

Kriging of Surface Normal Vectors

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Abstract

The problem to predict a polar unit vector at a given location from corresponding geocoded data is discussed and a general solution is presented including an explicit justification in terms of mathematical assumptions concerning stationarity/homogeneity and isotropy. The data are modelled by a stationary random field, and the spatial coherence is represented by modified multivariate variograms and covariance functions. Various types of isotropy assumptions can be distinguished, e.g. (i) isotropy of space, (ii) isotropy of measurements, (iii) isotropy of the random process, (iv) geographical isotropy of the random process, and lead to different simplifications of the general cross-covariance function. While the assumption of isotropy of measurements leads to great simplifications, but seems to be rather artificial, the assumption of geographical isotropy of the process implies less simplification but seems appropriate in many geological situations. Different kriging procedures referring to different assumptions of isotropy are applied to a set of unit surface normal vectors and the effects of these varying assumptions are empirically checked, in particular the surfaces modelled from the observed and estimated normal vectors are compared with special respect to the measure of confidence in the estimates provided by the method.

KEYWORDS: vector-kriging, co-kriging, manifolds, directions, isotropy assumptions

Introduction

The Problem

The actual problem is to predict a polar unit vector, i.e. a direction, at a given location from corresponding geocoded data like unit surface normal vectors. More specifically, our interest is in estimating a random manifold-value function of space $\mathbf{U} : \mathbb{R}^p \mapsto M \subset \mathbb{R}^q$ given data

$(\mathbf{x}_i, \mathbf{u}(\mathbf{x}_i)) \in \mathbb{R}^p \times M, i = 1, \dots, n$, where M is generally not a linear manifold. Since our special interest is in directions, the manifold $M = S^{q-1} = \{v \in \mathbb{R}^q \mid \|v\| = 1\}$ for regionalized directions.

Beyond spatial prediction we would like to provide a measure of confidence in the estimates. Therefore, the data $\mathbf{u}(\mathbf{x}_i) \in S^{q-1} \subset \mathbb{R}^q, \mathbf{x}_i \in D \subset \mathbb{R}^p, i = 1, \dots, n$, shall be modelled by a random field $\{\mathbf{U}(\mathbf{x}), \mathbf{x} \in D\}$, and the spatial correlation is represented by modified multivariate cross-variograms and cross-covariance functions, respectively. The method of choice is vector or co-kriging, respectively.

However, for spheres and other non-linear manifolds, known methods of linear prediction like kriging cannot be applied without some relaxations. Generally, the predicted objects obtained by this method will not be directions, i.e. being defined as linear combinations of elements of non-linear manifolds they will not be an element of this manifold themselves. However, the estimator should be close to the manifold if the prediction is sensible in practical terms.

Different kriging procedures corresponding to different types of isotropy are applied to sets of unit surface normal vectors and the effects of these varying assumptions are empirically checked, in particular the surfaces modelled from the observed and estimated normal vectors are compared with special respect to the measure of confidence in the estimates provided by the method.

Thematic vs. Geometric Vectors and Isotropy Assumptions

It should be noted that the vectors being observed or estimated by multivariate or co-kriging constitute geometric entities. A thematic vector of e.g. geophysical or geochemical properties conveys its information independently of the order of its components, while the information is changed if the components of a geometric vector are re-ordered. Therefore, kriging of geometric unit vectors has features to be distinguished from general vector-kriging. One of these features is that various types of isotropy assumptions can be distinguished

- isotropy of space,
- isotropy of measurements,
- isotropy of the random process,
- geographical isotropy of the random process

Any assumption of isotropy corresponds to a different physical understanding of the process and imposes different constraints on the possible variograms and covariance functions, and the kriging weights, and leads to different simplifications of the general cross-covariance function and the kriging procedure, respectively.

Kriging in Embedding Spaces

To apply kriging, an appropriate mapping $f : M \mapsto \mathbb{R}^q$ into an embedding space is defined, which preserves the canonical measure of distance in M and reproduces it correspondingly in the embedding space.

The mapping $f : S^{q-1} \mapsto \mathbb{R}^q$ into the embedding space \mathbb{R}^q is canonically provided by $f(\mathbf{u}) = \mathbf{u}$, preserving the measure of distance $\|f(\mathbf{u}_1) - f(\mathbf{u}_2)\| = 2 \sin \frac{\angle(\mathbf{u}_1, \mathbf{u}_2)}{2}$. The angle of two directions is the common canonical measure for their distance on the sphere as well as in the embedding space.

Then, kriging will be performed in embedding space and applied to the transformed objects

$$\mathbf{Z}(\mathbf{x}_i) := f(\mathbf{U}(\mathbf{x}_i)) = \mathbf{U}(\mathbf{x}_i)$$

The estimator can be projected onto the manifold by normalisation

$$\frac{\hat{\mathbf{U}}(\mathbf{x}_0)}{\|\hat{\mathbf{U}}(\mathbf{x}_0)\|}$$

Given a model for the expectation $E[\mathbf{U}_i(\mathbf{x}_k)] = \mu + \Sigma_{?}$, the

- best $E[(\hat{U}_i(\mathbf{x}_0) - U_i(\mathbf{x}_0))^2] \rightarrow \min, i = 1, \dots, q$
- linear $\hat{U}_i(\mathbf{x}_0) = \sum_{jk} \lambda_{ijk} U_j(\mathbf{x}_k)$
- unbiased $E[\hat{U}_i(\mathbf{x}_0) - U_i(\mathbf{x}_0)] = 0$

estimator $\hat{\mathbf{U}}(\mathbf{x}_0)$ of $\mathbf{U}(\mathbf{x}_0)$ is well defined.

The kriging weights λ_{ijk} are determined if the cross-covariance function

$$C(\mathbf{h}) = (\text{Cov}(U_i(\mathbf{x}), U_j(\mathbf{x} + \mathbf{h})))_{i,j=1,\dots,q} \in \mathbb{R}^{q \times q}$$

of the random field is known. Alternatively, the cross-variogram or generalized cross-covariance functions may be applied.

The result $\hat{\mathbf{U}}(\mathbf{x}_0)$ of kriging in the embedding space is generally not an element of the manifold. There are two different ways to use $\hat{\mathbf{U}}(\mathbf{x}_0)$ as a preliminary result. We could just project $\hat{\mathbf{U}}(\mathbf{x}_0)$ to the point of the manifold, which is closest to it. Since the true $\mathbf{U}(\mathbf{x}_0)$ belongs to the manifold, and the predicted $\hat{\mathbf{U}}(\mathbf{x}_0)$ is close to the true value $\mathbf{U}(\mathbf{x}_0)$, its projection onto the manifold should be close to the true value, too. Some special optimality criterion can be used to show that this prediction is actually sensible. The second possibility is to interpret the result of kriging directly. $\hat{\mathbf{U}}(\mathbf{x}_0)$ is not a member of the manifold itself, but it is close to the manifold. We can determine those points of the manifold which are close to $\hat{\mathbf{U}}(\mathbf{x}_0)$ and therefore probable values. We can investigate how well the datum at the location \mathbf{x}_0 can be predicted and whether there are ambiguities or not.

Notation

$\mathbf{Z}(\mathbf{x})$, $\mathbf{U}(\mathbf{x})$ denotes a stochastic process (field) of regionalized vectors or unit vectors, respectively, in q -dimensional space \mathbb{R}^q assigned to locations \mathbf{x} in p -dimensional geographic space \mathbb{R}^p , typically $p, q \in \{2, 3, 4\}$. $O(p)$ denotes the orthogonal group of dimension p , which is the group of rotations and orthogonal reflections.

