

# Bivariate Spatial Regression Model for Mixed-Response Lattice Data

MS Creative Component with Dr. Emily Berg

Steve Harms

Iowa State University  
Department of Statistics

*stharms@iastate.edu*

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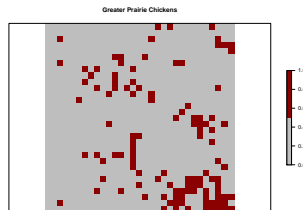
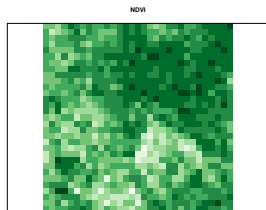
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# Data Description

- 2+ response variables, possibly correlated, distributions of mixed types
- Spatial data collected on a grid (discrete-indexed)
  - Model dependence in terms of adjacency rather than distance
- Study interested in both covariates and dependence relationships
  - Need interpretable dependence parameters

## Examples:

- ecology (presence/absence + environmental variables)
- agriculture (yield + categorical plant characteristics)
- weather/meteorology
- image pixel analysis



# Notation

- $\{s_i : i = 1, \dots, n\}$  : locations
- $Y(s_i)$  : Binary variable (0-1) at location  $s_i$
- $Z(s_i)$  : Gaussian variable at location  $s_i$
- $\mathbf{z} : \{z(s_i) : i = 1, \dots, n\}$  and  $\mathbf{y} : \{y(s_i) : i = 1, \dots, n\}$ : all obs. of the same type
- $\mathbf{z}(\bar{s}_i) : \{z(s_j) : i \neq j\}$  and  $\mathbf{y}(\bar{s}_i) : \{y(s_j) : i \neq j\}$ : all obs. of the same type except for location  $s_i$
- $N_i$  : Neighborhood of location  $s_i$ 
  - $j \in N_i$  if  $s_i$  and  $s_j$  are neighboring locations
- $M_i$  : Number of neighbors ( $|N_i|$ ) of location  $s_i$
- $\delta_i, \mu_i$  : Global/marginal mean parameters (node potentials)
- $\eta_y, \eta_z$  : Spatial dependence parameters for variables of the same type
- $\rho$  : Dependence parameter for variables of different types

# Background - Markov Random Field Models

Markov Random fields (auto-models) for lattice data from Besag (1974):

- One response variable from a one-parameter exponential family
- Specify expectation at each location conditionally on neighboring values:  $E[x(s_i)|x(\bar{s}_i)] = \mu_i + \sum_{j \neq i} \eta_{ij}x(s_j)$
- Sain, Furrer, and Cressie (2011): Extension to multivariate auto-normal model by "stacking" the univariate lattices
  - Direct extension of Besag's univariate conditional model rather than specifying MVN covariance of response variables
- Caragea and Berg (2014): Model two tree species' presence in bivariate autologistic model
  - Both response variables are binary

# Background - Mixed Graphical Models

Graphical models for learning the edge structure given  $n$  realizations of a set of mixed nodes (variables):

- Chen, et al. (2014): Edge potential parameter spaces for mixed one-parameter exponential family nodes corresponding to valid joint
- Lee and Hastie (2015): Specific case where any continuous variable is conditionally Gaussian, any discrete variable is conditionally logistic regression
- Gaussian nodes:

$$p(z(s_i)|z(\bar{s}_i), \mathbf{y}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left\{ \frac{-\sigma^{-2}}{2} \left[ \frac{\mu_i + \sum_{j=1}^n \rho_{ij} y(s_j) + \sum_{j=1}^n \eta_{y,ij} z(s_j)}{\sigma^{-2}} - z(s_i) \right]^2 \right\}$$

- Discrete nodes:

$$p(y(s_i)|\mathbf{y}(\bar{s}_i), \mathbf{z}) = \frac{\exp \left\{ y(s_i) \left( \delta_i + \sum_{j=1}^n \rho_{ij} z(s_j) + \sum_{j=1}^n \eta_{y,ij} y(s_j) \right) \right\}}{1 + \exp \left\{ y(s_i) \left( \delta_i + \sum_{j=1}^n \rho_{ij} z(s_j) + \sum_{j=1}^n \eta_{y,ij} y(s_j) \right) \right\}}$$

