Chap.4: Descriptive Spatio-Temporal Statistical Models（担当：秋田）

4.1 Additive Measurement Error and Process Models
4.2 Prediction for Gaussian Data and Processes
    4.2.1 Spatio-Temporal Covariance Functions
    4.2.2 Spatio-Temporal Semivariograms
    4.2.3 Gaussian Spatio-Temporal Model Estimation
4.3 Random-Effects Parameterizations
Lab 4.1: Spatio-Temporal Kriging with **gstat**

観測モデルと過程モデル

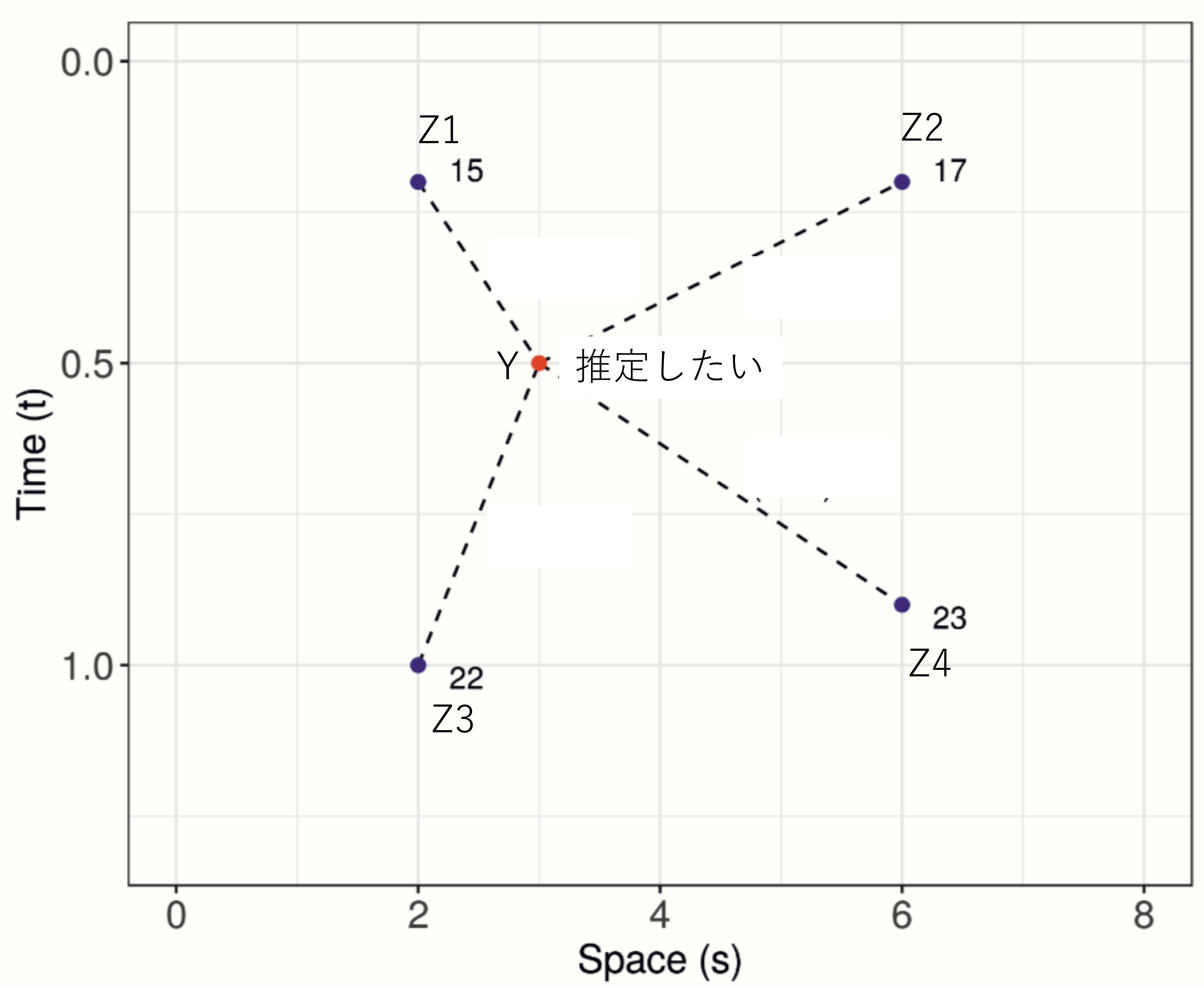
data (observation) model

$$\mathbf{Z} = \mathbf{Y} + \boldsymbol{\varepsilon},$$

process model

$$\mathbf{Y} = \boldsymbol{\mu} + \boldsymbol{\eta},$$

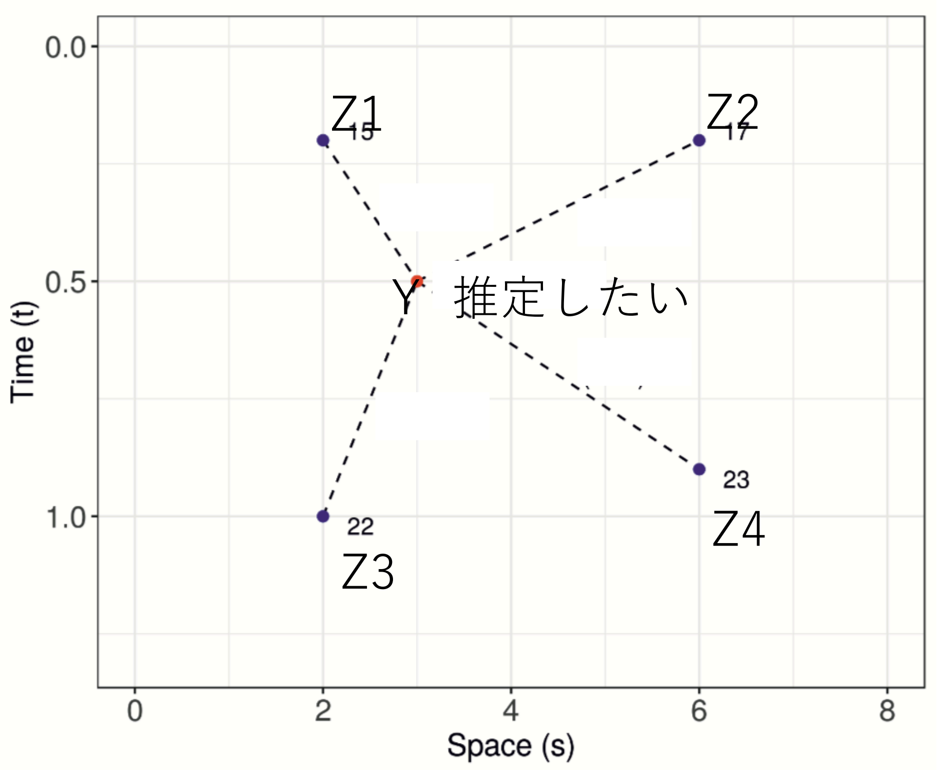
考えたい問題の例



$$\mathbf{Z} = \mathbf{Y} + \boldsymbol{\varepsilon},$$
$$\mathbf{Y} = \boldsymbol{\mu} + \boldsymbol{\eta},$$