Kriging Subject to Isotropy

Isotropy of Space

All finite-dimensional marginal probability laws remain unchanged when the geographic locations of the measurements are rotated

$$P(\mathbf{U}(\sigma\mathbf{x}_1), \dots, \mathbf{U}(\sigma\mathbf{x}_n)) = P(\mathbf{U}(\mathbf{x}_1), \dots, \mathbf{U}(\mathbf{x}_n)), \quad \sigma \in O(p) \quad (1)$$

It should be noted that the vectors $\mathbf{U}(\mathbf{x})$ are not subject to rotations.

Isotropy of space applies to thematic vectors \mathbf{U} , the components of which do not constitute a geometric entity and maybe re-ordered without changing their information content. The assumption of spatial isotropy conforms with the conventional assumption of isotropy as discussed by e.g. Cressie (1993) or Wackernagel (1998).

The assumption of spatial isotropy leads to the general theory of tensor kriging and to isotropic tensor valued variograms

$$\gamma_{ij}(\|\mathbf{h}\|) = E[(U_i(\mathbf{x}) - U_i(\mathbf{x} + \mathbf{h}))(U_j(\mathbf{x}) - U_j(\mathbf{x} + \mathbf{h}))] \in \mathbb{R}^{3 \times 3}$$

In this case a matrix valued (cross-)variogram, which is only a function of the scalar distance, is required to calculate the matrix-valued kriging weights. Spatial isotropy has been discussed for instance by Cressie (1993) and Wackernagel (1998).

The assumption of isotropy of space does generally not apply to geometric vectors \mathbf{U} , the components of which constitute geometric entities, and are likely to relate to the geographical coordinates of the locations, i.e. the components of which cannot be interchanged without changing their information content. A set scalar quantities, such as chemical composition data, are likely to have this or no isotropy.

Isotropy of Measurements

All finite-dimensional marginal probability laws remain unchanged when the geometric vectors $\mathbf{U}(\mathbf{x})$ are considered with respect to a rotated coordinate system

$$P(\sigma\mathbf{U}(\mathbf{x}_1), \dots, \sigma\mathbf{U}(\mathbf{x}_n)) = P(\mathbf{U}(\mathbf{x}_1), \dots, \mathbf{U}(\mathbf{x}_n)), \quad \sigma \in O(q) \quad (2)$$

Isotropy of measurements implicitly assumes that the geometric vectors may be rotated independently of their geographic locations. This assumption may be appropriate for geometrical directions which do not physically relate to directions in geographic space. Thus, it seems rather artificial; it was applied without explicit notion by Young (1987).

Isotropy of measurements transforms to the corresponding isotropy assumption in the embedding space and additionally implies $E[\mathbf{U}(x)] = 0$ there.

In this case

- the optimality criterion simplifies to

$$E[\|\hat{\mathbf{U}}(x_0) - \mathbf{U}(x_0)\|^2] \rightarrow \min$$

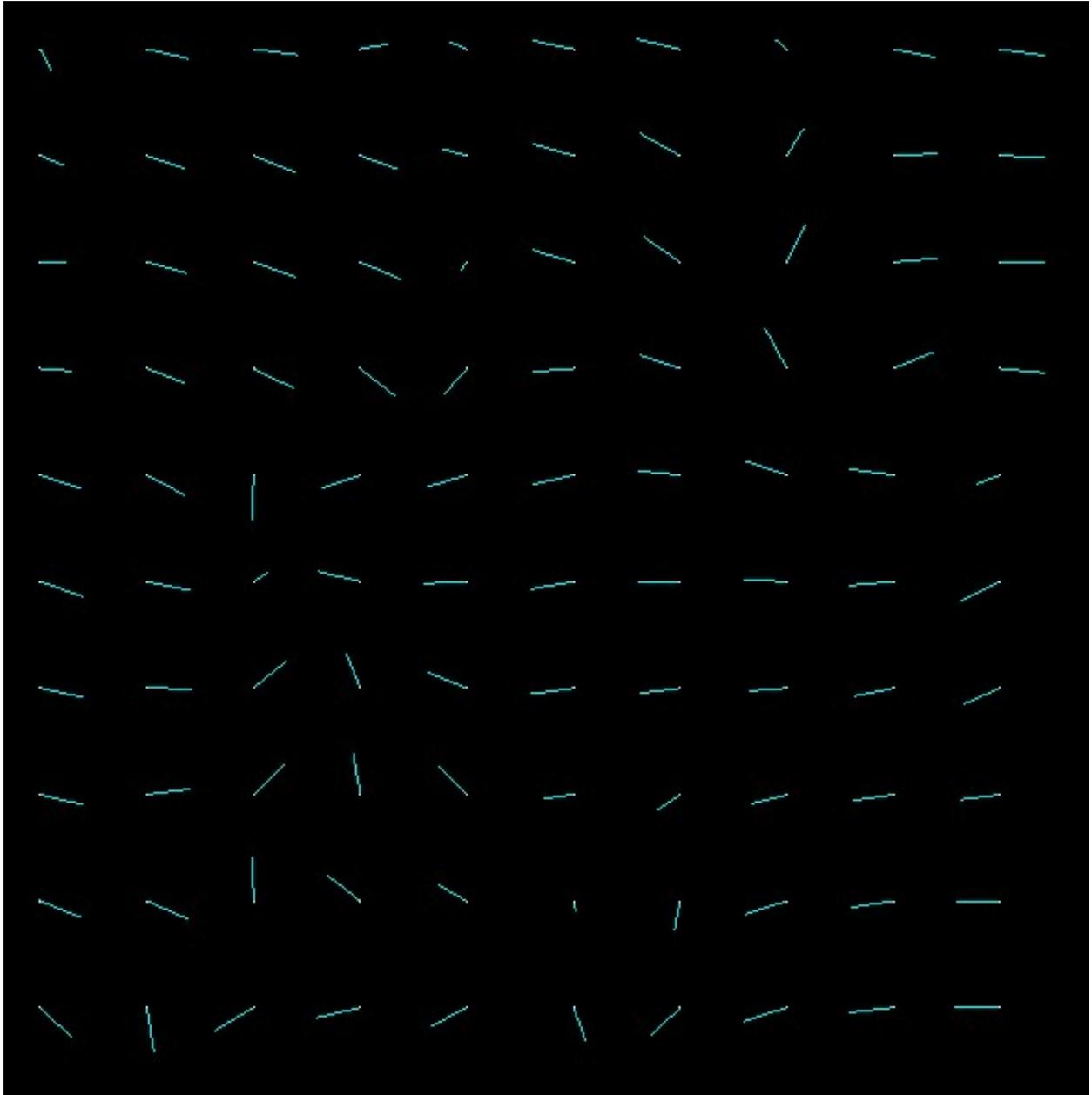


Figure 1a) The simulated data $\mathbf{U}(\mathbf{x}) \in \mathbb{R}^3$, $\mathbf{x} \in \mathbb{R}^2$ exhibit spatial isotropy without isotropy of measurements: A clearly preferred direction of the data is obvious while the spatial correlation is the same in any given direction.

