

Simultaneous Treatment of Random and Systematic Errors in the Historical Radiosonde Temperature Archive

Josh Browning

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Project Overview

Problem: Random and systematic errors exist in the radiosonde temperature archive, and no studies have addressed how to handle both types of errors simultaneously.

Solution: I studied the effect of applying various sequences of quality control algorithms on simulated data which was designed to have the same structure as true radiosonde data.

Problems with the radiosonde data: Random Errors

Random errors can occur because of

1. Faulty data transmission
2. Sporadic instrumentation problems
3. Keystroke entries
4. Errors in data management
5. Many other reasons

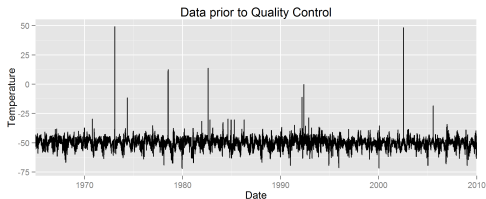


Figure: Data collected from Station 70219 in Bethel, Alaska.

Problems with the radiosonde data: Systematic Errors

Systematic errors can occur because of

1. Station location changes
2. Urbanization of the area surrounding the station
3. Changes in instrumentation
4. Many other reasons

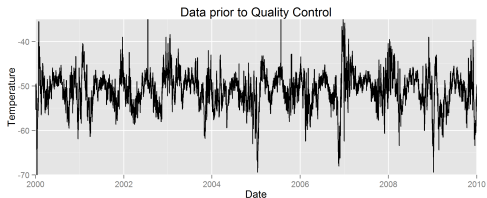


Figure: Data collected from Station 70219 in Bethel, Alaska.

Note on terminology

	Statistics	Climatology
Random Error	Any error which causes a measurement to differ from the true value. It does not necessarily lead to an extreme observation.	An observation which is incorrect and inconsistent with the rest of the data (in statistical terms, an outlier).
Systematic Error	The error for a set of observations whose mean value is biased from the true mean. The bias does not have to be constant but could follow some trend.	The error for a set of observations whose mean value has shifted from the true mean (i.e. a constant bias has been introduced). In statistical language, this is a “change point.”

For the rest of this presentation, I will use the climatological language.

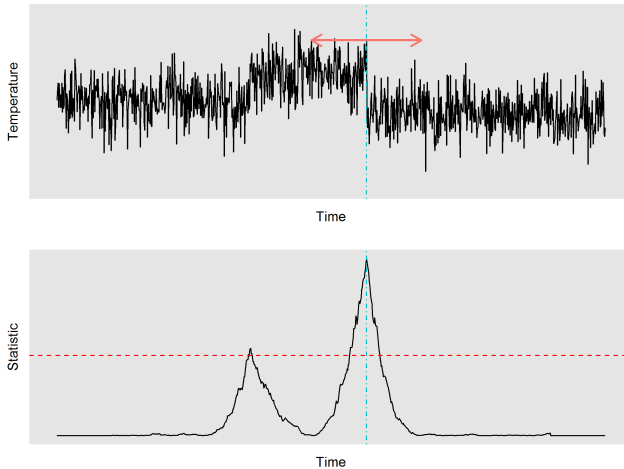
Random Error Detection Methods

- ▶ The simplest way to detect random errors is to estimate the mean and standard deviation of the data and then to label observations as random errors if they are more than k standard deviations from the mean (where k may be 5 or so).
- ▶ In Anderson et al. (2014), a better alternative is proposed which uses robust estimates of the mean and standard deviation.
- ▶ These estimators, called the winsorized mean and standard deviation(s), reduce the influence of extreme observations.

Systematic Error Correction (Homogenization)

