

Supplementary Document
for
A Bayesian Spatio-Temporal Geostatistical Model
with an Auxiliary Lattice for Large Datasets

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1. Proof of Proposition 1

Using (4), if all eigenvalues of $\Phi(\beta)$ have absolute value less than 1, then one has the representation

$$\vec{U}_t = \sum_{j=0}^{\infty} \Phi(\beta)^j \vec{\zeta}_{t-j},$$

which implies that the variance of \vec{U}_t is

$$\Sigma_U(\beta) = \sigma_q^2 \sum_{j=0}^{\infty} \Phi(\beta)^j \Lambda^{-1}(\beta) \Phi(\beta)^j.$$

By definition, $\Phi(\beta)$ and $\Lambda(\beta)$ are symmetric block circulant matrices, that have the same set of eigenvectors with all eigenvalues real (Rue and Held (2005), Chapter 2). Block circulant matrices also have the property that $\Phi(\beta)\Lambda(\beta) = \Lambda(\beta)\Phi(\beta)$. Then, straightforward algebra yields

$$\Sigma_U(\beta) = \sigma_q^2 \{(\mathbf{I} - \Phi^2(\beta))\Lambda(\beta)\}^{-1} = \sigma_q^2 \mathbf{Q}^{-1}(\beta),$$

which gives $\mathbf{Q}(\beta) = (\mathbf{I} - \Phi^2(\beta))\Lambda(\beta)$. □

2. MCMC algorithm details

Given an odd number K , let $\Phi_K(\beta)$ and $\Lambda_K(\beta)$ be the matrices obtained

by setting $m_1 = m_2 = K$ in (6) and (7), respectively. Take $d_K = (K - 1)/2$,

$$\vec{U}_{(-kl)t, \partial K} = (U_{(k-d_K)(l-d_K), t}, U_{(k-d_K)(l-d_K+1), t}, \dots, \underbrace{0}_{kl, t}, \dots, U_{(k+d_K)(l+d_K), t})^T,$$

$$\vec{U}_t^{(1)} = \mathbf{\Lambda}(\boldsymbol{\beta})\vec{U}_t, \quad \vec{U}_t^{(2)} = \mathbf{\Phi}(\boldsymbol{\beta})\vec{U}_t, \quad \vec{U}_t^{(3)} = \mathbf{\Lambda}(\boldsymbol{\beta})\mathbf{\Phi}(\boldsymbol{\beta})\vec{U}_t,$$

where we can show that the entry corresponding to the (k, l) th location in the lattice W is

$$\begin{aligned} \vec{U}_{kl, t}^{(1)} &= U_{kl, t} + \beta_{010}(U_{k(l+1), t} + U_{k(l-1), t}) + \beta_{100}(U_{(k+1)l, t} + U_{(k-1)l, t}) \\ &\quad + \beta_{110}(U_{(k+1)(l+1), t} + U_{(k-1)(l-1), t} + U_{(k-1)(l+1), t} + U_{(k+1)(l-1), t}), \\ \vec{U}_{kl, t}^{(2)} &= \beta_{001}U_{kl, t} + \beta_{011}(U_{k(l+1), t} + U_{k(l-1), t}) + \beta_{101}(U_{(k+1)l, t} + U_{(k-1)l, t}) \\ &\quad + \beta_{111}(U_{(k+1)(l+1), t} + U_{(k-1)(l-1), t} + U_{(k-1)(l+1), t} + U_{(k+1)(l-1), t}), \\ \vec{U}_{kl, t}^{(3)} &= U_{kl, t}^{(2)} + \beta_{010}(U_{k(l+1), t}^{(2)} + U_{k(l-1), t}^{(2)}) + \beta_{100}(U_{(k+1)l, t}^{(2)} + U_{(k-1)l, t}^{(2)}) \\ &\quad + \beta_{110}(U_{(k+1)(l+1), t}^{(2)} + U_{(k-1)(l-1), t}^{(2)} + U_{(k-1)(l+1), t}^{(2)} + U_{(k+1)(l-1), t}^{(2)}), \end{aligned}$$

for $k = 1, \dots, m_1, l = 1, \dots, m_2, t = 1, \dots, T$.

