Lecture 22

Spatio-temporal Models

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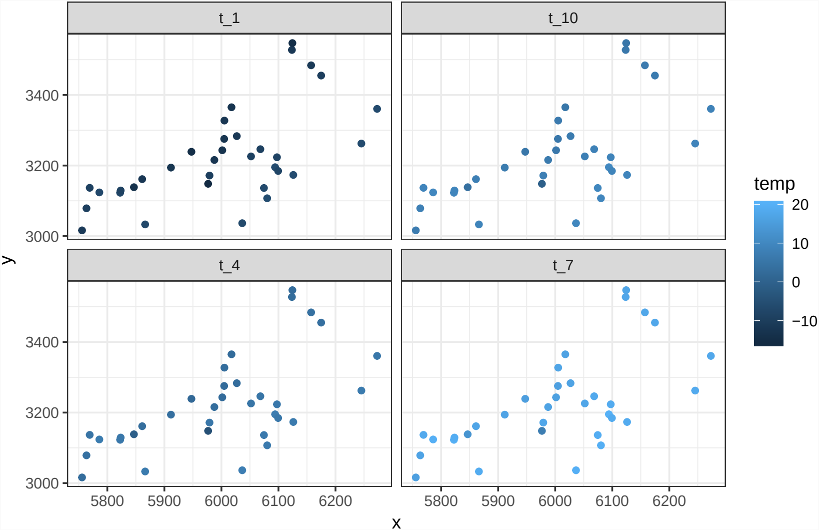
Spatial Models with AR time dependence

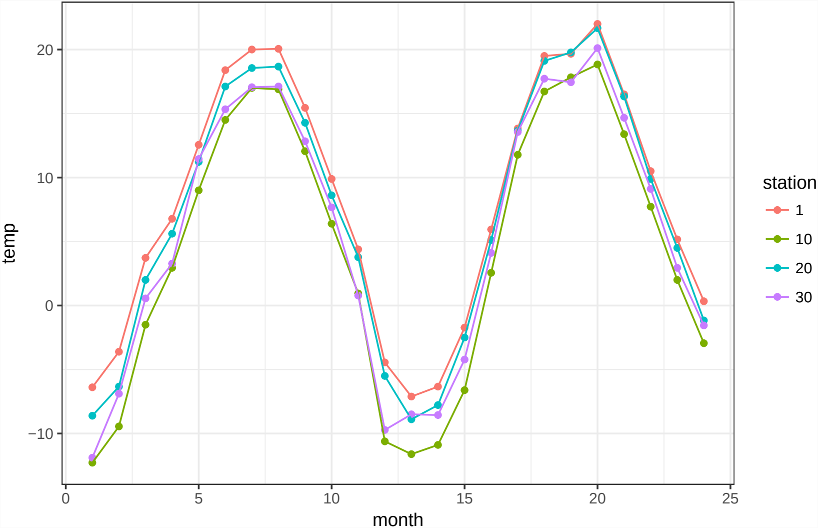
Example - Weather station data

Based on Andrew Finley and Sudipto Banerjee's notes from National Ecological Observatory Network (NEON) Applied Bayesian Regression Workshop, March 7 - 8, 2013 Module 6

