

Algorithms for Estimating Trends in Global Temperature Volatility

Author 1 and Author 2

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Abstract

Trends in terrestrial temperature variability are perhaps more relevant for species viability than trends in mean temperature. In this paper, we develop methodology for estimating such trends using multi-resolution climate data from polar orbiting weather satellites. We derive two novel algorithms for computation that are tailored for dense, gridded observations over both space and time. We evaluate our methods with a simulation constructed to mimic these data's features and on a large, publicly available, global temperature dataset with the eventual goal of tracking trends in cloud reflectance temperature variability.

1 Introduction

The amount of sunlight reflected from clouds is among the largest sources of uncertainty in climate prediction (Boucher et al. 2013). But climate models fail to reproduce global cloud statistics, and understanding the reasons for this failure is a grand challenge of the World Climate Research Programme (Bony et al. 2015). While numerous studies have examined the overall impacts of clouds on climate variability (Myers, Mechoso, and DeFlorio 2018; Grise et al. 2013; Bender, Ramanathan, and Tselioudis 2012), such investigations have been hampered by the lack of a suitable dataset. Ideal data would have global coverage at high spatial resolution, a long enough record to recover temporal trends, and be multispectral (Wielicki et al. 2013). Current work (Staten et al. 2016; Schreier et al. 2010; Kahn et al. 2007) seeks to create a spectrally-detailed dataset by combining radiance data from Advanced Very High Resolution Radiometer imagers with readings from High-resolution Infrared Radiation Sounders on board legacy satellites. In anticipation of this new dataset, our work develops novel methodology for examining the trends in variability of climate data across space and time.

1.1 Variability Rather Than Average

Trends in terrestrial temperature variability are perhaps more relevant for species viability than trends in mean temperature (Huntingford et al. 2013), because an increase in temperature variability will increase the probability of extreme hot outliers (Vasseur et al. 2014). Recent climate

literature suggests that it is more difficult for society to adapt to these extremes than to the gradual increase in the mean temperature (Hansen, Sato, and Ruedy 2012; Huntingford et al. 2013). Furthermore, the willingness of popular media to emphasize the prevalence extreme cold events coupled with a fundamental misunderstanding of the relationship between climate (the global distribution of weather over the long run) and weather (observed short-term, localized behavior) leads to public misunderstanding of climate change. In fact, a point of active debate is the extent to which the observed increased frequency of extreme cold events in the northern hemisphere can be attributed to increases in temperature variance rather than to increases in mean climate (Screen 2014; Fischer, Beyerle, and Knutti 2013; Trenberth et al. 2014).

Nevertheless, research examining trends in the volatility of spatio-temporal climate data is scarce. Hansen, Sato, and Ruedy (2012) studied the change in the standard deviation (SD) of the surface temperature in the NASA Goddard Institute for Space Studies gridded temperature data set by examining the empirical SD at each spatial location relative to that location's SD over a base period, and showed that these estimates are increasing. Huntingford et al. (2013) took a similar approach in analyzing the ERA-40 data set. They argued that, while there is an increase in the SDs from 1958-1970 to 1991-2001, it is much smaller than found in (Hansen, Sato, and Ruedy 2012). Huntingford et al. (2013) also computed the time-evolving global SD from the de-trended time-series at each position and argued that the global SD has been stable.

These and other related work (Rhines and Huybers 2013, e.g.,) have several shortcomings. First, no statistical analysis has been performed to examine if the changes in the SD are statistically significant. Second, the methodologies for computing the SDs are highly sensitive to the choice of base period. Third, and most importantly, temporal and spatial correlations between observations are completely ignored.

In the present work, we examine variance (rather than the mean) for a number of reasons. First, instrument bias in the satellites increases over time so examining the mean over time conflates that bias with any actual change in mean (though the variance is unaffected). Second, extreme weather events (hurricanes, droughts, wildfires in California, heat-waves in Europe) may be driven more strongly by increases in variance than by increases in mean. Finally, even if the global

mean temperature is constant, there may still be climate change. In fact, atmospheric physics suggests that, across space, average temperatures should not change (extreme cold in one location is offset by heat in another). But if swings across space are becoming more rapid, then, even with no change in mean global temperature over time, increasing variance can lead to increases in the prevalence of extreme events.

1.2 Main Contributions

The main contribution of this work is to develop a new methodology for detecting the trend in the volatility of spatio-temporal data. In this methodology, the variance at each position and time are estimated by maximizing penalized likelihood maximization. Following (Tibshirani 2014), we penalize the differences between the estimated variances which are temporally and spatially “close”, resulting in a generalized LASSO problem. However, in our application, the dimension of this optimization problem is massive, so the standard solvers are inadequate.

We develop two algorithms which are computationally feasible on extremely large data. In the first method, we adopt an optimization technique called alternating direction method of multipliers (ADMM, Boyd et al. 2011), to divide the total problem into several sub-problems of much lower dimension and show how the total problem can be solved by iteratively solving these sub-problems. The second method, called linearized ADMM (Parikh and Boyd 2014), solves the main problem by iteratively solving a linearized version of it. We will compare the benefits of each method.

Our main contributions are as follows:

1. We propose a model for nonparametric variance estimation for a spatio-temporal process and discuss the relationship between our methods and those existing in the machine learning literature (Section 2).
2. We derive two alternating direction method of multiplier algorithms (ADMM) to fit our estimator when applied to very large data (Section 3). We give situations under which each algorithm is most likely to be useful. Open-source Python code is available on [github](#).
3. Because the construction of satellite-based datasets is ongoing and currently proprietary, we illustrate our methods on a large, publicly available, global temperature dataset. The goal is to demonstrate the feasibility of these methods for tracking world-wide trends in variance in standard atmospheric data and a simulation constructed to mimic these data’s features (Section 4).

While the motivation for our methodology is its application to large, gridded climate data, we note that our algorithms are also applicable to neuroimaging, image denoising, or examining large collections of financial instruments.