To simulate samples from (19), we treat $\mathbf{U}_1, \dots, \mathbf{U}_T$ as missing data and use a Gibbs sampler as a data augmentation tool. The rest of the parameters are updated one by one using the Metropolis-Hasting (MH) algorithm. To facilitate the sampling, the parameters are grouped into subgroups after appropriate transformations: $\boldsymbol{\theta}_1 = (\boldsymbol{\beta}, \log \sigma_q^2)$, $\boldsymbol{\theta}_2 = (\log \phi, \boldsymbol{\xi}, \log \sigma_e^2)$. With samples at the b th iteration, say $\boldsymbol{\theta}_1^b, \boldsymbol{\theta}_2^b$ and $\mathbf{U}_1^b, \dots, \mathbf{U}_T^b$, let $\boldsymbol{\theta}_1^*, \boldsymbol{\theta}_2^*$ and $\mathbf{U}_1^*, \dots, \mathbf{U}_T^*$ denote the samples of $\boldsymbol{\theta}_1, \boldsymbol{\theta}_2$, and $\mathbf{U}_1, \dots, \mathbf{U}_T$, at the $(b + 1)$ th iteration. If we suppress the subscript b , the sampling process can be described as follows.

1. Update $(\mathbf{U}_1, \dots, \mathbf{U}_t)$: Generate $U_{kl, t}^*$ using the Gibbs sampler from the conditional density $f(U_{kl, t} | \mathbf{U}_{-(kl, t)})$, where $\mathbf{U}_{-(kl, t)}$ denotes the set of all elements of $(\mathbf{U}_1, \dots, \mathbf{U}_t)$ except for $U_{kl, t}$. With extensive algebra, we can show that $U_{kl, t}^* | \mathbf{U}_{-(kl, t)}, \boldsymbol{\theta}, \mathbf{Y} \sim N(E_{\partial}^2 F_{\partial}, E_{\partial}^2)$, where

$$E_{\partial}^2 = \left\{ \frac{1}{\sigma_q^2} (1 + h) + \sum_{i=1}^{n_t} I(w_{kl} \in \partial \mathbf{s}_{it}) \frac{c^2(\boldsymbol{\beta}) [(\mathbf{r}_{\partial \mathbf{s}_{it}}^T \boldsymbol{\Sigma}_{\partial}^{-1}(\boldsymbol{\beta}))]_{i(kl)}^2}{\sigma_e^2 + \sigma_{it\partial}^2} \right\}^{-1},$$

$$\begin{aligned}
F_{\partial} = & \left\{ \frac{1}{\sigma_q^2} \left(-\mathbf{b}_1^T \vec{U}_{(-kl)t, \partial 3} - \mathbf{b}_2^T \vec{U}_{(-kl)t, \partial 7} + \vec{U}_{kl, (t+1)}^{(3)} + \vec{U}_{kl, (t-1)}^{(3)} \right) \right\} \\
& + \sum_{i=1}^{n_t} I(w_{klt} \in \partial \mathbf{s}_{it}) \frac{c(\boldsymbol{\beta}) [(\mathbf{r}_{\partial \mathbf{s}_{it}}^T \boldsymbol{\Sigma}_{\partial}^{-1}(\boldsymbol{\beta}))]_{i(kl)}}{\sigma_e^2 + \sigma_{it\partial}^2} \\
& \quad \times \{Y(\mathbf{s}_{it}, t) - \mu(\mathbf{s}_{it}, t) - c(\boldsymbol{\beta}) \sum_{ab \neq kl} [\mathbf{r}_{\partial \mathbf{s}_{it}}^T \boldsymbol{\Sigma}_{\partial}^{-1}(\boldsymbol{\beta})]_{i(ab)} U_{ab,t}\}.
\end{aligned}$$