`NETemp.dat` - Monthly temperature data (Celsius) recorded across the Northeastern US starting in January 2000.

```
## # A tibble: 34 x 27
##        x     y  elev    t_1   t_2    t_3   t_4   t_5   t_6   t_7   t_8
##    <dbl> <dbl> <int>  <dbl> <dbl>  <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
##  1 6094. 3195.   102  -6.39 -3.61  3.72   6.78 12.6   18.4  20.0  20.1
##  2 6245. 3262.     1  -6.28 -4.11  2.61   6.56 11.4   16.8  18.4  18.7
##  3 6157. 3484.   157 -11.1  -9.44 -0.389  3.94  9.89  15.4  17.5  17.4
##  4 6124. 3528.   176 -11.6  -9.72 -1.17   2.89  9.67  14.8  17.4  16.9
##  5 6005. 3275.   400 -12.6  -9.06 -1.61   2.56  8.56  14.3  15.9  15.8
##  6 6052. 3226.   133  -9.11 -6.39  1.22   4.94 10.9   15.9  17.3  17.6
##  7 6099. 3185.    56  -7.94 -6.06  2.06   5.56 11.1   17.0  18.6  18.8
##  8 6075. 3136.    59  -6.56 -3.50  3.17   6.17 11.5   17.4  19.1  19.4
##  9 6175. 3455.   160  -9.94 -8.94 -0.278  3.56  9.61  15.3  17.7  17.3
## 10 6005. 3327.   360 -12.3  -9.44 -1.50   2.94  9.00  14.5  17.0  16.9
## # ... with 24 more rows, and 16 more variables: t_9 <dbl>, t_10 <dbl>,
## #   t_11 <dbl>, t_12 <dbl>, t_13 <dbl>, t_14 <dbl>, t_15 <dbl>,
## #   t_16 <dbl>, t_17 <dbl>, t_18 <dbl>, t_19 <dbl>, t_20 <dbl>,
## #   t_21 <dbl>, t_22 <dbl>, t_23 <dbl>, t_24 <dbl>
```


t_1
t_10
t_4
t_7
3400
3200
3000
5800
5900
6000
6100
6200
x
y
temp
20
10
0
−10



20
10
0
−10
temp
0
5
10
15
20
25
month
station
1
10
20
30

$$\underset{}{y_t} = \underset{1\times p}{\mathbf{F}_t'}\ \underset{p\times 1}{\boldsymbol{\theta}_t} + v_t \qquad \text{observation equation}$$

$$\underset{p\times 1}{\boldsymbol{\theta}_t} = \underset{p\times p}{\mathbf{G}_t}\ \underset{p\times 1}{\boldsymbol{\theta}_{t-1}} + \underset{p\times 1}{\boldsymbol{\omega}_t} \qquad \text{evolution equation}$$

$$\mathbf{v}_t \sim \mathcal{N}(0, \mathbf{V}_t)$$
$$\boldsymbol{\omega}_t \sim \mathcal{N}(0, \mathbf{W}_t)$$

ARMA / ARIMA are a special case of a dynamic linear model, for example an $AR(p)$ can be written as

$$F_t' = (1, 0, \ldots, 0)$$

$$G_t = \begin{pmatrix} \phi_1 & \phi_2 & \cdots & \phi_{p-1} & \phi_p \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & 0 \\ 0 & 0 & \cdots & 1 & 0 \end{pmatrix}$$

$$\omega_t = (\omega_1, 0, \ldots, 0), \qquad \omega_1 \sim \mathcal{N}(0,\, \sigma^2)$$

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$$G_t = \begin{pmatrix} \phi_1 & \phi_2 & \cdots & \phi_{p-1} & \phi_p \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & 0 \\ 0 & 0 & \cdots & 1 & 0 \end{pmatrix}$$

$$\omega_t = (\omega_1, 0, \dots, 0), \qquad \omega_1 \sim \mathcal{N}(0, \sigma^2)$$

$$\begin{aligned} y_t &= \theta_t + v_t, & v_t &\sim \mathcal{N}(0, \sigma_v^2) \\ \theta_t &= \sum_{i=1}^{p} \phi_i \, \theta_{t-i} + \omega_1, & \omega_1 &\sim \mathcal{N}(0, \sigma_\omega^2) \end{aligned}$$

The observed temperature at time t and location s is given by $y_t(s)$ where,

$$y_t(\mathbf{s}) = \mathbf{x}_t(\mathbf{s})\boldsymbol{\beta}_t + u_t(\mathbf{s}) + \epsilon_t(\mathbf{s})$$
$$\epsilon_t(\mathbf{s}) \overset{ind.}{\sim} \mathcal{N}(0, \tau_t^2)$$

$$\boldsymbol{\beta}_t = \boldsymbol{\beta}_{t-1} + \boldsymbol{\eta}_t$$
$$\boldsymbol{\eta}_t \overset{i.i.d.}{\sim} \mathcal{N}(0, \boldsymbol{\Sigma}_\eta)$$

$$u_t(\mathbf{s}) = u_{t-1}(\mathbf{s}) + w_t(\mathbf{s})$$
$$w_t(\mathbf{s}) \overset{ind.}{\sim} \mathcal{N}\left(\mathbf{0}, \Sigma_t(\phi_t, \sigma_t^2)\right)$$

