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Mathematical, methodological questions concerning the spatial interpolation of climate elements

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Abstract — The paper focuses on the basic mathematical and theoretical questions of spatial interpolation of meteorological elements. Nowadays, in meteorology the most often applied procedures for spatial interpolation are the geostatistical interpolation methods built also in GIS software. The mathematical basis of these methods is the geostatistics that is an exact but special part of the mathematical statistics. However, special meteorological spatial interpolation methods for climate elements also exist, such as Gandin optimum interpolation as well as the MISH method developed at the Hungarian Meteorological Service in the last few years. These meteorological interpolation methods are also based on the mathematical statistical theory. Therefore, the basic type of the interpolation formulas applied by the geostatistical and meteorological methods are similar. One of our intentions is to present some comparison of the various kriging formulas, such as ordinary, universal, regression, residual, detrended, etc., ones. In general, these formulas can be derived from the multiple linear regression formula by using the generalized-least-squares estimation for certain unknown parameters. But the main difference between the geostatistical and meteorological interpolation methods can be found in the amount of information used for modeling the necessary statistical parameters. In geostatistics, the usable information or the sample for modeling is only the system of predictors, which is a single realization in time, while in meteorology we have spatiotemporal data, namely the long data series which form a sample in time and space as well. The long data series is such a speciality of the meteorology that makes possible to model efficiently the statistical parameters in question.

Key-words: spatial interpolation, geostatistics, statistical climatology, data series, geostatistical interpolation, meteorological interpolation

1. Introduction

First let us consider the abstract scheme of the meteorological examinations. The initial stage is the meteorology that means the qualitative formulation of the given problem. The next stage is the mathematics in order to formulate the problem quantitatively. The third stage is to develop software on the basis of the mathematics. Finally, the last stage is again the meteorology that is the application of the developed software and evaluation of the obtained results. In the practice, however, the mathematics is sometimes neglected. Instead of adequate mathematical formulation of the meteorological problem, ready-made software are applied to solve the problem. Of course, in this case the results are not authentic either. Allow me a not word for word citation from John von Neumann: without quantitative formulation of the meteorological questions, we are not able to answer the simplest qualitative questions either.

Concerning our topic we have the following question. What kind of mathematics of spatial interpolation is adequate for meteorology? Nowadays, the geostatistical interpolation methods built in GIS software are applied in meteorology. The mathematical basis of these methods is the geostatistics that is an exact but special part of the mathematical statistics. The speciality is connected with the assumption that the data are purely spatial. To illustrate this problem, here are some quotations from the valuable book of Noel A.C. Cressie: "Statistics for Spatial Data" (*Cressie*, 1991). On page 29: "The first part of this book is concerned with modeling data as a (partial) realization of a random process $\{Z(\mathbf{s}):\mathbf{s}\in D\}$….". Explanation of the sentence is that the data are purely spatial data, since D is a space domain. On page 30: "It is possible to allow for spatiotemporal data by considering the variable $Z(\mathbf{s}, t)$, but for most of this book it will be assumed that the data are purely spatial…". Last, on page 53: "Statistically speaking, some further assumptions have to be made. Otherwise, the data represent an *incomplete* sampling of a *single* realization, making inference impossible." It means "*incomplete* sampling" in space, "*single* realization" in time.

Consequently, as we see it, the geostatistical methods can not efficiently use the meteorological data series, while the data series make possible to obtain the necessary climate information for the interpolation in meteorology.

2. Mathematical statistical model of spatial interpolation

In practice, many kinds of interpolation methods exist, therefore, the question is the difference between them. According to the interpolation problem, the unknown predictand $Z(\mathbf{s}_0, t)$ is estimated by use of the known predictors $Z(\mathbf{s}_i, t)$ $(i=1,...,M)$, where the location vectors $\mathbf{s}$ are the elements of the given space domain D, and t is the time. The vector form of predictors is $\mathbf{Z}^{\mathrm{T}}(t)=[Z(\mathbf{s}_1,t),.....,Z(\mathbf{s}_M,t)]$. The type of the adequate interpolation formula depends on the probability distribution of the meteorological element in question. In this paper only the linear or additive formula is described in detail, which is appropriate in case of normal probability distribution. However, perhaps it is worthwhile to remark that for case of a quasi lognormal distribution (e.g., precipitation sum), we deduced a mixed additive multiplicative formula which is used also in our MISH system, and it can be written in the following form,

