Lecture 13

Gaussian Process Models - Part 2

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EDA and GPs

Variogram

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Variogram:

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2\gamma(t_i, t_j) &= Var(Y(t_i) - Y(t_j)) \\
&= E([(Y(t_i) - \mu(t_i)) - (Y(t_j) - \mu(t_j))]^2)
\end{aligned}
$$

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

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

If the process has constant mean (e.g. $\mu(t_i) = \mu(t_j)$ for all i and j) then we can simplify to

$$2\gamma(t_i, t_j) = E([Y(t_i) - Y(t_j)]^2)$$

Some Properties of the theoretical Variogram / Semivariogram

- both are non-negative

$$\gamma(t_i, t_j) \geq 0$$

- both are 0 at distance 0

$$\gamma(t_i, t_i) = 0$$

- both are symmetric

$$\gamma(t_i, t_j) = \gamma(t_j, t_i)$$

- there is no dependence if

$$2\gamma(t_i, t_j) = Var(Y(t_i)) + Var(Y(t_j)) \quad \text{for all } i \neq j$$

- if the process *is not* stationary

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

- if the process *is* stationary

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

Empirical Semivariogram

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

Empirical Semivariogram:

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

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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.

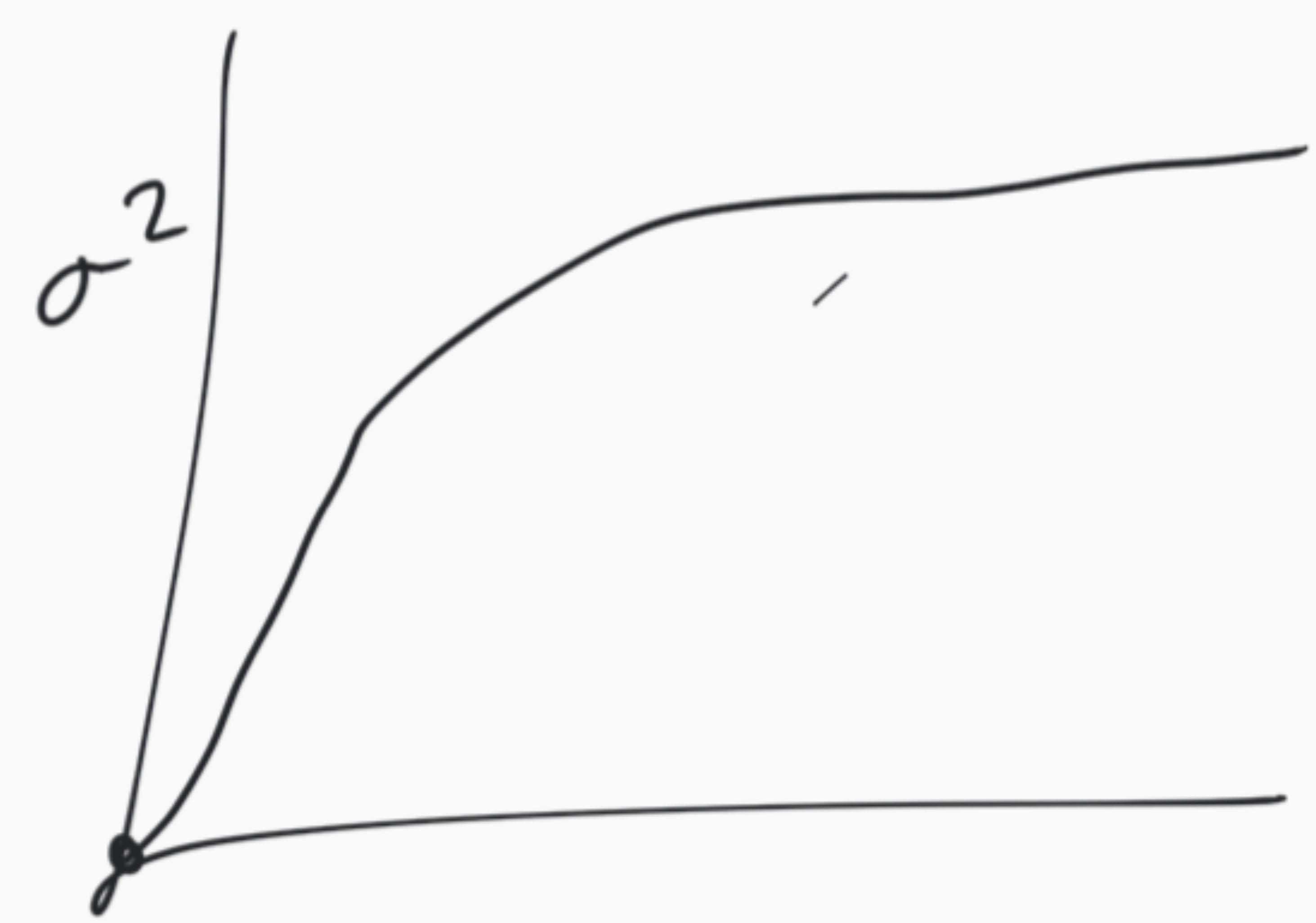
Connection to Covariance

In stationary case

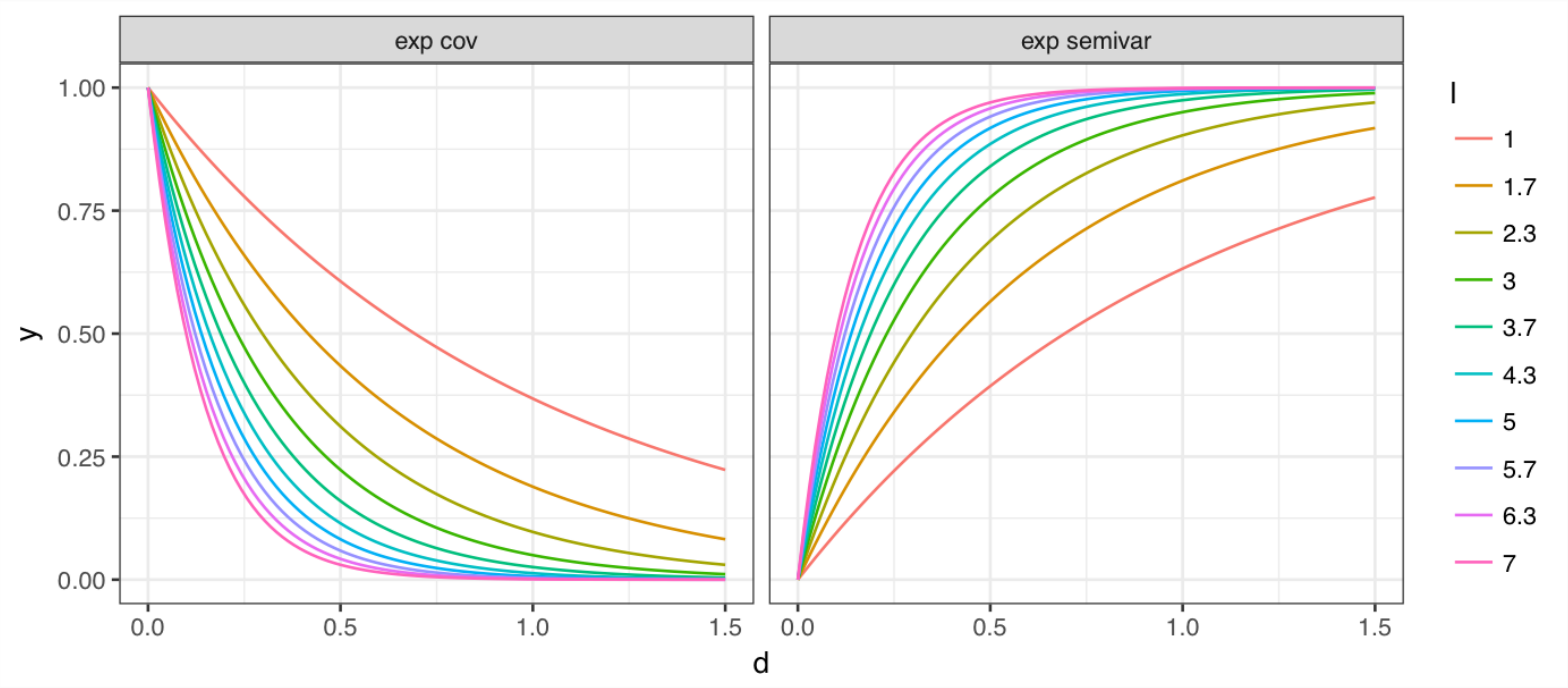
$$\gamma(h) = Var(y_t) - Cov(h)$$
$$= Cov(0) - Cov(h)$$
$$= \sigma^2 - \sigma^2 e^{-h\ell}$$

