

Multivariate localization

Benjamin Ménétrier

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1 Framework

1.1 State vector definition

The state vector $\mathbf{x} \in \mathbb{R}^n$ is split into Q concatenated sub-vectors \mathbf{x}_q (called “groups”), each one gathering P_q sub-vectors $\mathbf{x}_{p,q}$ of size n_q (called “variables”). Each sub-vector $\mathbf{x}_{p,q}$ corresponds to the data for a given physical variable (e.g. zonal wind, temperature, humidity, etc.). In a given group, all variables have the same size (n_q). Thus:

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_Q \end{pmatrix} \quad \text{and} \quad \mathbf{x}_q = \begin{pmatrix} \mathbf{x}_{1,q} \\ \vdots \\ \mathbf{x}_{P_q,q} \end{pmatrix} \quad (1)$$

As a consequence:

- The total number of variables is $P = \sum_{q=1}^Q P_q$.
- Each group \mathbf{x}_q has a size $P_q n_q$, so the full state vector size is $n = \sum_{q=1}^Q P_q n_q$.

The main idea behind this distribution of variables into groups is to apply the same localization to all variables within a given group.

1.2 Illustration setup

A simple example will be used as an illustration throughout this note. We define a vector \mathbf{x} with $Q = 3$ groups, where $P_1 = 3$, $P_2 = 1$ and $P_3 = 2$:

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_{1,1} \\ \mathbf{x}_{2,1} \\ \mathbf{x}_{3,1} \\ \mathbf{x}_{1,2} \\ \mathbf{x}_{1,3} \\ \mathbf{x}_{2,3} \end{pmatrix} \begin{matrix} \left. \vphantom{\begin{matrix} \mathbf{x}_{1,1} \\ \mathbf{x}_{2,1} \\ \mathbf{x}_{3,1} \end{matrix}} \right\} \mathbf{x}_1 \text{ (1st group of variables)} \\ \left. \vphantom{\begin{matrix} \mathbf{x}_{1,2} \end{matrix}} \right\} \mathbf{x}_2 \text{ (2nd group of variables)} \\ \left. \vphantom{\begin{matrix} \mathbf{x}_{1,3} \\ \mathbf{x}_{2,3} \end{matrix}} \right\} \mathbf{x}_3 \text{ (3rd group of variables)} \end{matrix} \quad (2)$$

1.3 Localization square-root

The localization matrix $\mathbf{L} \in \mathbb{R}^{n \times n}$ is applied to \mathbf{x} . The main issue is to design a positive semi-definite \mathbf{L} matrix, and the simplest solution is to build it as:

$$\mathbf{L} = \mathbf{U}\mathbf{U}^T \quad (3)$$

where $\mathbf{U} \in \mathbb{R}^{n \times m}$ is called a “square-root” of the localization matrix \mathbf{L} . The control vector $\mathbf{v} \in \mathbb{R}^m$ is such that:

$$\mathbf{x} = \mathbf{U}\mathbf{v} \quad (4)$$

We can define a square-root component $\mathbf{U}_q \in \mathbb{R}^{n_q \times m_q}$ for each group.

2 Possible implementations

2.1 Univariate localization

For the case where there is no cross-localization between variables, the square-root \mathbf{U} can be defined as:

$$\mathbf{U} = \left(\begin{array}{ccc|c|cc} \mathbf{U}_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{U}_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{U}_1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & \mathbf{U}_2 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \mathbf{U}_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{U}_3 \end{array} \right) \quad (5)$$

Thus:

$$\mathbf{L} = \left(\begin{array}{ccc|c|cc} \mathbf{U}_1 \mathbf{U}_1^T & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{U}_1 \mathbf{U}_1^T & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{U}_1 \mathbf{U}_1^T & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & \mathbf{U}_2 \mathbf{U}_2^T & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \mathbf{U}_3 \mathbf{U}_3^T & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{U}_3 \mathbf{U}_3^T \end{array} \right) \quad (6)$$

In this case, the total control vector size is $m = \sum_{q=1}^Q P_q m_q$

2.2 Duplicated localization

It is possible to define the cross-localization between the variables of a same group as duplicates of the diagonal localization, by defining \mathbf{U} as:

