mrbsizeR: Scale space multiresolution analysis in R

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1 Introduction

mrbsizeR is an R package based on the MRBSiZer method by Holmström et al. [2011]. The name is an abbreviation for MultiResolution Bayesian SIgnificant ZEro crossings of derivatives in R and the method extends the portfolio of Bayesian SiZer methods for images and spatial fields, originally introduced by Erästö and Holmström [2005].

In the analysis of spatial fields or images (i.e. an object), scale space methods are often useful. When observed on different scales, distinct features of the object can be detected. Imagine the concept of a branch of a tree (Lindeberg [1994]): This concept makes sense on a scale from a few centimeters to a few meters. On a much smaller scale, one could describe the molecules that form the branch and on a much larger scale, it would be possible to describe the forest the tree grows in. The goal in scale space analysis is therefore to represent an object on different scales, and this is done by dividing it into a family of smooths. The smooths are made on different smoothing levels and each smooth provides information relevant at a particular scale, which makes it possible to extract scale-dependent features from the object.

Significant Zero Crossings of Derivatives (SiZer) is a method based on scale space ideas and has originally been developed for smooths of curves and time series. The goal is to find out whether a certain feature of the curve is "really there" or if it is just a sampling artifact. For curves and time series this is usually done by investigating the significance of the increases and decreases of the derivatives. Within the last years, this concept has been extended to various directions.

In contrast to usual scale space procedures, where a wide range of smooths is used, mrbsizeR employs differences of smooths at neighboring scales. This attempts to separate the features into distinct scale categories more aggressively. In a next step, the resulting differences are investigated with a Bayesian version of SiZer to see which of the features found are "really there" and which are only artifacts of sampling.

For data on a regular grid, one can summarize the analysis procedure in three steps:

- 1. Bayesian signal reconstruction
- 2. Forming of scale-dependent details using differences of smooths at neighboring scales
- 3. Posterior credibility analysis of the differences of smooths

For spherical data, no Bayesian signal reconstruction is implemented. The analysis procedure for this type of data therefore consists of the forming of scale-dependent details and the subsequent credibility analysis. The single steps and their application in mrbsizeR are explained by the following three examples. For further theory and algorithm details, see Holmström et al. [2011] and Schuster [2017]. An extensive review of different statistical scale space methods including their applications is available in Holmström and Pasanen [2016].

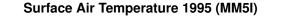
2 Example: Data On A Regular Grid

For the first example, data from the North American Regional Climate Change Assessment Program (NARCCAP) is analyzed. NARCCAP is an international program producing climate change simulations for Canada, the United States and northern Mexico. The data used for this example is based on the MM5I regional model [Mearns et al., 2007, updated 2014] and is a simulation of the surface air temperature during summer 1995 [Mearns et al., 2007, updated 2014], see also http://www2.mmm.ucar.edu/mm5/ and http://www.narccap.ucar.edu/index.html. The simulation was carried out on a 120-by-98 regular grid, therefore 11'760 data points are available in total. The data set is not part of the mrbsizeR package.

```
# Structure of the dataset
str(tas.su.1995.MM5I)
#> List of 3
#> $ lon: num [1:120, 1:98] 241 241 242 242 242 ...
#> $ lat: num [1:120, 1:98] 23 23.1 23.2 23.3 23.5 ...
#> $ su : num [1:120, 1:98] 21.8 21.7 21.7 21.7 21.7 ...
```

The variables lon and lat describe the longitude and latitude of each simulated surface air temperature in summer 1995 in degrees Celsius (su). The data covers the United States, the southern part of Canada and the northern part of Mexico.

As the output of the mrbsizeR analysis are plots on a rectangular grid, it makes sense to display Figure 1 also like this (compare Figure 2). By combining Figures 1 and 2, it is still possible to recognize all the important features such as coastlines, the Baja California or the Great Lakes.