Exp Cov

$$Cov(h) = \sigma^2 e^{-h\ell}$$

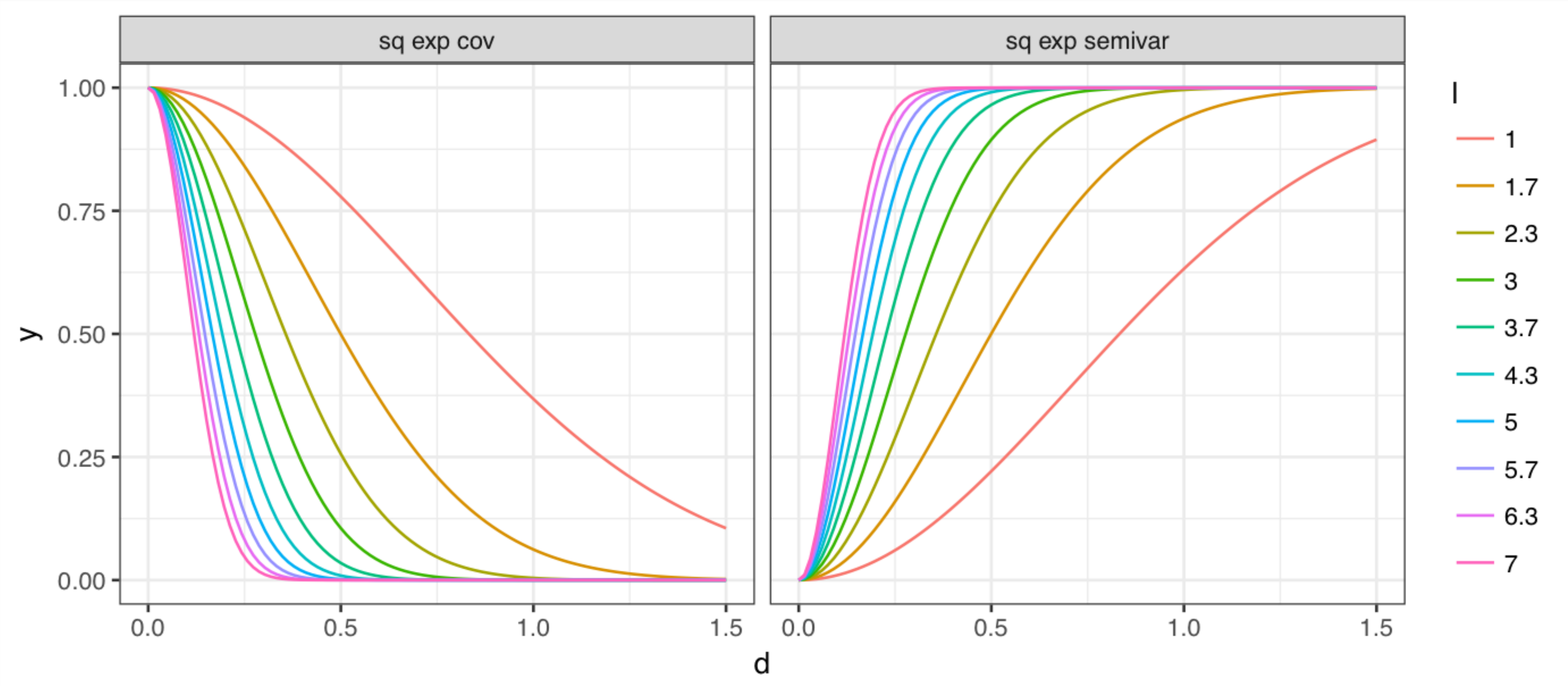


