Estimation and prediction of atmospheric state parameters using the Kalman filtering algorithm. Part 1. Methodic foundation

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The methods and algorithms for estimating and forecasting the atmospheric parameters with the Kalman filtering method are considered.

Introduction

In recent years, the procedure of data assimilation preceding numerical weather prediction, is widely used in practical processing of meteorological observations. This procedure is based on simultaneous consideration of both measurements themselves and the results predicted with a chosen mathematical model. The problem of data assimilation is usually solved with a dynamic-stochastic approach based on Kalman filtering theory.[1–7]

This approach assumes that the state of the atmosphere can be described by random fields, which are interconnected by some system of relations. Therefore, the process of forecasting in this approach consists of two stages:

– assimilation of the atmospheric state measurements and correction of parameters of a prediction model;

– prediction itself based on the corrected model.

It should be noted that application of the Kalman filter in the procedure of assimilation of meteorological data obtained with up-to-date prediction models faces certain problems while implementing an assimilation algorithm because of the high order of the covariance matrix of prediction errors.[5]

Taking into account this, as well as the need to solve the problem of forecast on the mesometeorological scale in the absence of global data, we propose a simplified model describing the behavior of meteorological parameters in space and time using the first-order stochastic differential equations. The distinctive feature of this approach is a possibility to dispense with the procedure of solution of a complex set of hydrodynamic equations. Every atmospheric parameter of interest is treated separately, and its change in space and time is considered as a stochastic process with known correlation properties. According to the chosen approach, the prediction is made for a certain point in space from observations of only several meteorological stations. In this case, the dimension of the state vector is limited, implementation of the filtering algorithm becomes simpler, and the stability of the algorithm itself increases.

Solution of the problem of space and time mesoscale forecasting is dictated by the need in meteorological support of various economic and national defense problems, such as

– assessment of spatial spread of technogenic pollution to small distances (up to 100 – 200 km) from the sources;

– diagnosis and prediction of the state of the atmosphere (first of all, temperature and wind) at the enemies territory for meteorological support of land and air forces during local military missions.

It should be noted here that the study of the problem of estimating and predicting the parameters of the atmosphere state with the use of the Kalman filter continues the earlier works,[8–12] in which the corresponding algorithms were based on the modified method of clustering of arguments (MMCA). In spite of marked advantages over the traditional methods of regression analysis, including the method of optimal extrapolation (these advantages include the possibility of realization of an algorithm using limited sampled data, multiple-criterion choice of the best model, orientation at obtaining models of optimal complexity, etc.), the MMCA has certain restrictions. They are connected mostly with the necessity of prior obtaining of some data sample with the total length about $N = k + 1$ (here k is the number of levels) and with the requirement that the forecast interval is equal to the measurement interval.

In this connection, it is necessary to develop the prediction methods free of such restrictions and allowing one to estimate a meteorological parameter at an arbitrary point in space from the data of single measurements at a local network of upper-air stations, as well as in the time interval between these measurements.

In this paper, we consider the methodic foundation and algorithms for solution of this problem based on the use of the Kalman filter.

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1. General theoretic aspects of the formulated problem

The general requirement in synthesis of algorithms for estimation of unknown parameters of a dynamic system is the possibility of their description by a set of differential or difference equations of the first order.[13] Difference equations can be written in the matrix form as

$$\mathbf{X}(k+1, L) = \mathbf{F}(k, L)\cdot\mathbf{X}(k, L) + \mathbf{C}(k, L)\cdot\mathbf{W}(k, L), \quad (1)$$