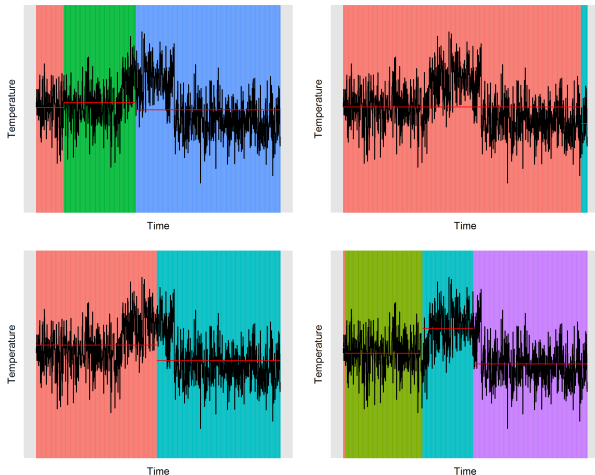
- ▶ Many homogenization methods have been proposed in the climate literature: Eskridge et al. (1995); Haimberger (2007); Lanzante (1996); Lanzante et al. (2003); Venema et al. (2012). However, these methods are not generally robust to outliers.
- ▶ Modern homogenization methods are also presented in the statistical literature Killick et al. (2012); Scott and Knott (1974).
- ▶ I'll compare the following methods:
 - ▶ Standard Normal Homogeneity Test (SNHT)
 - ▶ A proposed “Robust SNHT”, or the SNHT with robust estimators
 - ▶ Binary Segmentation (BinSeg)
 - ▶ Pruned Exact Linear Time (PELT)

Homogenization Methods: SNHT and Robust SNHT



- ▶ The SNHT statistic detects systematic errors by comparing the left and right mean to a threshold.
- ▶ The robust SNHT replaces the mean and standard deviation estimators with robust estimators.

Homogenization Methods: BinSeg and PELT



- ▶ Systematic errors can be detected by optimizing some cost function over all change point configurations.
- ▶ BinSeg optimizes this function greedily while PELT follows a more sophisticated approach.

Quality Control Algorithm Sequencing

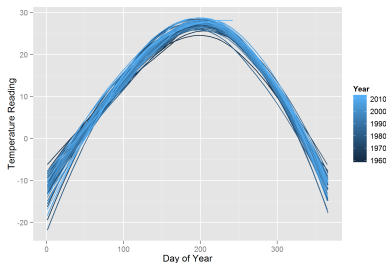
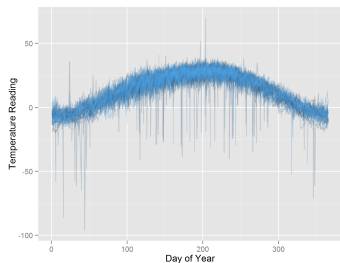
- ▶ I am also interested in understanding the effect that the sequence of the quality control algorithms has on the overall quality control procedure.
- ▶ Let “Ran” denote the random error detection algorithm and “Sys” the systematic error correction algorithm. Then, I investigate the following alternatives:
 - ▶ $\text{Ran} \rightarrow \text{Sys}$
 - ▶ $\text{Sys} \rightarrow \text{Ran}$
 - ▶ $\text{Ran} \rightarrow \text{Sys} \rightarrow \text{Ran}$
 - ▶ $\text{Sys} \rightarrow \text{Ran} \rightarrow \text{Sys}$

Overall Simulation Design

To understand the effect of these various algorithms/sequencings on the final quality controlled dataset, I used the following simulation design:

1. Model observed radiosonde data:
 - ▶ Fit a GAM to capture daily/seasonal/annual trends
 - ▶ Fit a skew- t distribution to the error terms
 - ▶ Model correlation in the error terms with an AR(1) model.
2. Simulate a dataset using the model from step 1, and contaminate it with systematic and random errors.
3. Apply the quality control algorithms described above to the simulated dataset, and determine
 - ▶ The best homogenization algorithms for sub-daily data in the presence of random errors
 - ▶ The best sequencing in the presence of both random and systematic errors
4. Repeat steps 2 and 3 1,000 times for each of 10 different radiosonde stations and 3 pressure levels.

Modeling Radiosonde Data



- ▶ During the proposal, a question was raised about our data-generating model and if the seasonal trend was consistent each year.
- ▶ The graphs above depict the yearly time series from station 51777 (left) and a scatterplot smoother fit to each year individually (right).