Covariance vs Semivariogram - Exponential

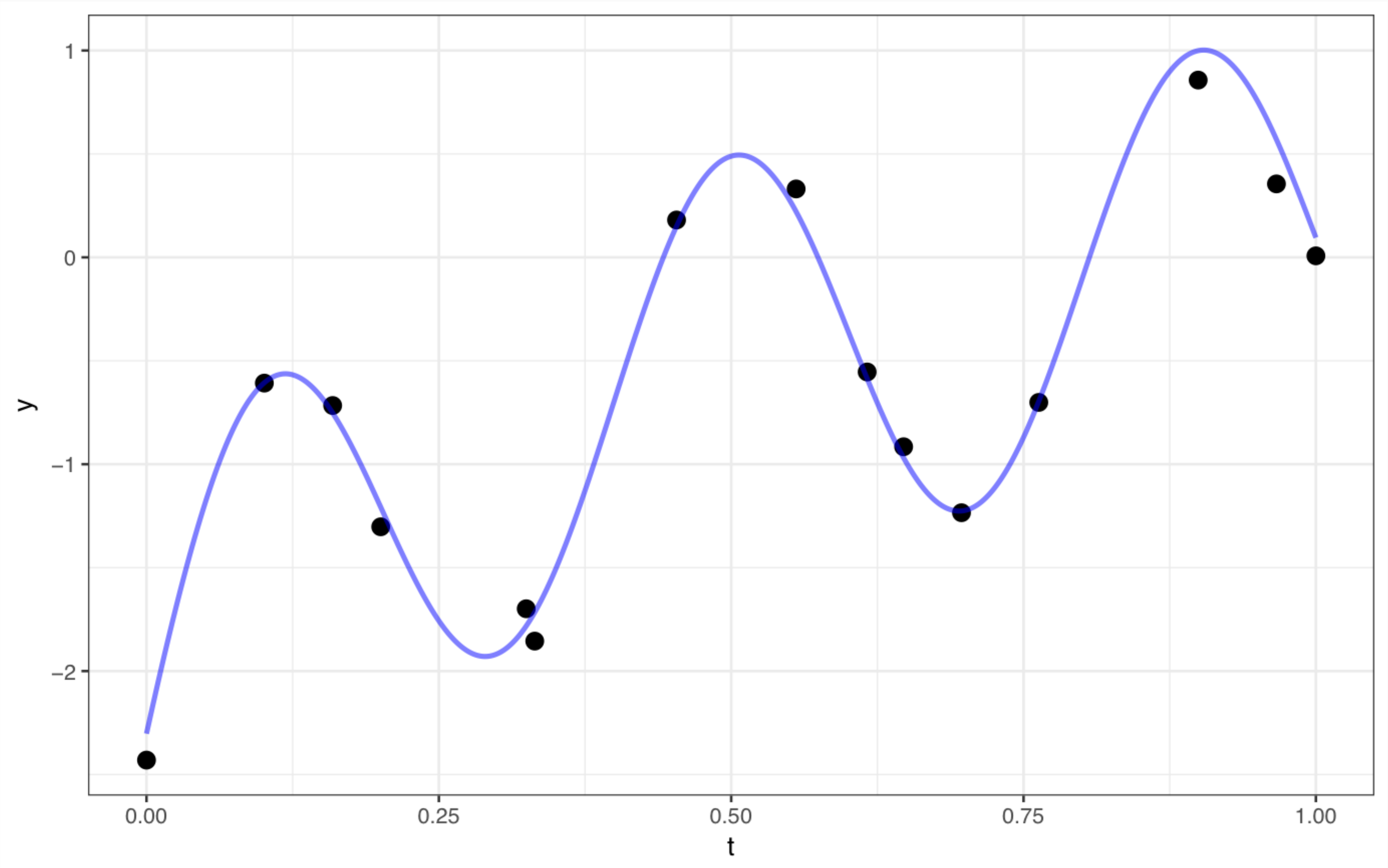


$\sigma^2 = 1$