$Y(s_0;t_0)$の予測子$\hat{Y}(s_0;t_0)$
(optimal linear predictor)
を見つける

考えたい問題の例



$$\mathbf{Z} = \mathbf{Y} + \boldsymbol{\varepsilon},$$
$$\mathbf{Y} = \boldsymbol{\mu} + \boldsymbol{\eta},$$

①：μ 既知
→**simple kriging**
②：μ は定数だが未知
→ordinary kriging
③：μ は変数で未知
→**universal kriging**

Prediction for Gaussian Data & Processes

$$\mathbf{Z} = \mathbf{Y} + \boldsymbol{\varepsilon},$$

$$\mathbf{Y} = \boldsymbol{\mu} + \boldsymbol{\eta},$$

$\boldsymbol{\mu} = \mathbf{X}\beta$

予測したい

$$\begin{bmatrix} \boxed{Y(\mathbf{s}_0; t_0)} \\ \boxed{\mathbf{Z}} \end{bmatrix} \sim Gau\left(\underbrace{\begin{bmatrix} \mathbf{x}(\mathbf{s}_0; t_0)' \\ \mathbf{X} \end{bmatrix} \boldsymbol{\beta}}_{\text{期待値}}, \underbrace{\begin{bmatrix} c_{0,0} & \mathbf{c}_0' \\ \mathbf{c}_0 & \mathbf{C}_z \end{bmatrix}}_{\text{分散共分散}} \right)$$

観測データ

スカラー

$C_z = C_\eta + C_\varepsilon$

重み　残差

$$Y(\mathbf{s}_0; t_0) \mid \mathbf{Z} \sim Gau(\mathbf{x}(\mathbf{s}_0; t_0)'\boldsymbol{\beta} + \underbrace{\mathbf{c}_0'\mathbf{C}_z^{-1}(\mathbf{Z} - \mathbf{X}\boldsymbol{\beta})}_{\text{観測データによる補正}}, \; c_{0,0} - \underbrace{\mathbf{c}_0'\mathbf{C}_z^{-1}\mathbf{c}_0}_{\text{観測データによる補正}}),$$

観測データZが与えられた時の
Yの分布（条件付き分布）

β が既知 / β を推定

$$Y(\mathbf{s}_0;t_0)\ \mid \mathbf{Z}\ \sim\ Gau\Big(\mathbf{x}(\mathbf{s}_0;t_0)'\boldsymbol{\beta}+\underbrace{\overset{\text{重み}}{\mathbf{c}_0'\mathbf{C}_z^{-1}}\overset{\text{残差}}{(\mathbf{Z}-\mathbf{X}\boldsymbol{\beta})}}_{\text{観測データによる補正}},\ c_{0,0}-\underbrace{\mathbf{c}_0'\mathbf{C}_z^{-1}\mathbf{c}_0}_{\text{観測データによる補正}}\Big),$$

観測データZが与えられた時の
Yの分布（条件付き分布）

β 既知

$$\widehat{Y}(\mathbf{s}_0;t_0)=\mathbf{x}(\mathbf{s}_0;t_0)'\boldsymbol{\beta}+\mathbf{c}_0'\mathbf{C}_z^{-1}(\mathbf{Z}-\mathbf{X}\boldsymbol{\beta})$$

$$\sigma^2_{Y,sk}(\mathbf{s}_0;t_0)=c_{0,0}-\mathbf{c}_0'\mathbf{C}_z^{-1}\mathbf{c}_0$$

β 未知

$$\widehat{\boldsymbol{\beta}}_{\mathrm{gls}}\equiv(\mathbf{X}'\mathbf{C}_z^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{C}_z^{-1}\mathbf{Z}.$$

$$\widehat{Y}(\mathbf{s}_0;t_0)=\mathbf{x}(\mathbf{s}_0;t_0)'\widehat{\boldsymbol{\beta}}_{\mathrm{gls}}+\mathbf{c}_0'\mathbf{C}_z^{-1}(\mathbf{Z}-\mathbf{X}\widehat{\boldsymbol{\beta}}_{\mathrm{gls}})$$

$$\sigma^2_{Y,\mathrm{uk}}(\mathbf{s}_0;t_0)=c_{0,0}-\mathbf{c}_0'\mathbf{C}_z^{-1}\mathbf{c}_0+\kappa,$$

$$\kappa\equiv(\mathbf{x}(\mathbf{s}_0;t_0)-\mathbf{X}'\mathbf{C}_z^{-1}\mathbf{c}_0)'(\mathbf{X}'\mathbf{C}_z^{-1}\mathbf{X})^{-1}(\mathbf{x}(\mathbf{s}_0;t_0)-\mathbf{X}'\mathbf{C}_z^{-1}\mathbf{c}_0)$$

β が既知

$$Y(\mathbf{s}_0;t_0)\ |\,\mathbf{Z}\ \sim\ Gau(\mathbf{x}(\mathbf{s}_0;t_0)'\boldsymbol{\beta}+\underbrace{\overset{\text{重み}}{\mathbf{c}_0'\mathbf{C}_z^{-1}}\overset{\text{残差}}{(\mathbf{Z}-\mathbf{X}\boldsymbol{\beta})}}_{\text{観測データによる補正}},\ c_{0,0}-\underbrace{\mathbf{c}_0'\mathbf{C}_z^{-1}\mathbf{c}_0}_{\text{観測データによる補正}}),$$

観測データZが与えられた時の
Yの分布（条件付き分布）

$$c(\mathbf{h};\tau)=\sigma^2\exp\{-b^2||\mathbf{h}||^2/(a^2\tau^2+1)\}/(a^2\tau^2+1)^{d/2}, \qquad (4.13)$$

