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Data assimilation for compartmental systems

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Summary

Compartmental systems are widely used to model dynamics of ecosystems, carbon, water, land surface, and other systems where the state variables are concentrations. Compartmental systems are linear in the state variables, but they often contain unknown parameters which can interact non-linearly with the state variables. We illustrate the smoothing process (in both state variables and parameters) for a simple system, and discuss avenues of research for data assimilation in these systems.

Compartmental systems

A compartmental dynamical system is governed by a linear ordinary differential equation of the form:

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}\mathbf{x},\ \mathbf{x}(t=0) = \mathbf{x}^0$$

$$\mathbf{x} \in \mathcal{R}^{N_x},\ \mathbf{F} \in \mathcal{R}^{N_x \times N_x}$$

where **x** is a vector of state variables and **F** is a matrix of coefficients. This matrix has the following properties:

$$F_{ii} < 0,\ F_{ij} > 0, i \neq j,\ \sum_{i=1}^{N_x} F_{ij} \leq 0\ \forall j$$

The state variables can be interpreted as concentrations, and the dynamics as fluxes between different compartments. These systems have have been used, for instance, in the context of carbon balance models, and they have well-studied mathematical properties [1].

Often both the initial concentrations and some elements in the matrix **F** are unknown. Let us illustrate the time evolution of a closed compartmental system (sum of columns equal zero) in the presence of both sources uncertainty. In particular we consider the element **F**(2,2) to be an unknown parameter.

Figure 1 shows the evolution of the concentrations for the 2 compartments (left and centre). Depending on both the initial concentrations and the parameter, the system evolves to different fixed points. These fixed points are Lyapunov stable but not attracting. Since the system is closed, the total concentration is fixed (right) and only depends on the initial conditions and not the parameter.

