Title
Web-based Supplementary Materials for Bayesian Modeling and Analysis for Gradients in Spatiotemporal Processes by Quick et al.

Permalink

Authors
Quick, Harrison
Banerjee, Sudipto
Carlin, Bradley P.

Publication Date
2015-01-28

Peer reviewed

Web-based Supplementary Materials for Bayesian Modeling and Analysis for Gradients in Spatiotemporal Processes by Quick et al.

A   The legitimacy of $\mathbf{C_W}(\boldsymbol{\Delta}, \delta)$

The legitimacy of the cross-covariance matrix, $\mathbf{C_W}(\boldsymbol{\Delta}, \delta)$, can be established by first constructing the associated finite-difference process and then passing to limits. To be precise, let $\mathbf{U}_h(\mathbf{s}, t) = (Z(\mathbf{s}, t), Z(\mathbf{s} + h\mathbf{e}_1, t), \ldots, Z(\mathbf{s} + h\mathbf{e}_d, t))^T$ be $(d+1) \times 1$ and let $\mathbf{W}_{1,h}(\mathbf{s}, t) = \mathbf{G}_h \mathbf{U}_h(\mathbf{s}, t)$, where $\mathbf{G}_h = \begin{bmatrix} 1 & \mathbf{0}' \\ -(1/h)\mathbf{1}_d & (1/h)\mathbf{I}_{d \times d} \end{bmatrix}$. Since $Z(\mathbf{s}, t)$ is a Gaussian process, $\mathbf{U}_h(\mathbf{s}, t)$ has a nondegenerate Gaussian law for every $h \neq 0$. Therefore, $\mathbf{W}_{1,h}(\mathbf{s}, t)$ is a well-defined multivariate Gaussian process because it is a nonsingular linear transformation of $\mathbf{U}_h(\mathbf{s}, t)$. If $\mathbf{C}_{1,h}(\boldsymbol{\Delta}, \delta)$ is the cross-covariance of $\mathbf{W}_{1,h}(\mathbf{s}, t)$, then $\lim_{h \to 0} \mathbf{W}_{1,h}(\mathbf{s}, t) = \mathbf{W}_1(\mathbf{s}, t)$ is a legitimate multivariate Gaussian process as long as $\lim_{h \to 0} \mathbf{C}_{1,h}(\boldsymbol{\Delta}, \delta) = \mathbf{C}_1(\boldsymbol{\Delta}, \delta)$ exists, which is, then, the valid cross-covariance matrix of $\mathbf{W}_1(\mathbf{s}, t)$. Assuming that our parent spatiotemporal covariance function $K(\boldsymbol{\Delta}, \delta)$ is such that $\mathbf{C}_1(\boldsymbol{\Delta}, \delta)$ exists, we further construct the $2(d+1) \times 1$ process

$$\mathbf{W}_{h,k}(\mathbf{s}, t) = \begin{bmatrix} \mathbf{I}_{d \times d} & \mathbf{O} \\ -(1/k)\mathbf{I}_{d \times d} & (1/k)\mathbf{I}_{d \times d} \end{bmatrix} \begin{bmatrix} \mathbf{W}_{1,h}(\mathbf{s}, t) \\ \mathbf{W}_{1,h}(\mathbf{s}, t + k) \end{bmatrix}$$

Therefore, for every nonzero h and k, $\mathbf{W}_{h,k}(\mathbf{s}, t)$ is a nonsingular linear transformation of a random vector with a nondegenerate Gaussian law and, hence, $\mathbf{W}_{h,k}(\mathbf{s}, t)$ is a well-defined process. Let $\mathbf{C}_{h,k}(\boldsymbol{\Delta}, \delta)$ be the cross-covariance function for $\mathbf{W}_{h,k}(\mathbf{s}, t)$. Then, $\lim_{h,k \to 0} \mathbf{W}_{h,k}(\mathbf{s}, t) = \mathbf{W}(\mathbf{s}, t)$ is a well-defined multivariate Gaussian process with cross-covariance function $\lim_{h,k \to 0} \mathbf{C}_{h,k}(\boldsymbol{\Delta}, \delta) = \mathbf{C_W}(\boldsymbol{\Delta}, \delta)$, whenever the latter limit exists. Our

choice of $K(\boldsymbol{\Delta}, \delta)$, so that its required derivatives exist, ensures that $\mathbf{C_W}(\boldsymbol{\Delta}, \delta)$ exists and the spatiotemporal gradient process is well-defined.