Dynamic spatio-temporal model

The observed temperature at time t and location s is given by $y_t(s)$ where,

$$y_t(\mathbf{s}) = \mathbf{x}_t(\mathbf{s})\boldsymbol{\beta}_t + u_t(\mathbf{s}) + \epsilon_t(\mathbf{s})$$
$$\epsilon_t(\mathbf{s}) \overset{ind.}{\sim} \mathcal{N}(0, \tau_t^2)$$

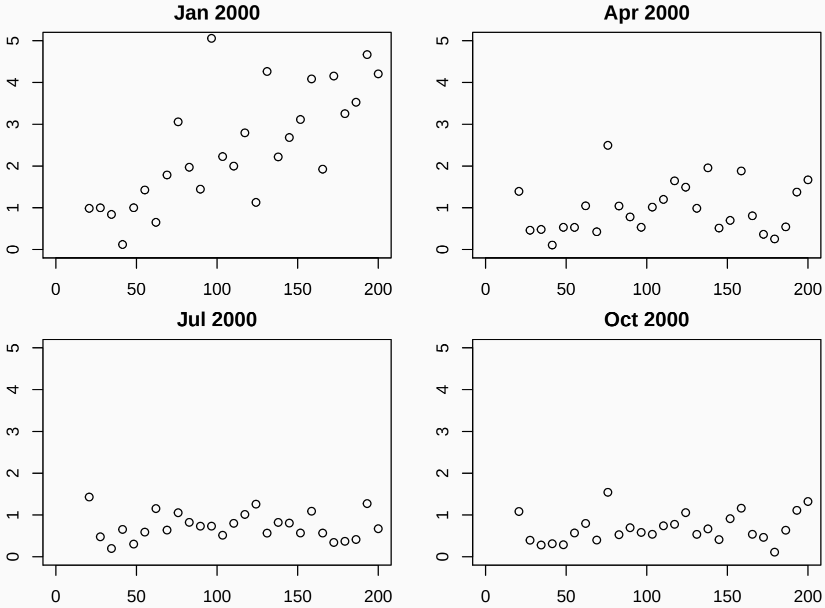
$$\boldsymbol{\beta}_t = \boldsymbol{\beta}_{t-1} + \boldsymbol{\eta}_t$$
$$\boldsymbol{\eta}_t \overset{i.i.d.}{\sim} \mathcal{N}(0, \boldsymbol{\Sigma}_\eta)$$

$$u_t(\mathbf{s}) = u_{t-1}(\mathbf{s}) + w_t(\mathbf{s})$$
$$w_t(\mathbf{s}) \overset{ind.}{\sim} \mathcal{N}\left(\mathbf{0}, \Sigma_t(\phi_t, \sigma_t^2)\right)$$

Additional assumptions for $t = 0$,

$$\boldsymbol{\beta}_0 \sim \mathcal{N}(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$$
$$u_0(\mathbf{s}) = 0$$

Variograms by time



Data and Model Parameters

Data:

```
max_d = coords %>% dist() %>% max()
n_t = 24
n_s = nrow(ne_temp)
```

Parameters:

```
n_beta = 2
starting = list(
  beta = rep(0, n_t * n_beta), phi = rep(3/(max_d/4), n_t),
  sigma.sq = rep(1, n_t), tau.sq = rep(1, n_t),
  sigma.eta = diag(0.01, n_beta)
)
tuning = list(phi = rep(1, n_t))
priors = list(
  beta.0.Norm = list(rep(0, n_beta), diag(1000, n_beta)),
  phi.Unif = list(rep(3/(0.9 * max_d), n_t), rep(3/(0.05 * max_d), n_t)),
  sigma.sq.IG = list(rep(2, n_t), rep(2, n_t)),
  tau.sq.IG = list(rep(2, n_t), rep(2, n_t)),
  sigma.eta.IW = list(2, diag(0.001, n_beta))
)
```