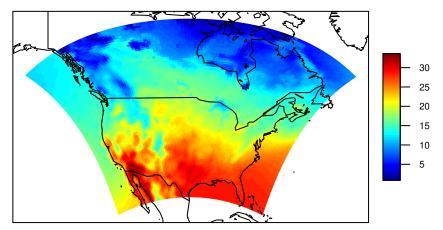
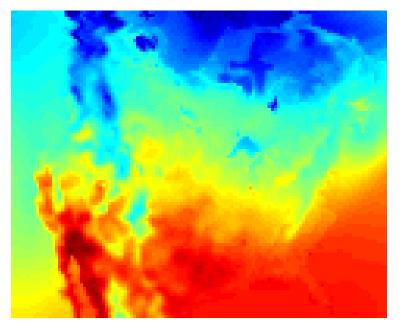


Figure 1: Simulated surface air temperature in summer 1995 for the United States, the southern part of Canada and the northern part of Mexico. The unit of the temperature is degrees Celsius.



Surface Air Temperature 1995 (MM5I)

Figure 2: Simulated surface air temperature in summer 1995 for the United States, the southern part of Canada and the northern part of Mexico on a rectangular grid. Red describes warmer areas, colder areas are colored blue.

2.1 Bayesian Signal Reconstruction

The first step of the mrbsizeR analysis is the Bayesian signal reconstruction. The data set is assumed to be a random signal which might be noisy. In order to account for this uncertainty in the data, a Bayesian model is used to reconstruct the original signal. The model used is

$$oldsymbol{y} = oldsymbol{x} + oldsymbol{arepsilon}$$

where \boldsymbol{y} is the observed random signal (compare Figures 1 and 2), \boldsymbol{x} is the unobserved underlying original signal and $\boldsymbol{\epsilon}$ is the noise. A \mathcal{N} -Inv- χ^2 prior distribution is assumed. In mrbsizeR, not the full posterior $p(\boldsymbol{x}, \sigma^2 | \boldsymbol{y})$ is of interest, but the marginal posterior $p(\boldsymbol{x} | \boldsymbol{y})$. This marginal posterior follows a multivariate *t*-distribution t_{ν} and sampling from it results in samples from the reconstructed original signal \boldsymbol{x} .

Depending on how much is known about the noise in \boldsymbol{y} , the prior distribution parameters can be adjusted. For the example of the surface air temperature, the parameters $\lambda_0 = 0.2$, $\nu_0 = 15$ and $\sigma_0^2 = 36^2$ were used. This prior has little influence on the posterior as no information about possible noise on \boldsymbol{y} is available. Using the function rmvtDCT(), samples from a t_{ν} -distribution can be generated. The sampling algorithm uses a discrete cosine transform (DCT) to speed up computations. For further information on the distributions and the sampling algorithm, see Holmström et al. [2011] and Schuster [2017].

1000 samples of the posterior distribution of the surface air temperature in Canada, Mexico and the United States were generated. These samples now form the reconstructed signal \boldsymbol{x} and are used for further analysis.

2.2 Forming of scale-dependent detail components

Now that the original signal has been reconstructed, one can start forming scale-depending detail components. For being able to create differences of smooths at neighboring scales z_1, \ldots, z_L , a set of appropriate smoothing levels $\lambda_1, \ldots, \lambda_L$ needs to be known. In contrast to other scale space methods, where a wide range of smoothing levels is used, mrbsizeR only requires a few of them. The goal is to separate the features of the object (here: the surface air temperature data) into scale-distinct categories. If too many smoothing levels are chosen, this will result in categories that do not feature relevant detail components. If, on the other hand, too few smoothing levels are chosen, detail components on different scales might mix up and are not recognizable anymore. It is therefore not only crucial to determine which smoothing levels are useful, but also the number of smoothing levels that should be used.

All methods proposed for the selection of smoothing levels have one thing in common: They offer a good starting point for finding useful smoothing levels - but to make sure that all detail components are captured optimally, user interaction is usually inevitable. Typically, a few iterations are necessary until satisfying smoothing levels are found.

