# Predicting Droughts in the Amazon Basin based on Global Sea Surface Temperatures

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Clustering

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Summary

```
## Lade nötiges Paket: sp
##
## Attache Paket: 'patchwork'
## Das folgende Objekt ist maskiert 'package:raster':
##
## area
```

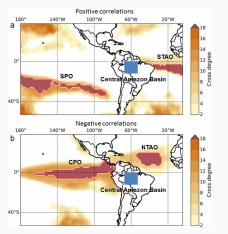
# Introduction

#### Motivation

- The Amazon basin is a key hotspot of biodiversity, carbon storage and moisture recycling
- Hydrological extremes affect ecosystem and populations tremendously
- Droughts in the Amazon rainforest can have severe biomass carbon impact
- Severe Amazon drought in 2010 had total biomass carbon impact of 2.2 PgC, affected area 3miokm<sup>2</sup>

#### Related work

 Ciemer et al. (2020) established an early warning indicator for water deficits in the central Amazon basin (CAB)



**Figure 1:** Cross degree between sea surface temperature and continental rainfall anomalies. For each grid cell of sea surface temperature in the

#### Our approach

- Inspect spatial and temporal characteristics in raw data
- Directly predict rain from SST
- Use lasso and fused lasso
- model evaluation with cross validation for time series

# Explorative analysis

#### The data

- Rain data from CHIRPS ()
- CHIRPS contains in-situ and satellite data
- SST data from ERSST (Extended Reconstructed Sea Surface Temperature)
- ERSST is reanalysis of observation data (made by ships and buoys for example), missing data filled by interpolation techniques
- These are the same data sets as in Ciemer et al. (2020)

# **Explorative analysis Rain**

- show area
- show mean and sd
- show glyph plots

# **Explorative analysis SST**

show mean and sd

# Correlation analysis

## **Correlation analysis**

show timelag 0, raw and de-seasonalized

# Clustering

# Motivation/ Overview

- explorative analysis has shown spatial and temporal differences in the precipitation data
- we explored this further using k-means clustering
- steps: find optimal k via pca and gap statistic
- apply k-means to original precipitation data
- we compared k-means and k-medoid with and without PCA via the gap statistic
- here show only k-means with PCA as it gave best results
- applying the regression models to separate clusters might improve predictions
- Using 3 principal components and 5 cluster centers with k-means gave best results on gap statistic

#### k-means

- Our objective is to find k internally homogeneous and externally heterogeneous clusters
- Similarity is measured by the euclidean distance

$$d(x_i, x_{i'}) = \sum_{i=1}^{p} (x_{ij} - x_{i'j})^2 = ||x_i - x_{i'}||^2 (\#eq : eucl - dist)$$
 (1)

And we want to minimize the sum of distances inside all clusters, given by:

$$W(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(i')=k} ||x_i - x_{i'}||^2 = \sum_{k=1}^{K} N_k \sum_{C(i)=k} ||x_i - \bar{x}_k||^2 (\#eq : w)$$
(2)

where  $\bar{x} = (\bar{x}_{1k}, ..., \bar{x}_{nk})$  stands for the mean vectors of the kth

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#### gap statistic

- number of clusters has to be defined beforehand
- we decided on the optimal number of k using the gap statistic
- Let  $W_k$  be W(C) for fix k
- We compare  $W_k$  from the precipitation data with average  $W_k^*$  from B Monte Carlo sampled data sets

$$Gap(k) = E\{log(W*_k)\} - log(W_k).(\#eq : gap)$$
 (3)

We choose k as smallest k such that

$$Gap(k) \ge Gap(k+1) - s_{k+1} \tag{4}$$

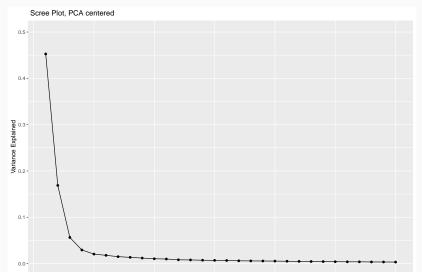
•  $s_{k+1}$  is  $sd_k\sqrt{1+1/B}$ , and sd the standard deviation of  $\log(W^*\_k)$ 