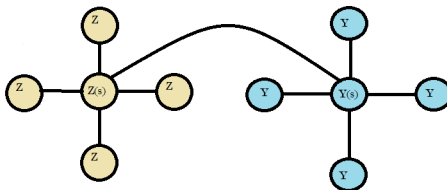
## Mixed Bivariate Markov Random Fields

Goal: Combine the interpretive properties of auto-models with compatible node-conditional specifications from mixed graphical models

- View each response variable at each location as a node, combine with (fixed/known) set of edges into an undirected graph with  $2n$  total nodes
- Use this graph structure in the context of auto-models

# Assumptions

- Simplifying assumptions for the models in this work:
  - Four-nearest neighbor structure (pairwise-only dependence):  $M = 4$
  - Binary and Gaussian nodes are only connected at each location
  - Isotropy:  $\eta_{Y,ij} = \eta_Y$  and  $\eta_{Z,ij} = \eta_Z$
  - Interior locations only: each node has same number of neighbors (no edge effects)
  - Common conditional variance for Gaussian nodes (variance =  $\sigma^2 \forall Z(s_i)$ )





# Conditional Distributions

- Gaussian node at location  $s_i$  has conditional distribution

$$p(z(s_i) | \mathbf{z}(\bar{s}_i), y(s_i)) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left\{ \frac{-1}{2\sigma^2} [z(s_i) - \alpha(s_i)]^2 \right\}$$

where

$$\alpha(s_i) = \mu_i + \frac{\eta_z}{M} \sum_{j \in N_i} (z(s_j) - \mu_j) + \rho \left( y(s_i) - \frac{\exp(\delta_i)}{1 + \exp(\delta_i)} \right)$$

# Conditional Distributions

- Binary node at location  $s_i$  has conditional distribution

$$p(y(s_i) | \mathbf{y}(\bar{s}_i), z(s_i)) = \frac{\exp \{y(s_i) (\phi(s_i))\}}{1 + \exp \{y(s_i) (\phi(s_i))\}}$$

where

$$\phi(s_i) = \delta_i + \frac{\eta_y}{M} \sum_{j \in N_i} \left[ y(s_j) - \frac{\exp(\delta_j)}{1 + \exp(\delta_j)} \right] + \frac{\rho}{\sigma^2} (z(s_i) - \mu_i)$$

- “Centering” in the auto-regressive terms allow separation of global and local effects for a more sensible interpretation of  $\eta_y$ ,  $\eta_z$ , and  $\rho$

# Properties of the Conditional Specification

- $\mu_i$  and  $\frac{\exp(\delta_j)}{1+\exp(\delta_j)}$  are independence expectations, i.e., marginal means
- Incorporate covariates  $\mathbf{X}_y, \mathbf{X}_z$  by setting  $\mu_i = \mathbf{X}_{z,i}\beta_z$  and  $\delta_i = \mathbf{X}_{y,i}\beta_y$
- The remaining terms in  $\alpha(s_i)$  and  $\phi(s_i)$  govern the clustering or “local” behavior due to dependence/auto-correlation
- Full set of node-conditionals combine into a negpotential function

$$\begin{aligned} Q(\mathbf{y}, \mathbf{z}) = & \sum_{i=1}^n \left[ \frac{\mu_i}{\sigma^2} z(s_i) - \frac{1}{2\sigma^2} z(s_i)^2 + \delta_i y(s_i) \right] + \frac{\rho}{\sigma^2} \sum_{i=1}^n \left[ (z(s_i) - \mu_i) \left( y(s_i) - \frac{\exp(\delta_i)}{1+\exp(\delta_i)} \right) \right] \\ & - \frac{1}{2\sigma^2} \sum_{i=1}^n \sum_{j \in N_i} \left[ \frac{\eta_z}{M} (z(s_i) - \mu_i)(z(s_j) - \mu_j) \right] \\ & + \frac{1}{2} \sum_{i=1}^n \sum_{j \in N_i} \left[ \frac{\eta_y}{M} \left( y(s_i) - \frac{\exp(\delta_i)}{1+\exp(\delta_i)} \right) \left( y(s_j) - \frac{\exp(\delta_j)}{1+\exp(\delta_j)} \right) \right] \end{aligned}$$

