Detecting changes in essential ecosystem and biodiversity properties - towards a Biosphere Atmosphere Change Index: BACI

Deliverable 5.3: Algorithms for Interactive User Feedback for Model Analysis and Improvement

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Contents

Summary

This deliverable is dedicated to the work done within the *WP5 - Synthetic Index and Attribution Scheme: the BACIndex*. WP5 is divided into 4 main tasks and this third report refers to the third one: *Task 5.3 - Incremental novelty detection, automatic dataset cleanup and going from novelty scores to direct detections*.

The focus of this third task of our WP was divided into two main objectives: on one hand we have developed an interactive software able to incorporate user feedback based on the Maximally Divergent Algorithm to detect anomalies and on the other hand we have been working on the improvement and novelty detection methods based on autoregressive models developed in Tasks 5.1 and 5.2 (see Deliverable 5.1 and 5.2) by improving the cleanup pretreatment of the data and extending the methodology to direct detection of anomalies.

Each section of this deliverable corresponds to one of these two objectives:

1. **Implementation of the Maximally Divergent Intervals Method for Anomaly Detection. Software Prototype.** In this section, we present the software prototype developed to run an algorithm able to detect abnormal intervals within multivariate time series based on a Kullback-Leibler divergence criteria. This algorithm was developed during Task 5.1 and extended during Task 5.2. The algorithm was extended to be able to deal with spatio-temporal data. Although the software can handle non-spatial time series and also spatio-temporal data; for non-spatial, purely temporal time series, we have developed a graphical user interface (GUI). This GUI facilitates the implementation with any kind of data and allows for interactive expert feedback and threshold adaptation. The software together with the GUI are publicly available under https://cvjena.github.io/libmaxdiv/.

2. **Advances in the Multivariate Autoregressive Models for Novelty Detection. First Version of the BACIndex.** In this section, we present the improvements and extensions for our methodology to detect extreme events in biosphere data based on autoregressive models developed during previous tasks. In terms of dataset cleanup we have improved our pretreatment step in the methodology by introducing a regionalization scheme and automatic selection of the autoregressive models to be applied at each location and variable. Additionally, at the event detection step of our methodology we have developed a spatio-temporal classification method of the novelty score (Mahalanobis distance in our method) that allows direct detection of the spatial and temporal extent of anomalies. By using the spatial and temporal regularity in neighboring locations, the method classifies the novelty score into three classes, intense anomaly, possible anomaly, and normal. Making the detection of the spatial and temporal extent of the anomalies straightforward.

1 Implementation of the Maximally Divergent Intervals Method for Anomaly Detection. Software Prototype.

While in the first task of this Work Package we developed the MDI algorithm, whose early prototype was described in details in Deliverable 5.1. Since the beginning, this method presented promising results but also suffered from some disadvantages. These shortcomings were successfully addressed during Task 5.2 and presented in Deliverable 5.2.

In this deliverable we present two final implementations done to the model. Initially, we have extended the MDI to be able to deal with spatio-temporal data. Additionally we also present a graphical user interface (GUI) for non-spatial time series that facilitates the experimentation with any kind of data. This interface allows for interactive experiments, anomaly thresholds testing and comparison between different approaches.

The software with the MDI algorithm, together with the graphical user interface and a user guide has been released and are publicly available.

The current status of the Maximally Divergent Intervals method for Anomaly Detection was selected to be presented within the Student Posters Competition organized within the MTS/IEEE OCEANS-17 Conference last June 2017 in Aberdeen, UK, [1].

1.1 Improvements and Extensions to the MDI Algorithm. Spatial Extension.

The extension of our MDI algorithm to spatio-temporal data is straightforward: Imagine the data as a hypercube $X_{t,x,y,z,d}$ with 5 axes: time, x, y, z and attribute. Instead of considering intervals of time only, we consider sub-blocks along the first four axes and compare the distribution of the data within a given sub-block with the distribution outside of the block using the KL divergence.