$$\hat{Z}(\mathbf{s}_0,t)=\vartheta\cdot\left(\prod_{q_i\cdot Z(\mathbf{s}_i,t)\geq\vartheta}\left(\frac{q_i\cdot Z(\mathbf{s}_i,t)}{\vartheta}\right)^{\lambda_i}\right)\cdot\left(\sum_{q_i\cdot Z(\mathbf{s}_i,t)\geq\vartheta}\lambda_i+\sum_{q_i\cdot Z(\mathbf{s}_i,t)<\vartheta}\lambda_i\cdot\left(\frac{q_i\cdot Z(\mathbf{s}_i,t)}{\vartheta}\right)\right), \quad (1)$$

where the interpolation parameters are $\vartheta>0,\ q_i>0,\ \lambda_i\geq 0\ (i=1,...,M)$, and $\sum_{i=1}^{M}\lambda_i=1$.

2.1. Statistical parameters

In general, the interpolation formulas have some unknown interpolation parameters which are known functions of certain statistical parameters. At the linear interpolation formulas the basic statistical parameters can be divided into two groups, such as the deterministic and the stochastic parameters.

The deterministic or local parameters are the expected values $\mathrm{E}(\mathbf{Z}(\mathbf{s}_i,t))(i=0,...,M)$. Let $\mathrm{E}(\mathbf{Z}(t))$ denote the vector of expected values of predictors, i.e., $\mathrm{E}(\mathbf{Z}(t))^{\mathrm{T}}=[\mathrm{E}(Z(\mathbf{s}_1,t)),....,\mathrm{E}(Z(\mathbf{s}_M,t))]$.

The stochastic parameters are the covariance or variogram values belonging to the predictand and predictors, such as

$\mathbf{c}$: predictand-predictors covariance vector,

$\mathbf{C}$: predictors-predictors covariance matrix,

$\boldsymbol{\gamma}$: predictand-predictors variogram vector,

$\boldsymbol{\Gamma}$: predictors-predictors variogram matrix.

The covariance is preferred in mathematical statistics and meteorology, while the variogram is preferred in geostatistics. Here is a quotation from the chapter "Geostatistics" of the mentioned book of Noel A.C. Cressie (*Cressie*, 1991, p. 30.). "The cornerstone is the variogram, a parameter that in the past has been either unknown or unfashionable among statisticians." In our opinion, the main reason of this reluctance is that the covariance is a more general statistical parameter than the variogram. The variogram values, can be written as functions of the covariance values and it is not true inversely.

2.2. Linear meteorological model for expected values

At the statistical modeling of the meteorological elements we have to assume, that the expected values of the variables are changing in space and time alike. The spatial change means that the climate is different in the regions. The temporal change is the result of the possible global climate change. Consequently, in case of linear modeling of expected values, we assume that

$$\mathrm{E}(Z(\mathbf{s}_i, t)) = \mu(t) + E(\mathbf{s}_i) \quad (i = 0, \ldots, M), \tag{2}$$

where $\mu(t)$ is the temporal trend or the climate change signal and $E(\mathbf{s})$ is the spatial trend. We emphasize, that this spatiotemporal model for expected values is different from the classic models used in geostatistics or by the multivariate statistical methods. As regards the geostatistics, there are purely spatial data assumed in general.

