Covariance Functions

Lecture 15

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sta344 package

Basics

The package is based on the course organizartion and can be installed with,

```r
remotes::install_github("sta344-fa22/sta344")
```

collects all of the utility functions from the host scripts (e.g. `util-crps.R`, `fix_pred_draw.R`, etc.)

```r
library(sta344)
ls("package:sta344")
```

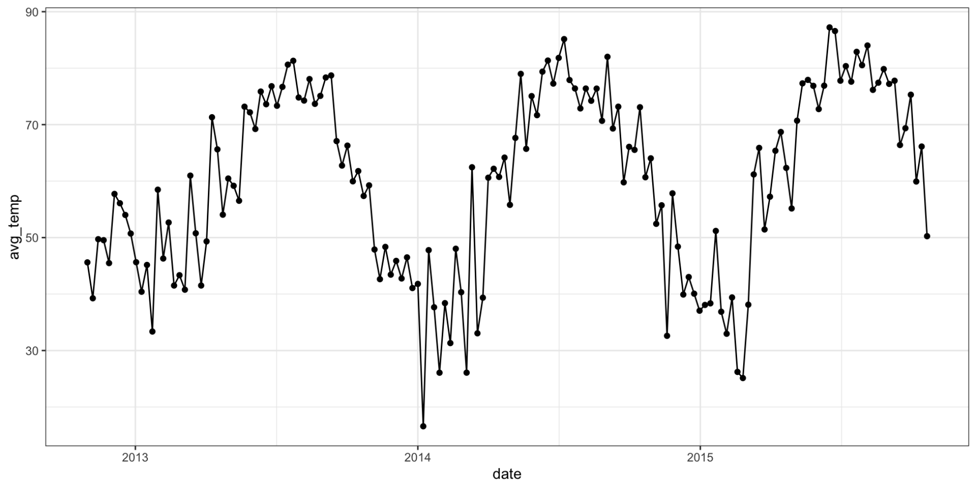
```
 [1] "avg_temp"            "calc_crps"           "cond_predict"
 [4] "emp_semivariogram"   "epred_draws_fix"     "exp_cov"
 [7] "exp_sv"              "gplm"                "linear_cov"
[10] "matern_cov"          "normalize_weights"   "nugget_cov"
[13] "periodic_cov"        "pow_exp_cov"         "pow_exp_sv"
[16] "predicted_draws_fix" "residual_draws_fix"  "rmvnorm"
[19] "rquad_cov"           "sphere_cov"          "sq_exp_cov"
[22] "sq_exp_sv"           "strip_attrs"
```

From last time

```r
( temp = readRDS("data/avg_temp_df.rds") %>%
    slice(1:(52*3)) %>%
    mutate(week = as.numeric(date - date[1])/
```

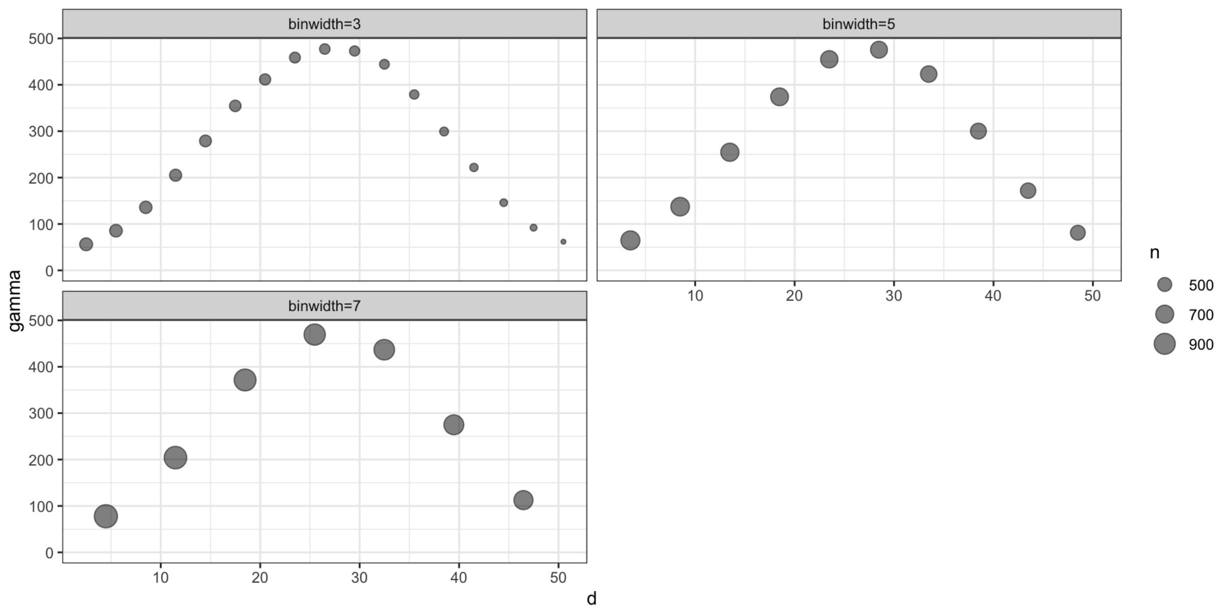
```
# A tibble: 156 × 3
   date       avg_temp  week
   <date>        <dbl> <dbl>
 1 2012-10-31     45.6     0
 2 2012-11-07     39.3     1
 3 2012-11-14     49.7     2
 4 2012-11-21     49.5     3
 5 2012-11-28     45.5     4
 6 2012-12-05     57.7     5
 7 2012-12-12     56.1     6
 8 2012-12-19     54.0     7
 9 2012-12-26     50.7     8
10 2013-01-02     45.6     9
# … with 146 more rows
```

```r
ggplot(temp, aes(x=date, y=avg_temp)) +
  geom_line() +
  geom_point()
```



Empirical semi-variogram

```
emp_semivariogram(
  d=temp, y=avg_temp, x=week,
  bin=TRUE, binwidth=c(3,5,7)
) %>%
  ggplot(aes(x=d, y=gamma, size=n)) +
    geom_point(alpha=0.5) +
    facet_wrap(~paste0("binwidth=",bw), ncol=2) +
    ylim(0,NA)
```

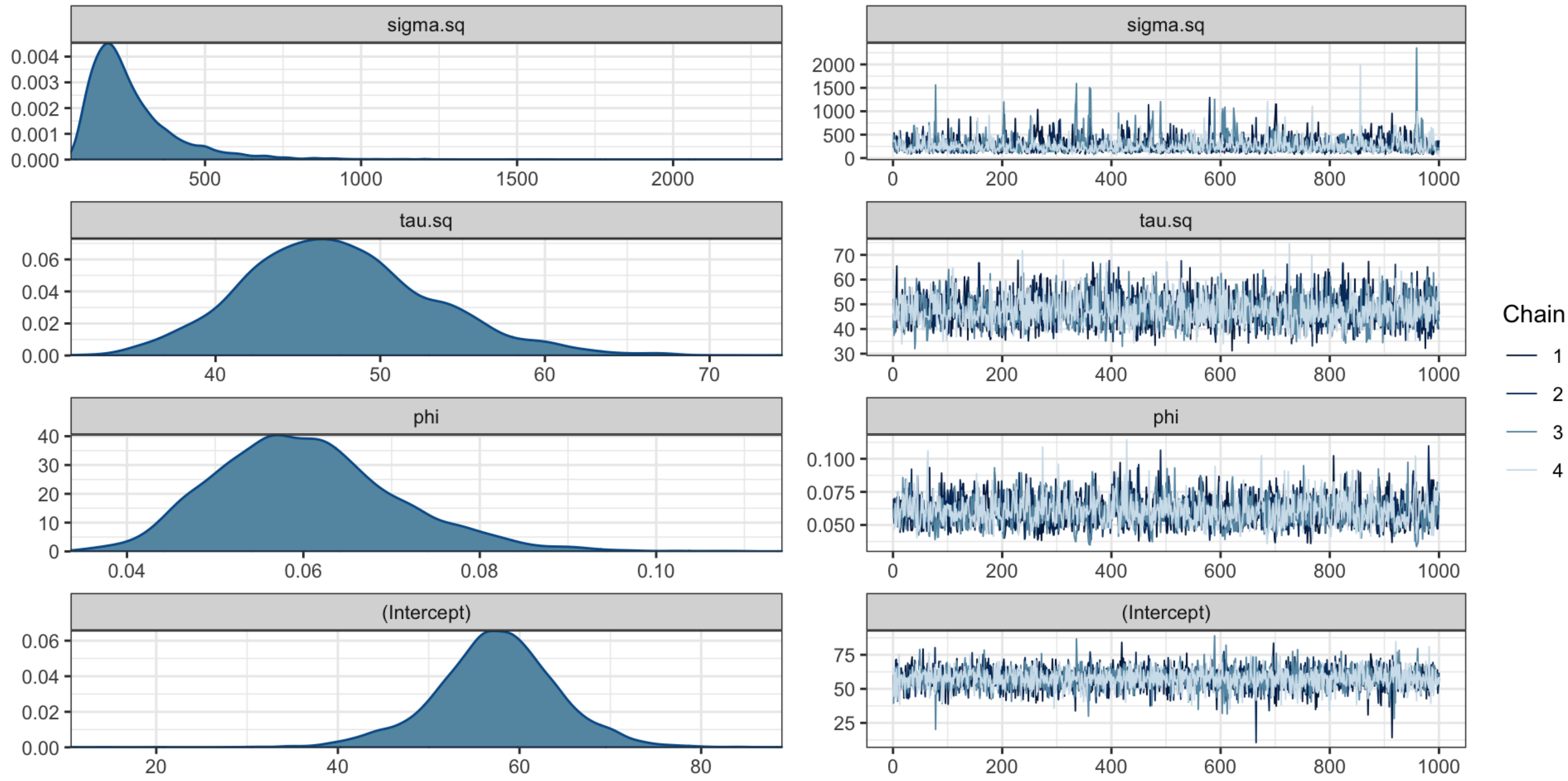


Model fitting

```
m = gplm(
  avg_temp~1, data = temp, coords = "week",
  cov_model = "gaussian",
  starting=list(
    "phi"=sqrt(3)/4, "sigma.sq"=1, "tau.sq"=1
  ),
  tuning=list(
    "phi"=1, "sigma.sq"=1, "tau.sq"=1
  ),
  priors=list(
    "phi.unif"=c(sqrt(3)/52, sqrt(3)/1),
    "sigma.sq.ig"=c(2, 1),
    "tau.sq.ig"=c(2, 1)
  ),
  thin = 5,
  n_batch = 100,
  batch_len = 100
)
```

Model plots

```
plot(m)
```



Prediction

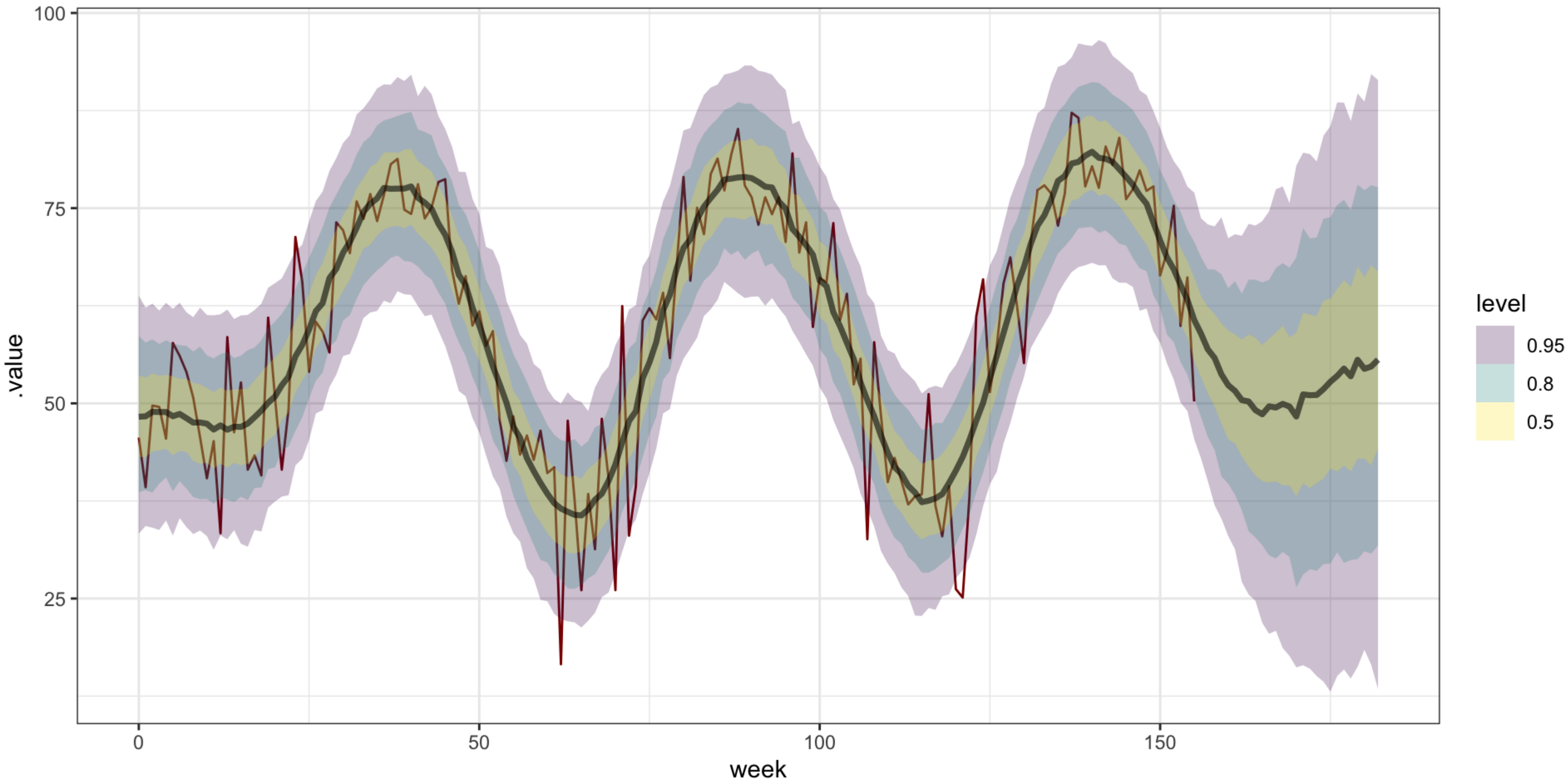
```
newdata = data.frame(
  week = seq(0,3.5*52) |> jitter()
)

(p = predict(m, newdata=newdata, coords = "week"))
```

```
# A draws_matrix: 1000 iterations, 4 chains, and 183 variables
    variable
draw y[1] y[2] y[3] y[4] y[5] y[6] y[7] y[8]
  1    38   45   57   42   43   47   43   55
  2    51   54   47   47   46   36   50   46
  3    42   56   45   57   36   54   48   60
  4    48   43   52   39   53   48   54   59
  5    39   38   39   46   50   50   49   48
  6    65   43   50   45   48   43   55   57
  7    43   52   56   60   54   71   40   58
  8    51   35   55   48   54   45   45   49
  9    50   48   42   44   38   52   58   40
```