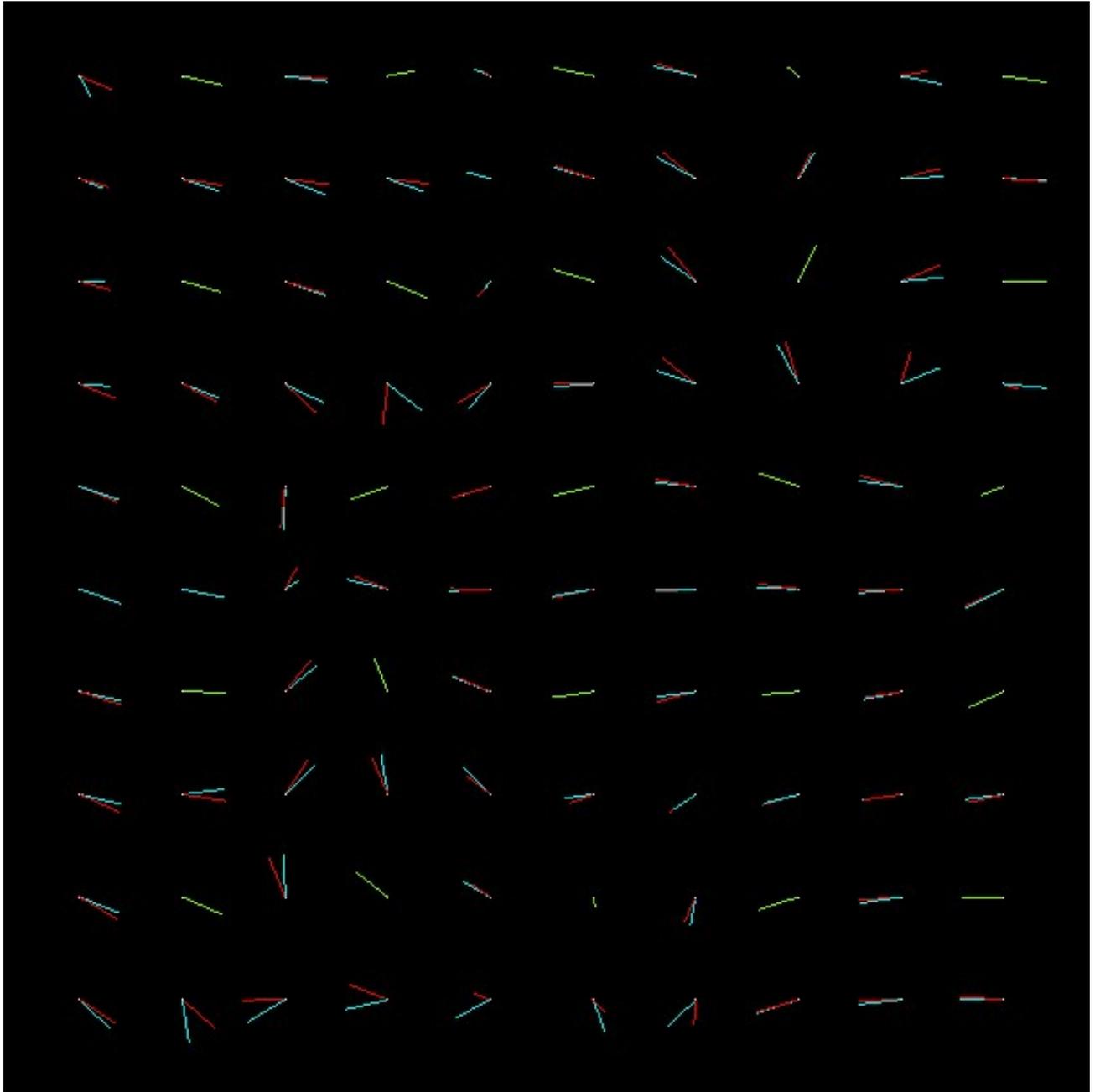


Figure 1b) Results of kriging with unit vector data subject to spatial isotropy; green arrows represent input data set selected form the simulated data shown in Fig. 1a, blue arrows represent the true (simulated) directions at test sites, red arrows represent the estimated directions.

- the estimator simplifies to

$$\hat{U}_i(x_0) = \sum_k^n \lambda_k U_i(x_k)$$

- the expectation is known and therefore simple kriging and the covariance function applies.
- the simplified covariance function

$$\tilde{C}(\mathbf{x}_i - \mathbf{x}_j) = \tilde{C}(\mathbf{x}_i, \mathbf{x}_j) = \text{trace Cov}(\mathbf{U}(\mathbf{x}_i), \mathbf{U}(\mathbf{x}_j))$$

is sufficient to determine the kriging weights λ .

- a simplified definition of the variogram which allows to use an ordinary real-valued variogram function can be used for this kind of geometrical vector kriging.

$$2\gamma(\mathbf{h}) = \text{E}[\|\mathbf{U}(\mathbf{x}) - \mathbf{U}(\mathbf{x} + \mathbf{h})\|^2] \in \mathbb{R}$$

It should be noted that it depends only on the vector difference $\mathbf{h} \in \mathbb{R}^p$ of the measurement locations.

- the kriging weights λ_k can actually be calculated according to the formulae of simple kriging

$$\lambda = \tilde{C}^{-1}c, \text{ with } c_i = \tilde{C}(\mathbf{x}_i - \mathbf{x}_0) \text{ and } \tilde{C}_{ij} = \tilde{C}(\mathbf{x}_i - \mathbf{x}_j)$$

At first sight it seems counter-intuitive that the estimator itself is not an object of the same kind as the data. However, in case of directions it can be shown that the length of the estimator is measure of the accuracy of the estimation which actually depends on the data. Moreover, the estimator satisfies a “strange” optimality criterion, e.g. for directions it reads

$$\tilde{\lambda} = \underset{\tilde{\mu}}{\text{argmax}} \text{E} \left[\|\hat{\mathbf{U}}(\mathbf{x}_0)\| \cos \left(\angle \left(\mathbf{U}(\mathbf{x}_0), \sum_i \tilde{\mu}_i \mathbf{U}(\mathbf{x}_i) \right) \right) \right]$$

Thus, the situation of “spherical” kriging is definitely different from real kriging.

The assumption of isotropy of measurements does not apply when the coordinate system of the geometric vectors is related to the coordinate system of the geographic locations. Then a phenomenon may be thought of as being isotropic with respect to simultaneous rotation (or reflection) of both coordinate systems.

Examples of this kind of isotropy are (i) water flow which changes its velocity more rapidly in the directions orthogonal to the downstream flow direction, since the water flowing has to go somewhere, or (ii)

Isotropy of the Process

All finite-dimensional marginal probability laws remain unchanged when the geometric vectors $\mathbf{U}(\mathbf{x}) \in \mathbb{R}^q$ and their geographic location vectors $\mathbf{x} \in \mathbb{R}^p$ are subject to a common rotation

$$P(\sigma\mathbf{U}(\sigma\mathbf{x}_1), \dots, \sigma\mathbf{U}(\sigma\mathbf{x}_n)) = P(\mathbf{U}(\mathbf{x}_1), \dots, \mathbf{U}(\mathbf{x}_n)), \quad \sigma \in O(p), \quad p = q \quad (3)$$