2 Smooth Spatio-temporal Variance Estimation

Kim et al. (2009) proposed ℓ_1 -trend filtering as a method for estimating a smooth, time-varying trend. It is formulated as

the optimization problem

$$\min_{\beta} \frac{1}{2} \sum_{t=1}^T (y_t - \beta_t)^2 + \lambda \sum_{t=1}^{T-2} |\beta_t - 2\beta_{t+1} + \beta_{t+2}|$$

or equivalently:

$$\min_{\beta} \frac{1}{2} \|y - \beta\|_2^2 + \lambda \|D_t \beta\|_1 \quad (1)$$

where $y = \{y_t\}_{t=1}^T$ is an observed time-series, $\beta \in \mathbb{R}^T$ is the smooth trend, D_t is a $(T-2) \times T$ matrix, and λ is a tuning parameter which balances fidelity to the data (small errors in the first term) with a desire for smoothness. Kim et al. (2009) proposed a specialized primal-dual interior point (PDIP) algorithm for solving (1). From a statistical perspective, (1) can be viewed as a constrained maximum likelihood problem with independent observations from a normal distribution with common variance, $y_t \sim N(\beta_t, \sigma^2)$, subject to a piecewise linear constraint on β . Alternatively, solutions to (1) are maximum a posteriori Bayesian estimators based on Gaussian likelihood with a special Laplace prior distribution on β . Note that the structure of the estimator is determined by the penalty function $\lambda \|D_t \beta\|_1$ rather than any parametric trend assumptions—autoregressive, moving average, sinusoidal seasonal component, etc. The resulting trend is therefore essentially nonparametric in the same way that splines are nonparametric. In fact, using squared ℓ_2 norm as the penalty instead of ℓ_1 results exactly in regression splines.

2.1 Modifications for Variance

Inspired by the ℓ_1 -trend filtering algorithm, we propose a non-parametric model for estimating the variance of a time-series. To this end, we assume that at each time step t , there is a parameter h_t such that the observations y_t are independent normal variables with zero mean and variance $\exp(h_t)$. The negative log-likelihood of the observed data in this model is $l(y | h) \propto -\sum_{t=1}^T h_t - y_t^2 e^{-h_t}$. Crucially, we assume that the parameters h_t vary smoothly and estimate them by minimizing the penalized, negative log-likelihood:

$$\min_h -l(y | h) + \lambda \|D_t h\|_1 \quad (2)$$

where D_t has the same structure as above.

As with (1), one can solve (2) using the PDIP algorithm (as in, e.g., [cvxopt](#), Andersen, Dahl, and Vandenberghe 2013). In each iteration of PDIP we need to compute a search direction by taking a Newton step on a system of nonlinear equations. For completeness, we provide the details in Appendix A of the Supplement, where we show how to derive the dual of this optimization problem and compute the first and second derivatives of the dual objective function.

2.2 Adding Spatial Constraints

The method in the previous section can be used to estimate the variance of a single time-series. Here we extend this method to the case of spatio-temporal data.

At a specific time t , the data are measured on a grid of points with n_r rows and n_c columns for a total of $S = n_r \times n_c$ spatial locations. Let y_{ijt} denote the value of the

observation at time t on the i^{th} row and j^{th} column of the grid, and h_{ijt} denote the corresponding parameter. We seek to impose both temporal and spatial smoothness constraints on the hidden variables. Specifically, we seek a solution for h which is piecewise linear in time and piecewise constant in space (although higher-order smoothness can be imposed with minimal alterations to the methodology). We achieve this goal by solving the following optimization problem:

$$\begin{aligned} \min_h \sum_{i,j,t} h_{ijt} + y_{ijt}^2 e^{-h_{ijt}} + \lambda_t \sum_{i,j} \sum_{t=1}^{T-2} |h_{ijt} - 2h_{i,j(t+1)} + h_{i,j(t+2)}| \\ + \lambda_s \sum_{t,j} \sum_{i=1}^{n_r-1} |h_{ijt} - h_{(i+1)jt}| + \lambda_s \sum_{t,i} \sum_{j=1}^{n_c-1} |h_{ijt} - h_{i(j+1)t}| \end{aligned} \quad (3)$$

The first term in the objective is proportional to the negative log-likelihood, the second is the temporal penalty for the time-series at each location (i, j) , while the third and fourth, penalize the difference between the estimated variance of two vertically and horizontally adjacent points, respectively. The spatial component of this penalty is a special case of trend filtering on graphs (Wang et al. 2016) which penalizes the difference between the estimated values of the signal on the connected nodes (though the likelihood is different). As before, we can write (3) in matrix form where h is a vector of length TS and D_t is replaced by $D \in \mathbb{R}^{(N_t+N_s) \times (T \cdot S)}$, where $N_t = S \cdot (T-2)$ and $N_s = T \cdot (2n_r n_c - n_r)$ are the number of temporal and spatial constraints, respectively. Then, as we have two different tuning parameters for the temporal and spatial components, we write $\Lambda = [\lambda_t \mathbf{1}_{N_t}^\top, \lambda_s \mathbf{1}_{N_s}^\top]^\top$ leading to:¹

$$\min_h -l(y | h) + \Lambda^\top |Dh|. \quad (4)$$

2.3 Related Work

Variance estimation for financial time series has a lengthy history, focused especially on parametric models like the generalized autoregressive conditional heteroskedasticity (GARCH) process (Engle 2002) and stochastic volatility models (Harvey, Ruiz, and Shephard 1994). These models (and related AR processes) are specifically for parametric modelling of short “bursts” of high volatility, behavior typical of financial instruments. Parametric models for spatial data go back at least to (Besag 1974) who proposed a conditional probability model on the lattice for examining plant ecology.

More recently, nonparametric models for both spatial and temporal data have focused on using ℓ_1 -regularization for trend estimation. Kim et al. (2009) proposed ℓ_1 -trend filtering for univariate time series, which forms the basis of our methods. These methods have been generalized to higher order temporal smoothness (Tibshirani 2014), graph dependencies (Wang et al. 2016), and, most recently, small, time-varying graphs (Hallac et al. 2017).