The first method for the smoothing level selection depends on the smoother implemented in mrbsizeR and

the dimension of the object analyzed only. By plotting so-called tapering functions of the eigenvalues of Q, a precision matrix used in the smoother of mrbsizeR, and the smoothing levels λ_i , it is possible to determine which λ 's could be useful. The eigenvalues and the smoothing parameters are related as follows:

- Small λ 's involve large eigenvalues of Q.
- Large λ 's involve small eigenvalues of Q.

The idea is to plot the tapering functions for different ranges of λ so that the functions are approximately disjoint. When using these λ -ranges for calculating the differences of smooths, this will result in orthogonal detail components. For detailed information about the smoother used and the properties of the tapering functions, see Holmström et al. [2011] and Schuster [2017].

The surface air temperature data was simulated on a 120-by-98 grid, and this information has to be passed to the plotting function TaperingPlot(). The vector lambdaSmoother contains the smoothing levels that should be used for drawing the tapering functions.

```
# Plot of signal-independent tapering functions
TaperingPlot(lambdaSmoother = c(1, 100, 10000), mm = 120, nn = 98)
```

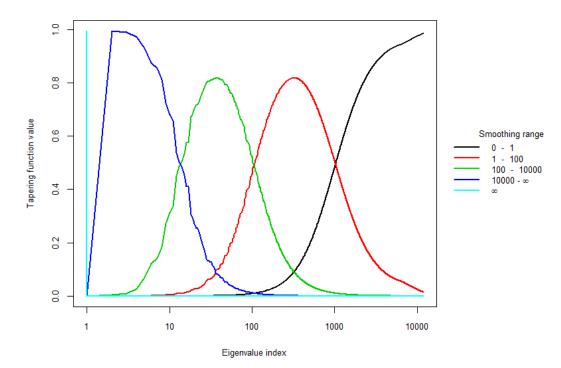


Figure 3: Signal-independent tapering functions for a 120-by-98 object with the smoothing level (λ) ranges 0–1, 1–100, 100–10000, 10000– ∞ and ∞ . The tapering functions are approximately disjoint.

The corresponding tapering functions are shown in Figure 3. The smoothing levels 0 and ∞ are added to the set of smoothing levels, as both of them have a special meaning. Whereas a smoother with $\lambda = 0$ is the so-called identity smoother ($S_0 x = x$), smoothing with $\lambda_L = \infty$ results in the global mean. The five tapering functions in Figure 3 are approximately disjoint and a good starting point when trying to find useful smoothing levels.

An even better starting point can be attained if the underlying signal x is also taken into account. TaperingPlot() allows to draw signal-dependent tapering functions using the (optional) argument Xmu. As the original signal x is unknown, it is replaced by its posterior mean.

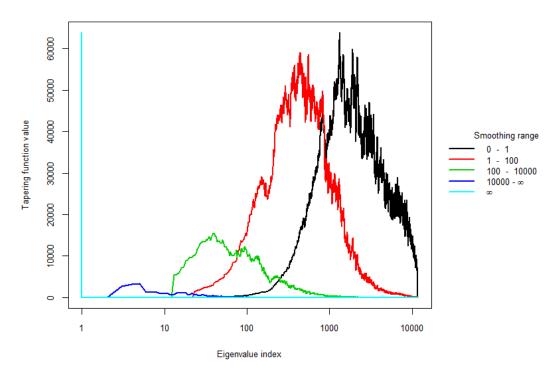


Figure 4: Moving average of the absolute values of signal-dependent tapering functions for the surface air temperature data with the smoothing level (λ) ranges 0–1, 1–100, 100–10000, 10000– ∞ and ∞ .

As signal-dependent tapering functions have values that vary wildly, visual inspection of these functions is difficult. TaperingPlot() therefore uses moving averages on the absolute values of these tapering functions to facilitate visual inspection. Figure 4 shows that the disjointedness of the smoothed tapering functions is not as pronounced as in Figure 3, but can still be observed.