Here $i(kl)$ signifies that $U_{kl,t}^*$ is the $i(kl)$ th element of $\vec{U}_{\partial \mathbf{s}_{it}, t}$, $[(\mathbf{r}_{\partial \mathbf{s}_{it}}^T \boldsymbol{\Sigma}_{\partial}^{-1}(\boldsymbol{\beta}))]_{i(kl)}$ is the $i(kl)$ th entry of the vector $\mathbf{r}_{\partial \mathbf{s}_{it}}^T \boldsymbol{\Sigma}_{\partial}^{-1}(\boldsymbol{\beta})$, h is the $(1, 1)$ th entry of $\mathbf{B}_7(\boldsymbol{\beta}) = \boldsymbol{\Phi}_7(\boldsymbol{\beta}_1) \boldsymbol{\Lambda}_7(\boldsymbol{\beta}) \boldsymbol{\Phi}_7(\boldsymbol{\beta})$, and \mathbf{b}_1 and \mathbf{b}_2 are the 5th and 25th columns of $\boldsymbol{\Lambda}_3(\boldsymbol{\beta})$ and $\mathbf{B}_7(\boldsymbol{\beta})$, respectively.

2. Update $\boldsymbol{\theta}_1$: Generate $\boldsymbol{\theta}_1^*$ using the MH algorithm from the density

$$f(\boldsymbol{\theta}_1 | \boldsymbol{\theta}_2, \mathbf{U}, \mathbf{Y}) \propto \pi(\boldsymbol{\theta}_1 | \boldsymbol{\theta}_2) \prod_{t=1}^T f(\mathbf{U}_t | \boldsymbol{\theta}_1) f(\mathbf{Y}_t | \mathbf{U}_t, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2).$$

3. Update $\boldsymbol{\theta}_2$: Generate $\boldsymbol{\theta}_2^*$ using the MH algorithm from the density

$$f(\boldsymbol{\theta}_2 | \boldsymbol{\theta}_1, \mathbf{U}, \mathbf{Y}) \propto \pi(\boldsymbol{\theta}_2 | \boldsymbol{\theta}_1) \prod_{t=1}^T f(\mathbf{Y}_t | \mathbf{U}_t, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2).$$

Remark. Since the number of parameters involved in the MCMC algorithm is not small (10 in the simplest case), it is important to start the sampling process with good initial values so that the Markov chain converges quickly and generates well-mixed samples. We recommend setting $\boldsymbol{\Phi}(\boldsymbol{\beta}) = \mathbf{0}$ and using data from only one time point to get rough estimates of the remaining parameters, that are then used as the initial values for the spatio-temporal hierarchical model. While the computation time of this step is negligible compared with that of the spatio-temporal kriging, our numerical examples indicate that initial values obtained in this way can greatly reduce the convergence time of the Markov chain while stabilizing the prediction performance.

