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Supplement of

Reconstruction of spatio-temporal temperature from sparse historical records using robust probabilistic principal component regression

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S Supplementary Material

S.1 Marginal distribution

Conditional on the unobserved latent principal components, we can write the robust Student's-t pPCR likelihood as

$$
\begin{aligned}
&\left[y_{it}\middle|\mathbf{Z}_i,\boldsymbol{\beta}_t,v_{it}^2\right]\left[\mathbf{X}_i|\mathbf{Z}_i,\sigma\right]\left[\mathbf{Z}_i\right]\\
&\qquad\propto \exp\left\{-\frac{(y_{it}-\mathbf{Z}_i\boldsymbol{\beta}_t)^2}{2v_{it}^2}-\frac{\left(\mathbf{X}_i-\hat{\mathbf{K}}\mathbf{Z}_i\right)'\left(\mathbf{X}_i-\hat{\mathbf{K}}\mathbf{Z}_i\right)}{2\sigma^2}-\frac{\mathbf{Z}_i'\mathbf{Z}_i}{2}\right\}\\
&\qquad\propto \exp\left\{-\frac{1}{2}\mathbf{Z}_i'\left(\frac{\boldsymbol{\beta}_t\boldsymbol{\beta}_t'}{v_{it}^2}+\frac{\hat{\mathbf{K}}'\hat{\mathbf{K}}}{\sigma^2}+\mathbf{I}\right)\mathbf{Z}_i+\mathbf{Z}_i'\left(\frac{\boldsymbol{\beta}_t y_{it}}{v_{it}^2}+\frac{\hat{\mathbf{K}}'\mathbf{X}_i}{\sigma^2}\right)\right\}\\
&\qquad\quad\times\exp\left\{-\frac{y_{it}^2}{2v_{it}^2}-\frac{\mathbf{X}_i'\mathbf{X}_i}{2\sigma^2}\right\}\\
&\qquad\propto \exp\left\{-\frac{1}{2}\left(\mathbf{Z}_i-\boldsymbol{\mu}_{Z_{it}}\right)'\boldsymbol{\Sigma}_{Z_{it}}^{-1}\left(\mathbf{Z}_i-\boldsymbol{\mu}_{Z_{it}}\right)-\frac{y_{it}^2}{2v_{it}^2}-\frac{\mathbf{X}_i'\mathbf{X}_i}{2\sigma^2}+\frac{\boldsymbol{\mu}_{Z_{it}}'\boldsymbol{\Sigma}_{Z_{it}}^{-1}\boldsymbol{\mu}_{Z_{it}}}{2}\right\}
\end{aligned}
$$

where $\boldsymbol{\Sigma}_{Z_{it}}=\left(\frac{\boldsymbol{\beta}_t\boldsymbol{\beta}_t'}{v_{it}^2}+\frac{\hat{\mathbf{K}}'\hat{\mathbf{K}}}{\sigma^2}+\mathbf{I}\right)^{-1}$ and $\boldsymbol{\mu}_{Z_{it}}=\boldsymbol{\Sigma}_{Z_{it}}\left(\frac{\boldsymbol{\beta}_t y_{it}}{v_{it}^2}+\frac{\hat{\mathbf{K}}'\mathbf{X}_i}{\sigma^2}\right)$. Integrating the above equation with respect to $\mathbf{Z}_i$ we get

$$
\begin{aligned}
\left[y_{it}\middle|\boldsymbol{\beta}_t,v_{it}^2,\sigma\right]&\propto\exp\left\{-\frac{y_{it}^2}{2v_{it}^2}+\frac{\boldsymbol{\mu}_{Z_{it}}'\boldsymbol{\Sigma}_{Z_{it}}^{-1}\boldsymbol{\mu}_{Z_{it}}}{2}\right\}\\
&\propto\exp\left\{-\frac{y_{it}^2}{2v_{it}^2}+\frac{\left(\boldsymbol{\Sigma}_{Z_{it}}\left(\frac{y_{it}\boldsymbol{\beta}_t}{v_{it}^2}+\frac{\hat{\mathbf{K}}'\mathbf{X}_i}{\sigma^2}\right)\right)'\boldsymbol{\Sigma}_{Z_{it}}^{-1}\left(\boldsymbol{\Sigma}_{Z_{it}}\left(\frac{y_{it}\boldsymbol{\beta}_t}{v_{it}^2}+\frac{\hat{\mathbf{K}}'\mathbf{X}_i}{\sigma^2}\right)\right)}{2}\right\}\\
&\propto\exp\left\{-\frac{1}{2}y_{it}^2\left(\frac{1}{v_{it}^2}-\frac{\boldsymbol{\beta}_t'\boldsymbol{\Sigma}_{Z_{it}}\boldsymbol{\beta}_t}{(v_{it}^2)^2}\right)+y_{it}\left(\frac{\boldsymbol{\beta}_t'\boldsymbol{\Sigma}_{Z_{it}}\hat{\mathbf{K}}'\mathbf{X}_i}{v_{it}^2\sigma^2}\right)\right\}
\end{aligned}
$$

which is $\mathrm{N}\left(\mu_{y_{it}},\sigma_{y_{it}}^2\right)$ with

$$
\begin{aligned}
\sigma_{y_{it}}^2&=\left(\frac{1}{v_{it}^2}-\frac{\boldsymbol{\beta}_t'\boldsymbol{\Sigma}_{Z_{it}}\boldsymbol{\beta}_t}{(v_{it}^2)^2}\right)^{-1}\\
\mu_{y_{it}}&=\left(\frac{1}{v_{it}^2}-\frac{\boldsymbol{\beta}_t'\boldsymbol{\Sigma}_{Z_{it}}\boldsymbol{\beta}_t}{(v_{it}^2)^2}\right)^{-1}\frac{\boldsymbol{\beta}_t'\boldsymbol{\Sigma}_{Z_{it}}\hat{\mathbf{K}}'\mathbf{X}_i}{v_{it}^2\sigma^2}
\end{aligned}
$$

To further simplify this equation, we use the Morrison-Woodbury matrix inversion formula

$$(\mathbf{A}+\mathbf{UDV})^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{U}\left(\mathbf{D}^{-1}+\mathbf{VA}^{-1}\mathbf{U}\right)^{-1}\mathbf{VA}^{-1}.$$

Then, defining $\mathbf{A} = v_{it}^2\mathbf{I}$, $\mathbf{U} = \boldsymbol{\beta}_t'$, $\mathbf{V} = \boldsymbol{\beta}_t$, and $\mathbf{D} = \left(\frac{\hat{\mathbf{K}}'\hat{\mathbf{K}}}{\sigma^2}+\mathbf{I}\right)^{-1}$,

$$\begin{aligned}
\sigma_{y_{it}}^2 &= \left(\frac{\mathbf{I}}{v_{it}^2} - \frac{\boldsymbol{\beta}_t'\boldsymbol{\Sigma}_{Z_{it}}\boldsymbol{\beta}_t}{(v_{it}^2)^2}\right)^{-1} \\
&= \left(\frac{\mathbf{I}}{v_{it}^2} - \frac{\boldsymbol{\beta}_t'}{v_{it}^2}\left(\frac{\boldsymbol{\beta}_t\boldsymbol{\beta}_t'}{v_{it}^2} + \frac{\hat{\mathbf{K}}'\hat{\mathbf{K}}}{\sigma^2}+\mathbf{I}\right)^{-1}\frac{\boldsymbol{\beta}_t}{v_{it}^2}\right)^{-1} \\
&= v_{it}^2 + \boldsymbol{\beta}_t'\left(\frac{\hat{\mathbf{K}}'\hat{\mathbf{K}}}{\sigma^2}+\mathbf{I}\right)^{-1}\boldsymbol{\beta}_t \\
&= v_{it}^2 + \boldsymbol{\beta}_t'\mathbf{M}_p^{-1}\boldsymbol{\beta}_t
\end{aligned}$$