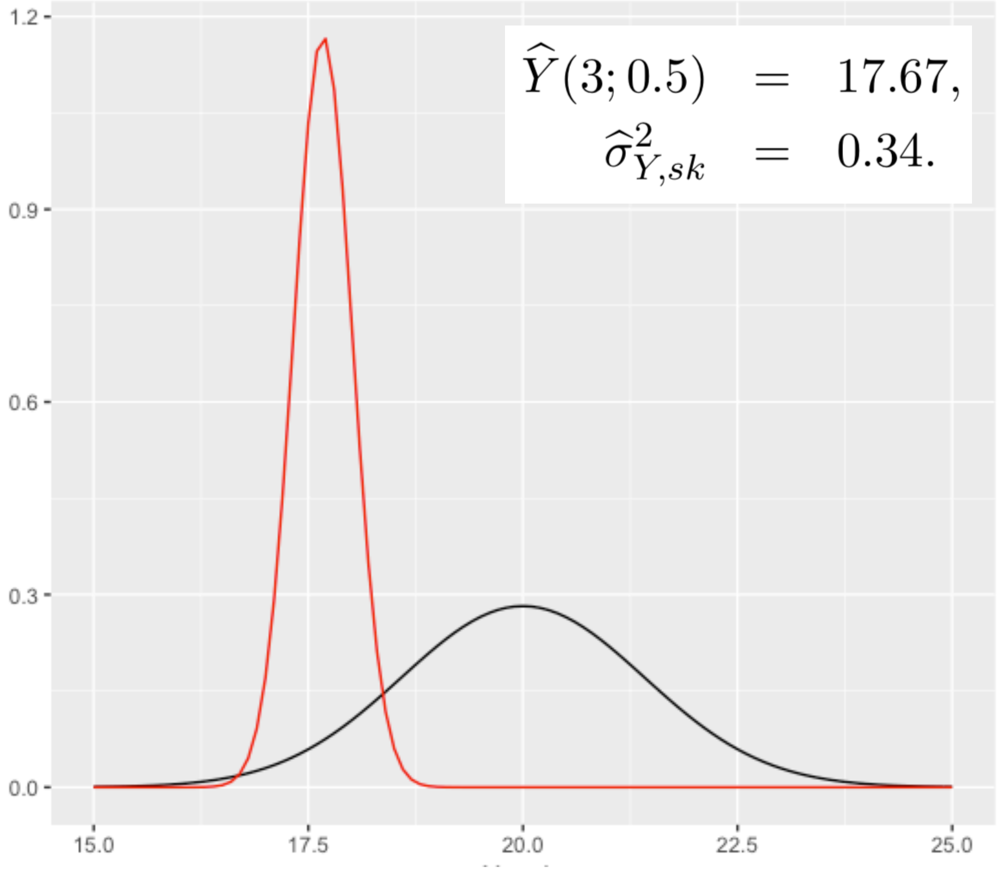
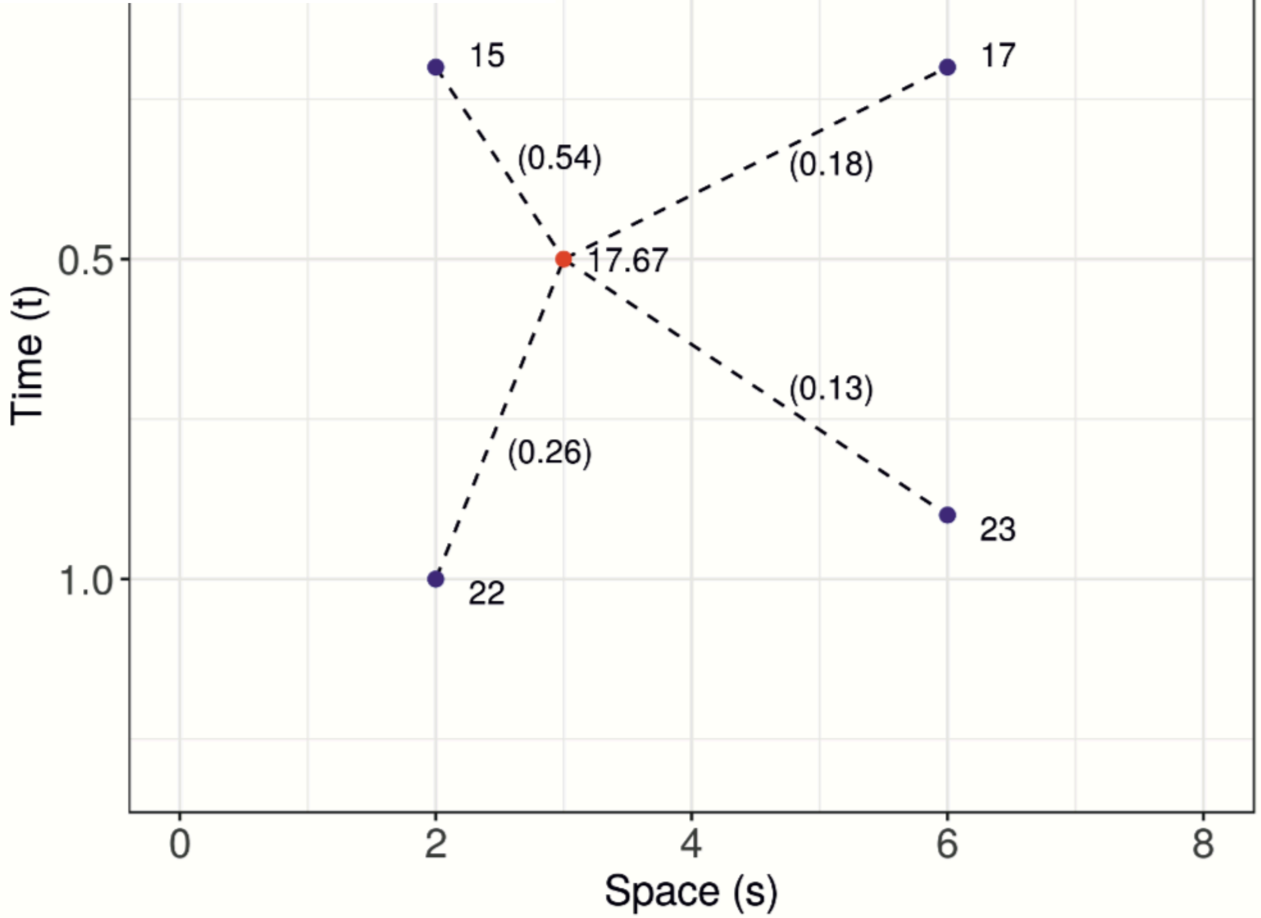