Performance Metrics

- ▶ **True Positive Rate:** The proportion of simulated errors correctly detected by the quality control algorithm.
- ▶ **False Positive Rate:** The proportion of valid data points incorrectly identified as errors by the quality control algorithm.
- ▶ **Efficiency:** Let \mathbf{x} , \mathbf{c} , and \mathbf{h} be the original, contaminated, and contaminated and homogenized time series, respectively and let the i -th observation be denoted by x_i , c_i , and h_i respectively. The Root Mean Square Error (RMSE) of \mathbf{h} is then defined as follows:

$$\text{RMSE}(\mathbf{h}) = \sqrt{\frac{1}{n} \sum_{i=1}^n (h_i - x_i)^2}.$$

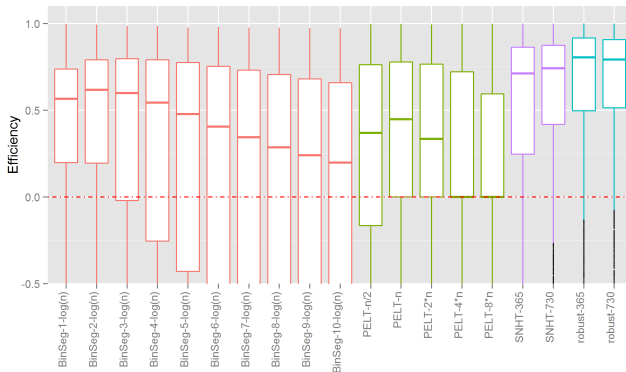
Then, the efficiency of the homogenized series, where 1 means perfect skill, 0 means no improvement, and negative values indicate degradation is

$$\text{Eff}(\mathbf{h}) = \frac{\text{RMSE}(\mathbf{c}) - \text{RMSE}(\mathbf{h})}{\text{RMSE}(\mathbf{c})}.$$

Tuning Parameters

- ▶ PELT: The cost function for PELT and BinSeg allow for an increase in the penalty as a function of the number of change points. Thus, I consider penalties of $\beta = n/2, n, 2n, 4n$, and $8n$.
- ▶ BinSeg: I use no penalty term and instead restrict the maximum number of change points that can occur, varying from 1 to 10.
- ▶ SNHT: This algorithm computes means of seasonal data, so periods which are multiples of a year should be considered. Thus, I use one and two year averaging windows with $N = 365$ or $N = 730$.
- ▶ Robust SNHT: I use $N = 365$ and $N = 730$.

Observed Efficiencies



- ▶ This plot depicts the observed efficiencies for the various homogenization algorithms.
- ▶ Most algorithms tend to have efficiencies above 0, but some of the BinSeg algorithms substantially overfit.
- ▶ This graph suggests that the SNHT and robust SNHT attain the highest efficiency, and that the robust version is slightly better than the traditional.

Logistic Regression Model Selection

- ▶ In order to analyze the results more effectively, and to understand the influence of different simulation parameters, I fit a logistic regression model to the results. Let Y_i be the probability that the efficiency is greater than 0 for the i th simulation, then

$$Y_i \sim \text{Bernoulli}(0, p_i), \quad g(p_i) = X_i \cdot \beta$$

where

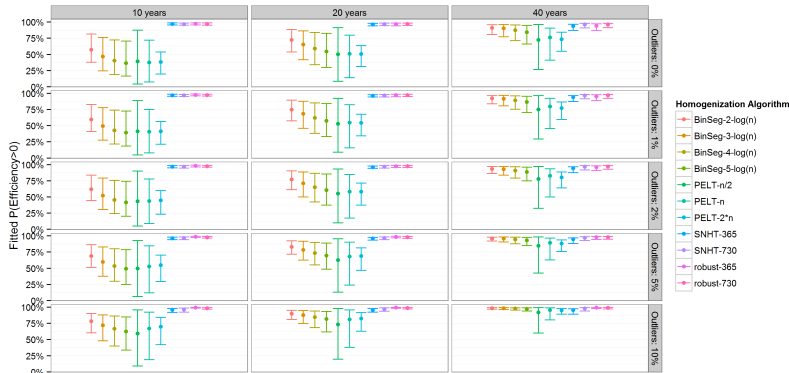
- ▶ $g(\cdot)$ is the logit link
- ▶ X is my design matrix consisting of sample size, outlier contamination rate, station, pressure, and homogenization algorithm.
- ▶ β is a vector of the estimated coefficients

Logistic Regression Model Selection

- ▶ I allowed for interaction effects, and considered models with only main effects up to models with all 5-way interactions.
- ▶ I used the deviance of these different models to assess model fit and choose which model to interpret.