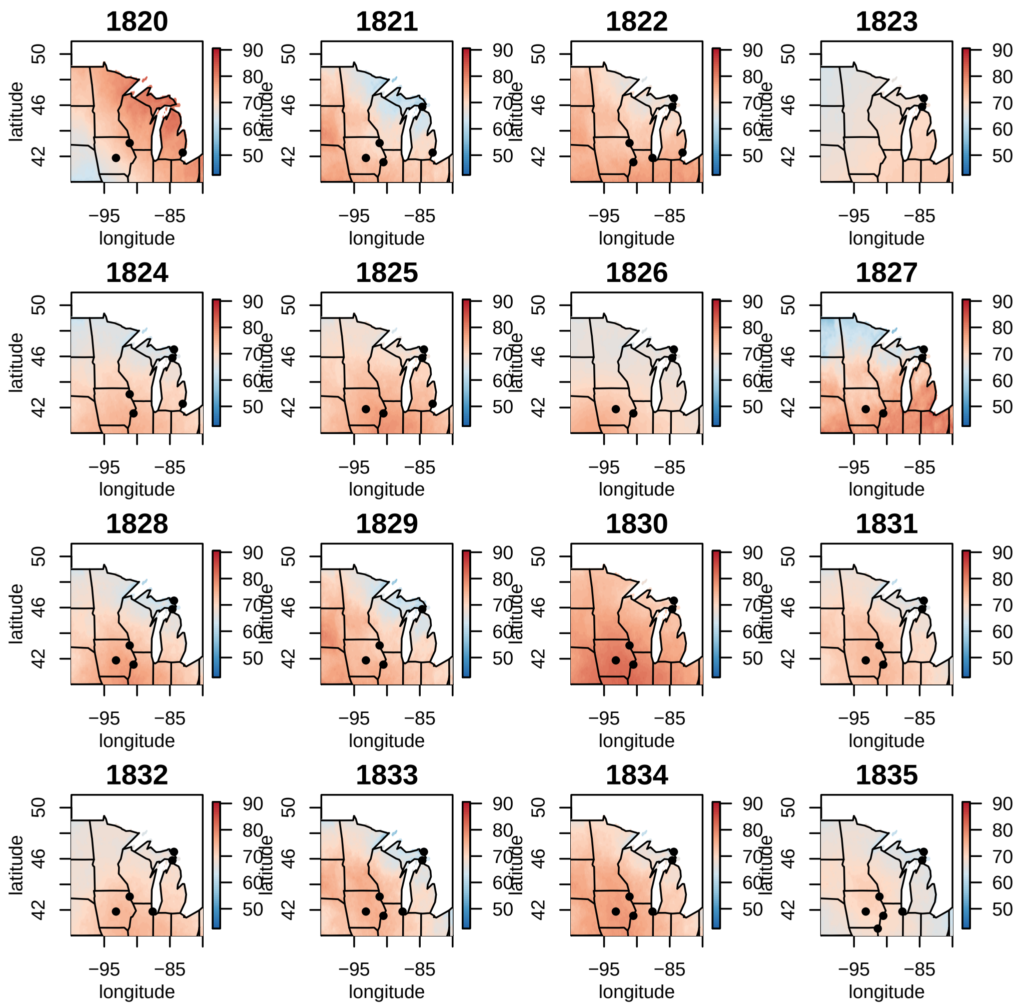
with $\mathbf{M}_p = \frac{\hat{\mathbf{K}}'\hat{\mathbf{K}}}{\sigma^2}+\mathbf{I}$.

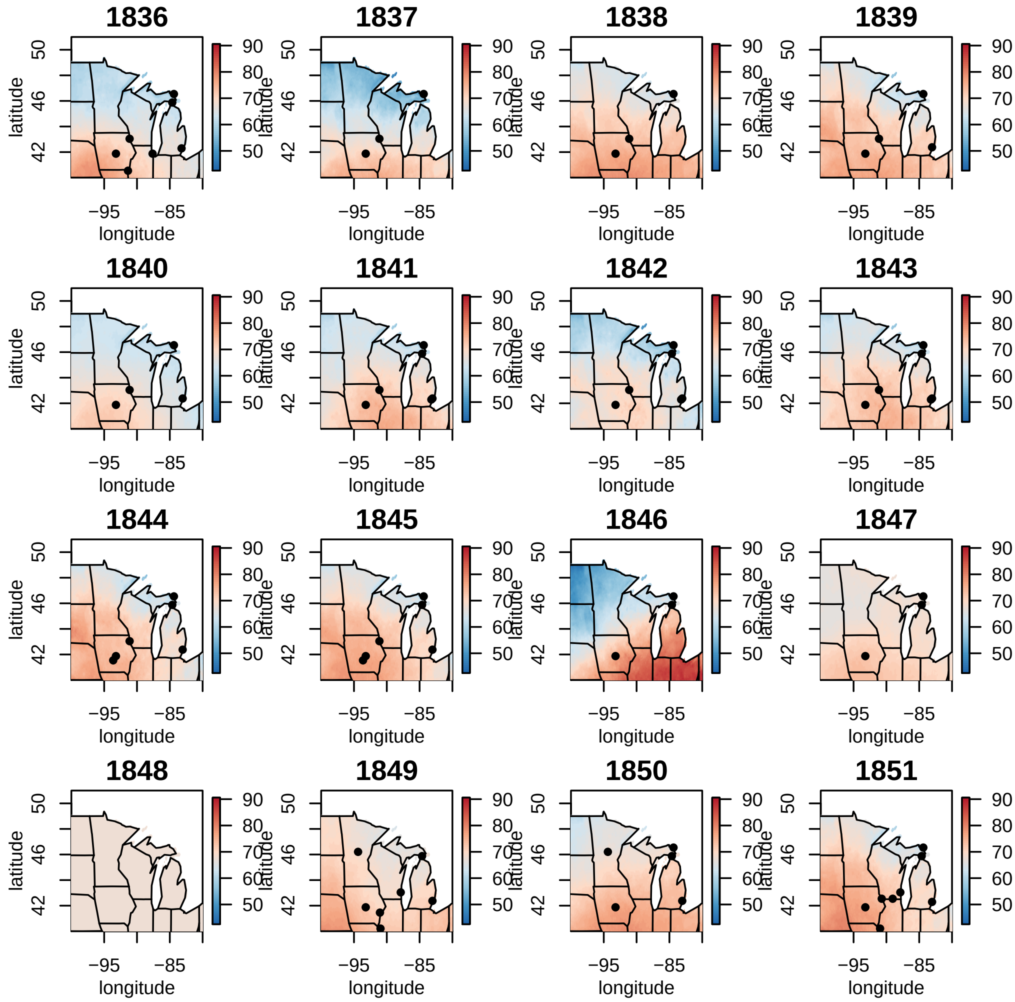
Then, letting $\mathbf{B}_t = \mathbf{M}_p^{-1/2}\boldsymbol{\beta}_t$ the conditional mean $\mu_{y_{it}}$ is

$$\begin{aligned}
\mu_{y_{it}} &= \left(\frac{1}{v_{it}^2} - \frac{\boldsymbol{\beta}_t'\boldsymbol{\Sigma}_{Z_{it}}\boldsymbol{\beta}_t}{(v_{it}^2)^2}\right)^{-1}\left(\frac{\boldsymbol{\beta}_t'\boldsymbol{\Sigma}_{Z_{it}}\hat{\mathbf{K}}'\mathbf{X}_i}{v_{it}^2\sigma^2}\right) \\
&= \left(v_{it}^2 + \boldsymbol{\beta}_t'\mathbf{M}_p^{-1}\boldsymbol{\beta}_t\right)\left(\frac{\boldsymbol{\beta}_t'}{v_{it}^2}\left(\frac{\boldsymbol{\beta}_t\boldsymbol{\beta}_t'}{v_{it}^2} + \frac{\hat{\mathbf{K}}'\hat{\mathbf{K}}}{\sigma^2}+\mathbf{I}\right)^{-1}\frac{\hat{\mathbf{K}}'\mathbf{X}_i}{\sigma^2}\right) \\
&= \left(v_{it}^2 + \mathbf{B}_t'\mathbf{B}_t\right)\left(\frac{\boldsymbol{\beta}_t'}{v_{it}^2}\left(\frac{\boldsymbol{\beta}_t\boldsymbol{\beta}_t'}{v_{it}^2} + \mathbf{M}_p\right)^{-1}\frac{\hat{\mathbf{K}}'\mathbf{X}_i}{\sigma^2}\right) \\
&= \left(v_{it}^2 + \mathbf{B}_t'\mathbf{B}_t\right)\left(\frac{\boldsymbol{\beta}_t'}{v_{it}^2}\left(\mathbf{M}_p^{\frac{1}{2}}\left(\frac{\mathbf{M}_p^{-\frac{1}{2}}\boldsymbol{\beta}_t\boldsymbol{\beta}_t'\mathbf{M}_p^{-\frac{1}{2}}}{v_{it}^2}+\mathbf{I}\right)\mathbf{M}_p^{\frac{1}{2}}\right)^{-1}\frac{\hat{\mathbf{K}}'\mathbf{X}_i}{\sigma^2}\right) \\
&= \left(v_{it}^2 + \mathbf{B}_t'\mathbf{B}_t\right)\frac{\mathbf{B}_t'}{v_{it}^2}\left(\frac{\mathbf{B}_t\mathbf{B}_t'}{v_{it}^2}+\mathbf{I}\right)^{-1}\mathbf{M}_p^{-\frac{1}{2}}\frac{\hat{\mathbf{K}}'\mathbf{X}_i}{\sigma^2} \\
&= \left(\mathbf{B}_t' + \frac{\mathbf{B}_t'\mathbf{B}_t\mathbf{B}_t'}{v_{it}^2}\right)\left(\frac{\mathbf{B}_t\mathbf{B}_t'}{v_{it}^2}+\mathbf{I}\right)^{-1}\mathbf{M}_p^{-\frac{1}{2}}\frac{\hat{\mathbf{K}}'\mathbf{X}_i}{\sigma^2} \\
&= \mathbf{B}_t'\left(\mathbf{I} + \frac{\mathbf{B}_t\mathbf{B}_t'}{v_{it}^2}\right)\left(\frac{\mathbf{B}_t\mathbf{B}_t'}{v_{it}^2}+\mathbf{I}\right)^{-1}\mathbf{M}_p^{-\frac{1}{2}}\frac{\hat{\mathbf{K}}'\mathbf{X}_i}{\sigma^2} \\
&= \mathbf{B}_t'\mathbf{M}_p^{-\frac{1}{2}}\frac{\hat{\mathbf{K}}'\mathbf{X}_i}{\sigma^2} \\
&= \frac{\boldsymbol{\beta}_t'\mathbf{M}_p^{-1}\hat{\mathbf{K}}'\mathbf{X}_i}{\sigma^2}
\end{aligned}$$

$$y_{it}|\boldsymbol{\beta}_t, v_{it}^2, \sigma \sim \mathrm{N}\left(\frac{\mathbf{X}_i'\hat{\mathbf{K}}\mathbf{M}_p^{-1}\boldsymbol{\beta}_t}{\sigma^2}, v_{it}^2 + \boldsymbol{\beta}_t'\mathbf{M}_p^{-1}\boldsymbol{\beta}_t\right).$$