Fig. 4.1



お手製コード

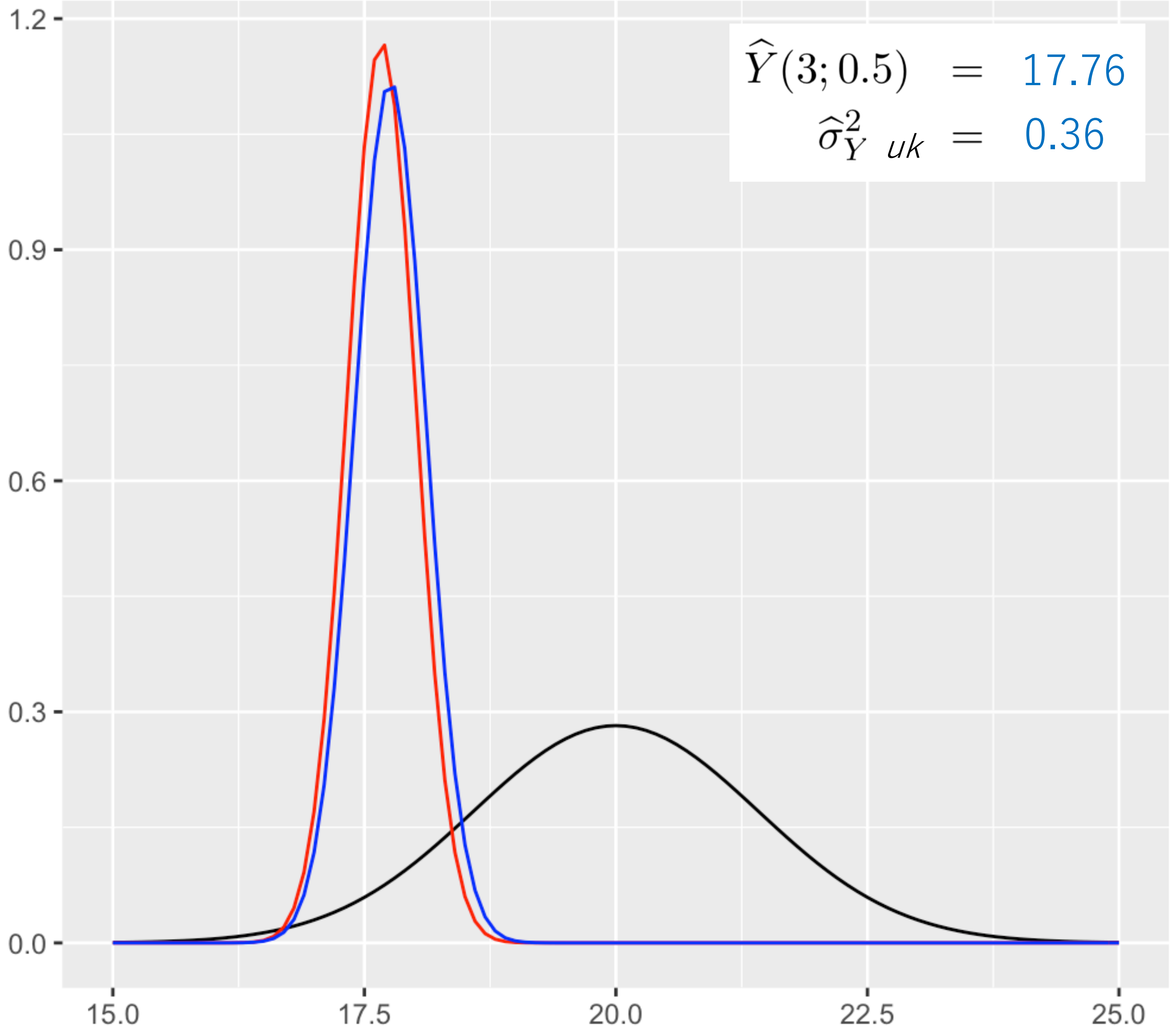
```
Z = tibble::tibble(s=c(2,2,6,6),t=c(0.2,1,0.2,0.9),n=c(15,22,17,23))
Y = tibble::tibble(s=c(3),t=c(0.5),n=c(NA))
cov_func = function(a=2,b=0.2,v=2,d=1,s,t){
  v * exp(-b^2*s^2/(a^2*t^2+1)) / (a^2*t^2+1)^(d/2)
}

Cz = as.matrix(cov_func(s=dist(Z$s,diag = T,upper = T),t=dist(Z$t,diag = T,upper = T)))
+ 2*diag(4) # cov_func does not return the diag elements...
c0 = cov_func(s=Z$s-Y$s, t=Z$t-Y$t)
w_t = t(c0) %*% solve(Cz)

beta = 20
X = c(1,1,1,1)
cond_mean = as.vector(t(Z$n) - X*beta)
Y_hat = beta + t(c0) %*% solve(Cz) %*% cond_mean
sigma_sk = 2- t(c0) %*% solve(Cz) %*% c0
cat("Y_hat =",Y_hat,"sigma_sk =",sigma_sk,"¥n")

ggplot(data=data.frame(X_axis=c(15,25)), aes(x=X_axis)) +
  stat_function(fun=dnorm, args=list(mean=beta, sd=2^0.5)) +
  stat_function(fun=dnorm, args=list(mean=Y_hat, sd=sigma_sk),col="red")
```

β を推定



$\widehat{Y}(3;0.5) = 17.76$
$\widehat{\sigma}^2_{Y\ uk} = 0.36$
1.2
0.9
0.6
0.3
0.0
15.0
17.5
20.0
22.5
25.0