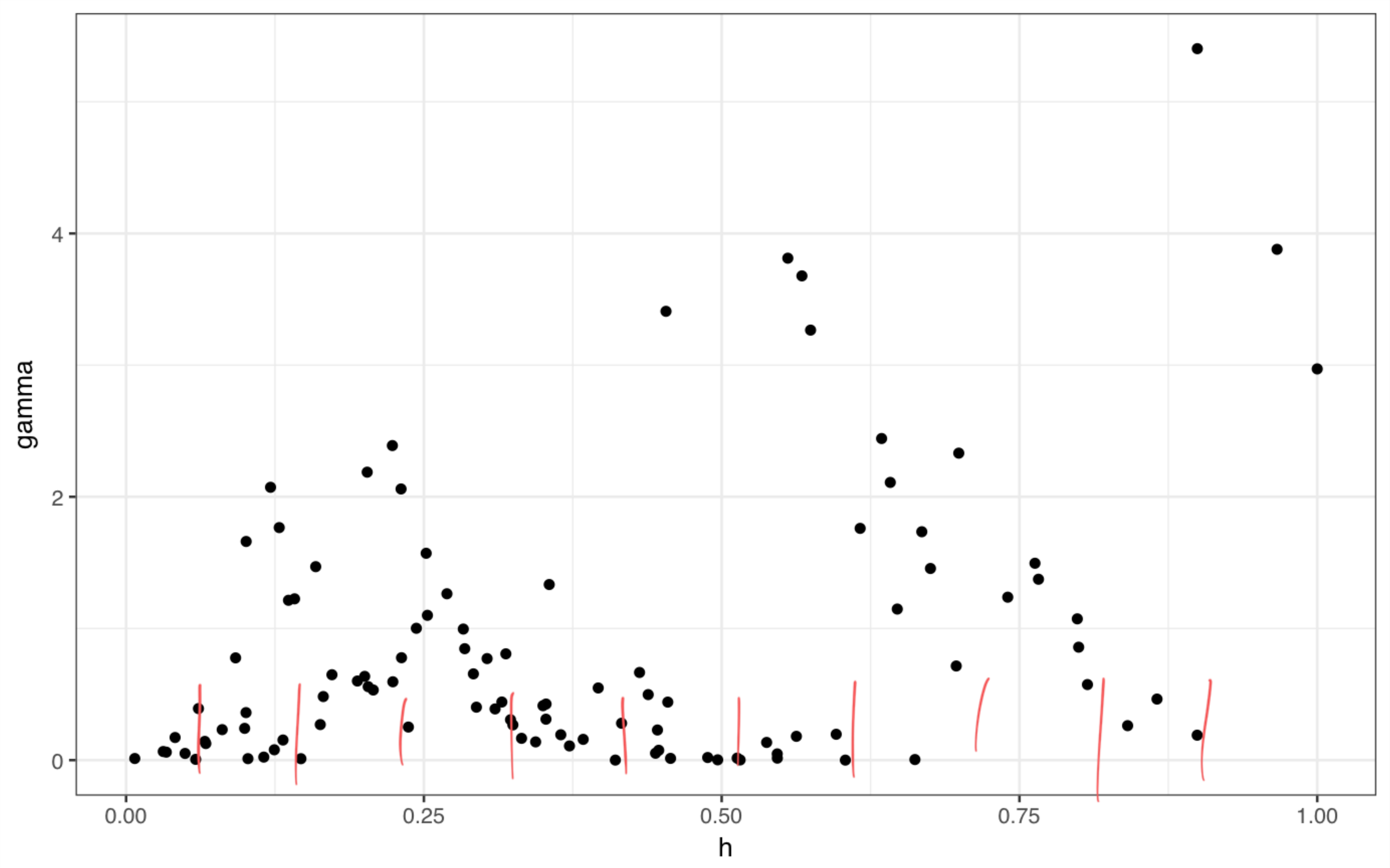
Covariance vs Semivariogram - Square Exponential



