

Bias correction in daily maximum and minimum temperature measurements through Gaussian process modeling

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Abstract

Climatological summary statistics based on daily temperature minima and maxima suffer from bias due to the observation time (Baker, 1975). We develop a novel approach to correcting this bias, by imputing hourly temperatures at the location of the measurements, which can then be used directly for summary purposes. The imputation strategy combines information from the observed minima and maxima, and from nearby meteorological stations that record hourly temperatures. A spatio-temporal Gaussian process model allows these two sources of information to be combined. Imputed samples are obtained using the Hamiltonian Monte Carlo algorithm implemented by the Stan probabilistic programming language (Carpenter et al., 2017). We develop approximations to the imputation model that enable the HMC sampler to efficiently draw samples that match the observed minima and maxima, and demonstrate the success of this approach in a simpler example where the imputation distribution is analytically tractable. We further validate our imputation pipeline using hourly temperature data from four meteorological stations in Iowa, of which one is hidden and the data replaced with daily minima and maxima, and show that the imputed temperatures closely match the hidden temperatures. We also demonstrate that this model and data allow the time of the daily measurements itself to be inferred.

Contents

1	Introduction	2
1.1	Illustration of bias induces by measurement hour	3
1.2	Proposed solution	4
2	First Spatiotemporal Model	5
2.1	Fitting the spatiotemporal model	6
3	Predictions using nearby data	6
4	Imputations	8
4.1	Imputing by Conditioning on Extrema	8
4.2	Illustration of Hamiltonian Monte Carlo with Smoothmax Approximation	10
4.3	Smoothmax Temperature Model	13
5	Model diagnostics	15
5.1	Variogram	15
5.2	Error and expected error	15
6	Improving model	16

7 Analysis	18
8 Inference on measurement hour	19
9 Conclusion	19
A Stan programs	22
A.1 Smoothmax toy example	22
A.1.1 Without smoothmax Approximation	22
A.1.2 With smoothmax Approximation	22
A.2 Temperature imputations	23
B Derivation of the analytic posterior for toy example	24

1 Introduction

Long, high-quality records of temperature provide an important basis for our understanding of climate variability and change. Historically, there has been a focus on monthly-average temperature records, which are sufficient for certain analyses, such as quantifying long-term changes in temperature. As our knowledge of climate change expands, however, there is increasing interest in understanding changes in temperature on shorter timescales, with a particular focus on extreme events. To do so, it is necessary to utilize higher-resolution temperature data.

Recent work has led to the development of the Global Historical Climatology Network-Daily (GHCND) database (Menne et al., 2012), which contains, among other variables, daily maximum and minimum temperatures from weather stations around the globe. The database draws from a range of different sources, and the data within it undergoes basic quality control to remove erroneous values.

The current quality control methodology, however, does not account for so-called ‘inhomogeneities’. Inhomogeneities result from changes in measurement practices that impact the recorded temperatures. For temperature, known inhomogeneities include (a) changes in the time of observation, (b) changes in the thermometer technology, (c) station relocation, and (d) changes in land use around a station (Menne et al., 2009). While these inhomogeneities have a small effect on, e.g., the estimation of global mean temperature, they can have a large effect on estimation of temperature variability and change at a more local scale.

There is a large body of work focused on homogenizing monthly-average temperatures (e.g., Karl et al., 1986; Easterling et al., 1996; Peterson et al., 1998; Ducré-Robitaille et al., 2003; Menne and Williams Jr, 2009; Vincent et al., 2012), resulting in widely available, large-scale homogenized monthly temperature datasets. Homogenization typically proceeds through identifying non-climatic ‘breakpoints’ in a given time series through comparison with neighboring stations. Once a breakpoint is identified, the measurements recorded after the breakpoint are adjusted in some way to reduce or remove the inhomogeneity. Most applications of these methods, however, focus on adjusting the mean state of the data rather than the shape of the distribution (see Della-Marta and Wanner, 2006, and references therein). While this may be sufficient for monthly data, it is known that certain changes in measurement practices affect different percentiles of daily temperature in different ways. To address this issue, some homogenization methods have also employed percentile matching techniques, wherein the adjustment to a timeseries after a breakpoint is a function of percentile (Della-Marta and Wanner, 2006; Trewin, 2013).

Here, we focus primarily on addressing the time of observation bias, as well as its time trend, because of its known impact on the distribution of daily maximum and minimum temperature (T_x and T_n) measurements. The bias exists because T_x and T_n are often recorded by an observer who visits a weather station every 24 hours, and notes the maximum and minimum temperatures measured by the thermometer over the previous 24 hours. Ideally, the observer would visit the station at midnight, and the highest and lowest temperatures over the past 24 hours would typically be representative of the high and low during the prior day. For convenience, however, most observers record data at a daytime hour instead. As can be seen in Fig. XX, measurements recorded in the early morning may not properly register the low of the night before if it was unusually warm. Similarly, measurements recorded in the late afternoon may not properly register

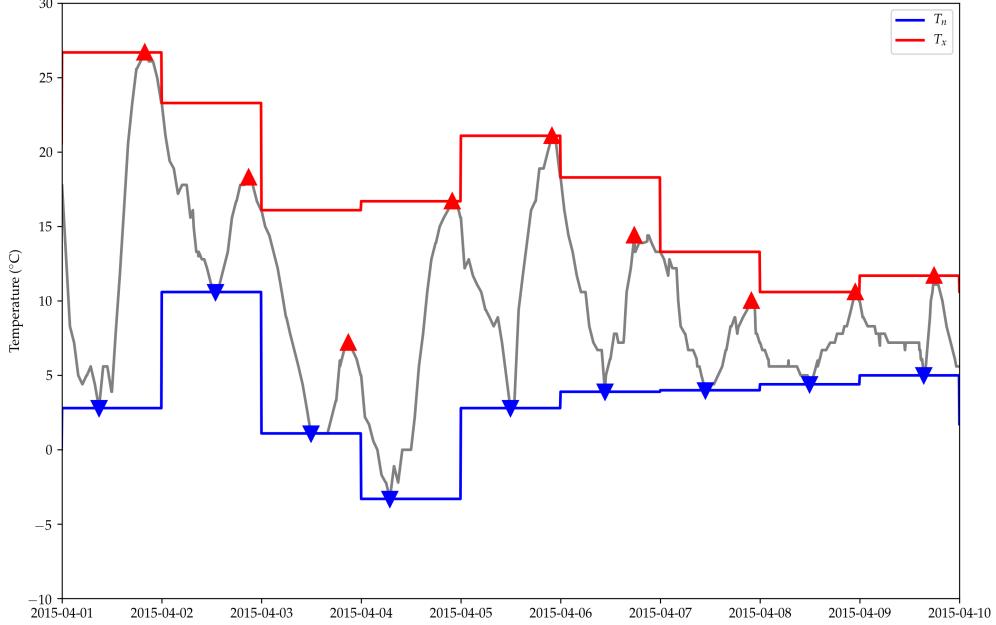


Figure 1: An extract of the temperature measurements made at the Waterloo Municipal Airport, with emulated measurements of daily minima and maxima shown in blue and red respectively, measured each day at 23:00 UTC. The blue and red triangles indicate the coldest and warmest point of each diurnal cycle. The occasional mismatches between the 24-hour extrema, and the peaks and troughs of the diurnal cycle induces a bias in the temperature record.

the high of the prior day if it was usually cool. In both cases, this will lead to a reduction in the variance of T_x and T_n distributions, but the effect will be greater at low (high) percentiles for T_x (T_n).

If the time of observation remained constant over time, the bias would still exist, but it would not be linked to spurious trends in the data. However, there have been known (and likely unknown) changes in the time of observation. In the United States, for example, observers were instructed to switch from recording data in the afternoon to recording data in the morning beginning in the 1950s. This change has led to an apparent decrease in both T_x and T_n over time (Menne et al., 2009).

The goal of our approach is to infer the true T_x and T_n values throughout the data records, thereby correcting both the variance biases and the spurious trends. This stands in contrast to previous work, which has focused primarily on addressing spurious trends. We approach the problem as a missing data problem, wherein we are trying to recover the values of T_x and T_n that may have been overwritten due to measurement practices. Furthermore, by employing a Gaussian process framework and nearby stations with hourly data, we are able to simulate multiple realizations of temperature timeseries at each station, thereby providing estimates of uncertainty.

1.1 Illustration of bias induces by measurement hour

We illustrate the measurement bias in daily maxima and minima with ten days of hourly temperature measurements from the Waterloo Municipal Airport station in Iowa. Ideally, T_x measurements should capture the peak of each diurnal cycle, and T_n its trough. In Figure 1, those ideal measurements are indicated by the red and blue triangles respectively. The actual measurements are obtained by dividing the data into 24 hour measurement windows, and extracting the minimum and maximum. For each window, we plot these extrema with a red and blue horizontal line.

On most days, the ideal measurement and the actual measurement coincide: the triangle is on that day's line. But there are also several misses. The most blatant example occurs on April 3rd, where the peak of the

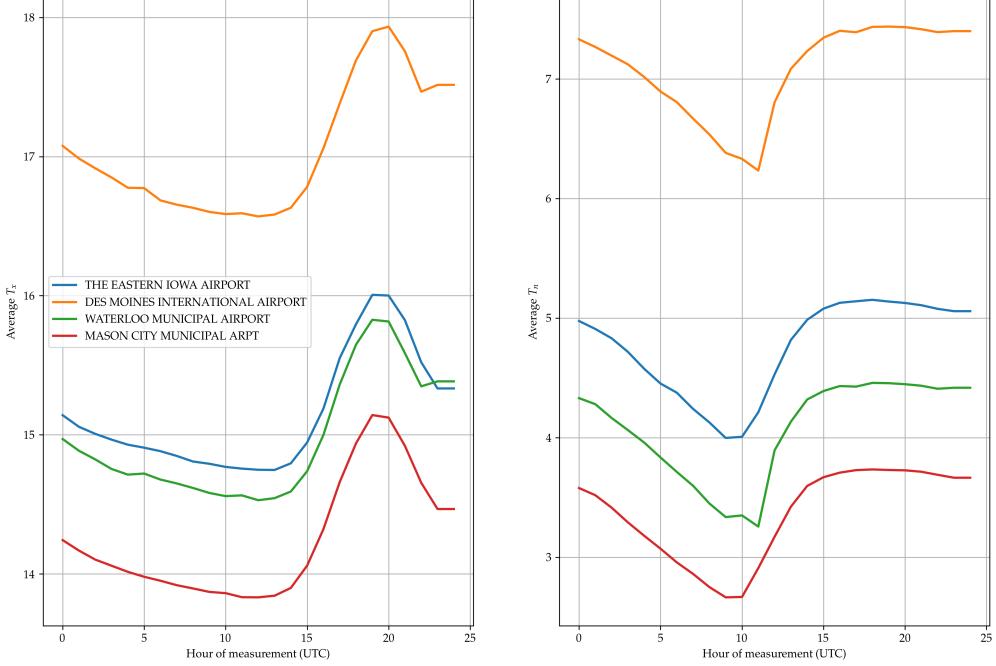


Figure 2: Mean daily maximum temperature (left) and mean daily minimum temperature (right) for 2015 as a function of measurement time (UTC), based on daily extrema emulated at four Iowa weather stations.

diurnal cycle is 7.2°C and occurs at 21:00 UTC. However, because the previous day was much warmer, the day's T_x record of 16.1°C is reached immediately after the previous day's measurement. The measured T_x therefore overestimates the diurnal cycle's peak by 8.9°C .