Results

```
p |>
  tidybayes::gather_draws(y[i]) |>
  mutate(week = i-1) |>
  filter(.chain == 1) |>
  ggplot(aes(x=week, y=.value)) +
    geom_line(data=temp, aes(y=avg_temp), color="darkred") +
    tidybayes::stat_lineribbon(alpha=0.25)
```


100
75
50
25
.value
0
50
100
150
week
level
0.95
0.8
0.5

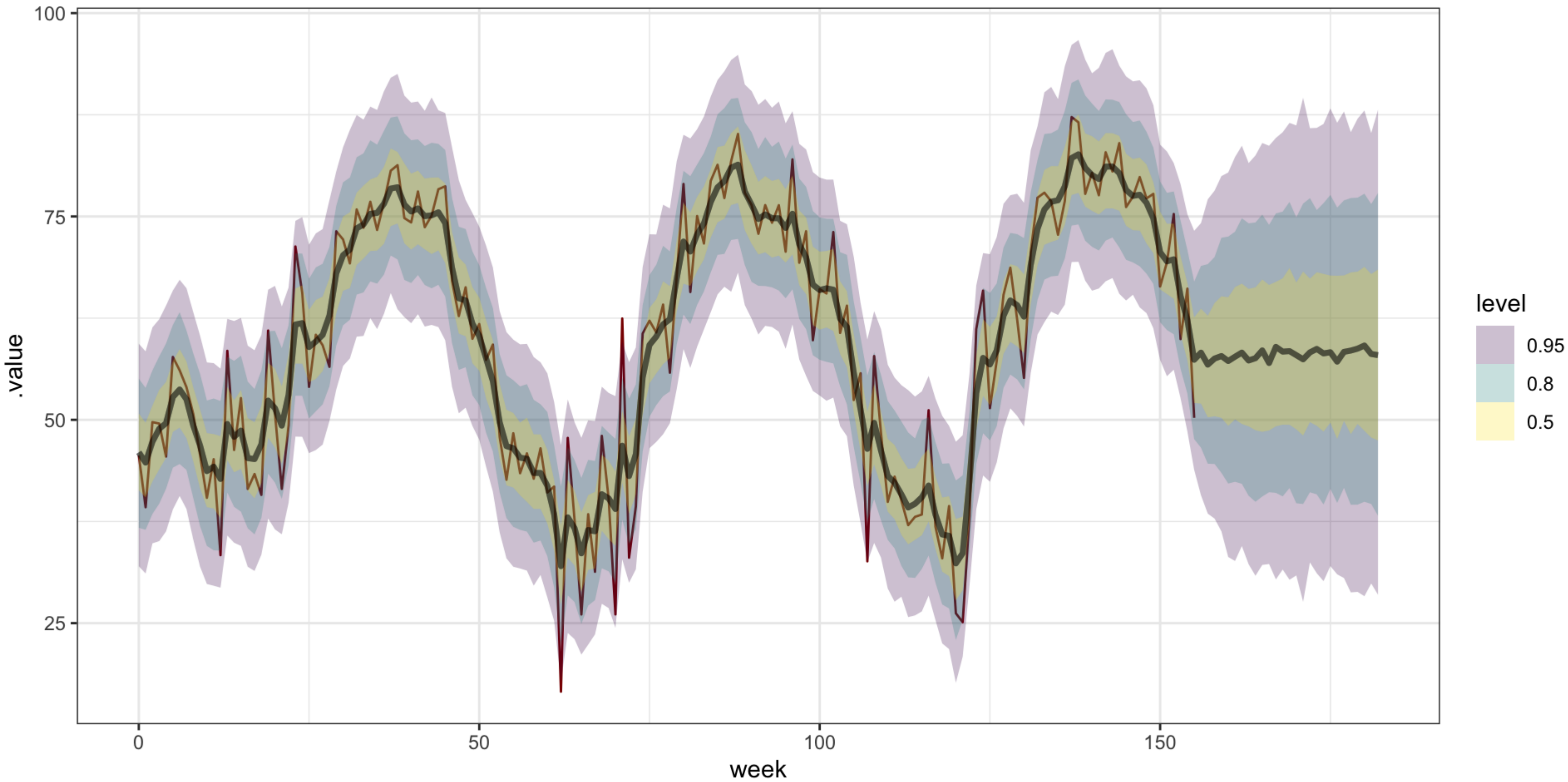
Exponential covariance

::: {.small}

```
m_exp = gplm(
  avg_temp~1, data = temp, coords = "week",
  cov_model = "exponential",
  starting=list(
    "phi"=3/4, "sigma.sq"=1, "tau.sq"=1
  ),
  tuning=list(
    "phi"=1, "sigma.sq"=1, "tau.sq"=1
  ),
  priors=list(
    "phi.unif"=c(3/52, 3/1),
    "sigma.sq.ig"=c(2, 1),
    "tau.sq.ig"=c(2, 1)
  ),
  thin = 5,
  n_batch = 100,
```

Results

```
p_exp |>
  tidybayes::gather_draws(y[i]) |>
  mutate(week = i-1) |>
  filter(.chain == 1) |>
  ggplot(aes(x=week, y=.value)) +
    geom_line(data=temp, aes(y=avg_temp), color="darkred") +
    tidybayes::stat_lineribbon(alpha=0.25)
```

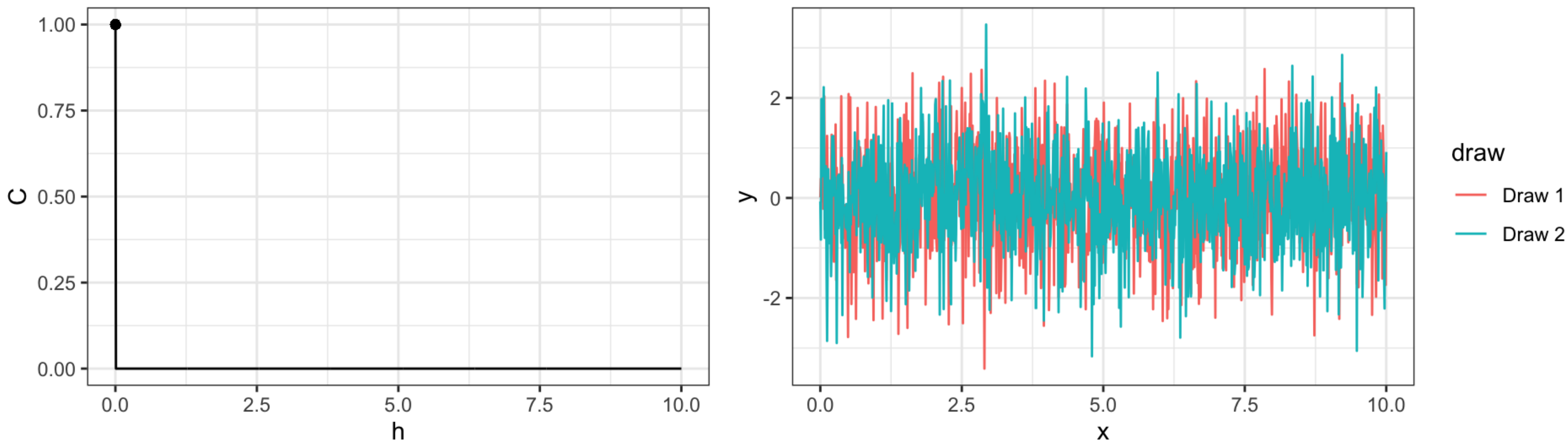


100
75
50
25
.value
0
50
100
150
week
level
0.95
0.8
0.5

More Covariance Functions

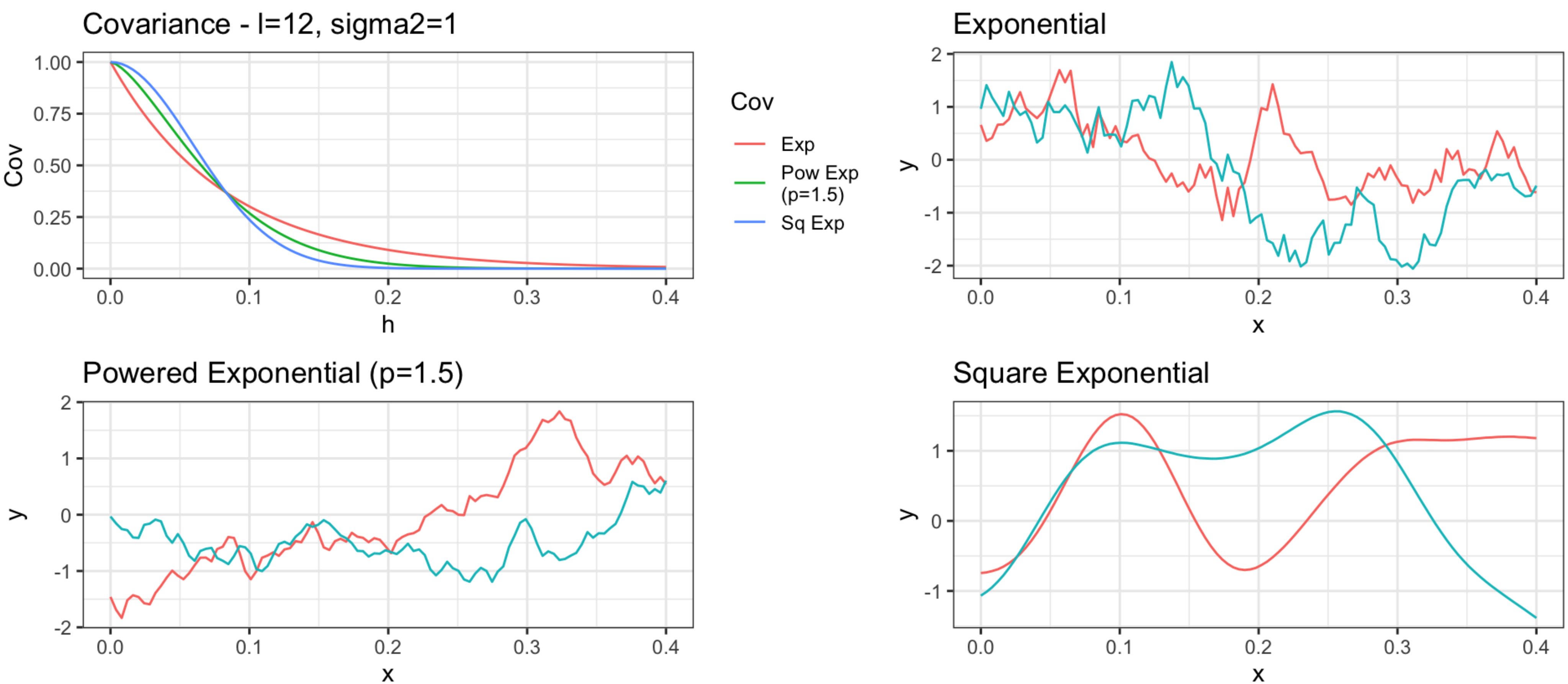
Nugget Covariance

$$\text{Cov}(y_{t_i}, y_{t_j}) = \sigma^2 \, 1_{\{h=0\}} \;\; \text{where } h = |t_i - t_j|$$



