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Spatiotemporal Kalman Filtering: a new approach to solving dynamical inverse problems

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Abstract—This paper discusses a new approach to state-space modelling of multivariate time series obtained from spatially extended dynamical systems. Since the assumed true states are unobserved and high-dimensional, their estimation poses an inverse problem. By discretising both time and space and assuming a stochastic autoregressive dynamics, it is possible to apply Kalman Filtering to this problem. Additional approximations are introduced into the filter in order to obtain an efficient implementation by properly exploiting the spatial structure of the problem. The model is fitted to time series data by using likelihood maximisation. Also the covariance of the stochastic component of the model may depend on time and space by a suitable autoregressive model. We demonstrate the feasibility of the proposed algorithm by presenting a numerical simulation designed to imitate the situation of the generation of electroencephalographic recordings (EEG) by the human cortex.

1. Introduction

In many fields of science (such as oceanography, geophysics or medicine) spatially extended systems are studied which evolve in time according to some possibly complicated dynamics. It is a typical situation that the relevant state variables of such systems cannot be observed directly, but only through an observation function; in many cases this function performs a projection of the high-dimensional true state space of the system onto an observation space of much lower dimension. The task of retrieving estimates of the true states from such observations represents a typical inverse problem. Due to the absence of a simple invertible relationship between state and observation such problems are ill-posed, i.e. the solutions ("inverse solutions") are unstable and ambiguous.

Let the unobserved true states of the system be given by a vector field $\boldsymbol{x}(\boldsymbol{r},t)$, where $\boldsymbol{r}$ and t denote space and time, respectively. By discretising space into a set of grid points and stacking the corresponding *local* state vectors a *global* state vector $\mathbf{X}(t)$ is defined [1]. Let $\mathbf{Y}(t)$ denote a vector of simultaneously recorded measurements; in this paper we assume a linear observation equation:

$$\mathbf{Y}(t) = \mathsf{K}\mathbf{X}(t) + \boldsymbol{\mathcal{E}}(t) \quad , \qquad \text{(a)}$$

where $\boldsymbol{\mathcal{E}}(t)$ denotes a vector of observational noise. K is assumed to be known and full-rank. Note that, albeit typically $\dim(\mathbf{X}) \gg \dim(\mathbf{Y})$, the task is to estimate the unknown states $\mathbf{X}$ from time series of $\mathbf{Y}$; this constitutes the *inverse problem.* Considering the example of the dynamics of human brain, the measurements may be given by a 18-dimensional vector of electroencephalographic recordings (EEG), whereas the "true" states (i.e. the unobserved sources) would be a (3433×3)-dimensional vector composed of local current density vectors on a set of 3433 grid points (voxels) covering the gray-matter parts of brain.

2. Spatiotemporal dynamics

For the dynamics of the global state $\mathbf{X}$ a general multivariate p^{th}-order autoregressive (AR) model

$$\mathbf{X}(k) = \mathcal{F}\big(\mathbf{X}(k-1), \mathbf{X}(k-2), \ldots, \mathbf{X}(k-p)\,|\,\boldsymbol{\vartheta}\big) + \boldsymbol{\mathcal{H}}(k) \quad \text{(b)}$$

is assumed, where k denotes discretised time, p denotes an integer model order, $\boldsymbol{\vartheta}$ denotes a vector of model parameters and $\boldsymbol{\mathcal{H}}$ denotes the global noise vector.

So far such inverse problems have been addressed almost exclusively within the framework of constrained least squares methods [2], and the temporal (i.e. dynamical) aspect of the problem has either been ignored entirely or included only through an arbitrary constraint without justification from the data [3].

In principle, it is possible to apply Kalman Filtering and maximum likelihood estimation directly to equations (a) and (b) (within a chosen model class), but due to the very high dimension of $\mathbf{X}$, the practical application will be infeasible in terms of computational time and memory consumption. However, we will now present a set of approximations which allows us to decompose this intractable high-dimensional filtering problem into a set of coupled tractable low-dimensional filtering problems, each of which is centred at one grid point [4]. For this purpose we are imposing the following assumptions on the function $\mathcal{F}$:

(α) $\mathcal{F}$ is linear:

$$\mathbf{X}(k) = \sum_{\kappa=1}^{p} \mathsf{A}(\kappa)\mathbf{X}(k-\kappa) + \boldsymbol{\mathcal{H}}(k) \ ,$$

where $\mathsf{A}(\kappa)$ is a set of parameter matrices (of size $\dim(\mathbf{X}) \times \dim(\mathbf{X})$), replacing $\boldsymbol{\vartheta}$. Such model shall be denoted as AR(p).