S.2 Robust PCR Model Posterior Mean July Temperature

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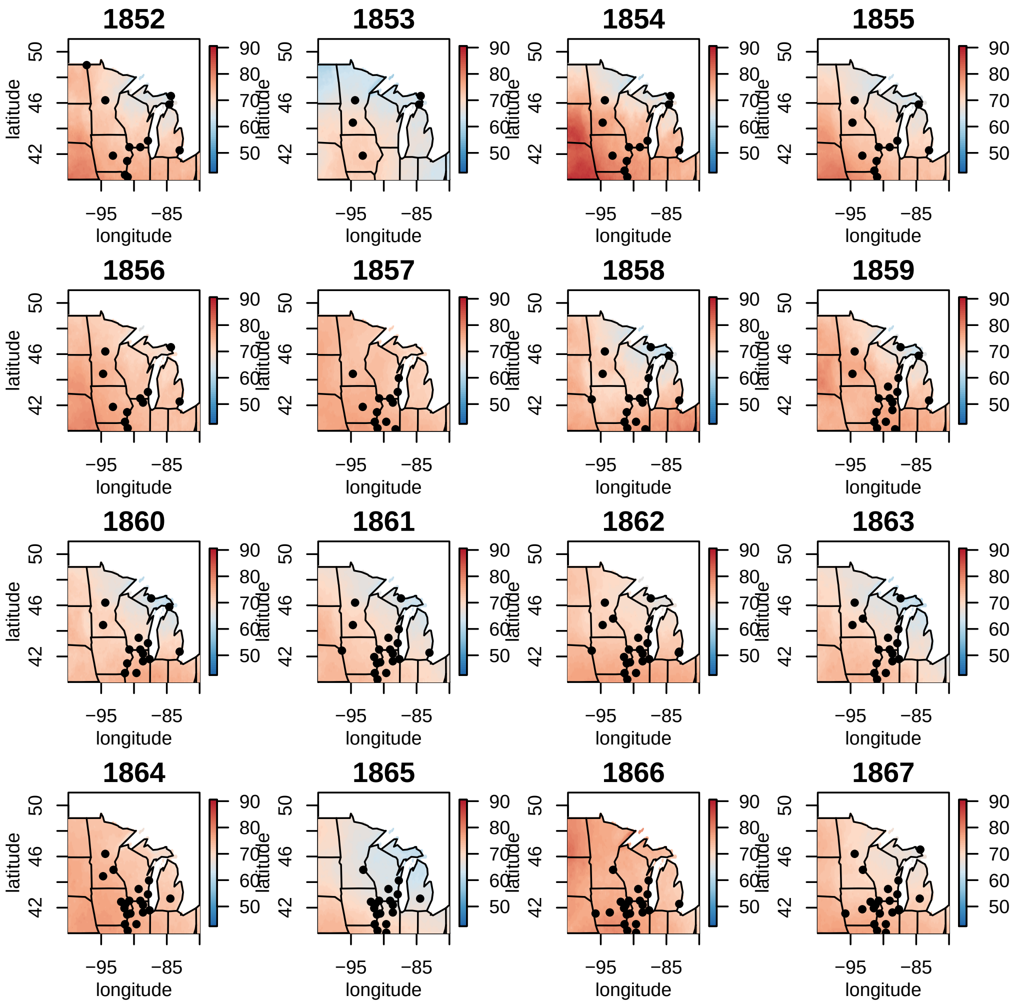
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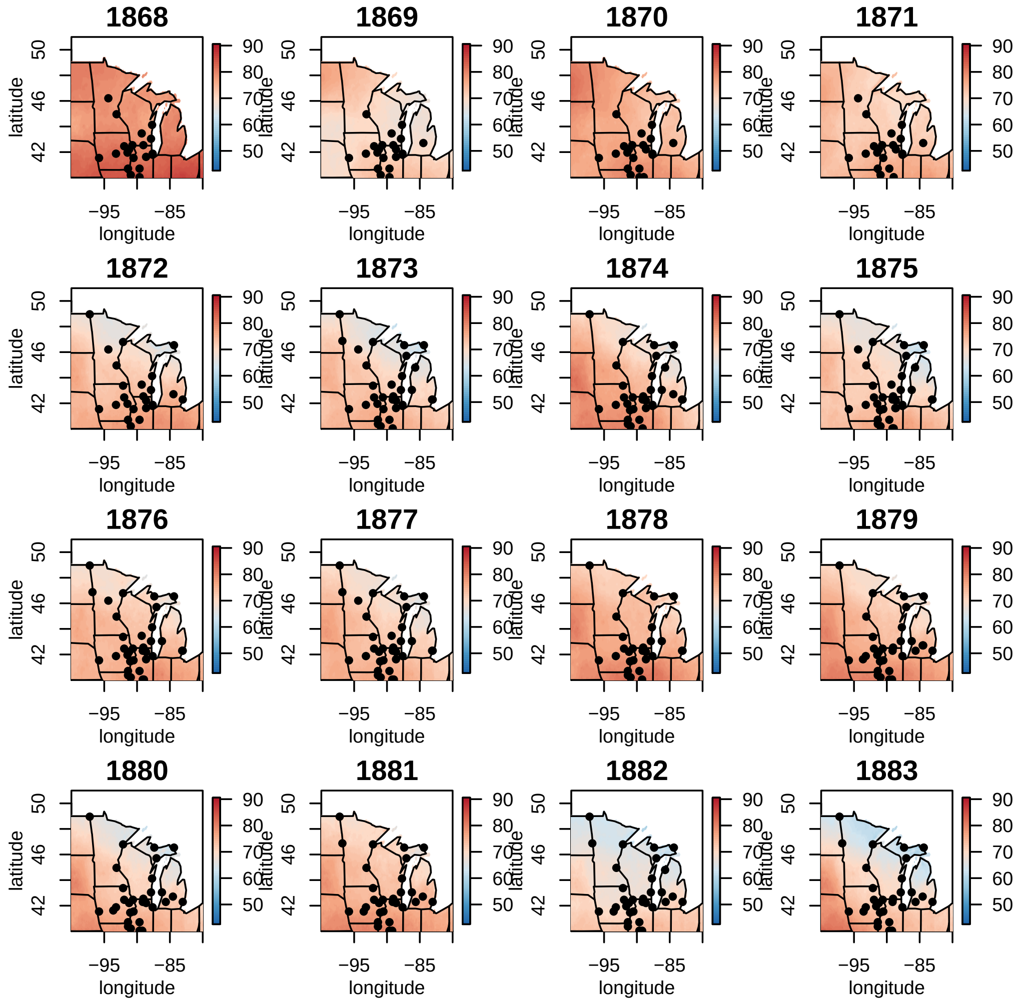