$$\begin{aligned} \mathbf{U} &= \left(\begin{array}{c|c|c} \mathbf{U}_1 & 0 & 0 \\ \mathbf{U}_1 & 0 & 0 \\ \mathbf{U}_1 & 0 & 0 \\ \hline 0 & \mathbf{U}_2 & 0 \\ \hline 0 & 0 & \mathbf{U}_3 \\ 0 & 0 & \mathbf{U}_3 \end{array} \right) \\ &= \left(\begin{array}{c|c|c} \mathbf{I}_1 & 0 & 0 \\ \mathbf{I}_1 & 0 & 0 \\ \mathbf{I}_1 & 0 & 0 \\ \hline 0 & \mathbf{I}_2 & 0 \\ \hline 0 & 0 & \mathbf{I}_3 \\ 0 & 0 & \mathbf{I}_3 \end{array} \right) \left(\begin{array}{c|c|c} \mathbf{U}_1 & 0 & 0 \\ \hline 0 & \mathbf{U}_2 & 0 \\ \hline 0 & 0 & \mathbf{U}_3 \end{array} \right) \end{aligned} \quad (7)$$

where $\mathbf{I}_q \in \mathbf{R}^{n_q, n_q}$ is the identity matrix of size n_q . Thus:

$$\mathbf{L} = \left(\begin{array}{ccc|c|cc} \mathbf{U}_1 \mathbf{U}_1^T & \mathbf{U}_1 \mathbf{U}_1^T & \mathbf{U}_1 \mathbf{U}_1^T & 0 & 0 & 0 \\ \mathbf{U}_1 \mathbf{U}_1^T & \mathbf{U}_1 \mathbf{U}_1^T & \mathbf{U}_1 \mathbf{U}_1^T & 0 & 0 & 0 \\ \mathbf{U}_1 \mathbf{U}_1^T & \mathbf{U}_1 \mathbf{U}_1^T & \mathbf{U}_1 \mathbf{U}_1^T & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & \mathbf{U}_2 \mathbf{U}_2^T & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \mathbf{U}_3 \mathbf{U}_3^T & \mathbf{U}_3 \mathbf{U}_3^T \\ 0 & 0 & 0 & 0 & \mathbf{U}_3 \mathbf{U}_3^T & \mathbf{U}_3 \mathbf{U}_3^T \end{array} \right) \quad (8)$$

In this case, the total control vector size is $m = \sum_{q=1}^Q m_q$

2.3 Duplicated and weighted localization

A variant of the previous case uses group-specific lower triangular matrices $\mathbf{S}^q \in \mathbb{R}^{P_q \times P_q}$ to define \mathbf{U} as:

$$\begin{aligned} \mathbf{U} &= \left(\begin{array}{ccc|ccc} S_{1,1}^1 \mathbf{U}_1 & 0 & 0 & 0 & 0 & 0 \\ S_{2,1}^1 \mathbf{U}_1 & S_{2,2}^1 \mathbf{U}_1 & 0 & 0 & 0 & 0 \\ S_{3,1}^1 \mathbf{U}_1 & S_{3,2}^1 \mathbf{U}_1 & S_{3,3}^1 \mathbf{U}_1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & S_{1,1}^2 \mathbf{U}_2 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & S_{1,1}^3 \mathbf{U}_3 & 0 \\ 0 & 0 & 0 & 0 & S_{2,1}^3 \mathbf{U}_3 & S_{2,2}^3 \mathbf{U}_3 \end{array} \right) \\ &= \left(\begin{array}{ccc|ccc} S_{1,1}^1 \mathbf{I}_1 & 0 & 0 & 0 & 0 & 0 \\ S_{2,1}^1 \mathbf{I}_1 & S_{2,2}^1 \mathbf{I}_1 & 0 & 0 & 0 & 0 \\ S_{3,1}^1 \mathbf{I}_1 & S_{3,2}^1 \mathbf{I}_1 & S_{3,3}^1 \mathbf{I}_1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & S_{1,1}^2 \mathbf{I}_2 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & S_{1,1}^3 \mathbf{I}_3 & 0 \\ 0 & 0 & 0 & 0 & S_{2,1}^3 \mathbf{I}_3 & S_{2,2}^3 \mathbf{I}_3 \end{array} \right) \left(\begin{array}{ccc|ccc} \mathbf{U}_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{U}_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{U}_1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & \mathbf{U}_2 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \mathbf{U}_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{U}_3 \end{array} \right) \quad (9) \end{aligned}$$

Thus:

$$\mathbf{L} = \left(\begin{array}{ccc|ccc} W_{1,1}^1 \mathbf{U}_1 \mathbf{U}_1^T & W_{1,2}^1 \mathbf{U}_1 \mathbf{U}_1^T & W_{1,3}^1 \mathbf{U}_1 \mathbf{U}_1^T & 0 & 0 & 0 \\ W_{2,1}^1 \mathbf{U}_1 \mathbf{U}_1^T & W_{2,2}^1 \mathbf{U}_1 \mathbf{U}_1^T & W_{2,3}^1 \mathbf{U}_1 \mathbf{U}_1^T & 0 & 0 & 0 \\ W_{3,1}^1 \mathbf{U}_1 \mathbf{U}_1^T & W_{3,2}^1 \mathbf{U}_1 \mathbf{U}_1^T & W_{3,3}^1 \mathbf{U}_1 \mathbf{U}_1^T & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & W_{1,1}^2 \mathbf{U}_2 \mathbf{U}_2^T & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & W_{1,1}^3 \mathbf{U}_3 \mathbf{U}_3^T & W_{1,2}^3 \mathbf{U}_3 \mathbf{U}_3^T \\ 0 & 0 & 0 & 0 & W_{2,1}^3 \mathbf{U}_3 \mathbf{U}_3^T & W_{2,2}^3 \mathbf{U}_3 \mathbf{U}_3^T \end{array} \right) \quad (10)$$

where $\mathbf{W}^q = \mathbf{S}^q \mathbf{S}^{qT}$ provides the weights applied to each covariance between variables within the group q . In practice, it is easier to set \mathbf{W}^q and to compute \mathbf{S}^q using a Cholesky decomposition. It also seems reasonable to set the diagonal elements of \mathbf{W}^q to one, even if it is not mandatory.

In this case, the total control vector size is $m = \sum_{q=1}^Q P_q m_q$

2.4 Multivariate localization

For the case where the cross-localization between variables is implicitly given as the product of square-roots, \mathbf{U} can be reduced to a column:

$$\begin{aligned} \mathbf{U} &= \begin{pmatrix} \mathbf{U}_1 \\ \mathbf{U}_1 \\ \mathbf{U}_1 \\ \hline \mathbf{U}_2 \\ \mathbf{U}_2 \\ \mathbf{U}_2 \\ \hline \mathbf{U}_3 \\ \mathbf{U}_3 \\ \mathbf{U}_3 \end{pmatrix} \\ &= \left(\begin{array}{c|c|c} \mathbf{I}_1 & 0 & 0 \\ \mathbf{I}_1 & 0 & 0 \\ \mathbf{I}_1 & 0 & 0 \\ \hline 0 & \mathbf{I}_2 & 0 \\ 0 & 0 & \mathbf{I}_3 \\ 0 & 0 & \mathbf{I}_3 \end{array} \right) \begin{pmatrix} \mathbf{U}_1 \\ \mathbf{U}_2 \\ \mathbf{U}_3 \end{pmatrix} \end{aligned} \quad (11)$$

An additional assumption is required here: the size of the group sub-vectors must be the same for all groups, i.e. $m_1 = \dots = m_Q = \bar{m}$. Thus:

$$\mathbf{L} = \left(\begin{array}{c|c|c|c|c|c} \mathbf{U}_1 \mathbf{U}_1^T & \mathbf{U}_1 \mathbf{U}_1^T & \mathbf{U}_1 \mathbf{U}_1^T & \mathbf{U}_1 \mathbf{U}_2^T & \mathbf{U}_1 \mathbf{U}_3^T & \mathbf{U}_1 \mathbf{U}_3^T \\ \mathbf{U}_1 \mathbf{U}_1^T & \mathbf{U}_1 \mathbf{U}_1^T & \mathbf{U}_1 \mathbf{U}_1^T & \mathbf{U}_1 \mathbf{U}_2^T & \mathbf{U}_1 \mathbf{U}_3^T & \mathbf{U}_1 \mathbf{U}_3^T \\ \mathbf{U}_1 \mathbf{U}_1^T & \mathbf{U}_1 \mathbf{U}_1^T & \mathbf{U}_1 \mathbf{U}_1^T & \mathbf{U}_1 \mathbf{U}_2^T & \mathbf{U}_1 \mathbf{U}_3^T & \mathbf{U}_1 \mathbf{U}_3^T \\ \hline \mathbf{U}_2 \mathbf{U}_1^T & \mathbf{U}_2 \mathbf{U}_1^T & \mathbf{U}_2 \mathbf{U}_1^T & \mathbf{U}_2 \mathbf{U}_2^T & \mathbf{U}_2 \mathbf{U}_3^T & \mathbf{U}_2 \mathbf{U}_3^T \\ \mathbf{U}_3 \mathbf{U}_1^T & \mathbf{U}_3 \mathbf{U}_1^T & \mathbf{U}_3 \mathbf{U}_1^T & \mathbf{U}_3 \mathbf{U}_2^T & \mathbf{U}_3 \mathbf{U}_3^T & \mathbf{U}_3 \mathbf{U}_3^T \\ \mathbf{U}_3 \mathbf{U}_1^T & \mathbf{U}_3 \mathbf{U}_1^T & \mathbf{U}_3 \mathbf{U}_1^T & \mathbf{U}_3 \mathbf{U}_2^T & \mathbf{U}_3 \mathbf{U}_3^T & \mathbf{U}_3 \mathbf{U}_3^T \end{array} \right) \quad (12)$$

In this case, the total control vector size is $m = \bar{m}$.

