# Lecture 13

## Gaussian Process Models - Part 2

3/06/2018

# EDA and GPs

# Variogram

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Variogram:

$$2\gamma(t_i, t_j) = Var(Y(t_i) - Y(t_j))$$

where $\gamma(t_i, t_j)$ is known as the semivariogram.

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- are non-negative

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$$2\gamma(t_i, t_j) = 2Var(Y(t_i)) - 2\,Cov(Y(t_i), Y(t_j))$$

# Empirical Semivariogram

We will assume that our process of interest is stationary, in which case we will parameterize the semivariagram in terms of $h = |t_i - t_j|$.

Empirical Semivariogram:

$$\hat{\gamma}(h) = \frac{1}{2\,N(h)} \sum_{|t_i - t_j| \in (h-\epsilon, h+\epsilon)} (Y(t_i) - Y(t_j))^2$$

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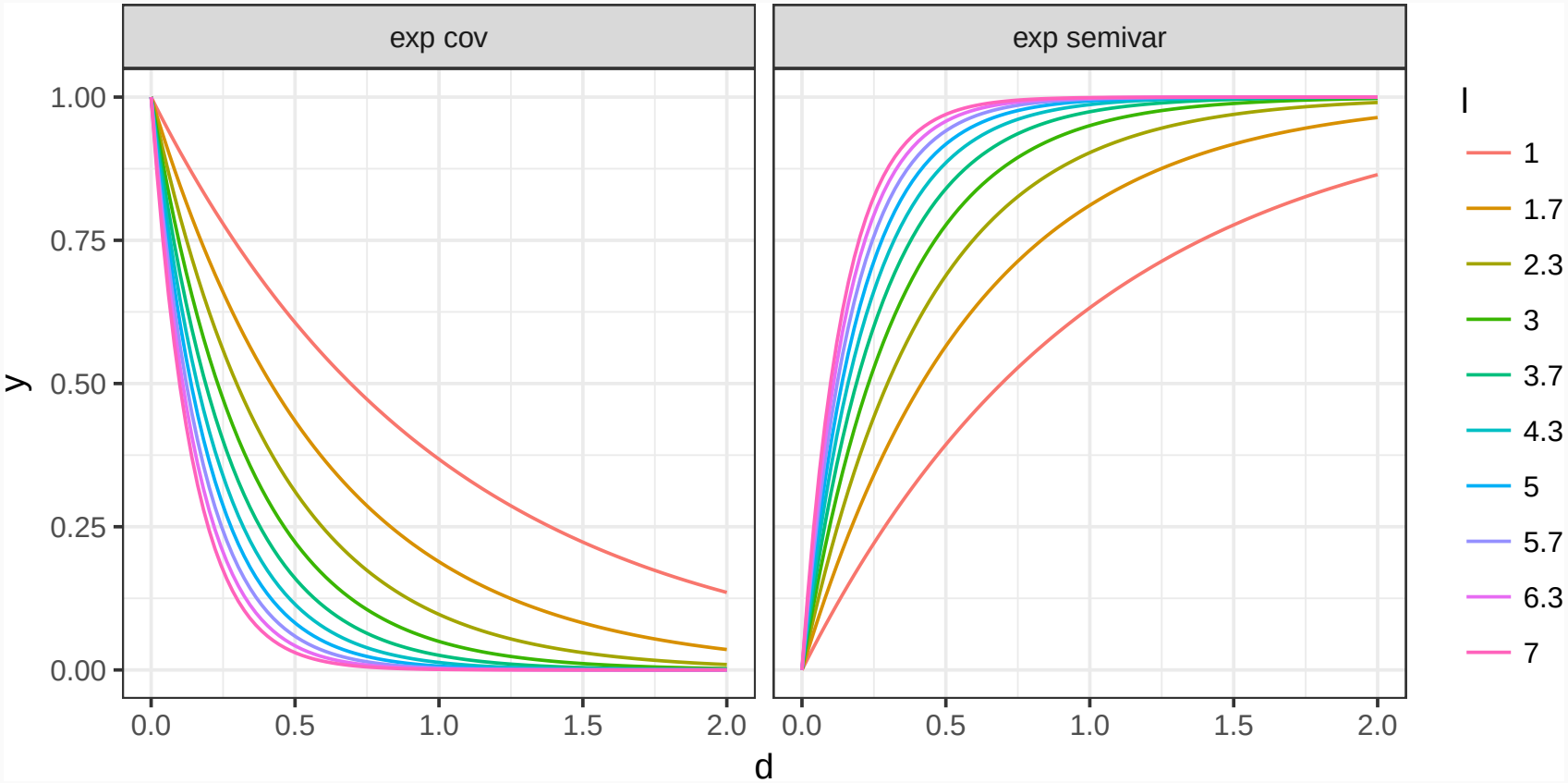
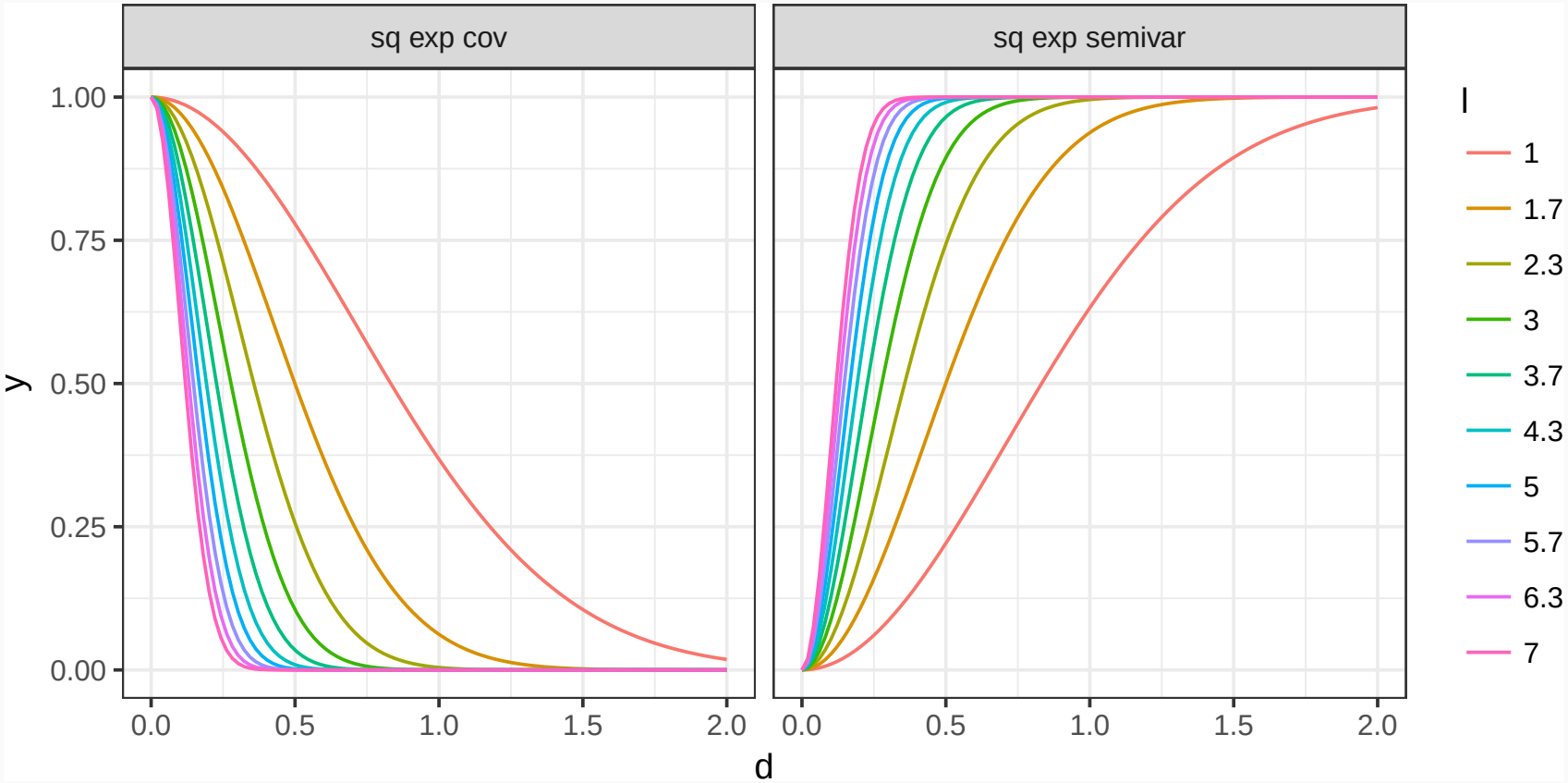
Practically, for any data set with $n$ observations there are $\binom{n}{2} + n$ possible data pairs to examine. Each individually is not very informative, so we aggregate into bins and calculate the empirical semivariogram for each bin.

# Connection to Covariance

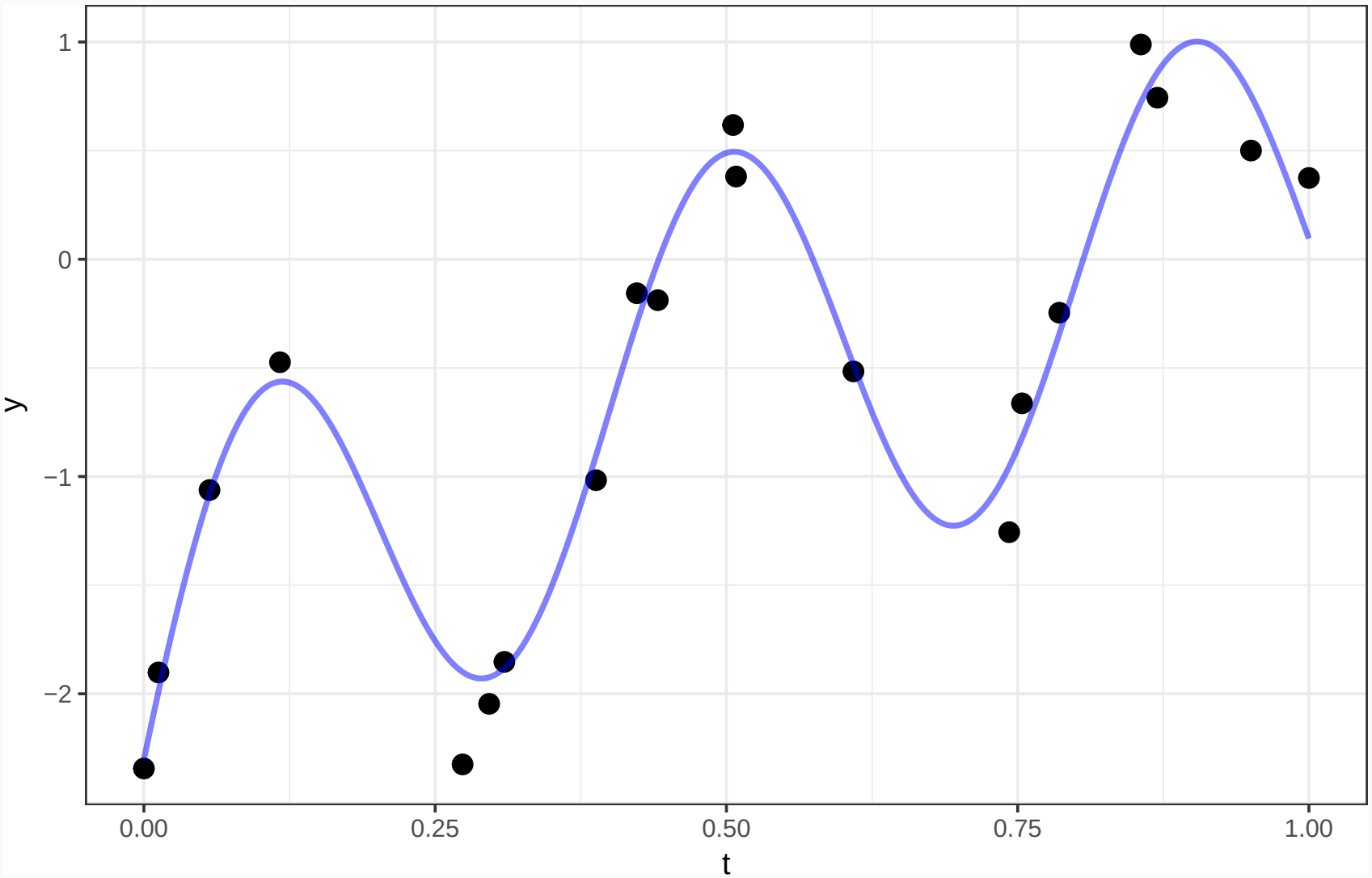
# Covariance vs Semivariogram - Exponential