The approach of cumulative sums (for more detailed information please see Deliverable 5.2) can be generalized as well. The extraction of the sum over a sub-block from a fourth-order tensor of cumulative sums $C_{t,x,y,z}$ follows the inclusion-exclusion principle and requires $2^4 = 16$ additions/subtractions:

$$\sum_{t=t_0}^{t_1} \sum_{x=x_0}^{x_1} \sum_{y=y_0}^{y_1} \sum_{z=z_0}^{z_1} X_{t,x,y,z} = \sum\nolimits_{(i,j,k,l)\in\{0,1\}^4} \left((-1)^{i+j+k+l} \cdot C_{t_i,x_j,y_k,z_l}\right) \tag{1}$$

In analogy to the Time-Delay Embedding implemented in Deliverable 5.2 for purely temporal time series, one might want to apply Spatial-Neighbour Embedding by augmenting the feature vector of each sample with the feature vectors of contiguous spatial locations. In combination with Time-Delay Embedding this usually leads to an explosion of dimensionality and becomes intractable quickly for data with many attributes.

Fortunately, this embedding is only necessary if one wants to detect spatial anomalies, but not if one is just interested in the spatial location of temporal anomalies.

Experiments on the Spatio-Temporal Anomaly Detection We have used Sea Level Pressure data from the NCEP-NCAR database [6] for the evaluation of our algorithm in the face of spatio-temporal data. It covers a larger area over the North Atlantic Sea, giving the Sea Level Pressure during 55 years from 1957 to 2011 at 476 spatial locations between 25° N, 52.5° W and 65° N, 15° E with a spatial resolution of 2.5° and a daily temporal resolution. Regarding the time dimension, we apply Time-Delay Embedding with $k = 3, T = 1$ and search for intervals of size between 3 and 10 days. Concerning space, we do not apply any embedding here and set a minimum size of $7.5° \times 7,5°$, but no maximum. We retrieve the top 20 detections with the unbiased Gaussian method and compared to a list of 89 historic storms compiled from several sources. Comparing our top 20 detections with the list of historic storms, we were able to match 7 of them.

A visual inspection of the results shows that our algorithm is not only capable of detecting occurrences of anomalous low-pressure fields over time, but also their spatial location. This can be seen in Figure 1, which shows the start, the middle and the end of the top 5 detections.

It is not necessary to apply Spatial-Neighbour embedding in this scenario, since we are not interested in spatial outliers, but only in the location of temporal outliers. If we do apply Spatial-Neighbour Embedding, some high-pressure fields surrounded by low-pressure fields are detected as well.

1.2 Software Prototype and Graphical User Interface

In order to make our algorithm available to a broad public, we have released the software. The software allows the detection of abnormal intervals in multivariate time series based on a divergence criteria.

Together with the release of the software we have also developed a Graphical User Interface (see Figure 2) and a user guide. Although the software support spatio-temporal data, the graphical interface support only non-spatial data, purely time series, and provides the user an immediate visualization of the intervals detected by the algorithm. The score of the detection is reflected by the intensity of the colour in the interactive figure, which can be zoomed, panned and exported. The raw list of detections may be exported as well. This ease of usage facilitates experimenting with different parameter combinations in order to achieve the best results for the respective application.

The software (libmaxdiv), together with the graphical user interface and a user guide was released around the beginning of 2017. All the documentation regarding the library and its installation can be found in https://cvjena.github.io/libmaxdiv/.