2.3. Linear regression formula

In essence, the multiple linear regression formula is the theoretical basis of the various linear interpolation methods. The multiple linear regression formula between predictand $Z(\mathbf{s}_0, t)$ and predictors $\mathbf{Z}(t)$ can be written as

$$\hat{Z}_{LR}(\mathbf{s}_0, t) = \mathrm{E}(\mathrm{Z}(\mathbf{s}_0, t)) + \mathbf{c}^{\mathrm{T}} \mathbf{C}^{-1} (\mathbf{Z}(t) - \mathrm{E}(\mathbf{Z}(t))) \tag{3}$$

and $\hat{Z}_{LR}(\mathbf{s}_0, t)$ is the best linear estimation that minimizes the mean-square prediction error. Consequently, the linear regression formula would be the optimal linear interpolation formula concerning the mean-square prediction error. In respect of application, however, problems arise from the unknown statistical parameters $\mathrm{E}(\mathrm{Z}(\mathbf{s}_0, t))(i = 0, \ldots, M)$ and $\mathbf{c}$, $\mathbf{C}$. Assuming the meteorological model, Eq. (2), for the expected values, Eq. (3) can be written as

$$\hat{Z}_{LR}(\mathbf{s}_0, t) = (\mu(t) + E(\mathbf{s}_0)) + \mathbf{c}^{\mathrm{T}} \mathbf{C}^{-1} (\mathbf{Z}(t) - (\mu(t)\mathbf{1} + \mathbf{E})), \tag{4}$$

where $\mathbf{E}^{\mathrm{T}} = [E(\mathbf{s}_1), \ldots.., E(\mathbf{s}_M)]$ and vector $\mathbf{1}$ is identically one. As it can be seen, the main problem is the estimation of the unknown climate change signal $\mu(t)$, if we want to apply the optimal linear regression interpolation formula.

3. Geostatistical interpolation methods

The various geostatistical interpolation formulas can be obtained from the linear regression formula, Eq. (3), by the application of the generalized-least-squares estimation for the expected values. The type of kriging formulas depends on the model assumed for the expected values.

3.1. Ordinary kriging formula

The ordinary kriging formula is a special case of the universal kriging formula. The assumed model for the expected values is $\mathrm{E}(Z(\mathbf{s}_i,t)) \equiv \mu(t)\ (i=0,\dots,M)$, thus, there is no spatial trend. The generalized-least-squares estimation for $\mu(t)$ by using only the predictors $\mathbf{Z}(t)$ may be expressed in the form $\hat{\mu}_{gls}(t) = (\mathbf{1}^{\mathrm{T}}\mathbf{C}^{-1}\mathbf{1})^{-1}\mathbf{1}^{\mathrm{T}}\mathbf{C}^{-1}\mathbf{Z}(t)$. Substituting the estimate $\hat{\mu}_{gls}(t)$ into the linear regression formula, Eq. (3), we obtain the ordinary kriging formula as

$$\hat{Z}_{OK}(\mathbf{s}_0,t) = \hat{\mu}_{gls}(t) + \mathbf{c}^{\mathrm{T}}\mathbf{C}^{-1}(\mathbf{Z}(t) - \hat{\mu}_{gls}(t)\mathbf{1}) = \sum_{i=1}^{M}\lambda_i Z(\mathbf{s}_i,t), \tag{5}$$

where $\sum_{i=1}^{M}\lambda_i = 1$.

The vector of weighting factors $\boldsymbol{\lambda}^{\mathrm{T}} = [\lambda_1,..,\lambda_M]$ can be written in covariance form

$$\boldsymbol{\lambda}^{\mathrm{T}} = \left(\mathbf{c}^{\mathrm{T}} + \mathbf{1}^{\mathrm{T}}\frac{(1-\mathbf{1}^{\mathrm{T}}\mathbf{C}^{-1}\mathbf{c})}{\mathbf{1}^{\mathrm{T}}\mathbf{C}^{-1}\mathbf{1}}\right)\mathbf{C}^{-1}, \tag{6}$$

or equivalently in variogram form

$$\boldsymbol{\lambda}^{\mathrm{T}} = \left(\boldsymbol{\gamma}^{\mathrm{T}} + \mathbf{1}^{\mathrm{T}}\frac{(1-\mathbf{1}^{\mathrm{T}}\boldsymbol{\Gamma}^{-1}\boldsymbol{\gamma})}{\mathbf{1}^{\mathrm{T}}\boldsymbol{\Gamma}^{-1}\mathbf{1}}\right)\boldsymbol{\Gamma}^{-1}. \tag{7}$$

The unknown variogram values $\boldsymbol{\gamma}$, $\boldsymbol{\Gamma}$ preferred in geostatistics are modeled according to the Section 3.3.