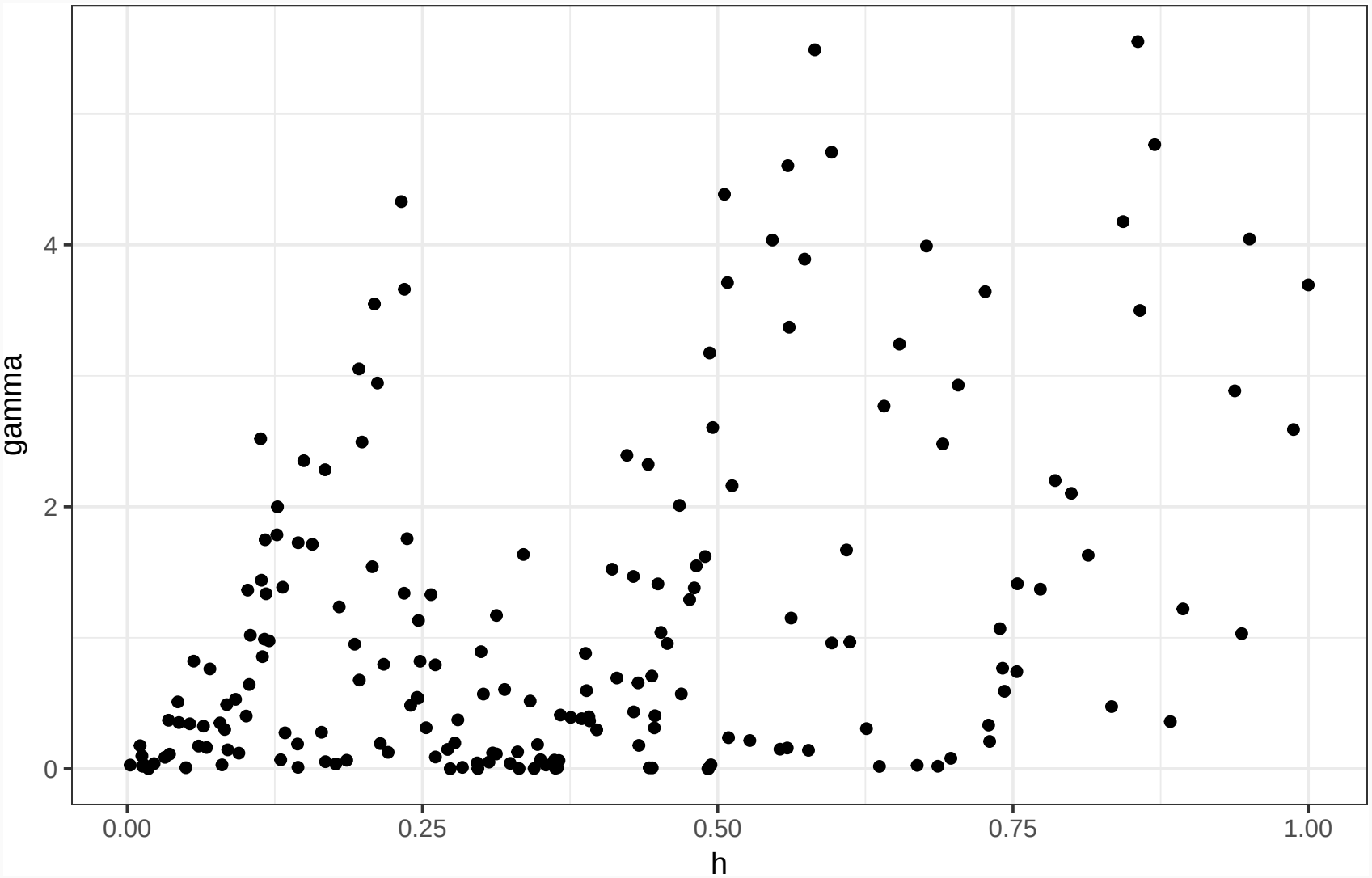
# Covariance vs Semivariogram - Square Exponential



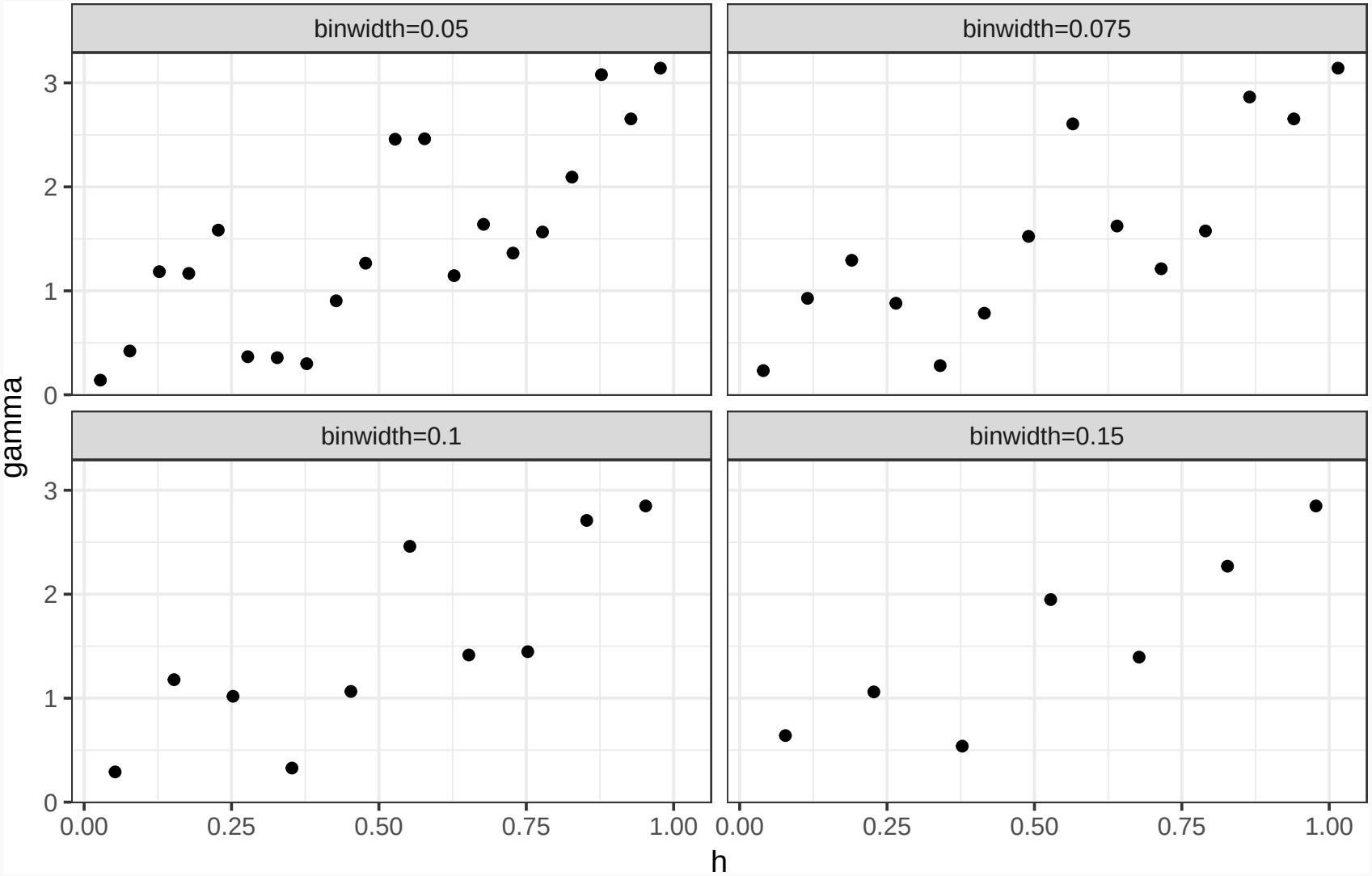
# From last time



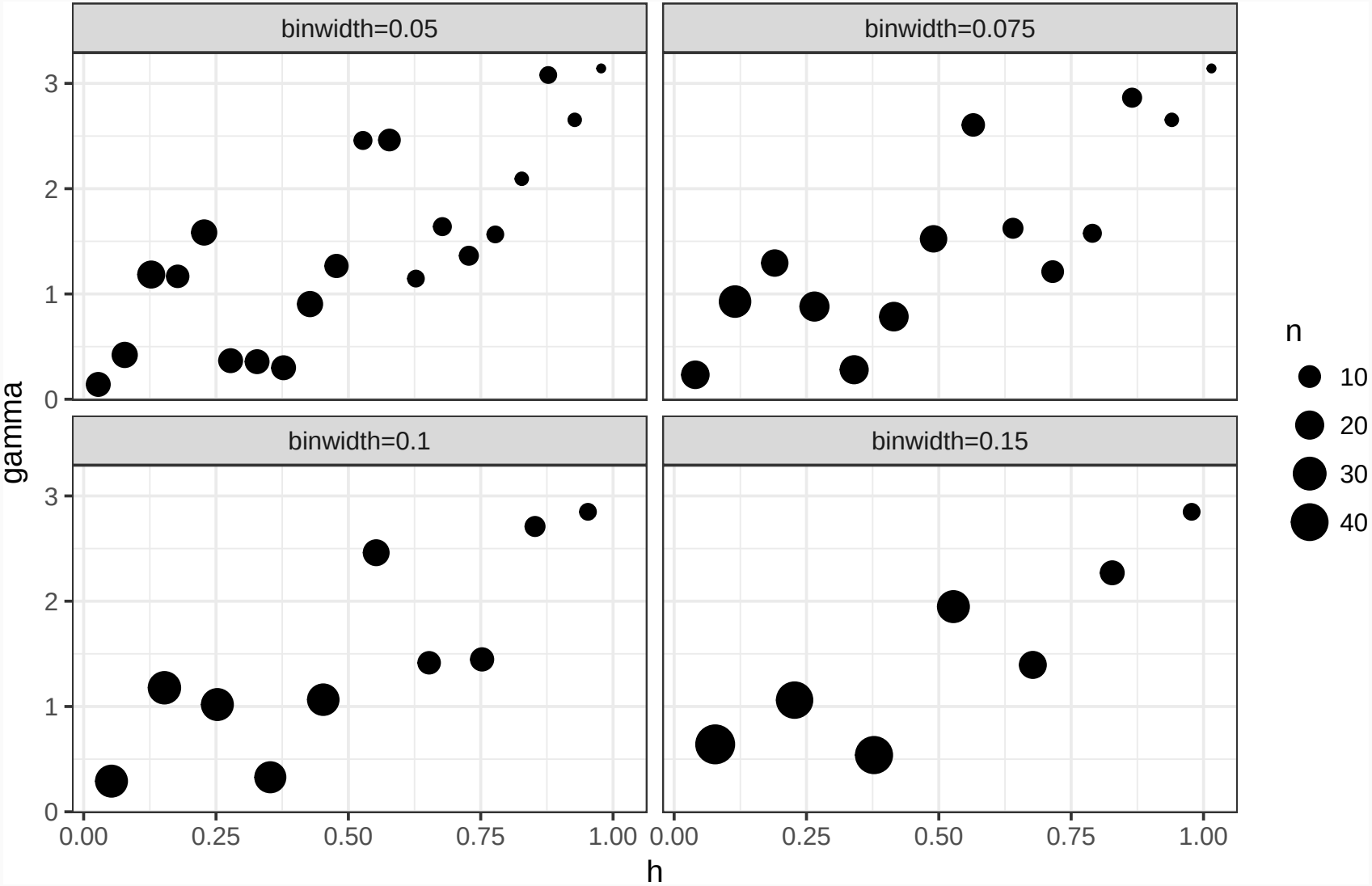
# Empirical semivariogram - no bins / cloud



# Empirical semivariogram (binned)



# Empirical semivariogram (binned + n)



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After fitting the model last time we came up with a posterior median of $\sigma^2 = 1.89$ and $l = 5.86$ for a square exponential covariance.