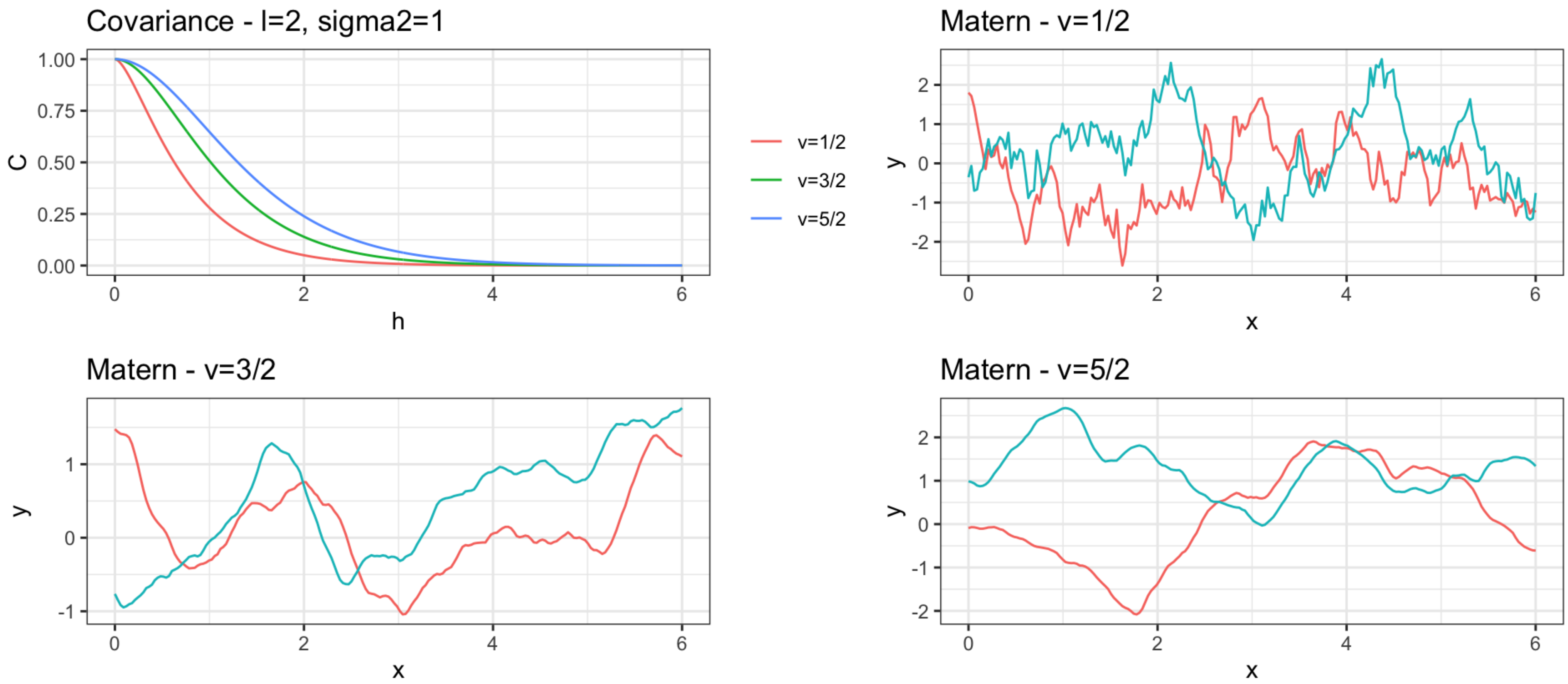
(- / Power / Square) Exponential Covariance

$$\text{Cov}(y_{t_i}, y_{t_j}) = \sigma^2 \exp\left(-(h\, l)^p\right) \text{ where } h = |t_i - t_j|$$



Matern Covariance

$$\text{Cov}(y_{t_i}, y_{t_j}) = \sigma^2 \; \frac{2^{1-\nu}}{\Gamma(\nu)} \; \left(\sqrt{2\nu}\, h \cdot l\right)^{\nu} K_\nu \left(\sqrt{2\nu}\, h \cdot l\right) \;\; \text{where } h = |t_i - t_j|$$

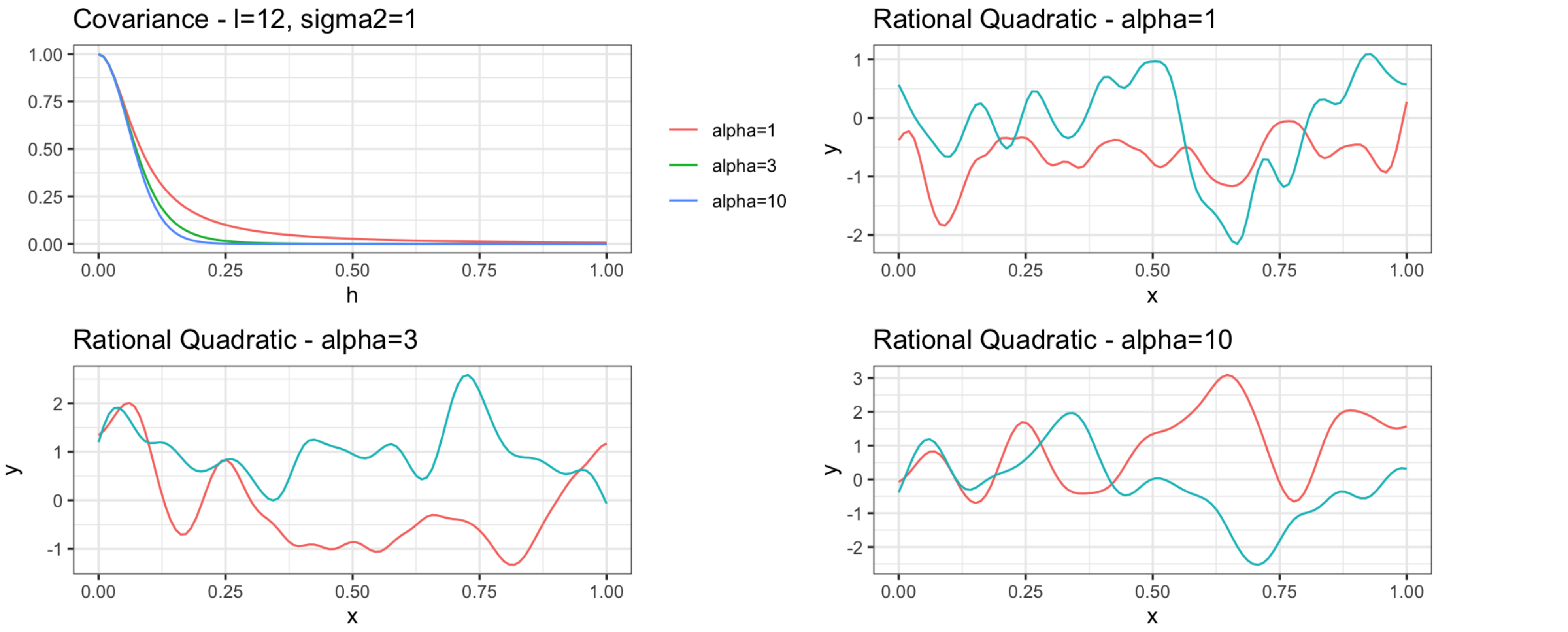


Matern Covariance

- $K_\nu()$ is the modified Bessel function of the second kind.
- A Gaussian process with Matérn covariance has sample functions that are $\lceil \nu - 1 \rceil$ times differentiable.
- When $\nu = 1/2 + p$ for $p \in \mathbb{N}^+$ then the Matern has a simplified form
- When $\nu = 1/2$ the Matern is equivalent to the exponential covariance.
- As $\nu \to \infty$ the Matern converges to the squared exponential covariance.

Rational Quadratic Covariance

$$\text{Cov}(y_{t_i}, y_{t_j}) = \sigma^2 \left(1 + \frac{h^2\, l^2}{\alpha}\right)^{-\alpha} \quad \text{where } h = |t_i - t_j|$$

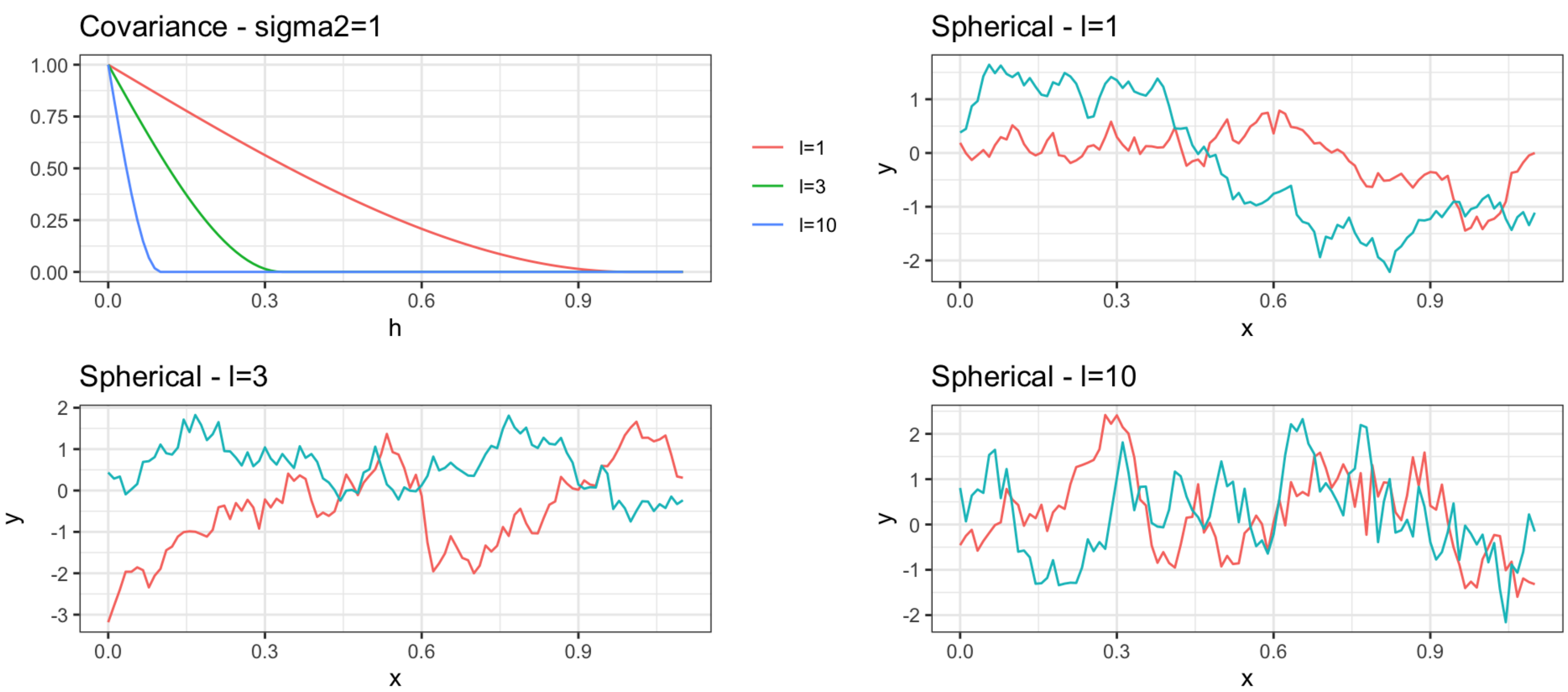


Rational Quadratic Covariance

- is a scaled mixture of squared exponential covariance functions with different characteristic length-scales (l).
- As $\alpha \longrightarrow \infty$ the rational quadratic converges to the square exponential covariance.
- Has sample functions that are infinitely differentiable for any value of α

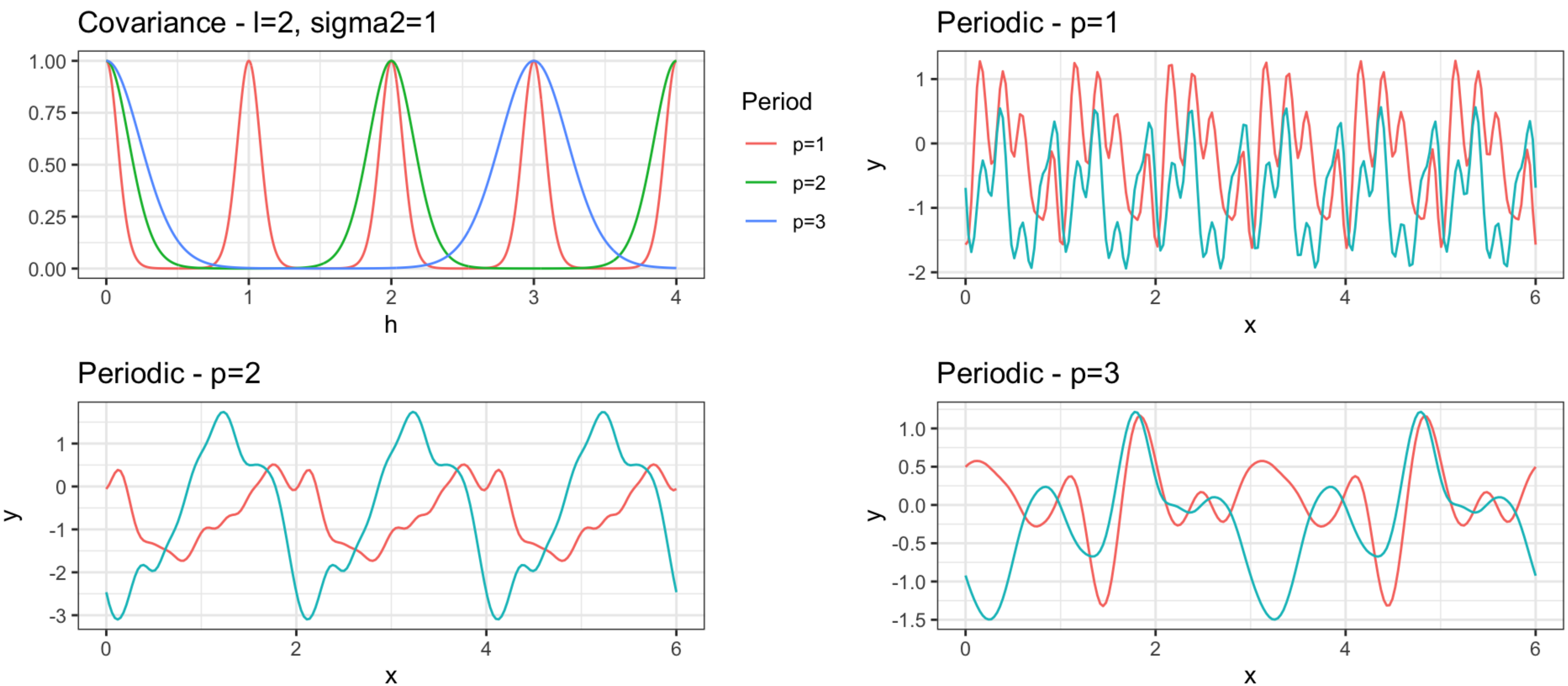
Spherical Covariance

$$\text{Cov}(y_{t_i}, y_{t_j}) = \begin{cases} \sigma^2 \left(1 - \frac{3}{2} h \cdot l + \frac{1}{2}(h \cdot l)^3\right) & \text{if } 0 < h < 1/l \\ 0 & \text{otherwise} \end{cases} \quad \text{where } h = |t$$