#### **PCA**

- Before running k-means we center the precipitation data and apply a PCA to reduce the large number of correlated variables to a few
- The new variables are linear combinations of the original variables
- Here: Each variable is a month of precipitation data in the CAB

### Scree Plot, PCA after centering

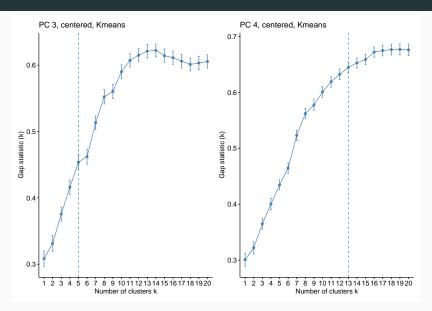
## Scale for 'y' is already present. Adding another scale :
## replace the existing scale.



#### Screeplot

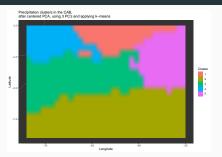
- The "elbow" be observe in the screeplot suggest 3 or 4 principal components
- The first 3 and 4 first PC explain 67.77 and 70.79 of the variance respectively.
- We compare the gap statistic results for 3 and 4 PC

#### **Gap statistic results**



• The k-means gap statistic on the first 3 PC proposes 5

## Clustering results



**Figure 3:** Spatial distribution of the found clusters in the CAB. We applied a centered PCA on the data and used 3 principal components before applying the k-means algorithm

- We find 5 clusters of different sizes
- The found clusters are almost completely spatially coherent although we did not include any spatial dependencies in the clustering

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# The lasso

#### **Definition of the lasso**

We now consider the lasso regression problem

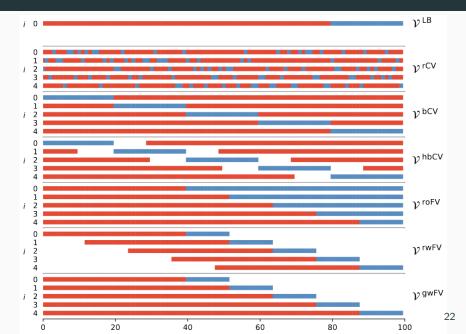
$$\min_{\beta_0,\beta} \frac{1}{N} \sum_{i=1}^{N} w_i I(y_i, \beta_0 + \beta^T x_i) + \lambda [(1-\alpha)||\beta||_2^2 / 2 + \alpha ||\beta||_1] (\#eq : glmnet)$$
(5)

- In our setting n « p, so lasso is natural choice
- The problem is solved using coordinate descent
- Due to the time dependencies in our data normal Cross Validation may be unjustified

#### Model evaluation

- Our goal is to train a model that can also predict well on new, unseen data
- We simulate the situation of unseen data by splitting our data into one part for model selection and another part for model evaluation
- Model evaluation is usually done via Cross Validation, but classic Cross Validation does not take into account the time dependency in our data

### Forward selection



#### Forward selection

- We compute a  $\lambda$ -vector for the complete training set
- For each fold we fit a model with this  $\lambda$ -vector
- We compute the prediction error for the cv-test set of each fold
- Choose  $\lambda_{\min}$ ,  $\lambda$  that minimizes average MSE over all folds
- $\blacksquare$  Fit model on complete selection data with  $\lambda_{\min}$  and compute MSE on evaluation data