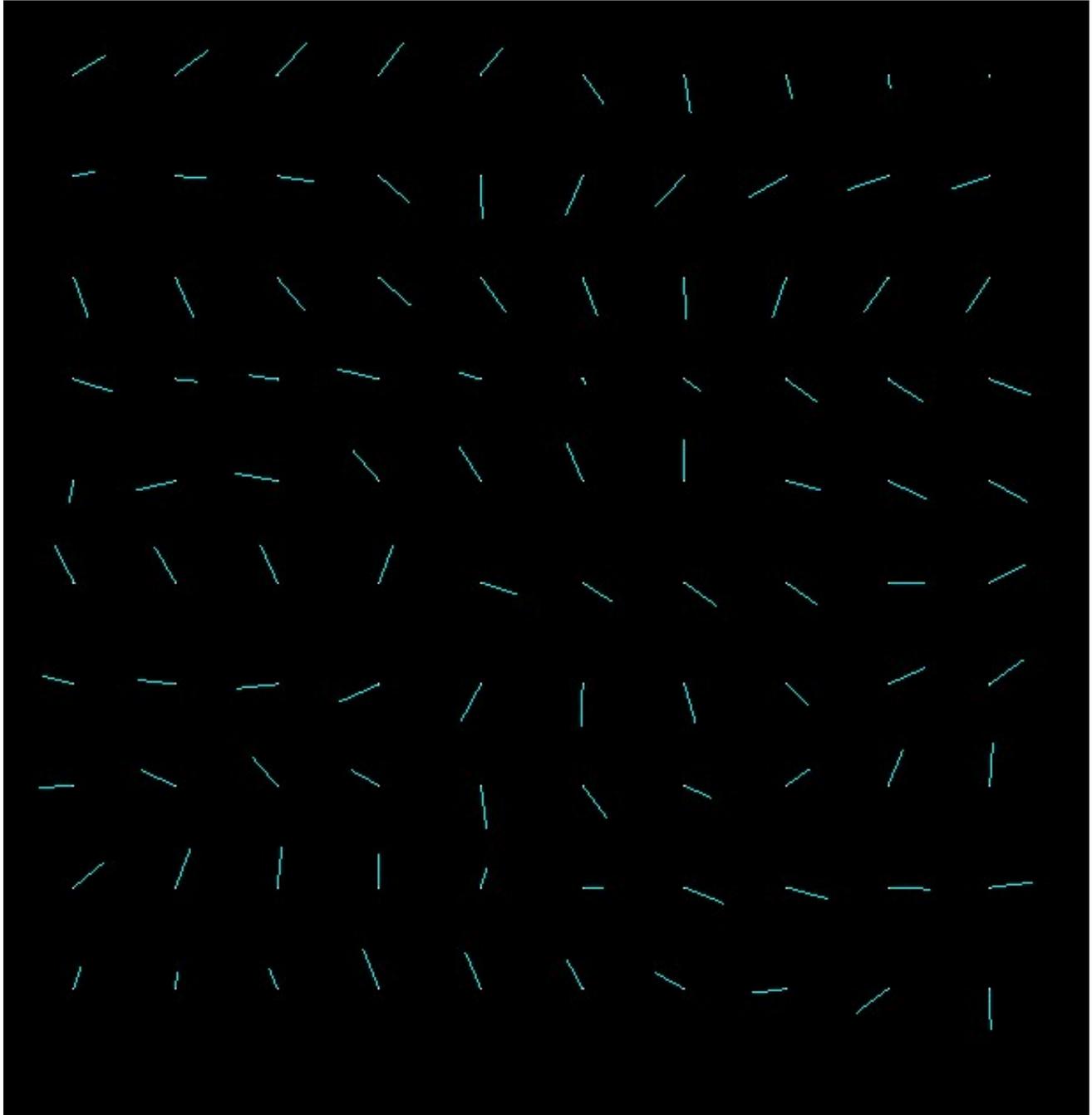


Figure 2a) The simulated data $\mathbf{U}(\mathbf{x}) \in \mathbb{R}^3$, $\mathbf{x} \in \mathbb{R}^2$ display isotropy of measurements without spatial isotropy: There is no preferred direction in the data, but the spatial correlation in West–East direction is more pronounced than in South–North direction.

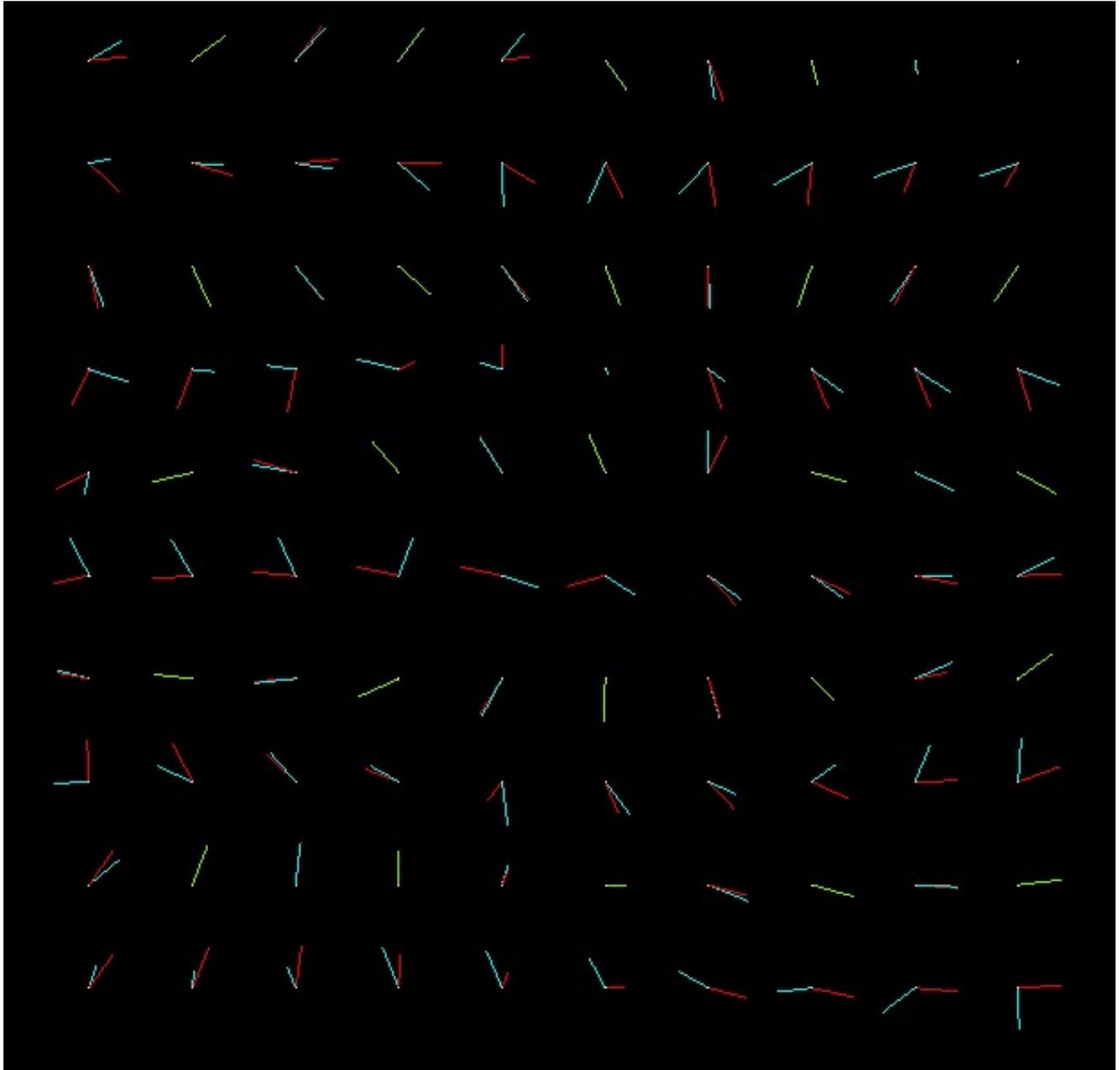


Figure 2b) Results of kriging with unit vector data subject to isotropy of measurements; green arrows represent input data set selected from the simulated data shown in Fig. 2a, blue arrows represent the true (simulated) directions at test sites, red arrows represent the estimated directions.

The assumption of process isotropy is adequate when geometric and geographic vectors are considered with respect to the same spatial coordinate systems, and when no spatial direction is physically preferred. Thus, it refers to physical isotropy when the directions are related to “geological space”. Indeed, the assumption of process isotropy seems to be the appropriate generalization of the usual kriging assumption of spatial isotropy to stochastic tensor fields.

More generally for tensors

$$\begin{aligned} & P(\sigma_{i_1}^{j_1} \dots \sigma_{i_r}^{j_r} U_{j_1 \dots j_r}(\sigma \mathbf{x}_1), \dots, \sigma_{i_1}^{j_1} \dots \sigma_{i_r}^{j_r} U_{j_1 \dots j_r}(\sigma \mathbf{x}_n)) \\ &= P(U_{i_1 \dots i_r}(\mathbf{x}_1), \dots, U_{i_1 \dots i_r}(\mathbf{x}_n)), \sigma \in O(p), p = q \end{aligned}$$

Isotropy of the process simplifies to the usual isotropy of space for scalar fields represented by a rank 0 tensor $U(\mathbf{x}) \in \mathbb{R}^1$.