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\begin{aligned}
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\gamma(h) &= \sigma^2 - \sigma^2 \exp\left(-(h\,l)^2\right) \\
&= 1.89 - 1.89 \exp\left(-(5.86\,h)^2\right)
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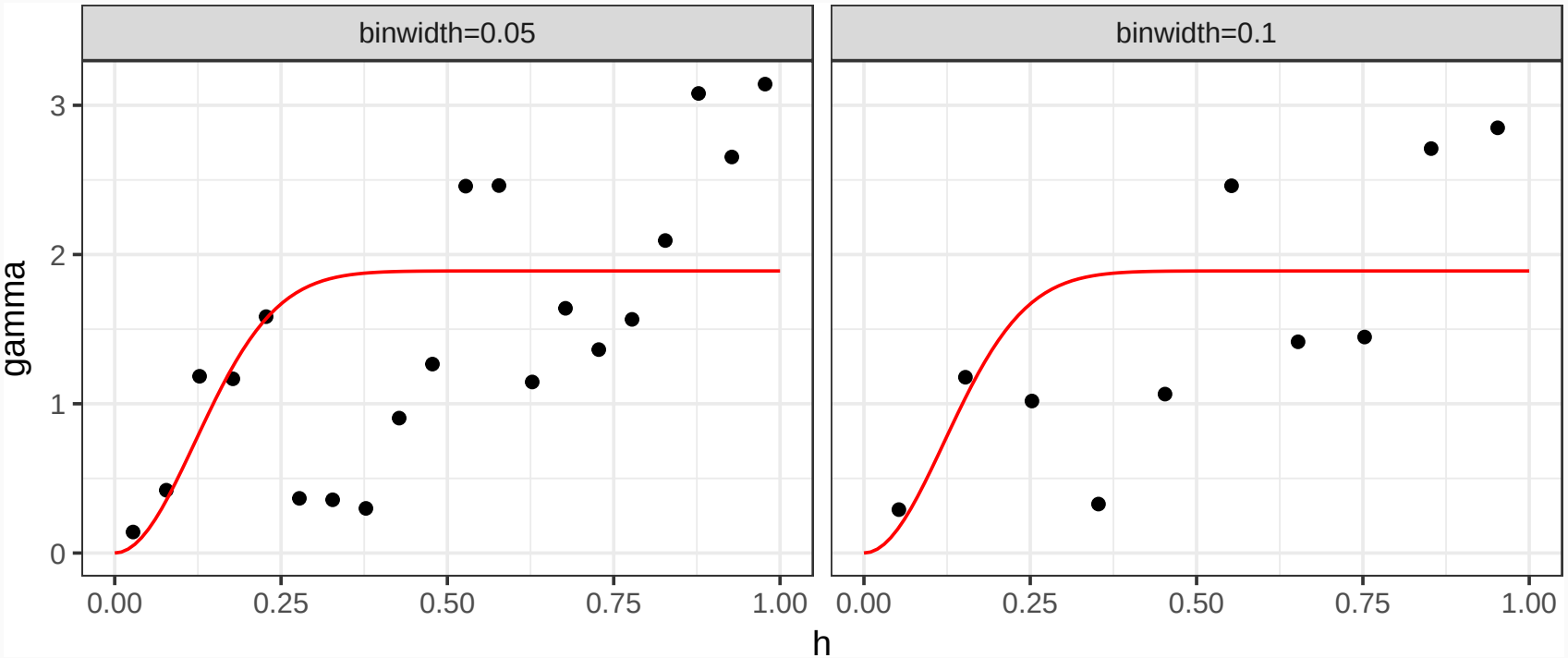
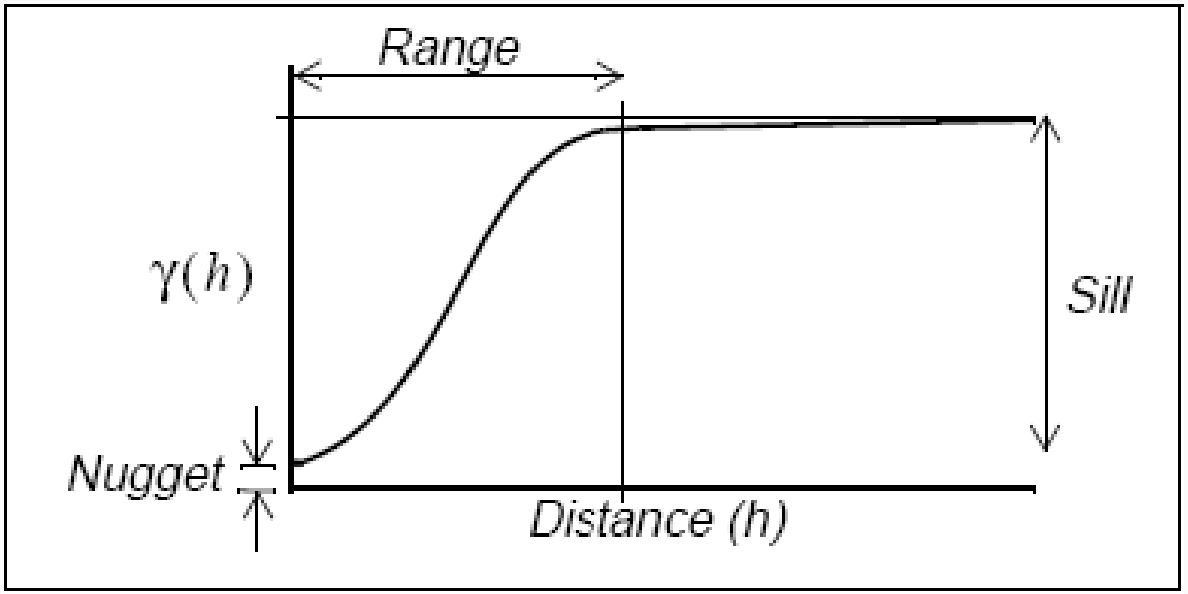