(β) The model order p is at most 2:

$$\mathbf{X}(k) = \mathsf{A}(1)\mathbf{X}(k-1) + \mathsf{A}(2)\mathbf{X}(k-2) + \boldsymbol{\mathcal{H}}(k)$$

(γ) Direct interactions exist only between neighbouring grid points: $\mathsf{A}(\kappa) = (a_\kappa + b_\kappa)\,\mathsf{I}_{\mathbf{X}} - b_\kappa \mathsf{L}$, where $\mathsf{I}_{\mathbf{X}}$ denotes the unity matrix of size $\dim(\mathbf{X}) \times \dim(\mathbf{X})$, and L is a discrete spatial 2^{nd}-order derivative matrix operator (*Laplacian*), acting on the spatial array of grid points. Most elements of $\mathsf{A}(\kappa)$ become zero by this assumption, thereby simplifying the model fitting. Through additional homogeneity and isotropy assumptions the parameters a_κ and b_κ become independent of the grid point index.

(δ) $\boldsymbol{\mathcal{E}}(k)$ is Gaussian white noise with diagonal covariance matrix $\mathsf{C}_\varepsilon = \sigma_\varepsilon^2\, \mathsf{I}_{\mathbf{Y}}$.

(ϵ) $\boldsymbol{\mathcal{H}}(k)$ is Gaussian white noise with (*non-diagonal*) covariance matrix $\mathsf{C}_{\mathcal{H}} = \sigma_{\mathcal{H}}^2 (\mathsf{L}^\dagger \mathsf{L})^{-1}$.

Assumptions (α), (β) and (δ) can be relieved during later work. Assumptions (γ) and (ϵ) are essential for the decomposition of the global high-dimensional filtering problem into spatially localised low-dimensional filtering problems. They can be interpreted as a direct consequence of discretising stochastic partial differential equations as given by

$$\frac{\partial^p\, \boldsymbol{x}(\boldsymbol{r},t)}{\partial t^{\,p}} = b\, \frac{\partial^2\, \boldsymbol{x}(\boldsymbol{r},t)}{\partial \boldsymbol{r}^{\,2}} + \boldsymbol{\eta}(\boldsymbol{r},t) \ , \qquad (1)$$

where $\partial^2/\partial \mathbf{r}^{\,2}$ corresponds to the Laplacian operator L, and $\boldsymbol{\eta}(\boldsymbol{r},t)$ is an integrable noise term. Obviously, a model order of $p = 1$ yields a diffusion equation, whereas a model order of $p = 2$ yields a wave equation.

The detailed definition of the spatiotemporal Kalman Filter, which corresponds to this model, is given in [1].

3. Parameter estimation

The modelling of actual multivariate time series by the class of spatiotemporal models described in the previous section can be shown to be equivalent to applying a *spatiotemporal* whitening filter, in analogy to the usual purely temporal whitening of time series data in statistical modelling. The particular choice for $\mathsf{C}_{\mathcal{H}}$, given in point (ϵ) above, corresponds to spatial whitening, since if the states X are replaced by LX, $\mathsf{C}_{\mathcal{H}}$ will be replaced by a *diagonal* covariance matrix [1].

Typically the parameter vector $\boldsymbol{\vartheta}$ which characterises the function $\mathcal{F}$, is unknown and has to be estimated from data. Under the assumptions outlined above we have for a 2^{nd}-order autoregressive model, AR(2), $\boldsymbol{\vartheta} = (a_1, a_2, b_1, b_2)$; furthermore the covariance parameters σ_ε^2 and $\sigma_{\mathcal{H}}^2$ also have to be estimated. This estimation step can be carried out by a maximum likelihood approach; the Kalman Filter is known to be a convenient tool for providing estimates of the likelihood $L(\boldsymbol{\vartheta}, \sigma_\varepsilon^2, \sigma_{\mathcal{H}}^2)$ of particular choices for the parameters [5].

More generally, we may also minimise the corresponding *Akaike Information Criterion*

$$\mathrm{AIC}(\boldsymbol{\vartheta}, \sigma_\varepsilon^2, \sigma_{\mathcal{H}}^2) = -2 \log L(\boldsymbol{\vartheta}, \sigma_\varepsilon^2, \sigma_{\mathcal{H}}^2) + 2\big(\dim(\boldsymbol{\vartheta}) + 2\big) \ ,$$

which is designed as an unbiased estimator of (-2) times Boltzmann entropy [6].