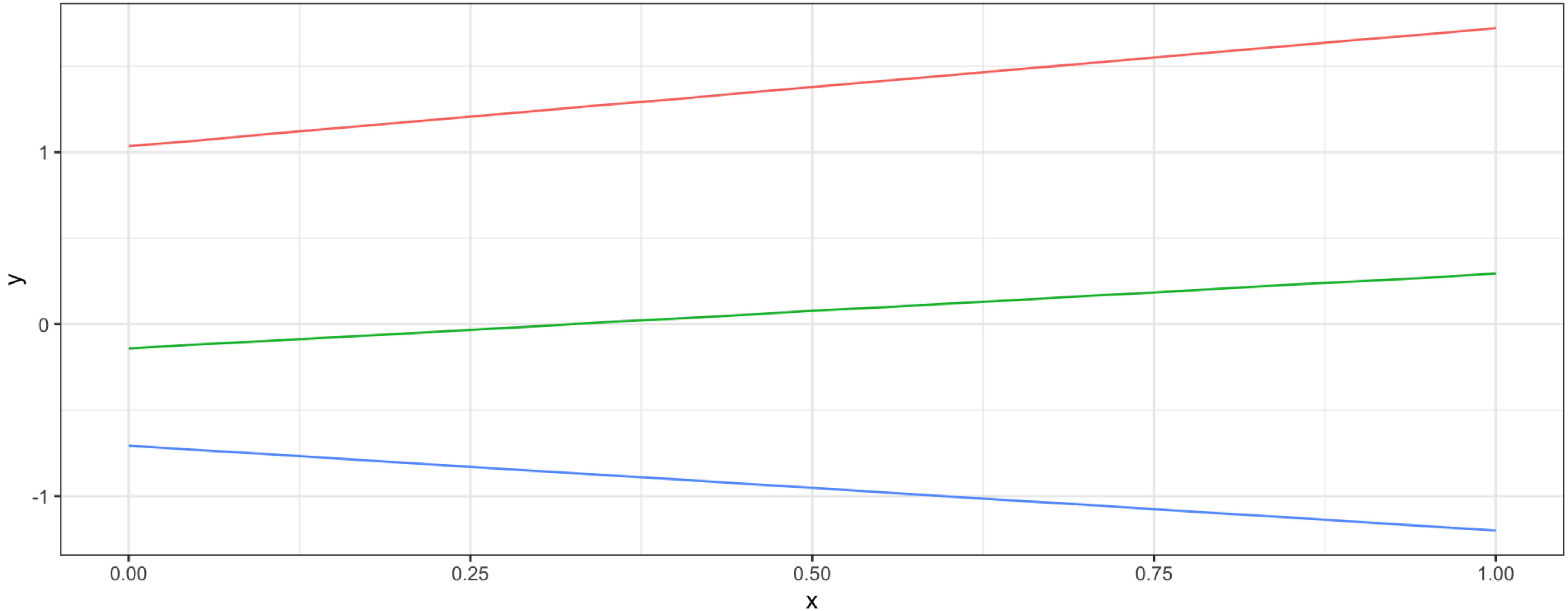
Periodic Covariance

$$\text{Cov}(y_{t_i}, y_{t_j}) = \sigma^2 \exp\left(-2\, l^2 \sin^2\left(\pi \frac{h}{p}\right)\right) \text{ where } h = |t_i - t_j|$$



Linear Covariance

$$\mathrm{Cov}(y_{t_i}, y_{t_j}) = \sigma_b^2 + \sigma_v^2\,(t_i - c)(t_j - c)$$



Combining Covariances

If we definite two valid covariance functions, $\text{Cov}_a(y_{t_i}, y_{t_j})$ and $\text{Cov}_b(y_{t_i}, y_{t_j})$ then the following are also valid covariance functions,

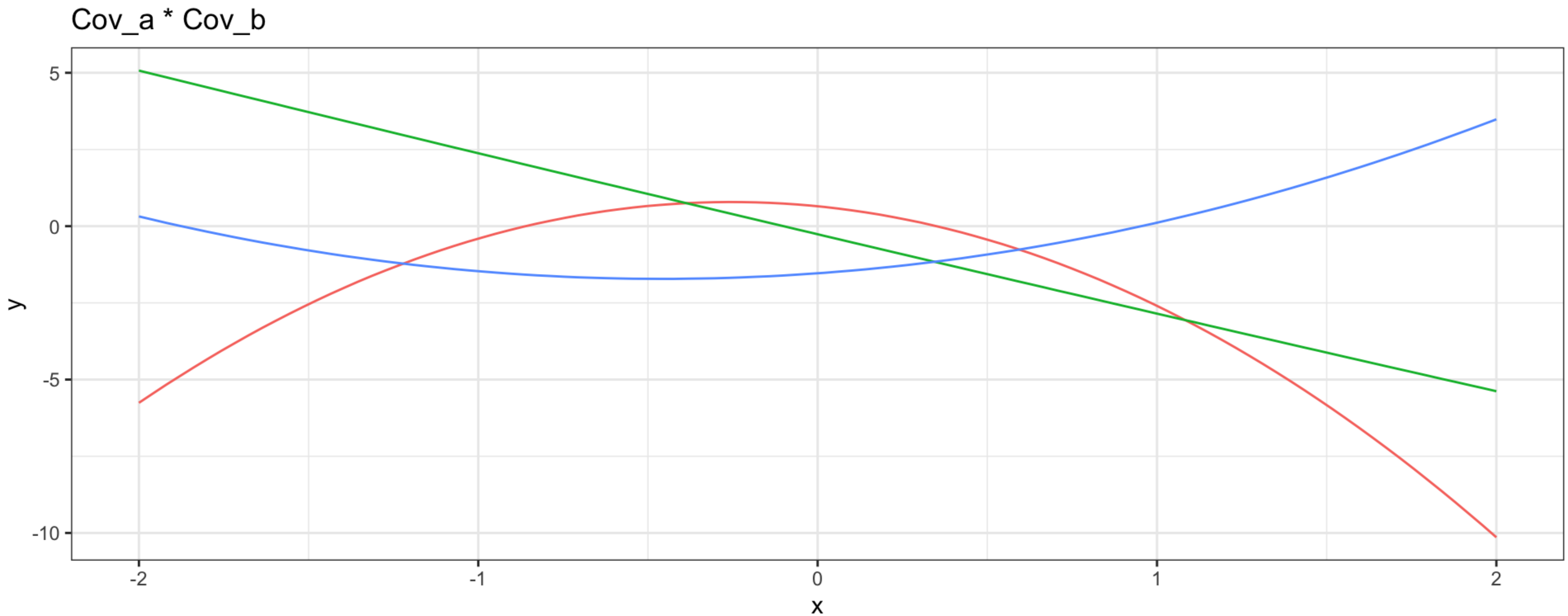
$$\text{Cov}_a(y_{t_i}, y_{t_j}) + \text{Cov}_b(y_{t_i}, y_{t_j})$$

$$\text{Cov}_a(y_{t_i}, y_{t_j}) \times \text{Cov}_b(y_{t_i}, y_{t_j})$$

Linear × Linear → Quadratic

$$\mathrm{Cov}_a(y_{t_i}, y_{t_j}) = 1 + 2\,(t_i \times t_j)$$

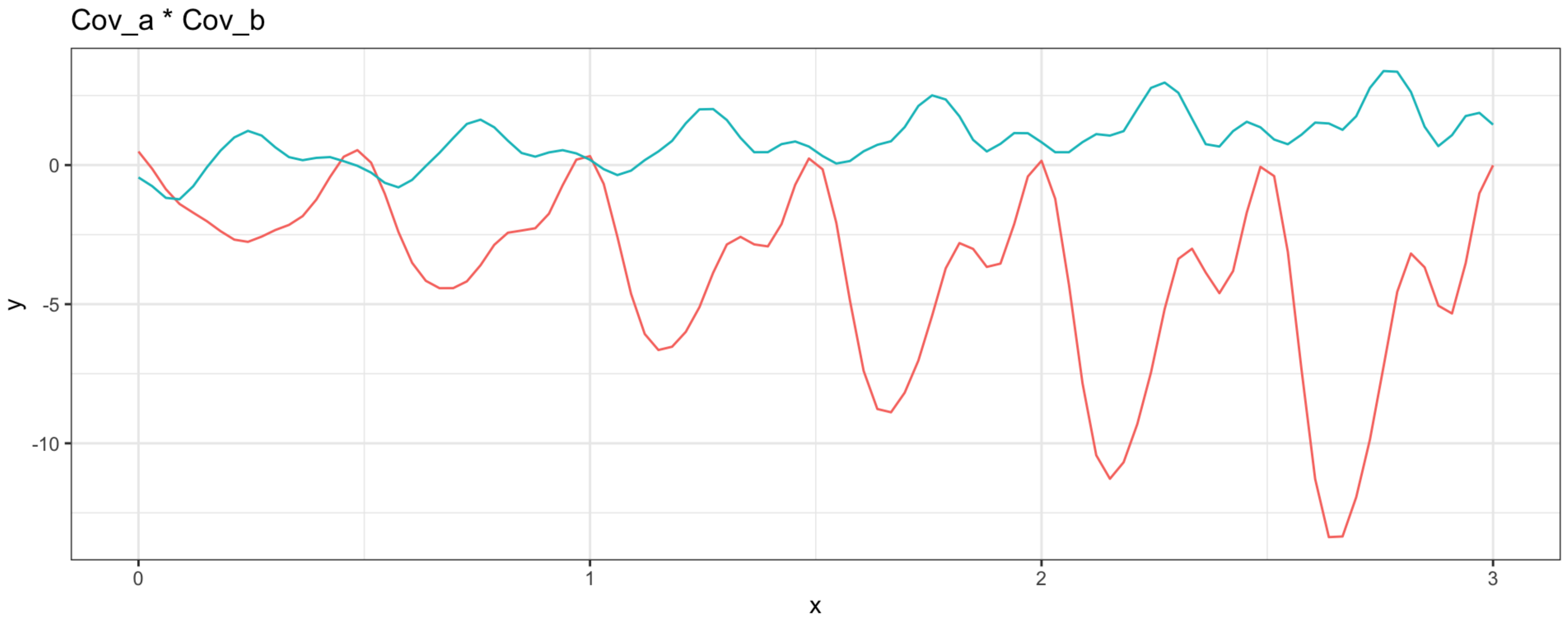
$$\mathrm{Cov}_b(y_{t_i}, y_{t_j}) = 2 + 1\,(t_i \times t_j)$$