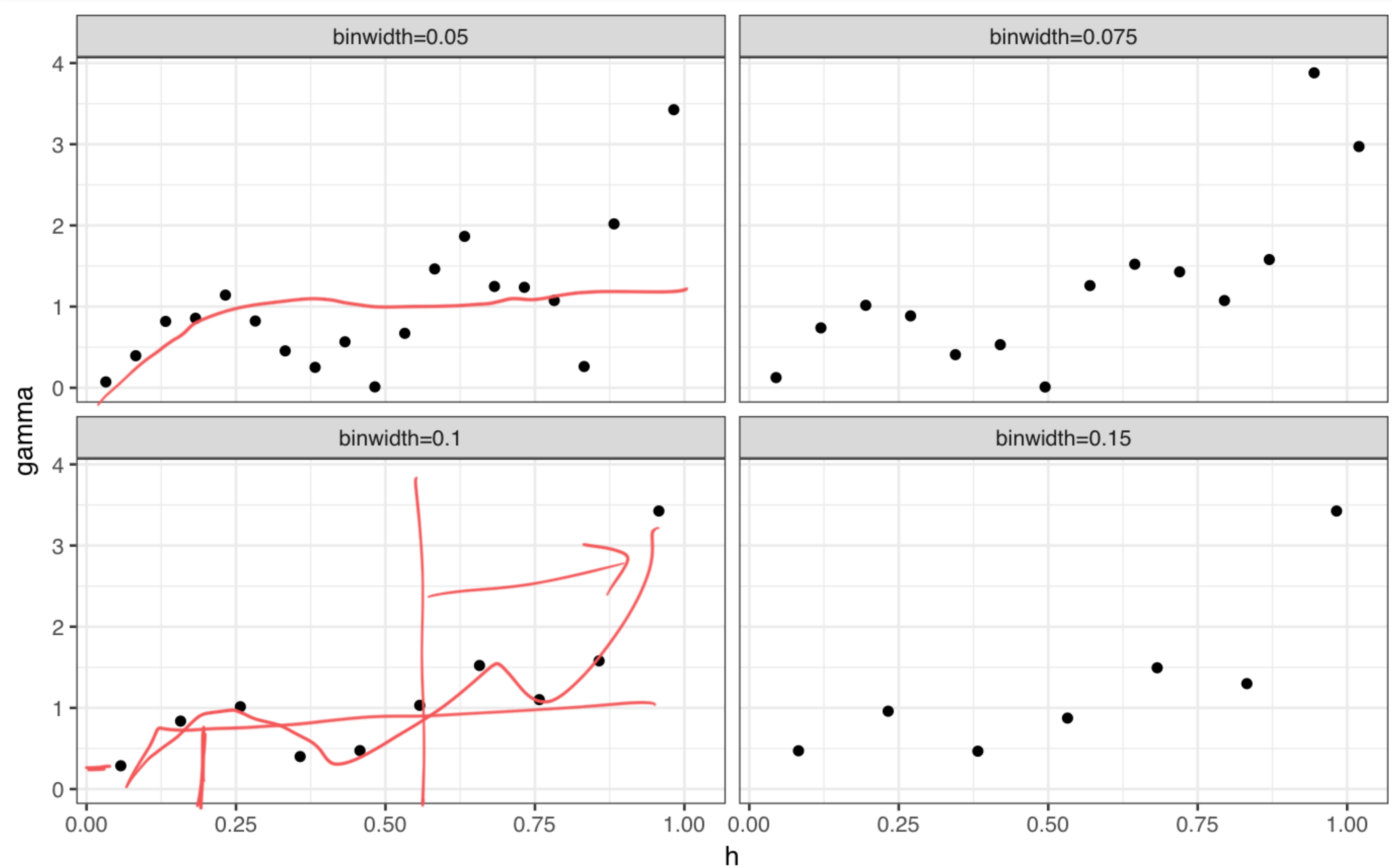
From last time



Empirical semivariogram - no bins / cloud