This subtle bias in the daily records can in turn bias long-term summary statistics that are of climatological interest. A measure as simple as the average daily maximum temperature for an entire year (2015) increases by over 1°C if the measurements are made at the warmest time of day 21:00 UTC rather than 14:00 UTC (see Figure 2). Conversely, the average T_n is colder by over 1°C if T_n is measured at 10:00 UTC (the coldest time of day on average) rather than 17:00 UTC.

A climatologist studying weather variability might be interested in summary statistics such as the average absolute change in the daily temperature maxima and minima from one day to the next. The answer to that question too depends on the time of day at which the temperatures are recorded. Collecting the measurements at the hottest time of day means that the peaks on a warm day gets recorded twice, erasing the diurnal peaks of the following colder day, and hence the variability gets underestimated. We can see this in Figure 3), where the respective variability estimates drop if the maxima get measured at the warmest time, or if the minima get measured at the coldest time.

1.2 Proposed solution

We have seen that the daily maxima and minima do not faithfully record each diurnal cycle's peak and trough. The peaks on a relatively cold day can get overwritten by temperatures at either end of the measurement window that properly belong to the previous or the next diurnal cycle. Troughs on relatively warm days can be similarly overwritten. Our goal is to undo this damage, and recover estimates of summary statistics, such as the average daily maximum temperature, that do not suffer from the consequent bias. We need to address the erasure of information caused by the measurement mechanism, and therefore view this as a missing data problem.

Taking the missing data perspective, we seek to impute the hourly temperatures that have been replaced by a maximum and minimum over a 24 hour period. To do so, we combine information from two sources:

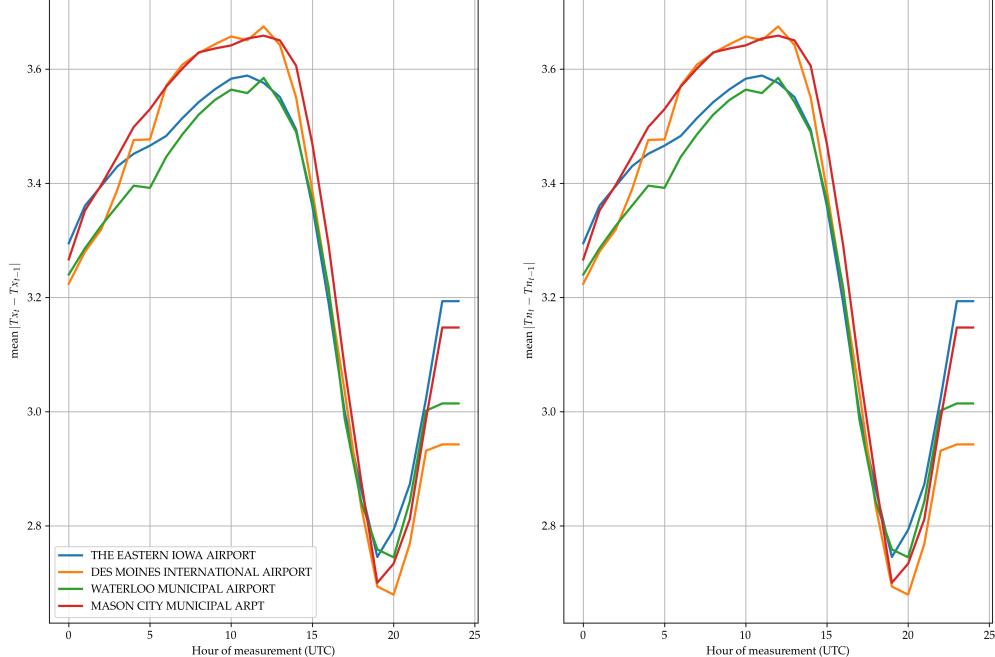


Figure 3: Mean absolute daily change in maximum temperature (left) and mean absolute daily change in minimum temperature (right) for 2015 as a function of measurement time (UTC), based on daily extrema emulated at four Iowa weather stations.

the recorded daily temperature extremes at the station of interest, and also hourly temperatures recorded at nearby meteorological stations. These hourly measurements are considered less reliable by climatologists, as they aren't as carefully documented, calibrated, and situated. The meteorological stations are often in locations (like airports) where human activity will affect temperatures. Therefore, summary statistics extracted directly from those measurements would not be directly usable for climatology, as they could suffer from systematic bias. However, even if miscalibrated, the meteorological data do contain valuable information about the hourly changes in temperatures on any given day. We therefore use them to inform the shape of the imputed temperature time-series at our location of interest, while we use the recorded temperature extrema to calibrate and constrain them.

2 First Spatiotemporal Model

To model measured temperatures at various locations and times, we use a spatio-temporal Gaussian process model. In its simplest form, we believe that temperatures from stations that are near each other are more correlated than distant stations, and that those correlations should also decay in time. In the spatial statistics literature, squared exponential covariance functions are commonly used to model correlations decaying as a function of distance. Ignoring the time dimension, we would model the simultaneous temperatures throughout a region as a Gaussian process, with the covariance of two locations \mathbf{x} and \mathbf{x}'

$$\text{cov}(\mathbf{T}(\mathbf{x}), \mathbf{T}(\mathbf{x}') | t) = k_{\text{space}}(\mathbf{x}, \mathbf{x}') = \sigma_{\text{GP}}^2 \exp\left(-\frac{(\mathbf{x} - \mathbf{x}')^\top (\mathbf{x} - \mathbf{x}')}{2\ell_x^2}\right). \quad (1)$$

Similarly, ignoring the spatial dimension, the time series of temperatures at a single location can be modeled as a Gaussian process with covariance between two moments t and t'

$$\text{cov} (T(t), T(t') | \mathbf{x}) = k_{\text{time}}(t, t') = \sigma_{\text{GP}}^2 \exp \left(-\frac{(t - t')^2}{2\ell_t^2} \right). \quad (2)$$

We then combine the spatial and temporal model by multiplying the covariance functions

$$k_{\text{st}}(\mathbf{x}, \mathbf{x}', t, t') = k_{\text{time}}(t, t') \cdot k_{\text{space}}(\mathbf{x}, \mathbf{x}'). \quad (3)$$

This gives us the covariance of the Gaussian process underlying the full spatio-temporal model of temperatures. To complete the model specification, we add a mean temperature for each station $\mu_{\text{station}[i]}$, and iid measurement noise ϵ_i .

$$\begin{aligned} T_i &= \mu_{\text{station}[i]} + f(\mathbf{x}_i, t_i) + \epsilon_i \\ f(\mathbf{x}_i, t_i) &\sim \mathcal{GP}(0, k_{\text{st}}(\mathbf{x}_i, \mathbf{x}_i, t_i, t_i)) \\ \epsilon_i &\stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma_\epsilon^2) \end{aligned} \quad (4)$$

2.1 Fitting the spatiotemporal model

Software is readily available in many programming languages for fitting Gaussian process models, including inference on the covariance parameters. We chose to use the Julia `GaussianProcesses.jl` package to fit the above spatiotemporal model to the hourly temperatures at four Iowa weather stations. However, the Iowa data includes 47,864 measurements, which is computationally infeasible to fit directly with a single Gaussian process. While approximation techniques exist to fit such large datasets, we chose the less efficient but simpler approach of dividing the data into 10-day chunks, modeled as independent Gaussian processes with shared hyperparameters. To simplify our implementation, we replaced the $\mu_{\text{station}[i]}$ terms by a spatial squared exponential component

$$k_\mu(\mathbf{x}, \mathbf{x}') = \sigma_\mu^2 \exp \left(-\frac{(\mathbf{x} - \mathbf{x}')^\top (\mathbf{x} - \mathbf{x}')}{2\ell_\mu^2} \right) \quad (5)$$

with large variance σ_μ^2 and low lengthscale ℓ_μ added to the covariance function so that the spatio-temporal kernel becomes

$$k_{\text{st}}(\mathbf{x}, \mathbf{x}', t, t') = k_{\text{time}}(t, t') \cdot k_{\text{space}}(\mathbf{x}, \mathbf{x}') + k_\mu(\mathbf{x}, \mathbf{x}'). \quad (6)$$

The model therefore has 4 free parameters: σ_{GP} , ℓ_t , ℓ_x and σ_ϵ . We optimize the marginal likelihood of the Iowa data as a function of these three parameters

$$\hat{\sigma}_{\text{GP}}, \hat{\ell}_t, \hat{\ell}_x, \hat{\sigma}_\epsilon = \arg \max_{\sigma_{\text{GP}}, \ell_t, \ell_x, \sigma_\epsilon} \{\mathbb{P}(Y | \sigma_{\text{GP}}, \ell_t, \ell_x, \sigma_\epsilon)\}, \quad (7)$$

and obtain $\hat{\sigma}_{\text{GP}} = 3.73^\circ \text{C}$, $\hat{\ell}_t = 2.7 \text{ hours}$, $\hat{\ell}_x = 176.4 \text{ km}$ and $\hat{\sigma}_\epsilon = 0.44^\circ \text{C}$.