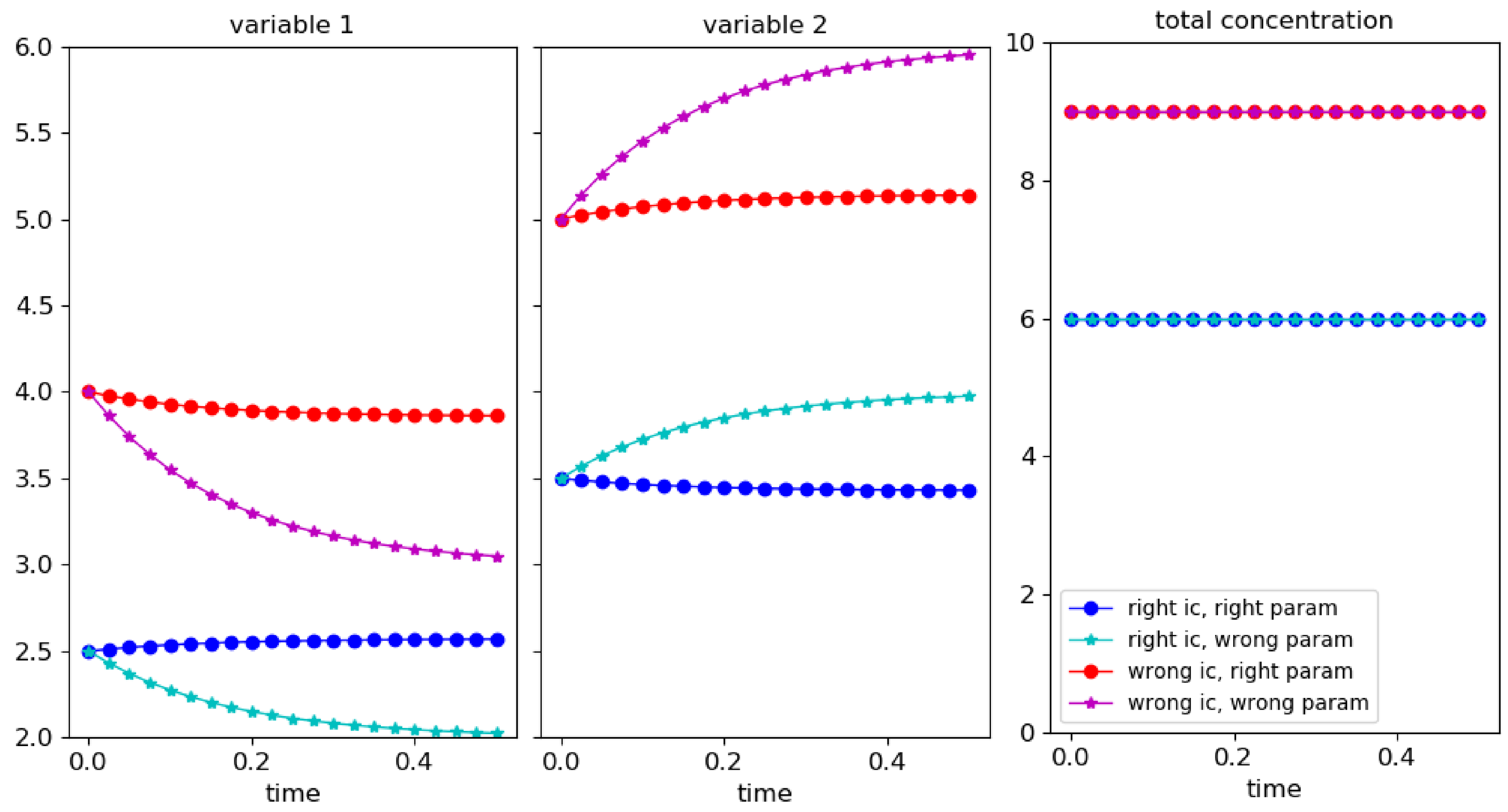

Figure 1. Evolution of a 2D compartmental system in the presence of uncertainty in initial conditions and one parameter (in particular one element of the matrix of coefficients).

Data assimilation

Smoothing has previously been achieved for both state and parameter estimation in carbon models, even in the presence of some complications like the lower bound of the (non-negative) concentrations.

Consider state estimation alone knowing (i) the real parameter and (ii) a guess for the parameter. We solve for initial concentrations using an imperfect observation at time *t=0.5*, and starting from a guess initial concentrations. The 4DVar process requires finding the minumum of a cost-function shown in figure 2. The cost-function is a perfect paraboloid (the model is linear in **x**) but it depends on the parameter. Each parameter leads to a different function and a different minimum.

