Dynamic-stochastic prediction of temperature and wind fields as applied to assessment of mesoscale atmospheric pollution

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New methods and algorithms of dynamic-stochastic prediction of temperature and wind fields are considered as applied to assessment of mesoscale atmospheric pollution. Based on data of many-year field observations, the proposed algorithm is studied for its use in spatial prediction of mean temperature and zonal and meridional components of the wind velocity.

Among numerous problems of applied meteorology, the problem on spatial prediction of mesometeorological fields (first of all, wind and temperature fields) for a territory not covered by observations based on measurements in neighboring regions has recently occupied one of the central places. This prediction is needed, in particular, for meteorological provision of ecological issues connected with assessment of air pollution on a local scale (for example, in big cities and industrial centers). Such provision is usually made for the planetary boundary layer with the use of the pollutant transport equation and based on the spatial distribution of wind and temperature above the territory of interest.

It is obvious that for meteorological provision of such issues the mesoscale wind and temperature fields should be extrapolated with high spatial and time resolution, as well as high accuracy. However, this requirement cannot be met when applying the widely used method of optimal extrapolation. Besides, this method requires in-depth study of an object modeled.

In this connection, to solve the problem on spatial prediction of mesoscale wind and temperature fields, we propose a dynamic-stochastic approach based on the use of the Kalman filtering and the generalized model of meteorological parameter behavior in space and time based on first-order stochastic differential equations.

It should be noted that this paper continues the study begun in Refs. 1 and 2, but its feature is the use of the mechanism of adaptation to unknown approximation parameters of correlation functions determining current properties of the processes.

Let us consider now the technique of solving the problem formulated.

Physically, the problem of spatial prediction of the field of a meteorological parameter is formulated as follows: using data of $S-1$ measurement stations, it is necessary to assess (predict) this parameter at the Sth point of a territory, for which measurements are lacking. Consider the solution of this problem for a mesoscale territory.

The specific feature of the mesoscale allows application of the splitting method, which, in its turn, allows the meteorological parameter to be assessed at some fixed height level neglecting its relations to the neighboring levels. In this case, the entire height range can be covered by N Kalman filters, and each filter uses measurements obtained for the given height and for all stations situated in the neighboring regions covered by the observations. Prediction is sought for the same height, but for the point with the coordinates (x_1, y_1) at the territory with no experimental data available. Further consideration deals only with one filter at an arbitrary height level.

According to the previous study, we can assert that the temporal and spatial correlation properties of the meteorological parameter $\xi(t)$ sought on the mesoscale are described by the following functions[1]:

$$\mu_\xi(\tau) = \exp(-\alpha\tau); \quad (1)$$

$$\mu_\xi(\rho) = \exp(-\beta\rho), \quad (2)$$

where τ is the time shift; ρ is the space shift; α and β are the approximating coefficients (in the general case, depending on the height h).

In accordance with Eqs. (1) and (2), let us introduce a system of generalized difference equations describing the behavior of a random process in space and time:

$$\begin{cases} X_1(k+1) = X_1(k)(1-\alpha\,\Delta t) + \omega_1(k), \\ X_2(k+1) = X_1(k)(1-\beta\Delta r_{12})(1-\alpha\,\Delta t) + \omega_2(k), \\ X_3(k+1) = X_1(k)(1-\beta\Delta r_{13})(1-\alpha\,\Delta t) + \omega_3(k), \\ \vdots \\ X_S(k+1) = X_1(k)(1-\beta\Delta r_{1S})(1-\alpha\,\Delta t) + \omega_S(k), \end{cases} \quad (3)$$

where

$$\mathbf{X}(k+1) = = |X_1(k+1), X_2(k+1), X_3(k+1), \ldots, X_S(k+1)|^{\mathrm{T}}$$

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is the state vector, whose elements are the values of the meteorological parameter ξ at the points with the coordinates x_i and y_i ($i = 1, 2, ..., S$) at the time moments $k + 1$ (and $X_1(k + 1)$ is the value of the meteorological parameter at the point (x_1, y_1) inaccessible for measurements;

$$\Delta r_{1i} = [(x_1 - x_i)^2 + (y_1 - y_i)^2]^{-1/2}$$

is the distance between the first point and the ith point ($i = 2, 3, ..., S$); Δt is the time discretization interval; $k = 0, 1, 2, ..., K$ is the iteration number (discrete time);

$$\mathbf{W}(k) = |\omega_1(k), \omega_2(k), \omega_3(k), ..., \omega_S(k)|^{\mathrm{T}}$$

is the column vector of the state noise.