- $p(\mathbf{y}, \mathbf{z}) = \frac{\exp(Q(\mathbf{y}, \mathbf{z}))}{\int_{\Omega} \exp(Q(\mathbf{y}, \mathbf{z})) d\mathbf{y} d\mathbf{z}}$  is a valid joint distribution if  $\int_{\Omega} \exp(Q(\mathbf{y}, \mathbf{z})) d\mathbf{y} d\mathbf{z} < \infty$ , which holds if  $\eta_z < 1$  and  $\sigma^2 > 0$

# Model Breakdown

- When dependence becomes too strong, no longer have clearly separated marginal (global) and conditional (local) effects
  - Large  $\eta_z$  or  $\eta_y$  cause local dependence to overwhelm global properties
  - Data are heavily clustered/chaotic
- Kaiser (2007) quantifies boundaries for “nicely behaved” models:
  - Auto-logistic models:  $\eta_y < 4$
  - Auto-normal models: Breakdown as  $\eta_z \rightarrow 1$ , especially  $\eta_z \geq 0.99$
- In bivariate case, we have 3 different dependence parameters ( $\eta_y, \eta_z, \rho$ ) and want all parameters to reflect appropriate properties of the data
- My rule of thumb:  $\rho > \sqrt{\sigma^2(1 - \eta_z)(4 - \eta_y)}$  implies strong dependence for bivariate model

# Estimation and Inference

# Maximum Pseudo-likelihood Estimation

- For most practical applications, maximizing full likelihood requires repeated evaluation of high-dimensional integral in full joint distribution
- Instead, minimize the negative of the log pseudo-likelihood  $\tilde{\ell}$ , which only uses lower-dimensional node-conditionals:

$$\tilde{\ell} = \sum_{i=1}^n \log(p(z(s_i) | \mathbf{z}(\bar{s}_i), y(s_i))) + \sum_{i=1}^n \log(p(y(s_i) | \mathbf{y}(\bar{s}_i), z(s_i)))$$

- Hughes, et al. (2011) show loss in efficiency for MPLE is negligible when the lattice is reasonably large ( $\sim 400$  points)
- Exact or asymptotic distributions for parameter estimates are not straightforward from pseudo-likelihood methods

- Use Gibbs sampling to simulate from full set of specified node-conditional distributions
  - Simulate sequentially node-by-node from each conditional distribution, update, iterate until convergence
- Relatively simple simulation algorithm enables ready implementation of parametric bootstrap for inference:
  - 1 For a set of parameters  $\hat{\Theta}$  estimated from the original data, use Gibbs sampling to simulate bootstrap replicates from  $\hat{\Theta}$
  - 2 Obtain MPLE estimates for each bootstrapped dataset to get an empirical distribution of parameters,  $\theta^* \in \Theta^*$
  - 3 Lower and upper bounds for a  $100(1-\alpha)\%$  confidence interval for a parameter  $\theta \in \Theta$  are:  
$$L_\alpha = 2\hat{\theta} - \theta_{1-\alpha/2}^* \text{ and } U_\alpha = 2\hat{\theta} - \theta_{\alpha/2}^*$$

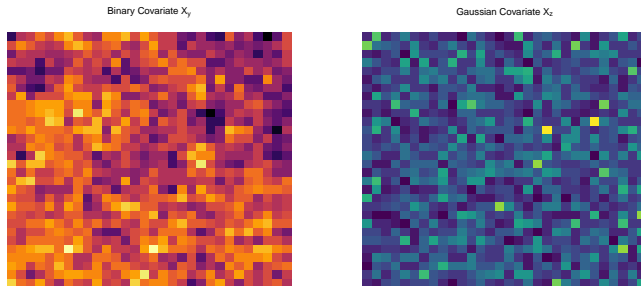
# Simulation Studies



# Study 1: MPLE Estimation Set-up

- Goal: Compare performance for full model vs. previous reduced models
- 3 different dependence regimes (weak, moderate, strong)
- For each dependence regime, obtain MPLE estimates (8 parameters for full model) for 1,000 simulated datasets on a  $30 \times 30$  lattice

**Figure:** Covariates used in simulation: Normal with spatial correlation  $\eta_z = 0.9$ ,  $\mu = 1$ ,  $\sigma^2 = 1$  (left) and  $\text{Gamma}(3, 4)$  (right)