The cross-covariance matrix in (8) can be constructed by first deriving the cross-covariance matrix of $\mathbf{W}_{h,k}(\mathbf{s}, t)$ and then passing to the limit as $h \to 0$ and $k \to 0$. The legitimacy of the finite difference processes ensure that $\mathbf{C_W}(\boldsymbol{\Delta}, \delta)$ in (8) is valid because it arises as limits of the valid finite-difference cross-covariances. For example, cross-covariance between the mixed spatial gradients $\mathrm{Cov}(\boldsymbol{\nabla}_{st} Z(\mathbf{s}, t), \boldsymbol{\nabla}_{st} Z(\mathbf{s} + \boldsymbol{\Delta}, t + \delta))$ is obtained as

$$
\lim_{h \to 0} \lim_{k \to 0} \mathrm{Cov} \left[\frac{Z(\mathbf{s} + h\mathbf{u}, t + h) - Z(\mathbf{s}, t)}{h}, \frac{Z(\mathbf{s} + \boldsymbol{\Delta} + k\mathbf{u}, t + \delta + k) - Z(\mathbf{s} + \boldsymbol{\Delta}, t + \delta)}{k} \right]
$$

$$
= \lim_{h \to 0} \lim_{k \to 0} \frac{1}{hk} \left[K(\boldsymbol{\Delta} + (k - h)\mathbf{u}, \delta + (k - h)) - K(\boldsymbol{\Delta} - h\mathbf{u}, \delta - h) - K(\boldsymbol{\Delta} + k\mathbf{u}, \delta + k) + K(\boldsymbol{\Delta}, \delta) \right]
$$

$$
= \lim_{h \to 0} \frac{1}{h} \left[\boldsymbol{\nabla}_{st} K(\boldsymbol{\Delta} - h\mathbf{u}, \delta - h) - \boldsymbol{\nabla}_{st} K(\boldsymbol{\Delta}, \delta) \right] = -\boldsymbol{\nabla}_{st} \boldsymbol{\nabla}_{st} K(\boldsymbol{\Delta}, \delta),
$$

whose (i, j) element is $-(\partial^4 / \partial t^2 \partial \Delta_i \partial \Delta_j) K(\boldsymbol{\Delta}, \delta)$. All the blocks in (8) are obtained similarly.

B   Details for deriving $\mathrm{Cov}\{\boldsymbol{\nabla} Z(\mathbf{s}_0, t_0), \mathbf{Z}\} = \boldsymbol{\nabla} \mathbf{K}_0$

To illustrate how to derive $\mathrm{Cov}\{\boldsymbol{\nabla} Z(\mathbf{s}_0, t_0), \mathbf{Z}\} = \boldsymbol{\nabla} \mathbf{K}_0$, we work out the details for deriving $\boldsymbol{\nabla}_s K(\boldsymbol{\Delta}_{i0}, \delta_{0j})$ using the covariance function in (10). In order to ease the notation, we again let $A_{0j} = \left(\phi_t^2 |\delta|_{0j}^2 + 1 \right)$. Then,

$$
\boldsymbol{\nabla}_s K(\boldsymbol{\Delta}_{i0}, \delta_{0j}) = \mathrm{Cov}(Z(\mathbf{s}_i, t_j), \boldsymbol{\nabla}_s Z(\mathbf{s}_0, t_0))
$$