3.2. Universal kriging formula

The universal kriging formula is the generalized case of the ordinary kriging formula. The model assumption is that the expected values may be expressed as $\mathrm{E}(\mathrm{Z}(\mathbf{s}_i,t)) = \sum_{k=1}^{K}\beta_k(t)x_k(\mathbf{s}_i)\ \ (i=0,\dots,M)$, that is in vector form

$\mathrm{E}(Z(\mathbf{s}_0,t))=\mathbf{x}^{\mathrm{T}}\boldsymbol{\beta}(t)$, $\mathrm{E}(\mathbf{Z}(t))=\mathbf{X}\boldsymbol{\beta}(t)$, where $\mathbf{x},\mathbf{X}$ are given supplementary deterministic model variables.

The generalized-least-squares estimation for coefficient vector $\boldsymbol{\beta}(t)$, by using only the predictors $\mathbf{Z}(t)$, can be written in the form $\hat{\boldsymbol{\beta}}_{gls}(t)=(\mathbf{X}^{\mathrm{T}}\mathbf{C}^{-1}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{C}^{-1}\mathbf{Z}(t)$. It is to be remarked, that in this way the spatial trend $E(\mathbf{s})$ according to Eq. (2) is modeled also by using only the predictors $\mathbf{Z}(t)$. Substituting the estimates $\mathbf{x}^{\mathrm{T}}\hat{\boldsymbol{\beta}}_{gls}(t)$, $\mathbf{X}\hat{\boldsymbol{\beta}}_{gls}(t)$ into the linear regression formula, Eq. (3), we obtain the universal kriging formula as

$$\hat{Z}_{UK}(\mathbf{s}_0,t)=\mathbf{x}^{\mathrm{T}}\hat{\boldsymbol{\beta}}_{gls}(t)+\mathbf{c}^{\mathrm{T}}\mathbf{C}^{-1}(\mathbf{Z}(t)-\mathbf{X}\hat{\boldsymbol{\beta}}_{gls}(t))=\sum_{i=1}^{M}\lambda_i Z(\mathbf{s}_i,t), \quad (8)$$

where $\boldsymbol{\lambda}^{\mathrm{T}}\mathbf{X}=\mathbf{x}^{\mathrm{T}}$.

The vector of weighting factors $\boldsymbol{\lambda}^{\mathrm{T}}=[\lambda_1,..,\lambda_M]$ can be written in covariance form

$$\boldsymbol{\lambda}^{\mathrm{T}}=\left\{\mathbf{c}+\mathbf{X}(\mathbf{X}^{\mathrm{T}}\mathbf{C}^{-1}\mathbf{X})^{-1}(\mathbf{x}-\mathbf{X}^{\mathrm{T}}\mathbf{C}^{-1}\mathbf{c})\right\}^{\mathrm{T}}\mathbf{C}^{-1},$$

or equivalently in variogram form

$$\boldsymbol{\lambda}^{\mathrm{T}}=\left\{\boldsymbol{\gamma}+\mathbf{X}(\mathbf{X}^{\mathrm{T}}\boldsymbol{\Gamma}^{-1}\mathbf{X})^{-1}(\mathbf{x}-\mathbf{X}^{\mathrm{T}}\boldsymbol{\Gamma}^{-1}\boldsymbol{\gamma})\right\}^{\mathrm{T}}\boldsymbol{\Gamma}^{-1}.$$

The unknown variogram values $\boldsymbol{\gamma}$, $\boldsymbol{\Gamma}$ preferred in geostatistics are modeled according to Section 3.3.

3.3. Modeling of unknown statistical parameters in geostatistics

In geostatistics, only the predictors $Z(\mathbf{s}_i,t)(i=1,...,M)$ constitute the usable information or the sample for modeling of variogram values $\boldsymbol{\gamma}$, $\boldsymbol{\Gamma}$. It means we have only a single realization in time for modeling of the statistical parameters in question. In order to solve the problem of absence of temporal data, some assumptions about the statistical structure are made that is some simplification of the problem. For example, such assumptions are the intrinsic stationarity or second-order (weak) stationarity, semivariogram $\gamma(Z(\mathbf{s}_i),Z(\mathbf{s}_j))=\gamma(\mathbf{s}_i-\mathbf{s}_j)$, etc.