where $\mathbf{X}(k+1, L) = |x_1, x_2, x_3, x_4, \dots, x_n|^{\mathrm{T}}$ is an $(n\times 1)$ column vector including unknown parameters of the state of a dynamic system (vector of states); $k = 0, \dots, K$ is the discrete current time with the discretization interval Δt $(t_k = k\Delta t)$; $L = 0, \dots,$ is the discrete value of coordinates in the range of definition with the step Δz_j (here: $z_{Lj} = L\,\Delta z_j$); $\mathbf{z} = |z_1, z_2, z_3|$ are coordinates of a point in the 3D space (z_1, z_2 are plane coordinates, z_3 is the height); j is the index determining the spatial coordinate $(j = 1, 2, 3)$; $\mathbf{F}(k, L)$ is the $(n\times n)$ transition matrix for the discrete system; $\mathbf{W}(k, L) = |w_1, w_2, w_3, w_4, \dots, w_m|^{\mathrm{T}}$ is the vector of accidental perturbations of the system (generating noise, state noise); $\mathbf{C}(k, L)$ is the $(n\times m)$ matrix of intensities of accidental perturbations.

The mathematical model of measuring channels, whose data are used for estimation of the system state, is described, in the general case, by an additive mixture of a useful message and measurement error:

$$\mathbf{Y}(k, L) = \mathbf{H}(k, L)\cdot\mathbf{X}(k, L) + \mathbf{V}(k, L), \quad (2)$$

where $\mathbf{Y}(k, L) = |y_1, y_2, y_3, y_4, \dots, y_s|^{\mathrm{T}}$ is the $(s\times 1)$ vector of actual changes; $\mathbf{H}(k, L)$ is the $(n\times s)$ matrix of observations determining the functional relation between the true values of state parameters and measuring channels of the system; $\mathbf{V}(k, L) = |v_1, v_2, v_3, v_4, \dots, v_s|^{\mathrm{T}}$ is the vector of measurement errors (measurement noise); T denotes transposition.

If the functions entering into Eqs. (1) and (2) are linear, the problem of estimation is solved with the use of the Kalman–Bucy linear filter[14,15] that provides estimation of the state vector from current measurements with a minimal root-mean-square (rms) errors. The equations of estimation in this case have the following form:

$$\hat{\mathbf{X}}(k+1, L) = \hat{\mathbf{X}}(k+1|k, L) + \mathbf{G}(k+1, L)\cdot[\mathbf{Y}(k+1, L) - \mathbf{H}(k+1, L)\cdot\hat{\mathbf{X}}(k+1|k, L)], \quad (3)$$

where $\hat{\mathbf{X}}(k+1, L) = |\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{x}_4, \dots, \hat{x}_n|^{\mathrm{T}}$ is the estimate of the vector of state at the time $(k+1)$; $\hat{\mathbf{X}}(k+1|k, L) = \mathbf{F}(k, L)\cdot\hat{\mathbf{X}}(k, L)$ is the matrix equation for calculation of the vector of forecast, $\hat{\mathbf{X}}(k+1|k, L)$ is the vector of predicted estimates at the time $(k+1)$ from the data at the kth step; $\mathbf{G}(k+1, L)$ is the $(n\times s)$ matrix of weighting factors.

Note that the vectors $\hat{\mathbf{X}}(k+1, L)$ and $\hat{\mathbf{X}}(k+1|k, L)$ have the dimension $(n\times 1)$.

In the classic Kalman–Bucy linear filter, calculation of weighting factors is a recurrent procedure independent of Eq. (3). This procedures includes a solution of the matrix equations for covariance of the estimation errors[16]:

$$\mathbf{G}(k+1, L) = \mathbf{P}(k+1|k)\mathbf{H}^{\mathrm{T}}(k+1, L)\times [\mathbf{H}(k+1, L)\mathbf{P}(k+1|k)\mathbf{H}^{\mathrm{T}}(k+1, L) + \mathbf{R}_V(k+1, L)]^{-1}; \quad (4)$$

$$\mathbf{P}(k+1|k) = \mathbf{F}(k, L)\mathbf{P}(k|k)\mathbf{F}^{\mathrm{T}}(k, L) + \mathbf{R}_W(k, L); \quad (5)$$

$$\mathbf{P}(k+1|k+1) = [\mathbf{I} - \mathbf{G}(k, L)\mathbf{H}(k, L)]\cdot\mathbf{P}(k+1|k), \quad (6)$$

where $\mathbf{P}(k+1|k)$ is the $(n\times n)$ *a posteriori* covariance matrix of prediction errors; $\mathbf{P}(k+1|k+1)$ is the $(n\times n)$ *a priori* covariance matrix of estimation errors; $\mathbf{R}_V(k+1, L)$ is the $(s\times s)$ diagonal covariance matrix of observation noise; $\mathbf{R}_W(k, L)$ is the $(n\times n)$ diagonal covariance matrix of state noise; $\mathbf{I}$ is the $(n\times n)$ unit matrix.