Model Type	Deviance	% Reduction
Intercept Only	672836	—
Main Effects	529612	21.29%
2-Way Interactions	501158	5.37%
3-Way Interactions	490553	2.12%
4-Way Interactions	487125	0.70%
5-Way Interactions	486493	0.13%

Logistic Regression Model Coefficients



- ▶ Error bars indicate the range of simulated efficiencies due to the different input time series.
- ▶ This graph shows the SNHT algorithms greatly outperform all other methods in most cases.
- ▶ A table of performance metrics is available in my thesis.

The SNHT Statistic

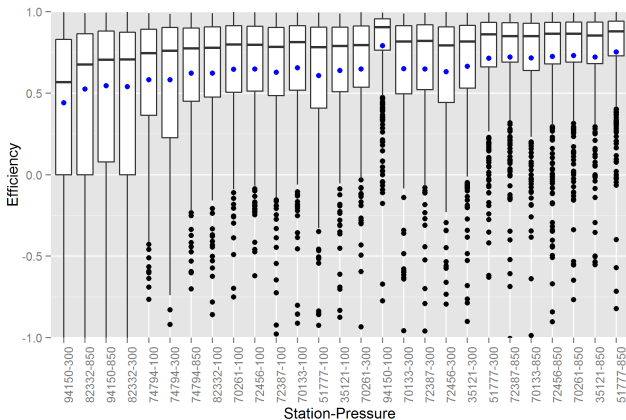
- ▶ For each time point, the SNHT test statistic is

$$T_i = \frac{N}{s_i} ((\bar{X}_{L,i} - \bar{X}_i)^2 + (\bar{X}_{R,i} - \bar{X}_i)^2),$$

where \bar{X}_i is the mean of $\bar{X}_{L,i}$ and $\bar{X}_{R,i}$, and s_i is the estimated standard deviation over the N days prior and N days following observation i .

- ▶ During my proposal, it was pointed out that T_i will depend on the variability of the time series, and that it might be more reasonable to replace s_i with s_i^2 .
- ▶ In Haimberger (2007), the above statistic is used. However, Haimberger (2007) references Alexandersson and Moberg (1997) for the SNHT, and in Alexandersson and Moberg (1997) the test statistic is defined with no s_i in the denominator because the X_i were already standardized.
- ▶ Thus, T_i is dependent on the variability of the time series and could be improved. However, it should be noted that the robust SNHT outperformed all other homogenization algorithms even with this lack of standardization.

More on the SNHT Statistic



- ▶ The above plot has station/pressure level combinations on the x-axis, with the standard deviation of the station/pressure level increasing from left to right.
- ▶ It is clear that the efficiency is dependent on the variability of the time series, and it will also depend on the autocorrelation of the time series.

More on the SNHT Statistic

- ▶ I plan on fixing this issue by replacing the original SNHT statistic with the correct statistic:

$$\begin{aligned} T_i &= \frac{N}{s_i^2} ((\bar{X}_{L,i} - \bar{X}_i)^2 + (\bar{X}_{R,i} - \bar{X}_i)^2) \\ &= \frac{2N}{s_i^2} (\bar{X}_{L,i} - \bar{X}_{R,i})^2 \end{aligned}$$

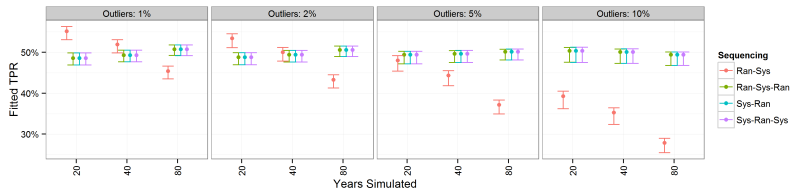
- ▶ Additionally, s_i will account for the autocorrelation of the time series \mathbf{X} , and thus T_i will be proportional to a χ_1^2 (provided \mathbf{X} is stationary and normal with a varying mean).

Logistic Model Deviances

Model Type	TPR		FPR		Efficiency	
	Deviance	% Reduction	Deviance	% Reduction	Deviance	% Reduction
Intercept Only	6240630	—	5835529	—	159942	—
Main Effects	4631181	25.79%	1244423	78.68%	136467	14.68%
2-Way Interactions	4101383	11.44%	279232	77.56%	132980	2.56%
3-Way Interactions	4058965	1.03%	258216	7.53%	132585	0.30%
4-Way Interactions	4049724	0.23%	255145	1.19%	132421	0.12%
5-Way Interactions	4047592	0.05%	254845	0.12%	132411	0.01%