Our methodology is similar in flavor to (Hallac et al. 2017) or related work in (Gibberd and Nelson 2017; Monti et al. 2014), but with several fundamental differences. These papers aim to discover the time-varying structure of a network.

¹Throughout the paper, we use $|x|$ for both scalars and vectors. For vectors we use this to denote a vector obtained by taking the absolute value of each entry of x .

To achieve this goal, they use Gaussian likelihood with unknown precision matrix and introduce penalty terms which (1) encourage sparsity among the off-diagonal elements and (2) discourage changes in the estimated inverse covariance matrix from one time-step to the next. Our goal in the present work is to detect the temporal trend in the variance of each point in the network, but the network is known (corresponding to the grid over the earth). To modify the objective function in (Hallac et al. 2017, Eq. 2), we would enforce complete sparsity on the off-diagonal elements (since they are not estimated) and add a new penalty to enforce spatial behavior across the diagonal elements. Thus, (4) is not simply a special case of these existing methods. Finally, these papers examine networks with hundreds of nodes and dozens to hundreds of time points. As discussed next, our data are significantly larger than these networks and attempting to estimate a full covariance would be prohibitive, were it required.

3 Optimization Methods

For a spatial grid of size S and T time steps, D in equation 4 will have $3Tn_r n_c - 2n_r n_c - Tn_r$ rows and $S \cdot T$ columns. For a $1^\circ \times 1^\circ$ grid over the entire northern hemisphere and daily data over 10 years, we have $S = 90 \times 360 \approx 32,000$ spatial locations and $T = 3650$ time points, so D has approximately 10^8 columns and 10^8 rows. In principal, we could solve (4) using PDIP as before, however, each iteration requires solving a linear system of equations which depends on $D^\top D$. Therefore, applying the PDIP directly is infeasible for our data.²

In the next section, we develop two ADMM algorithms for solving this problem efficiently. The first casts the problem as a so-called consensus optimization problem (Boyd et al. 2011) which solves smaller sub-problems using PDIP and then recombines the results. The second uses proximal methods to avoid matrix inversions.

3.1 Consensus Optimization

Consider an optimization problem of the form $\min_h f(h)$, where $h \in \mathbb{R}^n$ is the *global variable* and $f(h) : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{+\infty\}$ is convex. Consensus optimization breaks this problem into several smaller sub-problems that can be solved independently in each iteration.

Assume it is possible to define a set of local variables $x_i \in \mathbb{R}^{n_i}$ such that $f(h) = \sum_i f_i(x_i)$, where each x_i is a subset of the global variable h . More specifically, each entry of the local variables corresponds to an entry of the global variable. Therefore we can define a mapping $\mathcal{G}(i, j)$ from the local variable indices into the global variable indices: $k = \mathcal{G}(i, j)$ means that the j^{th} entry of x_i is h_k (or $(x_i)_j = h_k$). For ease of notation, define $\tilde{h}_i \in \mathbb{R}^{n_i}$ as $(\tilde{h}_i)_j = h_{\mathcal{G}(i,j)}$. Then, the original optimization problem is equivalent to the following

²We note that D is a highly structured, sparse matrix, but, unlike trend filtering alone, it is not banded. We are unaware of general linear algebra techniques for inverting such matrix, despite our best efforts to find them.

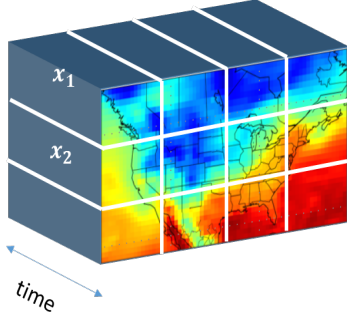


Figure 1: The cube represents the global variable h in space and time. The sub-cubes specified by the white lines are x_i .

problem:

$$\min_{\{x_1, \dots, x_N\}} \sum_{i=1}^N f_i(x_i) \quad \text{s.t.} \quad \tilde{h}_i = x_i. \quad (5)$$

It is important to note that each entry of the global variable may correspond to several entries of the local variables and so the constraints $\tilde{h}_i = x_i$ enforce the consensus between the local variables corresponding to the same global variable. The augmented Lagrangian corresponding to (5) is $L_\rho(x, h, y) = \sum_i (f_i(x_i) + u_i^\top (x_i - \tilde{h}_i) + (\rho/2) \|x_i - \tilde{h}_i\|_2^2)$. Now, we can apply ADMM to L_ρ . This results in solving N independent optimization problems followed by a step to achieve consensus among the solutions in each iteration. To solve the optimization problem (4) using this method, we need to address two questions: first, how to choose the local variables x_i , and second, how to update them.

In Figure 1, the global variable h is represented as a cube. We decompose h into sub-cubes as shown by white lines. Each global variable inside the sub-cubes corresponds to only one local variable. The global variables on the border (white lines), however, correspond to more than one local variable. With this definition of x_i , the objective (4) decomposes as $\sum_i f_i(x_i)$ where $f_i(x_i) = -l(y_i | x_i) + \Lambda_{(i)}^\top |D_{(i)} x_i|$, and $\Lambda_{(i)}$ and $D_{(i)}$ contain the temporal and spatial penalties corresponding to x_i only in one sub-cube along with its boundary. Thus, we now need to use PDIP to solve N problems each of size n_i , which is feasible for small enough n_i . Algorithm 1 gives the general version of this algorithm. A more detailed discussion of this is in Appendix B of the Supplement where we show how to compute the dual and the derivatives of the augmented Lagrangian.