お手製コード

```
# if beta is unknown...
beta_hat = solve( t(X) %*% solve(Cz) %*% X ) %*% t(X) %*% solve(Cz) %*% Z$n
cat("beta_hat =",beta_hat,"¥n")

X = c(1,1,1,1)
cond_mean = as.vector(t(Z$n) - X*c(beta_hat))
Y_hat_uk = beta_hat + t(c0) %*% solve(Cz) %*% cond_mean
kap = t(1 - t(X) %*% solve(Cz) %*% c0) %*% solve( t(X) %*% solve(Cz) %*% X ) %*% (1 - t(X)
%*% solve(Cz) %*% c0)
sigma_uk = 2- t(c0) %*% solve(Cz) %*% c0 + kap
cat("Y_hat_uk =",Y_hat_uk,"sigma_uk =",sigma_uk,"¥n")

ggplot(data=data.frame(X_axis=c(15,25)), aes(x=X_axis)) +
  stat_function(fun=dnorm, args=list(mean=beta, sd=2^0.5)) +
  stat_function(fun=dnorm, args=list(mean=Y_hat, sd=sigma_sk),col="red") +
  stat_function(fun=dnorm, args=list(mean=Y_hat_uk, sd=sigma_uk),col="blue")
```

分散共分散はどのように決めるか？

1. Spatio-Temporal Covariance function

$$c_*(\mathbf{s}, \mathbf{s}'; t, t') = c(\mathbf{s}' - \mathbf{s}; t' - t) = c(\mathbf{h}; \tau)$$

- (space-)isotoropy
- μ 一定（平均場近似？）

$$\begin{aligned}
\gamma_z(\mathbf{h}; \tau) &= \frac{1}{2}\mathrm{var}(Z(\mathbf{s} + \mathbf{h}; t + \tau) - Z(\mathbf{s}; t)) \\
&= C_z(\mathbf{0}; 0) - \mathrm{cov}(Z(\mathbf{s} + \mathbf{h}; t + \tau), Z(\mathbf{s}; t)) \\
&= C_z(\mathbf{0}; 0) - C_z(\mathbf{h}; \tau),
\end{aligned}$$

2. Spatio-Temporal Semivariogram

$$\mathrm{var}(Y(\mathbf{s}; t) - Y(\mathbf{s}'; t')) \equiv 2\gamma(\mathbf{s}, \mathbf{s}'; t, t')$$