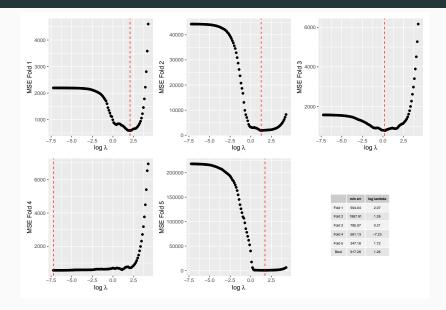
#### lasso settings

- lasso
- lasso with standardized features
- lasso with de-seasonalized SST
- lasso with differentiated SST
- lasso on clusters

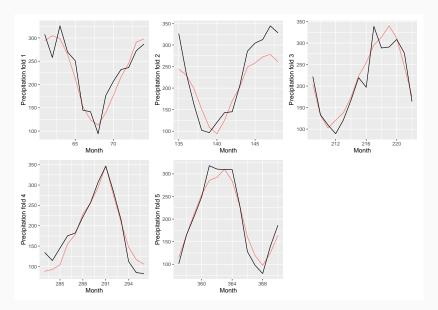
#### lasso results TODO

- Show only best model results
- lasso with standardized features
- show MSE in plots
- show predictions in plots
- show predictions
- show coefficients
- display table

#### MSE in each fold

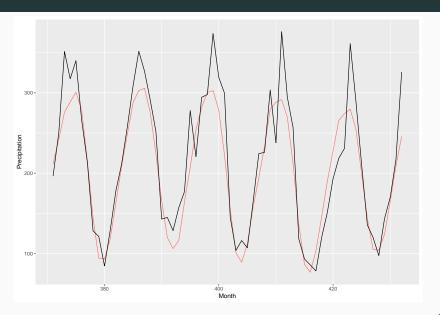


#### Predictions on test set, for each Fold

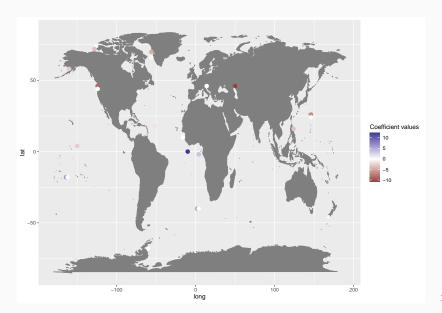


### **Predictions on External Test Set**

## **Predictions on External Test Set**



# SST Regions chosen by the lasso

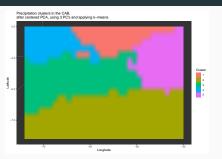


Lasso results all models

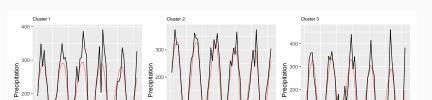
#### Lasso results all models

##		mse min	lambda min
##	stand	1214.49	3.52
##	original	1314.93	3.52
##	diff	1361.82	2.21
##	deseas	1809.45	1.75

#### Lasso on clusters results



**Figure 6:** Spatial distribution of the found clusters in the CAB. We applied a centered PCA on the data and used 3 principal components before applying the k-means algorithm



#### **Summary lasso results**

- We compared different settings for the lasso
- Lasso, lasso with standardization, de-seasonalizing, differentiation and on clusters
- Lasso with standardized SST worked best
- Can predict general seasonality, but still fails to predict peaks in precipitation
- Clustering the CAB improves only on one cluster, but on this cluster peaks can be predicted better than in the unclustered model
- Lasso chooses single "points" and not whole areas
- The points chosen as coefficients differ in the models, and can be very far away from the CAB

## Discussion Validation approach (maybe discuss this at the end)

- For the CAB we can not predict large values in the hold-out set, on cluster 2 it works a little better
- Possible explanations:
- Our validation approach works better when train and test set are similar in terms of seasonality and trend
- When train and test differ, predictions might not work so well (test of stationarity in folds)
- Differentiating and de-seasonalizing could not solve this problem
- Predictions work better when the precipitation remains fairly stable over time, see Cluster 2
- Final model uses complete model selection data, possibly some of that information is not useful anymore if it's toocfar away from hold-out time frame
- Our validation approach is a trade-off between efficient use of