3. Additional Simulation Results

$\phi = 20$				
Neighborhoods	$\tau = 2$		$\tau = 5$	
	2×2	3×3	2×2	3×3
β_{010}	-0.09(0.05)	-0.24(0.07)	-0.10(0.07)	-0.27(0.05)
β_{100}	-0.10(0.06)	-0.25(0.05)	-0.08(0.08)	-0.25(0.06)
β_{110}	-0.15(0.03)	0.00(0.05)	-0.16(0.04)	0.01(0.05)
β_{001}	0.56(0.04)	0.57(0.04)	0.77(0.04)	0.79(0.02)
β_{011}	0.02(0.03)	0.05(0.03)	0.02(0.02)	0.02(0.02)
β_{101}	0.03(0.03)	0.05(0.02)	0.02(0.03)	0.03(0.02)
β_{111}	0.00(0.02)	-0.03(0.02)	0.00(0.01)	-0.02(0.01)
ϕ	12.93(1.39)	13.61(1.25)	13.83(3.19)	13.18(1.47)
σ_0^2	7.4(1.02)	7.07(0.91)	7.64(1.80)	7.07(0.75)
σ_e^2	0.79(0.10)	0.99(0.09)	0.76(0.10)	0.82(0.07)
MSPE(24×24)	2.30(0.12)	2.29(0.12)	2.08(0.12)	2.07(0.11)
MSPE(28×28)	2.25(0.11)	2.24(0.11)	1.99(0.10)	2.00(0.11)
MSPE(32×32)	2.22(0.11)	2.22(0.11)	1.95(0.11)	1.95(0.11)
MSPE(35×35)	2.21(0.11)	2.20(0.11)	1.92(0.11)	1.92(0.10)
MSPE(SP)	2.38(0.12)	2.38(0.12)	2.37(0.14)	2.37(0.14)
MSPE(SPT)	2.07(0.09)	2.07(0.09)	1.77(0.08)	1.77(0.08)
CPU (m)	18.63	24.15	20.76	26.86
$\phi = 40$				
Neighborhoods	$\tau = 2$		$\tau = 5$	
	2×2	3×3	2×2	3×3
β_{010}	-0.09(0.05)	-0.27(0.05)	-0.09(0.05)	-0.25(0.05)
β_{100}	-0.09(0.05)	-0.25(0.06)	-0.08(0.05)	-0.26(0.06)
β_{110}	-0.16(0.04)	0.01(0.04)	-0.16(0.03)	0.01(0.04)
β_{001}	0.46(0.04)	0.50(0.05)	0.66(0.07)	0.69(0.05)
β_{011}	0.07(0.03)	0.06(0.03)	0.04(0.03)	0.06(0.03)
β_{101}	0.06(0.04)	0.07(0.03)	0.05(0.03)	0.05(0.03)
β_{111}	0.00(0.02)	-0.02(0.02)	0.00(0.02)	-0.02(0.02)
ϕ	19.70(4.33)	21.41(3.93)	25.75(9.17)	21.32(3.48)
σ_0^2	6.73(1.37)	6.41(0.87)	8.18(2.45)	6.88(1.28)
σ_e^2	0.81(0.08)	0.93(0.10)	0.79(0.07)	0.74(0.08)
MSPE(24×24)	1.76(0.09)	1.75(0.09)	1.61(0.08)	1.60(0.08)
MSPE(28×28)	1.75(0.10)	1.75(0.09)	1.59(0.07)	1.58(0.08)
MSPE(32×32)	1.74(0.09)	1.74(0.09)	1.57(0.07)	1.57(0.08)
MSPE(35×35)	1.75(0.10)	1.74(0.09)	1.57(0.07)	1.57(0.07)
MSPE(SP)	1.80(0.07)	1.80(0.07)	1.77(0.11)	1.77(0.11)
MSPE(SPT)	1.66(0.07)	1.66(0.07)	1.48(0.07)	1.48(0.07)
CPU (m)	18.76	23.41	18.45	26.86

Table S1: The mean of the estimated parameters averaged over 20 simulated datasets when the covariance function is correctly specified. The numbers in the parentheses are the standard errors of the estimates. The size of the auxiliary lattice is 32×32 .