# Study 1: MPLE Estimation

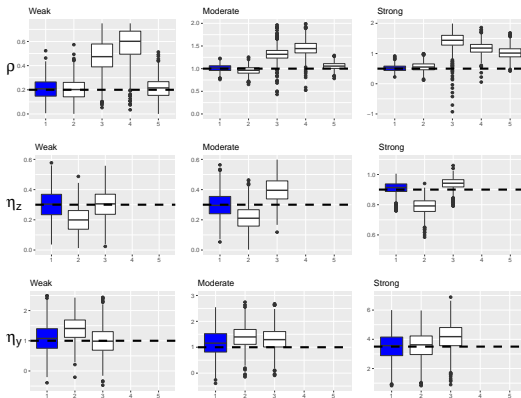
**Parameter Regimes Used to Simulate Data**

Dependence	$\rho$	$\eta_z$	$\eta_y$	$\beta_{0y}$	$\beta_{1y}$	$\beta_{0z}$	$\beta_{1z}$	$\sigma^2$
Weak	0.2	0.3	1	-1	0.5	1	0.5	1
Moderate	1	0.3	1	-1	0.5	1	0.5	1
Strong	0.5	0.9	3.5	-1	0.5	1	0.5	1

Model	Gaussian Cond. Mean Parameter $\alpha(s_i)$
Full (1)	$\beta_0 + \beta_1 X_{z,i} + \frac{\eta_z}{4} \sum_{j \in N_i} (z(s_j) - \mu_j) + \rho \left( y(s_i) - \frac{\exp(\delta_i)}{1 + \exp(\delta_i)} \right)$
Constant Mean (2)	$\beta_0 + \frac{\eta_z}{4} \sum_{j \in N_i} (z(s_j) - \mu_j) + \rho \left( y(s_i) - \frac{\exp(\delta_i)}{1 + \exp(\delta_i)} \right)$
Univariate Spatial (3)	$\beta_0 + \beta_1 X_{z,i} + \beta_\rho Y(s_i) + \frac{\eta_z}{4} \sum_{j \in N_i} (z(s_j) - \mu_j)$
Univariate Non-Spatial (4)	$\beta_0 + \beta_1 X_{z,i} + \beta_\rho Y(s_i)$
Bivariate Non-Spatial (5)	$\beta_0 + \beta_1 X_{z,i} + \rho \left( y(s_i) - \frac{\exp(\delta_i)}{1 + \exp(\delta_i)} \right)$

# MPLE Study Results - Dependence

- Only bivariate spatial models (1 and 2) capture the dependence structure adequately
- Strong dependence (far right column): only full bivariate spatial model obtains unbiased estimates for all three dependence parameters



# MPLE Study Results - Covariates

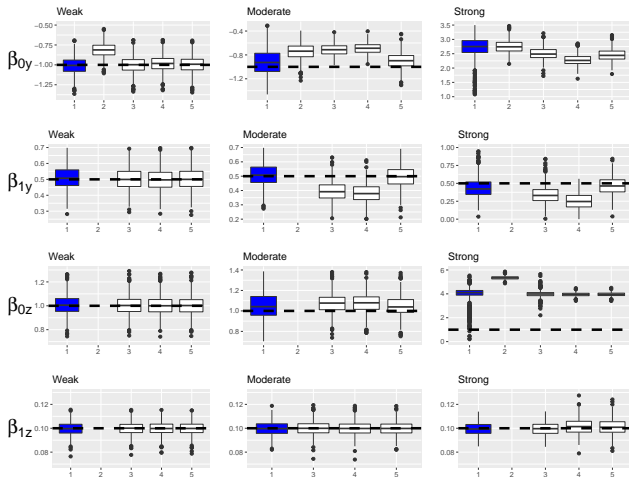


Figure: Mean Parameter Estimates for Simulated Data

## Summary

- Weak/Moderate dependence: all models provide unbiased estimates of the regression coefficients  $\beta$
- Strong dependence: only full model is remotely close to estimating the true parameter values
- The strong dependence regime "breaks" the data-generating mechanism:
  - Expected marginal behavior is not observed due to local dependence effects  
 $\implies$  Caution for parametric bootstrap if we encounter strong dependence

## Study 2: Bootstrap C.I. Coverage

Goal: Investigate empirical vs. nominal confidence interval coverage under different dependence

Set-up:

- No covariates
- 2 dependence regimes: weak/small variance and strong/large variance
- $30 \times 30$  lattice
- 95% confidence intervals via parametric bootstrap using 500 bootstrap replicates for 1,000 simulated datasets