$$
= \lim_{h \to 0} \frac{1}{h} \left[\mathrm{Cov}(Z(\mathbf{s}_i, t_j), Z(\mathbf{s}_0 + \mathbf{u}h, t_0) - Z(\mathbf{s}_0, t_0)) \right]
$$

$$
= \frac{1}{A_{0j}} \boldsymbol{\nabla}_s \left[\left(1 + \frac{\phi_s ||\boldsymbol{\Delta}_{i0}||}{A_{0j}^{1/2}} \right) \exp \left[-\frac{\phi_s ||\boldsymbol{\Delta}_{i0}||}{A_{0j}^{1/2}} \right] \right]
$$

$$
= -\frac{\phi_s^2}{A_{0j}^2} \exp \left[-\frac{\phi_s ||\boldsymbol{\Delta}_{i0}||}{A_{0j}^{1/2}} \right] \boldsymbol{\Delta}_{i0}.
$$

Expressions for $\nabla_t K(\boldsymbol{\Delta}_{i0}, \delta_{0j})$ and $\boldsymbol{\nabla}_{s,t} K(\boldsymbol{\Delta}_{i0}, \delta_{0j})$ can be derived in a similar fashion, where it is convenient to note that $\partial A_{0j}/\partial \delta = 2\phi_t^2 \delta$ and use the chain rule.

The cross-covariance matrix of $\boldsymbol{\nabla} Z(\mathbf{s}, t)$ at $(\mathbf{0}, 0)$, $\mathbf{C}_{\nabla Z}(\mathbf{0}, 0)$, is block diagonal (Section 4) and straightforward to derive. Now defining $A = (\phi_t^2|\delta| + 1)$, the first diagonal block of $\mathbf{C}_{\nabla Z}(\mathbf{0}, 0)$ is

$$
\begin{aligned}
\text{Cov}(\boldsymbol{\nabla}_s Z(\mathbf{s}, t), \boldsymbol{\nabla}_s Z(\mathbf{s} + \boldsymbol{\Delta}, t + \delta)) &= \lim_{h \to 0} \frac{1}{h} \left[\text{Cov}(Z(\mathbf{s} + h\mathbf{u}, t) - Z(\mathbf{s}, t), \boldsymbol{\nabla}_s Z(\mathbf{s} + \boldsymbol{\Delta}, t + \delta)) \right] \\
&= -\boldsymbol{\nabla}_s \left[\boldsymbol{\nabla}_s K(||\boldsymbol{\Delta}||, |\delta|) \right] \\
&= \frac{\phi_s^2}{A^2} \exp \left[-\frac{\phi_s ||\boldsymbol{\Delta}||^{1/2}}{A} \right] \left[I_2 - \frac{\phi_s}{A^{1/2}} \frac{\boldsymbol{\Delta}\boldsymbol{\Delta}^T}{||\boldsymbol{\Delta}||} \right] \\
&\to \phi_s^2 I_2 \text{ as } \boldsymbol{\Delta} \to \mathbf{0}, \ \delta \to 0 .
\end{aligned}
$$

The remaining diagonal blocks of $\mathbf{C}_{\nabla Z}(\mathbf{0}, 0)$ are obtained similarly.