- $\sigma^2(\mathbf{s}; t) \equiv \mathrm{var}(Y(\mathbf{s}; t))$
- μ 一定の仮定は不要？

Spatio-Temporal Covariance function

- Separable in space and time

$$c(\mathbf{h};\tau) \equiv c^{(s)}(\mathbf{h}) \cdot c^{(t)}(\tau)$$

  - Non-negative-definite
  - Pseudo-replication
  - 時間と空間の交互作用を無視
  - 逆行列の計算簡単

- Non-separable

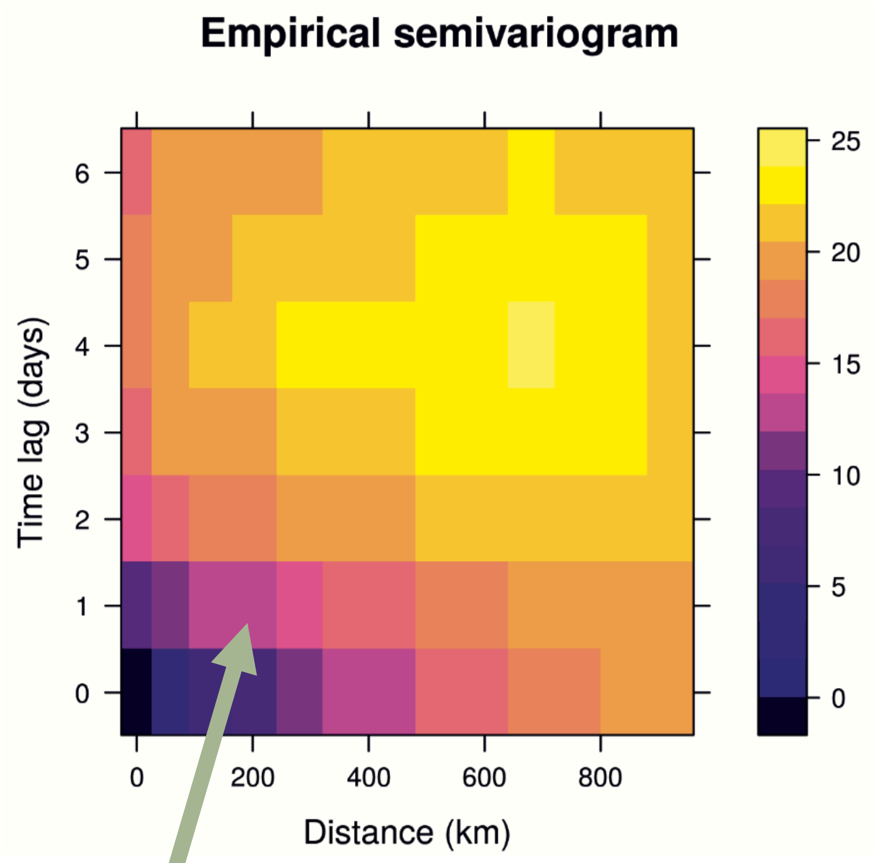
経験セミバリにoptim()でフィットさせる

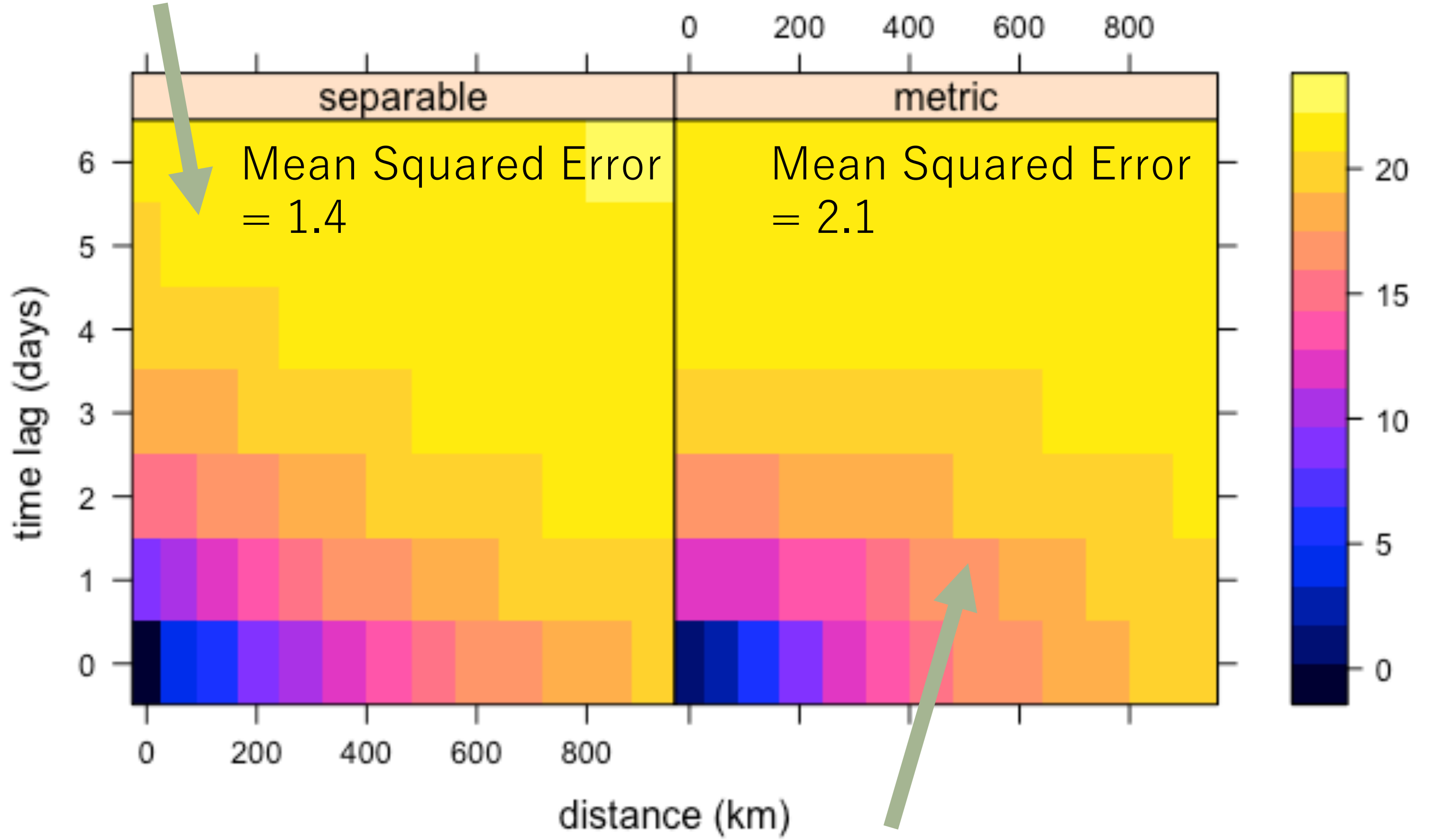
$$c^{(\mathrm{sep})}(\|\mathbf{h}\|;|\tau|) \equiv c^{(s)}(\|\mathbf{h}\|)\cdot c^{(t)}(|\tau|), \tag{4.18}$$

in which we let both covariance functions, $c^{(s)}(\cdot)$ and $c^{(t)}(\cdot)$, take the form

$$c^{(\cdot)}(h) = b_1 \exp(-\phi h) + b_2 I(h = 0), \tag{4.19}$$

Tmax 1993 7/1 - 7/31





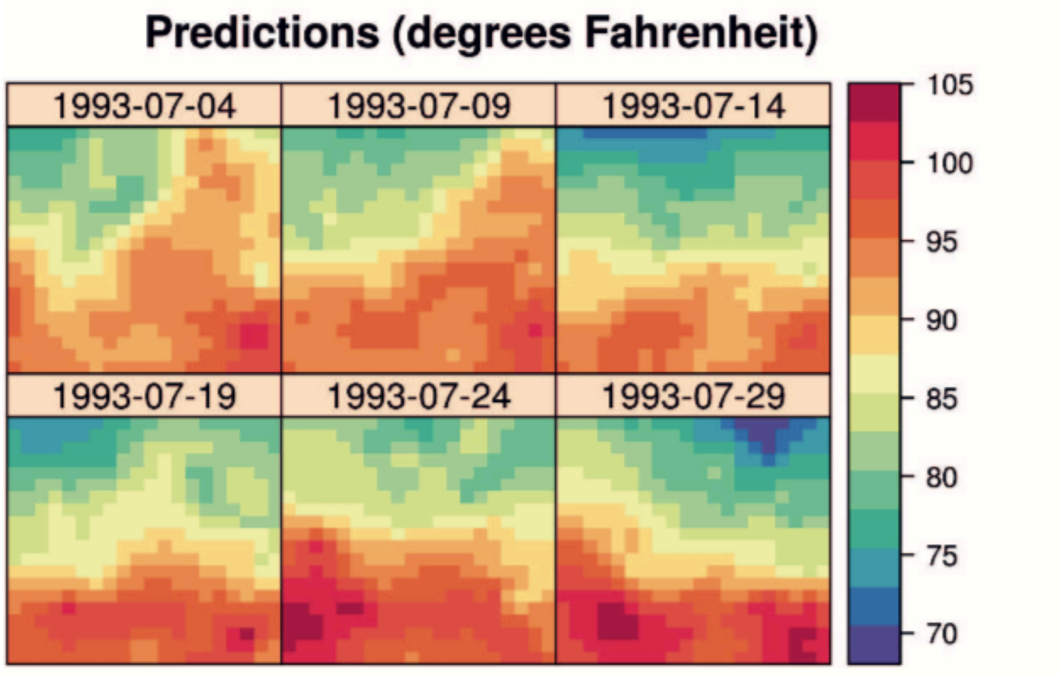
$$\widehat{\gamma}_z(\mathbf{h};\tau) = \frac{1}{|N_{\mathbf{s}}(\mathbf{h})|}\frac{1}{|N_t(\tau)|}\sum_{\mathbf{s}_i,\mathbf{s}_k \in N_{\mathbf{s}}(\mathbf{h})}\ \sum_{t_j,t_\ell \in N_t(\tau)} (Z(\mathbf{s}_i;t_j) - Z(\mathbf{s}_k;t_\ell))^2, \tag{2.8}$$