4. Meteorological interpolation

Similarly to the geostatistical interpolation formulas, an appropriate meteorological interpolation formula can be obtained from the linear regression formula, Eq. (3), by the application of the generalized-least-squares estimation for the expected values. The key-question is the model assumption for the expected values.

4.1. Meteorological interpolation formula

The meteorological model, Eq. (2), is assumed namely $\mathrm{E}(Z(\mathbf{s}_i,t))=\mu(t)+E(\mathbf{s}_i)\,(i=0,...,M)$, where $\mu(t)$ is the temporal trend and $E(\mathbf{s})$ is the spatial trend. Supposing that the spatial trend $E(\mathbf{s})$ is known, we apply the generalized-least-squares estimation for temporal trend $\mu(t)$ by using the predictors $\mathbf{Z}(t)$ and the spatial trend $\mathbf{E}^{\mathrm{T}}=[E(\mathbf{s}_1),.....,E(\mathbf{s}_M)]$. In this case, the generalized-least-squares estimate can be written in the form as $\hat{\mu}^{E}_{gls}(t)=(\mathbf{1}^{\mathrm{T}}\mathbf{C}^{-1}\mathbf{1})^{-1}\mathbf{1}^{\mathrm{T}}\mathbf{C}^{-1}(\mathbf{Z}(t)-\mathbf{E})$. Substituting the estimate $\hat{\mu}^{E}_{gls}(t)$ into the linear regression formula, Eq. (4), rewritten from Eq. (3) according to Eq. (2), we obtain the following interpolation formula:

$$\hat{Z}_{MI}(\mathbf{s}_0,t)=(\hat{\mu}^{E}_{gls}(t)+E(\mathbf{s}_0))+\mathbf{c}^{\mathrm{T}}\mathbf{C}^{-1}(\mathbf{Z}(t)-(\hat{\mu}^{E}_{gls}(t)\mathbf{1}+\mathbf{E}))=$$

$$=E(\mathbf{s}_0)+\sum_{i=1}^{M}\lambda_i(Z(\mathbf{s}_i,t)-E(\mathbf{s}_i)), \tag{9}$$

where $\sum_{i=1}^{M}\lambda_i=1$.

The vector of weighting factors $\boldsymbol{\lambda}^{\mathrm{T}}=[\lambda_1,..,\lambda_M]$ can be written equivalently in covariance and variogram form according to Eqs. (6) and (7). The obtained interpolation formula is a detrended or residual interpolation formula that includes the spatial trend and the theoretical ordinary kriging weighting factors. However, it is not identical with the detrended or residual interpolation method, because the interpolation formula as well as the modeling methodology of the necessary statistical parameters together defines an interpolation method. For example, at the detrended interpolation methods applied in the practice, the modeling procedure for the statistical parameters is based on only the predictors $Z(\mathbf{s}_i,t)(i=1,...,M)$.

4.2. Possibility for modeling of unknown statistical parameters in meteorology

According to Eq. (9), where the sum of weighting factors is equal to one, we have the following appropriate meteorological interpolation formula

$$\hat{Z}_{MI}(\mathbf{s}_0,t)=\sum_{i=1}^{M}\lambda_i(E(\mathbf{s}_0)-E(\mathbf{s}_i))+\sum_{i=1}^{M}\lambda_i Z(\mathbf{s}_i,t), \quad (10)$$

where $\sum_{i=1}^{M}\lambda_i=1$ and the covariance form of weighting factors is defined by Eq. (6). Consequently, the unknown statistical parameters are the spatial trend differences $E(\mathbf{s}_0)-E(\mathbf{s}_i)(i=1,...,M)$ and covariances $\mathbf{c},\mathbf{C}$. In essence, these parameters are climate parameters which in fact means that we could interpolate optimally if we knew the climate. The special possibility in meteorology is to use the long meteorological data series for modeling of the climate statistical parameters in question. The data series make possible to know the climate in accordance with the fundamentals of statistical climatology!