C Estimated Gradients from California Air Quality Data

This appendix includes maps of the posterior medians for each component of our spatiotemporal gradient process from the analysis of the California air quality data. Spatial gradient maps can be found in Figures 1 and 2, and the temporal gradient maps can be found in Figure 3. Maps of the mixed gradients can be found in Figures 4 and 5.
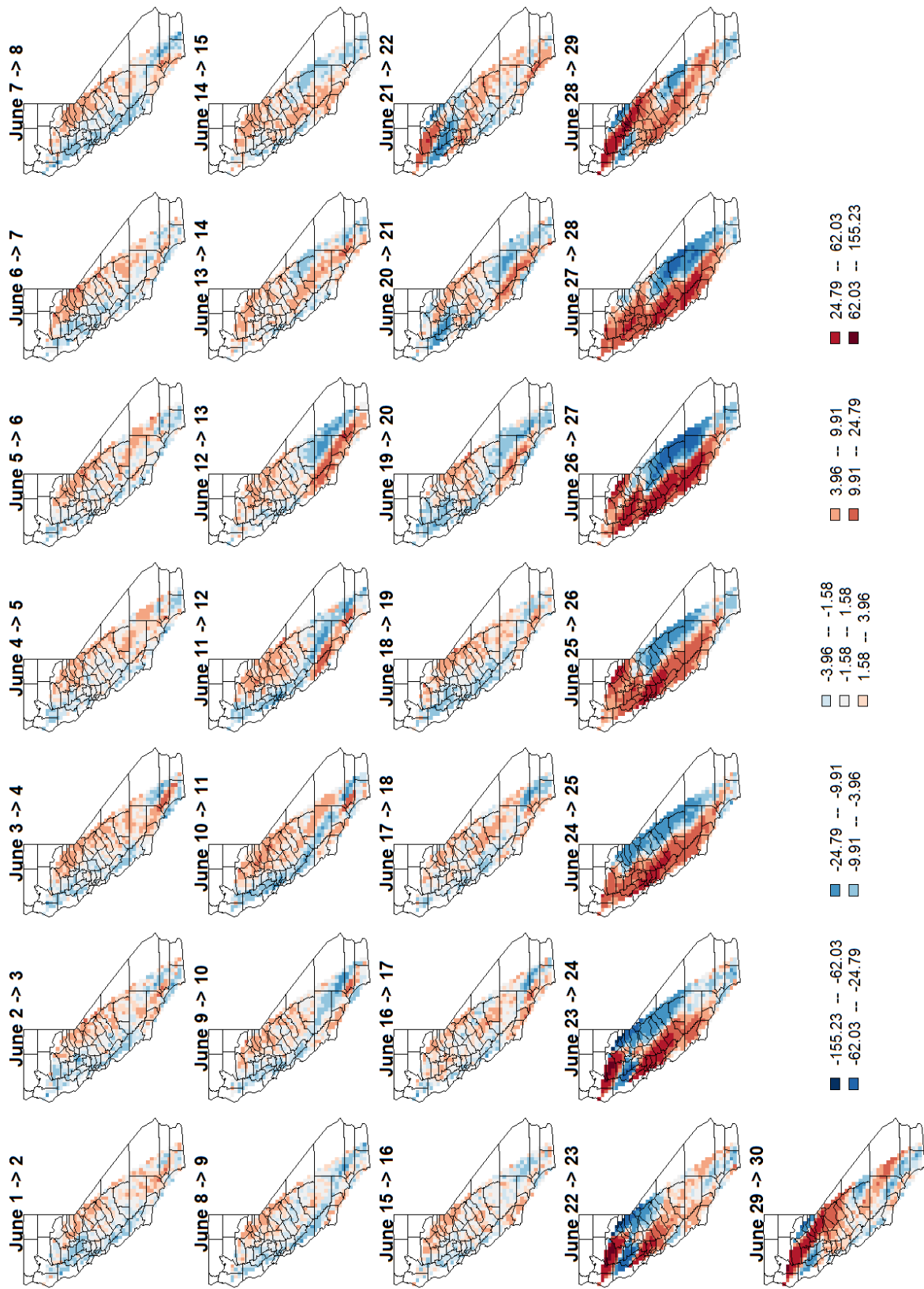
Figure 1: Estimated east/west spatial gradients from the California air quality data.
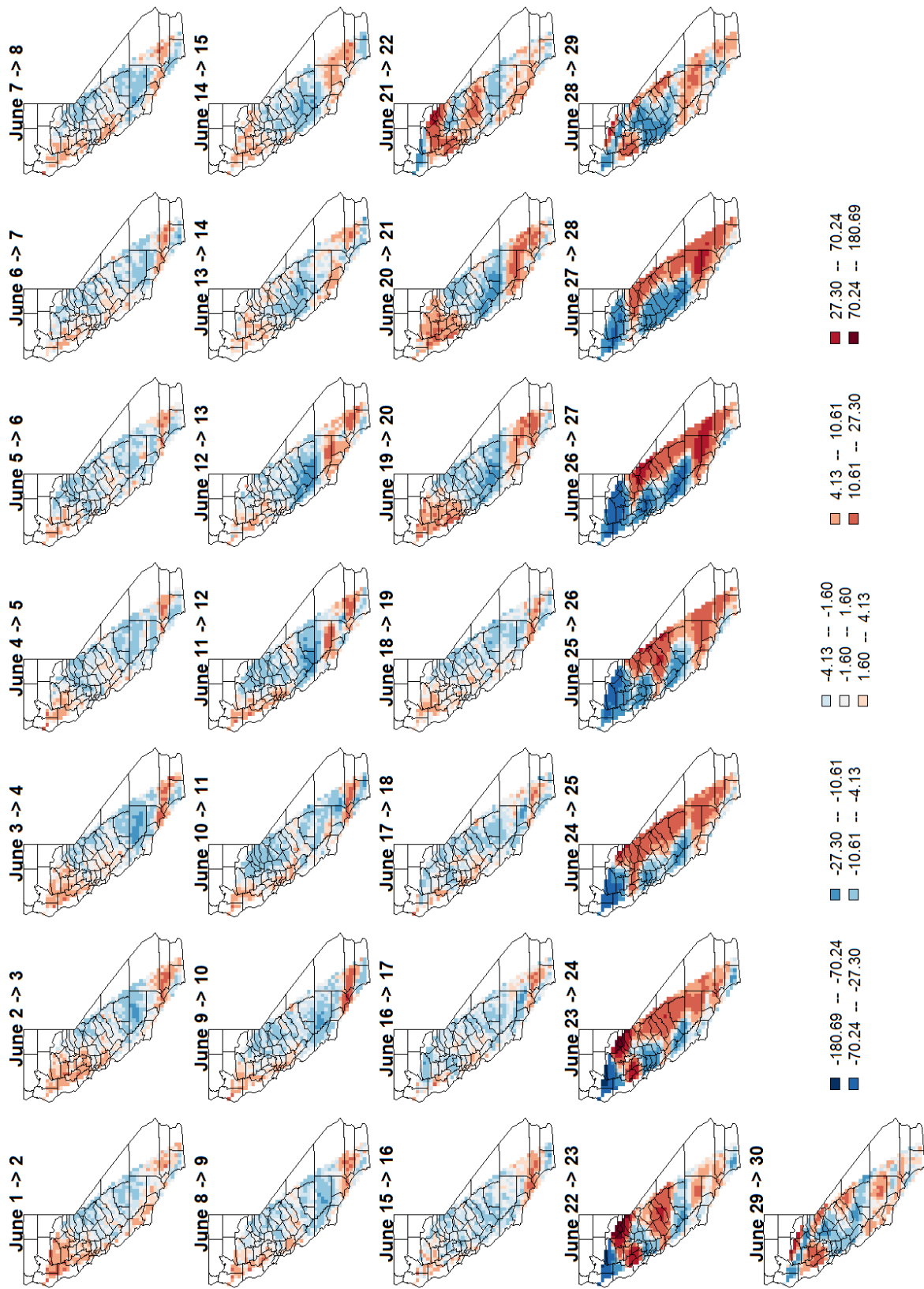
Figure 2: Estimated north/south spatial