3 Predictions using nearby data

Once we have a spatio-temporal Gaussian process model with optimized covariance parameters, we can use it to generate predictions at the station where we aim to generate imputations based on nearby measurements. Gaussian processes make this a closed-form procedure. We'll denote the temperatures we wish to impute as T_{miss} at times t_{miss} and location \mathbf{x}_{miss} and those observed at nearby stations as T_{nearby} at times t_{nearby} and locations $\mathbf{x}_{\text{nearby}}$. Under the spatio-temporal model, T_{miss} and T_{nearby} are jointly multivariate normal, with mean zero and covariance given by $k_{\text{st}}(\mathbf{x}, \mathbf{x}', t, t')$. Standard results for conditioning within multivariate normals then yields

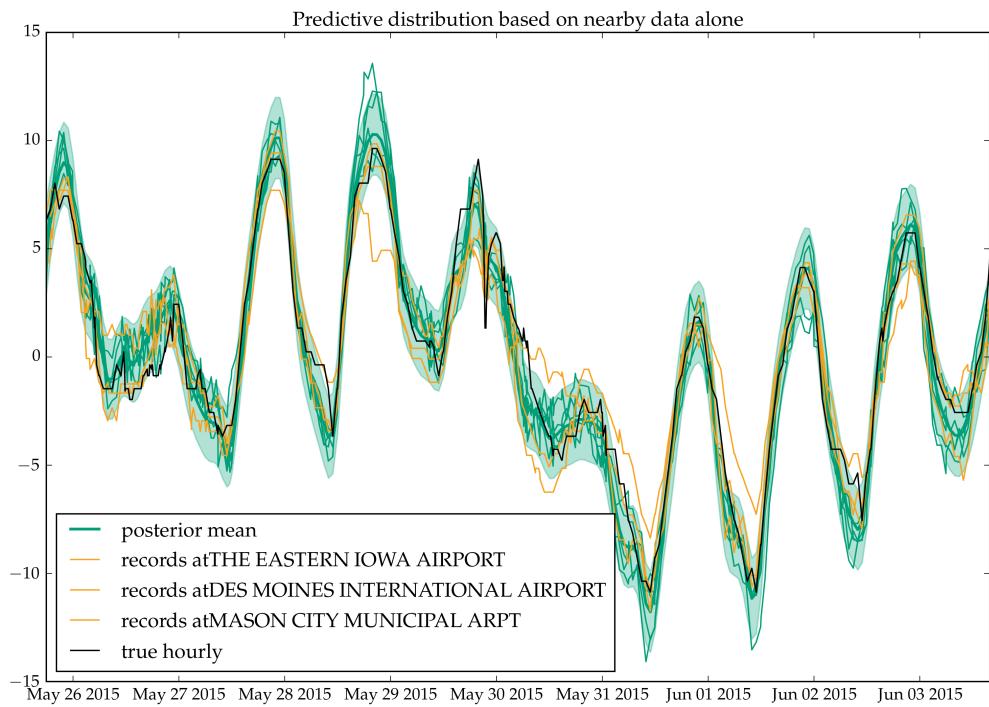


Figure 4: Predictive distribution using only nearby data and the simple product of square exponentials model. The orange lines are the measurements at nearby stations that are being used to inform the predictions. The black line is the true temperatures that have been withheld from the model, while the green line is the posterior mean of the predictions. The credible range (in green) is twice the standard deviations extracted from the diagonal entries of the posterior covariance matrix.

$$\begin{aligned}
T_{\text{miss}} \mid T_{\text{nearby}} &\sim \mathcal{N}(\mu_{\text{miss} \mid \text{nearby}}, \Sigma_{\text{miss} \mid \text{nearby}}), \\
\mu_{\text{miss} \mid \text{nearby}} &= \mathbb{E}(T_{\text{miss}} \mid T_{\text{nearby}}) \\
&= \text{cov}(T_{\text{miss}}, T_{\text{nearby}}) \text{cov}(T_{\text{nearby}}, T_{\text{nearby}})^{-1} T_{\text{nearby}}, \\
\Sigma_{\text{miss} \mid \text{nearby}} &= \text{var}(T_{\text{miss}} \mid T_{\text{nearby}}) \\
&= \text{cov}(T_{\text{miss}}, T_{\text{miss}}) - \text{cov}(T_{\text{miss}}, T_{\text{nearby}}) \text{cov}(T_{\text{nearby}}, T_{\text{nearby}})^{-1} \text{cov}(T_{\text{nearby}}, T_{\text{miss}}).
\end{aligned} \tag{8}$$

All covariance matrices can be obtained by plugging into k_{st} . For example, the ij th entry of $\text{cov}(T_{\text{miss}}, T_{\text{nearby}})$ is given by $k_{st}(x_{\text{miss}}, X_{\text{nearby}}[j], t_{\text{miss}}[i], t_{\text{nearby}}[j])$, where $X_{\text{nearby}}[j]$ gives the spatial covariates of the j th observation, and $t_{\text{nearby}}[j]$ its time.

In Figure 4, we show an example of predictions obtained from this spatio-temporal model. We withheld measurements from the Waterloo Municipal Airport, and then used data from three nearby stations between May 25, 2015 and June 3, 2015 to predict the Waterloo temperatures during the same time window. This allows us to assess the quality of the predictions on this example.

4 Implications

4.1 Imputing by Conditioning on Extrema

Our aim isn't simply to predict temperatures at a location with no measurements, but rather to impute hourly temperatures at a location with accurate measurements of the daily temperature extrema. This is an instance of a more general statistical problem: if a random p -vector $\{X_i : i = 1, \dots, p\}$ has a known distribution F_X , and its maximum $X_{\max} \equiv \max_i \{X_i\}$ and minimum $X_{\min} \equiv \min_i \{X_i\}$ are measured, how does one draw samples from $F_{X|X_{\max}, X_{\min}}$, the distribution of X conditional on X_{\max} and X_{\min} ? Conditional draws from $F_{X|X_{\max}, X_{\min}}$ need to respect three constraints: one component of X must be equal to X_{\min} , another to X_{\max} , and all other components must lie between X_{\min} and X_{\max} .

Conceptually, we could implement a valid imputation algorithm by drawing random samples F_X , and only keeping the samples that satisfy the three constraints. Unfortunately, if F_X is a continuous distribution, the probability of a random draw from F_X satisfying such sharp constraints is zero. One could envision adding some tolerance, so that samples with minimum and maximum within ϵ of X_{\max} and X_{\min} are retained, but as the dimensionality p grows, the rejection probability will rapidly go to 1, thus requiring huge sample sizes. Ultimately, this rejection sampling strategy is therefore bound to fail.

Markov Chain Monte Carlo (MCMC) techniques can also be used to draw samples from arbitrary distributions with densities known up to a constant. The density of $F_{X|X_{\max}, X_{\min}}$ is obtained up to a constant multiplier through a simple application of Bayes' theorem. It is proportional to the prior density of F_X multiplied by indicators ensuring that the extrema are respected.

$$\begin{aligned}
\mathbb{P}(X \mid X_{\max}, X_{\min}) &\propto \mathbb{P}(X) \mathbb{P}(X_{\max}, X_{\min} \mid X), \\
&\propto \mathbb{P}(X) \mathbb{I}\left(\max_i \{X_i\} = X_{\max}\right) \mathbb{I}\left(\min_i \{X_i\} = X_{\min}\right).
\end{aligned} \tag{9}$$

However, once again, this distribution is zero everywhere in \mathbb{R}^p , except in a $(p-2)$ dimensional subspace where the min and max constraints are met. This doomed the rejection sampler, and will also prevent any unmodified MCMC algorithm from converging onto $F_{X|X_{\max}, X_{\min}}$. We therefore approximate the constraint by replacing the likelihood term $\mathbb{P}(X_{\max}, X_{\min} \mid X)$ with two narrow independent normal distributions around the minimum and maximum of X . This "softens" the conditional distribution,

$$\mathbb{P}(X \mid X_{\max}, X_{\min}) \propto \mathbb{P}(X) \mathcal{N}\left(X_{\max} \mid \max_i \{X_i\}, \epsilon^2\right) \mathcal{N}\left(X_{\min} \mid \min_i \{X_i\}, \epsilon^2\right), \tag{10}$$

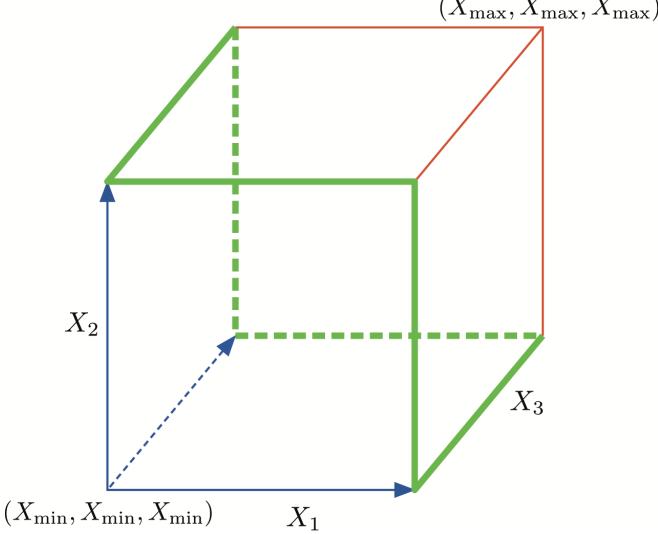


Figure 5: With three variables X_1 , and X_2 and X_3 , $F_{X|X_{\max}, X_{\min}}$ resides in the one-dimensional six-sided loop shown with thicker green lines. This is a 1D manifold embedded in 3D space, and possessing sharp corners, making it difficult for most MCMC algorithms to explore.

where $\mathcal{N}(x | \mu, \sigma^2)$ is the density of a normal distribution with mean μ and variance σ^2 evaluated at x . For small ϵ , this is a very tolerable approximation which enables the use of MCMC techniques.

This approximation to $F_{X|X_{\max}, X_{\min}}$ remains a difficult distribution to sample from. We illustrate the constraint in a 3-dimensional setting in Figure 5. The MCMC algorithm must travel efficiently along the six edges of the allowed subspace, and navigate corners when the index of the extremum components change. Hamiltonian Monte Carlo (HMC) has shown a remarkable ability to navigate complicated distributions, including distributions where the typical set has “pinch points” of strong curvature (Betancourt, 2017), similar to the “corners” in $F_{X|X_{\max}, X_{\min}}$. We therefore used HMC as implemented by the Stan probabilistic programming language (Carpenter et al., 2017) to obtain draws from $F_{X|X_{\max}, X_{\min}}$.

HMC’s efficient sampling relies on gradient information in order to move towards regions of high probability. The normal likelihood (10) softened the extrema constraints, but the maximum and minimum functions also remove information from the gradient. The partial derivative of the log-likelihood of the maximum term with respect to X_i is proportional to

$$\frac{\partial \log \mathcal{N}(X_{\max} | \max_i \{X_i\}, \epsilon^2)}{\partial X_i} \propto (X_{\max} - X_i) \mathbb{I} \left\{ \arg \max_j (X_j) = i \right\}, \quad (11)$$

where $\arg \max$ is the function that returns the index of the maximum component. In other words, the gradient pulls the maximum of the current sample towards X_{\max} , and ignores all other components. This makes it difficult for HMC to efficiently explore scenarios where other components are the maximum.