Because consensus ADMM breaks the large optimization into sub-problems that can be solved independently, it is amenable to a split-gather parallelization strategy via, e.g., the map reduce framework. In each iteration, the computation time will be equal to the time to solve each sub-problem plus the time to communicate the solutions on the master processor and perform the consensus step. Since each sub-problem is small, with parallelization, the computation time in each iteration will be small. In addition, our experiments with several values of λ_t and λ_s showed that the algorithm

Algorithm 1 Consensus ADMM

- 1: **Input:** data y , penalty matrix D , ϵ , ρ , λ_t , $\lambda_s > 0$.
 - 2: **Set:** $h \leftarrow 0$, $z \leftarrow 0$, $u \leftarrow 0$. ▷ Initialization
 - 3: **repeat**
 - 4: $x_i \leftarrow \underset{x_i}{\operatorname{argmin}} -l(y_i | x_i) + \Lambda_{(i)}^\top |D_{(i)} x_i| + (u_i)^\top x_i + (\rho/2) \|x_i - \tilde{h}_i\|_2^2$.
▷ Update local vars using PDIP
 - 5: $h_k \leftarrow (1/S_k) \sum_{\mathcal{G}(i,j)=k} (x_i)_j$. ▷ Global update.
 - 6: $u_i \leftarrow u_i + \rho(x_i - \tilde{h}_i)$. ▷ Dual update
 - 7: **until** $\max \{ \|h^{m+1} - h^m\|, \|h^m - x^m\| \} < \epsilon$
 - 8: **Return:** h .
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converges in a few hundred iterations. This algorithm is most useful if we can parallelize the computation over several machines with low communication cost between machines. In the next section, we describe another algorithm which makes the computation feasible on a single machine.

3.2 Linearized ADMM

Consider the generic optimization problem $\min_x f(x) + g(Dx)$ where $x \in \mathbb{R}^n$ and $D \in \mathbb{R}^{m \times n}$. Each iteration of the linearized ADMM algorithm (Parikh and Boyd 2014) for solving this problem has the form

$$\begin{aligned} x &\leftarrow \underset{\mu f}{\operatorname{prox}} (x - (\mu/\rho) D^\top (Dx - z + u)) \\ z &\leftarrow \underset{\rho g}{\operatorname{prox}} (z + u) \\ u &\leftarrow u + Dx - z \end{aligned}$$

where the algorithm parameters μ and ρ satisfy $0 < \mu < \rho / \|D\|_2^2$, $z, u \in \mathbb{R}^m$ and the proximal operator is defined as $\operatorname{prox}_{\alpha \varphi}(u) = \min_x \alpha \cdot \varphi(x) + \frac{1}{2} \|x - u\|_2^2$. Proximal algorithms are feasible when these proximal operators can be evaluated efficiently which, as we show next, is the case.

Lemma 1. Let $f(x) = \sum_k x_k + y_k^2 e^{-x_k}$ and $g(x) = \|x\|_1$. Then,

$$\begin{aligned} [\operatorname{prox}_{\mu f}(u)]_k &= \mathcal{W} \left(\frac{y_k^2}{\mu} \exp \left(\frac{1 - \mu u_k}{\mu} \right) \right) + \frac{1 - \mu u_k}{\mu}, \\ \operatorname{prox}_{\rho g}(u) &= S_{\rho \lambda}(u) \end{aligned}$$

where $\mathcal{W}(\cdot)$ is the Lambert W function (Corless et al. 1996), $[S_\alpha(u)]_k = \operatorname{sign}(u_k)(|u_k| - \alpha_k)_+$ and $(v)_+ = v \vee 0$.

The proof is fairly straightforward and given in Appendix B in the Supplement. Therefore, Algorithm 2 gives a different method for solving the same problem. For this algorithm, both the primal update and the soft thresholding step are performed elementwise at each point of the spatio-temporal grid. It can therefore be extremely fast to perform these steps. However, because there are now many more dual variables, this algorithm will require more outer iterations to achieve consensus. It therefore is highly problem and architecture dependent whether Algorithm 1 or Algorithm 2 will be more useful in any particular context. In our experience, Algorithm 1 converges in many fewer iterations, but each iteration is much slower unless carefully parallelized.

Algorithm 2 Linearized ADMM

1: **Input:** data y , penalty matrix D , ϵ , ρ , λ_t , $\lambda_s > 0$.
2: **Set:** $h \leftarrow 0$, $z \leftarrow 0$, $u \leftarrow 0$. \triangleright Initialization
3: **repeat**
4: $h_k \leftarrow \mathcal{W}\left(\frac{y_k^2}{\mu} \exp\left(\frac{1-\mu u_k}{\mu}\right)\right) + \frac{1-\mu u_k}{\mu}$ for all $k = 1, \dots, TS$. \triangleright Primal update
5: $z \leftarrow S_{\rho\lambda}(u)$. \triangleright Elementwise soft thresholding
6: $u \leftarrow u + Dh - z$. \triangleright Dual update
7: **until** $\max\{\|Dh - z\|, \|z^{m+1} - z^m\|\} < \epsilon$
8: **Return:** z .

Table 1: Parameters used to simulate data.

s	r_s	c_s	σ_s	α_s	ω_s	ϕ_s
1	0	0	5	0.5	0.121	0
2	0	5	5	0.1	0.121	0
3	3	0	5	-0.5	0.121	$\pi/2$
4	3	5	5	-0.1	0.121	$\pi/2$

4 Empirical Evaluation

In this section, we examine both simulated and real spatio-temporal climate data. All the computations were performed on a Linux machine with four 3.20GHz Intel i5-3470 cores.