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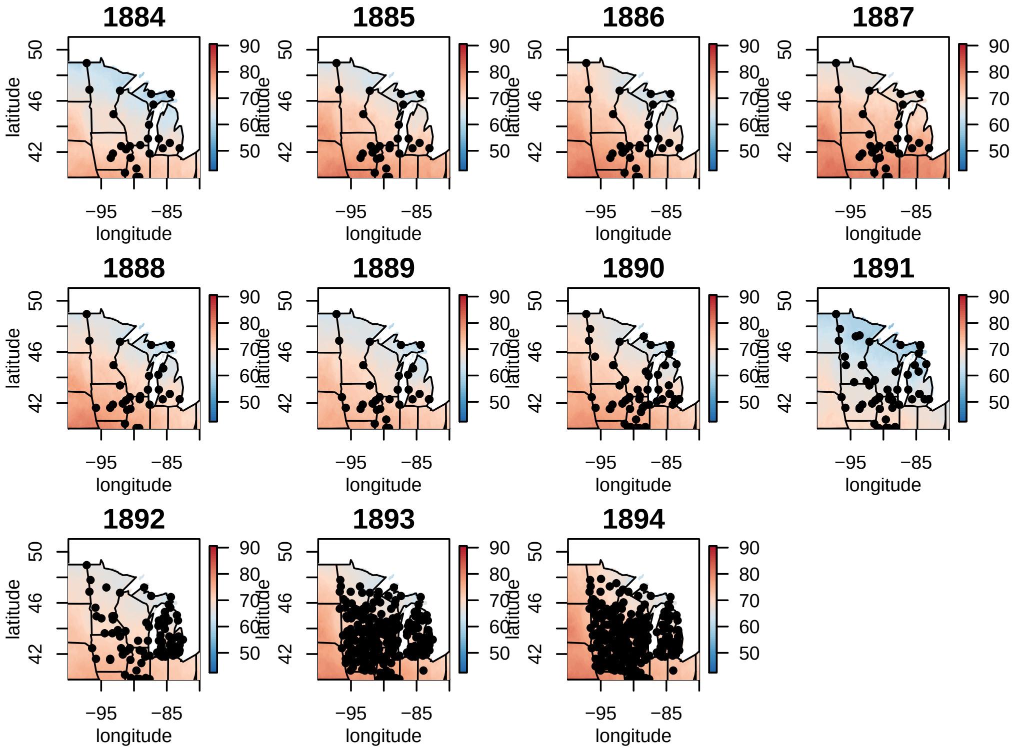
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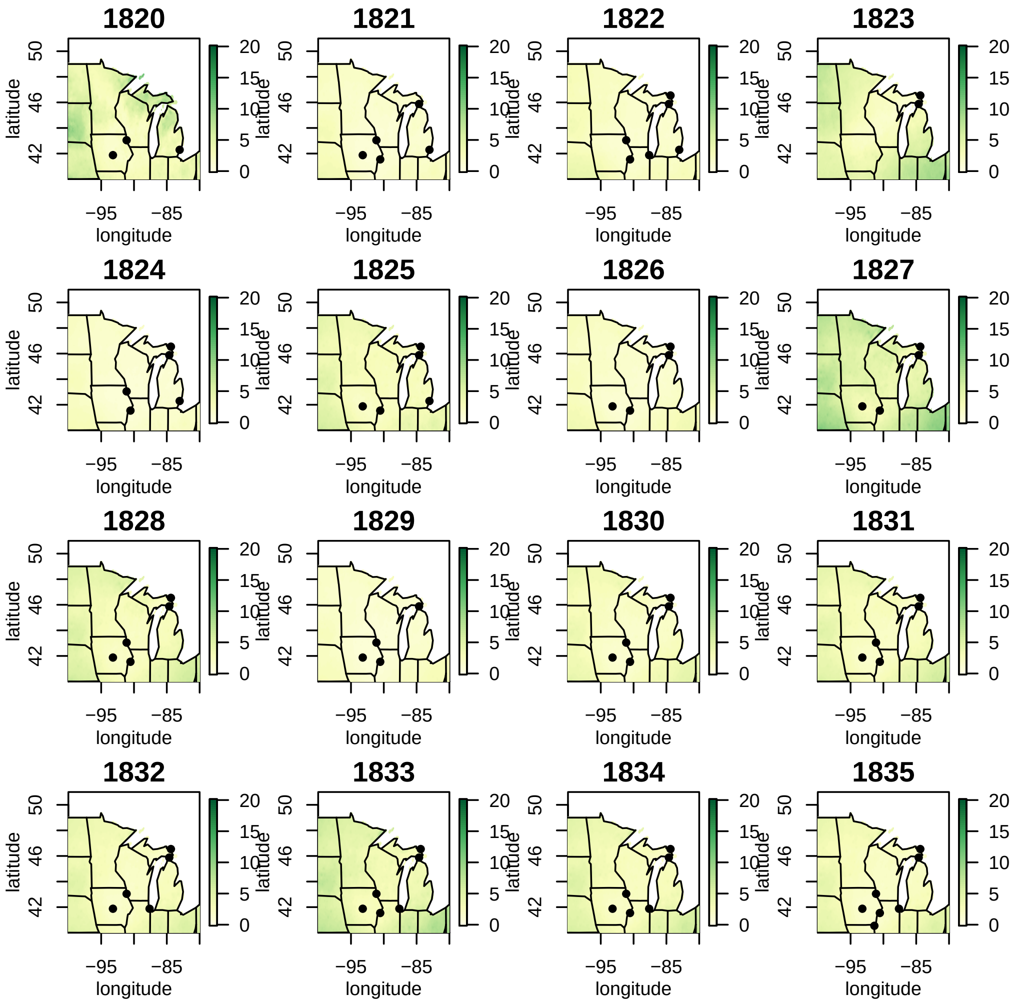
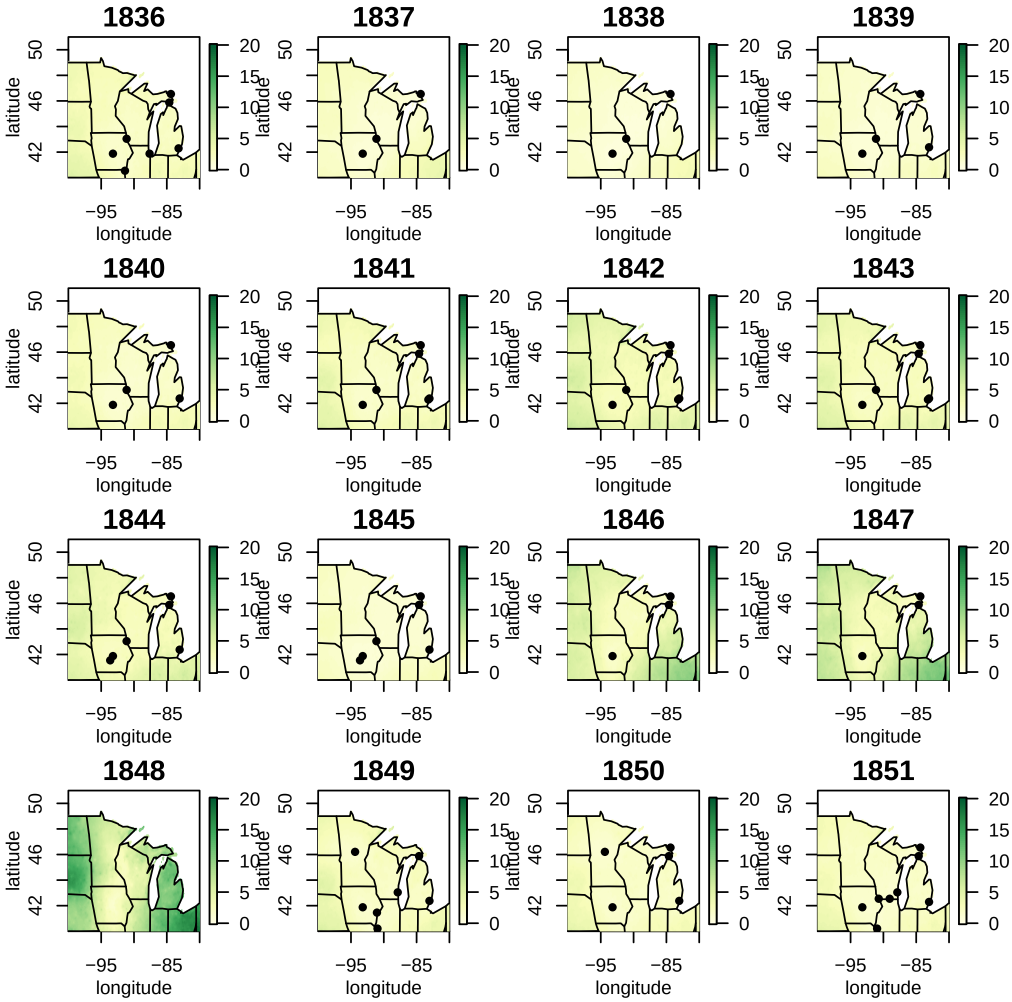
S.3 Robust PCR Model July Temperature Posterior Standard Deviations