We can assist the HMC algorithm with another approximation. We replace the max and min functions with the smoothmax and smoothmin functions, which take real inputs x_1, \dots, x_p and a sharpness parameter k and return

$$\begin{aligned} \text{smoothmax}(x_1, \dots, x_p; k) &= \frac{1}{k} \log \left(\sum_{i=1}^p e^{kx_i} \right) \\ \text{smoothmin}(x_1, \dots, x_p; k) &= -\text{smoothmax}(-x_1, \dots, -x_p; k) \end{aligned} \quad (12)$$

As $k \rightarrow \infty$, smoothmax becomes the maximum, and smoothmin becomes the minimum. When smoothmax replaces max and smoothmin replaces min, there is a small price in precision due to the ap-

proximation, but there is a huge computational benefit: the gradient is now informative for all components of X :

$$\frac{\partial \log \mathcal{N}(X_{\max} | \text{smoothmax}(X_{1:p}; k), \epsilon^2)}{\partial X_i} \propto (X_{\max} - \text{smoothmax}(X_{1:p}; k)) \frac{e^{kX_i}}{\sum_{j=1}^p e^{kX_j}}. \quad (13)$$

These modifications make HMC a viable algorithm to efficiently draw samples from the constrained posterior. Setting k and σ_ϵ is a compromise between exactness and efficiency; we found $k = 10$ and $\sigma_\epsilon = 0.1$ to perform well for this paper's application.

In the rest of this paper, we will refer to this use of HMC and a smoothmax approximation to the target distribution as SmoothHMC. SmoothHMC provides a generally applicable algorithm to draw from a multivariate distribution conditionally on the observed minimum and maximum of its components.

4.2 Illustration of Hamiltonian Monte Carlo with Smoothmax Approximation

We verify SmoothHMC's ability to obtain draws from $F_{X|X_{\max}, X_{\min}}$ in a simplified setting where the distribution function of $F_{X|X_{\max}, X_{\min}}$ can be derived analytically and also computed easily. In our application, F_X is the posterior predictive multivariate normal distribution $T_{\text{miss}} | T_{\text{nearby}}$ obtained from nearby measurements, with mean and marginal variance evolving smoothly from one prediction to the next. To retain a resemblance to this, we specify a random vector X with each component X_i normally distributed, and with sinusoidal means and variances, but without any correlations between them, so as to avoid a combinatorial explosion when obtaining the distribution function analytically:

$$\begin{aligned} X_i &\sim \mathcal{N}(\mu_i, \sigma_i), \\ X_i &\perp X_j \forall i \neq j, \\ X_{\max} &= \max_i \{X_i\}, \\ X_{\min} &= \min_i \{X_i\}, \\ \mu_i &= 10 + \sin(2\pi i / 50), \\ \sigma_i &= 0.1 + \cos^2(2\pi i / 50), \\ i &= 1, 2, \dots, 100. \end{aligned} \quad (14)$$

The unconstrained distribution of X_i is illustrated in Figure 6(a). In this example, we aim to sample from the distribution of X_i subject to the observation that $X_{\max} = 12.5$ and $X_{\min} = 8.8$. We chose this example to have an analytically and computationally constrained distribution $F_{X|X_{\max}, X_{\min}}$ (see derivation in Appendix B) so that we can verify the correctness of the imputations. The marginal quantiles of the analytical posterior are shown in Figure 6(b).

To obtain samples from $F_{X|X_{\max}, X_{\min}}$, we use the implementation of Hamiltonian Monte Carlo provided by the probabilistic programming language Stan. In Stan, the user specifies a probabilistic data-generating process for the observed data, based on parameters and latent variables with accompanying priors. Stan then compiles this model into a custom C++ program that implements posterior sampling using HMC. We implement two Stan models to draw from $F_{X|X_{\max}, X_{\min}}$. The Stan model code for both are available in appendix A.1. The first model implements equation (10), with the narrow normal likelihood term around the maximum and minimum, while the second model includes the smoothmax and smoothmin approximations to the maximum and minimum functions. For each Stan model, we obtain 4 HMC chains each with 10,000 warm-up samples followed by 10,000 samples. The quantiles of the samples obtained without the smoothmax approximation are shown in Figure 6(c). By default, Stan initializes each X_i uniformly at random between -2 and 2, and for most variables, the algorithm remains stuck near the initial values. Furthermore, most samples do not conform to the constraints imposed by the observed X_{\min} and X_{\max} values, which further invalidates these results. However, once we replace the maximum function with the smoothmax function, with quantiles shown in Figure 6(d), Stan is able to draw samples that respect the observed extrema. Furthermore, a visual comparison of the analytical quantiles in Figure 6(a) and the Stan

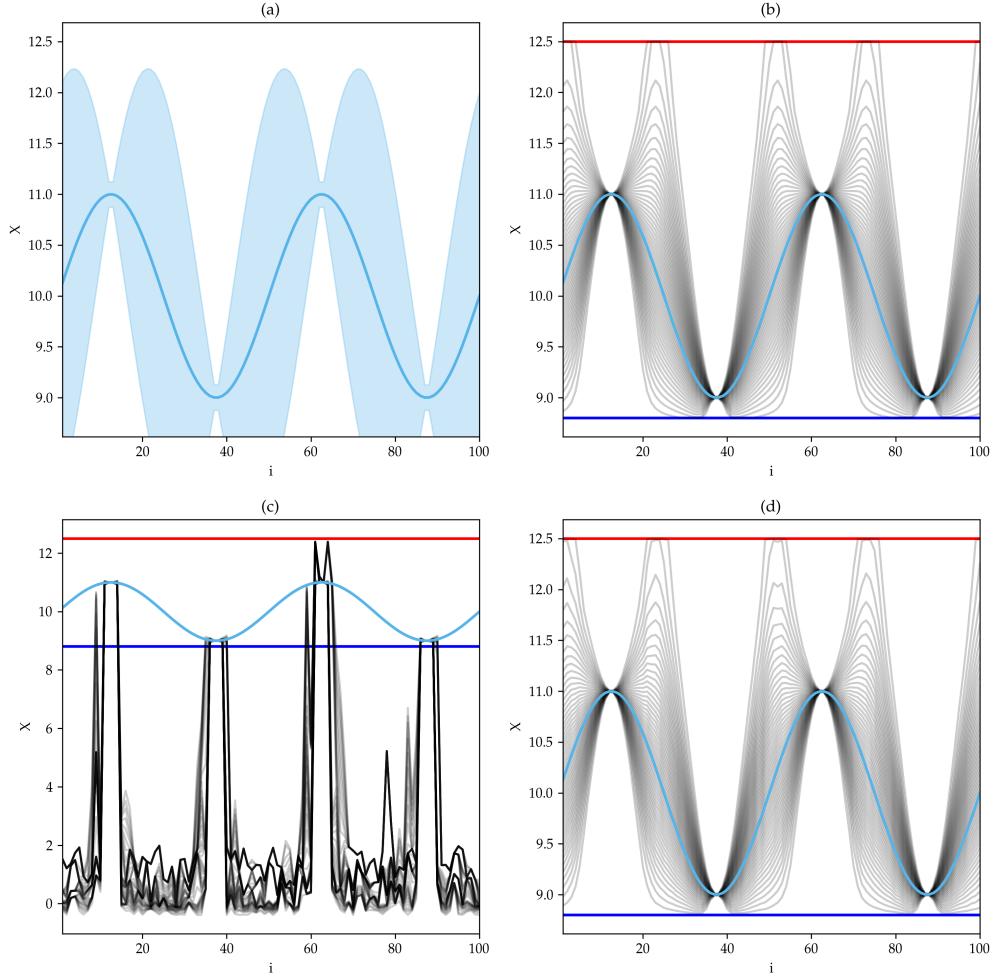


Figure 6: (a) Prior distribution of X_i displayed as mean function with 2σ envelope; (b) Quantiles of the analytically derived posterior $F_{X|X_{\max},X_{\min}}$ conditioned on X_{\min} and X_{\max} , with prior μ_i shown in blue; (c) Quantiles of the samples drawn from $F_{X|X_{\max},X_{\min}}$ using Stan without the smoothmax approximation, with prior μ_i shown in blue; (d) Quantiles of the samples drawn from $F_{X|X_{\max},X_{\min}}$ using Stan with the smoothmax approximation, with prior μ_i shown in blue.

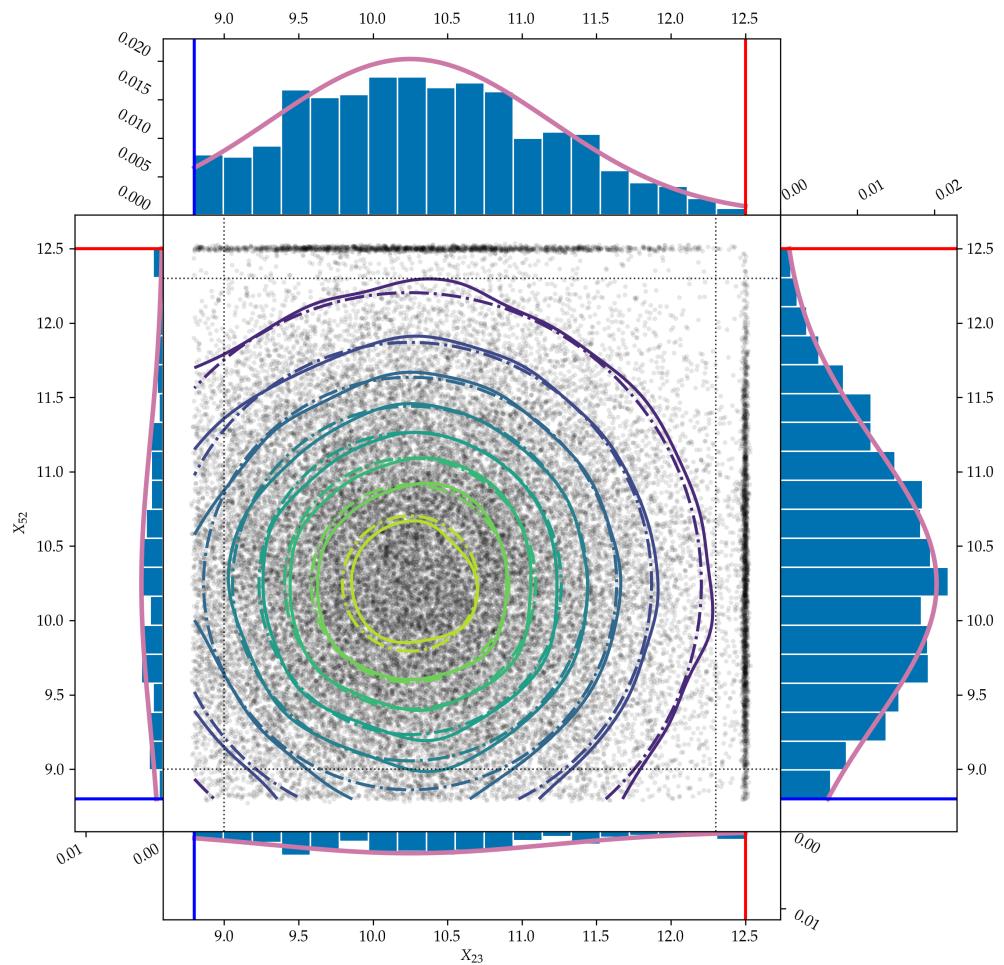


Figure 7: Comparison of the joint distribution of X_{23} and X_{52} obtained analytically and from Stan samples.

sample quantiles in Figure 6(d) confirms that this sampling algorithm delivers a close approximation of the marginal distribution of each variable X_i in $F_{X|X_{\max}, X_{\min}}$.