A more formal approach is the numerical optimization of a suitable objective function with respect to the smoothing parameters. With MinLambda() it is possible to conduct this optimization for 2 or 3 λ 's. The resulting smoothing levels are, in terms of disjointedness of the signal-dependent tapering functions, optimal. Still, it is often necessary to adjust the smoothing levels manually. For being able to extract also the smallest-scale details it can for instance be useful to include an additional, small λ . Furthermore, the number of "optimal" smoothing levels found with MinLambda() is limited. When optimizing over 3 λ 's, one ends up with a sequence of 5 smoothing levels in total (3 optimized λ 's, $\lambda_0 = 0$, $\lambda_L = \infty$). In cases where more smoothing levels are necessary, i.e. where the object contains details relevant on more distinct scales, it is

necessary to add smoothing levels manually. However, five smoothing levels turned out to be sufficient in many cases.

Most of the arguments of MinLambda() are already known from TaperingPlot(). In addition to this, it is necessary to specify nGrid (size of the grid the optimization should be carried out on, nGrid-by-nGrid), nLambda (either 2 or 3, number of λ 's to be optimized) and sphere (logical; is the analysis on spherical data?). The optimal λ values evaluated for the surface air temperature data are 3.16e-11, 1e+02 and 1e+04.

```
# Minimal smoothing parameter values
tas.min.lambda.out$lambda[tas.min.lambda.out$minind]
#> [1] 3.16e-11 1.00e+02 1.00e+04
```

The minimization result can also be shown visually. For each optimized pair of λ 's, a plot is drawn. Figure 5 shows the optimization for the surface air temperature example. The optimized λ 's have the indices λ_2 , λ_3 and λ_4 , because $\lambda_1 = 0$ and $\lambda_5 = \infty$.

```
# Plot of the minimization result
plot(x = tas.min.lambda.out)
```

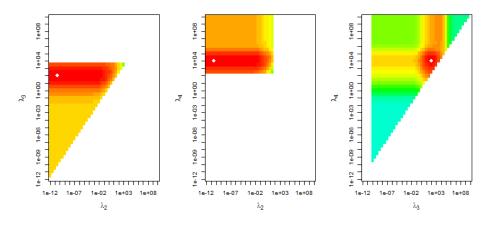


Figure 5: Minimization of the objective function for three smoothing levels λ . The minimum is indicated by a white point.

The smoothing levels found with the different methods can now be used as a starting point for finding scaledependent details in the analyzed object. Usually, a few iterations with some smoothing level adjustments are necessary until the results found are satisfying. For the surface air temperature example, the smoothing level sequence $[\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5] = [0, 0.1, 90, 16'000, \infty]$ turned out to be useful. Using mrbsizeRgrid(), differences of smooths at neighboring scales are created. For the surface air temperature example, the samples generated with rmvtDCT() are used as input. If other samples are already available and no Bayesian signal reconstruction is needed, it is important to store them as a matrix where each column vector represents one sample.

The resulting object tas.mrb.out is a list containing three sublists. smMean contains the mean of each difference of smooths z_i over all ns = 1000 samples from the posterior p(x|y). The lists hpout and ciout are relevant for the posterior credibility analysis, which is discussed in detail in the next subsection.

The smMean-plots for the surface air temperature example are displayed in Figure 6. With increasing smoothing level λ , the features are getting larger. The first component z_1 shows the smallest scale details of x. The contours of areas where a rapid change from warmer to colder temperature can be observed are clearly visible. In z_2 , larger-scale details are identifiable. The Great Lakes seem to be colder than the surrounding regions and the areas surrounding the Gulf of California are clearly warmer than the Gulf itself. z_3 shows that the Gulf of California is the hottest region in Northern America. Furthermore, the Rocky Mountains are identifiable as a cool, longish band across the map. The next difference of smooths z_4 shows a north-south temperature gradient, and z_5 is the mean across the whole map.