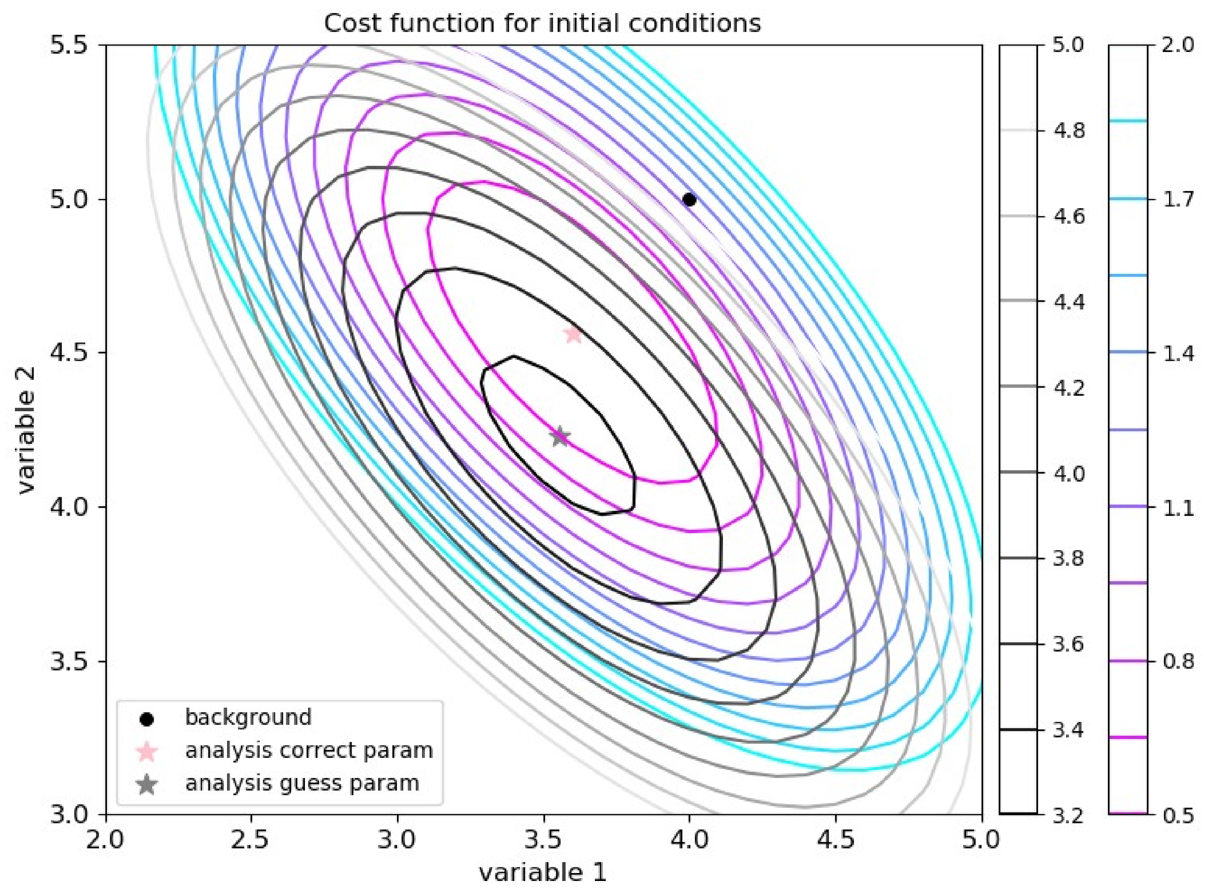

Figure 2. Cost-functions to be minimised in the 4DVar process to find initial concentrations based on an observation in the future. Two cost-functions are shown, one for each value of the parameter (exact and guess).

The solution of the extended problem is to perform the assimilation for both the state variables and the parameters [2]. This increases the dimensionality of the problem and it destroys the paraboloidal structure of the cost-function. In figure 3 we show cross-sections of the cost-function for different values of one of the variables.

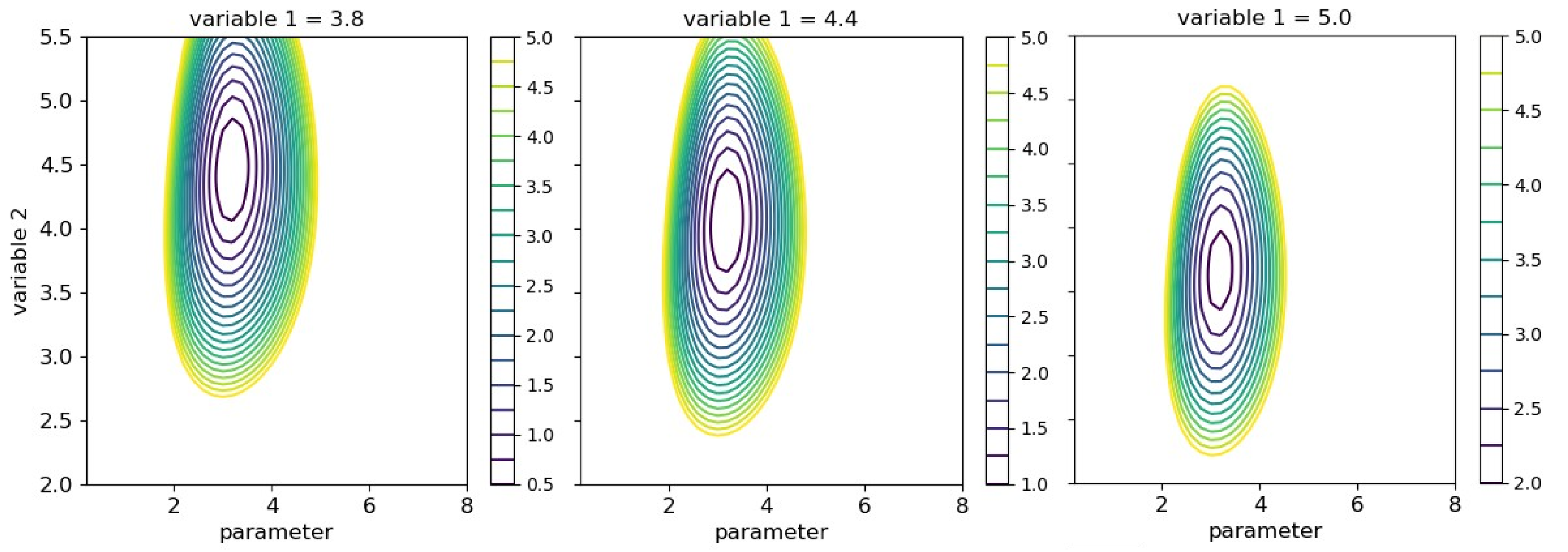

Figure 3. Cross-section of the cost-function of the extended problem in the space parameter vs variable 2 for three values of variable 1 (panels). Notice the deformation of the contours with respect to figure 2.

In figure 4 we illustrate the results --at initial time (left) and observation time (right)-- of performing DA in state space only for given guess values of the parameter (blue and pink families of points), versus performing the extended state-parameter estimation (red point).