We may also wish to verify that Stan samples correctly from the *joint* distribution of any combination of variables. We do this visually for a pair of variables, X_{23} and X_{52} , with results shown in Figure 7. In that figure, the central scatterplot shows the 40,000 Stan samples obtained using the smoothmax approximation. Superimposed on the scatterplot are a contour plot (with dash-dotted lines) of the probability distribution function of the analytical conditional distribution $F_{X|X_{\max}, X_{\min}}$ of X_{23} and X_{52} when neither X_{23} nor X_{52} is one of the extrema, multiplied by the probability of that being the case (which is $1 - (\mathbb{P}_{23\bullet} + \mathbb{P}_{52\bullet} + \mathbb{P}_{\bullet23} + \mathbb{P}_{\bullet52}) + (\mathbb{P}_{23,52} + \mathbb{P}_{23,52})$). This can be compared to the contour plot (solid lines) of the same probability distribution function obtained through a kernel density estimator of the subset of Stan samples where neither X_{23} and X_{52} is the minimum or maximum, using a normal kernel with bandwidth 0.2, and multiplied by the proportion of samples where that is the case. The kernel estimates are divided by the integrated probability mass of the kernel that is inside of the boundaries, in order to reduce boundary effects. The thin black dotted line are one kernel bandwidth away from the X_{\min}/X_{\max} boundaries. Outside the thin black dotted line, the kernel density estimates are less trustworthy. The four histograms around the scatter plot are of the Stan samples where one of the variables is an extremum, weighted so as to integrate to the fraction of samples that satisfy that condition. For example, the top histogram is of X_{23} for samples where X_{52} is the maximum, and integrates to the fraction of samples where that is the case. The super-imposed pink line is that of a truncated normal probability distribution function multiplied by the probability of the satisfied condition. For example, the pink line over the top histogram integrates to $\mathbb{P}_{\bullet52}$. Lastly, the blue and red lines are X_{\min} and X_{\max} respectively. There is a close match between the contours of the analytical joint distribution function (dash-dotted lines) and of the kernel density estimate of the Stan samples. Each of the four histogram of samples where X_{23} or X_{52} occupies the minimum or maximum position matches the corresponding analytical distribution function. This visual comparison of the sample and analytical distributions should reassure us that Stan is yielding a good approximation of a sample drawn from the true $F_{X|X_{\max}, X_{\min}}$ in this example. We did not examine the behavior of the sampling algorithm for the joint distribution of more than two variables due to the difficulty of visualizing such a distribution, but we see no reason to suspect that the algorithm suffers from pathological behavior that does not manifest itself in these univariate and bivariate inspections.

4.3 Smoothmax Temperature Model

Armed with the SmoothHMC algorithm implemented in Stan, we finally return to the problem of imputing hourly temperature measurements. To impute the missing temperatures, we need to draw from the posterior distribution $T_{\text{miss}} | T_{\text{nearby}}, T_n, T_x$. Bayes' theorem conditional on T_{nearby} gives

$$\mathbb{P}(T_{\text{miss}} | T_{\text{nearby}}, T_n, T_x) = \frac{\mathbb{P}(T_n, T_x | T_{\text{nearby}}, T_{\text{miss}}) \mathbb{P}(T_{\text{miss}} | T_{\text{nearby}})}{\mathbb{P}(T_n, T_x | T_{\text{nearby}})}. \quad (15)$$

The second term in the numerator is the posterior obtained in section 3 now acting as a prior. The denominator is a normalizing constant. The first term in the numerator is either zero or one, indicating whether T_{miss} satisfies the constraint imposed by the observed T_n and T_x . Therefore, the posterior distribution takes a similar form to (9), which motivates the use of SmoothHMC.

A small leap of faith is needed to accept that SmoothHMC's success in a toy example in section 4.2 will extend to this application. There are three important differences between the toy example and the temperature time series model. Firstly, $F_{X|X_{\max}, X_{\min}}$ is now a multivariate normal distribution with strong correlations obtained as the posterior distribution of a Gaussian process in section 3. Secondly, instead of a single minimum and maximum, we observe extrema for every 24 hour period. Thirdly, we allow for the mean temperature to be different at different locations, and so the imputed temperatures are shifted by an additional parameter μ_{miss} , to which we will attach a vague prior. To summarize, the probabilistic model that we wish to draw posterior imputations of T_{miss} from is given in (16).

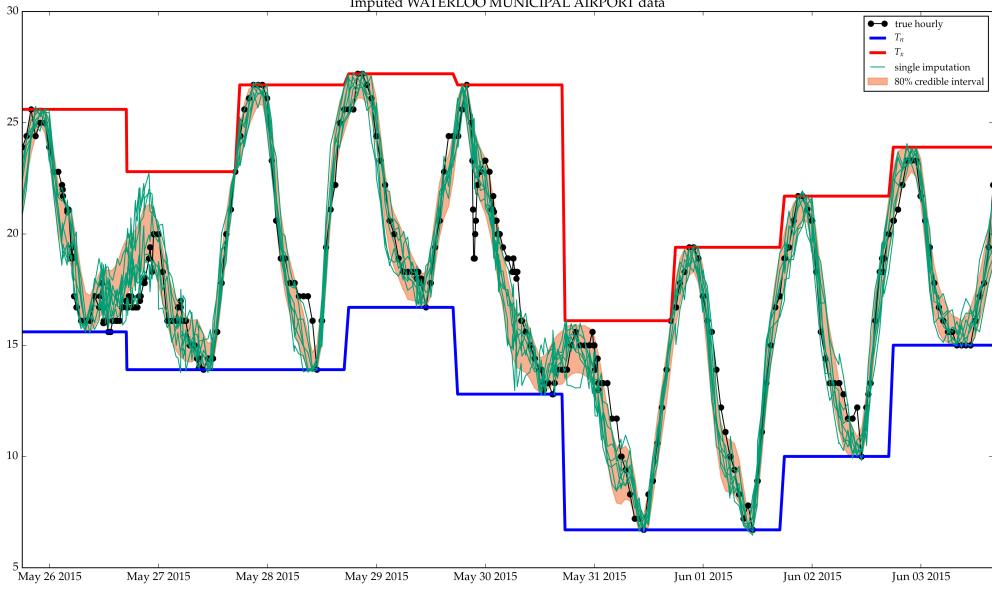


Figure 8: Imputations at Waterloo Airport from May 25, 2015 to June 3, 2015.

$$\begin{aligned}
 \mu_{\text{miss}} &\sim \mathcal{N}(0, 100) && \text{(vague prior on mean temperature)} \\
 f_{\text{miss}} &\sim \mathcal{N}(\mu_{\text{miss|nearby}}, \Sigma_{\text{miss|nearby}}) && \text{(posterior from } T_{\text{nearby}} \text{ becomes prior)} \\
 T_{\text{miss}} &= \mu_{\text{miss}} + f_{\text{miss}} \\
 T_x[\text{day}] &= \max_{i \in \{i\}_{\text{day}}} \{T_{\text{miss},i}\} && \text{(observe maximum in 24hr window)} \quad (16) \\
 T_n[\text{day}] &= \min_{i \in \{i\}_{\text{day}}} \{T_{\text{miss},i}\} && \text{(observe minimum in 24hr window)} \\
 \{i\}_{\text{day}} &= \left\{ i : \text{day} - 1 + \frac{\text{hour}}{24} < t_{\text{miss},i} \leq \text{day} + \frac{\text{hour}}{24} \right\} && \text{(indices of times in the 24hr window)}
 \end{aligned}$$

To sample from this model, we modify it with the smoothmax approximation to the maximum, and a normal likelihood. The resulting model is shown in (17), and the corresponding Stan code is in Appendix A.2.

$$\begin{aligned}
 \mu_{\text{miss}} &\sim \mathcal{N}(0, 100) \\
 f_{\text{miss}} &\sim \mathcal{N}(\mu_{\text{miss|nearby}}, \Sigma_{\text{miss|nearby}}) \\
 T_{\text{miss}} &= \mu_{\text{miss}} + f_{\text{miss}} \\
 T_x[\text{day}] &\sim \mathcal{N} \left(\text{smoothmax}_{i \in \{i\}_{\text{day}}} \{T_{\text{miss},i}; k = 10\}, 0.1^2 \right) \\
 T_n[\text{day}] &\sim \mathcal{N} \left(\text{smoothmin}_{i \in \{i\}_{\text{day}}} \{T_{\text{miss},i}; k = 10\}, 0.1^2 \right) \quad (17)
 \end{aligned}$$

Example imputations from this procedure are shown in Figure 8. From May 25, 2015 to June 3, 2015, hourly temperatures are imputed at Waterloo Airport, using the hourly temperature measurements from nearby stations to inform the course of the temperatures, and using the daily minima and maxima “measurements” to constrain the imputed temperatures. One can verify visually that the imputations respect the T_n and T_x constraints, reaching but not exceeding each extreme on each day. Because we actually have

hourly data for Waterloo, yet only fed our algorithm a reduction of this data to daily extremes, we can also plot the hidden temperatures, and see how faithfully the imputations reproduce them. We see that the imputations indeed track the true measurements very closely. On May 27th, we can see that the imputations capture the fact that the T_x record *could* have been set early in the measurement window, but more likely at its very end, just before the measurement. This success demonstrates that the “leap of faith” was justified, and that SmoothHMC is capable of imputing temperature time series from the posterior distribution $T_{\text{miss}} \mid T_{\text{nearby}}, T_n, T_x$.