Fitting with spDynLM from spBayes

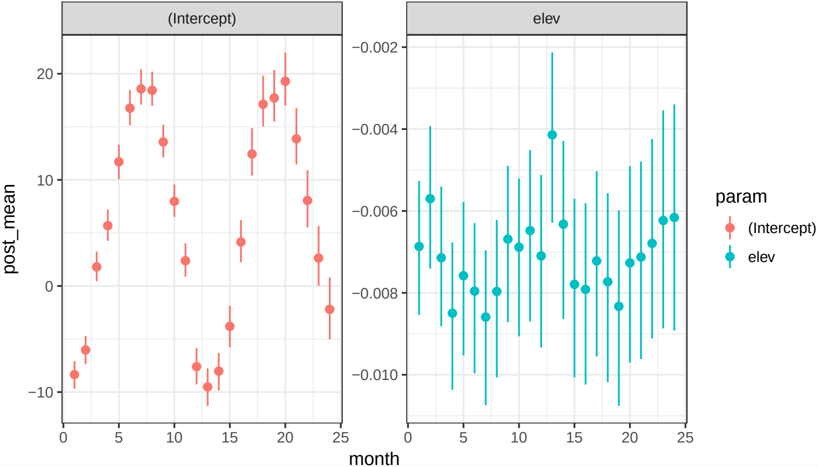
```
n_samples = 10000
models = lapply(paste0("t_",1:24, "~elev"), as.formula)

m = spBayes::spDynLM(
  models, data = ne_temp, coords = coords, get.fitted = TRUE,
  starting = starting, tuning = tuning, priors = priors,
  cov.model = "exponential", n.samples = n_samples, n.report = 1000)

m = clean_spdynlm(m, n_samples/2+1, n_samples, (n_samples/2)/1000)
save(m, file="dynlm.Rdata")

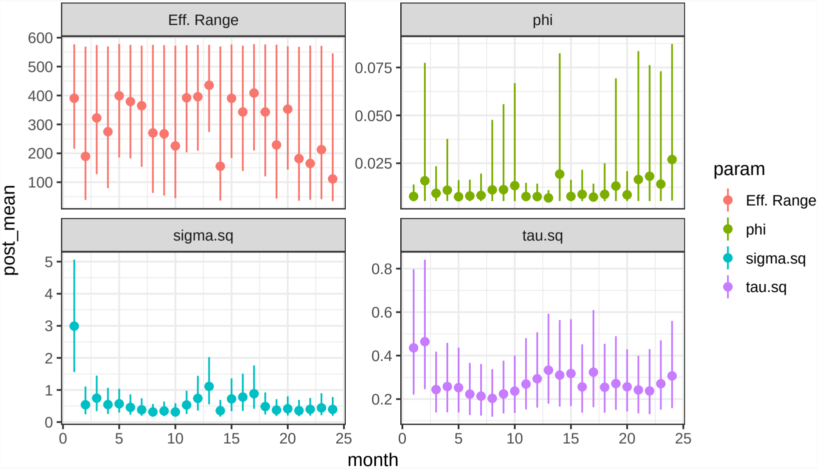
## ----------------------------------------
##     General model description
## ----------------------------------------
## Model fit with 34 observations in 24 time steps.
##
## Number of missing observations 0.
##
## Number of covariates 2 (including intercept if specified).
##
## Using the exponential spatial correlation model.
##
## Number of MCMC samples 10000.
##
## ...
```