To start the filtering algorithm (4)–(6) at the time $k = 0$ (time of initiation), the following initial conditions should be set: the initial estimation vector $\hat{\mathbf{X}}(0, L) = \mathbf{M}\{\mathbf{X}(0, L)\}$ (here $\mathbf{M}$ is the operator of mathematical expectation); initial covariance matrix of estimation errors $\mathbf{P}(0\,|\,0) = \mathbf{M}\{[\mathbf{X}(0, L) - \mathbf{M}\{\mathbf{X}(0, L)\}]\times[\mathbf{X}(0, L) - \mathbf{M}\{\mathbf{X}(0, L)\}]^{\mathrm{T}}\}$, as well as the values of the covariance matrices of noises $\mathbf{R}_V(0, L)$ and $\mathbf{R}_W(0, L)$. In practice, the values of $\hat{\mathbf{X}}(0, L)$ and $\mathbf{P}(0\,|\,0)$ can be set based on the minimum information on the actual properties of the system; in the case of complete absence of useful information, it is assumed that $\hat{\mathbf{X}}(0, L) = 0$ and $\mathbf{P}(0\,|\,0) = \mathbf{I}$.

2. Statement of the estimation problem in terms of the Kalman filter

To formulate the problem of estimation in terms of the Kalman filter, according to Eqs. (1)–(2), we should represent the meteorological parameters varying in space and time as a dynamic system. We begin the formulation of the problem with the assumption that the meteorological parameters of our interest (for example, pressure, temperature, humidity, orthogonal wind velocity components, or others) are continuously distributed in some space. This space is limited below by the ground (see the figure) and limited above by the height of the considered atmospheric layer (h); the dimensions in the bottom cross section are determined by the chosen mesoscale polygon. This polygon includes $(S-1)$ arbitrarily arranged upper-air stations providing measurement of the meteorological parameters within the entire considered atmospheric layer with the height resolution Δz_3. These measurements for some fixed time t_k can be presented as N-dimension profile (vector) with each its component corresponding to a certain height level $z_{i3} = h_1, h_2, h_3, \dots, h_N$. It should be underlined that the accuracy and frequency of measurements, as well as height resolution are determined by parameters of measuring instrumentation, and they are not considered in this paper.

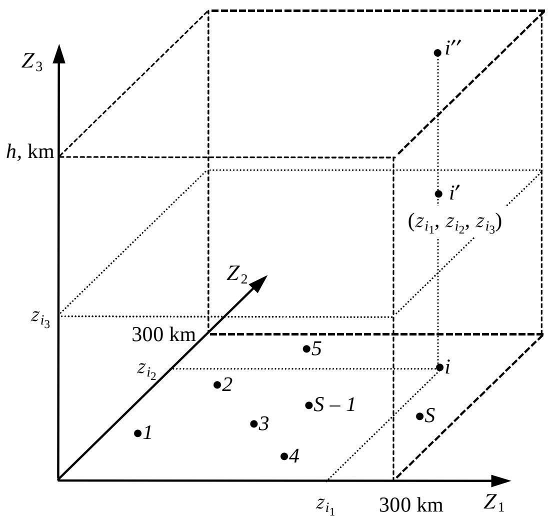

Fig. 1. Arrangement of measuring stations.

Physically, the task is to estimate (predict) a meteorological parameter at the Sth point of a given space, at which measurements are absent or impossible, from the data of $(S - 1)$ measuring stations. We will consider solution of this task on the mesometeorological scale.