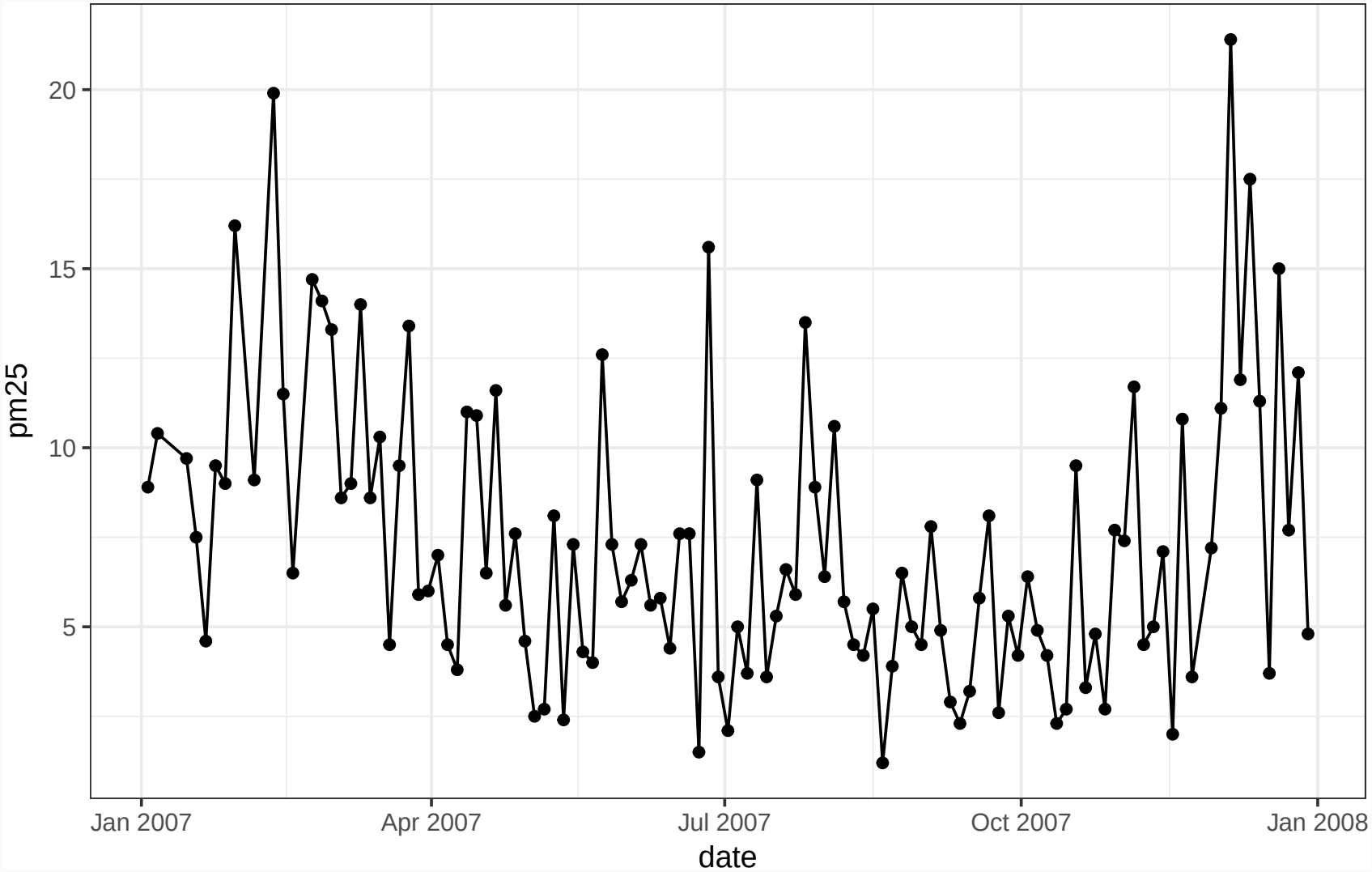
# Variogram features



# PM2.5 Example

# FRN Data

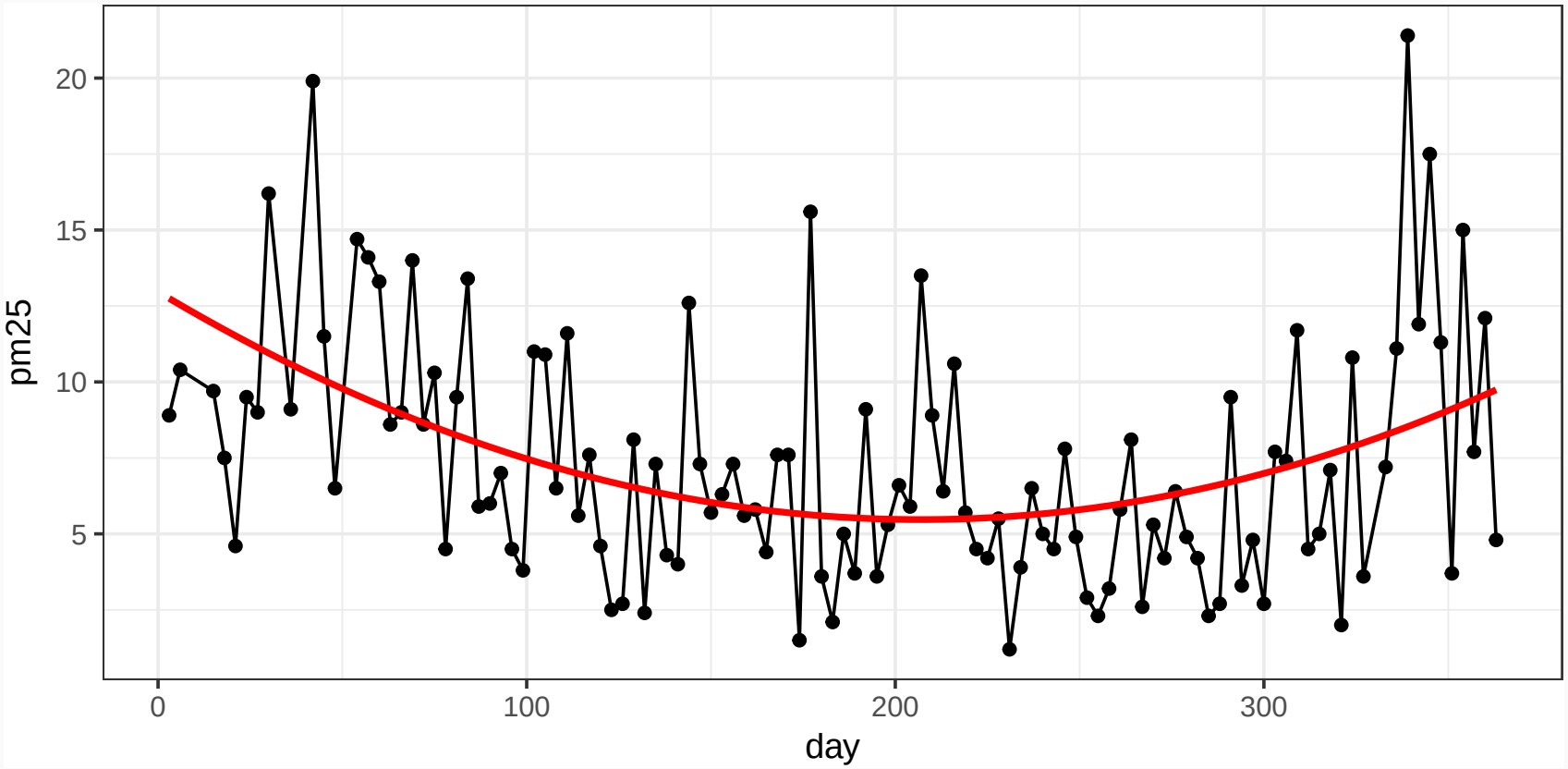
Measured PM2.5 data from an EPA monitoring station in Columbia, NJ.



# FRN Data

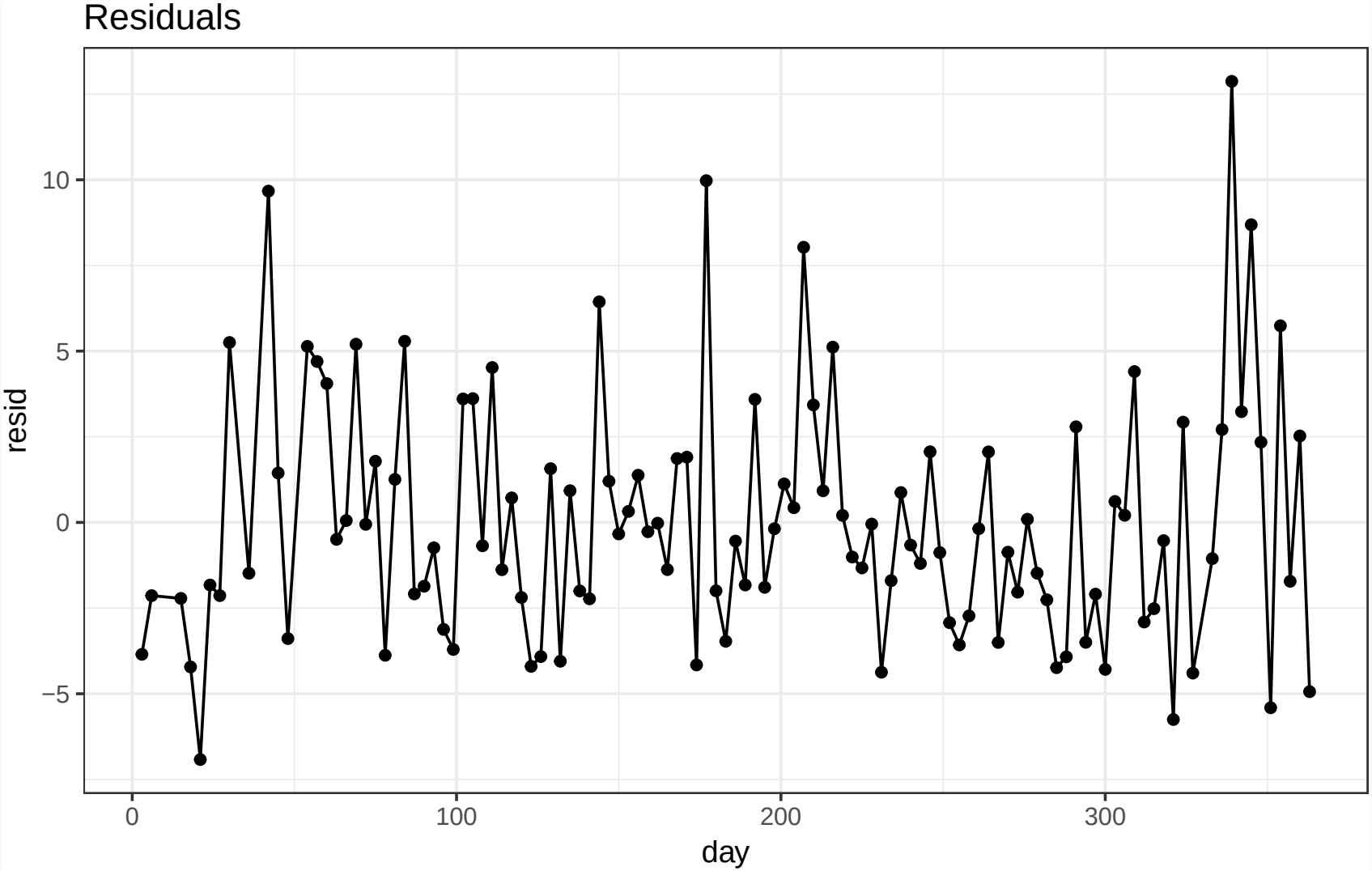
| site | latitude | longitude | pm25 | date | day |
|---|---|---|---|---|---|
| 230031011 | 46.682 | -68.016 | 8.9 | 2007-01-03 | 3 |
| 230031011 | 46.682 | -68.016 | 10.4 | 2007-01-06 | 6 |
| 230031011 | 46.682 | -68.016 | 9.7 | 2007-01-15 | 15 |
| 230031011 | 46.682 | -68.016 | 7.5 | 2007-01-18 | 18 |
| 230031011 | 46.682 | -68.016 | 4.6 | 2007-01-21 | 21 |
| 230031011 | 46.682 | -68.016 | 9.5 | 2007-01-24 | 24 |
| 230031011 | 46.682 | -68.016 | 9.0 | 2007-01-27 | 27 |
| 230031011 | 46.682 | -68.016 | 16.2 | 2007-01-30 | 30 |
| 230031011 | 46.682 | -68.016 | 9.1 | 2007-02-05 | 36 |
| 230031011 | 46.682 | -68.016 | 19.9 | 2007-02-11 | 42 |
| 230031011 | 46.682 | -68.016 | 11.5 | 2007-02-14 | 45 |
| 230031011 | 46.682 | -68.016 | 6.5 | 2007-02-17 | 48 |
| 230031011 | 46.682 | -68.016 | 14.7 | 2007-02-23 | 54 |
| 230031011 | 46.682 | -68.016 | 14.1 | 2007-02-26 | 57 |
| 230031011 | 46.682 | -68.016 | 13.3 | 2007-03-01 | 60 |
| 230031011 | 46.682 | -68.016 | 8.6 | 2007-03-04 | 63 |
| 230031011 | 46.682 | -68.016 | 9.0 | 2007-03-07 | 66 |
| 230031011 | 46.682 | -68.016 | 14.0 | 2007-03-10 | 69 |
| 230031011 | 46.682 | -68.016 | 8.6 | 2007-03-13 | 72 |
| 230031011 | 46.682 | -68.016 | 10.3 | 2007-03-16 | 75 |

# Mean Model

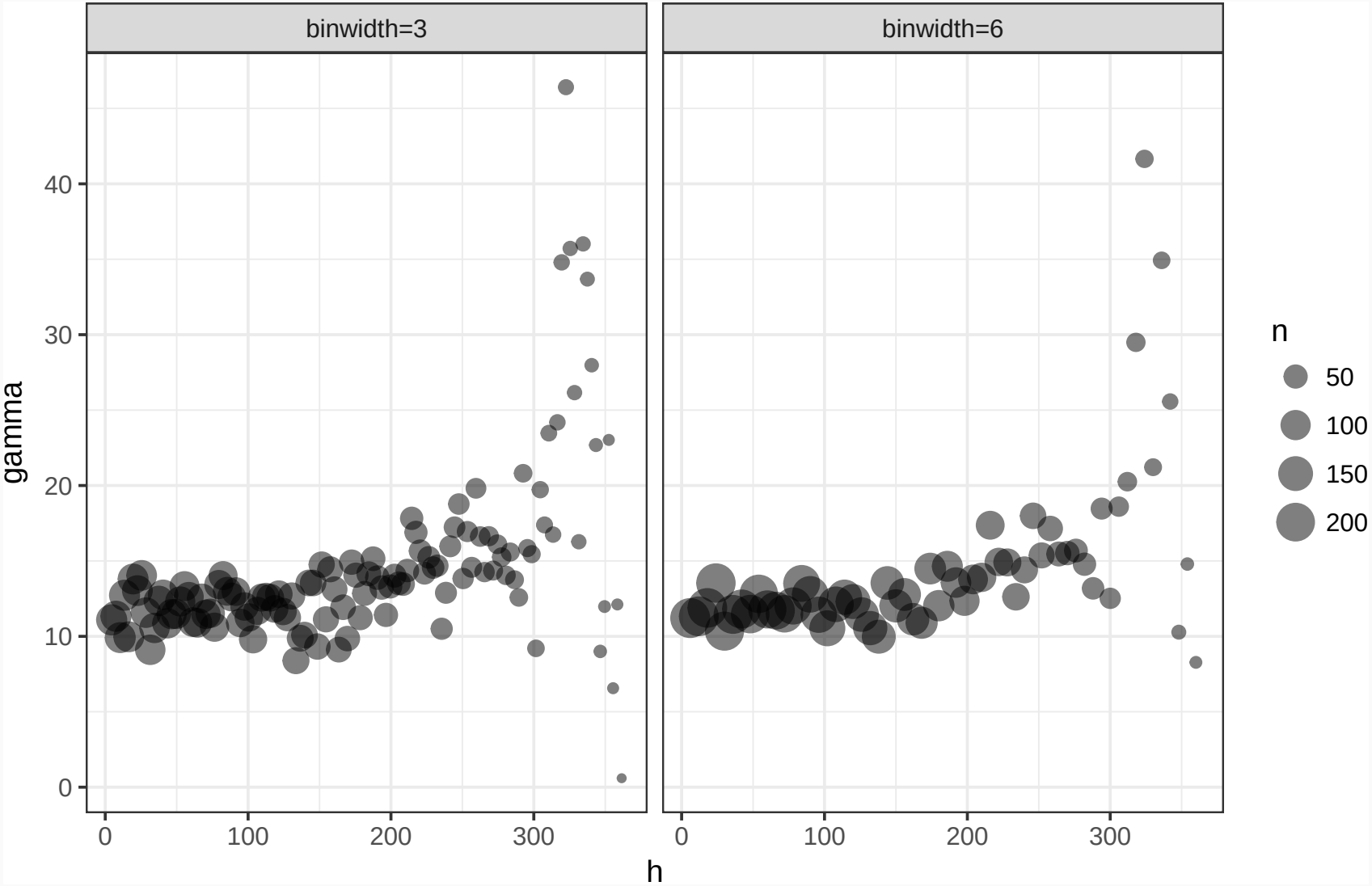



```
##
## Call:
## lm(formula = pm25 ~ day + I(day^2), data = pm25)
##
## Coefficients:
## (Intercept)          day     I(day^2)
##  12.9644351   -0.0724639    0.0001751
##
```