The amplitude of cross-localization is not one in this case. For $1 \leq q, q' \leq Q$, we denote \mathbf{u} the k^{th} column of \mathbf{U}_q and \mathbf{u}' the k^{th} column of $\mathbf{U}_{q'}$. The k^{th} diagonal coefficient of $\mathbf{U}_q \mathbf{U}_{q'}^T$ is given by $\langle \mathbf{u}, \mathbf{u}' \rangle$, where $\langle \cdot, \cdot \rangle$ denotes the canonical inner product. The Cauchy-Schwartz inequality requires that:

$$|\langle \mathbf{u}, \mathbf{u}' \rangle| \leq \sqrt{\langle \mathbf{u}, \mathbf{u} \rangle \langle \mathbf{u}', \mathbf{u}' \rangle} \quad (13)$$

Thus, the cross-localization amplitude between groups q and q' is necessarily smaller than the geometric mean of the auto-localization amplitudes for groups q and q' . Besides, the more the vectors \mathbf{u} and \mathbf{u}' have different shapes, the smaller their inner product and the smaller the cross-localization amplitude.

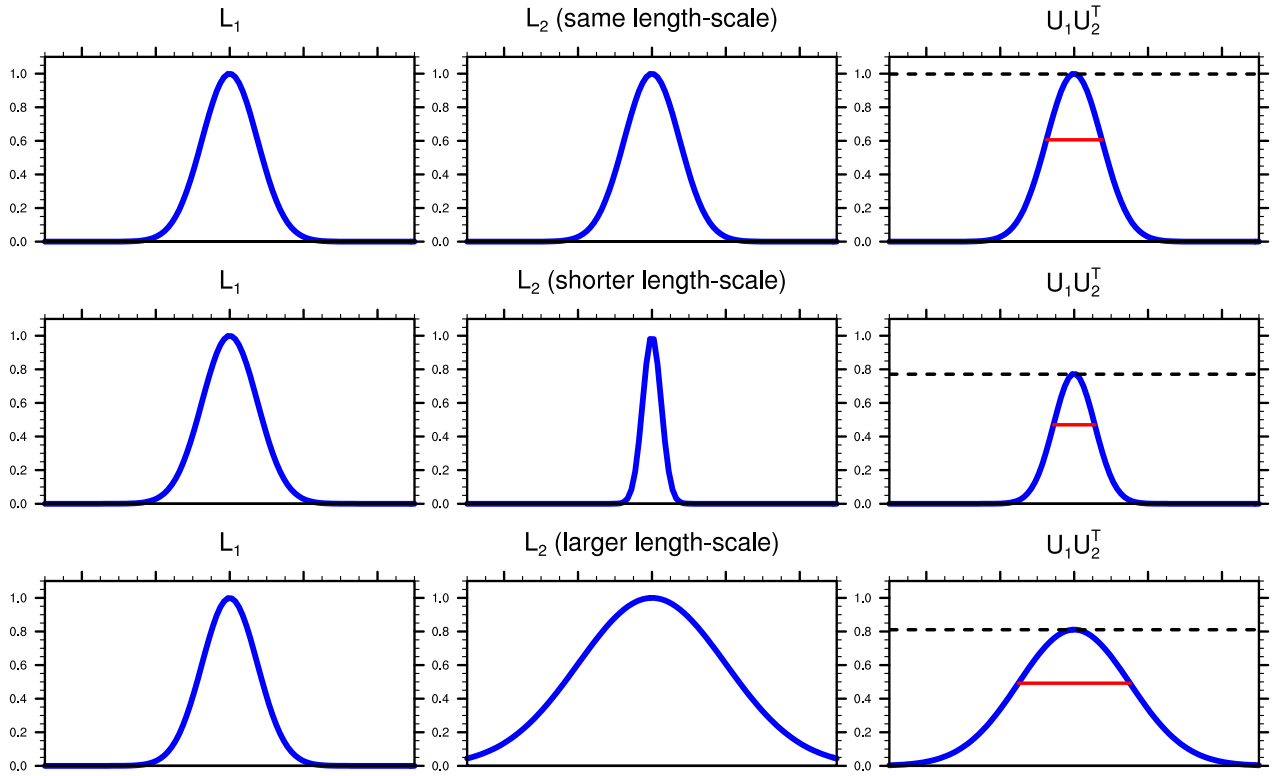


Figure 1: 1D illustration of the product of two localization square-root, with Gaussian localization functions. The dashed black line shows the function amplitude, while the solid red line shows the function length-scale.