4.1 Simulations

Before examining real data, we apply our model to some synthetic data. This example was constructed to mimic the types of spatial and temporal phenomena observable in typical climate data. We generate a complete spatio-temporal field wherein observations at all time steps and all locations are independent Gaussian random variables with zero mean. However, the variance of these random variables follows a smoothly varying function in time and space given by the following parametric model:

$$\sigma^2(t, r, c) = \sum_{k=1}^K W_k(t) \cdot \exp\left(\frac{(r - r_k)^2 + (c - c_k)^2}{2\sigma_k^2}\right)$$

$$W_k(t) = \alpha_k \cdot t + \exp(\sin(2\pi\omega_k t + \phi_k)).$$

The variance at each time and location is computed as the weighted sum of K bell-shaped functions where the weights are time-varying, consist of a linear trend $\alpha_k \cdot t$ and a periodic term $\beta_k \cdot \sin(2\pi\omega_k t + \phi_k)$. The bell-shaped functions impose spatial smoothness while the linear trend and the periodic terms enforce the temporal smoothness similar to the seasonal component in the real climate data. We simulated the data on a 5 by 7 grid and for 780 time steps with $K = 4$. This yields a small enough problem so that it can be evaluated many times while still mimicking important properties of climate data. Specific parameter choices of the variance function are shown in Table 1. For illustration, we also plot the variance function for all locations at $t = 25$ and $t = 45$ (Figure 2, top panel) as well as the variance across time at $(0, 0)$ (bottom panel, orange).

We estimated the linearized ADMM for all combinations of values of λ_t and λ_s from the sets $\lambda_t \in$

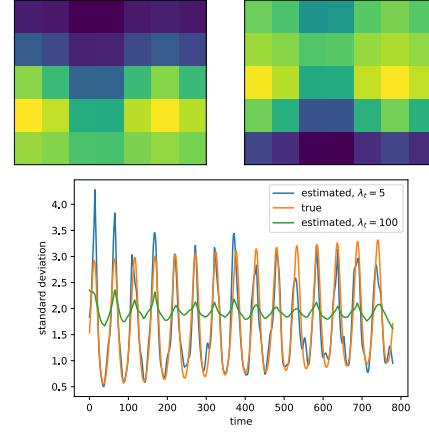


Figure 2: Top: Variance function at $t = 25$ (left) and $t = 45$ (right). Bottom: The true (orange) and estimated standard deviation function at the location $(0,0)$. The estimated values are obtained using linearized ADMM with $\lambda_s = 0.1$ and two values of λ_t : $\lambda_t = 5$ (blue) and $\lambda_t = 100$ (green).

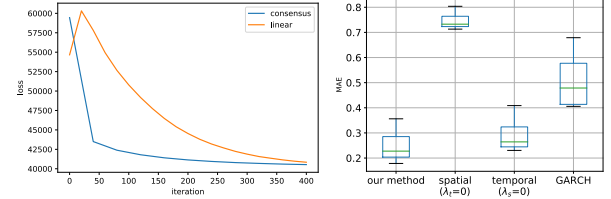


Figure 3: Left: Value of the objective function for linearized (orange) and consensus (blue) ADMM against iteration. Right: MAE for (1) our method with optimal values of λ_t and λ_s (2) spatial penalty only (3) temporal penalty only and (4) a GARCH(1,1).

$\{0, 1, 5, 10, 50, 100\}$ and $\lambda_s \in \{0, 0.05, 0.1, 0.2, 0.3\}$. For each pair, we then compute the mean absolute error (MAE) between the estimated variance and the true variance at all locations and all time steps. For $\lambda_t = 5$ and $\lambda_s = 0.1$, the MAE was minimized. The bottom panel of Figure 2 shows the true and the estimated standard deviation at location $(0,0)$ and $\lambda_t = 5$ (blue) and $\lambda_t = 100$ (green) ($\lambda_s = 0.1$). Larger values of λ_t lead to estimated values which are “too smooth”. The left panel of Figure 3 shows the convergence of both methods as a function of iteration. It is important to note that each iteration of the linearized algorithm takes 0.01 seconds on average while each iteration of the consensus ADMM takes about 20 seconds. Thus, where the lines meet at 400 iterations requires about 4 seconds for the linearized method and 2 hours for the consensus method.

To further examine the performance of the proposed model, we next compare it to three alternatives: a model which does not consider the spatial smoothness (equivalent to fitting the model in Section 2.1 to each time-series separately), a model which only imposes spatial smoothness, and a GARCH(1,1) model. We simulated 100 datasets using the method explained

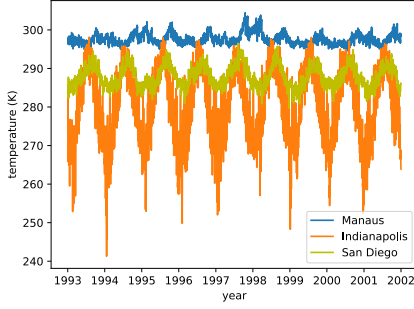


Figure 4: Time-series of the temperature (in Kelvin) of three cities.

above with $\sigma_s \sim \text{uniform}(4, 7)$. The right panel of Figure 3 shows the boxplot of the MAE for these models. As discussed above, using an algorithm akin to (Hallac et al. 2017) ignores the spatial component and thus gives results which are similar to the second column when the covariances are shrunk to zero and massively worse otherwise.

4.2 Data Analysis

Consensus ADMM in Section 3.1 is appropriate when we can easily parallelize over multiple machines. Otherwise, it is significantly slower, so all the results reported in this section are obtained using Algorithm 2. We applied this algorithm to the Northern Hemisphere of the ERA-20C dataset available from the European Center for Medium-Range Weather Forecasts³. We use the 2 meter temperature measured daily at 12 p.m from January 1, 1960 to December 24, 2010.

Preprocessing and other considerations Examination of the time-series alone demonstrates strong differences between trend and cyclic behavior across spatial locations (the data are not mean-zero). One might try to model the cycles by the summation of sinusoidal terms with different frequencies. However, for some time-series this may need many terms to be included in the summation to achieve a reasonable level of accuracy. In addition, such a model cannot capture the non-stationarity in the cycles.

Figure 4 shows the time-series of the temperature of three cities: Indianapolis (USA), San Diego (USA) and Manaus (Brazil). The time-series of Indianapolis and San Diego show clear cyclic behavior, though the amplitude of the cycles changes. The time-series of Manaus does not show any regular cyclic behavior. For this reason, we first apply trend filtering to remove seasonal terms and de-trend every time series. For each time-series, we found the optimal value of the penalty parameter using 5-fold cross-validation with $k = 5$. The blue curve in the left panel of Figure 5 shows the time-series of the temperature of Indianapolis after detrending using this method.