# Detrended Residuals



# Empirical Variogram



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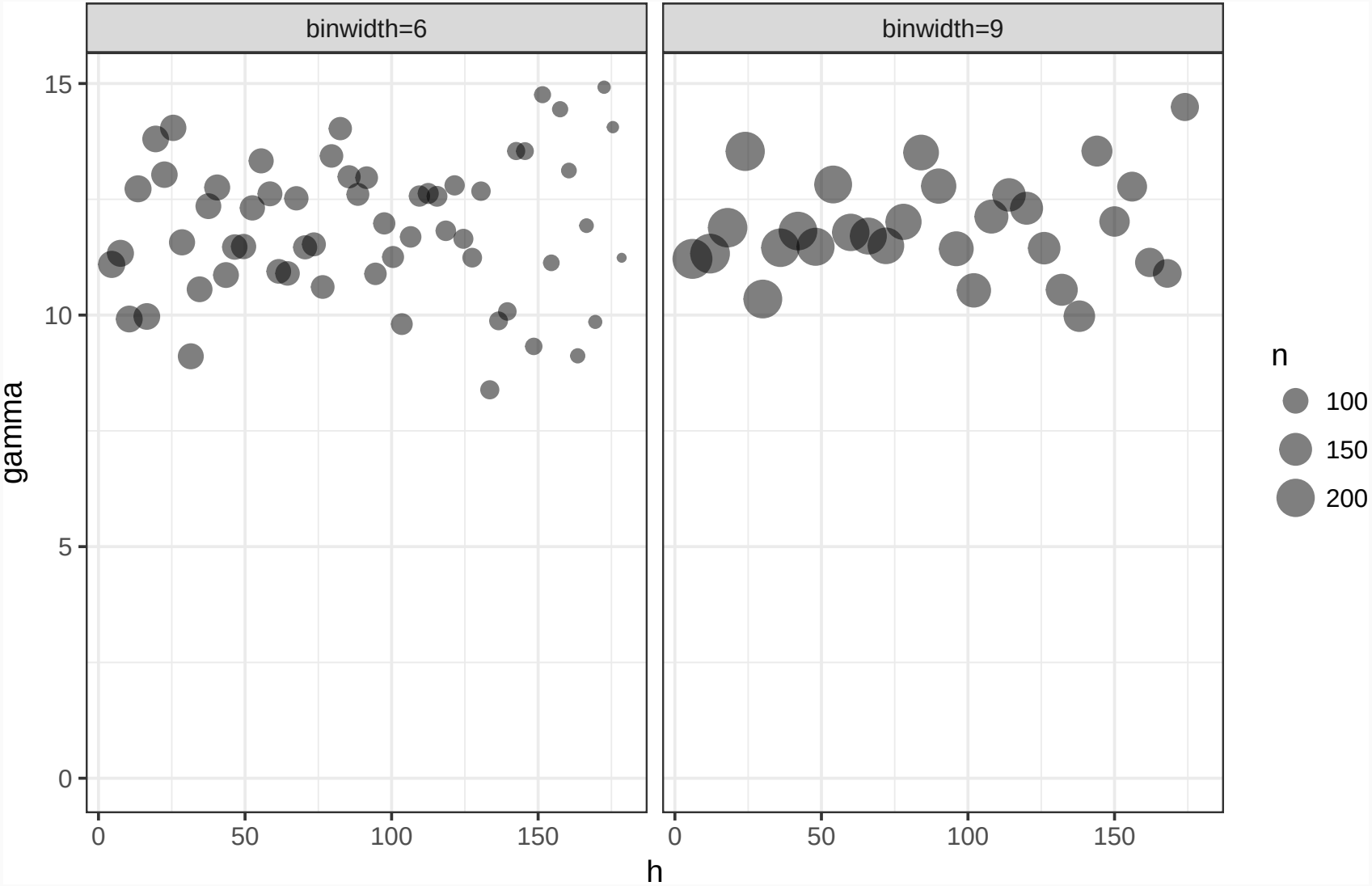

# Model

What does the model we are trying to fit actually look like?

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What does the model we are trying to fit actually look like?

$$y(t) = \mu(t) + w(t) + \epsilon(t)$$

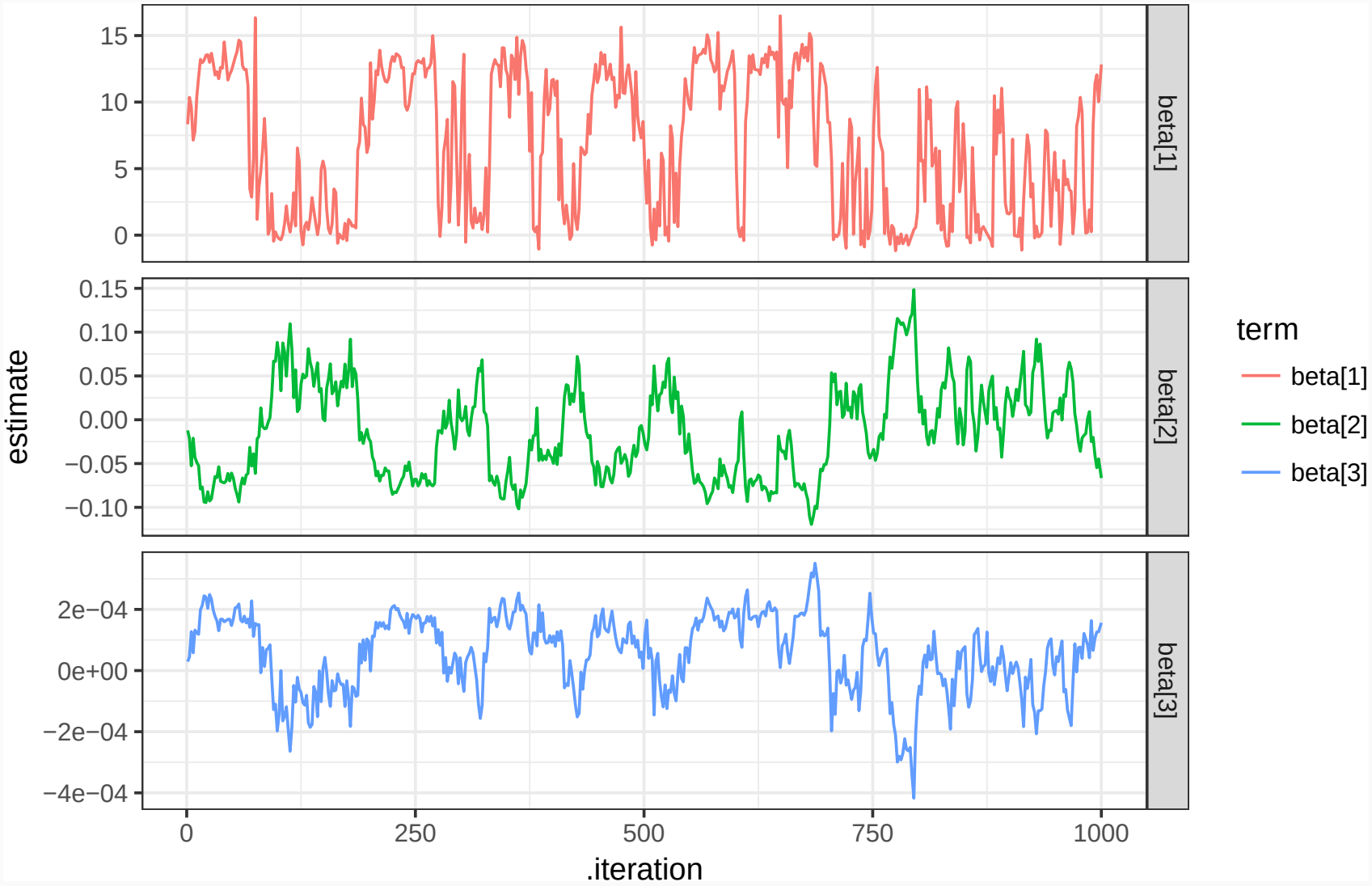
where

$$\begin{aligned}
\boldsymbol{\mu}(\mathbf{t}) &= \beta_0 + \beta_1\,\mathbf{t} + \beta_2\,\mathbf{t}^2 \\
\mathbf{w}(\mathbf{t}) &\sim \mathcal{GP}(0, \boldsymbol{\Sigma}) \\
\epsilon(t) &\sim \mathcal{N}(0, \sigma_w^2)
\end{aligned}$$

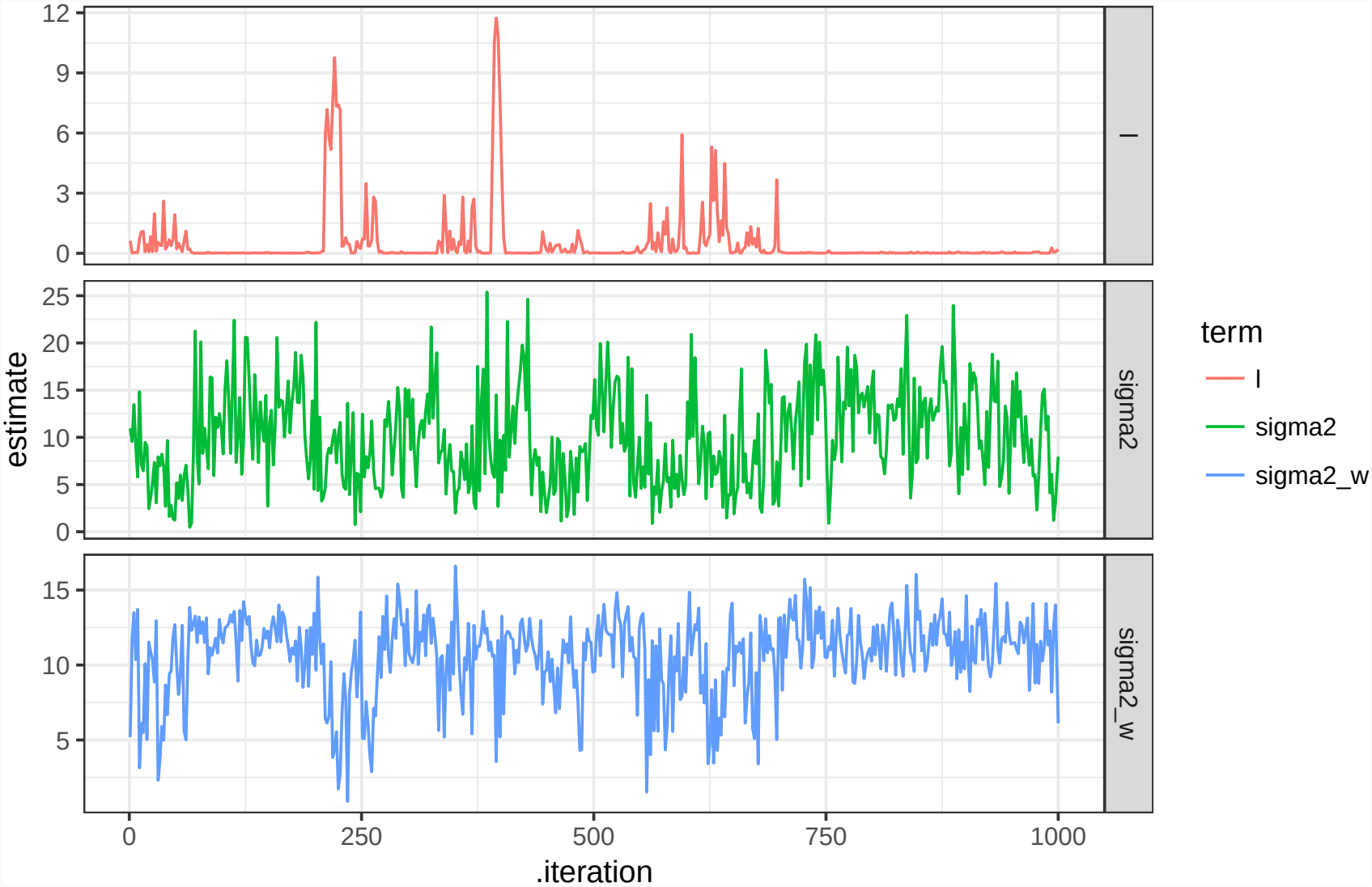
# JAGS Model

```
gp_exp_model = "model{
  y ~ dmnorm(mu, inverse(Sigma))

  for (i in 1:N) {
    mu[i] <- beta[1]+ beta[2] * x[i] + beta[3] * x[i]^2
  }

  for (i in 1:(N-1)) {
    for (j in (i+1):N) {
      Sigma[i,j] <- sigma2 * exp(- pow(l*d[i,j],2))
      Sigma[j,i] <- Sigma[i,j]
    }
  }

  for (k in 1:N) {
    Sigma[k,k] <- sigma2 + sigma2_w
  }

  for (i in 1:3) {
    beta[i] ~ dt(0, 2.5, 1)
  }
  sigma2_w ~ dnorm(10, 1/25) T(0,)
  sigma2   ~ dnorm(10, 1/25) T(0,)
  l        ~ dt(0, 2.5, 1) T(0,)
}"
```