The assumption of process isotropy leads to a simplification and constraint for the variogram

$$\sigma C(\sigma(\mathbf{x} - \mathbf{y}))\sigma^t = C(\mathbf{x} - \mathbf{y})$$

due to Equation (3)

Analysing this condition in greater detail reveals that if the function C is known for one direction $\mathbf{v} = (h \ 0 \ \dots 0)^t$, then it can be calculated for all other directions by virtue of Equation (.). Furthermore, for all σ which leave \mathbf{v} fixed it must hold

$$\sigma C \sigma^t = C$$

Thus, using transformations $\{\sigma \in O(p) \mid \sigma \mathbf{v} = \mathbf{v}\}$, it holds

$$C(\sigma(\mathbf{x} - \mathbf{y}))_{ij} = \begin{cases} 0 & , \text{ if } i \neq j, i, j > 1 \\ c_{22} & , \text{ for } i = j, i, j > 1 \\ c_{21} & , \text{ for } i = 1, j > 1 \text{ or } i > 1, j = 1 \\ c_{11} & , \text{ for } i = j = 1 \end{cases}$$

Thus C has the structure

$$C(h\mathbf{v}) = \begin{pmatrix} c_{11}(h) & c_{21}(h) & c_{21}(h) & \dots & c_{21}(h) \\ c_{21}(h) & c_{22}(h) & 0 & \dots & 0 \\ c_{21}(h) & 0 & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & 0 \\ c_{21}(h) & 0 & \dots & 0 & c_{22}(h) \end{pmatrix}, h \in \mathbb{R}$$

Eventually, only three functions of distance are required to represent the covariance structure sufficiently well. Analogous results hold for the variogram.

Isotropy of Space and Measurements

Combining any two of these three types of isotropy assumptions (isotropy of space, isotropy of measurements, isotropy of the process) leads to independent isotropy of space and measurements

$$P(\tau \mathbf{U}(\sigma \mathbf{x}_1), \dots, \tau \mathbf{U}(\sigma \mathbf{x}_n)) = P(\mathbf{U}(\mathbf{x}_1), \dots, \mathbf{U}(\mathbf{x}_n)), \sigma \in O(p), \tau \in O(q) \quad (4)$$

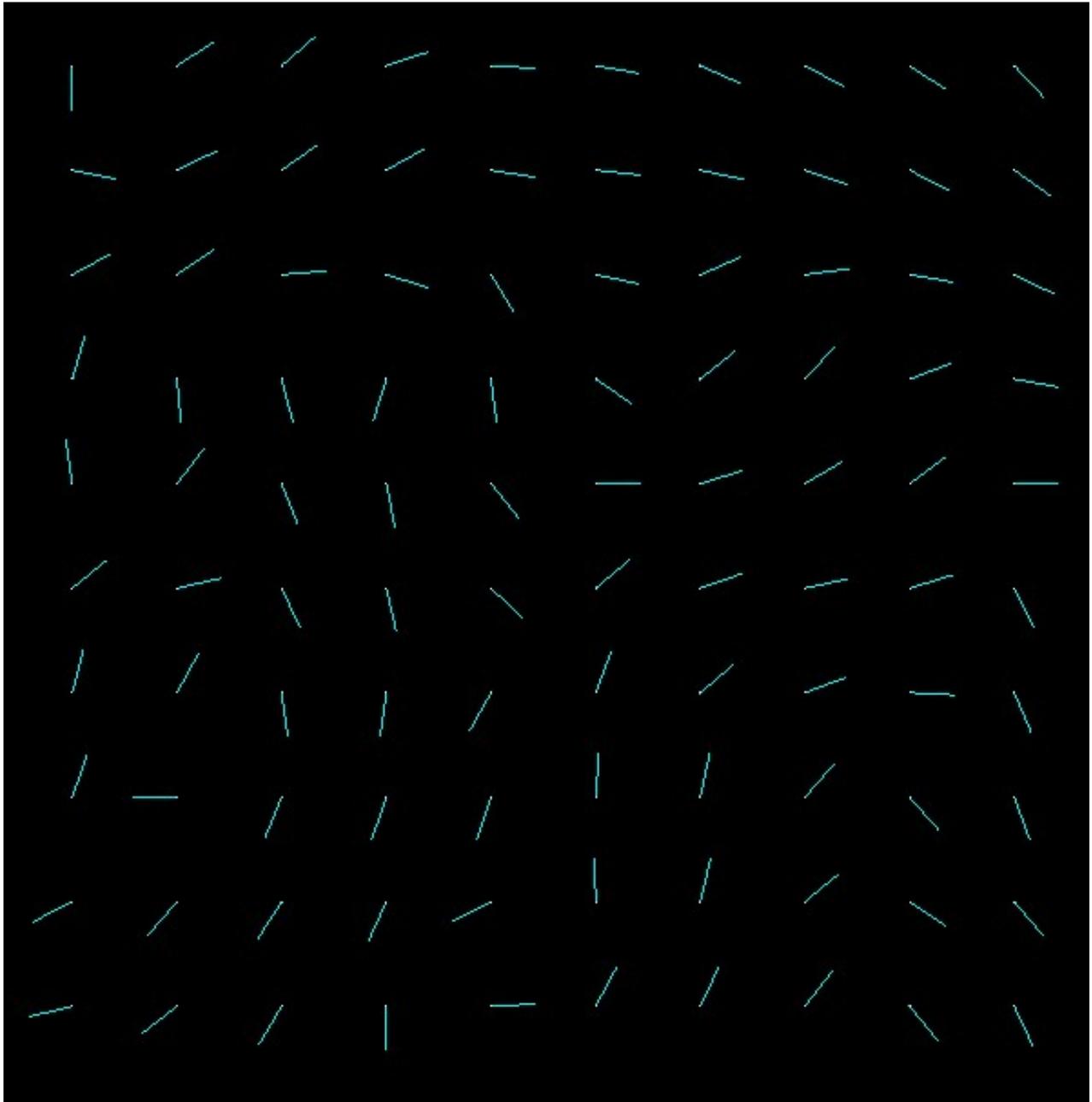


Figure 3a) The simulated data $\mathbf{U}(\mathbf{x}) \in \mathbb{R}^3$, $\mathbf{x} \in \mathbb{R}^2$ display an instance of process isotropy without either isotropy of space nor of measurements. It is hard to detect visually, there does not seem to exist any preferred direction neither in the data nor in the spatial correlation. Yet, there seem to be indications that some contiguous directions may be connected to form smooth curves.