The red curve shows the estimated SD (which is $\exp(h_t/2)$) obtained from our proposed model. For ease of

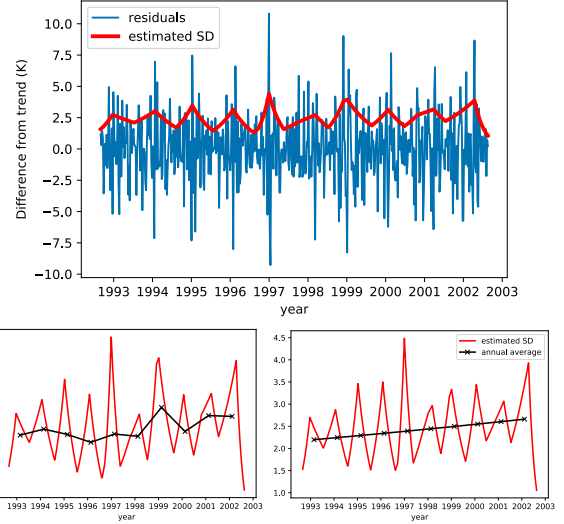


Figure 5: Top: The variability of the time-series of Indianapolis (weekly) and the estimated SD obtained from the method of Section 2.1 (red). Lower left: the estimated SDs (red) and their annual average (black) without imposing the long horizon penalty. Lower right: the same but with the long horizon penalty is imposed.

analysis, we compute the average of the estimated SD for each year. Both are shown in the lower left panel of Figure 5.

In addition to the constraints discussed in Section 2.2, we add a long horizon penalty to smooth the annual trend. $\sum_{i=1}^{N_{year}-2} |\sum_t h_{t_1} - 2h_{t_2} + h_{t_3}|$ where N_{year} is the number of years, $t_1 = 52(i-1) + t$, $t_2 = 52i + t$ and $t_3 = 52(i+1) + t$. Finally, because the observations are on the surface of a hemisphere rather than a grid, we add extra spatial constraints with the obvious form to handle the boundary between 180°W and 180°E as well as the region near the North Pole. The estimated SDs for Indianapolis are shown the right panel of Figure 5. The annual average of the estimated SDs shows a linear trend with a positive slope.

As shown in Algorithm 2, we evaluated convergence using $\epsilon = 0.001\%$ of the MSE of the data. Our simulation experiments indicated that the convergence speed depends on the value of λ_t and λ_s . For the temperature data, we used the solutions obtained for smaller values of these parameters as a warm start for the larger values resulting in faster convergence.

Model Selection One common method for choosing the penalty parameters in the Lasso problems is to find the solution for a range of the values of these parameters and then choose the values which minimize a model selection criterion. However, such analysis needs the computation of the degrees of freedom. Several previous work have investigated the degrees of freedom in generalized lasso problems with Gaussian likelihood (Tibshirani and Taylor 2012; Hu, Zeng, and Lin 2015; Zeng, Hu, and Li 2017). However, similar computations for non-Gaussian likelihood remains an open

³<https://www.ecmwf.int>

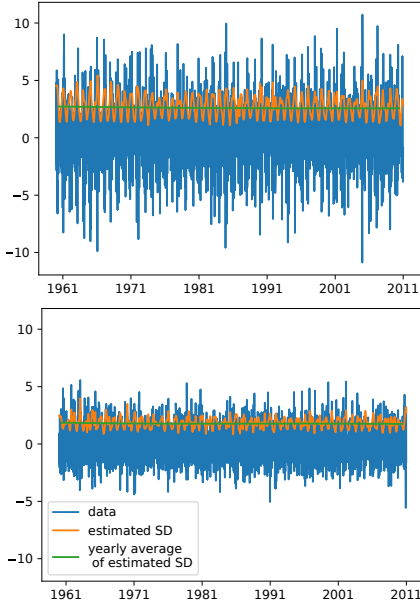


Figure 6: Difference in observed data from the estimated trend (blue), the estimated SDs (orange), and annual average SD (green) for Indianapolis (top) and San Diego (bottom). The y -axis shows K° .

problem. In this paper, therefore, we use a heuristic method for choosing λ_t and λ_s : we compute the solutions for a range of values of these parameters and choose the values which minimize $\mathcal{L}(\lambda_t, \lambda_s) = -l(y|h) + \sum \|D_{total}h\|$. This objective is a compromise between the negative log likelihood ($-l(y|h)$) and the complexity of the solution ($\sum \|D_{total}h\|$). For smoother solutions the value of $\sum \|D_{total}h\|$ will be smaller but with the cost of larger $-l(y|h)$. We computed the optimal solution for all the combinations of the following sets of values: $\lambda_t \in \{0, 2, 4, 8, 10, 15, 200, 1000\}$, $\lambda_s \in \{0, .1, .5, 2, 5, 10\}$. The best combination was $\lambda_t = 4$ and $\lambda_s = 2$.

Analysis of Trends in Temperature Volatility Figure 6 shows the detrended data, the estimated standard deviation and the yearly average of these estimates for two cities in the US: Indianapolis (top) and San Diego (bottom). The estimated SD captures the periodic behavior in the variance of the time-series. In addition, the number of linear segments changes adaptively in each time window depending on how fast the variance is changing.