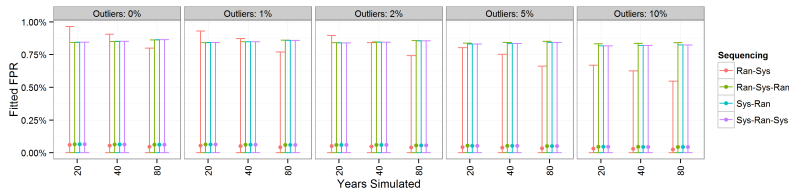
- ▶ Similar to the homogenization algorithm comparison, I fit a logistic regression model to the true positive, false positive, and efficiency results for the sequencing study.
- ▶ In all cases, I chose to use the 2-way interaction model, as that model seemed to attain a good deviance without too much complexity.

True Positive Rate Results



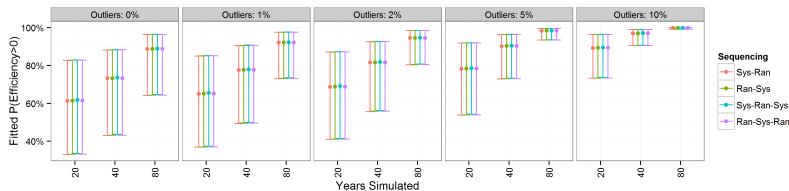
- ▶ In most cases, the true positive rate is maximized with a sequencing that has a random error check following a systematic error correction.
- ▶ The few exceptions are with small datasets and small contamination rates.
- ▶ There are very few differences between the other 3 sequencings considered.

False Positive Rate Results



- ▶ I again see more variability in the “Ran-Sys” sequencing.
- ▶ All false positive rates are extremely low, and I see no reason for choosing one sequencing over another based on these False Positive Rate alone.

Efficiency Results

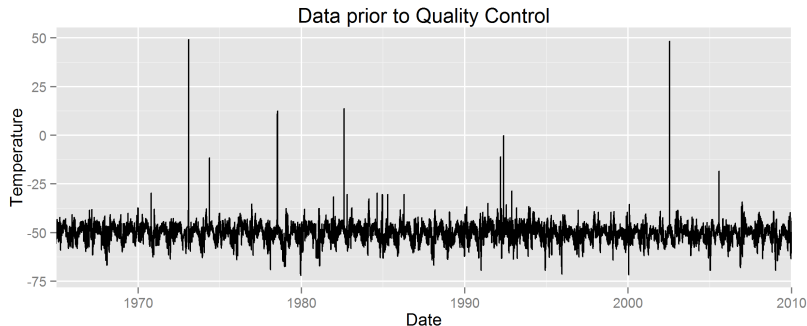


- ▶ Again, there are very little differences between the four proposed sequencings.

Conclusion

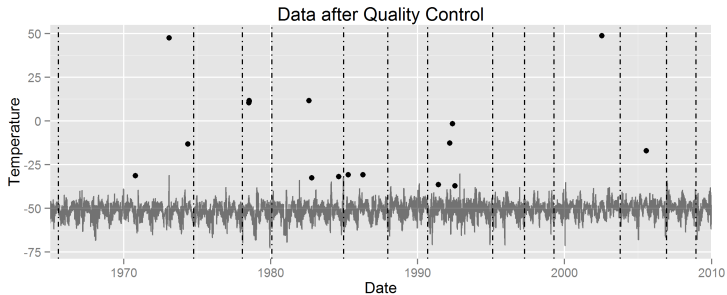
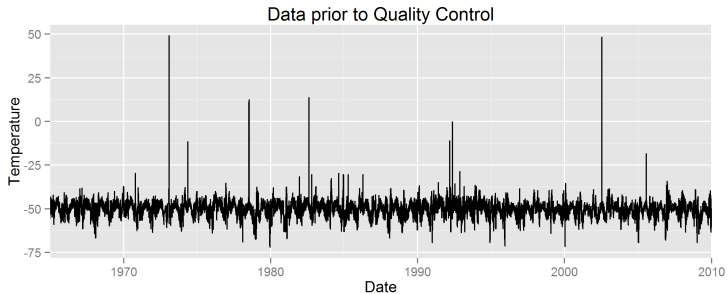
- ▶ The Robust SNHT achieves the highest efficiency across all homogenization algorithms.
- ▶ I recommend the sequence “Sys-Ran” for quality controlling radiosonde data. It outperforms “Ran-Sys” at detecting true errors, and is comparable in all other cases.
- ▶ I do not recommend the sequencings “Sys-Ran-Sys” or “Ran-Sys-Ran” as they do not appear to show any improvement over “Sys-Ran” and are certainly more computationally expensive.