$\phi = 20$				
Neighborhoods	$\tau = 2$		$\tau = 5$	
	2×2	3×3	2×2	3×3
β_{010}	-0.17(0.06)	-0.26(0.05)	-0.18(0.10)	-0.28(0.05)
β_{100}	-0.18(0.07)	-0.26(0.05)	-0.17(0.10)	-0.27(0.06)
β_{110}	-0.06(0.07)	0.03(0.04)	-0.06(0.09)	0.04(0.04)
β_{001}	0.62(0.03)	0.62(0.03)	0.82(0.03)	0.82(0.05)
β_{011}	0.00(0.03)	0.02(0.02)	0.00(0.02)	0.01(0.03)
β_{101}	0.00(0.03)	0.02(0.02)	0.00(0.02)	0.01(0.03)
β_{111}	0.01(0.01)	-0.02(0.01)	0.00(0.01)	-0.02(0.02)
ϕ	9.75(0.48)	9.32(0.43)	9.75(0.65)	9.07(3.48)
σ_0^2	7.65(0.37)	7.22(0.37)	7.53(0.66)	6.86(1.28)
σ_e^2	0.55(0.16)	0.72(0.15)	0.58(0.12)	0.61(0.08)
MSPE(24×24)	2.70(0.13)	2.70(0.13)	2.35(0.10)	2.34(0.10)
MSPE(28×28)	2.59(0.12)	2.60(0.14)	2.20(0.08)	2.21(0.08)
MSPE(32×32)	2.54(0.12)	2.54(0.13)	2.12(0.07)	2.13(0.08)
MSPE(35×35)	2.52(0.12)	2.50(0.12)	2.09(0.07)	2.10(0.07)
MSPE(SP)	2.92(0.13)	2.92(0.13)	2.91(0.13)	2.91(0.13)
MSPE(SPT)	2.40(0.12)	2.40(0.12)	1.97(0.06)	1.97(0.07)
CPU (m)	21.15	26.87	23.03	24.28
$\phi = 40$				
Neighborhoods	$\tau = 2$		$\tau = 5$	
	2×2	3×3	2×2	3×3
β_{010}	-0.07(0.05)	-0.26(0.07)	-0.10(0.04)	-0.25(0.05)
β_{100}	-0.06(0.05)	-0.27(0.07)	-0.08(0.04)	-0.24(0.07)
β_{110}	-0.18(0.03)	0.02(0.05)	-0.16(0.02)	0.00(0.05)
β_{001}	0.41(0.04)	0.47(0.06)	0.64(0.05)	0.69(0.10)
β_{011}	0.09(0.03)	0.06(0.05)	0.06(0.03)	0.03(0.02)
β_{101}	0.09(0.03)	0.06(0.05)	0.06(0.03)	0.04(0.02)
β_{111}	-0.02(0.02)	-0.01(0.03)	0.00(0.02)	0.00(0.05)
ϕ	15.73(2.61)	16.69(2.49)	21.88(5.17)	21.25(8.32)
σ_0^2	7.24(1.07)	6.93(1.15)	8.98(2.29)	8.88(3.69)
σ_e^2	0.61(0.06)	0.73(0.04)	0.63(0.10)	0.68(0.11)
MSPE(24×24)	1.73(0.08)	1.71(0.08)	1.65(0.09)	1.63(0.09)
MSPE(28×28)	1.73(0.09)	1.70(0.08)	1.61(0.09)	1.59(0.09)
MSPE(32×32)	1.74(0.09)	1.70(0.09)	1.60(0.09)	1.59(0.08)
MSPE(35×35)	1.74(0.10)	1.69(0.09)	1.61(0.09)	1.58(0.09)
MSPE(SP)	1.80(0.10)	1.80(0.10)	1.83(0.11)	1.83(0.11)
MSPE(SPT)	1.63(0.08)	1.63(0.08)	1.53(0.08)	1.53(0.08)
CPU (m)	18.22	21.30	15.23	21.50

Table S2: The mean of the estimated parameters averaged over 20 simulated datasets when the covariance function is mis-specified. The numbers in the parentheses are the standard errors of the estimates. The size of the auxiliary lattice is 32×32 .

4. Precipitation Data

To illustrate the effectiveness of our method, we used annual total precipitation data. The longitudes of the stations ranged from -124.6 to -67.0 and the latitudes ranged from 24.55 to 49.00 . Besides the longitude and latitude, there was also elevation (in meters) information available for each location. We made a square root transform of the original data to make them more normal. Let $Y(\mathbf{s}, t)$ be the square root of the annual precipitation for location \mathbf{s} in year t . We used model (1) to analyze the observed process, where an intercept term, ξ_0 , and the elevation, $elev(\mathbf{s}, t)$ (calculated as the elevation (in meters) divided by 100), were included in the mean structure $\mu(\mathbf{s}, t)$. Since the region of interest can be roughly considered as flat, we used a grid of size 115×55 to cover the region $[-125, -65] \times [20, 50]$; for comparison, we took the grid sizes 100×50 , 120×60 and 125×65 . The ratio of the grid numbers in longitude and latitude roughly close to $2 : 1$ so that the grid points are evenly spaced in the spatial region. For prediction performance of the proposed method, we created 20 datasets by randomly taking 90% of the available data as the training dataset and the rest as prediction locations. For each dataset, we ran 23,000 MCMC iterations and took 1000 samples from the last 20,000 iterations at equally-spaced time points to do the estimation and prediction. The estimation results are summarized in Table S3. As the maximum likelihood approach brings prohibitive computation cost, we compared the purely spatial prediction accuracy using our method (by assuming that $T = 1$ and $\Phi(\boldsymbol{\beta}) = 0$ in (4) and the spatio-temporal prediction accuracy using the proposed STAR model. The ability of using the auxiliary GMRF to approximate the Gaussian random field in a purely spatial scenario was discussed and illustrated by Park and Liang (2012). The results are summarized in Table S3. The results indicate that, by taking into account the temporal dependence, the STAR model spatio-temporal kriging yields better prediction results with either a 2×2 or a 3×3 neighborhood structure. Increasing the grid size will give better prediction performance.