Let $\Delta\mathbf{Y}(k)$ denote the observation prediction error of the Kalman Filter at time t, $|\mathsf{R}(k\,|\,k-1)|$ the determinant of the observation prediction error covariance matrix, N_k the length of the time series and $n_c = \dim(\mathbf{Y})$, then the AIC is given by

$$\mathrm{AIC}(\boldsymbol{\vartheta}, \sigma_\varepsilon^2, \sigma_{\mathcal{H}}^2) = -2\sum_{k=1}^{N_k}\Big(\log|\mathsf{R}(k\,|\,k-1)| + \Delta\mathbf{Y}(k)^\dagger\, \mathsf{R}(k\,|\,k-1)^{-1}\, \Delta\mathbf{Y}(k) + n_c \log(2\pi)\Big) + 2\big(\dim(\boldsymbol{\vartheta}) + 2\big) \ .$$

We have found that numerical minimisation of this expression with respect to $(\boldsymbol{\vartheta}, \sigma_\epsilon^2, \sigma_{\mathcal{H}}^2)$ is a computationally demanding but feasible task for EEG time series of a few hundred time points and brain models of several thousand voxels [1]. The model corresponding to the minimum of AIC represents the most likely model for explaining the data and can therefore be expected to provide the best dynamical inverse solutions which are available for the data, within the constraint of the chosen model class. Since estimates of the state estimation error covariance matrix of the unobserved states are a central component of Kalman Filtering, it is easily possible to provide error estimates for the inverse solutions [1].

4. Covariance dynamics

As a generalisation of the case that the covariance structure of the noise driving the dynamics is described by a single constant parameter $\sigma_{\mathcal{H}}^2$, we now consider allowing this parameter to depend on space (i.e. on the grid point index v) and on time. More specifically, following the example of GARCH modelling in financial time series analysis [7], we explore the following model:

$$\log \sigma^2_{\mathcal{H}}(v,k) = \log \sigma^2_c + s_1 \log \sigma^2_{\mathcal{H}}(v,k-1) + s_2 \log \sum_i \left[\mathsf{g}(v,k-1)\, \Delta\mathbf{Y}(k-1)\right]^2_i \ ,$$

where $\mathsf{g}(v,k-1)$ denotes the local Kalman gain matrix at grid point v; the sum extends over all vector components of the local state. In GARCH modelling the residuals of previous state predictions are used as random elements of the assumed covariance dynamics, but since in the case of inverse problems these are not directly available, we have replaced them by the local state prediction error of Kalman Filtering, i.e. the difference between predicted and filtered local states. Three new parameters σ^2_c, s_1 and s_2 need to be chosen; further work will be required for designing a systematic approach to their choice, which may be possible by maximum likelihood, as well.

5. Simulation study

We will now present results for the estimation of inverse solutions for a simulated spatiotemporal system which imitates the typical situation given for the generation of the human EEG. A model cortex is discretised into 3433 grid points, using an average probabilistic brain atlas [8], and at each grid point (voxel) a time-dependent 3-dimensional current density vector is assumed to represent the local state. A highly simplified dynamics is implemented for these states by using locally coupled autoregressive processes; however, for two spherical regions within the cortex, one being located in frontal brain and the other in occipital brain, the parameters of these processes are not constant, but time-dependent, following a sine-wave pattern, chosen in a way such that the local dynamics becomes periodically unstable within these two regions, and the corresponding activation spreads out into the cortical grid, where it gradually damps out. These spatially extended oscillations are intended to imitate rhythmic activity, like alpha activity, which is known to be typical of cortical dynamics. By using an appropriate transfer matrix K (which can be estimated from electromagnetic theory [9]) simulated EEG time series are generated, shown in Fig. 1. A more detailed description of this simulation can be found in [1].

As can be seen, the simulated EEG clearly displays two oscillations (with different frequencies), corresponding to the two oscillating source regions, but in a quite blurred fashion. From this data set inverse solutions are computed by

- cLS: a constrained least-squares method [2] which is applied independently at each time point;

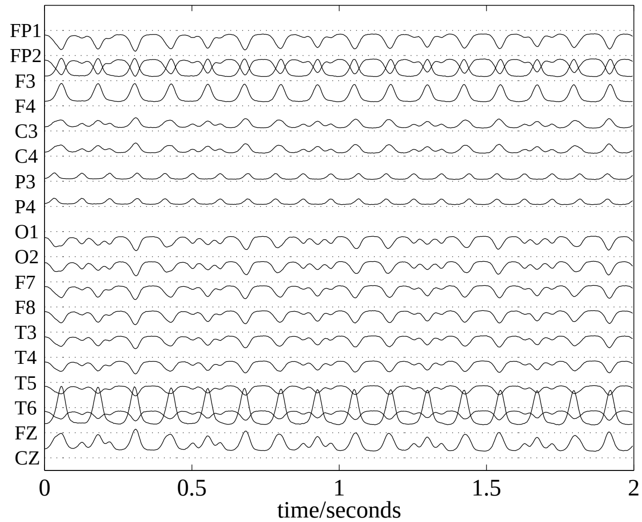

Figure 1: *Simulated EEG recording for 18 standard electrodes; electrode abbreviations are given on the vertical axis. The EEG potential is measured in arbitrary units versus average reference, time is measured in seconds, assuming a sampling rate of the simulated dynamics of 256 Hz.*

- KF1: spatiotemporal Kalman Filtering with the simplest possible dynamical model, i.e. AR(1) with constant homogeneous covariance;
- KF2g: spatiotemporal Kalman Filtering with an AR(2) model and GARCH modelling of covariances;
- KFp: spatiotemporal Kalman Filtering with the perfect model, i.e. the model employed in generating the simulated data.