Station 70219- Bethel, Alaska, USA

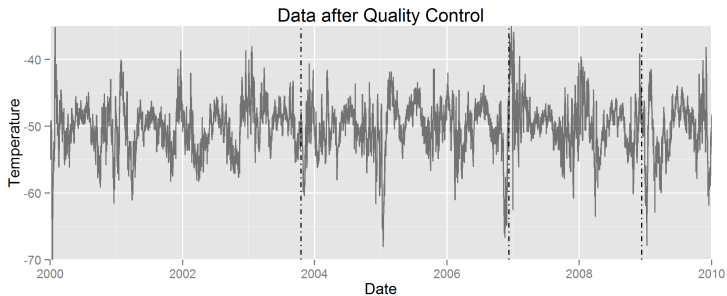
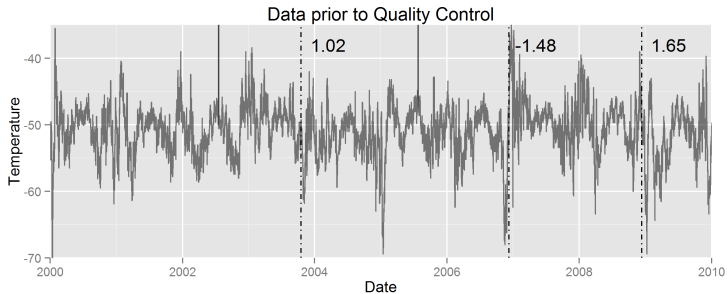


- ▶ This plot shows several obvious random errors in a radiosonde temperature dataset.
- ▶ Systematic errors are harder to detect my eye, especially at this scale.

Random Errors Removed



Systematic Errors Corrected



Future Work

- ▶ Redefine the SNHT statistic to
 - ▶ Correctly standardize by s^2 instead of s .
 - ▶ Robustly estimate the variance.
 - ▶ Model the temporal dependence and the influence this has on the variability of the sample means.
- ▶ Determine the sampling distribution of the test statistic in order to determine a threshold for systematic error detection.
- ▶ Apply the Benjamini-Hochberg correction for multiple dependent tests in order to appropriately adjust the threshold.

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Appendix

Radiosonde Data

Robust Mean and Standard Deviation

Homogenization Methods

Modeling Radiosonde Data

Variance of the SNHT Statistic

Radiosonde Data



Figure: Sample
Radiosonde

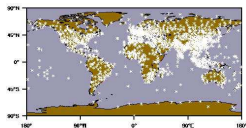


Figure: Global
Radiosonde Network

- ▶ Small instruments are suspended below 2m hydrogen or helium balloons.
- ▶ They measure atmospheric variables such as temperature, wind speed, etc.
- ▶ Balloons are launched twice daily at roughly 00 UTC and 12 UTC, and at 700 sites worldwide.
- ▶ More than 1,300 additional launch sites exist in the historical archive.
- ▶ Considering the number of launch sites, multiple observations for different pressure levels, and the total number of launches, there are between 50 and 90 million historical soundings.

Robust Mean and Standard Deviation

1. First, the estimates of the mean, $\hat{\mu}$, and standard deviation, $\hat{\sigma}$, are initialized to

$$\hat{\mu} = \text{median}(\mathbf{x})$$

$$\hat{\sigma} = \text{MAD}(\mathbf{x}),$$

where \mathbf{x} is a vector of the data, and MAD is the median absolute deviation, defined as

$$\text{MAD} = \text{median}(|x_i - \text{median}(\mathbf{x})|).$$

2. Then, Winsorized values, y_i , are computed. These are defined as

$$y_i = \begin{cases} \hat{\mu} - k\hat{\sigma} & : x_i \leq \hat{\mu} - k\hat{\sigma} \\ x_i & : \hat{\mu} - k\hat{\sigma} < x_i \leq \hat{\mu} + k\hat{\sigma} \\ \hat{\mu} + k\hat{\sigma} & : x_i > \hat{\mu} + k\hat{\sigma} \end{cases}$$

3. Updated estimates of $\hat{\mu}$ and $\hat{\sigma}$ are computed as the mean of \mathbf{y} and the standard deviation of \mathbf{y} , respectively.
4. Steps 2 and 3 are repeated until $\hat{\mu}$ changes by less than $10^{-6}\hat{\sigma}$.