The specificity of the mesoscale allows the splitting method to be applied, i.e., allows the meteorological parameters at some fixed height level to be estimated (predicted) neglecting interconnection between neighboring levels. Thus, the entire height range can be covered by N Kalman filters. Each filter uses measurements obtained for a given height level at all upper-air stations. The estimation (prediction) is made for the same height level and for the point with the plane coordinates (z_1, z_2).

Further reasoning is given for one filter meant to an arbitrary height level.

Because the meteorological parameters have random values, their statistical properties can be described by the corresponding correlation functions $\mu(\tau)$ in time and $\mu(\rho)$ in space. We can go from correlation functions to differential equations describing the dynamics of variability of random processes using the well-known methods[17,18] through the Laplace transformation.

The correlation functions describing the time and space dependence of random components of meteorological parameters, including temperature and wind velocity, can be described by exponential equations of the form:

$$\mu(\tau) = \exp(-\alpha\tau), \quad (7)$$

$$\mu(\rho) = \exp(-\beta\rho), \quad (8)$$

where $\alpha = 1/\tau_0$ is the coefficient inversely proportional to the time correlation interval τ_0; $\beta = 1/\rho_0$ is the coefficient inversely proportional to the space correlation interval ρ_0.

Assume that we need to estimate (predict) the values of a meteorological parameter at the point S (see the figure) with the coordinates (z_{S_1}, z_{S_2}); the stations, at which this parameter is measured, are at the points *1*, *2*, *3*, ..., $(S - 1)$ with known coordinates. Assuming that the values of τ_0 and ρ_0 are constant on the mesoscale, we write the system of generalized difference equations describing the behavior of a random process in space and time :

$$\begin{cases} x_1(k+1) = x_n(k)(1 - \beta\,\Delta r_{1S})(1 - \alpha\,\Delta t) + w_1(k); \\ x_2(k+1) = x_n(k)(1 - \beta\,\Delta r_{2S})(1 - \alpha\,\Delta t) + w_2(k); \\ \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \\ x_n(k+1) = x_n(k)(1 - \alpha\,\Delta t) + w_n(k), \end{cases} \quad (9)$$

where $\mathbf{X}(k) = |x_1(k), x_2(k), x_3(k), \dots, x_n(k)|^{\mathrm{T}}$ is the vector of the space of states in accordance with Eq. (1); $\mathbf{W}(k) = |w_1(k), w_2(k), w_3(k), \dots, w_n(k)|^{\mathrm{T}}$ is the column vector of state noise; $\Delta r_{iS} = [(z_{S_1} - z_{i_1})^2 + (z_{S_2} - z_{i_2})^2]^{-1/2}$ is the separation between the points S and $\mathbf{i}$ $(i = 1, 2, 3, \dots, S - 1)$; (z_{i_1}, z_{i_2}) are the coordinates of the point $\mathbf{i}$.

Note that the dimension of the state vector in such a formulation is larger by one than the number of measuring stations, i.e., $n = 1, 2, 3, \dots, S$.

We present the system of equations (9) in the matrix form:

$$\mathbf{X}(k+1) = \mathbf{F}(\Delta t, \Delta r) \cdot \mathbf{X}(k) + \mathbf{W}(k),$$

where

$$\mathbf{F}(\Delta t, \Delta r) = (1 - \alpha\Delta t) \begin{vmatrix} 0 & 0 & \dots & 0 & (1 - \beta\Delta r_{1S}) \\ 0 & 0 & \dots & 0 & (1 - \beta\Delta r_{2S}) \\ 0 & 0 & \dots & 0 & (1 - \beta\Delta r_{3S}) \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & 1 \end{vmatrix}$$

is the $(n \times n)$ transfer matrix, in which all parameters α, β, Δt, and Δr_{iS} are thought known $(i = 1, 2, 3, \dots, S - 1)$.

The system (9) allows us to introduce additional state equations refining the mathematical model of the dynamic system. Introduction of new variables into the state vector $\mathbf{X}(k)$ and their corresponding description lead to a change of the transfer matrix $\mathbf{F}(\Delta t, \Delta r)$.