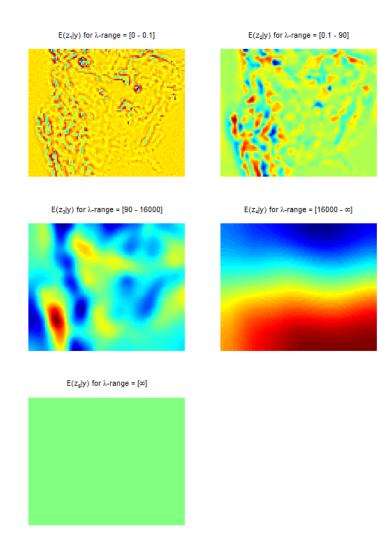


Figure 6: Decomposition of Figure 2 into differences of smooths at neighboring scales. The details z_1, \ldots, z_5 are summarized by their posterior means. Warmer areas are colored red, colder areas are colored blue.

2.3 Posterior Credibility Analysis

As the detail components z_i are random samples from the posterior distribution $p(\boldsymbol{x}|\boldsymbol{y})$, a credibility analysis has to be done. The goal is to infer which details are truly there and which are only artifacts of random variation. Three different methods for posterior credibility analysis are implemented in mrbsizeR:

- Pointwise Maps (PW): Each location / pixel is tested separately for credibility.
- Highest Pointwise Probability Maps (HPW): The inference is done jointly over all locations. In comparison to PW maps, this results in more non-credible areas. The advantage of HPW maps is that the credible areas are better connected than in PW maps. Small credibility islands with low expressiveness do appear less frequently and simplify the interpretation of the results.

• Simultaneous Credible Intervals (CI): Inference is also done jointly over all locations. Here, simultaneous credible intervals centered on the posterior means are calculated. CI maps flag locations as credible more conservatively than PW or HPW maps.

For more detailed information about the three methods, see Holmström et al. [2011] and Schuster [2017]. By default, credible regions of all three methods are calculated when executing mrbsizeRgrid(). The corresponding lists in the output of mrbsizeRgrid() are hpout and ciout.

```
# Plot of pointwise (PW) maps
plot(x = tas.mrb.out$hpout, plot_which = "PW", aspRatio = 98/120,
       color = c("dodgerblue3", "gainsboro", "firebrick1"), turnOut = FALSE)
                                  PW-Map for z_1 with \lambda-range = [0 - 0.1]
                                                                            PW-Map for z_2 with \lambda-range = [0.1 - 90]
                                         χ.,
                                PW-Map for z_3 with \lambda-range = [90 - 16000]
                                                                           PW-Map for z_4 with \lambda-range = [16000 - \infty]
                                   PW-Map for z_s with \lambda-range = [\infty]
```

Figure 7: Pointwise (PW) maps for the surface air temperature example. Credibly warmer areas are colored red, credibly colder areas blue. Areas without credibility are gray.

The pointwise credibility maps in Figure 7 do show little credibility for the difference of smooths z_1 . In z_2 , the Gulf of California is credibly colder than Baja California and the Mexican mainland on the eastern side of the Gulf. In z_3 , nearly everything is credible. This confirms that the Rocky Mountains are really colder and that the whole area of the Gulf of California is credibly warmer than surrounding regions. With z_4 , it gets clear that the northern part of the map is credibly colder than the southern part. z_5 simply shows that the whole global mean is credible.

```
# Plot of highest pointwise probability (HPW) maps
plot(x = tas.mrb.out$hpout, plotWhich = "HPW", aspRatio = 98/120,
       color = c("dodgerblue3", "gainsboro", "firebrick1"), turnOut = FALSE)
                                 HPW-Map for z_4 with \lambda-range = [0 - 0.1]
                                                                          HPW-Map for z_2 with \lambda-range = [0.1 - 90]
                                         ۰.
                               HPW-Map for z_3 with \lambda-range = [90 - 16000]
                                                                         HPW-Map for z_4 with \lambda-range = [16000 - \infty]
                                  HPW-Map for z_s with \lambda-range = [\infty]
```

Figure 8: Highest pointwise probability (HPW) maps for the surface air temperature example. Credibly warmer areas are colored red, credibly colder areas blue. Areas without credibility are gray.