Linear × Periodic

$$\text{Cov}_a(y_{t_i}, y_{t_j}) = 1 + 1\ (t_i \times t_j)$$

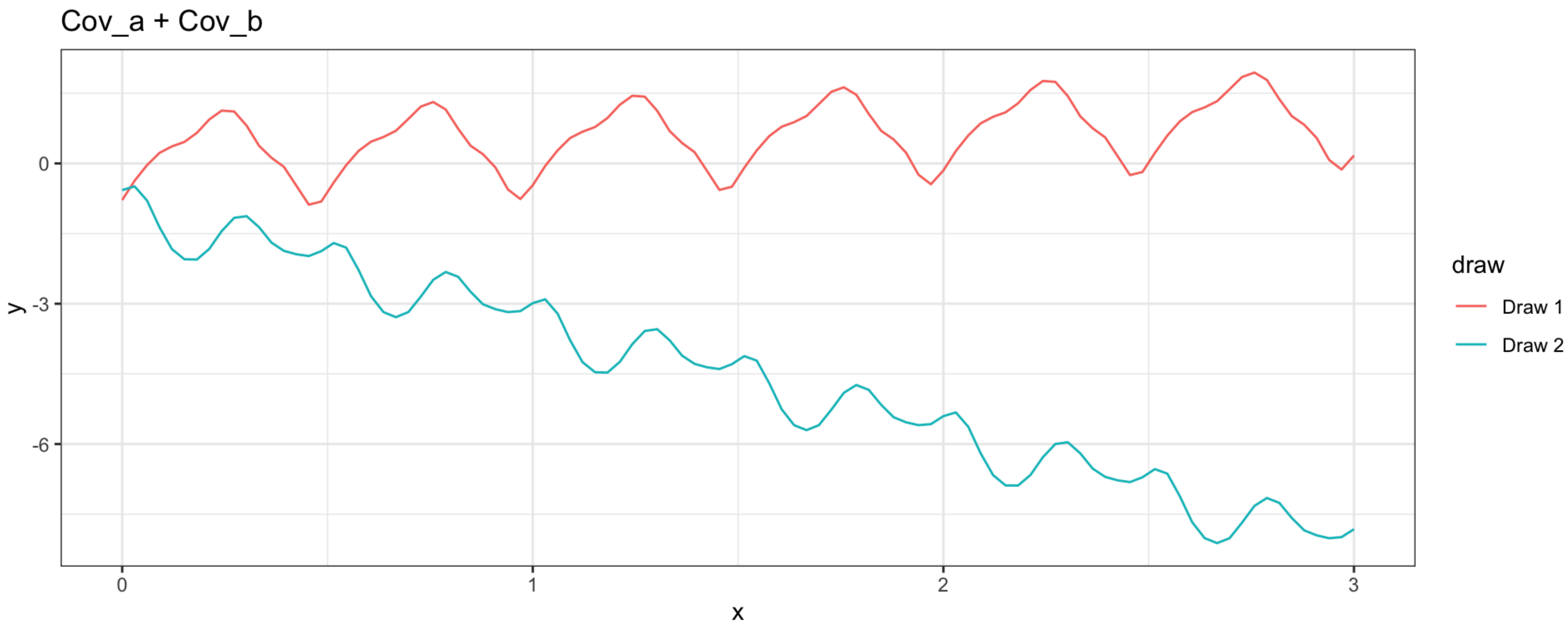
$$\text{Cov}_b(y_{t_i}, y_{t_j}) = \exp\left(-2\ \sin^2(2\pi\, h)\right)$$



Linear + Periodic

$$\text{Cov}_a(y_{t_i}, y_{t_j}) = 1 + 1\ (t_i \times t_j)$$

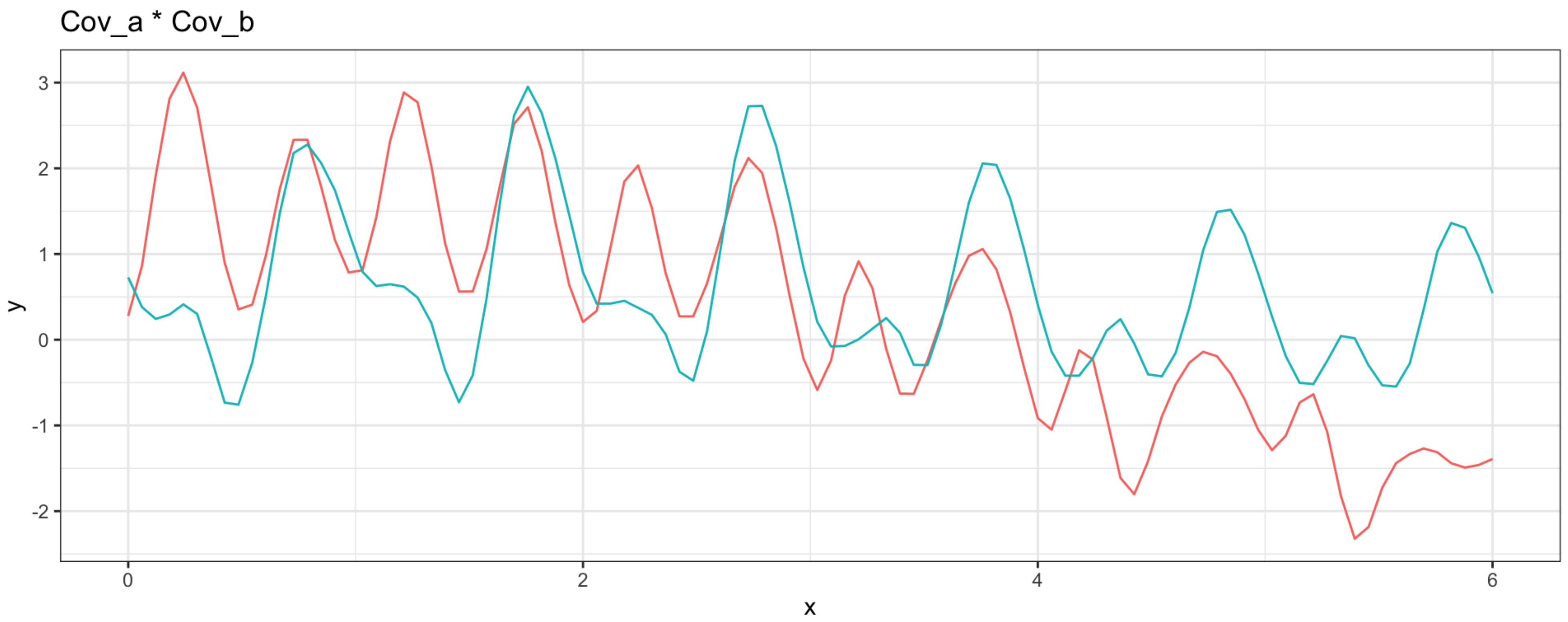
$$\text{Cov}_b(h = |t_i - t_j|) = \exp\left(-2\ \sin^2(2\pi\, h)\right)$$



Sq Exp × Periodic ⟶ Locally Periodic

$$\text{Cov}_a(h = |t_i - t_j|) = \exp(-(1/3)h^2)$$

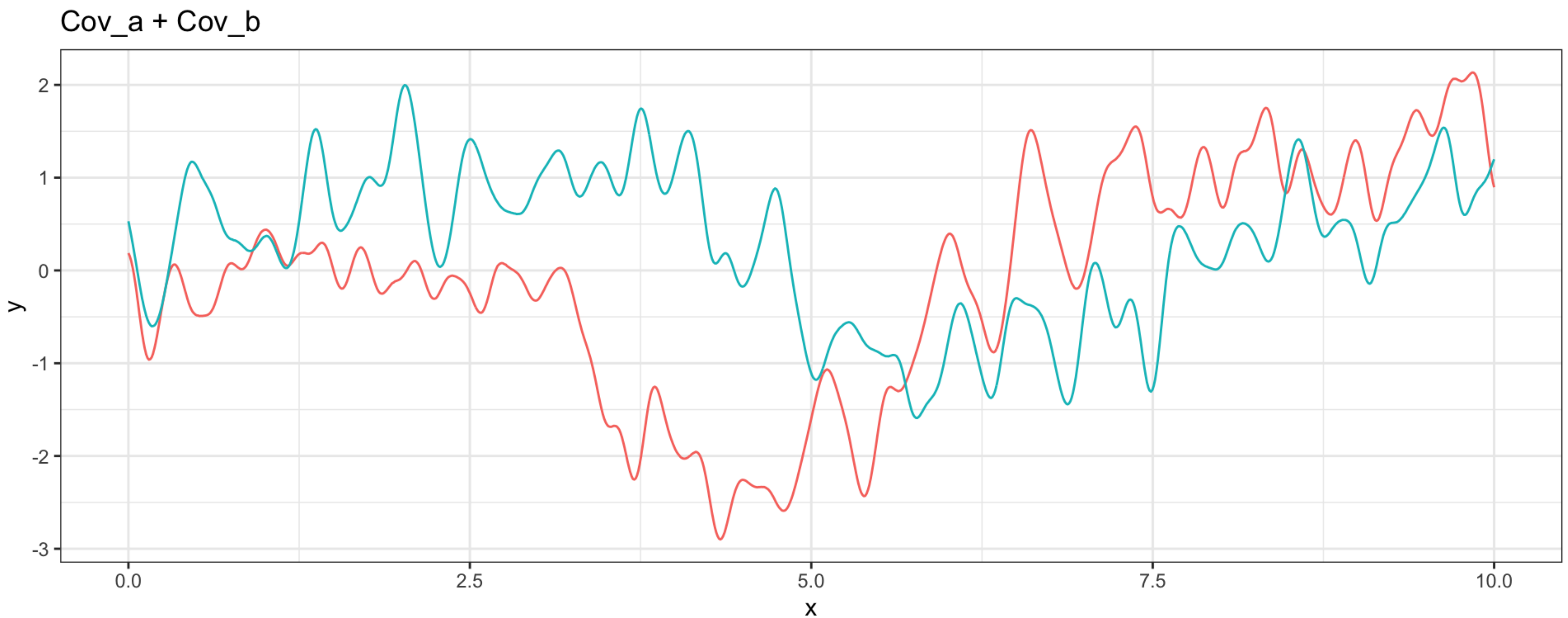
$$\text{Cov}_b(h = |t_i - t_j|) = \exp\left(-2\ \sin^2(\pi\, h)\right)$$



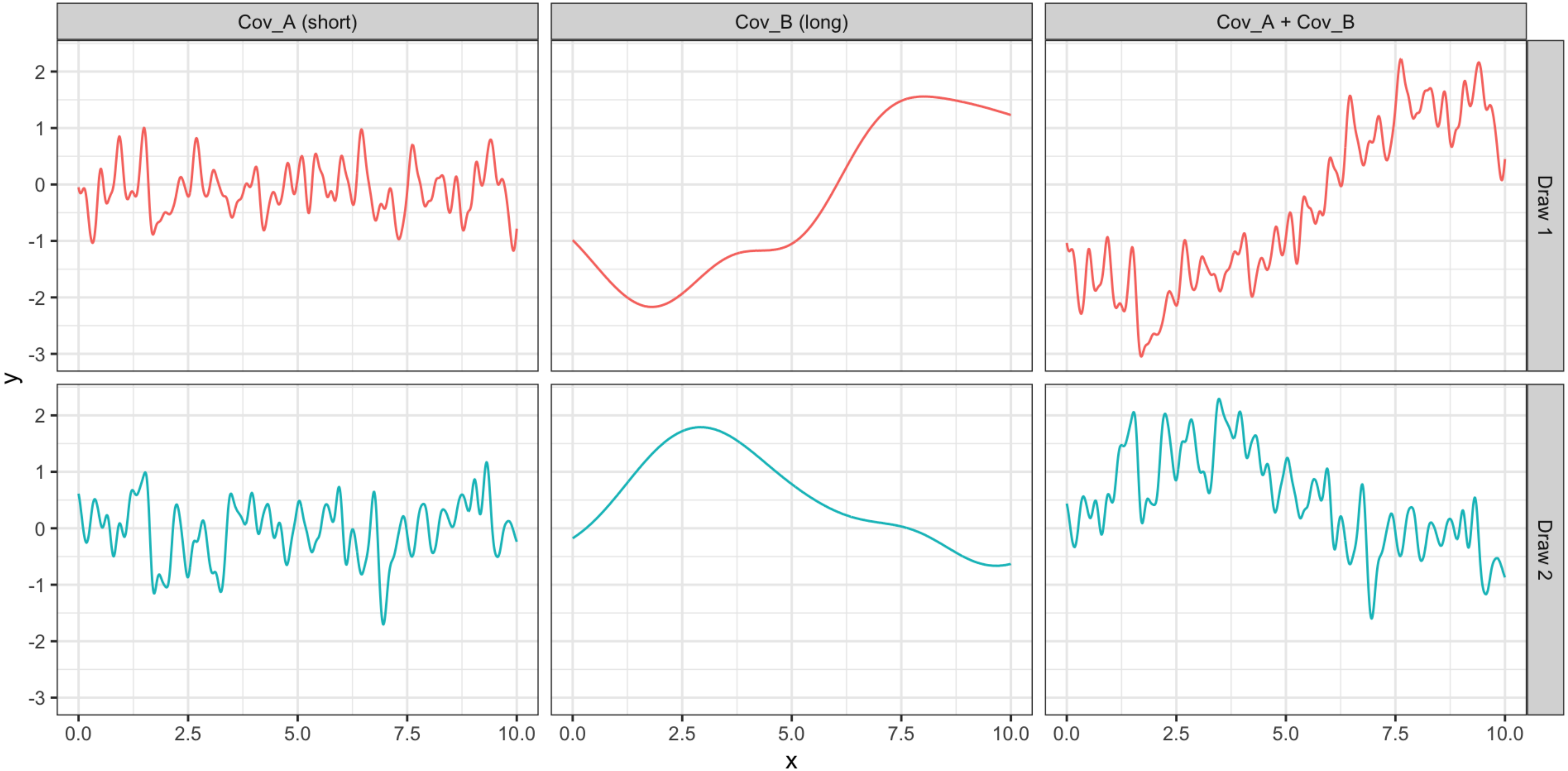
Sq Exp (short) + Sq Exp (long)