The system of equations (3) can be used as a model of the space of states at synthesizing the algorithm for estimation of the current values of meteorological parameters of interest within the framework of the Kalman filtering theory.[3] Application of Eq. (3) is limited due to the uncertain parameters α and β and their dependence on height and time. This limitation can be lifted by introducing additional variables $X_{S+1}(k) = \alpha(t, h)$ and $X_{S+2}(k) = \beta(t, h)$ in the state vector $\mathbf{X}(k)$ and passing to the extended system of difference equations:

$$\begin{cases} X_1(k+1) = X_1(k)[1 - X_{S+1}(k)\Delta t] + \omega_1(k), \\ X_2(k+1) = X_1(k)[1 - X_{S+2}(k)\Delta r_{12}][1 - X_{S+1}(k)\Delta t] + \\ \qquad + \omega_2(k), \\ X_3(k+1) = X_1(k)[1 - X_{S+2}(k)\Delta r_{13}][1 - X_{S+1}(k)\Delta t] + \\ \qquad + \omega_3(k), \\ \vdots \\ X_S(k+1) = X_1(k)[1 - X_{S+2}(k)\Delta r_{1S}][1 - X_{S+1}(k)\Delta t] + \\ \qquad + \omega_S(k), \\ X_{S+1}(k+1) = X_{S+1}(k), \\ X_{S+2}(k+1) = X_{S+2}(k). \end{cases} \quad (4)$$

It should be noted that the state space (4) is written based on the assumption of constant $X_{S+1}(k)$ and $X_{S+2}(k)$ within the whole observation interval.

The equations of observations at direct measurement of the meteorological parameter $\xi(k)$ at the points $i = 2, 3, ..., S$ can be presented as an additive mixture of the true value $X_i(k)$ and the measurement error

$$\begin{cases} \tilde{Y}_1(k) = X_2(k) + \varepsilon_1(k), \\ \tilde{Y}_2(k) = X_3(k) + \varepsilon_2(k), \\ \vdots \\ \tilde{Y}_{S-1}(k) = X_S(k) + \varepsilon_{S-1}(k), \end{cases} \quad (5)$$

where

$$\tilde{\mathbf{Y}}(k) = \left|\tilde{Y}_1(k), \tilde{Y}_2(k), ..., \tilde{Y}_{S-1}(k)\right|^{\mathrm{T}}$$

is the measurement vector at the selected (fixed) height level h;

$$\boldsymbol{\varepsilon}(k) = |\varepsilon_1(k), \varepsilon_2(k), \varepsilon_3(k), ..., \varepsilon_{S-1}(k)|^{\mathrm{T}}$$

is the vector of measurement errors (noise).

Let us present Eqs. (4) and (5) in the matrix form:

$$\mathbf{X}(k + 1) = \mathbf{\Phi}[\mathbf{X}(k)] + \mathbf{\Gamma} \cdot \mathbf{W}(k), \quad (6)$$

$$\tilde{\mathbf{Y}}(k) = \mathbf{H} \cdot \mathbf{X}(k) + \varepsilon(k), \quad (7)$$

where

$$\mathbf{\Phi}[\mathbf{X}(k)] = \begin{vmatrix} X_1(k)[1 - X_{S+1}(k)\Delta t] \\ X_1(k)[1 - X_{S+2}(k)\Delta r_{12}][1 - X_{S+1}(k)\Delta t] \\ X_1(k)[1 - X_{S+2}(k)\Delta r_{13}][1 - X_{S+1}(k)\Delta t] \\ \vdots \\ X_1(k)[1 - X_{S+2}(k)\Delta r_{1S}][1 - X_{S+1}(k)\Delta t] \\ X_{S+1}(k) \\ X_{S+2}(k) \end{vmatrix}$$

is the transition vector-function of states;

$$\mathbf{H} = \begin{vmatrix} 0 & 1 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \end{vmatrix}$$

is the $(S - 1) \times (S + 2)$ observation matrix;

$$\mathbf{\Gamma} = \begin{vmatrix} 1 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & \dots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \end{vmatrix}$$

is the $(S + 2) \times S$ transition noise matrix.