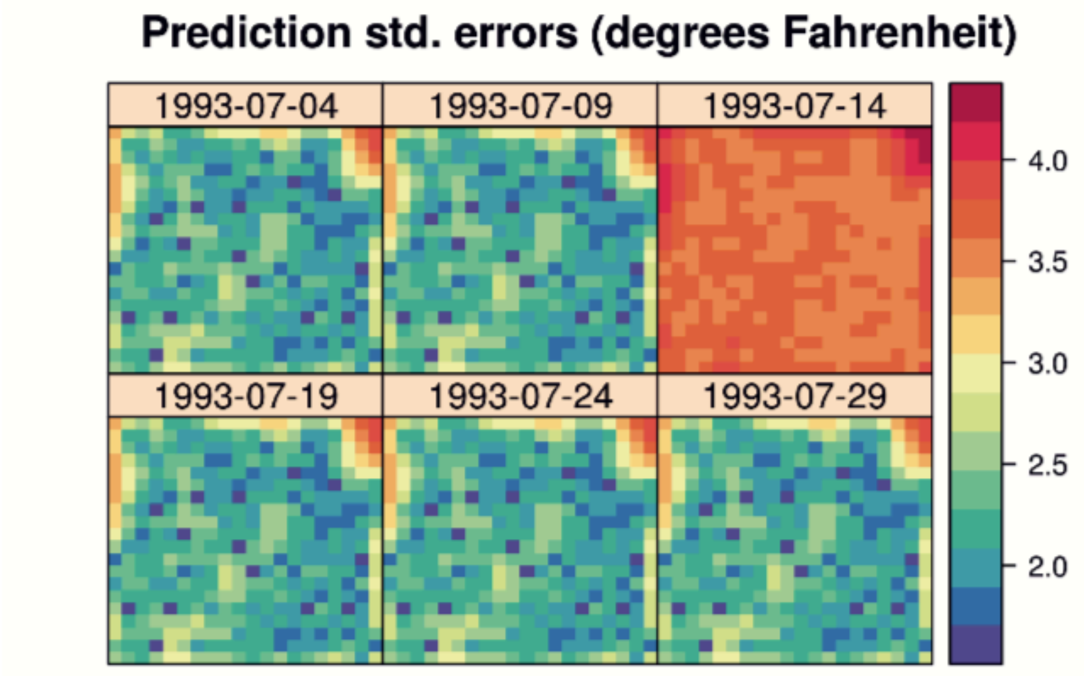
$$c^{(\mathrm{st})}(\|\mathbf{v}_a\|) \equiv b_1 \exp(-\phi\|\mathbf{v}_a\|) + b_2 I(\|\mathbf{v}_a\| = 0), \tag{4.20}$$

where $\mathbf{v}_a \equiv (\mathbf{h}', a\tau)'$, and recall that $||\mathbf{v}_a|| = (\mathbf{h}'\mathbf{h} + a^2\tau^2)^{1/2}$. Here, a is the scaling factor

フィットさせたSeparableモデルからS-Tkriging補間

Tmax 1993 7/1 - 7/31のデータから推定したモデルから補間
（7/14のTmaxは使わない）





Random-Effects Parameterizations

- 時空間共分散行列Czの特定は困難
- 階層モデリングができるように条件付けすると良い

- 秋田は、周辺化を繰り返す方面の研究の方が好み…

$$\pi|k_1,\ldots,k_N = \sum_{i=1}^{N}\frac{k_i(k_i-1)}{(\sum_{j=1}^N k_j)(\sum_{j=1}^N k_j-1)} = \frac{\sum_{i=1}^N k_i^2-\sum_{i=1}^N k_i}{(\sum_{j=1}^N k_j)^2-\sum_{j=1}^N k_j}.$$

$$\pi|\lambda_1,\ldots,\lambda_N = \mathbb{E}[\pi|k_1,\ldots,k_N] \approx \frac{\sum_{i=1}^N \mathbb{E}[k_i^2|\lambda_i]-\sum_{i=1}^N \mathbb{E}[k_i|\lambda_i]}{\mathbb{E}[(\sum_{j=1}^N k_j)^2|\lambda_1,\ldots,\lambda_N]-\sum_{j=1}^N \mathbb{E}[k_j|\lambda_j]} = \frac{\sum_{i=1}^N (1+\phi^{-1})\lambda_i^2}{\sum_{i=1}^N (1+\phi^{-1})\lambda_i^2+2\sum_{i>j}\lambda_i\lambda_j}.$$

$$\pi = \mathbb{E}[\pi|\lambda_1,\ldots,\lambda_N] \approx \frac{(1+\phi^{-1})\mathbb{E}[\lambda^2]}{(1+\phi^{-1})\mathbb{E}[\lambda^2]+(N-1)(\mathbb{E}[\lambda])^2}.$$

(Akita in revision)

$$\Pr[k_i|\lambda_i] = \frac{\Gamma[k_i+\phi]}{k_i!\Gamma[\phi]}\left(\frac{\lambda_i}{\phi+\lambda_i}\right)^{k_i}\left(\frac{\phi}{\phi+\lambda_i}\right)^{\phi}$$