$$Cov_a(h = |t_i - t_j|) = (1/4)\exp(-4\sqrt{3}h^2)$$

$$Cov_b(h = |t_i - t_j|) = \exp(-(\sqrt{3}/2)h^2)$$

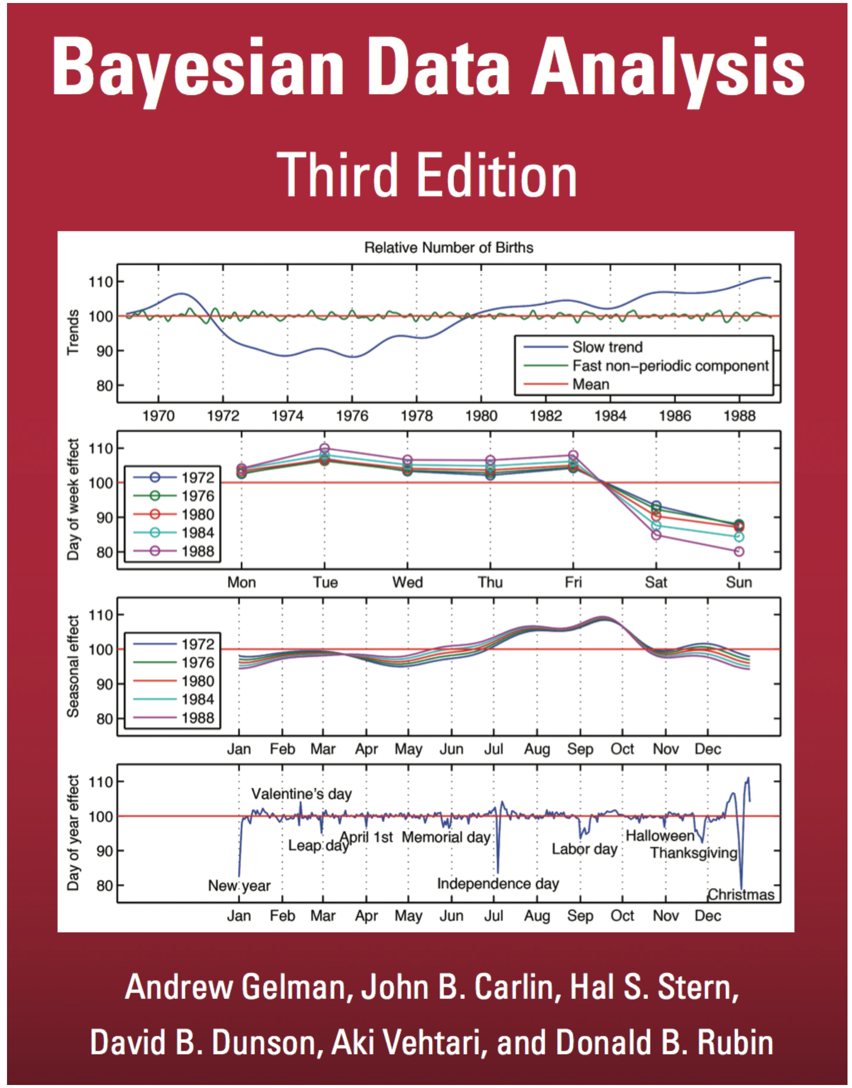


Seen another way



BDA3 example

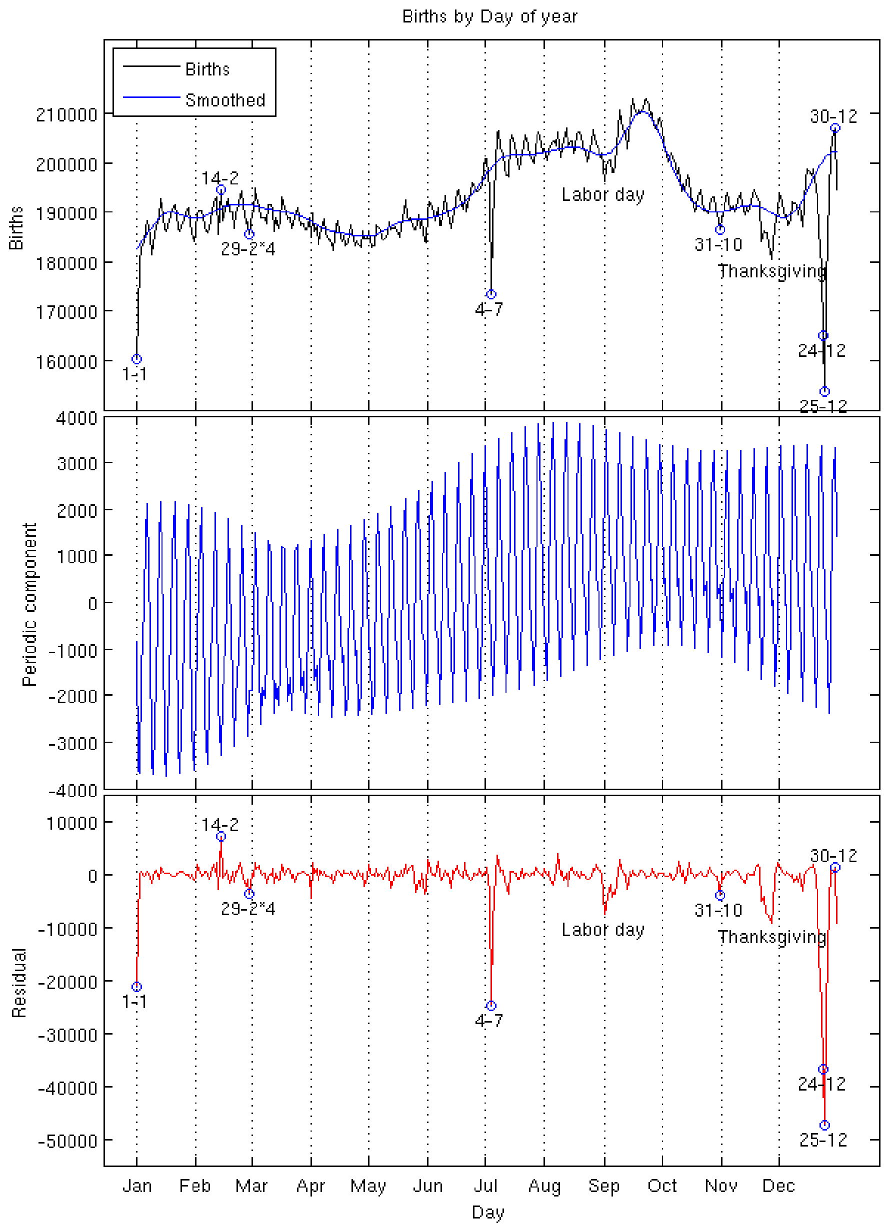
BDA3



Bayesian Data Analysis
Third Edition
Relative Number of Births
Trends
Slow trend
Fast non–periodic component
Mean
Day of week effect
Seasonal effect
Day of year effect
Valentine's day
Leap day
April 1st
Memorial day
Labor day
Halloween
Thanksgiving
New year
Independence day
Christmas
Andrew Gelman, John B. Carlin, Hal S. Stern,
David B. Dunson, Aki Vehtari, and Donald B. Rubin

Source

Births (one year)



1. Smooth long term trend (*sq exp cov*)
2. Seven day periodic trend with decay (*periodic x sq exp cov*)
3. Constant mean

Component Contributions

We can view our GP in the following ways (marginal form),

$$\boldsymbol{y} \sim \mathrm{N}(\boldsymbol{\mu},\ \boldsymbol{\Sigma}_1 + \boldsymbol{\Sigma}_2 + \sigma^2 \boldsymbol{I})$$

but with appropriate conditioning we can also think of $\boldsymbol{y}$ as being the sum of multiple independent GPs (latent form)

$$\boldsymbol{y} = \boldsymbol{\mu} + \mathrm{w}_1(\boldsymbol{t}) + \mathrm{w}_2(\boldsymbol{t}) + \mathrm{w}_3(\boldsymbol{t})$$

where

$$\begin{aligned}
\mathrm{w}_1(\boldsymbol{t}) &\sim \mathrm{N}(0, \boldsymbol{\Sigma}_1) \\
\mathrm{w}_2(\boldsymbol{t}) &\sim \mathrm{N}(0, \boldsymbol{\Sigma}_2) \\
\mathrm{w}_3(\boldsymbol{t}) &\sim \mathrm{N}(0, \sigma^2 \boldsymbol{I})
\end{aligned}$$

Decomposition of Covariance Components

$$\begin{bmatrix} \mathrm{y} \\ \mathrm{w}_1 \\ \mathrm{w}_2 \end{bmatrix} \sim \mathrm{N}\left(\begin{bmatrix} \boldsymbol{\mu} \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \Sigma_1 + \Sigma_2 + \sigma^2 \boldsymbol{I} & \Sigma_1 & \Sigma_2 \\ \Sigma_1 & \Sigma_1 & 0 \\ \Sigma_2 & 0 & \Sigma_2 \end{bmatrix}\right)$$

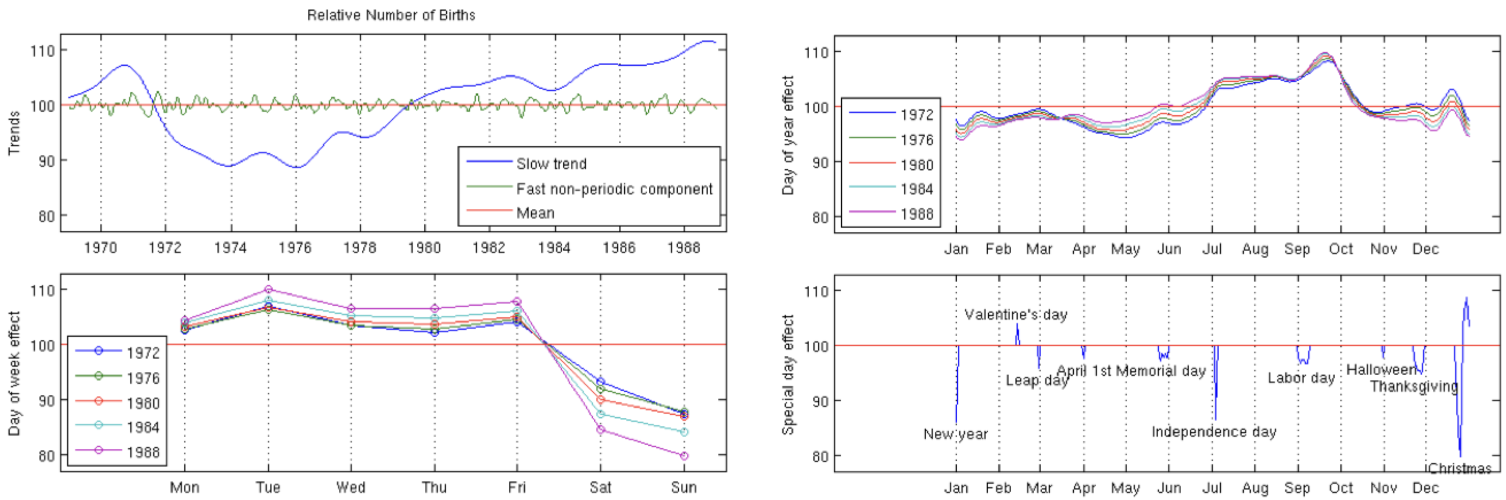
therefore

$$\mathrm{w}_1 \mid \boldsymbol{y}, \boldsymbol{\mu}, \boldsymbol{\theta} \sim \mathrm{N}(\boldsymbol{\mu}_{\text{cond}}, \boldsymbol{\Sigma}_{\text{cond}})$$

$$\boldsymbol{\mu}_{\text{cond}} = 0 + \Sigma_1 \, (\Sigma_1 + \Sigma_2 + \sigma^2 \mathrm{I})^{-1} (\boldsymbol{y} - \boldsymbol{\mu})$$

$$\boldsymbol{\Sigma}_{\text{cond}} = \Sigma_1 - \Sigma_1 (\Sigma_1 + \Sigma_2 + \sigma^2 \boldsymbol{I})^{-1} \Sigma_1{}^{\mathrm{t}}$$

Births (multiple years)

