this biharmonic equation is necessary. You are already minimizing a cost function in (6). Equation (7) gives you an immediate way to calculate  $|c|$  required by (6). Computing discretized  $ddc/ddx+ddc/ddy$  and computing the Euclidian norm should give you (6) without the need for higher derivatives in the definition of the problem. To efficiently solve (6) one might

need higher derivatives depending on the chosen algorithm (e.g. Gauss-Newton), but your paper does not detail this part very well.

Please describe in detail by which algorithm (6) is solved and how (9) plays a role in that.

line 169:

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Again, the regularization weight typically depends on diffusion coefficients and measurement errors and is often a tuning parameter. The grid size should directly be implemented in the finite difference equations.

line 180:

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What interpolation applied after the reconstruction process? The pixel-based algorithm assumes constant values over constant pixels. There is no smoothing interpolation, which would not deteriorate the fit to the measurements, i.e. deteriorate the results.

line 186

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Here  $c$  is defined, for the first time, as a continuous function! Please properly distinguish the "different"  $c$ 's.

line 189

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What source number? (10) defines only a single source. If you use multiple sources, please accommodate this in (10).

line 189

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You state that the peak width was set randomly. Was it chosen randomly from the listed peak width of line 187f?

line 195

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You were using  $c_{i,j}$  above for the 2-D fields, why now only  $c_i$ ?

line 201

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How was the location of the highest peak located?

line 210

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Why did you not apply the other algorithm on your fields for better comparability?

line 215

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While it seems to work, the pixel based algorithm derives pixels, not a continuous field. It is straightforward to derive a spline interpolated field directly, if desired for the higher accuracy. One simply needs to compute the integrals over the spline interpolated field for the coefficients when computing the error to the measurements. This can be accomplished by a linear matrix multiplication. I expect this to deliver similar results as the other methods at maybe even faster speed due to the smaller number of involved equations. Please discuss the choice of your simpler forward model.

line 243

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Why does the necessary computation time scale with the number of sources?

Shouldn't it be proportional to the problem size?

line 283

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"oversmooth issue" - necessarily, the amount of information cannot increase between the measurements and the solution. Due to the chosen regularization, the result will be necessarily smooth. If it is "oversmooth" depends on whether the a priori assumption of smooth fields is correct or not.

In case that this assumption does not hold, "better" (less smooth) results can be achieved by Total-variation minimization (isotropic or anisotropic) and primal dual methods, e.g. Split-Bregman. I doubt this would fit better to your problem, though.

MINOR REMARKS

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line 55

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"question". This is called an "inverse problem".

line 74

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grids -> grid points?

line 85

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necessary -> necessity

line 144

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-> "third-order forward difference operator"

line 160

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Which "multiple items"?

line 174:

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"For pixel-based"->"For conventional pixel-based", posted->posed