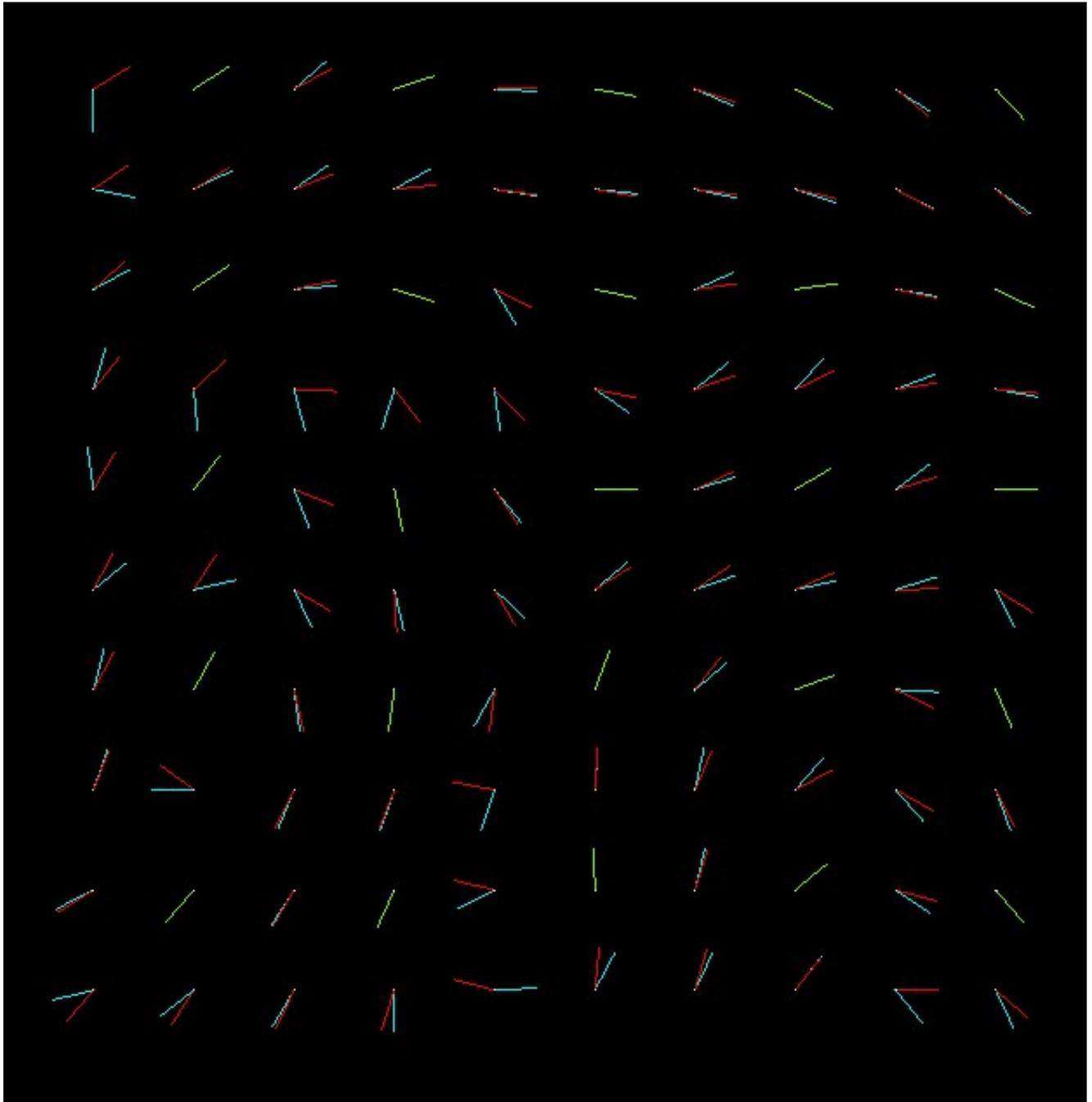


Figure 3b) Results of kriging with unit vector data subject to isotropy of the process; green arrows represent input data set selected from the simulated data shown in Fig. 3a, blue arrows represent the true (simulated) directions at test sites, red arrows represent the estimated directions.

It results in the most extensive simplification, i.e. to ordinary real-valued and isotropic covariance functions and variograms

$$\gamma(\|\mathbf{h}\|) = E[\|\mathbf{U}(\mathbf{x}) - \mathbf{U}(\mathbf{x} + \mathbf{h})\|^2] \in \mathbb{R}$$

Geographical Isotropy of the Process

In most real world applications of geostatistics in the geosciences there is indeed one physically distinguished direction: The downward direction with respect to the gravity field of the earth is clearly preferential for many geological processes.

Therefore, it seems reasonable to restrict isotropy assumptions concerning the stochastic process such that all finite-dimensional marginal probability laws are invariant with respect to rotations and reflections in the two dimensional geographic space orthogonal the “vertical” direction defined by gravity

$$P\left(\begin{pmatrix} \sigma & \\ & 1 \end{pmatrix} \mathbf{U}(\sigma \mathbf{x}_1), \dots, \begin{pmatrix} \sigma & \\ & 1 \end{pmatrix} \mathbf{U}(\sigma \mathbf{x}_n)\right) = P(\mathbf{U}(\mathbf{x}_1), \dots, \mathbf{U}(\mathbf{x}_n)), \quad (5)$$

$$\sigma \in O(p), \quad p = 2, q = 3$$

The assumption of geographical isotropy of the process imposes specific constraints on the variogram

$$\gamma(\mathbf{x} - \mathbf{y}) = \begin{pmatrix} \sigma & \\ & 1 \end{pmatrix} \gamma(\sigma(\mathbf{x} - \mathbf{y})) \begin{pmatrix} \sigma^t & \\ & 1 \end{pmatrix}$$

Then only variograms in direction $\mathbf{v} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ are required

$$\gamma(\mathbf{h}) = \begin{pmatrix} \sigma & \\ & 1 \end{pmatrix} \gamma(\|\mathbf{h}\|\mathbf{v}) \begin{pmatrix} \sigma^t & \\ & 1 \end{pmatrix} = \begin{pmatrix} \sigma & \\ & 1 \end{pmatrix} \gamma_{\mathbf{v}}(\|\mathbf{h}\|) \begin{pmatrix} \sigma^t & \\ & 1 \end{pmatrix}$$

with $\sigma(\mathbf{x} - \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|\mathbf{v}$

$$\sigma = \frac{1}{\|\mathbf{h}\|} \begin{pmatrix} h_1 & -h_2 \\ h_2 & h_1 \end{pmatrix}$$

Unfortunately, geographical isotropy of the process being the most realistic assumption for most geo-phenomena, it actually does not lead to a great simplification but only to additional constraints.

Conclusions and Discussion

Any assumption of isotropy leads to different simplifications of the general cross-covariance function and the kriging procedure. Effectively, isotropy assumptions are used to replace the ordinary distance of two directional objects in an equivalent way by an appropriately defined angle.