Note: In step 3, one may choose to estimate $\hat{\sigma}_L$ and $\hat{\sigma}_R$ using only observations to the left and right, respectively, of the mean. This allows for improved outlier detection with skewed data.

Homogenization Methods: SNHT

This algorithm is commonly used in the climate literature. The algorithm works as follows:

1. For each observation, two means are computed: one for the N days prior to observation i , $\bar{X}_{L,i}$, and one for the N days following, $\bar{X}_{R,i}$
2. Then, the test statistic

$$T_i = \frac{N}{s_i} ((\bar{X}_{L,i} - \bar{X}_i)^2 + (\bar{X}_{R,i} - \bar{X}_i)^2), \quad (1)$$

is computed where \bar{X}_i is the mean of $\bar{X}_{L,i}$ and $\bar{X}_{R,i}$, and s_i is the estimated standard deviation over the N days prior and N days following observation i .

3. If the largest T_i exceeds some threshold at time $i = i^*$, I conclude that a change point occurred at time i^* , and I adjust all observations after time i^* by $\bar{X}_{L,i^*} - \bar{X}_{R,i^*}$. A threshold of 100 is recommended in Haimberger (2007).
4. Repeat steps 1-3 until no test statistic exceeds the threshold.

Homogenization Methods: Robust SNHT

- ▶ The previous algorithm is not robust to random errors, as the influence function for the sample mean is unbounded.
- ▶ The Winsorized estimator of center and scale discussed previously is robust against random errors.
- ▶ Thus, to create a robust SNHT statistic, I propose replacing the means and standard deviation in Equation (1) with these estimators.

Homogenization Methods: BinSeg

- ▶ Several homogenization methods work by optimizing a cost function:

$$\sum_{i=1}^{m+1} [\mathcal{C}(y_{(\tau_{i-1}+1):\tau_i})] + \beta f(m), \quad (2)$$

where τ_i is the i th change point; m is the number of change points; \mathcal{C} is a cost function; $y_{(\tau_{i-1}+1):\tau_i}$ is the observed data between the $(i-1)$ and i th change point; and $\beta f(m)$ is a penalty term on the number of change points, see Killick et al. (2012).

- ▶ Often, \mathcal{C} is chosen to be twice the negative log likelihood, and $f(\cdot)$ is linear.
- ▶ Binary Segmentation (BinSeg) uses a greedy algorithm: at each step, a changepoint is selected which minimizes the cost function. The data is then partitioned in two, and optimization continues iteratively.

Homogenization Methods: PELT

- ▶ Pruned Exact Linear Time (PELT) is another algorithm for optimizing Equation (2), but it computes the exact minimum.
- ▶ It proceeds recursively as follows: first, the optimal number and location of change points is determined for observations 1 and 2 only. The optimal number and location of change points for the first three observations is then determined using this information, and more generally the optimal number and location of change points for the first $k + 1$ observations is determined by considering the optimal configurations for the first $2, 3, \dots, k$ observations.
- ▶ PELT is computationally efficient, and is implemented in the changepoint package in R Killick and Eckley (2014).

Modeling Radiosonde Data- Part 1

1. In order to capture seasonal and hourly trends, I plan on fitting a Generalized Additive Model (GAM) to the radiosonde temperature data.
2. GAMs are flexible, non-parametric models that allow the response variable to be a linear combination of smoothed functions of the input variables, see Hastie and Tibshirani (1990).
3. The particular model I'll fit is

$$t_i = \beta_0 + s_1(h_i) + s_2(d_i) + \beta_1 y_i + \epsilon_i, \quad (3)$$

where t_i is the temperature at a given station and pressure level; h_i , d_i and y_i are the hour, day, and year of the i -th observation, respectively; β_0 is the intercept; β_1 is the coefficient for the long term trend; and $s_1(\cdot)$ and $s_2(\cdot)$ are cubic regression splines.