Equations (6) and (7) completely determine the structure of the assessment algorithm.[3]

As the Eqs. (6) are nonlinear, the extended Kalman filter should be used as a method for algorithm synthesis. In this case, the equations of the optimal estimation of the state vector $\mathbf{X}(k)$ have the following form:

$$\hat{\mathbf{X}}(k + 1) = \hat{\mathbf{X}}(k + 1|k) + \mathbf{G}(\hat{\mathbf{X}}, k + 1) \times$$
$$\times [\tilde{\mathbf{Y}}(k + 1) - \mathbf{H} \cdot \hat{\mathbf{X}}(k + 1|k)], \quad (8)$$

where

$$\hat{\mathbf{X}}(k+1) = |\hat{X}_1, \hat{X}_2, \ldots, \hat{X}_{S+2}|$$

is the estimate of the state vector at the time $(k + 1)$;

$$\hat{\mathbf{X}}(k+1|k) = \mathbf{\Phi}[\hat{\mathbf{X}}(k)] \qquad (9)$$

is the vector of predicted estimates at the time $(k + 1)$ from the data at the step k; $\mathbf{G}(\hat{\mathbf{X}}, k+1)$ is the $(S+2)\times(S-1)$ matrix of weighting coefficients.

The weighting coefficients in the extended Kalman filter are calculated by recurring matrix equations of the following form:

$$\mathbf{G}(\hat{\mathbf{X}}, k+1) = \mathbf{P}(k+1|k)\cdot\mathbf{H}^{\mathrm{T}} \times$$

$$\times [\mathbf{H}\cdot\mathbf{P}(k+1|k)\cdot\mathbf{H}^{\mathrm{T}} + \mathbf{R}_{\varepsilon}(k+1)]^{-1}, \qquad (10)$$

$$\mathbf{P}(k+1|k) = \mathbf{F}\,[\hat{\mathbf{X}}(k)]\cdot\mathbf{P}(k|k)\cdot\mathbf{F}^{\mathrm{T}}\,[\hat{\mathbf{X}}(k)] +$$

$$+ \mathbf{\Gamma}\cdot\mathbf{R}_{\omega}(k)\cdot\mathbf{\Gamma}^{\mathrm{T}}, \qquad (11)$$

$$\mathbf{P}(k+1|k+1) =$$

$$= [\mathbf{I} - \mathbf{G}(\hat{\mathbf{X}}, k+1)\cdot\mathbf{H}]\cdot\mathbf{P}(k+1|k), \qquad (12)$$

where $\mathbf{P}(k+1|k)$ is the *a posteriori* $(S+2)\times(S+2)$ correlation matrix of the prediction errors; $\mathbf{P}(k+1|k+1)$ is the *a priori* $(S+2)\times(S+2)$ correlation matrix of the prediction errors; $\mathbf{R}_{\varepsilon}(k+1)$ is the $(S-1)\times(S-1)$ diagonal correlation matrix of the observation noise; $\mathbf{R}_{\omega}(k)$ is the $S\times S$ diagonal correlation matrix of the state noise; $\mathbf{I}$ is the $(S+2)\times(S+2)$ unit matrix; $\mathbf{F}\,[\hat{\mathbf{X}}(k)] = \dfrac{\partial\mathbf{\Phi}\,[\hat{\mathbf{X}}(k)]}{\partial\hat{\mathbf{X}}(k)}$ is the $(S+2)\times(S+2)$ Jacoby matrix of the transition vector-function.

To start the filtering algorithm (8)–(12) at the time $k = 0$ (initiation time), we should specify the following initial conditions:

$\hat{\mathbf{X}}(0) = \mathbf{M}\{\mathbf{X}(0)\}$ – the initial estimation vector, where $\mathbf{M}$ is the mathematical expectation vector;

$$\mathbf{P}(0|0) = \mathbf{M}\{[\mathbf{X}(0) - \mathbf{M}\{\mathbf{X}(0)\}][\mathbf{X}(0) - \mathbf{M}\{\mathbf{X}(0)\}]^{\mathrm{T}}\}$$

– the initial correlation matrix of the estimation errors; as well as the elements of the correlation noise matrices $\mathbf{R}_{\varepsilon}(0)$ and $\mathbf{R}_{\omega}(0)$.