The yearly average of the estimated SD captures the trend in the temperature volatility. For example, we can see that the variance in Indianapolis displays a small positive trend. To determine how the volatility has changed in each location, we subtract the average of the estimated variance in 1961 from the average in the following years and compute their sum. The average estimated variance at each location is shown in the top panel of Figure 7 while the change from 1961 is depicted in bottom panel. Since the optimal value of the spatial penalty is rather large ($\lambda_s = 2$) the estimated variance

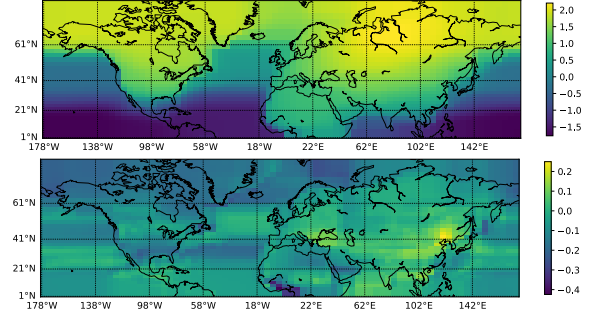


Figure 7: The average of the detrended estimated variance over the northern hemisphere (top) and the change in the variance from 1961 to 2011 (bottom).

is spatially very smooth.

The SD in most locations on the northern hemisphere had a negative trend in this time period, though spatially, this decreasing pattern is localized mainly toward the extreme northern latitudes and over oceans. In many ways, this is consistent with climate change predictions: oceans tend to operate as a local thermostat, regulating deviations in local temperature, while warming polar regions display fewer days of extreme cold. The most positive trend can be observed in Asia and particularly in south-east Asia.

5 Discussion

In this paper, we proposed a new method for estimating the variance of spatio-temporal data with the goal of analyzing global temperature data. The main idea is to cast this problem as a constrained optimization problem where the constraints enforce smooth changes in the variance for neighboring points in time and space. In particular, the solution is piecewise linear in time and piecewise constant in space. The resulting optimization is in the form of a generalized LASSO problem with high-dimension, and so applying the PDIP method directly is infeasible. We therefore developed two ADMM-based algorithms to solve this problem: the consensus ADMM and linearized ADMM.

The consensus ADMM algorithm converges in a few hundred iterations but each iteration takes much longer than the linearized ADMM algorithm. The appealing feature of the consensus ADMM algorithm is that if it is parallelized on enough machines the computation time per iteration remains constant as the problem size increases. The linearized ADMM algorithm on the other hand converges in a few thousand iterations but each iteration is performed in a split second. However, since the algorithm converges in many iterations it is not very appropriate for parallelization. The reason is that after each iteration the solution computed in each machine should be broadcast to the master machine and this operation takes some time which depends on the speed of the network connecting the slave machines to the master. A direction for future research would be to combine these two algorithms in the following way: the problem should be split into the sub-problems (as in the consensus ADMM) but each sub-problem can be solved using linearized ADMM.

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A PDIP for ℓ_1 Trend Filtering of variance

In this appendix we provide more details on how to solve the optimization problem with the objective specified in equation 2 using PDIP. The objective function is convex but not differentiable. Therefore, to be able to use PDIP we first need to derive the dual of this problem. We note that this is a generalized LASSO problem (Tibshirani and Taylor 2011). The dual of a generalized LASSO with the objective $f(x) + \lambda \|Dx\|_1$ is:

$$\min_{\nu} f^*(-D^\top \nu) \quad \text{s.t.} \quad \|\nu\|_\infty \leq \lambda$$

where $f^*(\cdot)$ is the Fenchel conjugate of f : $f^*(u) = \max_x u^\top x - f(x)$. It is simple to show that for the objective function of Equation 2

$$f^*(u) = \sum_t (u_t - 1) \log \frac{y_t^2}{1 - u_t} + u_t - 1.$$

Each iteration of PDIP involves computing a search direction by taking a Newton step for the system of nonlinear equations $r_w(v, \mu_1, \mu_2) = 0$, where $w > 0$ is a parameter and

$$r_w(v, \mu_1, \mu_2) := \begin{bmatrix} r_{dual} \\ r_{cent} \end{bmatrix} = \begin{bmatrix} \nabla f^*(-D^\top v) + \mu_1 - \mu_2 \\ -\mu_1(v - \lambda \mathbf{1}) + \mu_2(v + \lambda \mathbf{1}) - w^{-1} \mathbf{1} \end{bmatrix}$$

where μ_1 and μ_2 are dual variables for the ℓ_∞ constraint. Let $A = [\nabla r_{dual}^\top, \nabla r_{cent}^\top]^\top$. The newton step takes the following form

$$r_w(v, \mu_1, \mu_2) + A \begin{bmatrix} \nabla v \\ \nabla \mu_1 \\ \nabla \mu_2 \end{bmatrix} = 0$$

with

$$A = \begin{bmatrix} \nabla^2 f^*(-D^\top v) & I & -I \\ -\text{diag}(\mu_1) \mathbf{1} & -v + \lambda \mathbf{1} & \mathbf{0} \\ \text{diag}(\mu_2) \mathbf{1} & v + \lambda \mathbf{1} & \mathbf{0} \end{bmatrix}.$$

Therefore, to perform the Newton step we need to compute $\nabla f^*(-D^\top v)$ and $\nabla^2 f^*(-D^\top v)$.

It is straightforward to show that

$$\begin{aligned} \nabla f^*(-D^\top v) &= -\nabla_u f^*(u) D^\top, \\ u &= -D^\top v, \end{aligned}$$

$$(\nabla_u f^*(u))_j = \log \left(\frac{y_j^2}{1 - u_j} \right),$$

$$\nabla^2 f^*(-D^\top v) = D \nabla_u^2 f^*(u) D^\top,$$

$$(\nabla_u^2 f^*(u))_j = \text{diag} \left(\frac{1}{1 - u_j} \right).$$

Having computed the conjugate function and its gradient and Jacobian, now we can use a number of convex optimization software packages which have an implementation of PDIP to solve the optimization problem with the objective function (2). We chose the python API of the `cvxopt` package (Andersen, Dahl, and Vandenberghe 2013).