Posterior Inference - βs

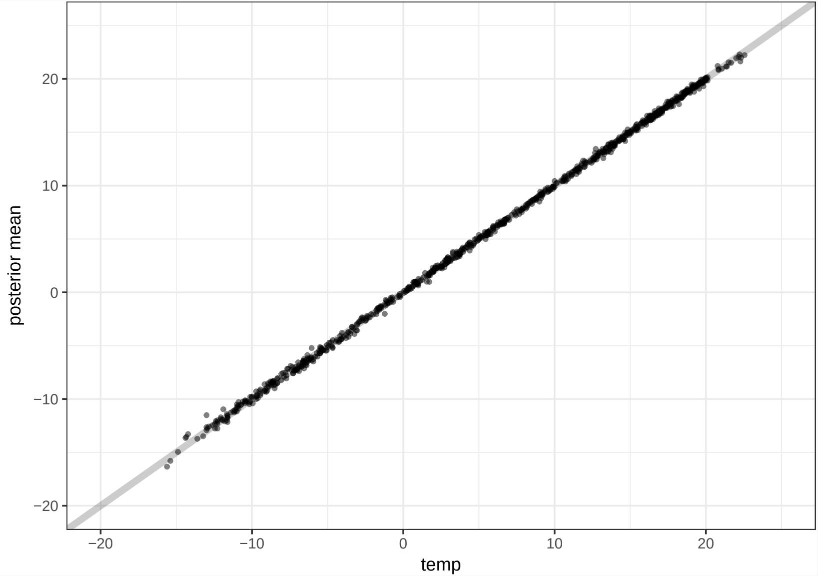


Lapse Rate $\approx -9.8\,^{\circ}C/km.$

Posterior Inference - θ



Posterior Inference - Observed vs. Predicted



Prediction

`spPredict` does not support `spDynLM` objects but it will impute missing values.

```
r = raster(xmn=5750, xmx=6300, ymn=3000, ymx=3550, nrow=20, ncol=20)

pred = xyFromCell(r, 1:length(r)) %>%
  as.data.frame() %>%
  mutate(type="pred") %>%
  bind_rows(
    ne_temp %>% mutate(type = "obs"),
    .
  )
```

Prediction

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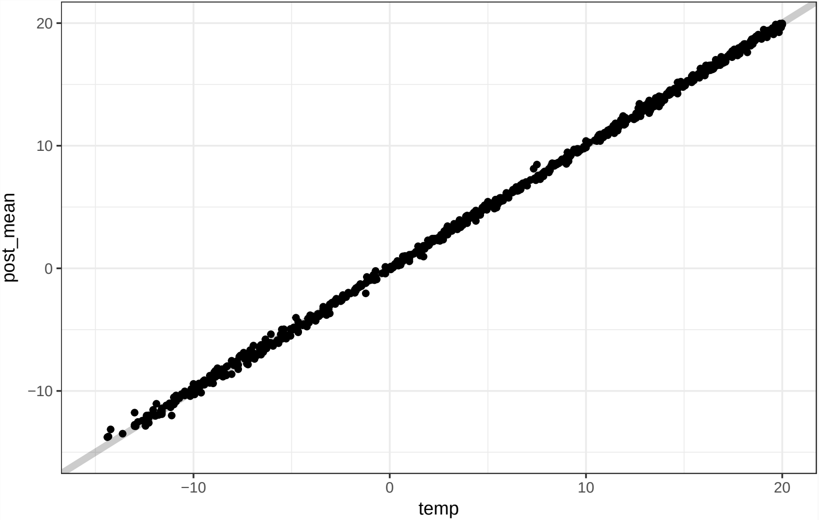
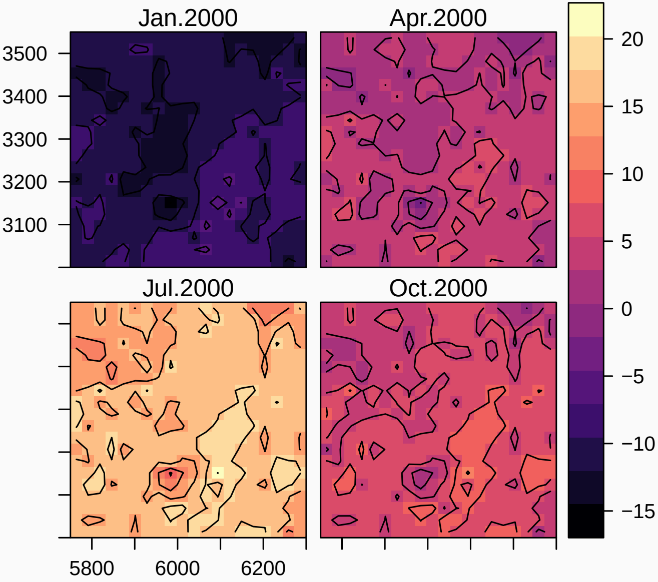
pred = xyFromCell(r, 1:length(r)) %>%
  as.data.frame() %>%
  mutate(type="pred") %>%
  bind_rows(
    ne_temp %>% mutate(type = "obs"),
    .
  )