We also used the univariate Bayesian dynamic space-time regression models proposed in Finley, Banerjee, and Gelfand (2012) to do spatio-temporal kriging on the same dataset. The implementation was carried out using the function `sp-DynLM()` in the R package `spBayes` (Finley and Banerjee (2013)). The variable

“elevation” was used as the only predictor in the regression model. Predictions were made based on 5,000 MCMC samples with a burn in period of 5,000 iterations. Knots were chosen as the grid points on 10×5 , 14×7 , and 20×10 lattices, which give the MSPE for the hold out data as 0.67, 0.53 and 0.42, respectively. As expected, the MSPE decreases as the number of knots increases. Using 200 knots gives roughly the prediction accuracy of our method, but its computation time for each iteration is almost 7 times as much as ours using a 115×55 grid size and a 2×2 neighborhood.

In Figure S1, we present the spatio-temporal prediction of the annual total precipitation in 1982 for all 11,918 stations. There are 6595 stations that have records in 1982. The locations of these stations are plotted as green dots in Figure S1(a). The red dots in Figure S1(a) represent stations that do not have records in 1982. An image of the observed precipitation data is shown in Figure S1(b). Figures S1(c) and (d) present images of the predicted precipitation for all 11,918 stations in 1982 using the STAR model spatio-temporal kriging with 2×2 and 3×3 neighborhood structures, respectively. The observations from the 6,595 stations with data from year 1982 are also used in the model estimation step. The similarity between Figure S1(b) and Figures S1(c) and (d) indicates that our method yields good prediction performance. Figures S1(e) and (f) give the prediction standard errors calculated using MCMC samples for all 11,918 locations.

Neighborhoods	2×2		3×3	
	SPTKrig	SPKrig	SPTKrig	SPKrig
β_{010}	-0.08(0.05)	-0.08(0.05)	-0.10(0.06)	-0.10(0.05)
β_{100}	-0.12(0.04)	-0.12(0.04)	-0.15(0.05)	-0.14(0.06)
β_{110}	-0.15(0.03)	-0.15(0.03)	-0.11(0.04)	-0.12(0.04)
β_{001}	0.69(0.06)	0	0.55(0.18)	0
β_{011}	0.05(0.03)	0	0.05(0.06)	0
β_{101}	0.05(0.03)	0	0.07(0.04)	0
β_{111}	0.01(0.02)	0	0.03(0.03)	0
ξ_0	7.21(0.34)	7.36(0.42)	6.95(0.20)	7.70(0.28)
<i>elev</i>	0.30(0.00)	0.29(0.01)	0.28(0.03)	0.18(0.04)
ϕ	9.90(2.22)	2.94(0.33)	4.43(1.87)	1.61(0.21)
σ_q^2	0.37(0.04)	0.97(0.15)	0.55(0.28)	1.35(0.21)
σ_e^2	0.19(0.04)	0.22(0.03)	0.15(0.06)	0.28(0.06)
MSPE(100×50)	0.44(0.03)	0.53(0.02)	0.47(0.05)	0.64(0.06)
MSPE(115×55)	0.43(0.02)	0.52(0.02)	0.46(0.07)	0.64(0.05)
MSPE(120×60)	0.40(0.01)	0.49(0.02)	0.43(0.05)	0.63(0.06)
MSPE(125×65)	0.40(0.01)	0.49(0.01)	0.41(0.02)	0.65(0.07)
CPU (m)	75.34	23.80	121.10	64.20

Table S3: The mean of the estimated parameters averaged over 20 datasets drawn from the precipitation data. The numbers in the parentheses are the standard errors of the estimates. The size of the auxiliary lattice is 115×55 .