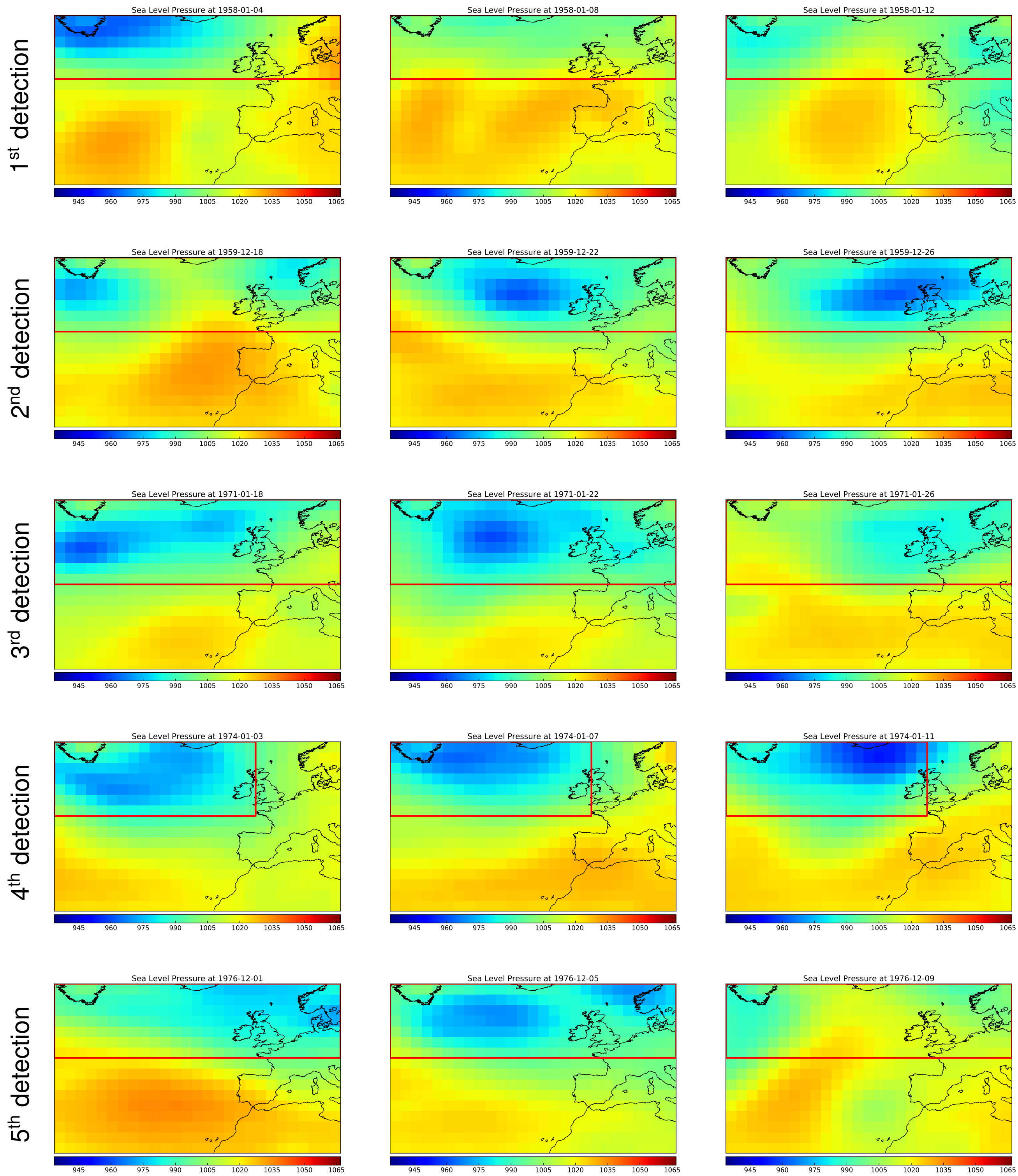


Figure 1: Sea Level Pressure during the start, the middle and the end of the top 5 detections on the SLP dataset. The red frame spans the region detected by the algorithm.