For two selected voxels, one of which ("OV") was chosen out of the frontal region displaying high-amplitude oscillations, while the other ("NOV") was chosen from a non-oscillating region, the estimated time series of the inverse solutions (modulus of local current density vector) are shown in Fig. 2; for comparison, the true evolution of local states is also shown (top panels). In the figure the inverse solutions are shown only for the first second (256 points) of the data displayed in Fig. 1.

From the figure it can be seen that the solution obtained from cLS correctly retrieves the oscillation in OV, but underestimates its true amplitude by a factor of approximately 2; in NOV spurious oscillations are found. Both these errors are typical for the well-known tendency of non-dynamical inverse solutions to produce "blurred" solutions. The KF1 solution seems not to offer obvious improvements over the instantaneous solution in this respect, although it can be shown to be superior with respect to likelihood maximisation [1]; we remark that the same holds true for an AR(2) model (results not shown). The KF2g solution starts at the beginning of the data with similar estimates as also the other inverse solutions, but then after a

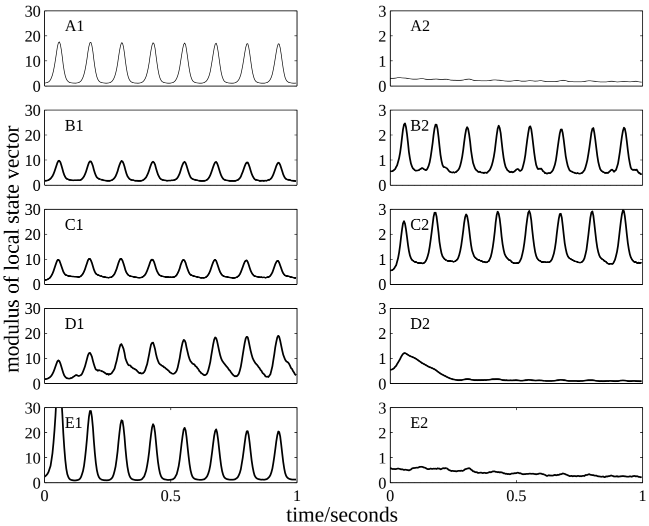

Figure 2: *True and reconstructed local states (modulus of local current density) for the first half of the data shown in Fig. 1 vs. time, for an oscillating voxel (left) and a non-oscillating voxel (right). Note the different vertical scale for left and right columns of figures. True local states are shown (A1, A2), state estimates from* cLS *(B1, B2), from* KF1 *(C1, C2), from* KF2g *(D1, D2) and from* KFp *(E1, E2); see text for details.*

transient of approximately 0.25-0.5 seconds arrives at much better estimates: The oscillation amplitude for OV is retrieved much better (although the wave shape is somewhat distorted), and no spurious oscillation is induced for NOV. The initial transient was to be expected for the GARCH dynamics. Finally, for comparison also the case of the perfect model, KFp, is shown in the figure, i.e. the case of providing the spatiotemporal Kalman Filter with the exact model which had been used for generating the data. It can be seen that, after an initial transient, for both grid points very good estimates are achieved. Of course, in real applications the perfect model will never be available; nevertheless this result is not trivial, since also in this case the Kalman Filter has to estimate $3 \times 3433 = 10299$ unobserved state variables from only 18 measurements. These results suggest that the identification of an appropriate model forms a crucial precondition for obtaining inverse solutions of improved quality.

6. Conclusion

In this paper we have discussed and extended a general framework for obtaining inverse solutions for spatially extended dynamical systems through a recently proposed new variant of Kalman Filtering [1]; in particular, we have proposed to link this methodology with the concept of GARCH modelling of covariance.

Through a simulation study, taken from the field of EEG source analysis, we have demonstrated the feasibility of this new approach and its potential for providing considerably improved inverse solutions.

We have only been able to present the core ideas and first results, while many questions still remain open. First, we are not yet able to propose a systematic approach for choosing the parameters of the GARCH dynamics, (σ_c^2, s_1, s_2); it is clear that they need to be chosen properly, otherwise the GARCH effect will not be initiated. So far we have not succeeded to employ the maximum-likelihood method for this task, although in principle this should be possible. A similar remark applies to the estimation of variances for inverse solutions, i.e. the estimation of error intervals; while for the spatiotemporal Kalman Filter with homogeneous covariance it was shown to be possible to obtain credible estimates of the error (as demonstrated in [1]), this has not yet been achieved for the generalisation to GARCH modelling of covariance. These issues remain to be addressed in future work.

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