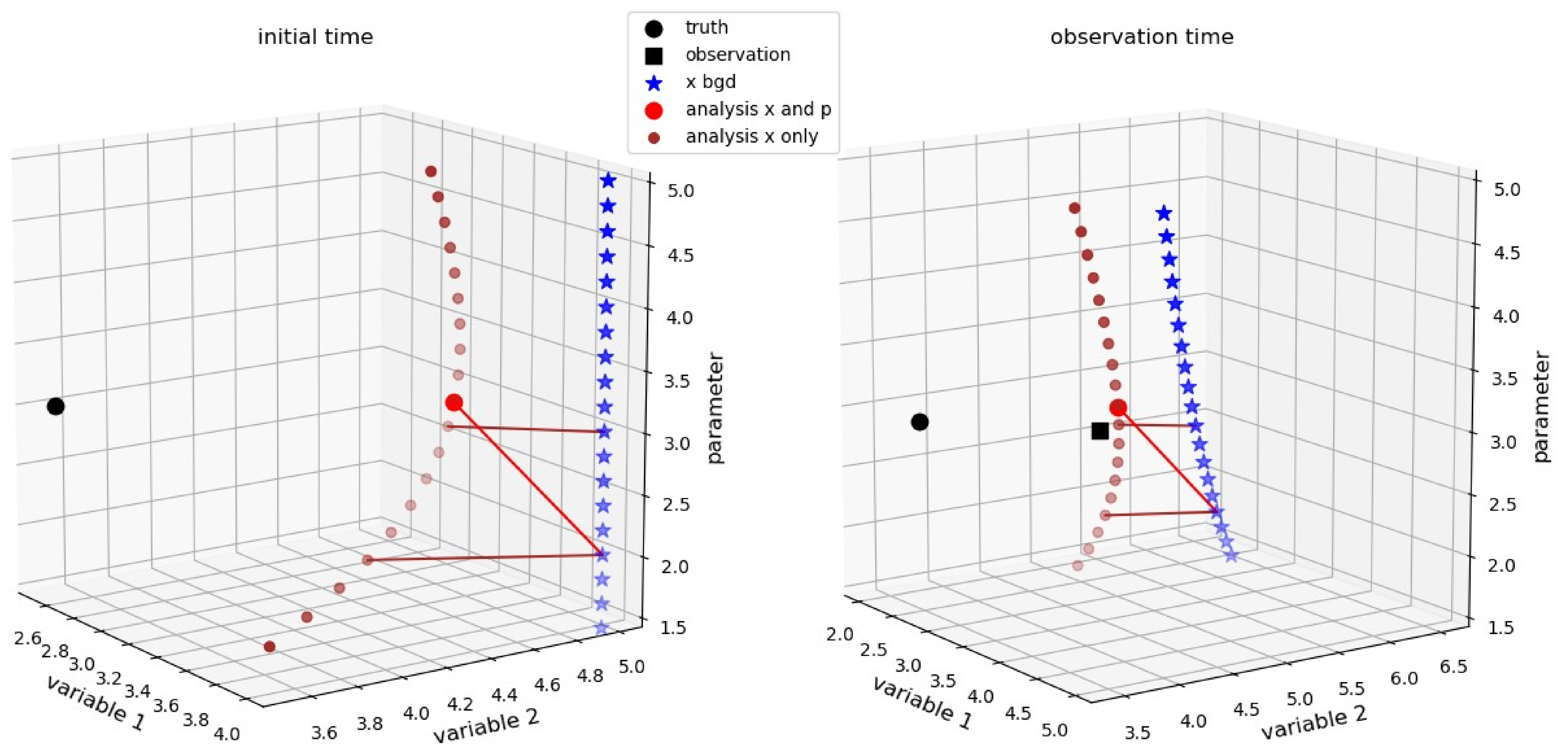

Figure 4. Elements of the DA procees at the initial time (left) and the observation time (right): truth, observation, background and analysis. The differences of performing only state estimation with a given parameter (pink and blue families), vs performing state-parameter estimation (red) are clear.

The future

Compartmental systems are well-studied, and it seems plausible that their properties can provide guidance on the type of DA methods that can be used in them. Some questions are: (a) under what conditions does the cost-function develop multiple minima, (b) can iterative methods (e.g. outer loops) jump between different fixed points?, (c) what about the non-autonomous systems?, (d) how far can we extend the validity of our Gaussian-based methods before having to use e.g. multinomial distributions for the concentrations? These are questions answered in [3] and to be applied in carbon balance models.

References

[1] H. Metzler, M. Müller, and C. Sierra, 2018. Transit-time and age distributions for nonlinear time-dependent compartmental systems. PNAS, 115, 61150-1155.

[2] E. Pinnington, E. Casella, S. Dance, A. Lawless, J. Morison, N. Nichols, M. Wilkinson, T. Quaife, 2016. Investigating the role of prior and observation error correlations in improving a model forecast of forest carbon balance using Four-dimensional Variational data assimilation. Agricultural and forest meteorology, 228, 299-314.

[3] J. Amezcua. Data Assimilaton for compartmental systems. In preparation.

Acknowledgements

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