For example, the parameters α and β thought to be constant and unknown can be introduced into the state variables. The difference equations for these parameters have the form

$$\begin{aligned} \alpha(k+1) &= \alpha(k); \\ \beta(k+1) &= \beta(k). \end{aligned} \quad (10)$$

In this case, a filter can be synthesized that provides simultaneous estimation of the meteorological parameter and its intervals of space and time correlation. This filter is nonlinear because the state equations acquire nonlinearity. Similarly to Eq. (10), the mean value of the meteorological parameter (within the mesoscale) can be introduced into the state variables. In this case, random components of the state vector determine variations of the process about the mean.

Now we consider models of measurement channels. As the measurement channel, we mean the measurements obtained from the meteorological station **i** ($i = 1, 2, 3, \ldots, S - 1$) located at a point with known coordinates. Assume that measurements of some meteorological parameter are the additive mixture of its true value and the measurement error:

$$\begin{aligned} y_1(k) &= x_1(k) + v_1(k); \\ y_2(k) &= x_2(k) + v_2(k); \\ y_3(k) &= x_3(k) + v_3(k); \\ &\ldots\ldots\ldots\ldots \\ y_{S-1}(k) &= x_{n-1}(k) + v_{S-1}(k), \end{aligned} \tag{11}$$

where $\mathbf{Y}(k) = |y_1(k), y_2(k), y_3(k), \ldots, y_{S-1}(k)|^{\mathrm{T}}$ is the vector of measured values of the meteorological parameter obtained from $(S - 1)$ meteorological stations; $x_1(k), x_2(k), x_3(k), \ldots, x_{n-1}(k)$ are true values of the same meteorological parameter that actually exist at measurement points $i = 1, 2, 3, \ldots, n - 1$, and $n = S$; $\mathbf{V}(k) = |v_1(k), v_2(k), v_3(k)|^{\mathrm{T}}, \ldots, v_{S-1}(k)|^{\mathrm{T}}$ is the vector of measurement errors.

Let us present the system of equations (11) in the matrix form

$$\mathbf{Y}(k) = \mathbf{H}\cdot\mathbf{X}(k) + \mathbf{V}(k), \tag{12}$$

where

$$\mathbf{H} = \begin{Vmatrix} 1 & 0 & \ldots & 0 & 0 \\ 0 & 1 & \ldots & 0 & 0 \\ 0 & 0 & \ldots & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & 1 & 0 \end{Vmatrix} \tag{13}$$

is the $(S-1)\times n$ matrix of observations. Equations (9), (11)–(13) or more exactly, the matrices $\mathbf{F}(\Delta t, \Delta r)$ and $\mathbf{H}$ completely determine the structure of the linear Kalman filter (4)–(6) used for estimation of meteorological parameters. However, for the atmospheric boundary layer, where periodic (diurnal) changes of meteorological parameters (first of all, temperature of air) are observed, the use of Eqs. (11) is possible only at a limited time interval. To consider this process, an additional function taking into account regular diurnal variability of temperature should be introduced into description of the measurement channel. Under mesoscale conditions, because of temperature stability in the horizontal plane, it is worth using the mathematical model taking into account its mean value at the considered height level. Introduction of the additional variable should be taken into account by expansion of the state vector and change of the matrices $\mathbf{F}(\Delta t, \Delta r)$ and $\mathbf{H}$. Let us make the corresponding changes in state equations (9) and equations (11) describing the measurement channels.

We introduce the expanded state vector with the dimension $n = (S + 1)$:

$$\mathbf{X}^{\mathrm{T}}(k) = |x_1(k), x_2(k), \ldots, x_{n-2}(k), x_{n-1}(k), x_n(k)|,$$

which is the vector of the space of states, where $x_1(k) - x_{n-2}(k)$ is the amplitude of the diurnal variability of temperature at the measurement points $i = 1, 2, \ldots, (S - 1)$; $x_{n-1}(k)$ is the amplitude of the diurnal variability of temperature at the point S to be estimated; $x_n(k)$ is the mean value of temperature for the chosen level on the mesoscale.