The HPW maps in Figure 8 exhibit less credibility than the PW maps, especially for small-scale details.

However, the interpretation of the results stays the same. Due to the joint inference over all locations, small islands of credibility are less frequent.



Figure 9: Simultaneous credible interval maps for the surface air temperature example. Credibly warmer areas are colored red, credibly colder areas blue. Areas without credibility are gray.

Detail component z_1 of the simultaneous credible interval maps in Figure 9 does not exhibit any credibility. CI maps are generally the most conservative credibility analysis method. It therefore is not surprising that in details z_2 and z_3 more gray areas can be observed than in the PW or HPW maps (compare Figures 7 and 8). Still, especially for the larger-scale details, the interpretation of the results does not change.

3 Example: Comparison to Matlab software

The mrbsizeR methodology was first implemented in the Matlab program MRBSiZer [Holmström and Pasanen, 2011], which is available at http://cc.oulu.fi/~lpasanen/MRBSiZer/. In order to ensure that the results obtained with R and Matlab are concordant, the sketch pad example from the original paper [Holmström et al., 2011] is reconstructed (compare Figure 10. The digital image is of the size 284-by-400 and the prior parameters λ_0 , σ_0^2 and ν_0 had the values $0.2, 8.9^2$ and 10, respectively. The set of smoothing levels used in the multiresolution analysis was $[0, 1, 30, 6 \times 10^5, \infty]$. 3000 samples of the posterior $p(\boldsymbol{x}|\boldsymbol{y})$ were generated.

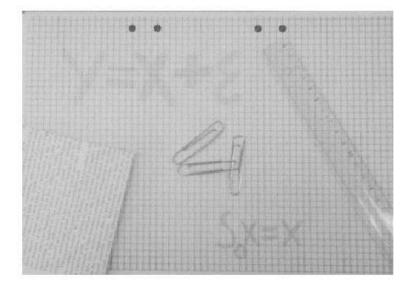
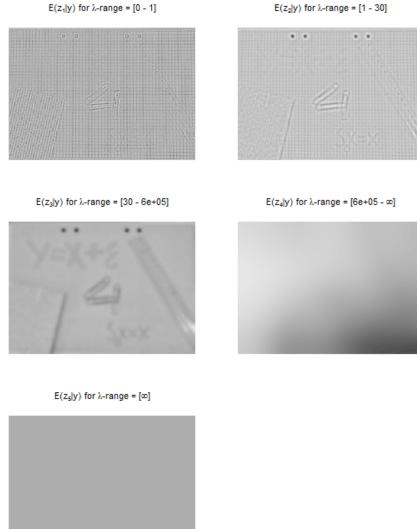


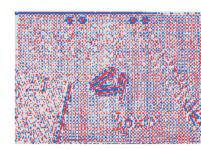
Figure 10: Original sketch pad image.

The detail components z_i are shown in Figure 11. As the output of mrbsizeRgrid() is based on random samples, small differences between two executions are inevitable. When compared to the Matlab figures in Holmström et al. [2011], no big differences can be detected. More differences can be found in the HPW maps, especially in detail component z_3 (compare Figure 12). It seems that in the **R** implementation, a slightly larger part of the component was flagged as credible. Nevertheless, the detail components look very similar to their Matlab pendants and the interpretation of the results stays the same. The differences can be explained by random sampling and one can be confident that concordance across the systems holds.



 $E(z_1|y)$ for λ -range = [0 - 1]

Figure 11: Posterior mean of detail components \boldsymbol{z}_i from the sketch pad example.