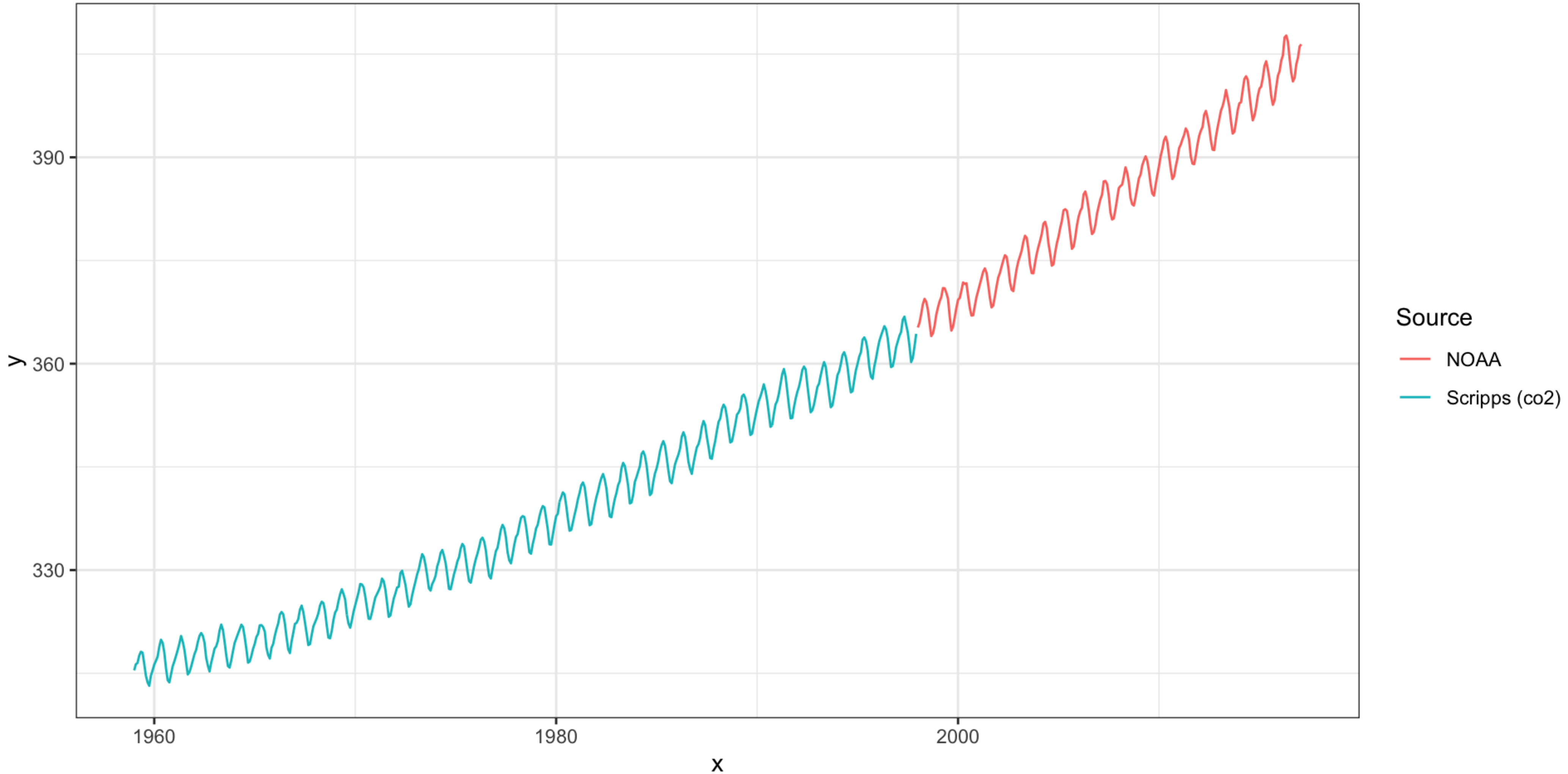


Full stan case study here with code here

1. slowly changing trend - yearly (*sq exp cov*)
2. small time scale trend - monthly (*sq exp cov*)
3. 7 day periodic - day of week effect (*periodic* $\times$ *sq exp cov*)
4. 365.25 day periodic - day of year effect (*periodic* $\times$ *sq exp cov*)
5. special days and interaction with weekends (*linear cov*)
6. independent Gaussian noise (*nugget cov*)
7. constant mean

Mauna Loa Example

Atmospheric CO_2



GP Model

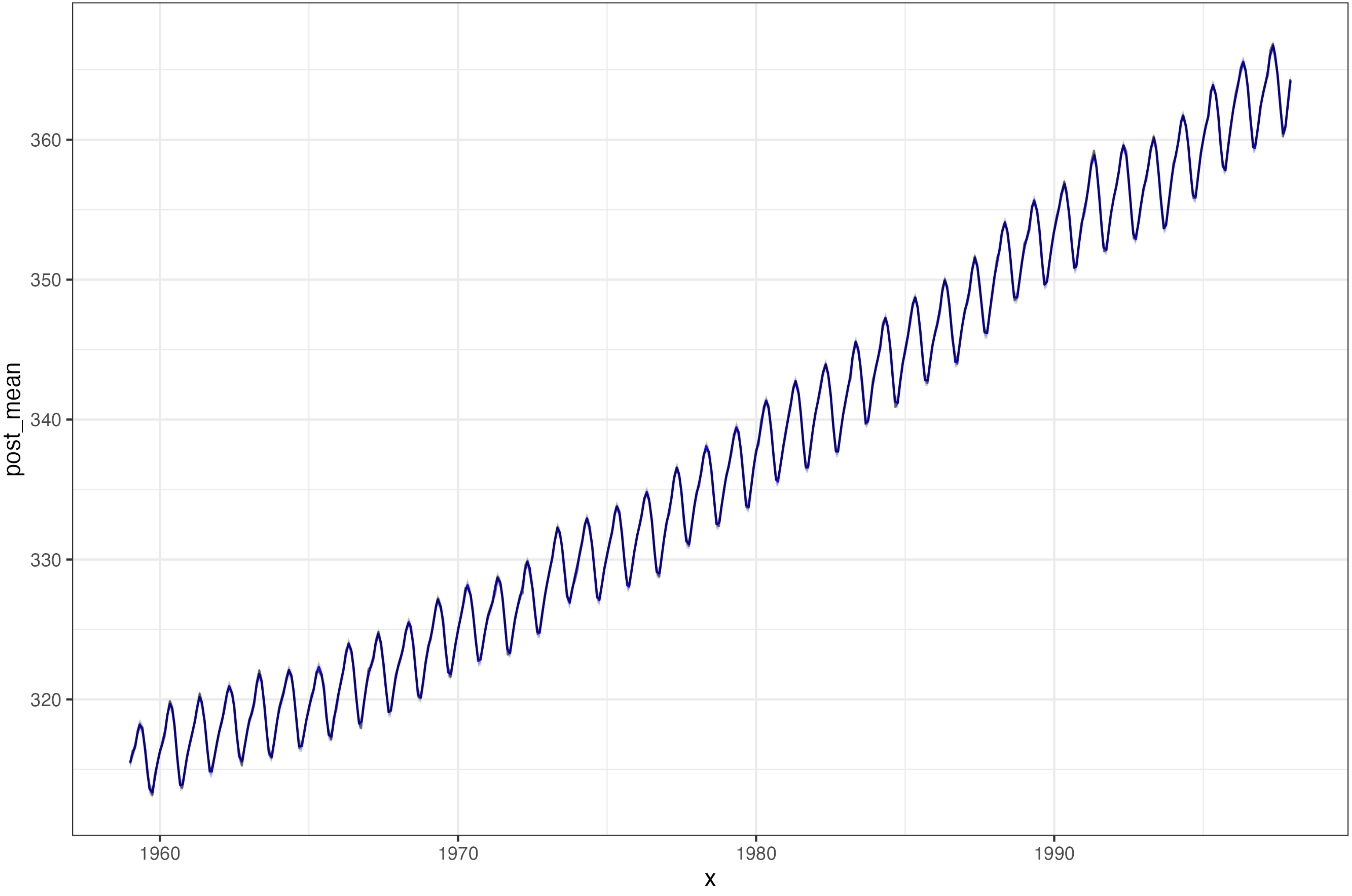
Based on Rasmussen 5.4.3 (we are using slightly different data and parameterization)

$$\boldsymbol{y} \sim \quad (\boldsymbol{\mu},\ \boldsymbol{\Sigma}_1 + \boldsymbol{\Sigma}_2 + \boldsymbol{\Sigma}_3 + \boldsymbol{\Sigma}_4 + \sigma^2 \mathrm{I}\,)$$

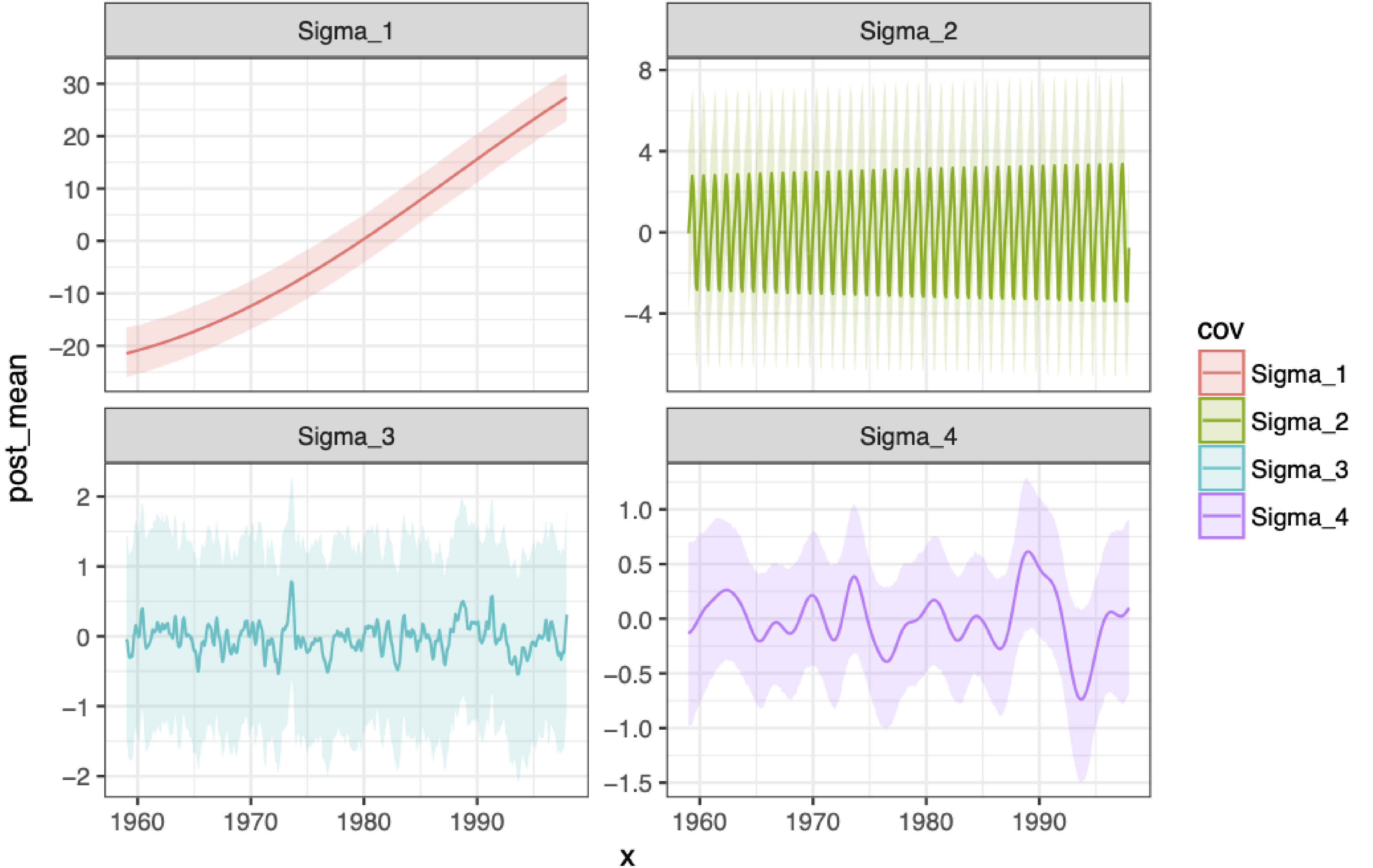
$$\{\boldsymbol{\mu}\}_i = y$$

$$\{\boldsymbol{\Sigma}_1\}_{ij} = \sigma_1^2 \exp\left(-(l_1 \cdot d_{ij})^2\right)$$
$$\{\boldsymbol{\Sigma}_2\}_{ij} = \sigma_2^2 \exp\left(-(l_2 \cdot d_{ij})^2\right) \exp\left(-2\,(l_3)^2 \sin^2(\pi\, d_{ij}/p)\right)$$
$$\{\boldsymbol{\Sigma}_3\}_{ij} = \sigma_3^2 \left(1 + \frac{(l_4 \cdot d_{ij})^2}{\alpha}\right)^{-\alpha}$$
$$\{\boldsymbol{\Sigma}_4\}_{ij} = \sigma_4^2 \exp\left(-(l_5 \cdot d_{ij})^2\right)$$