## Study 2: Bootstrap C.I. Coverage

- Generate  $m = 1,000$  datasets from the true parameter values,  $\Theta = \{\rho, \eta_z, \eta_y, \delta, \mu, \sigma^2\}$
- For each of the  $i = 1, \dots, 1000$  simulated datasets:
  - Estimate the parameters using MPLE to get  $\hat{\Theta}_i$
  - Use  $\hat{\Theta}_i$  to generate 500 bootstrap replicates for each dataset
  - For each of the bootstrap replicates, obtain MPLE estimates of the parameters and collect into empirical distribution  $\Theta_i^*$  of  $\Theta_i$  for data set  $i$
  - Obtain  $C = 95\%$  confidence intervals for  $\theta \in \Theta$  by taking  $U_i = 2 \cdot \hat{\theta}_i - \theta_{i,.025}^*$  and  $L_i = 2 \cdot \hat{\theta}_i - \theta_{i,.975}^*$  as the bounds.
- For a Monte Carlo sample of size  $m = 1000$ , the empirical coverage is  $C^* = \left(\frac{1}{1000}\right) \sum_{i=1}^{1000} \mathbb{1}\{\theta \in (L_i, U_i)\}$

## Study 2: Bootstrap C.I. Coverage

- Under weak or moderate dependence conditions, empirical coverage is close to 95%
- Slight undercoverage matches the results for the bivariate autologistic model from Caragea and Berg (2014)

Weak Dependence				
Parameter	True Value	MC Estimate	MC Std. Error	95% CI Coverage
$\rho$	0.2	0.202	0.073	92.9%
$\eta_z$	0.5	0.493	0.083	93.2%
$\eta_y$	1	0.959	0.419	94.5%
$\delta$	0.5	0.508	0.090	94.1%
$\mu$	1	1.001	0.052	93.6%
$\sigma^2$	1	0.996	0.053	92.9%

**Table:** Bootstrap confidence interval coverage for weak dependence regime



## Study 2: Bootstrap C.I. Coverage

- Strong dependence: empirical coverage is further from the nominal 95% value for the unbiased dependence parameters
- Unable to obtain unbiased estimates or reliable confidence intervals for mean parameters  $\delta$  and  $\mu$

Strong Dependence				
Parameter	True Value	MC Estimate	MC Std. Error	95% CI Coverage
$\rho$	5	5.024	0.911	96.9%
$\eta_z$	0.9	0.901	0.042	86.5%
$\eta_y$	3	3.031	0.710	98.0%
$\delta$	0.5	-1.683	1.103	49.4%
$\mu$	1	-17.845	10.419	50.0%
$\sigma^2$	100	99.622	5.582	92.6%

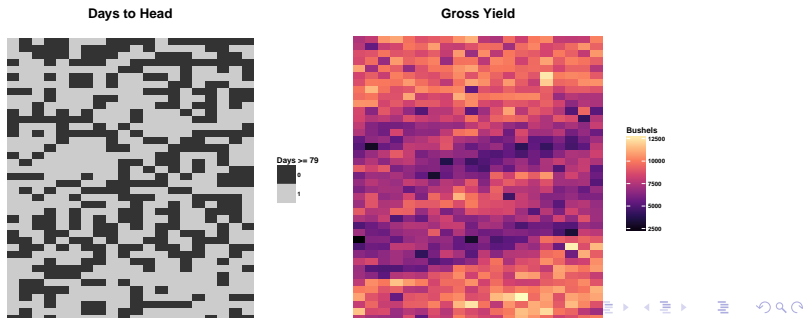
Table: Bootstrap confidence interval coverage for strong dependence regime

# Illustrative Examples

## Illustrative Example 1: Model Estimation and Selection

# Agricultural Field Trials - Set-Up

- Lado, et al. (2013) used basic spatial adjustments to aid in prediction of wheat yields
- Re-purpose yield data to implement bivariate mixed MRF model
- Goal: Evaluate model performance for full model vs. reduced models
  - Gaussian response  $Z(s_i)$  : Gross Yield (1000s of bushels)
  - Binary response  $Y(s_i)$ : Slow/Fast Growth (1 if  $> 78$  days to head)
  - Thousand-Kernel Weight (g) used a covariate for both responses
  - Fields arranged on a  $40 \times 20$  lattice