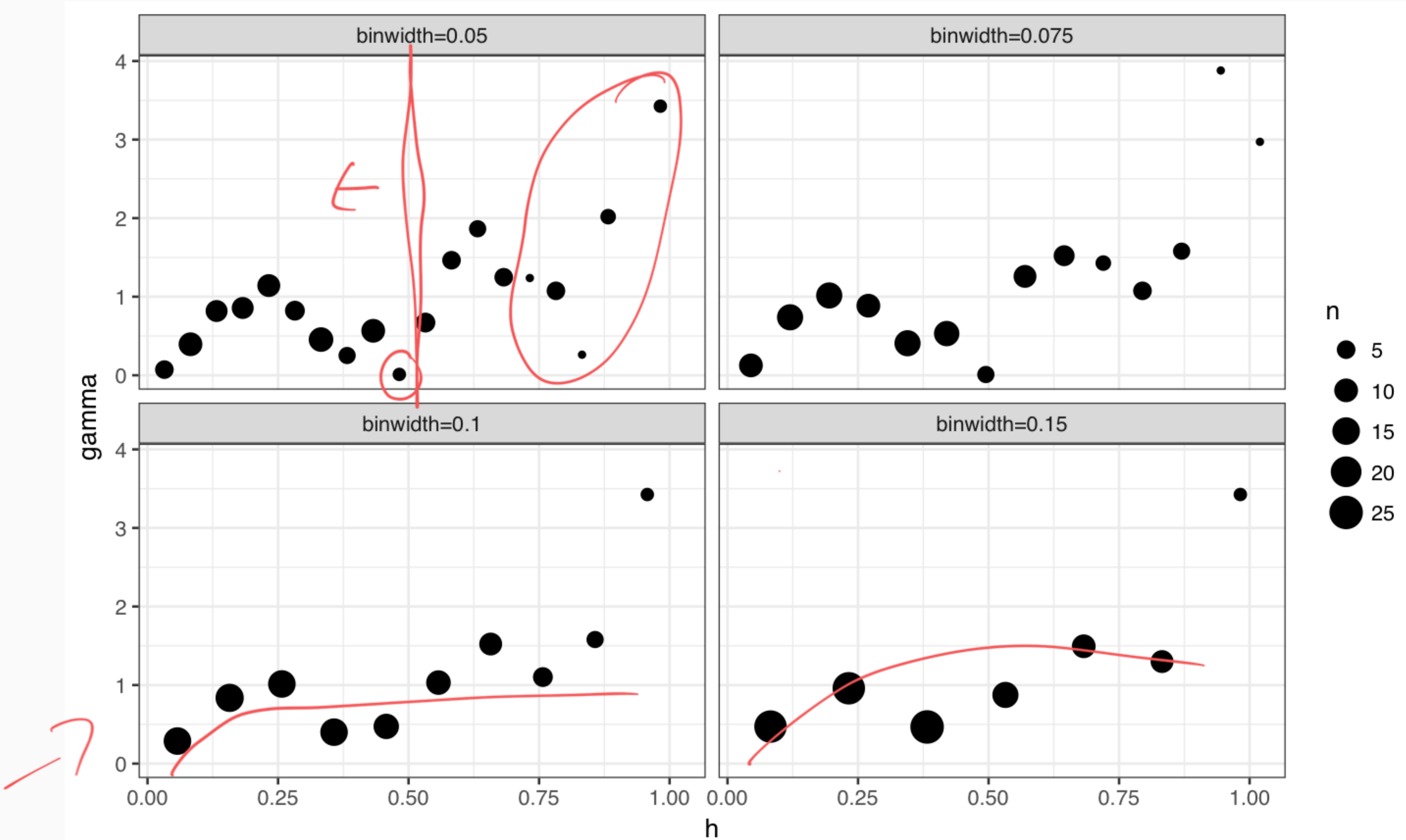


Empirical semivariogram (binned)