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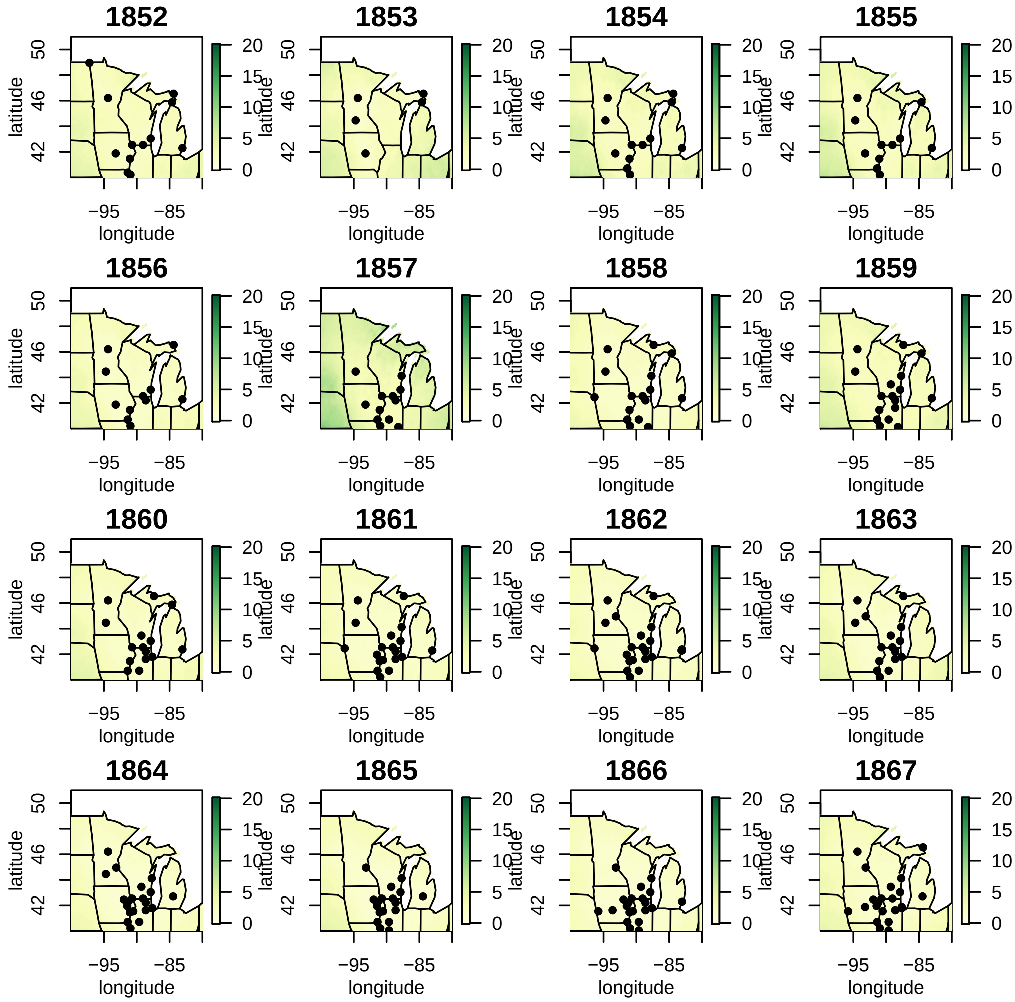
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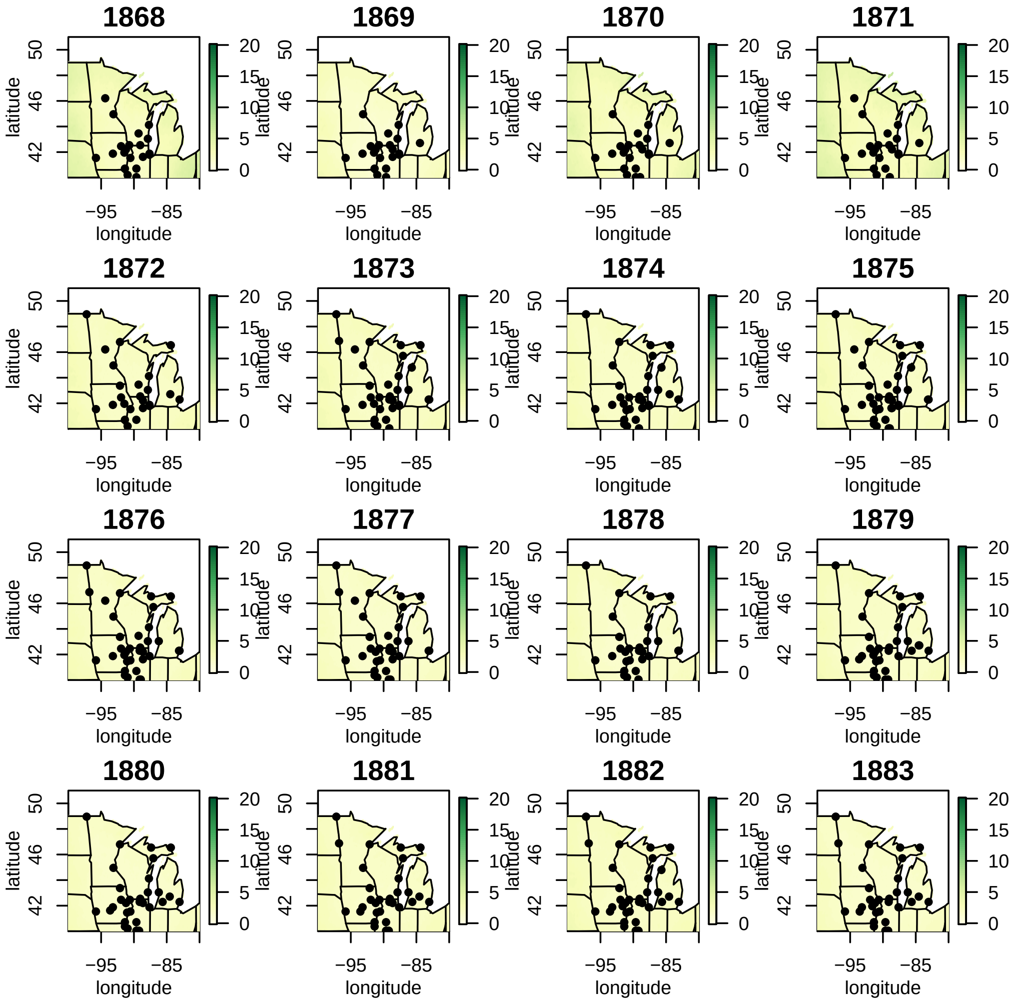
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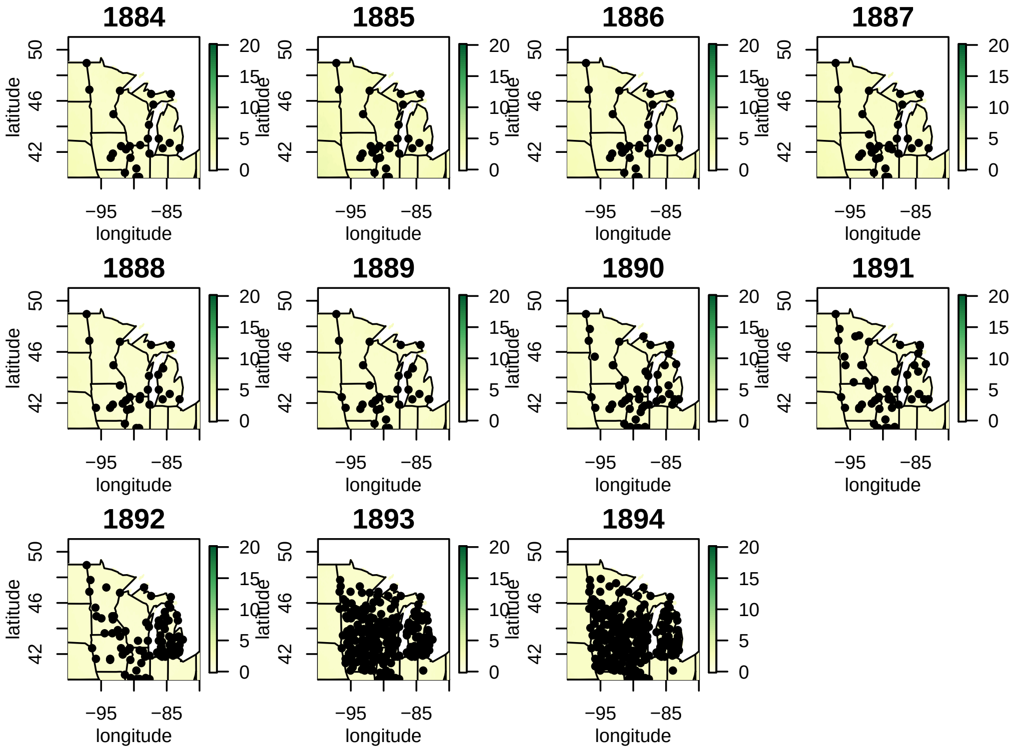
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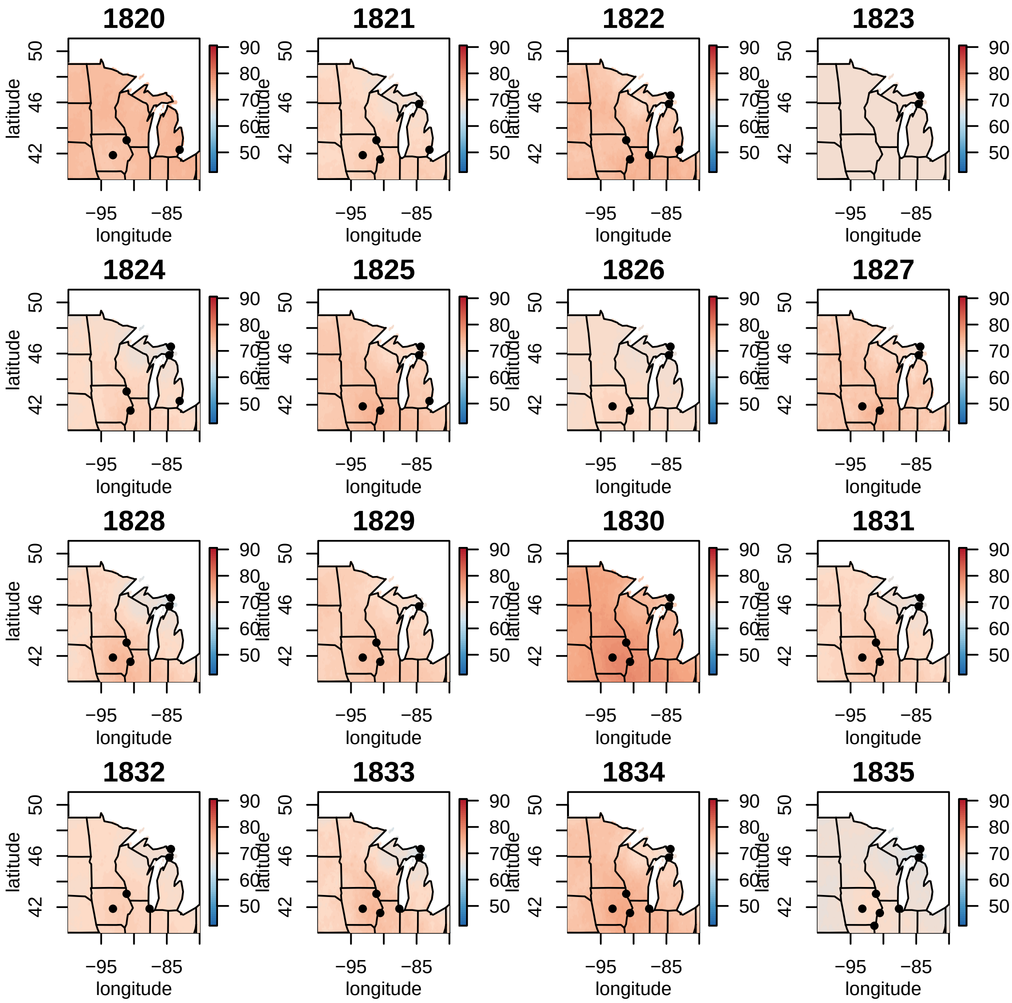
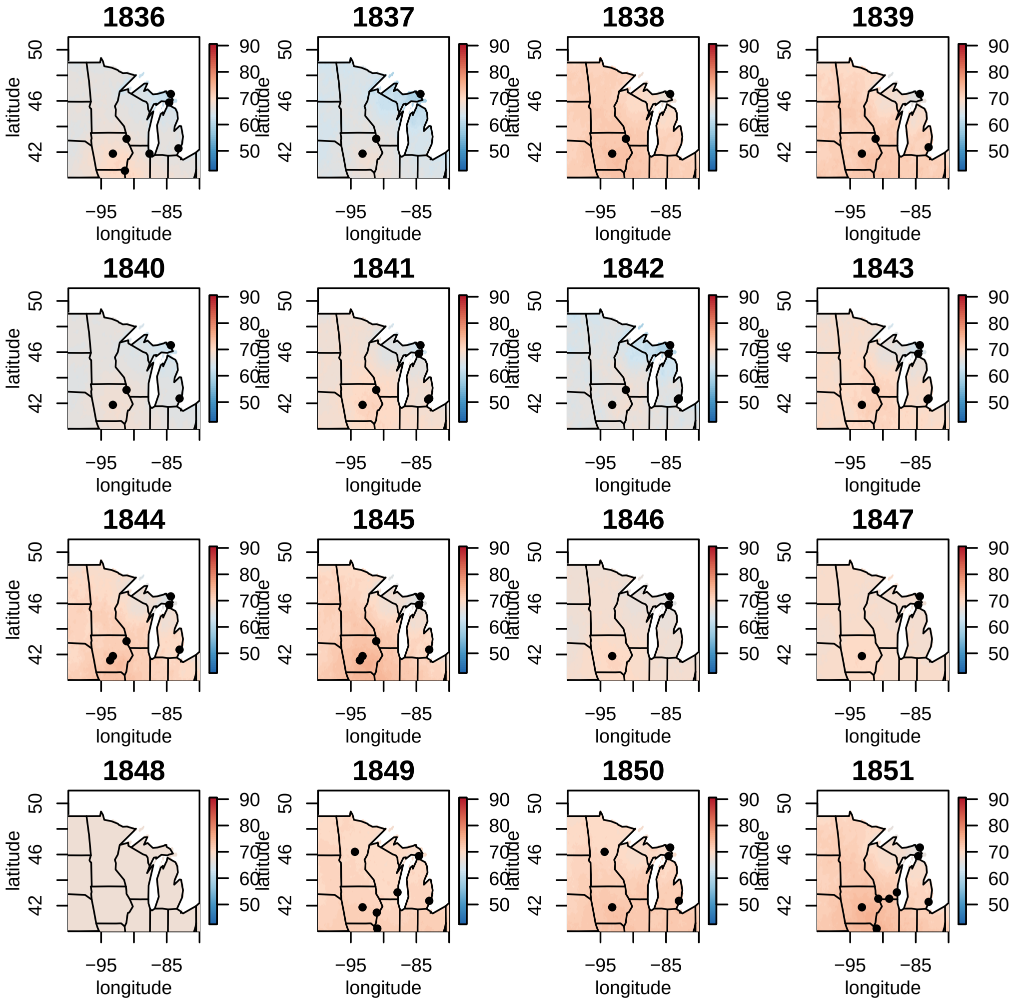
S.4 Robust Probabilistic PCR Model Posterior Mean July Temperature