5 Model diagnostics

5.1 Variogram

We can visually inspect our model by plotting temporal and spatial semi-variograms. The semi-variogram of a stationary spatio-temporal function $Y(x, t)$ is a function of the spatial lag h and the temporal lag r

$$\gamma(h, r) = \frac{1}{2} \mathbb{E} [(Y(x, t) - Y(x + h, t + r))^2] = \text{var}(Y(x, t)) - \text{cov}((Y(x, t)), Y(x + h, t + r)). \quad (18)$$

For a Gaussian Process model, with a stationary kernel $k(h, r) = k(x, x + h, t, t + r)$ this can be expressed in terms of the observation noise σ_ϵ and kernel function $k(\cdot, \cdot)$, as

$$\gamma(h, r) = \sigma_\epsilon^2 + k(0, 0) - k(h, r). \quad (19)$$

From the data, the semi-variogram can also be estimated empirically, by averaging the square differences of any two observations that are separated by h in space, and r in time (or, in practice, within half a bin width of h and r). By comparing the empirical variogram to the variogram of our fitted GP model, we obtain a visual diagnosis of the model.

In our Iowa example, there are only four possible locations. For each location, we plot the empirical temporal variogram $\hat{\gamma}(0, r)$. For any pair of stations separated by h (fixed), we can also plot $\hat{\gamma}(h, r)$. We then overlay the model’s semi-variogram obtained through equation (19), resulting in Figure 9.

We notice that the variogram of the simple SE \times SE model tracks the empirical variogram well at short lags, but fails to capture the diurnal cycle, and the fit degrades at long lag. We attempt to improve the model in section 6.

5.2 Error and expected error

The variogram gives us a visual diagnostic of the overall model fit. To quantify the model’s predictive ability in the Iowa example, we compare the posterior mean temperature to the withheld truth, and obtain the empirical mean squared error as

$$\text{MSE}(\text{err} \mid T_{\text{nearby}}, T_x, T_n) = \frac{1}{N} \sum_{i=1}^N [\mathbb{E}(T_{\text{miss},i} \mid T_{\text{nearby}}, T_x, T_n) - T_{\text{miss},i}]^2. \quad (20)$$

This equation is for the final predictions obtained using nearby hourly temperatures and local daily maxima and minima. A similar diagnostic can be computed for the intermediary predictions, which exclude the local T_x and T_n information. At that stage, we are not concerned with any overall bias in the predicted temperatures, so we instead compute the sample variance of the errors as

$$\text{var}(\text{err} \mid T_{\text{nearby}}) = \text{var}_i \{\mathbb{E}(T_{\text{miss},i} \mid T_{\text{nearby}}) - T_{\text{miss},i}\}. \quad (21)$$

Model	Log Likelihood	Var(err)	$\mathbb{E}(\text{Var}(\text{err}))$	MSE(err)	$\mathbb{E}(\text{MSE}(\text{err}))$
SE \times SE	-55,614	1.589	0.875	1.104	0.614
SExSE + diurnal	-54,472	1.633	0.974	1.137	0.697

Model	Log Likelihood	Var(err)	$\mathbb{E}(\text{Var}(err))$	MSE(err)	$\mathbb{E}(\text{MSE}(err))$
Sum of products, fixed variance	-48,589	4.991	8.791		
SoP, fixed temporal, free var	-47,082	1.314	2.321	1.150	0.897
SoP, completely free	-46,184	1.423	1.765	1.152	0.950
SoP, simpler	-45,945	1.319	1.190	1.069	0.823

For our purposes, it isn't sufficient for the spatio-temporal model to yield good predictions; we also require a good estimate of its own accuracy. We estimate the expected MSE and predictive variance by sampling K random draws T_{miss}^k from the posterior distribution, again conditioned firstly on just T_{nearby} after fitting the spatio-temporal Gaussian process model, and then additionally on T_{nearby}, T_x and T_n after incorporating the local data using Stan. The draws are obtained from the posterior multivariate normal distribution in the first case, and the MCMC samples obtained through Stan in the second case. We then evaluate the variance or MSE between the samples and the posterior mean as

$$\begin{aligned}\mathbb{E}(\text{var}(\text{err} | T_{\text{nearby}})) &\approx \frac{1}{K} \sum_{k=1}^K \text{var}_i \left\{ T_{\text{miss},i}^{(k)} - \mathbb{E}(T_{\text{miss},i} | T_{\text{nearby}}) \right\} \\ \mathbb{E}(\text{MSE}(\text{err} | T_{\text{nearby}}, T_x, T_n)) &\approx \frac{1}{K} \sum_{k=1}^K \text{MSE}_i \left\{ T_{\text{miss},i}^{(k)} - \mathbb{E}(T_{\text{miss},i} | T_{\text{nearby}}, T_x, T_n) \right\}\end{aligned}\quad (22)$$

When evaluating models, we want the errors to be small, and so the empirical error variance and MSE to be low. A well-calibrated model should also have the expected error variances $\mathbb{E}(\text{var}(\text{err} | \cdot))$ close to their empirical values.

These diagnostics for our first spatio-temporal model, the product of squared exponentials, are found in the first row of Table X. The empirical error variance using only nearby measurements is already fairly low, with typical errors of order $\sqrt{1.589} = 1.26^\circ\text{C}$. Incorporating the local measurements reduces it further to $\sqrt{1.104} = 1.05^\circ\text{C}$. However, the model is overly optimistic, and the expected errors underestimate the true errors.

6 Improving model

In this section, we develop more sophisticated Gaussian process models than the simple product of squared exponential kernels. We then assess whether these models improve the variogram and the predictive diagnostic measures that we developed in the previous sections.

The most salient feature of the empirical variogram that isn't captured by the `SESE` model is the oscillation with a 24-hour period. It is intuitively obvious that the diurnal cycle induces this periodic covariance, and that our model should be improved by incorporating this feature. Gaussian process models allow for periodic components of the covariance, for example the periodic squared exponential kernel, which we will use with a 24-hour period

$$k_{24}(t, t') = \sigma_{24}^2 \exp \left[-\frac{2}{\ell_{24}^2} \sin^2 \left(\pi \frac{t - t'}{24 \text{ hrs}} \right) \right]. \quad (23)$$

We modify the spatiotemporal model by adding this diurnal component to it, with its own spatial decay kernel $k_{\text{space}24}$ (with the same specification as k_{space} in (1)).

$$k_{\text{SESE}_24}(\mathbf{x}, \mathbf{x}', t, t') = k_{\text{time}}(t, t') \cdot k_{\text{space}}(\mathbf{x}, \mathbf{x}') + k_{24}(t, t') \cdot k_{\text{space}24}(\mathbf{x}, \mathbf{x}') + k_\mu(\mathbf{x}, \mathbf{x}'). \quad (24)$$

We also develop a more complex model, which breaks up k_{time} into short-term, medium-term and long-term correlation components, each with their own spatial decay.

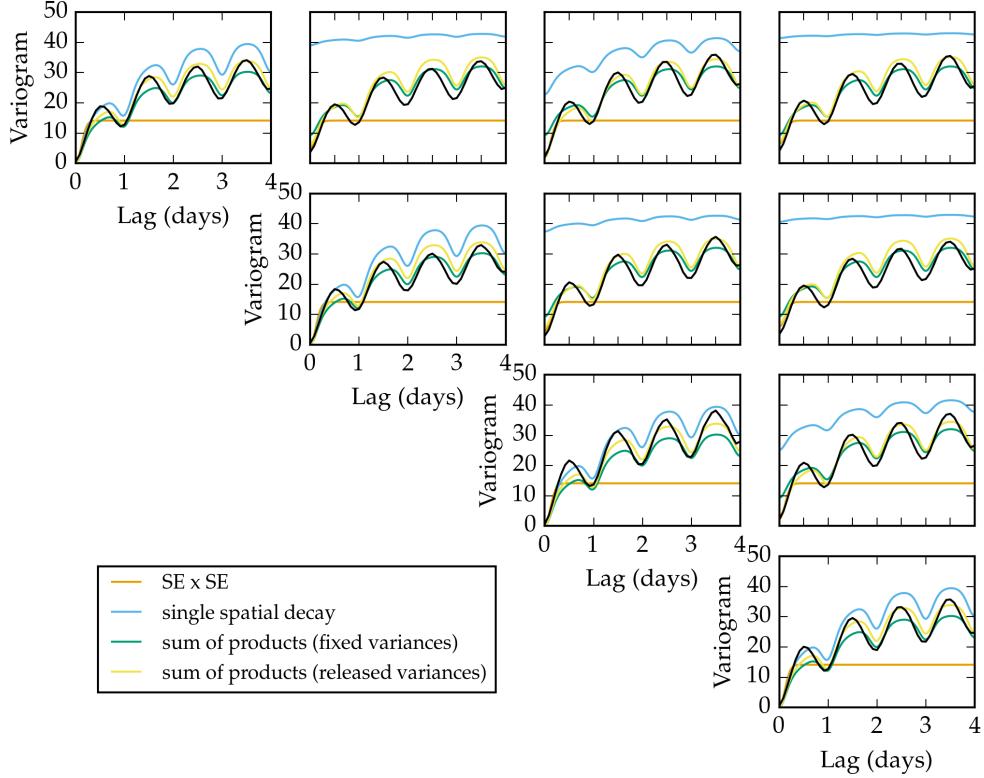


Figure 9: Semi-variogram

$$\begin{aligned}
 k_{\text{sumprod}}(x, x', t, t') &= k_{\text{time}1}(t, t') \cdot k_{\text{space}1}(x, x') && \text{(short-term variation)} \\
 &+ k_{\text{time}2}(t, t') \cdot k_{\text{space}2}(x, x') && \text{(medium-term variation)} \\
 &+ k_{\text{time}3}(t, t') \cdot k_{\text{space}3}(x, x') && \text{(long-term variation)} \\
 &+ k_{24}(t, t') \cdot k_{\text{space}24}(x, x') && \text{(diurnal cycle)} \\
 &+ k_{\mu}(x, x') && \text{(station mean)}
 \end{aligned} \tag{25}$$

Each of $k_{\text{time}1}$, $k_{\text{time}2}$, and $k_{\text{time}3}$, is a rational quadratic kernel

$$k_{\text{RQ}}(t, t') = \sigma^2 \left(1 + \frac{(t - t')^2}{2\alpha\ell^2} \right)^{-\alpha} \tag{26}$$

which is accompanied by its spatial decay kernel, specified as a squared exponential covariance. This more complicated kernel therefore has $3 \times 3 \times 2 + 2 \times 2 = 22$ free parameters, in addition to the noise parameter σ_ϵ^2 .