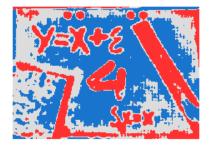


HPW-Map for z_4 with λ -range = [6e+05 - ∞]

HPW-Map for z_1 with λ -range = [0 - 1]



HPW-Map for z_3 with λ -range = [30 - 6e+05]



HPW-Map for z_s with λ-range = [∞]



Figure 12: Highest pointwise probabilities maps of detail components z_i from the sketch pad example. Credibly darker areas are red, credibly brighter areas are blue.

HPW-Map for z_2 with λ -range = [1 - 30]

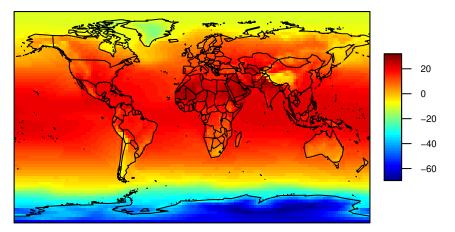
4 Example: Data On A Sphere

The third example in this vignette demonstrates how mrbsizeR can be used to analyze spherical data. In contrast to the analysis of data on a grid, no Bayesian signal reconstruction is implemented. To form scale-dependent details, data samples need to be available beforehand. The analysis procedure for spherical data can therefore be summarized in two steps:

- 1. Forming of scale-dependent details using differences of smooths at neighboring scales
- 2. Posterior credibility analysis of the differences of smooths

Data from the Community Climate System Model 4.0 (CCSM4, see http://www.cesm.ucar.edu/models/ ccsm4.0/ccsm/) is used to illustrate mrbsizeR on spherical data. CCSM4 is a climate model simulating the earth's climate system, see Gent et al. [2011]. For this analysis, the simulated surface air temperature in June of the years 1870–2100 was considered. Instead of using the surface air temperature itself, its deviation to the yearly mean has been used. This detrends the data and makes the simulations of 231 consecutive years comparable. The resulting data set consisting of 231 observations is then used as samples for the mrbsizeR analysis. The data is not part of the mrbsizeR package.

Figure 13 summarizes the samples by their mean. It is clearly visible that the temperature is higher in areas around the equator and gets lower closer to the Polar Regions. The unit of the surface air temperature deviation is degrees Kelvin.



Deviation of Mean from Surface Air Temperature (CCSM4)

Figure 13: Deviation from mean of simulated air temperature measurements (CCSM4) for the years 1870–2100 in degrees Kelvin. The deviations are summarized by their mean.

For conducting scale space multiresolution analysis with mrbsizeR, useful smoothing parameters need to be evaluated first. As explained in the NARCCAP data example, MinLambda() offers the possibility to find useful smoothing parameters numerically. The function call for spherical data is nearly identical to the call for non-spherical data, the only difference is the argument sphere which has to be TRUE.

Once useful smoothing levels have been selected, differences of smooths at neighboring scales can be created using the function mrbsizeRsphere().

For creating the differences of smooths at neighboring scales in Figure 14, the smoothing level sequence $[\lambda_1, \ldots, \lambda_3] = [0, 0.0026, \infty]$ was used. Only one smoothing level was added to the default sequence $[0, \infty]$. This is enough to capture features at all different scales. Whereas z_1 shows small-scale details like colder regions in Tibet or Chile, z_2 reveals a large red-colored area around the equator and large blue-colored areas at the Polar Regions. z_3 shows the global mean.

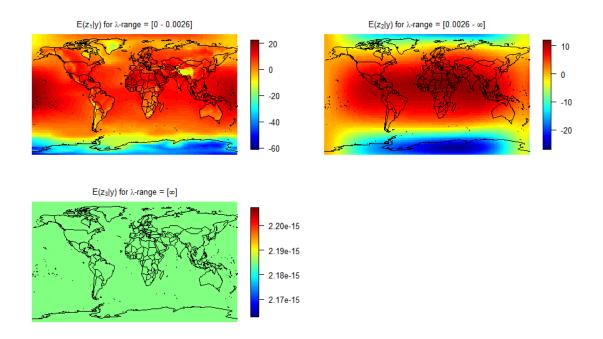
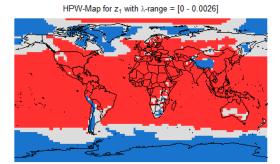
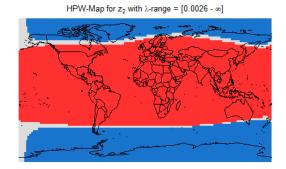