models_pred = lapply(paste0("t_",1:n_t, "~1"), as.formula)

n_samples = 5000
m_pred = spBayes::spDynLM(
  models_pred, data = pred, coords = coords_pred, get.fitted = TRUE,
  starting = starting, tuning = tuning, priors = priors,
  cov.model = "exponential", n.samples = n_samples, n.report = 1000)

m_pred = clean_spdynlm(m_pred, n_samples/2+1, n_samples, thin = 5)
```

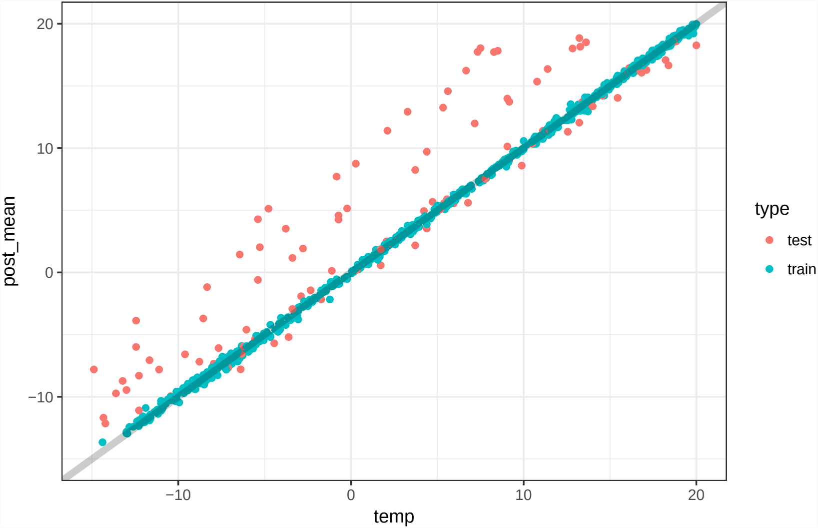

post_mean
20
10
0
−10
−10
0
10
20
temp



Jan.2000
Apr.2000
Jul.2000
Oct.2000
3500
3400
3300
3200
3100
5800
6000
6200
20
15
10
5
0
−5
−10
−15

Out-of-sample validation