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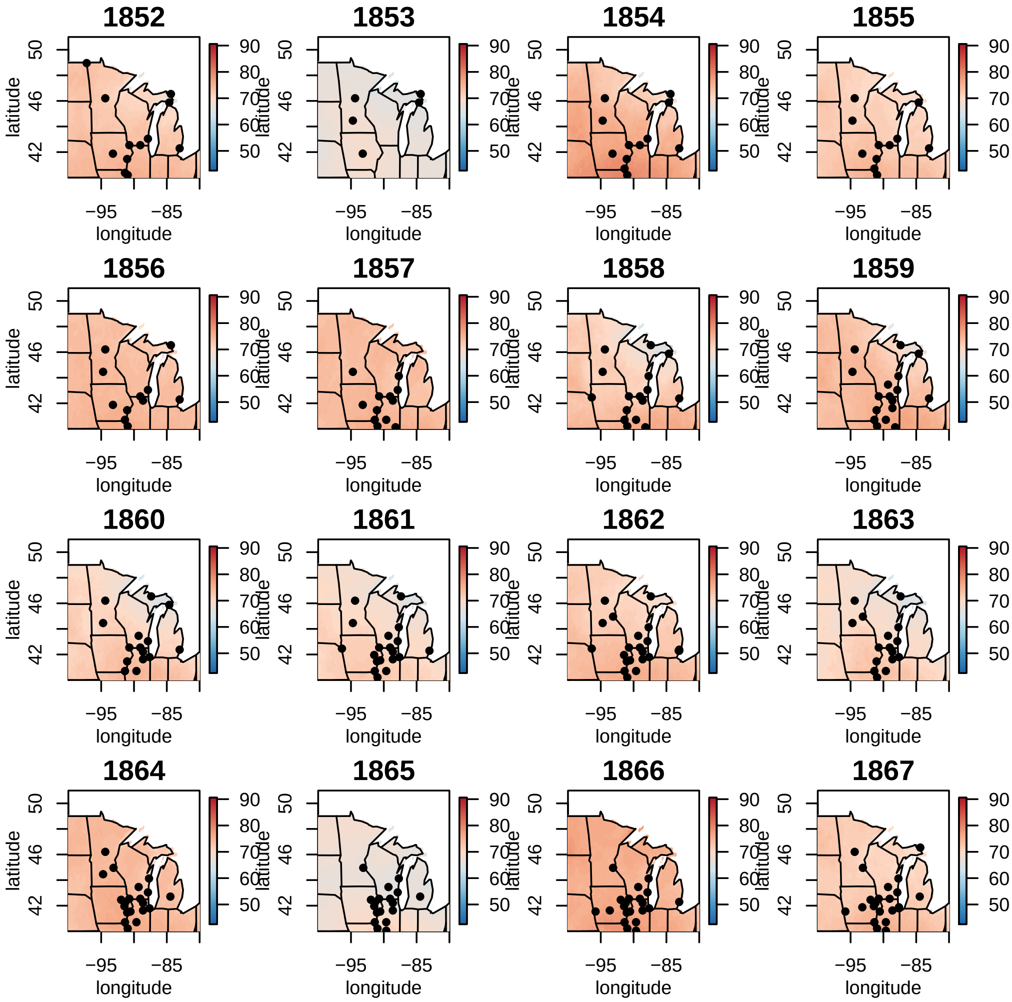
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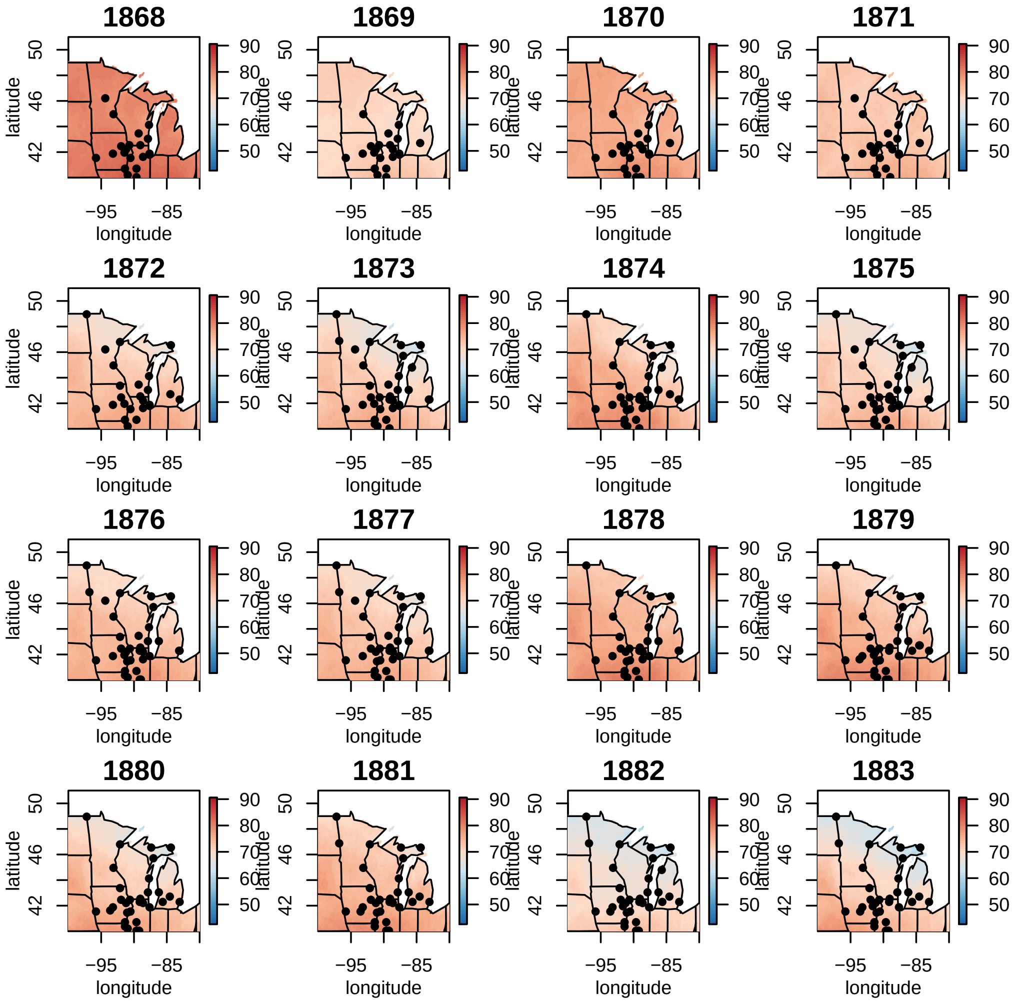
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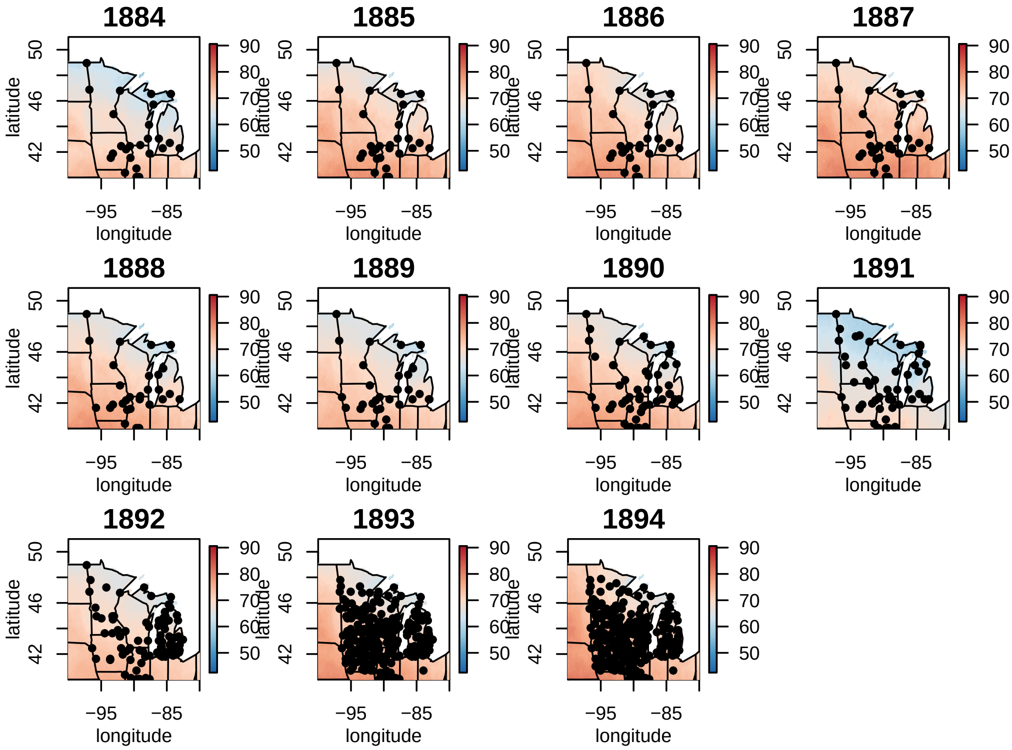