## The fused lasso

#### Definition of the fused lasso

- Fused lasso, "fuses" predictors together
- It penalizes the difference of close predictores
- Therefore close predictors should be similar

$$\min_{\beta} 1/2 \sum_{i=1}^{n} (y_i - x_i^T \beta_i)^2 + \lambda \sum_{i,j \in E} |\beta_i - \beta_j| + \gamma \cdot \lambda \sum_{i=1}^{p} |\beta_i|, (\#eq : fused-lasso)$$
(6)

- with  $x_i$  being the ith row of the predictor matrix and E is the edge set of an underlying graph.
- The third term  $\gamma \cdot \lambda \sum_{i=1}^{p} |\beta_i|$ , controls the sparsity of the coefficients.
- $\gamma=0$  leads to complete fusion of the coefficients (no sparsity) and  $\gamma>0$  introduces sparsity to the solution, with higher values placing more priority on sparsity.

#### **Fused lasso optimization**

 Lets consider the problem in the notation of the generalizes lasso problem

$$\hat{\beta} = \underset{\beta \in \mathbb{R}^p}{\arg\min} \frac{1}{2} \|y - X\beta\|_2^2 + \lambda \|D\beta\|_1, (\#eq : gen - lasso)$$
 (7)

- where  $y \in \mathbb{R}^n$  is the vector of the outcome,  $X \in \mathbb{R}^{n \times p}$  a predictor matrix,  $D \in \mathbb{R}^{m \times p}$  denotes a penalty matrix, and  $\lambda \geq 0$  is a regularization parameter.
- The dual path algorithm solves not the primal but the dual solution of the problem and computes the solution for a whole path instead of single values of  $\lambda$ .

Let's consider the case when X = I and rank(X) = p (this is called the "signal approximator" case), the dual problem of @ref(eq:gen-lasso) is then:

$$\hat{u} \in \underset{u \in \mathbb{R}^{\omega}}{\operatorname{arg\,min}} \frac{1}{2} \left\| y - D^{T} u \right\|_{\frac{2}{2}} \text{ subject to } \|u\|_{\infty} \le \lambda. (\#eq: dual)$$
(8)

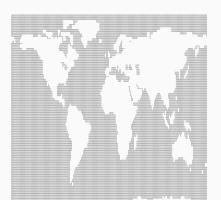
• The primal and dual solutions,  $\hat{\beta}$  and  $\hat{u}$  are related by:

$$\hat{\beta} = y - D^{\mathsf{T}} \hat{u}.(\#eq : dual - relate)$$
 (9)

 For general X and D with exploitable structure (as in our case), specialized implementations exist

## **Graph structure**

- We can use a graph as input in the fusedlasso function
- We created a grid and deleted all nodes that were land regions
- This induced subgraphs



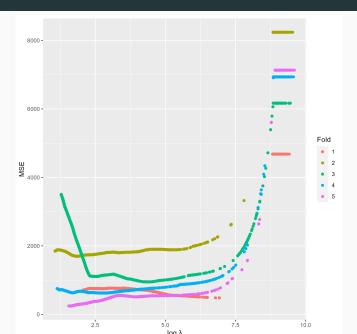
#### **Graph structure and implications**

- Results showed that removing the sub-graphs improved performance, although some of the regions were included in the final lasso models
- If we don't remove the clusters and also add sparsity (i.e  $\gamma>0$ ) the clusters dominate the results even more
- Possible explanations: Sub-graphs are less penalized, because they have fewer edges.
- Removing the clusters improved results more than f.e standardization