# Posterior - Betas



# Posterior - Covariance Parameters



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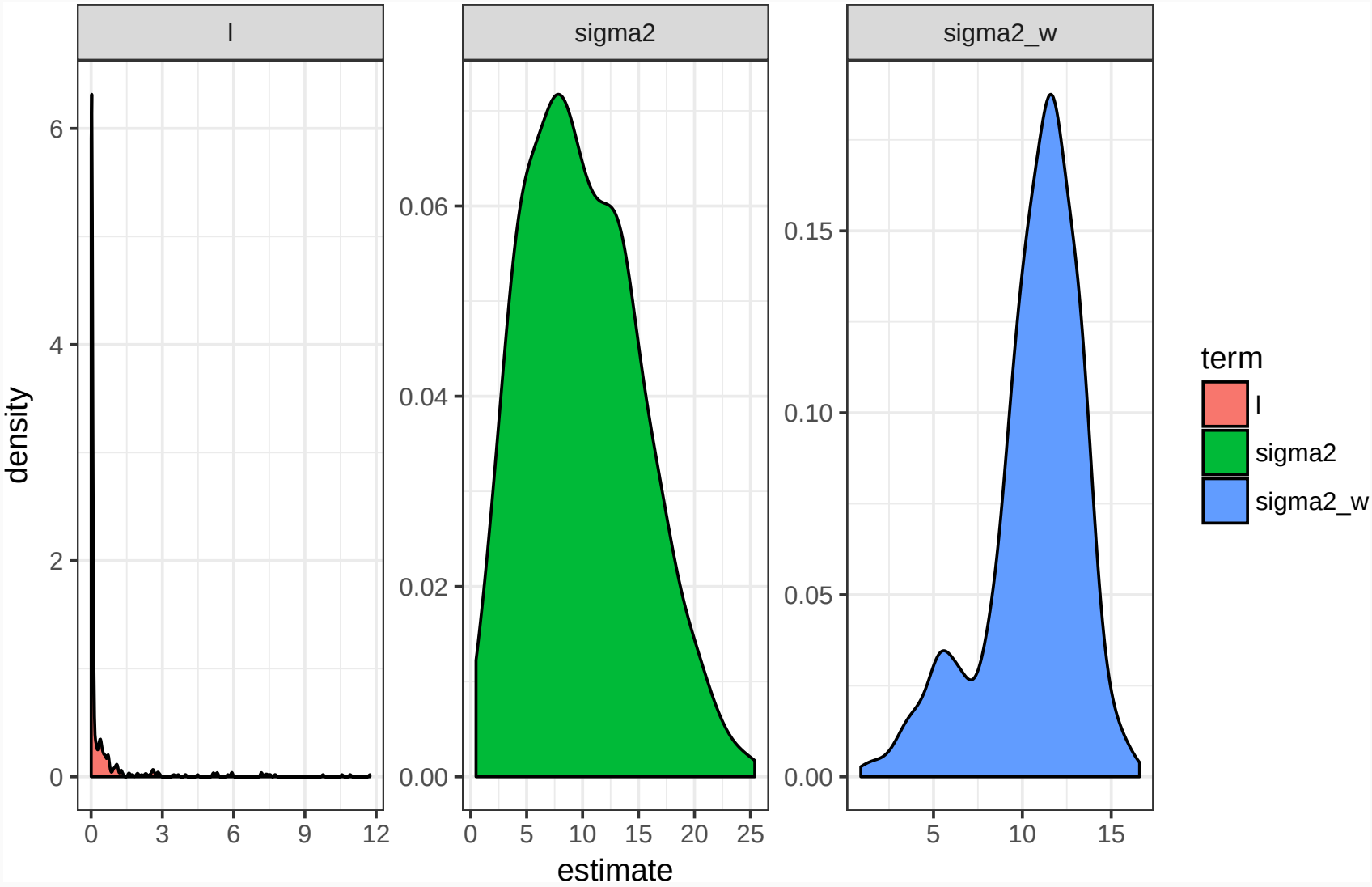
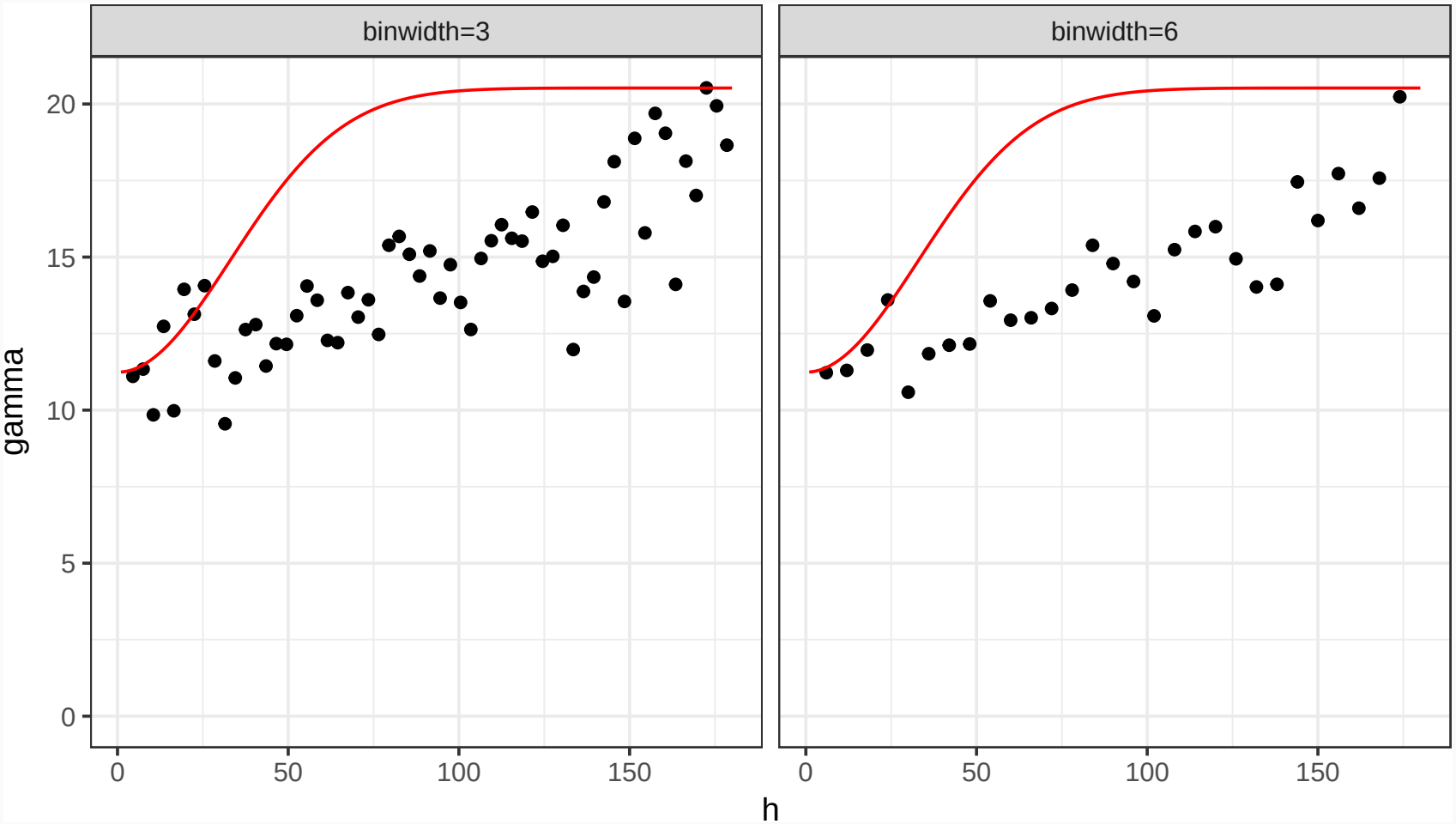