gradients from the California air quality data.
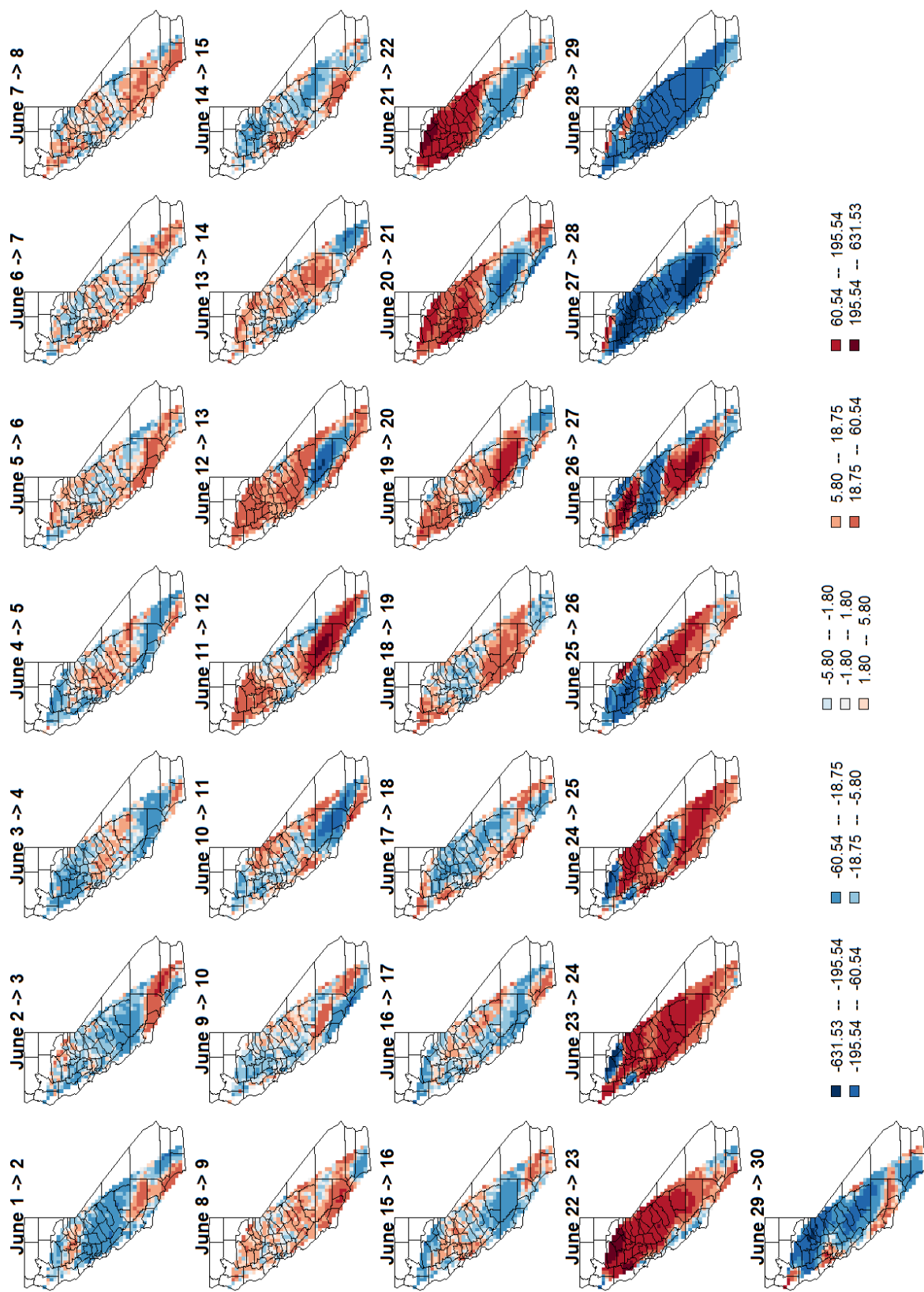
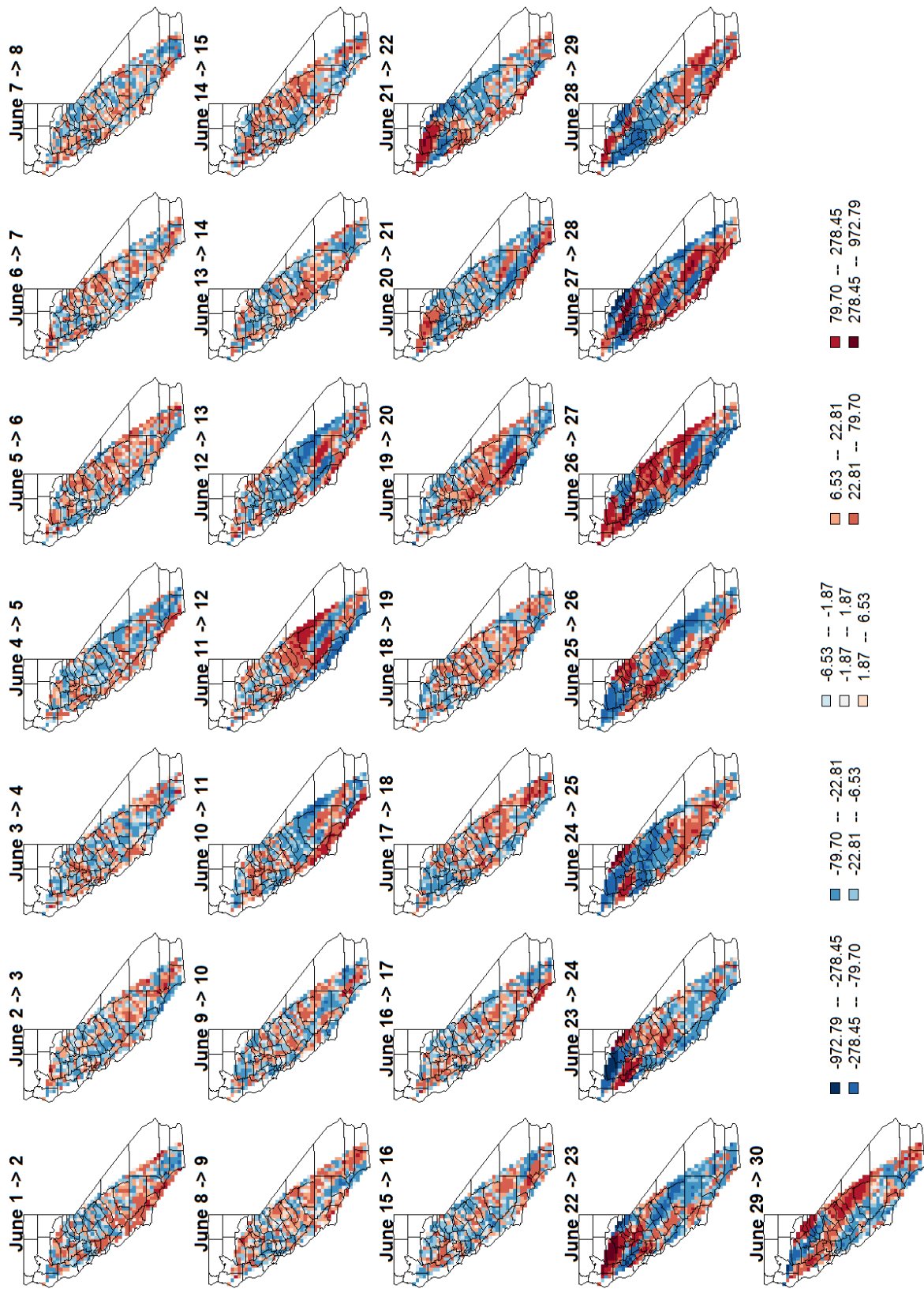Figure 3: Estimated temporal gradients from the California air quality data.