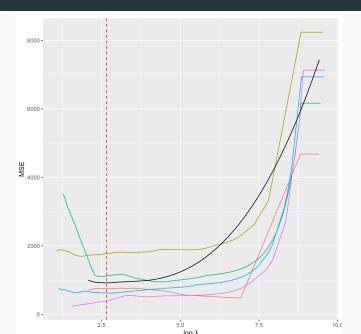
#### **Fused lasso settings**

- The considered fused lasso settings are: Fused lasso with clusters, fused lasso without clusters, fused lasso without clusters and sparsity (gamma: 0.01, 0.05, 0.1)
- Fused lasso without clusters and no sparsity showed best results

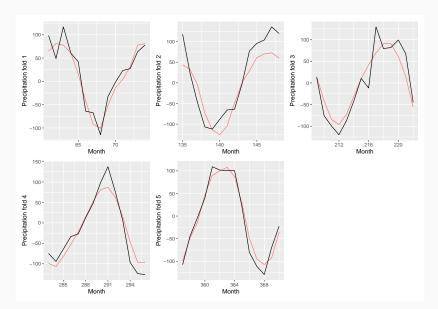
## Fused lasso results, clusters removed



## Fused lasso results, clusters removed



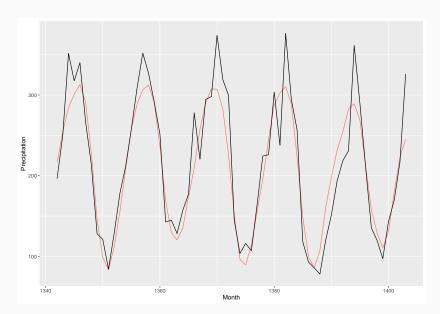
### **Prediction plots**



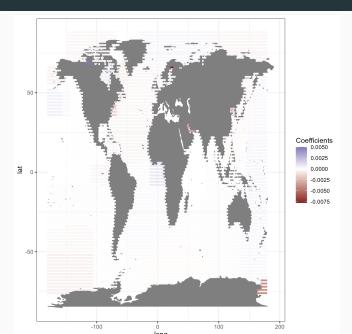
### **Prediction plot**

The predictions inside the folds are very similar to lasso without standardization, the same holds for the predictions from the full model, but the MSE improves here.

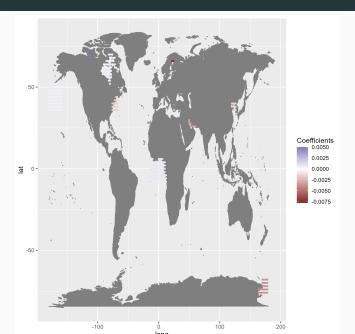
## **Full predictions**



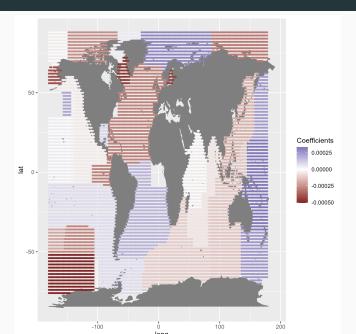
## Coefficient plot



## Coefficient plot, highest values only



## Coefficient plot, lowest values only



### Fused evaluation (maybe explain this when showing resutls)

- Generally same setting as for lasso, 5 folds with train and test, choose  $\lambda_{\min}$ , refit with  $\lambda_{\min}$ , get MSE on hold-out test set.
- But for the fused lasso we can not define the  $\lambda$  vector beforehand.
- $\lambda$ -path is found by dual path algorithm and the range of the paths can vary a lot!
- So to find  $\lambda_{\min}$  we search over the common range of all folds and interpolate to lines
- $\lambda_{\min}$  is then the  $\lambda$  that minimize MSE over all  $\lambda$  of that common range

## Graph structure

## Fused results

# Summary

# Important test

#### Important test

Ciemer, Catrin, Lars Rehm, Juergen Kurths, Reik V Donner, Ricarda Winkelmann, and Niklas Boers. 2020. "An Early-Warning Indicator for Amazon Droughts Exclusively Based on Tropical Atlantic Sea Surface Temperatures." Environmental Research Letters 15 (9): 094087.