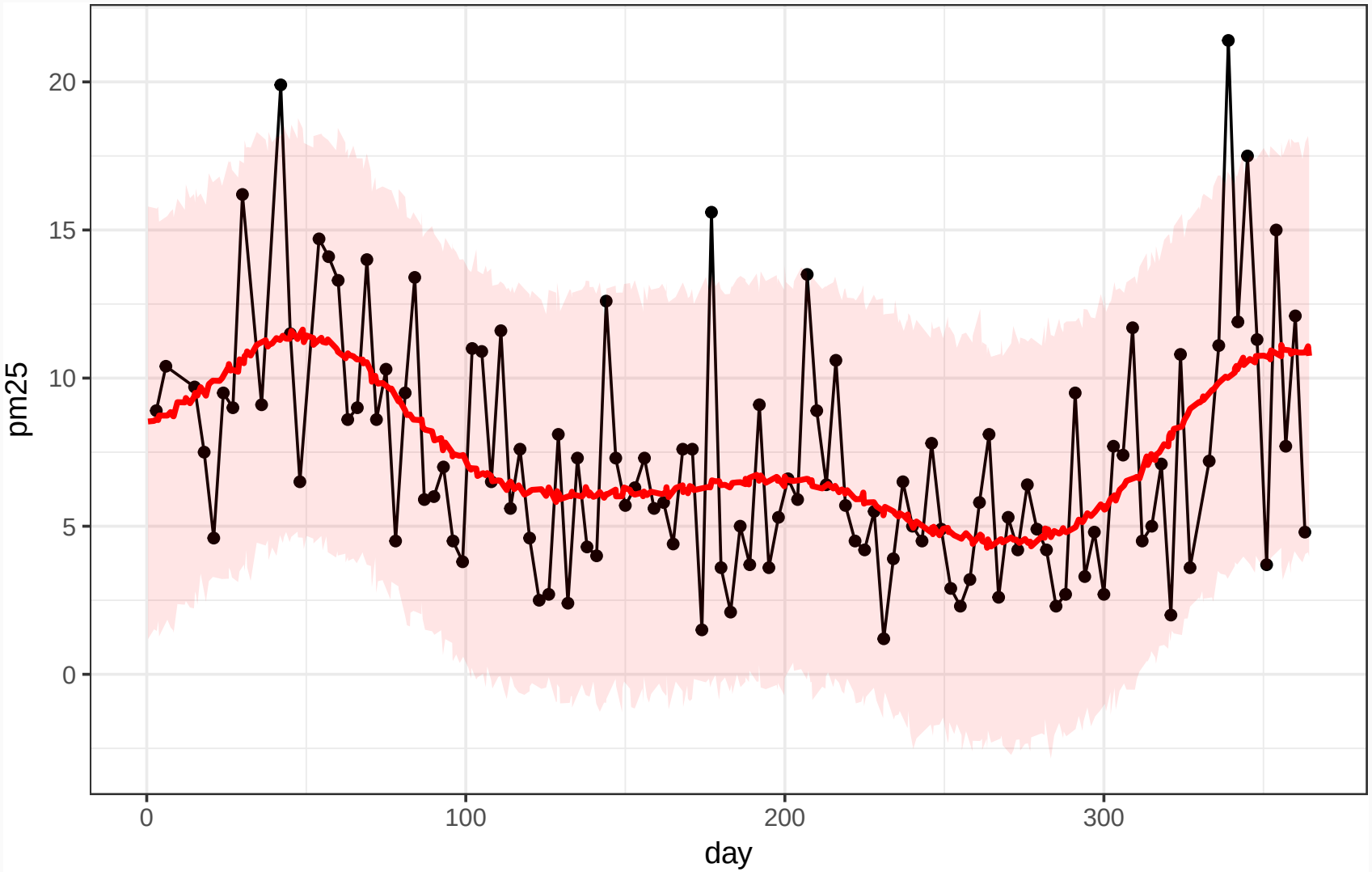
# Posterior

| term | post_mean | post_med | post_lower | post_upper |
|---|---|---|---|---|
| beta[1] | 6.922 | 7.624 | -0.720 | 14.369 |
| beta[2] | -0.015 | -0.018 | -0.091 | 0.092 |
| beta[3] | 0.000 | 0.000 | 0.000 | 0.000 |
| l | 0.462 | 0.021 | 0.007 | 5.303 |
| sigma2 | 9.862 | 9.284 | 1.610 | 20.555 |
| sigma2_w | 10.748 | 11.239 | 3.832 | 14.693 |