Modeling Radiosonde Data- Part 2

1. Typically the error term, ϵ_i , in the GAM model would be modeled as normal with some unknown variance, but the distribution of the error terms could be skewed or have heavier tails than a normal distribution.
2. Thus, I'll use a skew- t distribution for the errors of this model, which has 4 parameters, ξ, σ, α , and ν which are useful in controlling the first four moments of the distribution, see Azzalini and Capitanio (2003).

Modeling Radiosonde Data- Part 3

1. Additionally, I expect there to be temporal correlation in the error terms.
2. Since I have already included hourly and seasonal terms in the model, I expect most of this autocorrelation to be explained, and so an AR(1) time series model is sufficient to account for the remaining structure in the residuals.
3. For radiosonde data, observations are not equally spaced in time: Launches are scheduled globally at 0 and 12 UTC, but many deviations from this pattern are observed.
4. Thus, to estimate the lag- h autocorrelation, $\phi(h)$, in hours, I must use only those observations that are h time steps apart:

$$\hat{\phi}(h) = \frac{1}{|\mathcal{P}_h|} \sum_{(\hat{\epsilon}_i, \hat{\epsilon}_j) \in \mathcal{P}_h} \frac{(\hat{\epsilon}_i - \bar{\epsilon}_i)(\hat{\epsilon}_j - \bar{\epsilon}_j)}{\sqrt{s_{\epsilon_i} s_{\epsilon_j}}}, \quad (4)$$

where \mathcal{P}_h is the set of all pairs of residuals that are h hours apart (or within some window), and $\hat{\epsilon}_i$ is the observed residual from Equation (3).

5. For an AR(1) model, I need only estimate $\phi(\cdot)$ at $h = 12$ hours, and I plan on using a window of 5% of 12 hours, or 0.6 hours.

Modeling Radiosonde Data- Part 4

1. After a simulated dataset is generated, it is contaminated with random and systematic errors.
2. Random errors are generated by sampling 1, 2, 5 or 10% of the observations and adding or subtracting a random error following a distribution of $N(10\sigma, 1\sigma^2)$, where σ^2 is the standard deviation of the simulated series, estimated from the GAM model.
3. Systematic errors are generated by sampling 1, 2, or 3 observations uniformly per simulated decade and then drawing a break size from a $N(0, 0.04\sigma^2)$. The break size is then added to all observations after the change point.

Variance of the SNHT Statistic

- ▶ The new test statistic is

$$T_i = \frac{2N}{s_i^2} (\bar{X}_{L,i} - \bar{X}_{R,i})^2$$

where s_i^2 is the variance of $\bar{X}_{Li} - \bar{X}_{Ri}$.

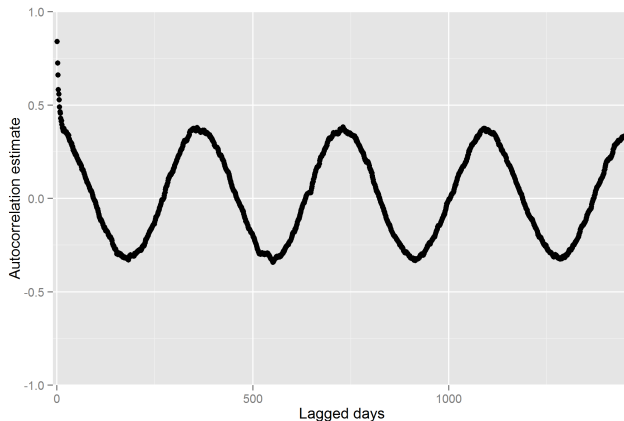
- ▶ I will assume the X_i are normal with some mean that depends on the hour of the day and the day of the year.
- ▶ $\bar{X}_{Li} - \bar{X}_{Ri}$ will then be normal with mean 0 (assuming \mathbf{X} is stationary) with variance

$$\frac{1}{N^2} (\mathbf{1}, -\mathbf{1}) \Sigma (\mathbf{1}, -\mathbf{1})^T$$

where $\mathbf{1}$ is a vector of N 1's and Σ is the $2N \times 2N$ covariance matrix for

$X_{i-N}, X_{i-N+1}, \dots, X_{i-2}, X_{i-1}, X_{i+1}, X_{i+2}, \dots, X_{i+N}$.

Modeling Σ



- ▶ To estimate Σ (from the previous slide), I'll model the autocorrelation function individually for each series.
- ▶ The plot above depicts the autocorrelation estimated at one particular station.