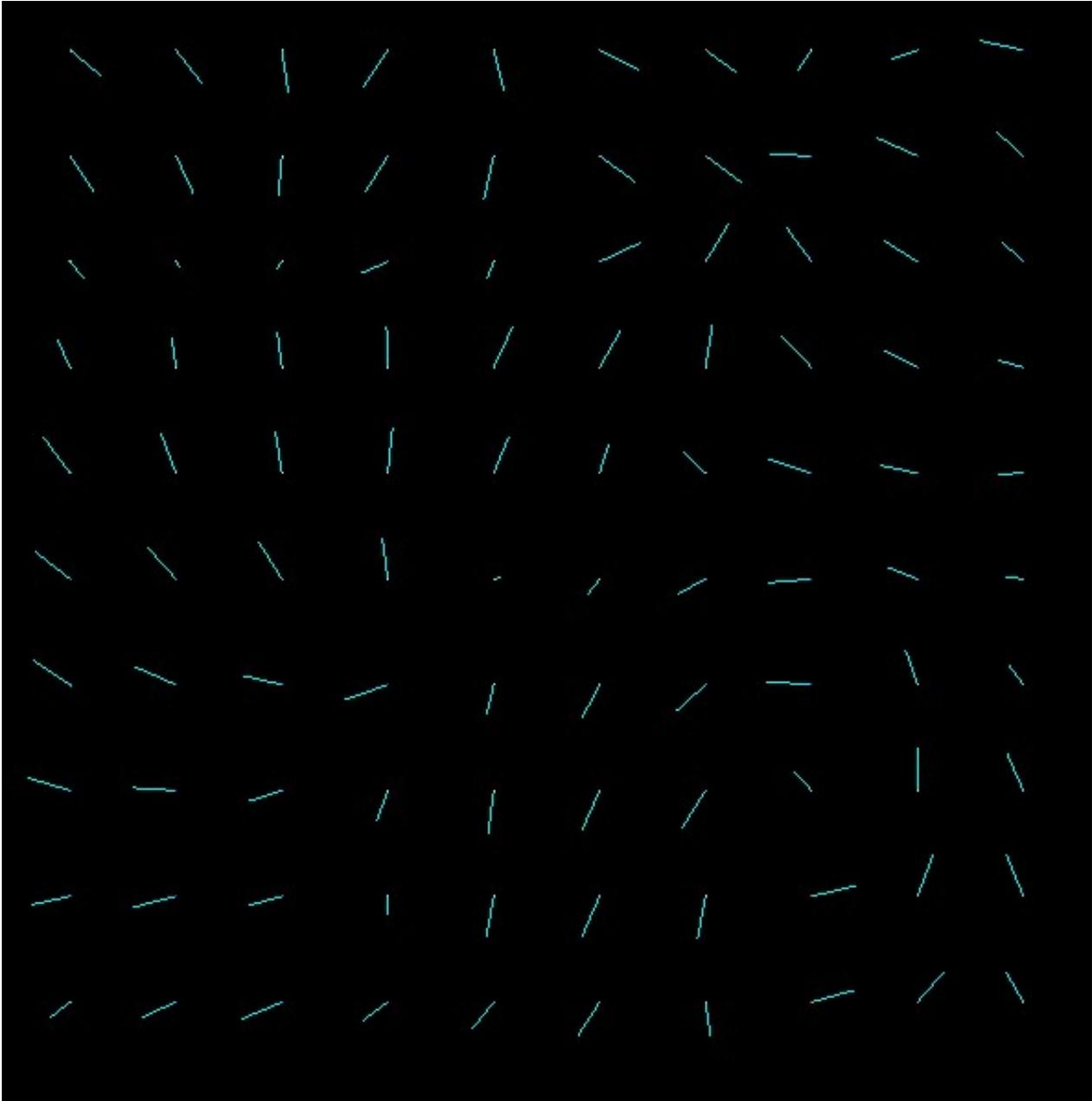


Figure 4a) The simulated data $\mathbf{U}(\mathbf{x}) \in \mathbb{R}^3$, $\mathbf{x} \in \mathbb{R}^2$ show full isotropy, i.e. isotropy of space and measurements. There is no preferred direction.

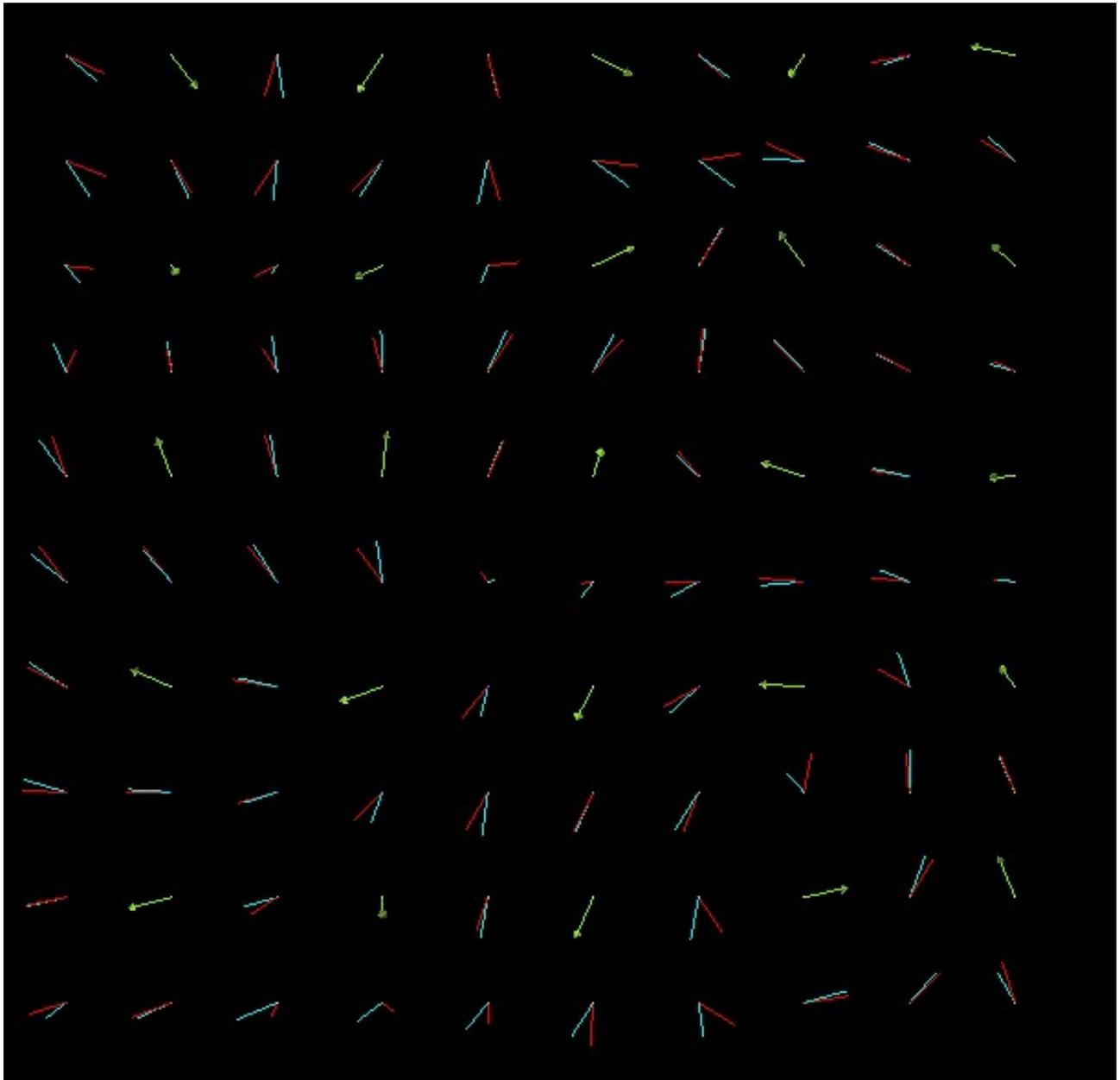


Figure 4b) Results of kriging with unit vector data subject to full isotropy; green arrows represent input data set selected from the simulated data shown in Fig. 4a, blue arrows represent the true (simulated) directions at test sites, red arrows represent the estimated directions.