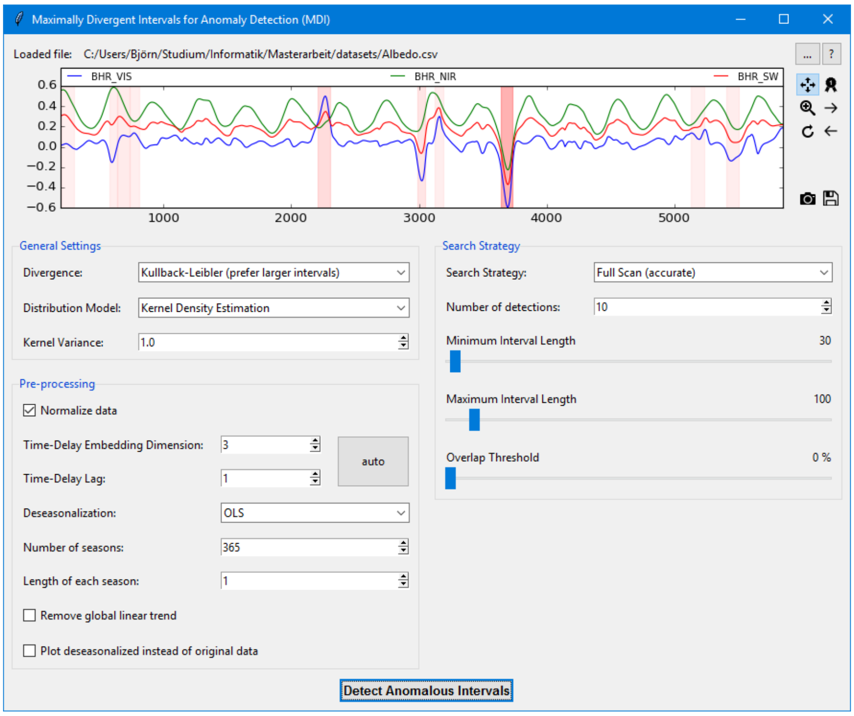


Figure 2: Screenshot of the MDI GUI.

1.3 Conclusions

In this section we have presented the advances developed for the Maximally Divergent Intervals algorithm together with the release of its software prototype. There have been two main implementations in this method:

- The MDI algorithm has been extended to be able to deal with spatio-temporal data. This extension has been done by considering sub-blocks along the 3 spatial axis and the temporal one and comparing them with the distribution outside the block.
- Additionally it has been developed a graphical user interface (GUI) for non-spatial time series. This GUI will help the experimentation and ease the use of the algorithm. Threshold testing and interactive experiments comparing the different approaches is now available for the user.
- The software with the MDI algorithm, together with a graphical user interface and a user guide has been released and are publicly available.

2 Advances in the Multivariate Autoregressive Models for Novelty Detection. First Version of the BACIndex.

The first version of our methodology on *Multivariate Novelty Detection with Autoregressive Models* was described in Deliverable 5.2. It yielded promising results, but still suffered from some major shortcomings:

- A similar order of autoregressive model (ARMA(p, q)) was assumed for all the variables involved. In Deliverable 5.2 it was assumed an ARMA(3,1), with $p = 3$ and $q = 1$ in the model:

$$X_t = \varepsilon_t + \sum_{i=1}^{p} \varphi_i X_{t-i} + \sum_{i=1}^{q} \theta_i \varepsilon_{t-i} \tag{2}$$

  where $\varphi_1, ..., \varphi_p$ and $\theta_1, ..., \theta_q$ are parameters of the model and ε_t is assumed to be white noise.

- In the global application presented in Deliverable 5.2, all the points of the grid were assumed to follow the same order of ARMA, independently of their spatial location. This was already pointed out as a weakness of the approach presented and could be the reason of a systematic overestimation of extremes seen in the northern latitudes.
- When detecting the abnormal events, two approaches were considered: extreme residual coexceedances and Mahalanobis distance. The use of coexceedances relies on a very simplistic assumption for the multivariate case. Therefore we have rejected this approach and followed with the use of the Mahalanobis distance.

We have tackled all those problems and implemented some improvements to the algorithm which will be described in the following sections. We have also tested these new implementations in the method on a new version of the Earth System Data Cube at the BACI area of interest, obtaining very promising results.

This work has been presented at the European Geosciences Union (EGU) General Assembly last April 2017 in Vienna [4] and has been accepted for presentation at the 3rd International Conference on Advances in Extreme Value Analysis and Application to Natural Hazards (EVAN) recently hosted in September by the University of Southampton, UK [5].

2.1 Improvements and Extensions to the Multivariate Novelty Detection with Autoregressive Models

In order to test the improvements and extensions developed, data from the Earth System Data Cube (ESCD) were used. From this database, 5 biosphere variables were selected:

- Gross Primary Productivity (GPP)

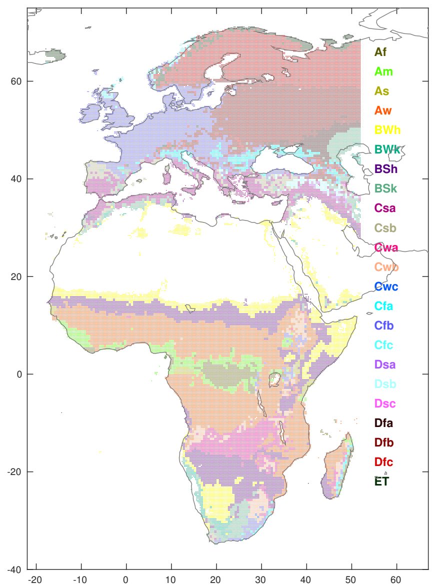
- Latent Energy (LE)
- Net Ecosystem Exchange (NEE)
- Sensible Heat (SH)
- Terrestrial Ecosystem Respiration (TER)