# Agricultural Field Trials - Estimation Results

## Regression Coefficient Estimates (and 95% Confidence Intervals):

- Estimates are similar across models
- In 3 out of 4 models, Thousand-Kernel Weight has significant relationship with both response variables

Model	Binary (Y) Intercept ( $\beta_{0,y}$ )	1000-Kernel Wt $\beta_{1,y}$	Gaussian (Z) Intercept ( $\beta_{0,z}$ )	1000-Kernel Wt ( $\beta_{1,z}$ )
Full	6.591 (5.109, 7.794)	-0.137 (-0.162, -0.106)	6.842 (5.915, 7.606)	0.022 (0.008, 0.036)
Bivariate No Covariates	0.336 (0.130, 0.534)	-	8.014 (7.496, 8.384)	-
Univariate	6.600 (4.319, 7.104)	-0.135 (-0.145, -0.087)	7.065 (6.969, 8.370)	0.019 (-0.011, 0.019)
Univariate Non-Spatial	6.561 (5.177, 7.818)	-0.134 (-0.161, -0.105)	5.330 (4.435, 6.250)	0.057 (0.038, 0.077)
Bivariate Non-Spatial	6.873 (5.328, 8.266)	-0.141 (-0.171, -0.110)	5.442 (4.485, 6.507)	0.055 (0.032, 0.076)

# Agricultural Field Trials - Estimation Results

## Dependence Parameters:

- Estimates are quite different between bivariate and univariate models
- Moderate within-type (spatial) dependence
- Significant cross-dependence for 2/3 models

Model	$\rho$	$\eta_z$	$\eta_y$
Full	0.299	0.888	0.846
Bivariate	(0.127 , 0.474)	(0.795 , 1.008)	(0.000 , 1.947)
Bivariate No Covariates	0.126 (-0.026 , 0.264)	0.900 (0.809, 0.996)	1.001 (0.135 , 2.001)
Univariate Spatial	-	0.618 (0.634 , 0.921)	1.232 (0.622 , 2.710)
Univariate Non-Spatial	-	-	-
Bivariate Non-Spatial	0.233 (0.282 , 0.487)	-	-

# Agricultural Field Trials - Model Selection

- We use continuous-ranked probability score to compare in-sample predictive capability of each model:

$$CRPS(F(x(s_i)|\mathbf{x}(\bar{s}_i), \hat{\Theta}), x_i) = \int_{-\infty}^{\infty} (F(x(s_i)) - \mathbb{1}_{[x(s_i) \geq x]})^2 dx(s_i)$$

where  $F(x(s_i)|\mathbf{x}(\bar{s}_i), \hat{\Theta})$  is the conditional CDF at each node

- Sum CRPS over all points to get  $CRPS(M)$  for the model
- Corresponding skill score for model  $M$  vs. constant mean model  $c$  is

$$Skill = 100 \cdot \left[ 1 - \frac{CRPS(M)}{CRPS(c)} \right]$$

- Minimize CRPS or maximize Skill to select best model

# Agricultural Field Trials - Model Selection

Model	$CRPS_y$	$Skill_y$	$CRPS_z$	$Skill_z$
Full	0.20	16.74	0.66	34.23
Intercept-Only Spatial	0.24	1.62	0.66	33.46
Univariate	0.21	14.82	0.70	29.57
Univariate Non-Spatial	0.22	8.11	0.97	2.59
Bivariate Non-Spatial	0.22	10.44	0.96	3.37

- Full bivariate spatial model with covariate has best in-sample prediction for both response variables
- Spatial models outperform non-spatial models for Gaussian response (Gross Yield)
- Covariate (Thousand-Kernel Weight) important for fitting the binary data



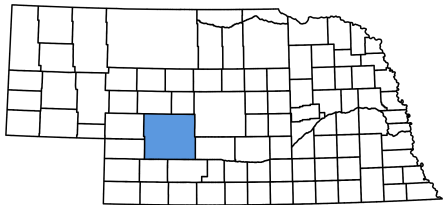
## Illustrative Example 2: Strong Spatial Dependence

# Greater Prairie Chickens - Data

Setting: Lincoln County (Western Nebraska)

Data from three sources:

- Greater Prairie Chicken observations (March-May, since 1990) from Cornell Lab of Ornithology
- Vegetative Cover: April 2018 NDVI (Normalized Difference Vegetation Index) collected via satellite, from USDA National Agricultural Statistics Survey's VegScape API
- Soil properties (covariates) from NRCS Web Soil Survey



# Greater Prairie Chickens - Data

- Data sources overlaid/combined/aggregated onto  $31 \times 31$  lattice (each point  $\sim 2$  square miles)
- NDVI (continuous response) has very strong spatial autocorrelation
- Prairie Chicken nesting sites (binary response) has visible spatial autocorrelation, but somewhat sparse

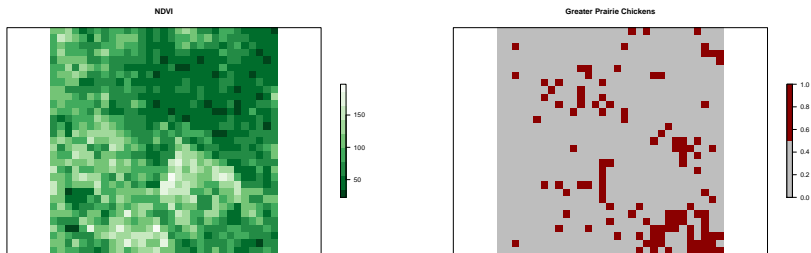


Figure: NDVI (left) and Greater Prairie Chicken observations (right)

# Greater Prairie Chickens - Methodology

## Methodology:

- NDVI as continuous response  $Z(s_i)$
- Greater Prairie Chicken observations (1 if observed since 1990, 0 if not) as binary response  $Y(s_i)$
- Exploratory analysis to select possible soil covariates
- Estimate the full bivariate MRF model use 90% confidence intervals for inference
- Can we find any evidence for:
  - Either response being related to soil properties?
  - Spatial dependence or cross-dependence among NDVI and nesting sites?

# Greater Prairie Chickens - Estimation Results

Parameter	Estimate	Std. Err.	90% Bootstrap C.I.
Y-Intercept( $\beta_{0,y}$ )	-0.417	1.962	(-2.343 , 4.183)
Wind Erodibility Index ( $\beta_{1,y}$ )	-0.005	0.006	(-0.017 , 0.002)
% Sand ( $\beta_{2,y}$ )	0.024	0.018	( 0.003 , 0.063)
Water Supply ( $\beta_{3,y}$ )	0.019	0.045	(-0.061 , 0.083)
Z-Intercept( $\beta_{0,z}$ )	204.543	15.970	(-43.172 , 66.560)

## Covariates:

- Soil variables not significantly related with either response, even with reduced confidence level
- Standard errors quite large for all variables except % Sand composition as covariate for Greater Prairie Chicken presence

# Greater Prairie Chickens - Estimation Results

Parameter	Estimate	Std. Err.	90% Bootstrap C.I.
$\eta_y$ (Presence-Absence)	3.613	0.697	(2.356 , 4.614)
$\eta_z$ (NDVI)	0.991	0.017	(0.955 , 1.012)
$\rho$ (Cross-dependence)	0.446	0.260	(0.000 , 0.844)
$\sigma^2$	16.765	0.949	(15.246 , 18.245)

## Dependence Parameters:

- Moderate/Strong spatial correlation (near 4) for Greater Prairie Chicken presence
- NDVI spatial correlation is near the boundary of the parameter space (very strong dependence)
- Some cross-dependence among response variables
  - Weak evidence supporting a positive dependence between vegetative cover and probability of observing a Greater Prairie Chicken nest
- In-sample predictive capability was poor for Prairie Chicken presence-absence (Skill < 0)

# Conclusions and Future Work

The proposed bivariate Gaussian-Binary Markov random field model:

- Provides interpretable dependence parameters in terms of conditional means by modeling dependence directly
- Allows for flexible specification of covariates related to each response
- Has easy-to-implement estimation and inference procedures from conditional specification
- Outperforms previous univariate auto-models in simulations and application
- Introduces mixed-response multivariate auto-models that can be extended to more complex applications



# Conclusions and Future Work

## Areas for future work:

- Formally quantifying/defining/interpreting/remedying strong dependence settings
- Expanded/irregular neighborhood structures
- Extension to other distributions and higher-dimensional responses
- Faster/more exact inference methods

# QUESTIONS?

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