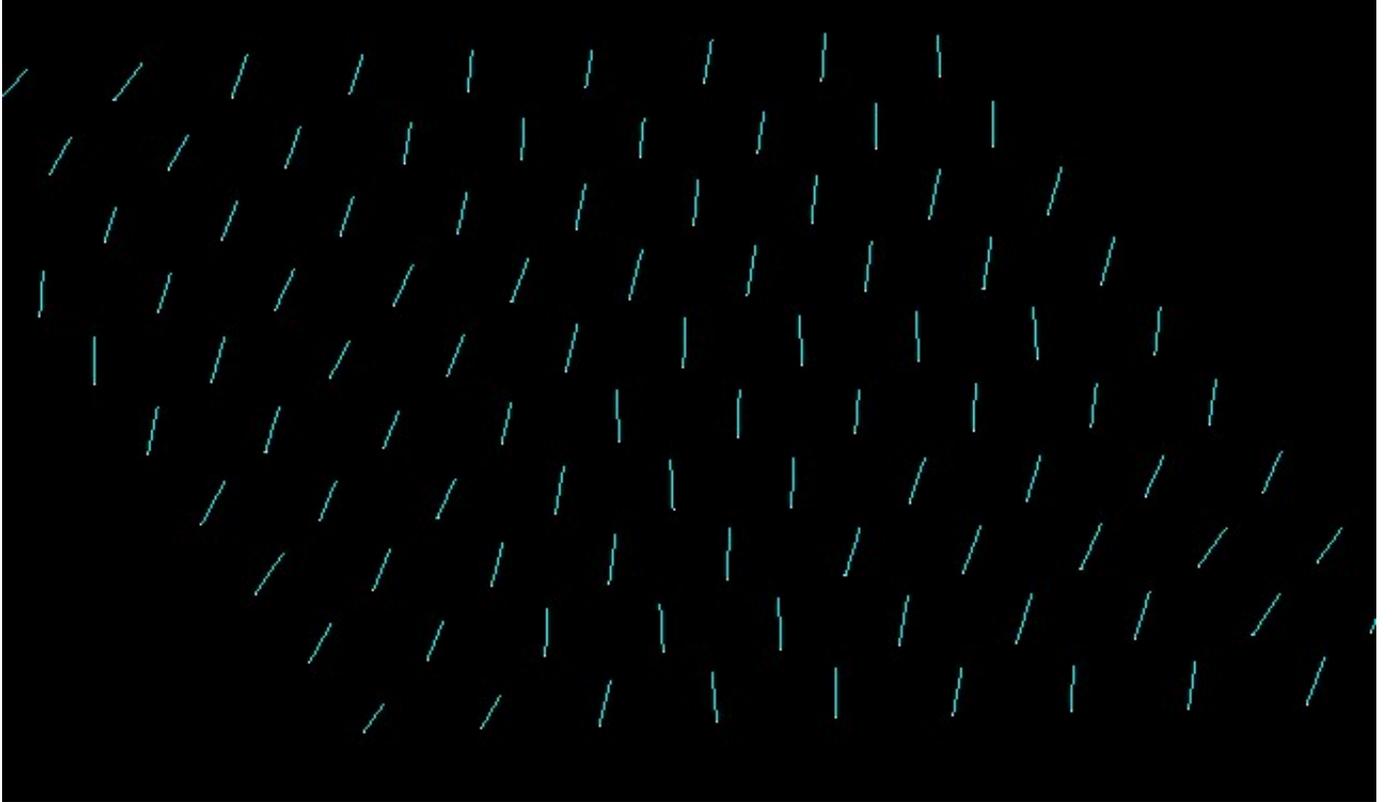


Figure 5a) Perspective view of the simulated data $\mathbf{U}(\mathbf{x}) \in \mathbb{R}^3$, $\mathbf{x} \in \mathbb{R}^3$ exhibit an instance of geographical process isotropy. The z -direction is clearly preferred, and the correlation in this direction is more pronounced than in the (x, y) -plane. The data restricted to the (x, y) do not show any preference, and their spatial correlation does not either.

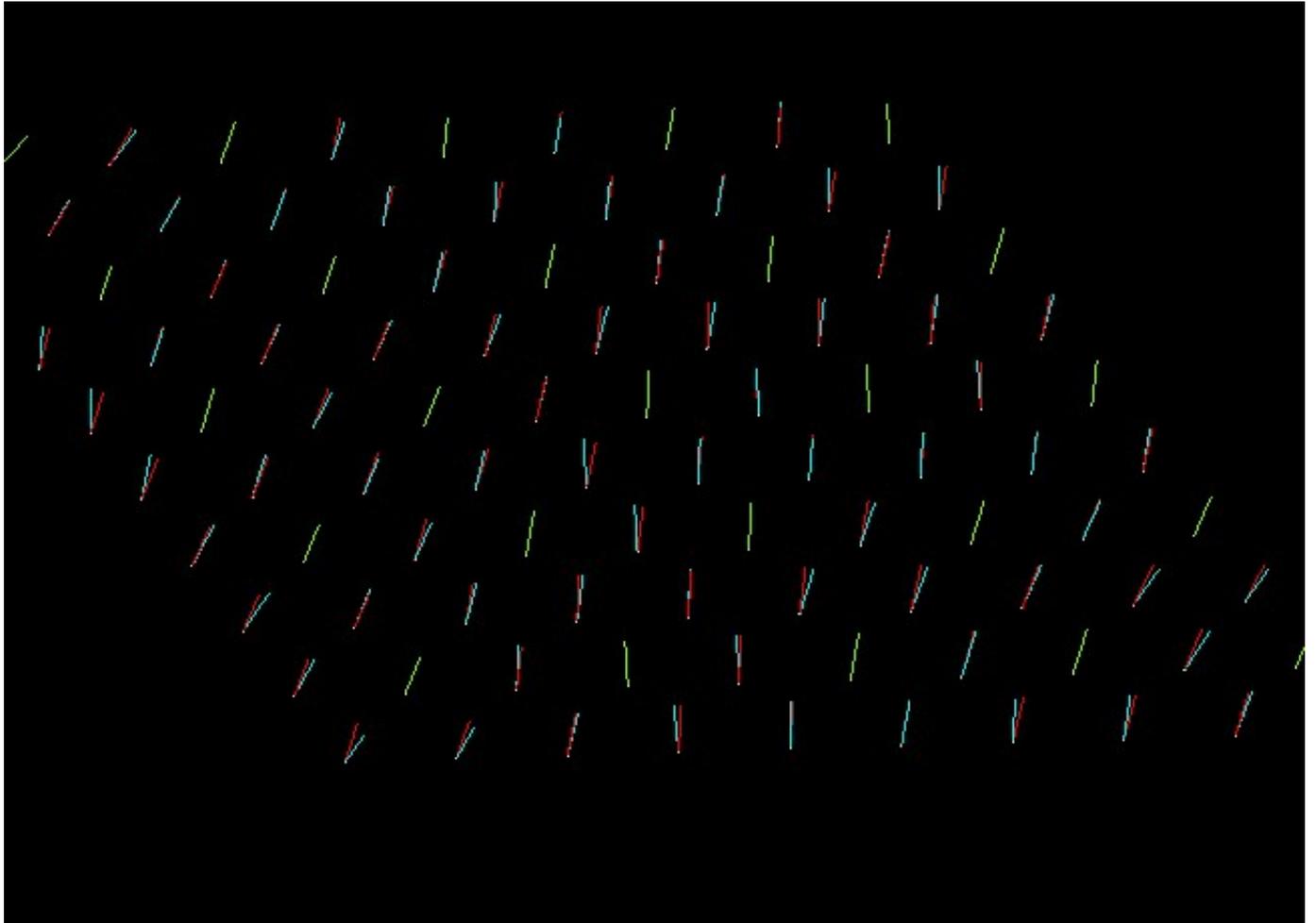


Figure 5b) Results of kriging with unit vector data subject to geographical isotropy of the process; green arrows represent input data set selected from the simulated data shown in Fig. 5a, blue arrows represent the true (simulated) directions at test sites, red arrows represent the estimated directions.

Viewing the isotropy assumptions from a pragmatic point of view, it can be stated that different types of isotropy assumptions impose just different constraints on the possible variograms and on the kriging weights. The constraints on the variogram exactly correspond to the constraints on the weights, in such a way that they guarantee that the optimal kriging weights have the specified form. In turn, the constraints on the weights reduce the linear combinations of the second order properties of the process to those which can be determined from the constrained variograms.

Thus, if too strong an assumption of isotropy is applied, then the class of linear predictors from which we want to determine the best predictor becomes too small and only the optimum within this restricted class can be found. The resulting predictor is typically not as good as the best one but it is still optimum within a smaller class. If too weak an assumption of isotropy is applied, then the estimated variogram should still represent the actual isotropy of the observed process up to a random estimation error of the variogram, i.e. the optimum kriging weights will be accomplished up to the estimation error in the variogram. Then, the estimation error of the variogram is the crucial problem of the method.

When the variogram can be estimated in a very stable way, then any isotropy assumptions are obsolete, as they will enter the analysis by themselves in the way they are present in the data. If the true isotropy is unknown, and the experimental variogram is supposed to be only a poor estimate of the true one, then the introduction of any likely isotropy assumption helps to stabilize the variogram estimation providing still reasonable predictors even when the process is not of the presumed type of isotropy.

Of course, the best results will be achieved if the correct type of isotropy is known and applied provided the estimation of the variogram is sufficiently stable.

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