These variables have a temporal coverage of 11 years, from January 2001 to December 2012 with 8-daily observations and a spatial grid of 0.25° covering the main area selected for BACI, which comprises Europe and Africa (see Figure 3). This new version of the ESDC used has a higher spatial resolution of 0.25°. In Deliverable 5.2 an older version with 1° spatial resolution was used.

At each point of the grid, and for all the variables separately, the mean seasonal cycle was subtracted and the remaining variables were standarized ($\mu = 0$ and $\sigma = 1$).

2.1.1 Pre-treatment: Dataset Cleanup

Regionalization We have clustered the spatial grid into regions of similar climate conditions. This regionalization was done according to the climate types defined by the Köppen Climate Classification [3]. The Köppen Climate Classification is a widely used vegetation-based empirical clustering that divides the world in up to 31 climate regions. From these 31 climate regions, 23 of them are present in our area of application. In Figure 3 the 23 climate regions present in our area of study with the legend explaining the codes that define them are depicted.



1^{st} letter	2^{nd} letter	3^{rd} letter
A: Tropical	f: fully humid	h: hot arid
B: Dry	m: monsoon	k: cold arid
C: Mild temperate	s: dry summer	a: hot summer
D: Snow	w: dry winter	b: warm summer
E: Polar	W: dessert	c: cool summer
	S: steppe	d: cold summer
	T: tundra	
	F: frost	

Figure 3: BACI area of study clustered according to the Köppen Climate Classification.

ARMA Model Selection For each climate region it has been selected a representative point. At this point it has been fitted a univariate ARMA model for each of the 5 variables. To select the best coefficients (p, q), a Bayesian Criteria [8] was applied to all the possible combinations between (0,0) and (5,5). Table 1 shows the kind of model selected for each region and variable. Note that there are some variables where the ARMA model selected is (0,0), in those cases, the Bayesian Criteria tells us that is better to work directly with the variables themselves instead of working with an ARMA.

Table 1: ARMA parameters, (p, q), selected for each climate region and variable.

Region	**Variables**				
	GPP	LE	NEE	SH	TER
Af	[0,0]	[0,0]	[0,0]	[0,0]	[0,0]
Am	[1,0]	[0,0]	[1,0]	[0,0]	[1,0]
As	[1,0]	[0,0]	[1,0]	[0,0]	[0,1]
Aw	[1,0]	[2,2]	[1,0]	[0,0]	[1,0]
BWh	[1,1]	[1,1]	[1,1]	[1,0]	[2,0]
BWk	[1,1]	[1,1]	[1,1]	[1,0]	[0,0]
BSh	[1,0]	[0,0]	[1,0]	[0,0]	[0,0]
BSk	[1,0]	[1,0]	[1,0]	[0,0]	[1,1]
Csa	[1,1]	[1,0]	[1,1]	[1,0]	[1,0]
Csb	[0,0]	[0,0]	[0,0]	[0,0]	[0,0]
Cwa	[1,1]	[1,1]	[1,1]	[1,0]	[1,1]
Cwb	[1,0]	[1,1]	[0,0]	[1,0]	[1,1]
Cwc	[1,1]	[1,1]	[1,1]	[1,1]	[1,1]
Cfa	[0,0]	[3,2]	[0,0]	[0,0]	[0,0]
Cfb	[4,2]	[1,0]	[1,1]	[1,1]	[1,0]
Cfc	[0,3]	[1,0]	[4,0]	[1,0]	[1,0]
Dsa	[4,2]	[1,1]	[2,0]	[1,1]	[1,1]
Dsb	[1,0]	[1,0]	[1,0]	[1,0]	[1,0]
Dsc	[0,0]	[0,0]	[0,0]	[0,1]	[0,0]
Dfa	[1,1]	[1,1]	[1,1]	[1,1]	[1,1]
Dfb	[1,0]	[1,0]	[1,0]	[0,0]	[1,0]
Dfc	[1,0]	[0,1]	[1,0]	[1,0]	[0,1]
ET	[1,0]	[0,0]	[0,0]	[0,0]	[0,1]

Now we are ready to proceed with the entire spatial grid. For each point an ARMA (p_{ij}, q_{ij}) is fitted for each variable, where i refers to the climate region the point belongs to and j refers to the used variable.