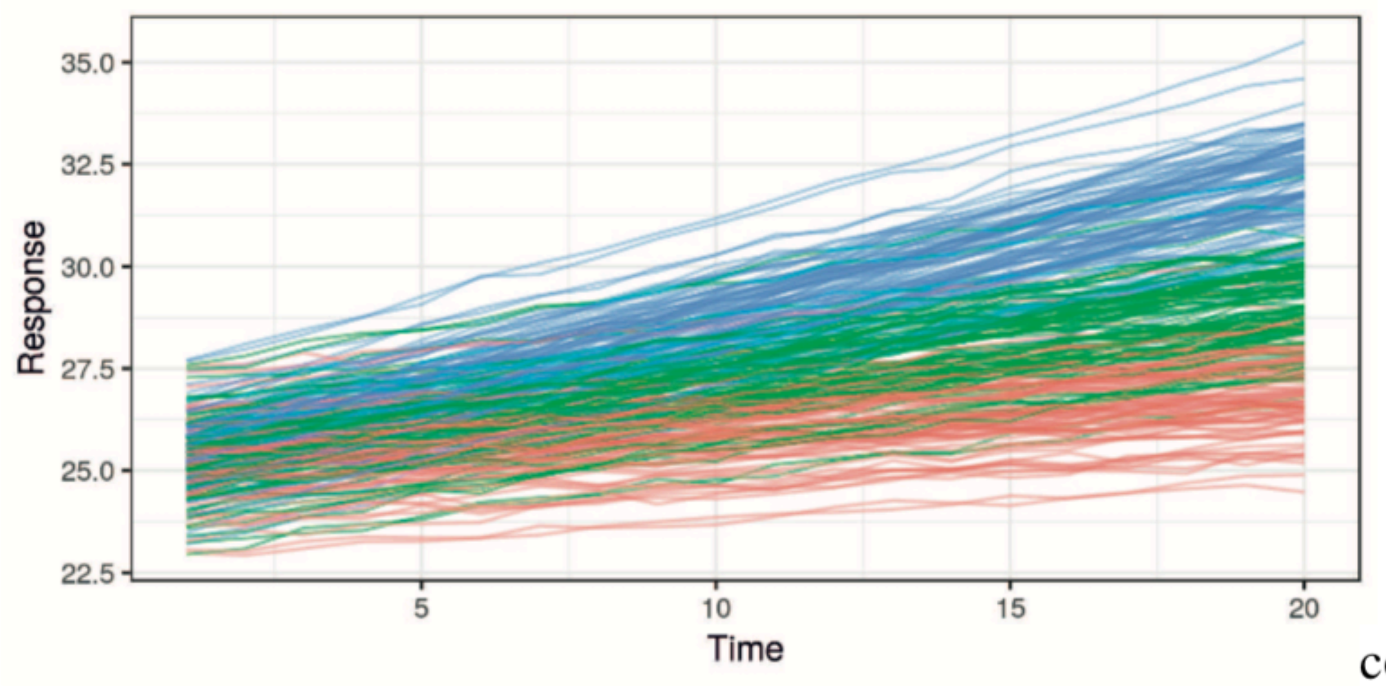
Kで周辺化してλの関数へ

λで周辺化

Random-Effects Parameterizations

$$\alpha_{0,i} \sim Gau(0, \sigma_1^2) \quad \alpha_{1,i} \sim Gau(0, \sigma_2^2)$$

$$Z_{ij} = \begin{cases} (\beta_0 + \alpha_{0i}) + (\beta_1 + \alpha_{1i})t_j + \epsilon_{ij}, & \text{if the subject receives the control,} \\ (\beta_0 + \alpha_{0i}) + (\beta_2 + \alpha_{1i})t_j + \epsilon_{ij}, & \text{if the subject receives treatment 1,} \\ (\beta_0 + \alpha_{0i}) + (\beta_3 + \alpha_{1i})t_j + \epsilon_{ij}, & \text{if the subject recieves treatment 2,} \end{cases}$$



β_0: Fixed intercept
β_i: Fixed time-trend
α_0: Indvidual-specific random intercept
α_1: Indvidual-specific random slope

興味があるのは
個体効果ではなく
treatmentの影響

$$\mathrm{cov}(Z_{ij}, Z_{ik}) = \sigma_1^2 + t_j t_k \sigma_2^2 + \sigma_\epsilon^2 I(j = k)$$

Figure 4.5: Simulated longitudinal data showing the response of individuals through time. The red lines are the simulated responses for a control group, the green lines are the simulated responses for treatment 1, and the blue lines are the simulated responses for treatment 2.

お手製コード（データ作成）

```
n_max = 90
t_max = 20
sigma_1 = 1
sigma_2 = 1
sigma_ep = 1
b_0 = 25
b_1 = 1
b_2 = 1.5
b_3 = 2
```

```
param = tibble::tibble(
  n = seq(1,n_max),
  alpha_1 = rnorm(n = n_max, mean = 0, sd = sigma_1^0.5),
  alpha_2 = rnorm(n = n_max, mean = 0, sd = sigma_2^0.5),
  intecept =  b_0 + rnorm(n = n_max, mean = 0, sd = sigma_1^0.5))
df = tidyr::crossing(
  n = seq(1,n_max),
  t = seq(1,t_max)) %>%
  dplyr::mutate(condition = assign_condtion(n_max,t_max)) %>%
  dplyr::mutate(epsilon =  rnorm(n = n_max*t_max, mean = 0, sd =
sigma_ep^0.5)) %>%
  dplyr::mutate(intercept = purrr::map_dbl(n, ~ {param$intecept[.]})) %>%
  dplyr::mutate(slope = if_else(condition == "control",
                                true = purrr::map2_dbl(n, t, function(x,y){
                                  (b_1 + param$alpha_2[x]) * y}),
                                false = if_else(condition == "treatment_1",
                                                true = purrr::map2_dbl(n, t, function(x,y){
                                                  (b_2 + param$alpha_2[x]) * y
                                                  }),
                                                false = purrr::map2_dbl(n, t, function(x,y){
                                                  (b_3 + param$alpha_2[x]) * y
                                                }))))) %>%
  dplyr::mutate(Z = intercept + slope + epsilon)
ggplot(df,aes(x=t,y=Z,colour=condition,group=n)) + geom_line()
```

vignette(“spatio-temporal-kriging”)より

The *separable covariance model* assumes that the spatio-temporal covariance function can be represented as the product of a spatial and temporal term:

$$C_{\text{sep}}(h,u) = C_{\text{s}}(h)C_{t}(u)$$

Its variogram is given by (see Appendix for details):

$$\gamma_{\text{sep}}(h,u) = \text{sill} \cdot (\bar{\gamma}_s(h) + \bar{\gamma}_t(u) - \bar{\gamma}_s(h)\bar{\gamma}_t(u))$$

where $\bar{\gamma}_s$ and $\bar{\gamma}_t$ are standardised spatial and temporal variograms with separate nugget effects and (joint) sill of 1. The overall sill parameter is denoted by ”sill”.

7 Appendix

7.1 Derivation of the separable covariance and variogram identities

The separable covariance and variogram identity is readily available through

$$\begin{aligned}
C_{\text{sep}}(h,u) &= C_{\text{s}}(h)C_{\text{t}}(u) = sill \cdot \bar{c}_s(h)\bar{c}_t(u) \\
\gamma_{\text{sep}}(h,u) &= C_{\text{sep}}(0,0) - C_{\text{sep}}(h,u) \\
&= sill\,(1 - \bar{c}_s(h) \cdot \bar{c}_t(u)) \\
&= sill\,(1 - (1 - \bar{\gamma}_s(h))\,(1 - \bar{\gamma}_t(u))) \\
&= sill\,(1 - (1 - \bar{\gamma}_s(h) - \bar{\gamma}_t(u) + \bar{\gamma}_s(h)\bar{\gamma}_t(u))) \\
&= sill\,(\bar{\gamma}_s(h) + \bar{\gamma}_t(u) - \bar{\gamma}_s(h)\bar{\gamma}_t(u))
\end{aligned}$$

where $\bar{c}$ and $\bar{\gamma}$ are normalised correlation and correlogram functions respectively.