In accordance with the new state vector $\mathbf{X}^{\mathrm{T}}(k)$, the system (9) is complemented with one equation for the mean temperature and takes the form:

$$\begin{cases} x_1(k+1) = x_{n-1}(k)(1 - \beta\Delta r_{1S})(1 - \alpha\Delta t) + w_1(k) \\ x_2(k+1) = x_{n-2}(k)(1 - \beta\Delta r_{2S})(1 - \alpha\Delta t) + w_2(k) \\ \ldots\ldots\ldots\ldots\ldots\ldots \\ x_{n-2}(k+1) = x_{n-1}(k)(1 - \beta\Delta r_{(n-2)S})(1 - \alpha\Delta t) + w_{n-2}(k) \\ x_{n-1}(k+1) = x_{n-1}(k)(1 - \alpha\Delta t) + w_{n-1}(k) \\ x_n(k+1) = x_n(k) \end{cases}. \tag{14}$$

The $(n\times n)$ transfer matrix in this case takes the form

$$\mathbf{F}(\Delta t, \Delta r) = \begin{Vmatrix} 0 & 0 & \ldots & 0 & (1 - \alpha\Delta t)(1 - \beta\Delta r_{1S}) & 0 \\ 0 & 0 & \ldots & 0 & (1 - \alpha\Delta t)(1 - \beta\Delta r_{2S}) & 0 \\ 0 & 0 & \ldots & 0 & (1 - \alpha\Delta t)(1 - \beta\Delta r_{3S}) & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & 0 & (1 - \alpha\Delta t) & 0 \\ 0 & 0 & \ldots & 0 & 0 & 1 \end{Vmatrix}, \tag{15}$$

where the parameters α, β, and Δt, as well as the distances Δr_{iS} between the measurement points $i = 1, 2, 3, \ldots, (S - 1)$ and the sought point S are assumed to be known.

The law of temperature change during a day corresponds to the cosine function, therefore the measurement channels can be described by the following equations:

$$\begin{cases} y_1(k) = x_n(k) + x_1(k)\cos\left(\frac{2\pi}{24}t_k - \pi\right) + v_1(k) \\ y_2(k) = x_n(k) + x_2(k)\cos\left(\frac{2\pi}{24}t_k - \pi\right) + v_2(k) \\ \ldots\ldots\ldots\ldots\ldots\ldots, \\ y_{S-2}(k) = x_n(k) + x_{S-2}(k)\cos\left(\frac{2\pi}{24}t_k - \pi\right) + v_{S-2}(k) \\ y_{S-1}(k) = x_n(k) + x_{S-1}(k)\cos\left(\frac{2\pi}{24}t_k - \pi\right) + v_{S-1}(k) \end{cases} \tag{16}$$

where

$$\mathbf{Y}^{\mathrm{T}}(k+1, L) = |y_1(k), y_2(k), \ldots, y_{S-2}(k), y_{S-1}(k)|$$

is the measurement vector; $v_1(k)$, ..., $v_{S-1}(k)$ are measurement errors; t_k is the local time at the measurement k.

The $(S-1)\times n$ matrix of observations in terms of the introduced state vector has the form

$$\mathbf{H} = \left| \begin{array}{cccccc} \cos(\frac{2\pi}{24}t_k - \pi) & 0 & \ldots & 0 & 0 & 1 \\ 0 & \cos(\frac{2\pi}{24}t_k - \pi) & \ldots & 0 & 0 & 1 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & \cos(\frac{2\pi}{24}t_k - \pi) & 0 & 1 \end{array} \right| . \quad (17)$$

It is assumed that measurements are taken synchronously at the time moments k at regular time intervals Δt.

Equations (14), (16) and matrices (15), (17) fully determine the structure of the Kalman filter for estimation of temperature at the point S.

In conclusion, it should be noted that the efficiency of the proposed methodic approach to estimation and prediction of mesometeorological fields can be judged from the data of the field experiment. The results of research with invoking many-year upper-air measurements obtained at a typical European mesometeorological polygon are the subject of the second part of this paper.

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