In practice, the values $\hat{\mathbf{X}}(0)$ and $\mathbf{P}(0|0)$ can be specified based on minimum information about the actual properties of the system, and in the case of complete lack of useful information it is usually specified that $\hat{\mathbf{X}}(0) = 0$ and $\mathbf{P}(0|0) = \mathbf{I}$.

Consider now the results of studying the performance of the Kalman filtering algorithm as applied to the problem on spatial prediction of layer-mean values of temperature ($\langle T\rangle_{h_0,h}$) and zonal ($\langle U\rangle_{h_0,h}$) and meridional ($\langle V\rangle_{h_0,h}$) wind velocity components, which are usually used in making practical calculations of the spread of pollutant clouds[4] and calculated with the following equations:

$$\langle\xi\rangle_{h_0,h} = \frac{1}{h-h_0}\int_{h_0}^{h}\xi(z)\,\mathrm{d}z,$$

where <...> denote vertical averaging over some atmospheric layer $h - h_0$ (h_0 and h are the heights of its lower and upper boundaries, and $h_0 = 0$ corresponds to the ground level); ξ is the value of the meteorological parameter.

It should be noted here that to assess the performance of the Kalman filtering algorithm, we used many-year (1971–1975) two-time (00:00 and 12:00 GMT) observations at five radiosonde stations: Warsaw (52°11′N, 20°58′E), Kaunas (54°53′N, 23°53′E), Brest (52°07′N, 23°41′E), Minsk (53°11′N, 27°32′E), and Lvov (49°49′N, 23°57′E) that form a typical mesometeorological area. As a control station (for which spatial prediction was made), the Warsaw Station was used. This station is separated by 180 km from the nearest Station in Brest. An important circumstance is that under conditions of zonally average west-to-east transport, Lvov Station is at the territory lying to the west from the region covered by the observations, that is, we consider the case that the problem on spatial prediction cannot be solved based on the hydrodynamic model.

Table. Standard (δ) and relative (θ, %) errors of spatial prediction of layer-mean temperature and zonal and meridional wind based on Kalman filtering algorithm, as well as the rms deviations (σ) of estimates of these parameters

Layer, m	Temperature, °C			Zonal wind, m/s			Meridional wind, m/s		
	δ	σ	θ	δ	σ	θ	δ	σ	θ
0–100	1.7	4.6	37	1.6	3.4	47	1.6	3.1	52
0–200	1.7	4.6	37	1.7	3.6	47	1.7	3.3	52
0–400	1.5	4.5	33	1.8	3.8	47	1.7	3.5	49
0–800	1.3	4.3	30	1.8	4.1	44	1.8	3.7	49
0–1200	1.2	4.1	29	1.8	4.3	43	1.8	3.9	46
0–1600	1.2	4.0	30	1.9	4.4	43	1.8	4.0	45

As an example, the Table presents the results of statistical estimation of the performance of the Kalman filtering algorithm in the procedure of spatial prediction of the parameters $(<T>_{h_0,h})$, $(<U>_{h_0,h})$, and $(<V>_{h_0,h})$ with the use of standard δ and relative θ errors of such prediction ($\theta = \delta/\sigma$, in %; σ is the standard deviation of the parameter).

It should be noted that the Table presents the results of statistical estimation only for summer season, when spatial correlations in the midlatitudes of the Northern Hemisphere are much weaker than in winter.[5]

References

1. V.S. Komarov and Yu.B. Popov, Atmos. Oceanic Opt. **14**, No. 4, 230–234 (2001).
2. V.S. Komarov and Yu.B. Popov, Atmos. Oceanic Opt. **14**, No. 4, 235–238 (2001).
3. C.T. Leondes, ed., *Control and Dynamic Systems: Advances in Theory and Applications* (Academic Press, New York, 1976), Vol. 12.
4. F.F. Bryukhan', *Methods of Climatic Processing and Analysis of Aerological Information* (Gidrometeoizdat, Moscow, 1983), 112 pp.
5. L.S. Gandin, V.I. Zakhariev, and R. Tselman, eds., *Statistical Structure of Meteorological Fields* (Budapest, 1976), 365 pp.