4.3. Difference between geostatistics and meteorology in respect of spatial interpolation

The main difference can be found in the amount of information used for modeling the statistical parameters. In geostatistics, the usable information or the sample for modeling is only the predictors $Z(\mathbf{s}_i,t)(i=1,...,M)$ which belong to a fixed instant of time, that is a single realization in time. „Statistically speaking, some further assumptions about Z have to be made. Otherwise, the data represent an *incomplete* sampling of a *single* realization, making inference impossible." (*Cressie*, 1991, p. 53.). The assumptions are, e.g., intrinsic stationarity or second-order (weak) stationarity, semivariogram $\gamma(Z(\mathbf{s}_i),Z(\mathbf{s}_j))=\gamma(\mathbf{s}_i-\mathbf{s}_j)$, covariogram $\mathrm{cov}(Z(\mathbf{s}_i),Z(\mathbf{s}_j))=\mathbf{C}(\mathbf{s}_i-\mathbf{s}_j)=C(\mathbf{0})-\gamma(\mathbf{s}_i-\mathbf{s}_j)$, which are some simplifications in order to solve the problem of absence of temporal data. While in meteorology, we have spatiotemporal data, namely long data series which form a sample in time and space as well make the modeling of the climate statistical parameters in question possible. If the meteorological stations $\mathbf{S}_k\ (k=1,..,K)\ (\mathbf{S}\in D)$ have long data series, then spatial trend differences $E(\mathbf{S}_k)-E(\mathbf{S}_l)\ (k,l=1,...,K)$ as well as the covariances $\mathrm{cov}(Z(\mathbf{S}_k),Z(\mathbf{S}_l))$ $(k,l=1,...,K)$ can be estimated statistically. Consequently, these parameters are essentially known and provide much more information for modeling than the predictors $Z(\mathbf{s}_i,t)(i=1,...,M)$ only.

5. Software and connection of topics

Our method MISH (Meteorological Interpolation based on Surface Homogenized Data Basis) for the spatial interpolation of surface meteorological elements was developed (*Szentimrey* and *Bihari*, 2007a,b) according to the mathematical background that is outlined in Section 4. This is a meteorological system not only in respect of the aim but in respect of the tools as well. It means that using all the valuable meteorological information – e.g., climate and possible background information – is required.

The new software version MISHv1.02 consists of two units that are the modeling and the interpolation systems. The interpolation system can be operated on the results of the modeling system. In the following paragraphs we summarize briefly the most important facts about these two units of the developed software.

Modeling system for climate statistical (deterministic and stochastic) parameters:

- Based on long homogenized data series and supplementary deterministic model variables. The model variables may be height, topography, distance from the sea, etc.. Neighborhood modeling, correlation model for each grid point.
- Benchmark study, cross-validation test for interpolation error or representativity.
- Modeling procedure must be executed only once before the interpolation applications!

Interpolation system:

- Additive (e.g., temperature) or multiplicative (e.g., precipitation) model and interpolation formula can be used depending on the climate elements.
- Daily, monthly values and many years' means can be interpolated.
- Few predictors are also sufficient for the interpolation and there is no problem if the greater part of daily precipitation predictors is equal to 0.
- The interpolation error or representativity is modeled too.
- Capability for application of supplementary background information (stochastic variables), e.g., satellite, radar, forecast data.
- Data series complementing that is missing value interpolation, completion for monthly or daily station data series.
- Interpolation, gridding of monthly or daily station data series for given predictand locations. In case of gridding, the predictand locations are the nodes of a relatively dense grid.

As it can be seen, modeling of the climate statistical parameters is a key issue to the interpolation of meteorological elements, and that modeling can be based on the long homogenized data series. The necessary homogenized data series can be obtained by our homogenization software MASHv3.02 (Multiple

Analysis of Series for Homogenization; *Szentimrey*, 1999, 2007). Similarly to the connection of interpolation and homogenization, in our conception the meteorological questions can not be treated separately. We present a block diagram (*Fig. 1*) to illustrate the possible connection between various important meteorological topics.