2.1.2 Event Detection: from Novelty Scores to Direct Detections

In Deliverable 5.2, we proposed two main methods to detect the extreme events after the residuals (difference between the original data and the ARMA models' estimation) are calculated: Extreme Residual Coexceedances and Mahalanobis distance. Back then we already pointed out the limitations that the coexceedances method proposed, therefore we have continued using the Mahalanobis distance as a metric that allow us to detect extreme events. For more detailed explanation about this metric and its application to the residuals please refer to Deliverable 5.2.

Once we have the novelty scores, *i.e.* the Mahalanobis distance, estimated for all the points of the grid, arises the following question: how could we discern between normal and abnormal behavior of this metric? The first and easiest option is to fix a threshold and look for the events surpassing this threshold, but then we would have a secondary question: how do we fix that threshold? We have tried two options: on a first approach we have used a fixed threshold at a certain percentile of the Mahalanobis distance distribution and as a second and more complex approach we have also explored an automatic manner to define the abnormal events based on a Markov Random Field model.

Fixed Threshold As said, the easiest way to distinguish between normal and abnormal events is to set a threshold. To do so, we have set the threshold at the 97.5th percentile of the Mahalanobis distance distribution (all the Mahalanobis distance values along the entire region). This is a common percentile chosen in extreme value analysis. We have then looked for the events above this threshold, it means the highest 2.5$\%$ observations. Figure 4 shows the 20 largest events in size detected. The red line shows the contour of the extreme event detected and the number in red measures the intensity of the Mahalanobis distance within the contour line.

This approach does not consider any spatial cross-correlation, the points of the spatial grid are treated independently. Additionally, no temporal dependencies have been considered to define the events, these are just the 20 observations were the Mahalanobis distance presents the 20 largest events in size above the threshold defined.

This approach still needs to be improved to be able to detect events that extend in time more than one timestep. That is the reason why within this 20 observations plotted there are some timesteps very close in time (please note that the database used provides data on an 8-daily basis). For example there are up to 4 observations within this Top 20 that occurred during summer 2010; these observations surely belong to the same event that expanded in time for some weeks during that summer: the *Russian Heat Wave of 2010*.

Multi-temporal Spatio-contextual Markov Random Field Model So far, in all the steps of the presented methodology, the time series of each location in the grid was processed independently. However, the neighboring locations are most likely to have spatially similar local statistics. Markov Random Field (MRF) spatio-contextual models have the ability to quantify the spatial dependency among neighboring locations by a mathematically well established methodology. These contextual dependencies can be modeled by conditional probabilities within the neighborhood system [7]. Hence, to tackle the spatio-temporal dependencies of biosphere data, the obtained Mahalanobis distance over all BACI area is treated as an image time series. These images are then classified into three classes namely, 'intense anomaly', 'possible anomaly' and 'normal' using MRF model. We used an adaptation of the muti-layer fusion MRF model proposed in [2] for the classification of the Mahalanobis distance images. The adapted