Figure 14: Decomposition of Figure 13 into differences of smooths at neighboring scales. The details z_1, \ldots, z_3 are summarized by their posterior means. Areas with larger data values are colored red, areas with smaller values are colored blue.

The posterior credibility analysis of detail component z_1 using highest pointwise probability (HPW) maps (compare Figure 15) reveals that regions like Chile or the eastern part of South Africa are credibly colder than surrounding areas. The large-scale components in z_2 are mostly credible and hence "really there". The global mean in z_3 is not credible in this example. The reason is the data used: Instead of considering the yearly surface air temperature, its deviations to the yearly mean are considered. z_3 is therefore not the average surface air temperature, but the average mean deviation, which always equals 0.



HPW-Map for z_3 with λ -range = $[\infty]$



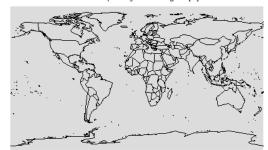


Figure 15: Highest pointwise probability maps. Areas with credibly larger data values are colored red, areas with credibly smaller values are blue. Areas without credibility are gray.

5 What If Not Enough Computing Power Is Available?

Especially for analyses with a large analysis object and/or many samples, an mrbsizeR analysis is resourceintensive. For cases where due to computational reasons not enough samples can be generated, the additional argument smoothOut has been added to mrbsizeRgrid() and mrbsizeRsphere(). If smoothOut = TRUE, the output list will also contain a sublist smoothSamples, which includes the differences of smooths for all samples. This makes it possible to manually increase the number of samples and get HPW maps and CI maps with a higher confidence. An example is provided in the following code chunk.

```
# Generate samples from posterior distribution
tas.post.samp <- rmvtDCT(object = tas.su.1995.MM5I$su,</pre>
                          lambda = 0.2, sigma = 36, nu0 = 15, ns = 1000)
# Do mrbsizeR analysis and output the differences of smooths for all samples
tas.mrb.out.1 <- mrbsizeRgrid(posteriorFile = tas.post.samp$sample, mm = 120,
                               nn = 98, lambdaSmoother = c(0.1, 90, 15000),
                               prob = 0.95, smoothOut = TRUE)
# Do the same procedure again
tas.post.samp <- rmvtDCT(object = tas.su.1995.MM5I$su,</pre>
                          lambda = 0.2, sigma = 36, nu0 = 15, ns = 1000)
tas.mrb.out.2 <- mrbsizeRgrid(posteriorFile = tas.post.samp$sample, mm = 120,</pre>
                               nn = 98, lambdaSmoother = c(0.1, 90, 15000),
                               prob = 0.95, smoothOut = TRUE)
# Combine all differences-of-smooths-samples and call CImap manually
smoothSamples <- list(); ciout <- list()</pre>
for(i in 1:length(tas.mrb.out.1$smoothSamples)) {
  smoothSamples <- cbind(tas.mrb.out.1$smoothSamples[[i]],</pre>
                          tas.mrb.out.2$smoothSamples[[i]])
  ciout[[i]] <- CImap(smoothVec = smoothSamples, mm = 120, nn = 98, prob = 0.95)
}
# Set the class correctly for visualizing the output.
# Titles need to be defined in this case!
# Class name CI maps: "CImapGrid" or "CImapSphere"
# Class name PW / HPW maps: "HPWmapGrid" or "HPWmapSphere"
class(ciout) <- "CImapGrid"</pre>
plot(ciout, title = c("Diff_1", "Diff_2", "Diff_3", "Diff_4", "Diff_5"))
```

6 Data Acknowledgments

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