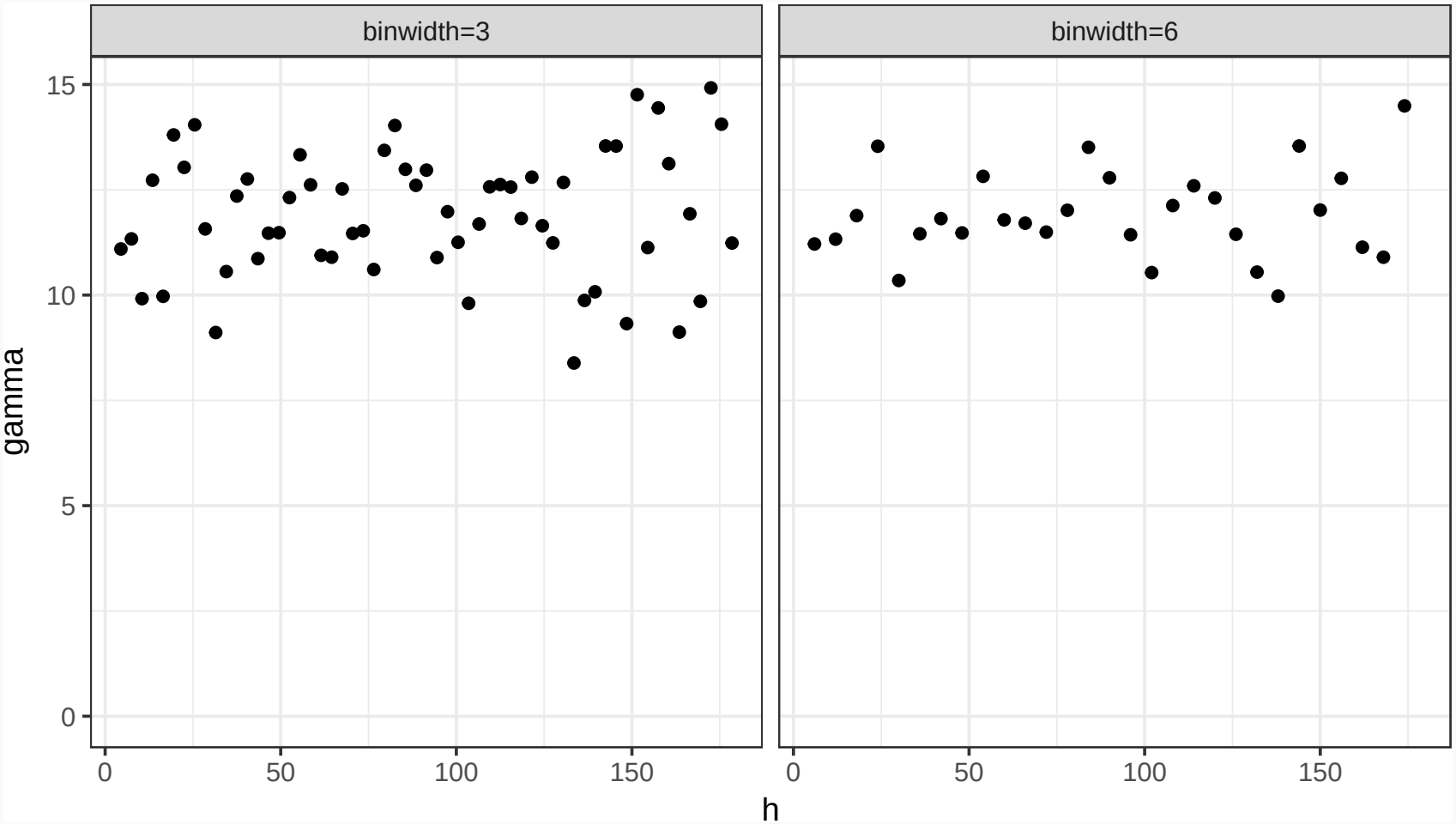
# Empirical + Fitted Variogram



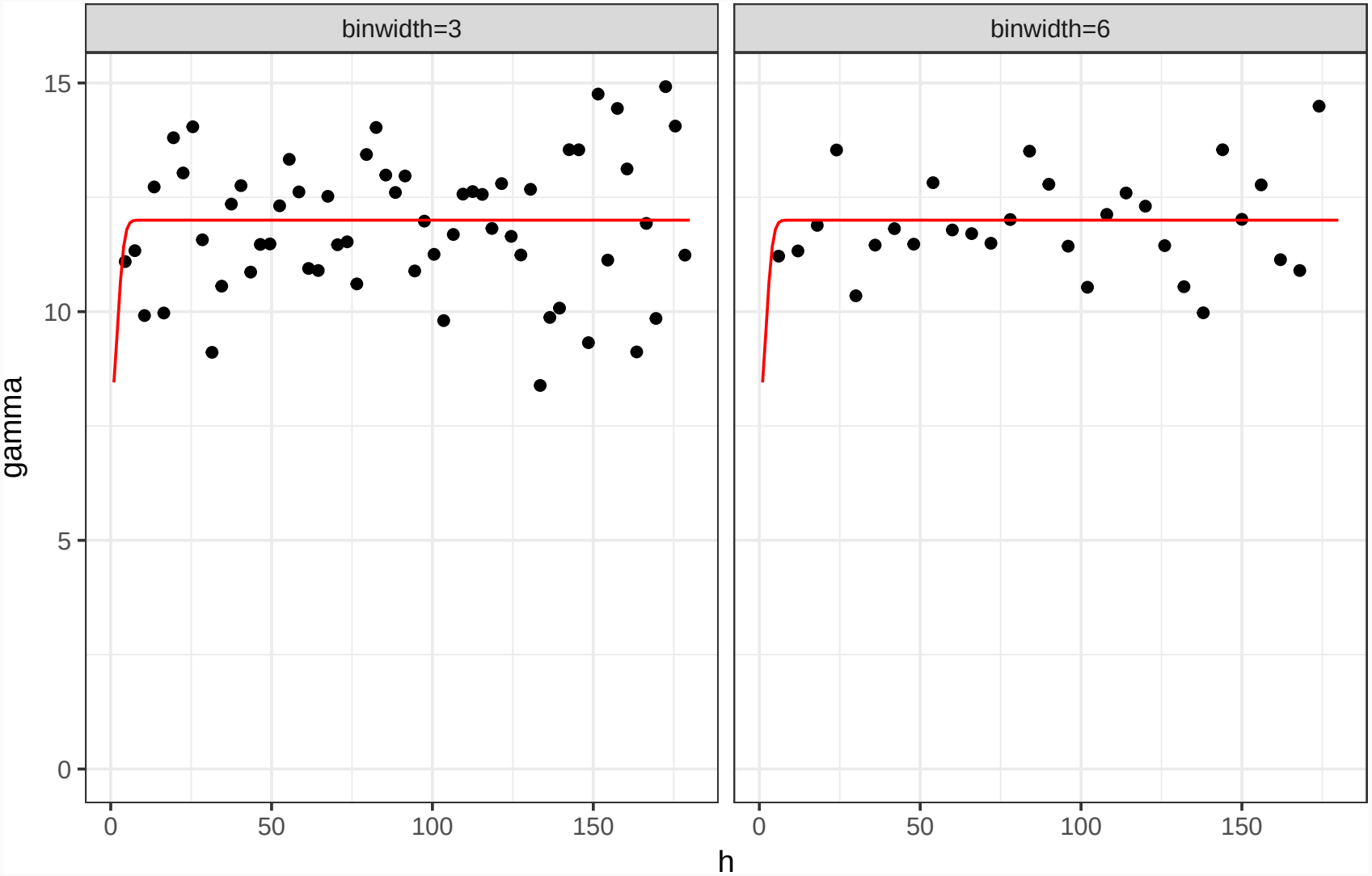
# Fitted Model + Predictions



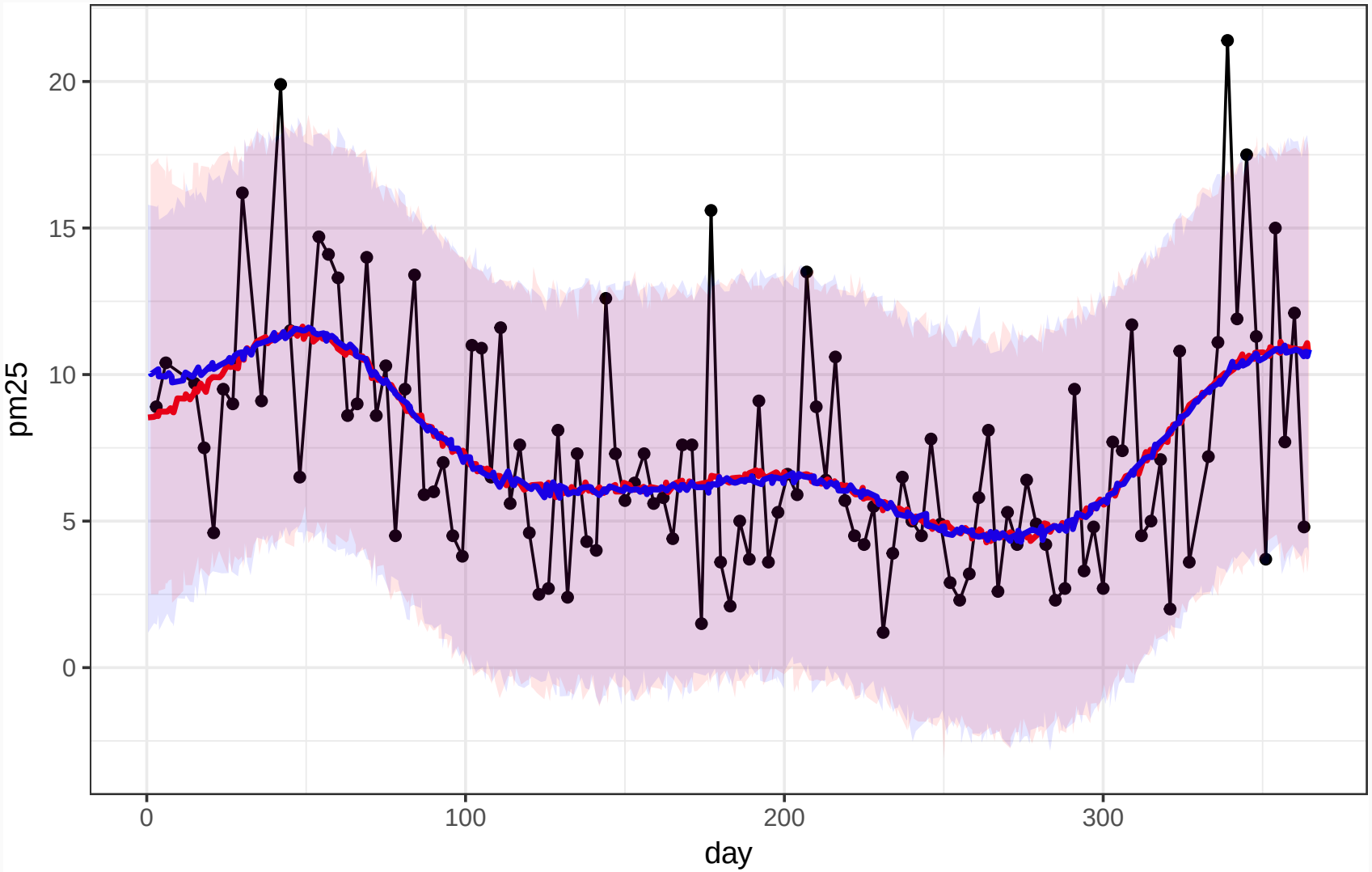
# Empirical Variogram Model



# Fit



# Predictions



# Full Posterior Predictive Distribution

# Plug in Prediction

```
l        = filter(post, term == 'l')        %>% pull(post_med)
sigma2   = filter(post, term == 'sigma2')   %>% pull(post_med)
sigma2_w = filter(post, term == 'sigma2_w') %>% pull(post_med)
beta0    = filter(post, term == 'beta[1]') %>% pull(post_med)
beta1    = filter(post, term == 'beta[2]') %>% pull(post_med)
beta2    = filter(post, term == 'beta[3]') %>% pull(post_med)

reps=1000

x = pm25$day
y = pm25$pm25
x_pred = 1:365 + rnorm(365, 0.01)

mu = beta0 + beta1*x + beta2*x^2
mu_pred = beta0 + beta1*x_pred + beta2*x_pred^2

dist_o = fields::rdist(x)
dist_p = fields::rdist(x_pred)
dist_op = fields::rdist(x, x_pred)
dist_po = t(dist_op)

cov_o  = sq_exp_cov(dist_o,  sigma2 = sigma2, l = l) + nugget_cov(dist_o, sigma2 = sig
cov_p  = sq_exp_cov(dist_p,  sigma2 = sigma2, l = l) + nugget_cov(dist_p, sigma2 = sig
cov_op = sq_exp_cov(dist_op, sigma2 = sigma2, l = l) + nugget_cov(dist_op, sigma2 = si
cov_po = sq_exp_cov(dist_po, sigma2 = sigma2, l = l) + nugget_cov(dist_po, sigma2 = si

inv = solve(cov_o, cov_op)
cond_cov = cov_p - cov_po %*% inv
```

# Full Posterior Predictive Distribution

Our posterior consists of samples from

$$l, \sigma^2, \sigma_w^2, \beta_0, \beta_1, \beta_2 \mid \mathbf{y}$$

and for the purposes of generating the posterior predictions we sampled

$$\mathbf{y}_{pred} \mid l^{(m)}, {\sigma^2}^{(m)}, {\sigma_w^2}^{(m)}, {\beta_0}^{(m)}, {\beta_1}^{(m)}, {\beta_2}^{(m)}, \mathbf{y}$$

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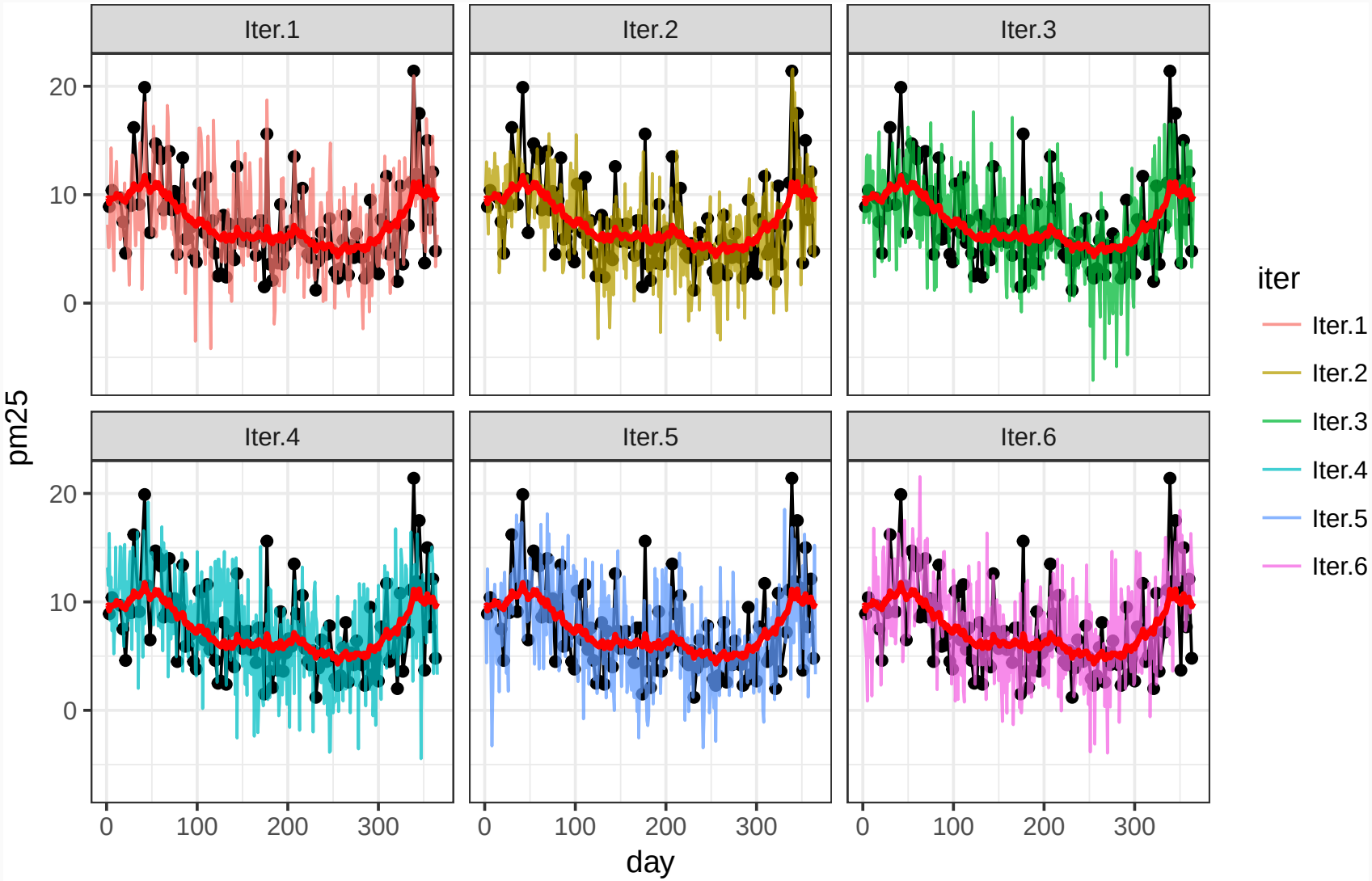
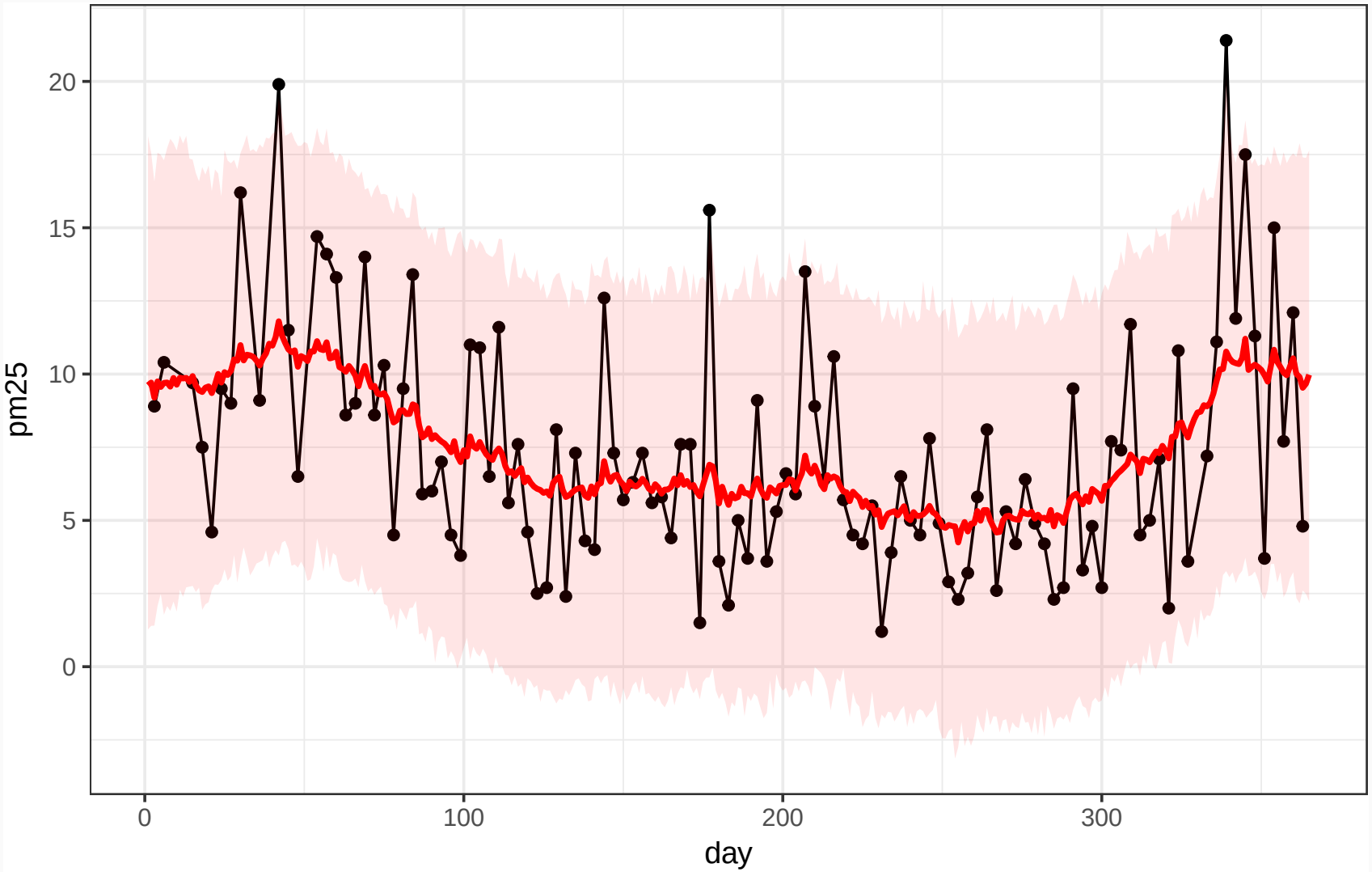
In practice we should instead be sampling

$$\mathbf{y}_{pred}^{(i)} \mid l^{(i)}, {\sigma^2}^{(i)}, {\sigma_w^2}^{(i)}, {\beta_0}^{(i)}, {\beta_1}^{(i)}, {\beta_2}^{(i)}, \mathbf{y}$$

since this takes into account the additional uncertainty in the model parameters.

# Full Posterior Predictive Distribution - Plots



# Full Posterior Predictive Distribution - Median + CI