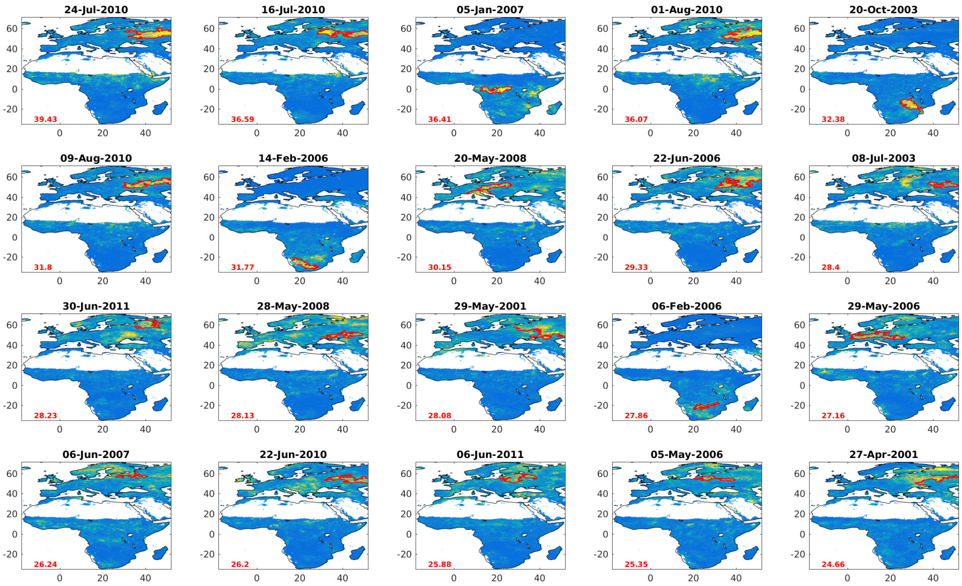


Figure 4: Contour lines of the 20 largest events detected.

method consists of unsupervised Kmeans clustering followed by multi-temporal MRF based segmentation applied recursively on each N $\geq$ 1 consecutive images. The selection of the value of N is based on the temporal resolution of the data. In our experiments, we set N=3 ensuring that the data belongs to similar season.

Experimental results are shown in Figure 5. The spatial and temporal extents of detected extreme events can be directly deduced from the classified images' label maps.

2.2 First Version of the BACIndex

From the methods detailed explained before we have provided two initial versions of the BACIndex. These two products serve to other WPs to work on the validation and socio-economic and biodiversity impacts.

The first product is the Mahalanobis distance of the ARMA residuals estimated for every point at every timestep of the time series. This value is related to the possibility of an abnormal event happening, in other words, this distance is already an index that shows the anomalies in the biosphere.

The second product comes as a result of the first one. For each timestep the Mahalanobis distance has been clustered into 3 levels: 'normal', 'possible anomaly' and 'intense anomaly'. This segmentation has been done by means of a Kmeans clustering followed by a multi-temporal Markov Random Field.

Both products have been storaged in netCDF files and uploaded to the BACI data exchange portal so it is easily accessible for other partners of the consortium.

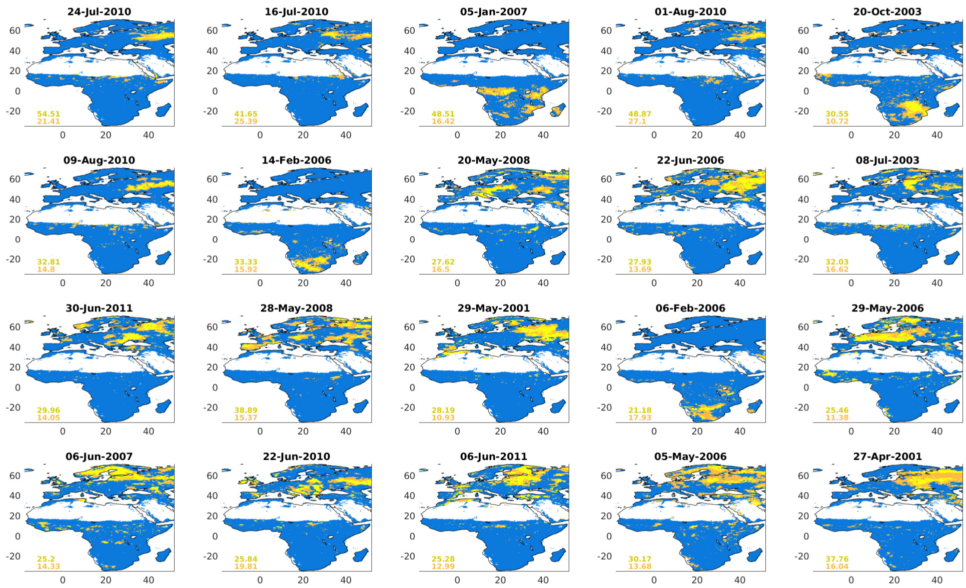


Figure 5: The classification of the images corresponding to the top 20 largest events shown in Figure 4. The legend shows the mean of the 'possible anomaly' and 'intense anomaly' clusters in orange and yellow colours respectively, the 'normal' class is shown in blue.