B Proof of Lemma 1

Proof. If $f(x) = \sum_k f_k(x_k)$ then $[\text{prox}_{\mu f}(x)]_k = \text{prox}_{\mu f_k}(u_k)$. So $[\text{prox}_{\mu f}(u)]_k = \min_{x_k} \mu(x_k + y_k^2 e^{-x_k}) + \frac{1}{2}(x_k - u_k)^2$. Setting the derivative to 0 and solving for u_k gives the result. Similarly, $[\text{prox}_{\rho g}(u)]_\ell = \rho \lambda_\ell |z_\ell| + 1/2(z_\ell - u_\ell)^2$. This is not differentiable, but the solution must satisfy $\rho \cdot \lambda_\ell \cdot \partial(|z_\ell|) = u_\ell - z_\ell$ where $\partial(|z_\ell|)$ is the sub-differential of $|z_\ell|$. The solution is the soft-thresholding operator $S_{\rho \lambda_\ell}(u_\ell)$. \square

C PDIP Update in Algorithm 1

In this section we give more details on performing the x -update step in Algorithm 1. We need to solve the following optimization problem:

$$\hat{x} := \underset{x}{\text{argmin}} \left(\sum_{j=1}^{n_b} (x_j + y_j^2 e^{-x_j}) + (\rho/2) \|x - \tilde{z} + u\|_2^2 + \Lambda^\top |Dx| \right)$$

where n_b is the number of local variables in each sub-cube in Figure 1, and for ease of notation we have dropped the subscript i and superscript m .

The matrix D has the following form: $D^t = [D_{temp}^t | D_{spat}^t]$. The matrix D_{temp} is the following block-diagonal matrix and corresponds to the temporal penalty:

$$D_{temp} = \begin{bmatrix} D_t & & \\ & \ddots & \\ & & D_t \end{bmatrix},$$

where D_t was first introduced in Section 2 of the main text and has the following form:

$$D_t = \begin{bmatrix} 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 & 1 \end{bmatrix}.$$

The number of the diagonal blocks in D_{temp} is equal to the grid size $n_r \times n_c$. Each row of the matrix D_{spat} corresponds to one spatial constraint in Equation (3) in the text. For example, the first T rows correspond to $|h_{11t} - h_{21t}|$ for $t = 1, \dots, T$, the next T rows correspond to $|h_{11t} - h_{12t}|$, and so on.

This optimization problem, is again a generalized LASSO problem with $f(x) = \sum_{j=1}^{n_b} (x_j + y_j^2 e^{-x_j}) + (\rho/2) \|x - \tilde{z} + u\|_2^2$.

As it was explained in Appendix A, the dual of this optimization problem is: $\min_{\nu} f^*(-D^\top \nu)$ with the constraints $|\nu_k| \leq \Lambda_k$. To use PDIP we first need to compute the conjugate function $f^*(\cdot)$. We have:

$$\begin{aligned} f^*(\xi) &= \max_x \xi^\top x - f(x) \\ &= \max_x \sum_{j=1}^{n_b} (\xi_j x_j - x_j - y_j^2 e^{-x_j} - (\rho/2)(x_j - \tilde{z}_j + u_j)) \end{aligned}$$

Setting the derivative of the terms inside the summation to 0, we obtain:

$$\xi_j - y_j^2 e^{-x_j^*} - \rho x_j^* + \rho(\tilde{z}_j - u_j) = 0 \quad (6)$$

where x^* is the maximizer in C. Then, it can be shown that x_j^* which satisfies (6) can be obtained as follows:

$$\begin{aligned} x_j^* &= \mathcal{W} \left(\frac{y_j^2}{\rho} e^{\phi_j} \right) - \phi_j \\ \phi_j &= \frac{1 - \xi_j - \rho(\tilde{z}_j - u_j)}{\rho} \end{aligned}$$

In this equation, $\mathcal{W}(\cdot)$ is the *Lambert function* (Corless et al. 1996). Finally, the conjugate function is: $f^*(\xi) = \sum_{j=1}^{n_b} (\xi_j x_j^* - x_j^* - y_j^2 e^{-x_j^*} - (\rho/2)(x_j^* - \tilde{z}_j + u_j))$.

To use PDIP, we also need to evaluate ∇f^* and $\nabla^2 f^*$. First note that $\frac{\partial \mathcal{W}(q)}{\partial q} = \frac{\mathcal{W}'(q)}{q(1+\mathcal{W}'(q))}$ and $\frac{\partial^2 \mathcal{W}(q)}{\partial q^2} = -\frac{\mathcal{W}''(q)(\mathcal{W}'(q)+q)}{q^2(1+\mathcal{W}'(q))^3}$. Using the chain rule we get:

$$\frac{\partial f^*(\xi)}{\partial \xi_j} = x_j^* + \frac{\partial x_j^*}{\partial \xi_j} \left[\xi_j - 1 + y_j^2 e^{-x_j^*} + \rho(\tilde{z}_j - u_j - x_j^*) \right]$$

where we have:

$$\frac{\partial x_j^*}{\partial \xi_j} = \frac{1}{\rho(1 + \mathcal{W}'((y_j^2/\rho)e^{-\phi_j}))}$$

By some tedious but straightforward computation we can obtain the second derivatives:

$$\begin{aligned} \frac{\partial^2 f^*(\xi)}{\partial \xi_j^2} &= \frac{\partial x_j^*}{\partial \xi_j} - \rho \frac{\partial^2 x_j^*}{\partial \xi_j^2} \left[\phi_j + x_j^* - \tilde{z}_j + u_j \right] \\ &\quad + \frac{\partial x_j^*}{\partial \xi_j} \left[1 - y_j^2 \frac{\partial x_j^*}{\partial \xi_j} e^{-x_j^*} - \rho \frac{\partial x_j^*}{\partial \xi_j} \right] \\ \frac{\partial^2 x_j^*}{\partial \xi_j^2} &= \frac{\mathcal{W}''((y_j^2/\rho)e^{-\phi_j})}{\rho^2(1 + \mathcal{W}'((y_j^2/\rho)e^{-\phi_j}))^3} \end{aligned}$$