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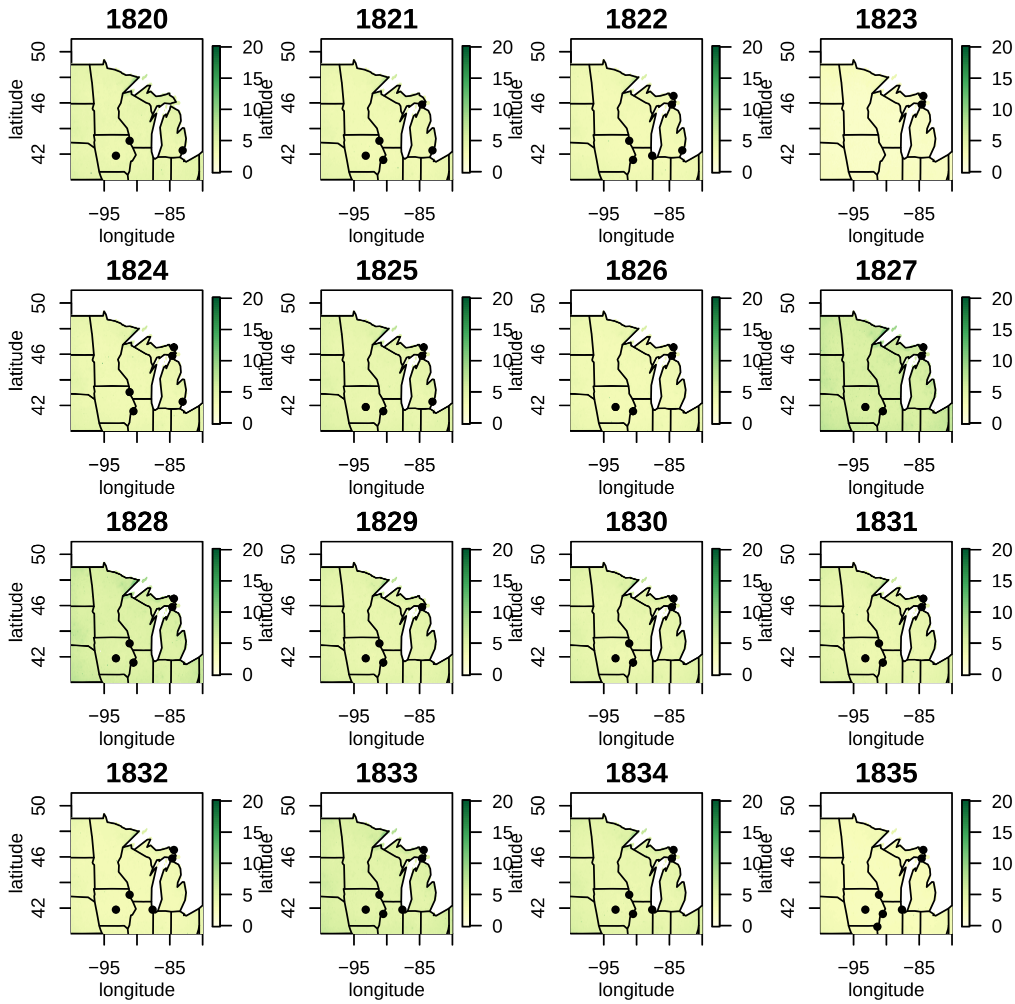
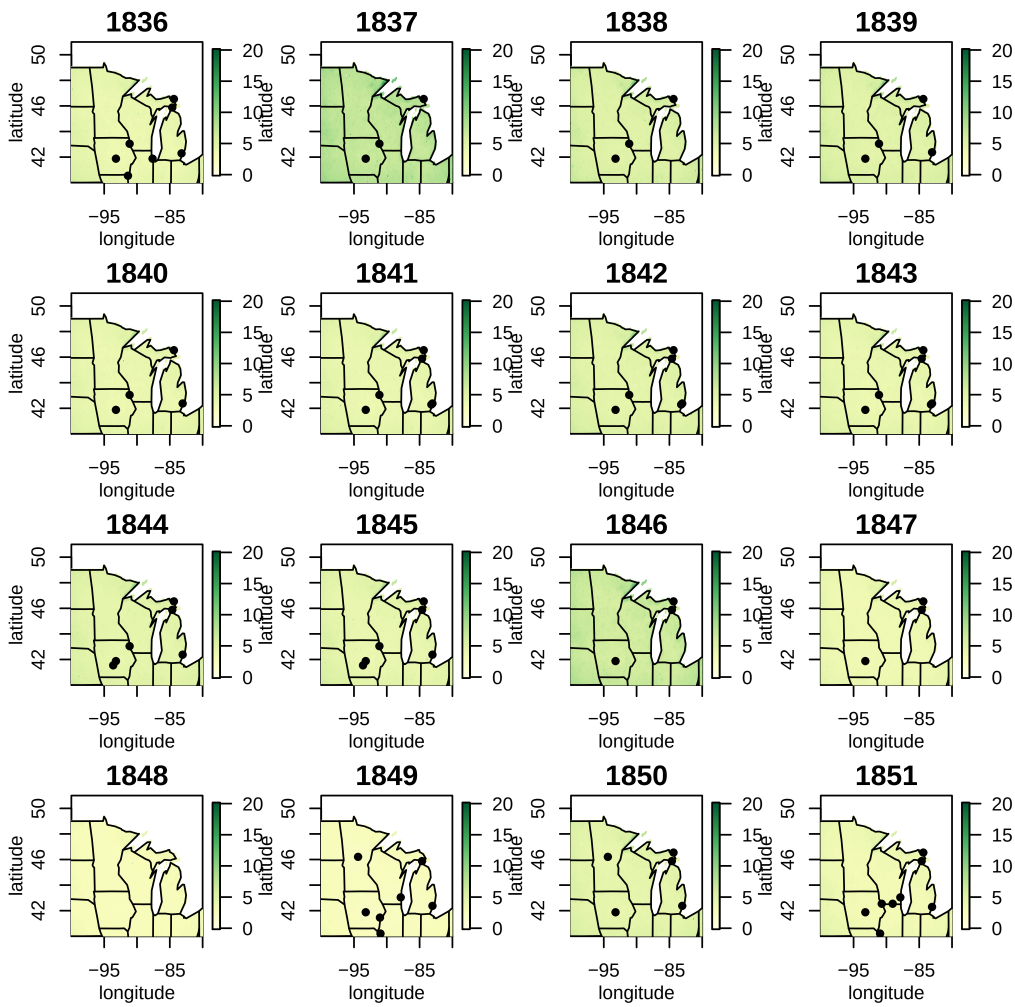
S.5 Robust Probabilistic PCR Model July Temperature Posterior Standard Deviations