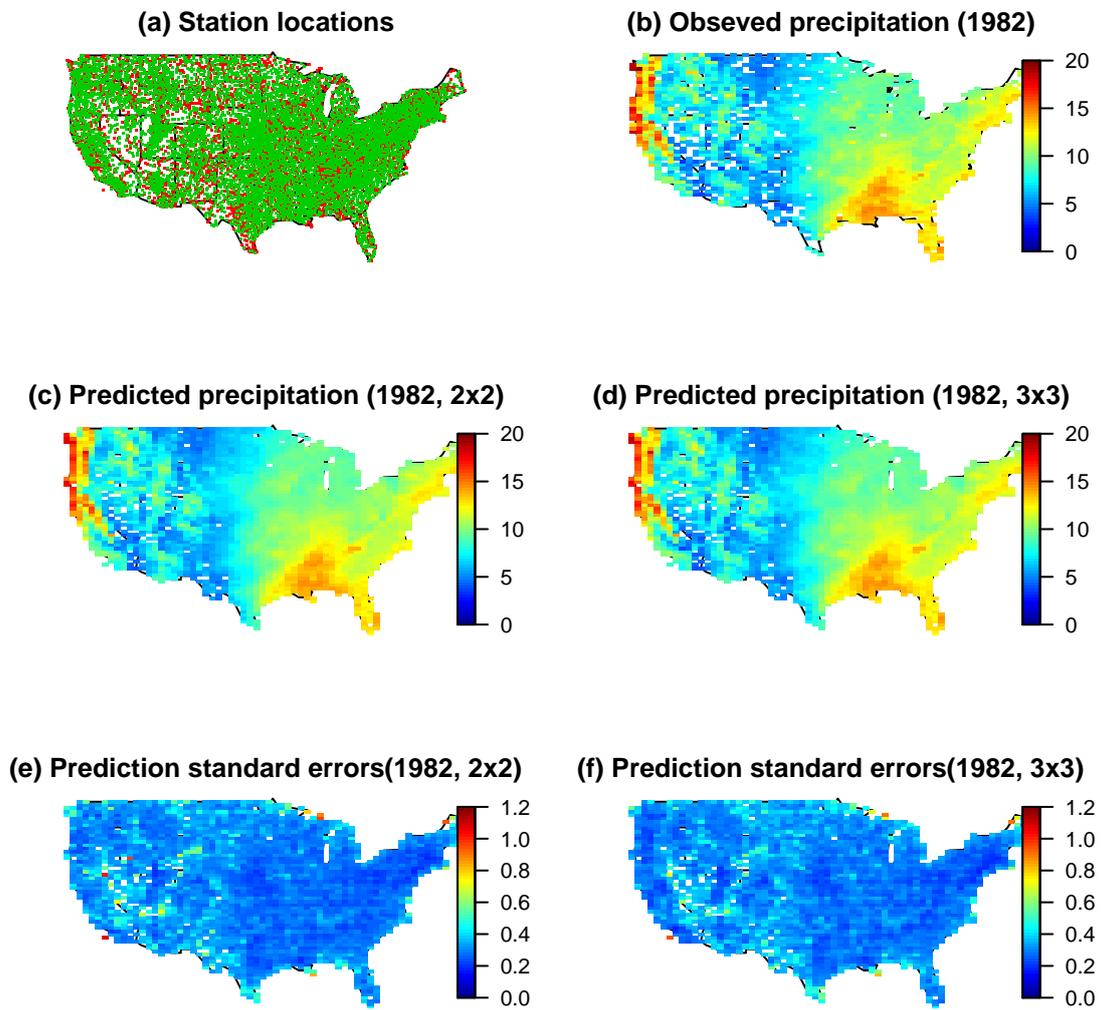


Figure S1: (a) Station locations: red dots are stations without observations; green dots are stations with observations. (b) Annual total precipitation reported from 6595 stations (stations with green dots in Fig. 3(a)). (c) Predicted annual total precipitation for 11,918 stations using a 2×2 neighborhood structure. (d) Predicted annual total precipitation for 11,918 stations using a 3×3 neighborhood structure. (e) Estimated prediction standard errors for 11,918 stations using a 2×2 neighborhood structure. (f) Estimated prediction standard errors for 11,918 stations using a 3×3 neighborhood structure.

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