```
## # A tibble: 34 x 29
##         x     y  elev type  station    t_1  t_10   t_11   t_12   t_13
##     <dbl> <dbl> <int> <chr>   <int>  <dbl> <dbl>  <dbl>  <dbl>  <dbl>
##  1 6094. 3195.   102 test        1   NA    NA    NA       NA     NA
##  2 6245. 3262.     1 train       2   -6.28  8.89  3.89   -4.22  -7.11
##  3 6157. 3484.   157 train       3 -11.1   6.44  1.94   -8.72 -11.6
##  4 6124. 3528.   176 train       4 -11.6   5.94  1.67   -9.17 -11.8
##  5 6005. 3275.   400 train       5 -12.6   5.67  0.278 -10.7  -11.9
##  6 6052. 3226.   133 train       6   -9.11  7.56  2.44   -7.11  -9.44
##  7 6099. 3185.    56 test        7   NA    NA    NA       NA     NA
##  8 6075. 3136.    59 train       8   -6.56  9.61  4.17   -4.89  -6.06
##  9 6175. 3455.   160 train       9   -9.94  6.67  1.72   -8.44 -12.1
## 10 6005. 3327.   360 train      10 -12.3   6.39  0.944 -10.6  -11.6
## # ... with 24 more rows, and 19 more variables: t_14 <dbl>, t_15 <dbl>,
## #   t_16 <dbl>, t_17 <dbl>, t_18 <dbl>, t_19 <dbl>, t_2 <dbl>, t_20 <dbl>,
## #   t_21 <dbl>, t_22 <dbl>, t_23 <dbl>, t_24 <dbl>, t_3 <dbl>, t_4 <dbl>,
## #   t_5 <dbl>, t_6 <dbl>, t_7 <dbl>, t_8 <dbl>, t_9 <dbl>
```



post_mean
temp
type
test
train
20
10
0
−10
−10
0
10
20

Spatio-temporal models for continuous time

In general, spatiotemporal models will have a form like the following,

$$\begin{aligned} y(\mathbf{s},t) &= \underset{\text{mean structure}}{\mu(\mathbf{s},t)} + \underset{\text{error structure}}{e(\mathbf{s},t)} \\ &= \underset{\text{Regression}}{\mathbf{x}(\mathbf{s},t)\,\boldsymbol{\beta}(\mathbf{s},t)} + \underset{\text{Spatiotemporal RE}}{w(\mathbf{s},t)} + \underset{\text{Error}}{\epsilon(\mathbf{s},t)} \end{aligned}$$

Additive Models

In general, spatiotemporal models will have a form like the following,

$$\begin{aligned} y(\mathbf{s},t) &= \underset{\text{mean structure}}{\mu(\mathbf{s},t)} + \underset{\text{error structure}}{e(\mathbf{s},t)} \\ &= \underset{\text{Regression}}{\mathbf{x}(\mathbf{s},t)\,\boldsymbol{\beta}(\mathbf{s},t)} + \underset{\text{Spatiotemporal RE}}{w(\mathbf{s},t)} + \underset{\text{Error}}{\epsilon(\mathbf{s},t)} \end{aligned}$$

The simplest possible spatiotemporal model is one were assume there is no dependence between observations in space and time,

$$w(\mathbf{s},t) = \alpha(t) + \omega(\mathbf{s})$$

these are straight forward to fit and interpret but are quite limiting (no shared information between space and time).

Spatiotemporal Covariance

Lets assume that we want to define our spatiotemporal random effect to be a single stationary Gaussian Process (in 3 dimensions*),

$$\mathbf{w}(\mathbf{s},\mathbf{t}) \sim \mathcal{N}\big(\mathbf{0}, \boldsymbol{\Sigma}(\mathbf{s},\mathbf{t})\big)$$

where our covariance function depends on both $\|s - s'\|$ and $|t - t'|$,

$$\text{cov}(\mathbf{w}(\mathbf{s},\mathbf{t}), \mathbf{w}(\mathbf{s}',\mathbf{t}')) = c(\|s - s'\|, |t - t'|)$$

- Note that the resulting covariance matrix Σ will be of size $n_s \cdot n_t \times n_s \cdot n_t$.
  - Even for modest problems this gets very large (past the point of direct computability).
  - If $n_t = 52$ and $n_s = 100$ we have to work with a 5200×5200 covariance matrix

Separable Models

One solution is to use a seperable form, where the covariance is the product of a valid 2d spatial and a valid 1d temporal covariance / correlation function,