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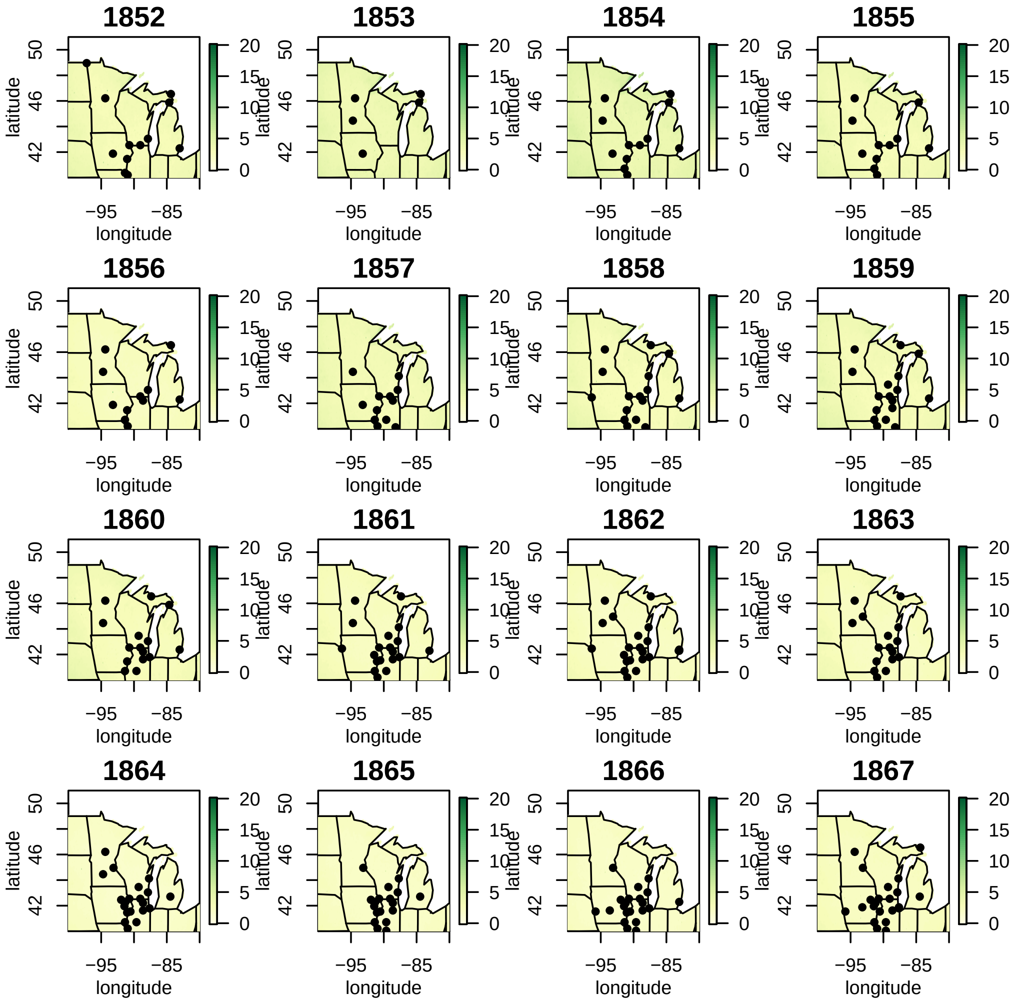
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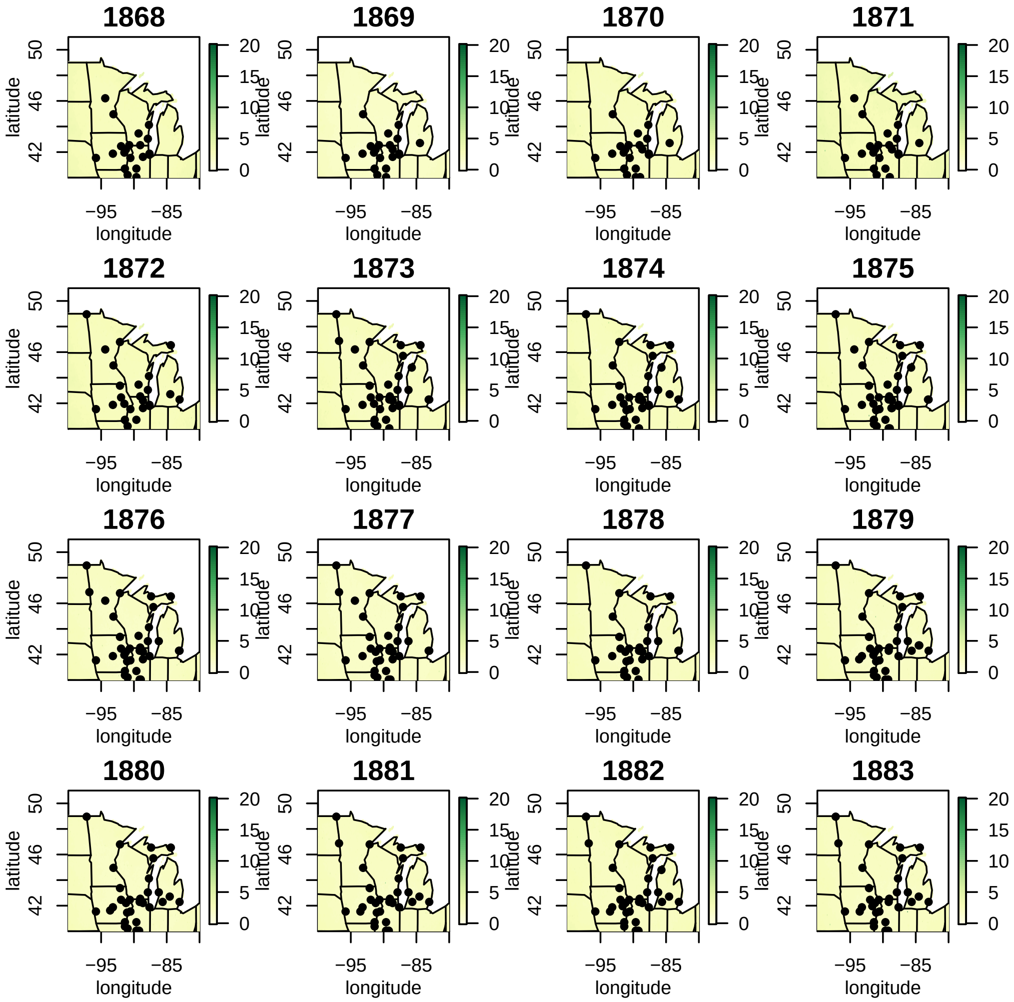
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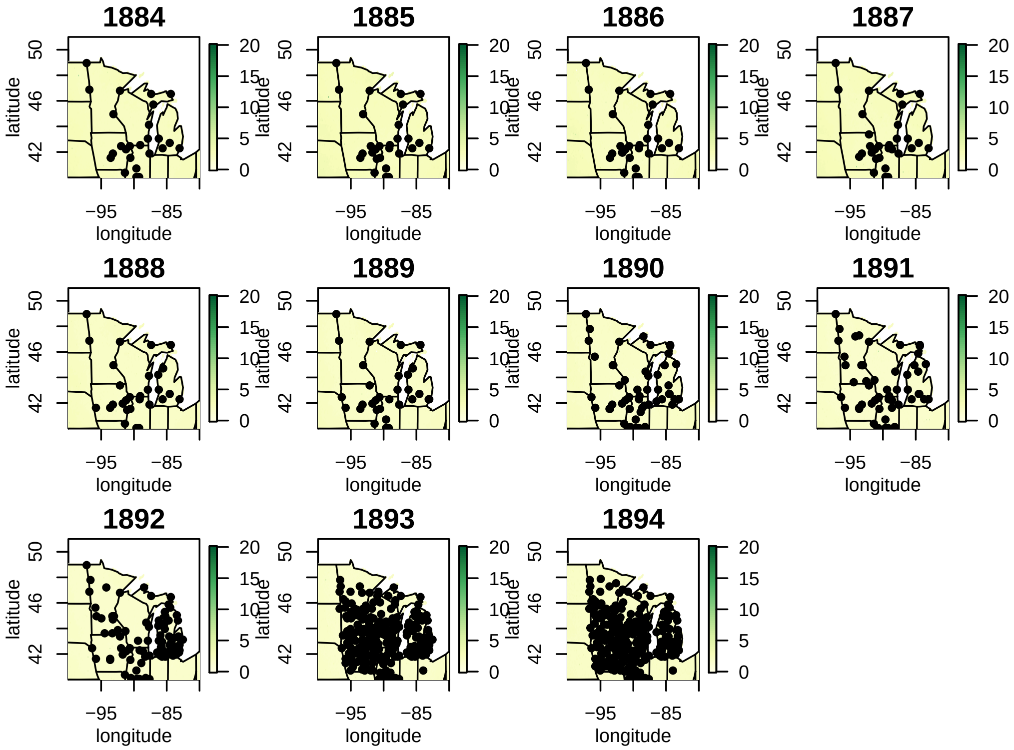
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