We now have three competing Gaussian process models, with covariance functions $k_{\text{SE} \times \text{SE}}$, k_{SESE_4} , and k_{sumprod} respectively. We can compare them in three ways. Firstly, the marginal log-likelihood is the quantity maximized by the parameter fitting procedure in (7). The maximized log-likelihood can be found in the second column of Table XX, and we see that the more complex models indeed yield a much higher log-likelihood, promising a better model fit which should yield better predictions. Secondly, we compare the variance of the error in the predicted temperatures specified in (21) when withholding all the data from a test station. Averaged over all of 2015, this is given in the third column, and shows more mixed results. The diurnal model k_{SESE_4} performs worse than the simple $k_{\text{SE} \times \text{SE}}$ model, and k_{sumprod} only yields a small improvement. Thirdly, we can reintroduce the daily minima and maxima from the withheld station, and compare the mean squared error specified in (20) for predictions at the test station. Results in the fifth column show even more modest improvements for the more complex models.

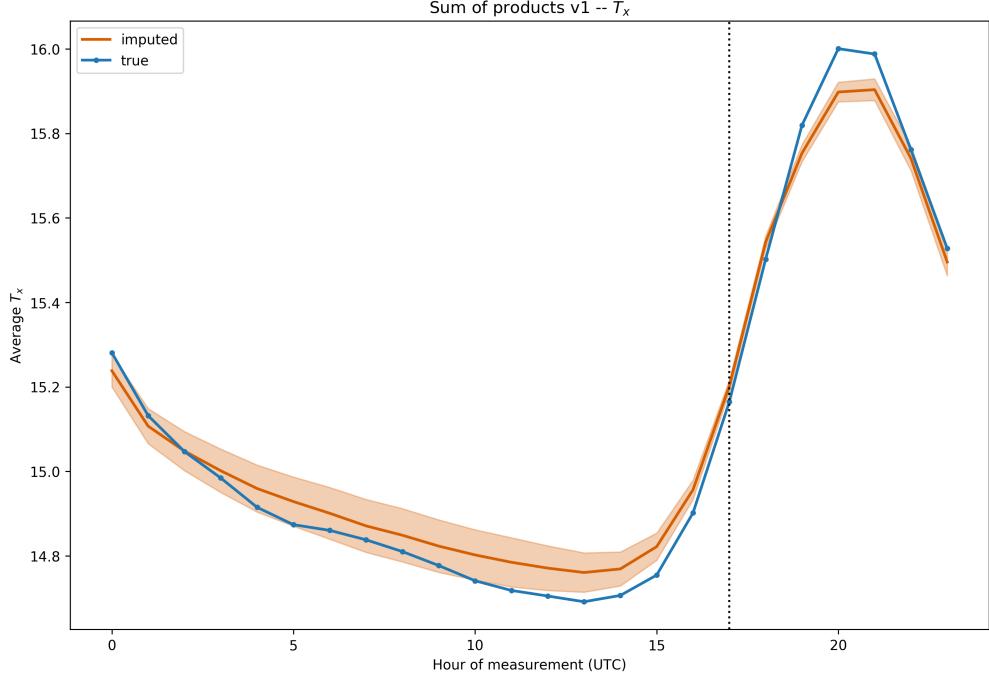


Figure 10

We interpret these results as a reminder that predictions using Gaussian process are sensitive to model specification when extrapolating, but fairly insensitive to the model when interpolating (Stein, 2012). Since our imputations interpolate the temperatures from nearby stations, further aided by the constraints imposed by the daily T_n and T_x measurements, the choice of model does not have a large impact on the performance of our procedure. This insensitivity can be seen as reassuring, as it (to an extent) reduces our need to worry about the incorrectness of our model.

7 Analysis

- show imputations on interesting days
- show imputations can capture two possible explanations for a measurement
- look at summary statistics applied to imputations
 - how to get correct uncertainty when we've carved the data into overlapping chunks? could correct for covariance by looking accounting for covariance (assuming X_3 independent of X_1 given X_2)...

Figure ?? shows the imputations produced under the sum of products kernel (25). This is the primary output of our imputation method, and it shows promising behavior. Firstly, just like in the toy example presented in 4.2, the individual imputations meet the three constraints imposed by the measured minimum and maximum. Each day, the imputations stay between T_n and T_x , and the temperatures always drop to T_n and rise to T_x at some time of the day. The imputations reflect the uncertainty in the time at which the extrema are reached. Notably, on some days, the posterior distribution of the warmest (or coldest) time is bimodal. For example this can be seen on May 31st, where some imputations reach T_x at the start of the measurement window, while others reach it at the end (which in this particular case is the correct choice). We view as a particular strength of our approach that the imputations are able to capture this bimodality.

These imputations however are not the final aim of this paper. Rather, the scientific goal is to undo, or at least account for, the sensitivity to measurement time seen in Figure 2. Equipped with these imputations, is it possible to infer what the value of the summary statistic would have been for different measurement

hours? This capability is demonstrated in Figure 10, which shows the same summary statistic as in Figure 2 applied to the individual imputations instead of the (withheld) hourly data at Waterloo Airport. The thick orange line shows the mean of the summary statistic over all imputations, while the envelope is double their standard deviation. [need to explain how posterior variance is obtained] It can be seen that the imputed summary statistics track within about 0.1°C of the true values, while the posterior standard deviation gives a fair estimate of the imputation error.

TODO: acknowledge it's not perfect (but rerun first).

8 Inference on measurement hour

Our analysis so far has focused on the case where the hour of measurement `hour` is known in advance. This is an unrealistic assumption in practice, and so inference on `hour` is a desirable feature. It is conceptually straightforward to modify the measurement model (17) with a uniform prior on `hour`. However, because we obtain our imputations in ten-day windows, in most windows precise information about `hour` will not be available, as moving the measurement time one hour earlier or later rarely affects the measured T_n and T_x . Furthermore, `hour` affects which observations are attributed to each day's measurements. This effect is discontinuous (observations suddenly jump from one day to the next) and non-differentiable, and so Hamiltonian Monte Carlo becomes unviable. This issue is similar to that caused by the non-differentiability of the minimum and maximum functions. We therefore do not consider the introduction of a uniform prior on `hour` in Stan to be feasible.

Our procedure allows us to obtain imputation samples of T_{miss} conditional on T_{nearby} , T_n , T_x and `hour`. If we do so for $\text{hour} = 1, 2, \dots, 24$, is there information available in these samples to infer `hour`? We will examine sample imputations to answer this question. Figure 11 shows mean imputation for temperatures over nine days starting on February 27, 2015. The orange line is the mean using only nearby temperatures (shifted by a constant to match the true temperatures), while the green line is additionally conditional on T_n and T_x ; the true temperatures are shown in grey. The top plot shows the imputation under the correct daily measurement time (17 UTC), while the bottom plot is under an incorrect measurement time (5 UTC). The first unsurprising observation is that assuming an incorrect measurement time can lead to wildly inaccurate imputations. But we then also notice that assuming the wrong time also causes the mean constrained imputation to depart further from the unconstrained imputation (that is, the green and orange lines are further apart). This can be interpreted as an indication of an incompatibility between T_{nearby} and the daily extremes, caused by assuming the wrong `hour`. To quantify this discrepancy, we propose to calculate the probability of the mean constrained imputation under the unconstrained posterior given by (8):

$$\begin{aligned}\mu(\text{hour}) &\equiv \mathbb{E}(T_{\text{miss}} | T_{\text{nearby}}, T_n, T_x, \text{hour}) \quad (\text{the mean imputed temperature}), \\ \delta_{\text{hour}} &\equiv \mathbb{P}(T_{\text{miss}} = \mu(\text{hour}) | T_{\text{nearby}}).\end{aligned}\tag{27}$$

Our intuition is that δ_{hour} will drop sharply when the wrong `hour` is assumed, and we may be able to infer the true `hour` by maximizing δ_{hour} .

9 Conclusion

- reiterate what we were trying to do
 - correct bias in T_n T_x
 - imputation strategy
- summarize work done:
 - modeling
 - Gaussian process prediction
 - constraining GP using Stan

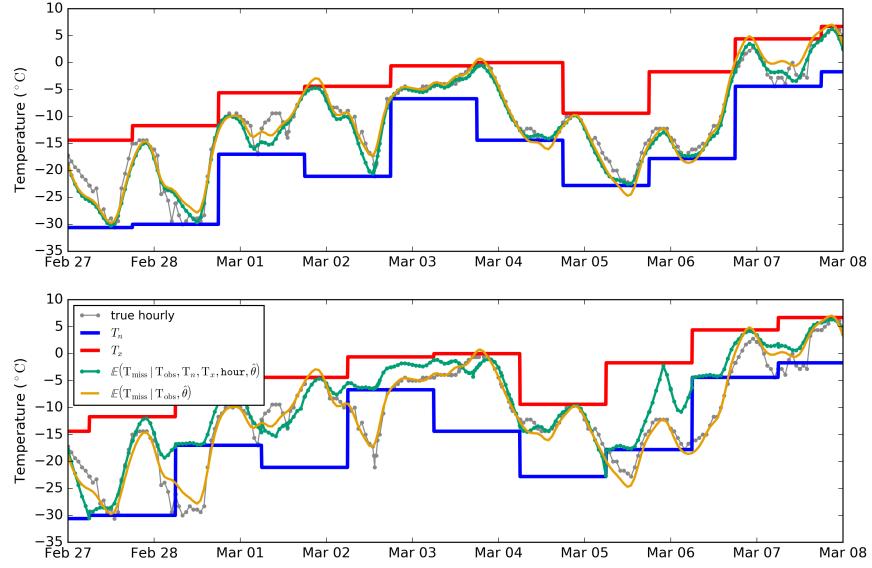


Figure 11: A sample window showing constrained and unconstrained imputations assuming (top) the correct measurement hour (17 UTC), and (bottom) the wrong measurement hour (5 UTC). Assuming the wrong measurement time drives the constrained mean imputation away from the unconstrained mean imputation.