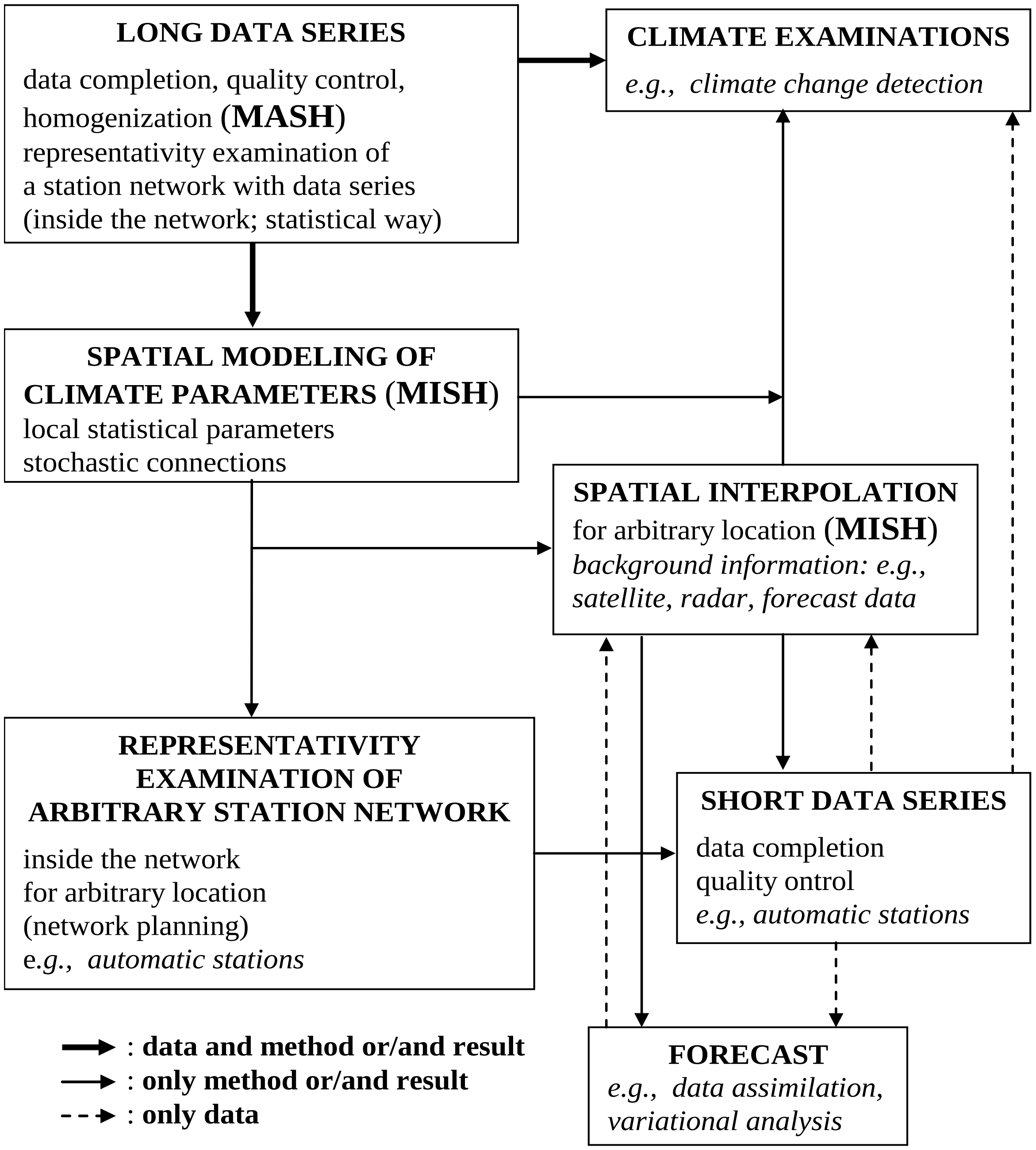

Fig. 1. Block diagram for the possible connections between various basic meteorological topics and systems.

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