2.3 Conclusions

We have presented the advances implemented in the methodology proposed to detect abnormal events in multivariate time series based on regressive models. A preliminary version of this methodology was already presented in the Deliverable 5.2. Since then we have improved it in several aspects:

- A regionalization scheme was introduced. This regionalization consists on a clusterization of the spatial grid into regions of similar climate conditions. This clusterization was done based on the Köppen Climate Classification. The implementation of this regionalization scheme has partially solved the issue of overestimation of extreme events in the northern latitudes. Anyways, the heteroscedastic nature of the time series in extreme northern latitudes is not an easy problem to solve, we have also tried to remove the seasonality by removing the harmonics instead of by removing the mean seasonal cycle to check if that would improve our results, but it did not work better.
- An automatic selection of the ARMA models based on a Bayesian Criteria was implemented: this allow us to automatically select a different kind of ARMA model (number of parameters to be fitted) for each variable and region.
- Two methods to go from novelty scores to direct detections have been analyzed and compared. The first one considers an event to be abnormal when it surpasses a previously fixed threshold. The threshold has been set to be at the 97.5th percentile of the distribution. The second method is based on a combination of a clustering method (k-means) with a Markov Random Field model. The

main advantage of this second method is that it takes into account spatial correlation between the points that conform the grid, while the fixed threshold approach presented doesn't.

- A preliminary BACIndex has been already created and is accessible for the rest of the partners of the consortium. Two different versions of this index have been provided: the first one is the Mahalanobis distance estimated in each point of the grid and each timestep and the second version is a segmentation of these Mahalanobis distances into three classes: 'normal', 'possible anomaly' and 'intense anomaly' at each timestep.

There are still some open questions we need to work on. We will keep on working on them to make our methodology more robust and with general applicability. Therefore, our next duties comprise:

- Application of the methodology proposed to the satellite data that will be provided by the WP2. We will try to apply the methodology as it is right now, but it might be needed some adaptations to fit to the different data that will be provided by the BACI partners. We have worked with some preliminary data already provided by WP2, but due to some artifacts and biases in the data we have not been able to apply our methods to this data. These issues have been accordingly reported and discussed with WP2.
- Further research on the events detection to select which is the optimal method to apply. The method presented so far is a good approach, but we would like to test some adaptations or improvements to tailor them to our problem.
- Attribution scheme. This step is crucial to understand the processes causing abnormal events. This will be our main focus for the next months: (*Task 5.4 - Attribution Scheme*).

3 Conclusions

This deliverable refers to the works done within the *Task 5.3 - Incremental novelty detection, automatic dataset cleanup and going from novelty scores to direct detections* within the *Work Package 5 - Synthethic Index and Attribution Scheme: the BACIndex*.

The work done along this task can be divided into two main parts:

We have been working on the development of the library to run our Maximally Divergent Intervals algorithm for anomaly detection. This algorithm was already presented in the Deliverable 5.1 and extended in the Deliverable 5.2. At this point, a main improvements was shown in this deliverable: the algorithm has been extended to be able to deal with spatio-temporal data. Parallel to this, a software prototype with the algorithm has been released. Together with software it has been also provided a graphical user interface and a user guide. These tools ease the use of the algorithm and allow for experimentation, threshold selection and interactive user feedback.

In parallel, our methodology to detect extreme events based on autoregressive models has been improved and further developed. These improvements where mostly focused on two main parts of the method:

- Pretreatment; dataset cleanup: *i)* we have worked on a regionalization scheme where the spatial grid of data is clustered into subregions of similar climate conditions and *ii)* an automatic ARMA model selection has been implemented making the entire methodology more flexible to the particular conditions that each variable might present at each location.
- Event detection; from novelty scores to direct detections: two method that allow the definition of detections from novelty scores have been analyzed and compared. A simple one considering a fixed threshold and a more complex one that combines a clustering method with a Markov Random Field model.

This developments lead to the creation of a first version of the BACIndex that has been already distributed among the BACI consortium.

With this deliverable is ratified the achievement of Task 5.3.

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