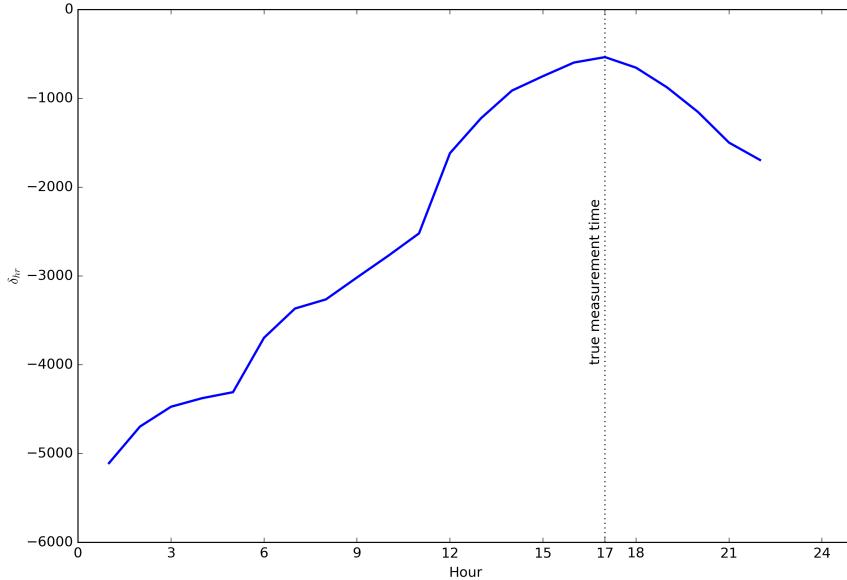


Figure 12: Discrepancy measure for imputations of temperatures at Waterloo Municipal Airport assuming measurement hours $\text{hour} = 1, 2, \dots, 24$. The true hour of measurement is 17, and obtains the highest δ_{hour} .

- model diagnostics and improvement: not hugely significant
- reiterate that we don't believe in this model, it's a tool to pool different sources of information
- we mostly test the validity of the method by withholding data from a station
- and show we can correct TnTx bias in summary statistics?

Climatological research relies on the ability to track small changes over long periods. For this reason, the subtle bias induced by the measurement time exposed by (Baker, 1975) could lead to wrong estimates and conclusions regarding long-term trends in temperature records. In this paper, this is illustrated in section 1.1, which demonstrates using temperature records from a meteorological station in Iowa, that the answer to a simple question such as "what was the average daily maximum temperature in 2015?" can change by about 1° C depending on the time of measurement. A drift in the time of measurement from one year to the next could therefore result in misleading conclusions.

We reframed the source of the bias as a missing data problem. If we had access to the full time series of temperatures, we could choose retrospectively to emulate the measurements of daily extremes at any time of day. For example, we may wish to emulate measurements of T_x at an hour that is typically cold, and T_n at a warm hour, in order to maximize our chances of measuring the true peaks of each diurnal cycle. This missing data perspective motivated our approach, which is to impute the temperature time series, by combining the information available from the record of daily temperature extremes, and from nearby records of hourly temperatures.

The hourly records are typically at meteorological stations that aren't always sufficiently well-calibrated or their equipment and procedures sufficiently well-documented to be directly used for climate science. Often they are located near airports and urban areas, which further affects the trustworthiness of their data. This precludes directly relying on meteorological records to estimate climatological trends. However, even if the hourly records are miscalibrated and biased, they can tell us how the temperature changed over the course of a day. This is the information that is missing from daily measurements of temperature extremes made at research-quality weather stations.

We therefore have two pieces of the puzzle — shape and daily extremes of the time series — but they are obtained at separate locations. To combine them, we needed a spatio-temporal model, and proposed a Gaussian process with squared exponential kernels (4) in space and time. While this is not a realistic physical model, it is very flexible, and is generally adequate for the task of interpolating temperatures between nearby locations and times. Misspecification of spatial models is much more troublesome for extrapolation tasks (Stein, 2012). Indeed, more complex kernels (with a diurnal component and a sum of short-range and long-range components) showed only modest improvements in the mean squared error of the imputations compared to a withheld hourly temperature record.

The GP specification and multivariate normal theory allow us to derive analytical predictions (8) of temperatures at the location of a climatological station given hourly measurements from nearby meteorological stations. But to further condition on the daily T_x and T_n , we developed SmoothHMC, a general algorithm based on Hamiltonian Monte Carlo with a smoothed approximation of the target distribution that can sample from a multivariate distribution conditionally on its observed minimum and maximum. It showed an excellent ability to sample from the conditional distribution in an example where the distribution function can also be obtained analytically. We believe this method could find applications beyond the present setting. We used this method to obtain imputations of the temperature time series that satisfied the constraints imposed by the measured T_n and T_x .

The imputed time series are the primary output of this work, but they are intended as a starting point for further analyses motivated by different scientific goals. Various summary statistics can be applied to the imputations. For example, one can now answer questions such as "what would the average T_x have been in 2015 if the measurements had instead been made at midnight?" by extracting and averaging daily maxima from each imputation, for 24 hour periods starting and ending at midnight each day. Using imputations obtained for the withheld time series at Waterloo airport, we have demonstrated a good ability to recover this information, though the resulting posterior variance seems to underestimate the error.

The average T_x is an example of a possible follow-up analysis, chosen mostly as an illustrative proof of concept. We plan to use this method to compare the average temperature to the average of the measured T_n and T_x for a given location and year, with the former obtained from imputed time series.

A Stan programs

A.1 Smoothmax toy example

A.1.1 Without **smoothmax** Approximation

```
data {
    int<lower=0> N; // number of observations
    real Xmax;
    real Xmin;
    vector[N] mu_i;
    real<lower=0> sigma_i[N];
}
parameters {
    vector[N] X_i; // latent variables
}
model {
    X_i ~ normal(mu_i, sigma_i);
    Xmax ~ normal(max(X_i), 0.01);
    Xmin ~ normal(min(X_i), 0.01);
}
```

A.1.2 With **smoothmax** Approximation

```
functions {
    real smoothmax(vector x, real k, real maxkx) {
        return (maxkx+log(sum(exp(k*x - maxkx))))/k;
    }
    real smoothmin(vector x, real k, real minkx) {
        return -smoothmax(-x, k, -minkx);
    }
}
data {
    int<lower=0> N; // number of observations
    real Xmax;
    real Xmin;
    real mu_i[N];
    real<lower=0> sigma_i[N];
    real<lower=0> k;
}
parameters {
    vector[N] X_i; // latent variables
}
transformed parameters {
    real Xsmoothmax;
    real Xsmoothmin;
    Xsmoothmax = smoothmax(X_i, k, k*Xmax);
    Xsmoothmin = smoothmin(X_i, k, k*Xmin);
}
model {
    X_i ~ normal(mu_i, sigma_i);
    Xmax ~ normal(Xsmoothmax, 0.01);
    Xmin ~ normal(Xsmoothmin, 0.01);
}
```

A.2 Temperature imputations

```

functions {
    real smoothmax(vector x, real k, real maxkx) {
        return (maxkx+log(sum(exp(k*x - maxkx))))/k;
    }
    real smoothmin(vector x, real k, real minkx) {
        return -smoothmax(-x, k, -minkx);
    }
}
data {
    // Tn Tx data
    int<lower=1> N_TxTn; //
    vector[N_TxTn] Tx;
    vector[N_TxTn] Tn;

    // imputation points (for which we have )
    int<lower=1> Nimpt;
    int<lower=1,upper=N_TxTn> day_impute[Nimpt];
    // number of hours recorded within each day
    int<lower=1> impt_times_p_day[N_TxTn];

    // prior
    vector[Nimpt] predicted_mean;
    matrix[Nimpt,Nimpt] predicted_cov;
    matrix[Nimpt,Nimpt] predicted_cov_chol;

    // control soft max hardness
    real<lower=0> k_smoothmax;
}
parameters {
    vector[Nimpt] w_uncorr;
    real mu;
}
transformed parameters {
    vector[Nimpt] temp_impt;
    real Tsmoothmax[N_TxTn];
    real Tsmoothmin[N_TxTn];
    temp_impt = mu + predicted_mean + predicted_cov_chol*w_uncorr;
{
    int istart;
    istart = 1;
    for (i in 1:N_TxTn) {
        int ntimes;
        ntimes = impt_times_p_day[i];
        Tsoftmin[i] = smoothmin(segment(temp_impt,istart,ntimes),
                                k_smoothmax,
                                k_smoothmax*Tn[i]);
        Tsoftmax[i] = smoothmax(segment(temp_impt,istart,ntimes),
                                k_smoothmax,
                                k_smoothmax*Tx[i]);
        istart = istart + ntimes;
    }
}

```

```

}
model {
  w_uncorr ~ normal(0,1);
  mu ~ normal(0, 100.0);
  Tn ~ normal(Tsmoothmin, 0.1);
  Tx ~ normal(Tsmoothmax, 0.1);
}

```

B Derivation of the analytic posterior for toy example

We first derive and compute $F_{X|X_{\max}, X_{\min}}$ for this example. We denote by $f_i(\cdot)$ and $F_i(\cdot)$ the prior probability distribution function and cumulative distribution function of X_i , i.e. the normal PDF and CDF with means and variances given by (14). Let \mathbb{P}_{ij} be the probability that X_i is the minimum of X , and X_j is its maximum. We also define $\mathbb{P}_{i\bullet} = \sum_{j=1}^{100} \mathbb{P}_{ij}$, the probability that X_i is the minimum, and $\mathbb{P}_{\bullet j} = \sum_{i=1}^{100} \mathbb{P}_{ij}$, the probability that X_j is the maximum. The cumulative distribution function of X_i is then given by

$$\mathbb{P}(X_i \leq x | X_{\max}, X_{\min}) = \begin{cases} 0 & \text{when } x < X_{\min}, \\ \mathbb{P}_{i\bullet} + (1 - \mathbb{P}_{i\bullet} - \mathbb{P}_{\bullet i}) \left[\frac{F_i(x) - F_i(X_{\min})}{F_i(X_{\max}) - F_i(X_{\min})} \right] & \text{when } X_{\min} \leq x < X_{\max}, \\ 1 & \text{when } x \geq X_{\max}. \end{cases} \quad (28)$$

Meanwhile, \mathbb{P}_{ij} is proportional to

$$f_i(X_{\min}) f_j(X_{\max}) \prod_{k \neq i, j}^{100} (F_k(X_{\max}) - F_k(X_{\min})) , \quad (29)$$

which we compute for all i, j and renormalize to obtain the 100×100 matrix of probabilities. We sum over its rows and columns to obtain $\mathbb{P}_{\bullet j}$ and $\mathbb{P}_{i\bullet}$. While this algorithm has cubic complexity in the dimensionality p of X , for $p = 100$ computers only take seconds to compute the entries of \mathbb{P} and evaluate $\mathbb{P}(X_i \leq x | X_{\max}, X_{\min})$ over a range of x . Figure 6(b) shows the analytical quantiles of $F_{X|X_{\max}, X_{\min}}$. Roughly speaking, we see that the prior distribution F_X is stretched to fit between X_{\min} and X_{\max} .

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