$$\text{cov}(\mathbf{w}(\mathbf{s},\mathbf{t}),\mathbf{w}(\mathbf{s}',\mathbf{t}')) = \sigma^2\,\rho_1(\|\mathbf{s}-\mathbf{s}'\|;\boldsymbol{\theta})\,\rho_2(|\mathbf{t}-\mathbf{t}'|;\boldsymbol{\phi})$$

One solution is to use a seperable form, where the covariance is the product of a valid 2d spatial and a valid 1d temporal covariance / correlation function,

$$\text{cov}(\mathbf{w}(\mathbf{s},\mathbf{t}),\mathbf{w}(\mathbf{s}',\mathbf{t}')) = \sigma^2\,\rho_1(\|\mathbf{s}-\mathbf{s}'\|;\boldsymbol{\theta})\,\rho_2(|\mathbf{t}-\mathbf{t}'|;\boldsymbol{\phi})$$

If we define our observations as follows (stacking time locations within spatial locations)

$$\mathbf{w}(\mathbf{s},\mathbf{t}) = \big(w(\mathbf{s}_1,t_1),\,\cdots,\,w(\mathbf{s}_1,t_{n_t}),\,\cdots,\,w(\mathbf{s}_{n_s},t_1),\,\cdots,\,w(\mathbf{s}_{n_s},t_{n_t})\big)^t$$

then the covariance can be written as

$$\underset{n_s n_t \times n_s n_t}{\boldsymbol{\Sigma}_w(\sigma^2,\theta,\phi)} = \sigma^2\,\underset{n_s\times n_s}{\mathbf{H}_s(\theta)} \otimes \underset{n_t\times n_t}{\mathbf{H}_t(\phi)}$$

where $\mathbf{H}_s(\theta)$ and $\mathbf{H}_t(\theta)$ are correlation matrices defined by

$$\{\mathbf{H}_s(\theta)\}_{ij} = \rho_1(\|\mathbf{s}_i-\mathbf{s}_j\|;\theta)$$

Kronecker Product

Definition:

$$\underset{[m\times n]}{\mathbf{A}} \otimes \underset{[p\times q]}{\mathbf{B}} = \underset{[m\cdot p\times n\cdot q]}{\begin{pmatrix} a_{11}\mathbf{B} & \cdots & a_{1n}\mathbf{B} \\ \vdots & \ddots & \vdots \\ a_{m1}\mathbf{B} & \cdots & a_{mn}\mathbf{B} \end{pmatrix}}$$

Kronecker Product

Definition:

$$\underset{[m\times n]}{\mathbf{A}} \otimes \underset{[p\times q]}{\mathbf{B}} = \underset{[m\cdot p\times n\cdot q]}{\begin{pmatrix} a_{11}\mathbf{B} & \cdots & a_{1n}\mathbf{B} \\ \vdots & \ddots & \vdots \\ a_{m1}\mathbf{B} & \cdots & a_{mn}\mathbf{B} \end{pmatrix}}$$

Properties:

$$\mathbf{A} \otimes \mathbf{B} \neq \mathbf{B} \otimes \mathbf{A} \qquad \text{(usually)}$$
$$(\mathbf{A} \otimes \mathbf{B})^t = \mathbf{A}^t \otimes \mathbf{B}^t$$

$$\begin{aligned} \det(\mathbf{A} \otimes \mathbf{B}) &= \det(\mathbf{B} \otimes \mathbf{A}) \\ &= \det(\mathbf{A})^{\text{rank}(\mathbf{B})} \det(\mathbf{B})^{\text{rank}(\mathbf{A})} \end{aligned}$$

$$(\mathbf{A} \otimes \mathbf{B})^{-1} = \mathbf{A}^{-1}\mathbf{B}^{-1}$$

If we have a spatiotemporal random effect with a separable form,

$$\mathbf{w}(\mathbf{s},\mathbf{t}) \sim \mathcal{N}(\mathbf{0},\, \mathbf{\Sigma}_w)$$

$$\mathbf{\Sigma}_w = \sigma^2\,\mathbf{H}_s \otimes \mathbf{H}_t$$

then the likelihood for $\mathbf{w}$ is given by

$$-\frac{n}{2}\log 2\pi - \frac{1}{2}\log|\Sigma_w| - \frac{1}{2}\mathbf{w}^t{\mathbf{\Sigma_w}}^{-1}\mathbf{w}$$

$$= -\frac{n}{2}\log 2\pi - \frac{1}{2}\log\left[(\sigma^2)^{n_t \cdot n_s}|H_s|^{n_t}|H_t|^{n_s}\right] - \frac{1}{2\sigma^2}\mathbf{w}^t(\mathbf{H}_s^{-1}\otimes\mathbf{H}_t^{-1})\mathbf{w}$$

Non-seperable Models

- Additive and separable models are still somewhat limiting
- Cannot treat spatiotemporal covariances as 3d observations
- Possible alternatives:
  - Specialized spatiotemporal covariance functions, i.e.

$$\gamma(\mathbf{s}, \mathbf{s}', t, t') = \sigma^2(|t - t'| + 1)^{-1} \exp\left(-\|\mathbf{s} - \mathbf{s}'\|(|t - t'| + 1)^{-\beta/2}\right)$$

  - Mixtures of separable covariances, i.e.

$$w(\mathbf{s}, t) = w_1(\mathbf{s}, t) + w_2(\mathbf{s}, t)$$