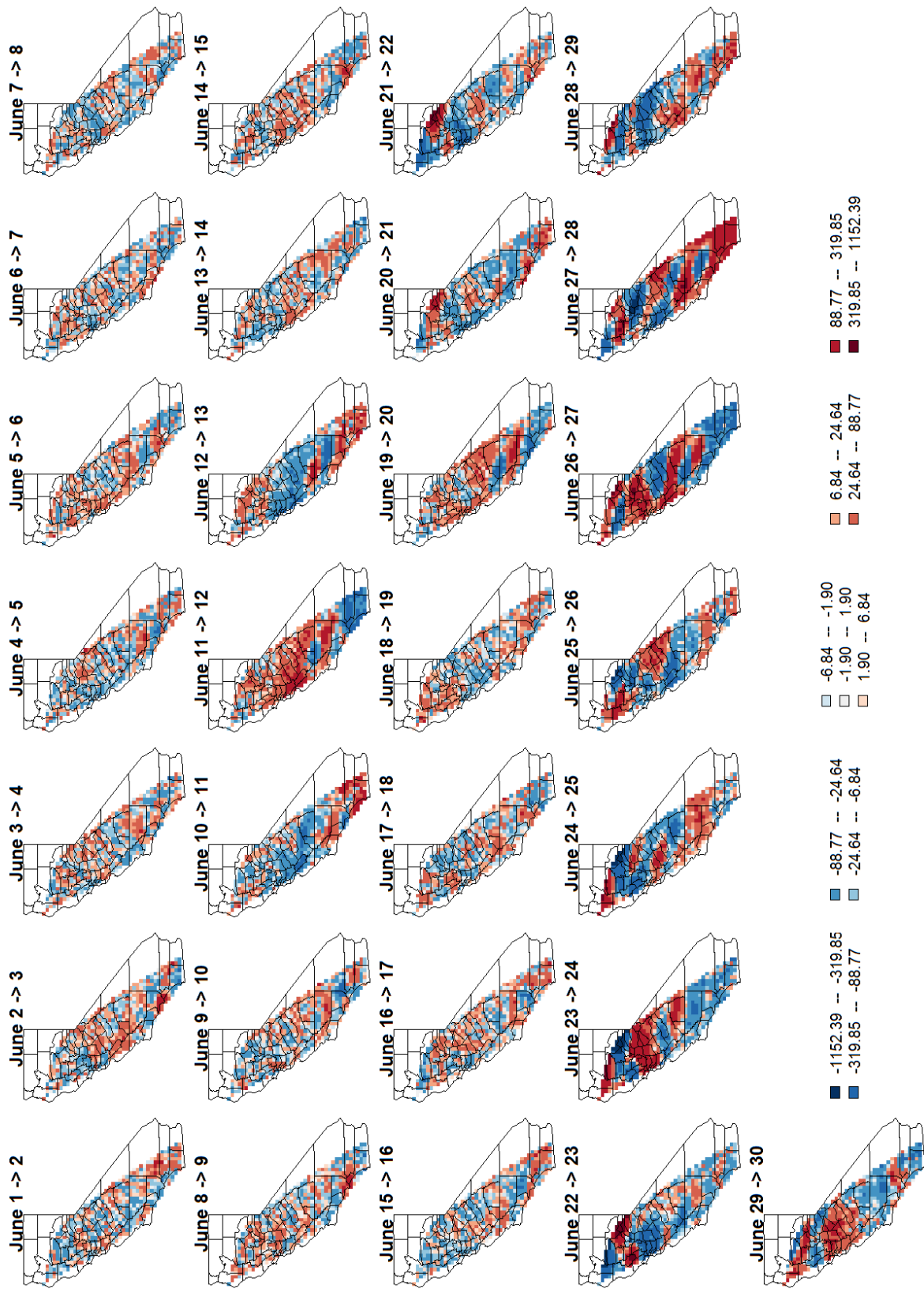Figure 4: Estimated east/west mixed gradients from the California air quality data.

Figure 5: Estimated north/south mixed gradients from the California air quality data.