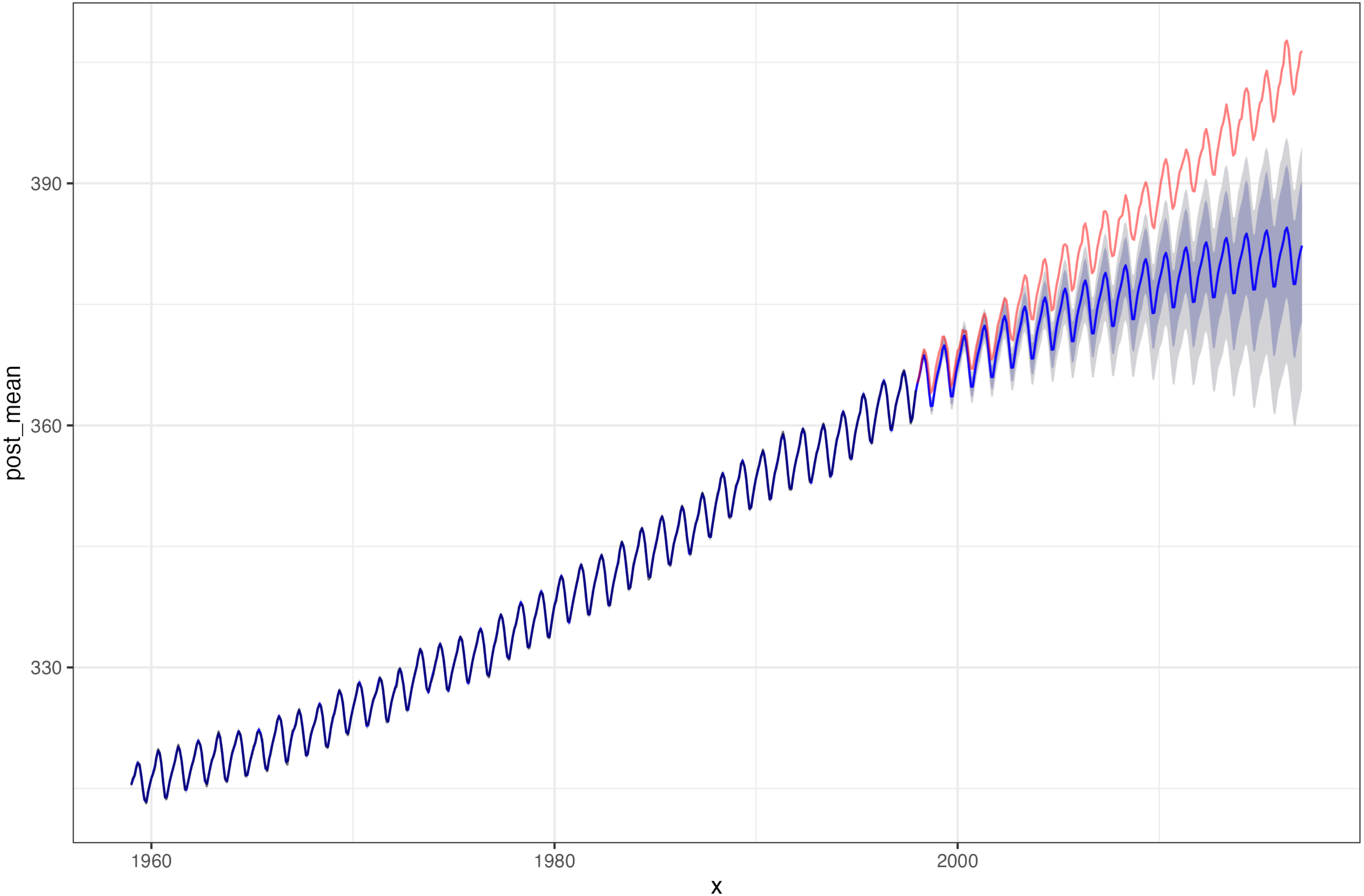
Model fit



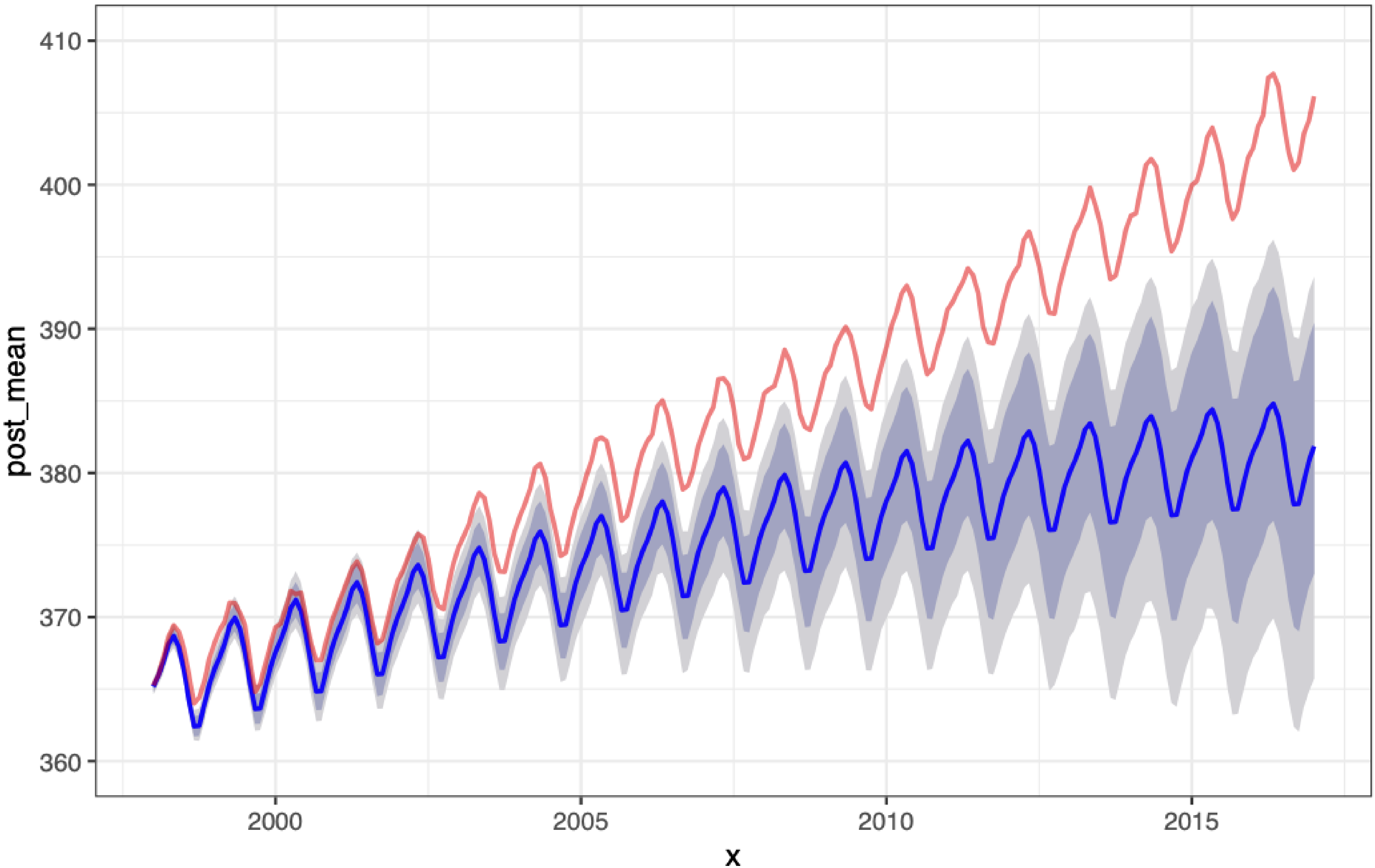
Fit Components



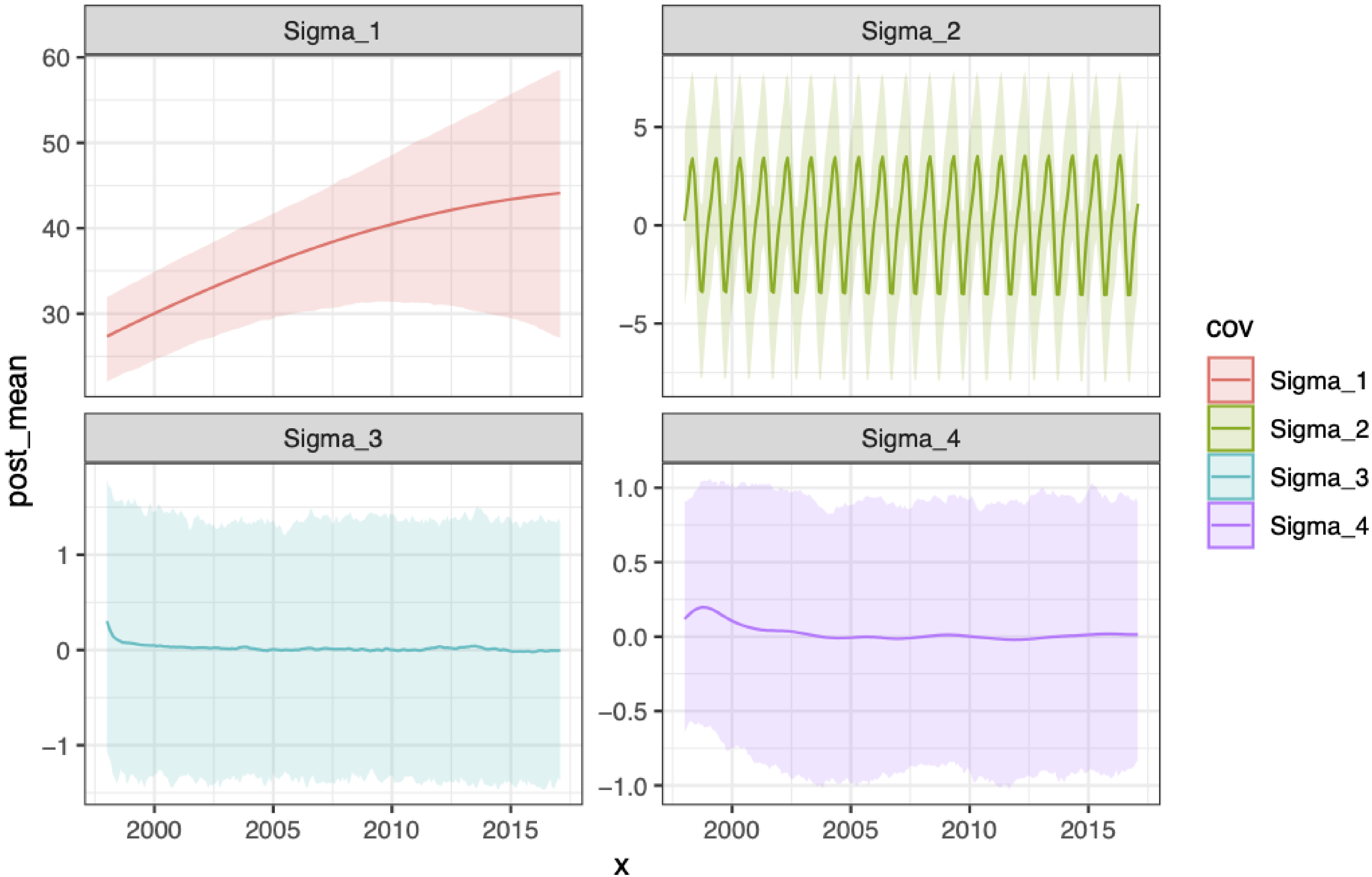
Model fit + forecast



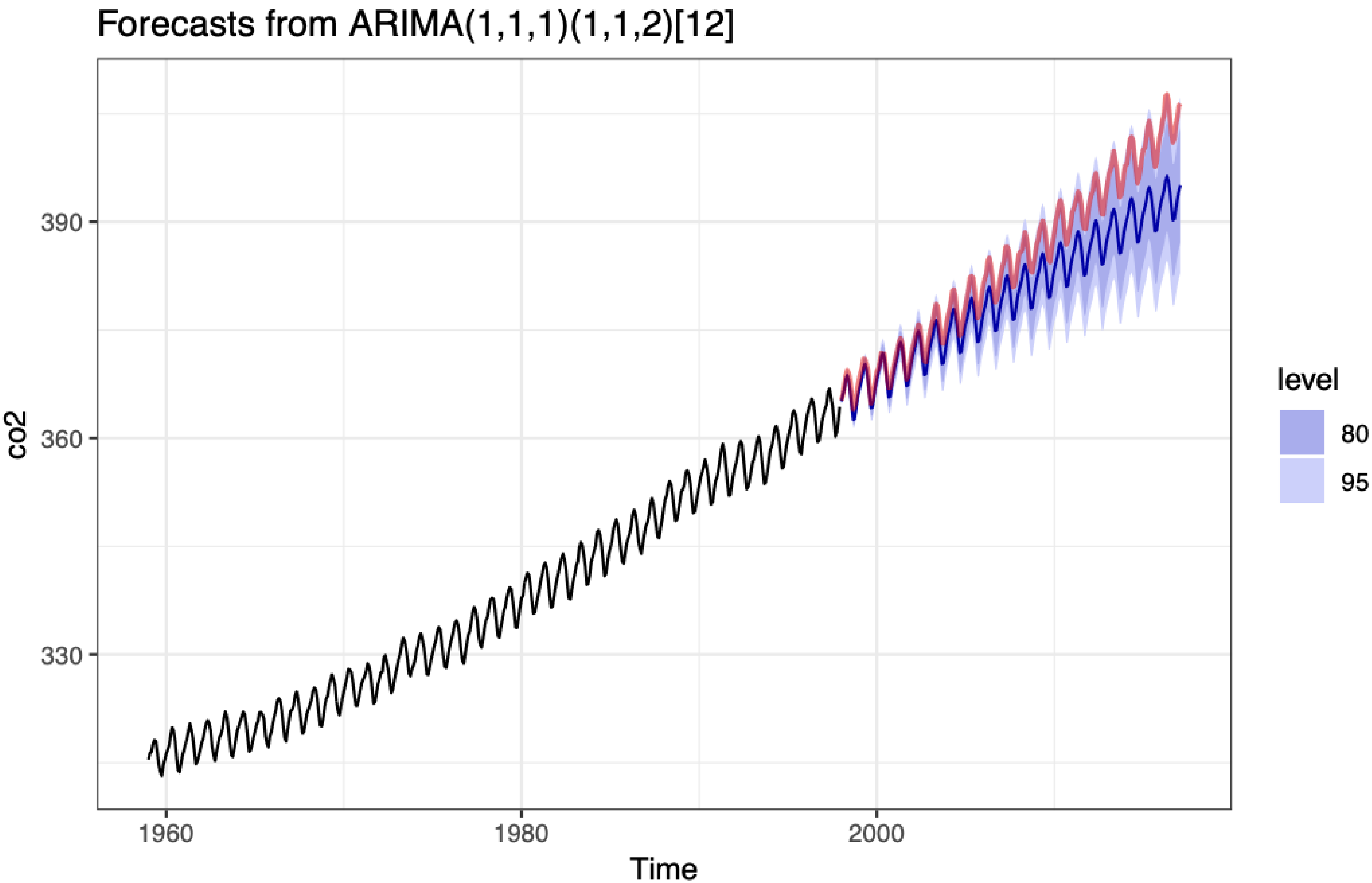
Forecast



Forecast components



ARIMA forecast



Model performance

Forecast dates	arima RMSE	gp RMSE
Jan 1998 - Jan 2003	1.10	1.91
Jan 1998 - Jan 2008	2.51	4.58
Jan 1998 - Jan 2013	3.82	7.71
Jan 1998 - Mar 2017	5.46	11.40