$\sigma_v^2 \approx 0.25$ $\quad$ $\sigma^2 = 0.5$ $\quad$ $\ell = \frac{\sqrt{3}}{0.2}$

Empirical semivariogram (binned + n)



Theoretical vs empirical semivariogram

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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\gamma(h) &= \sigma^2 - \sigma^2 \exp\Big(-(h\, l)^2 \Big) \\
&= 1.89 - 1.89 \exp\Big(-(5.86\, h)^2 \Big)
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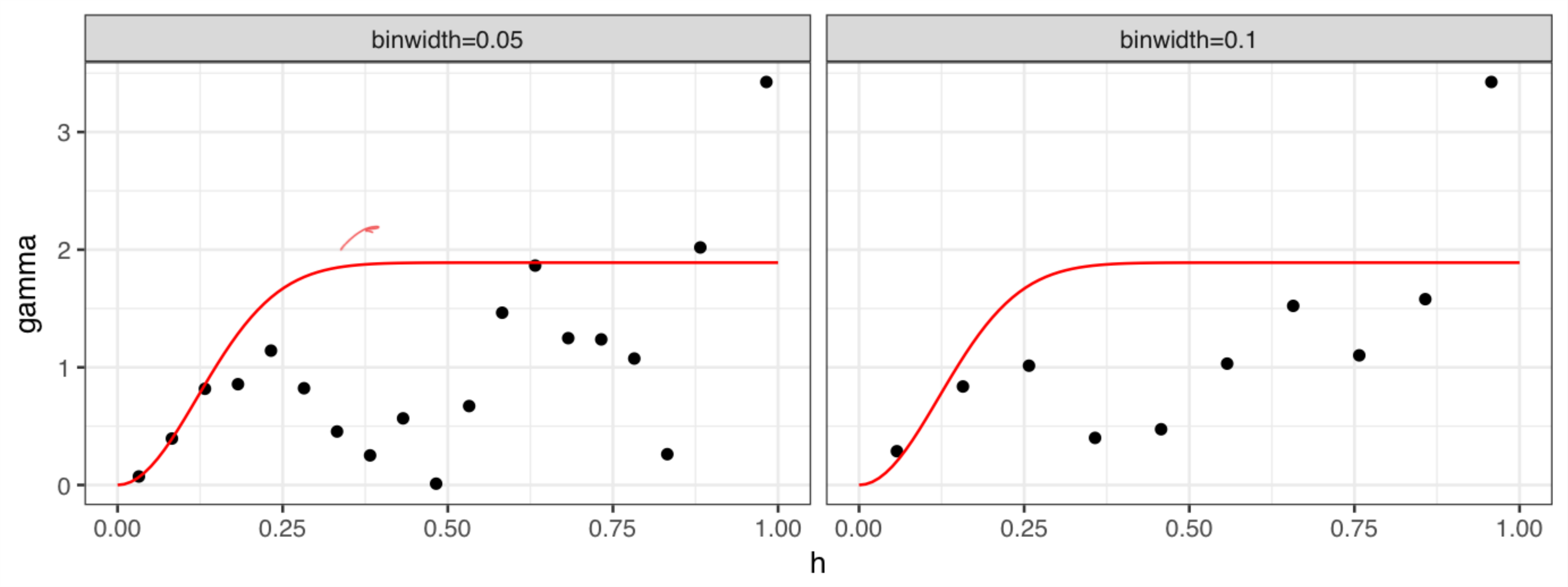
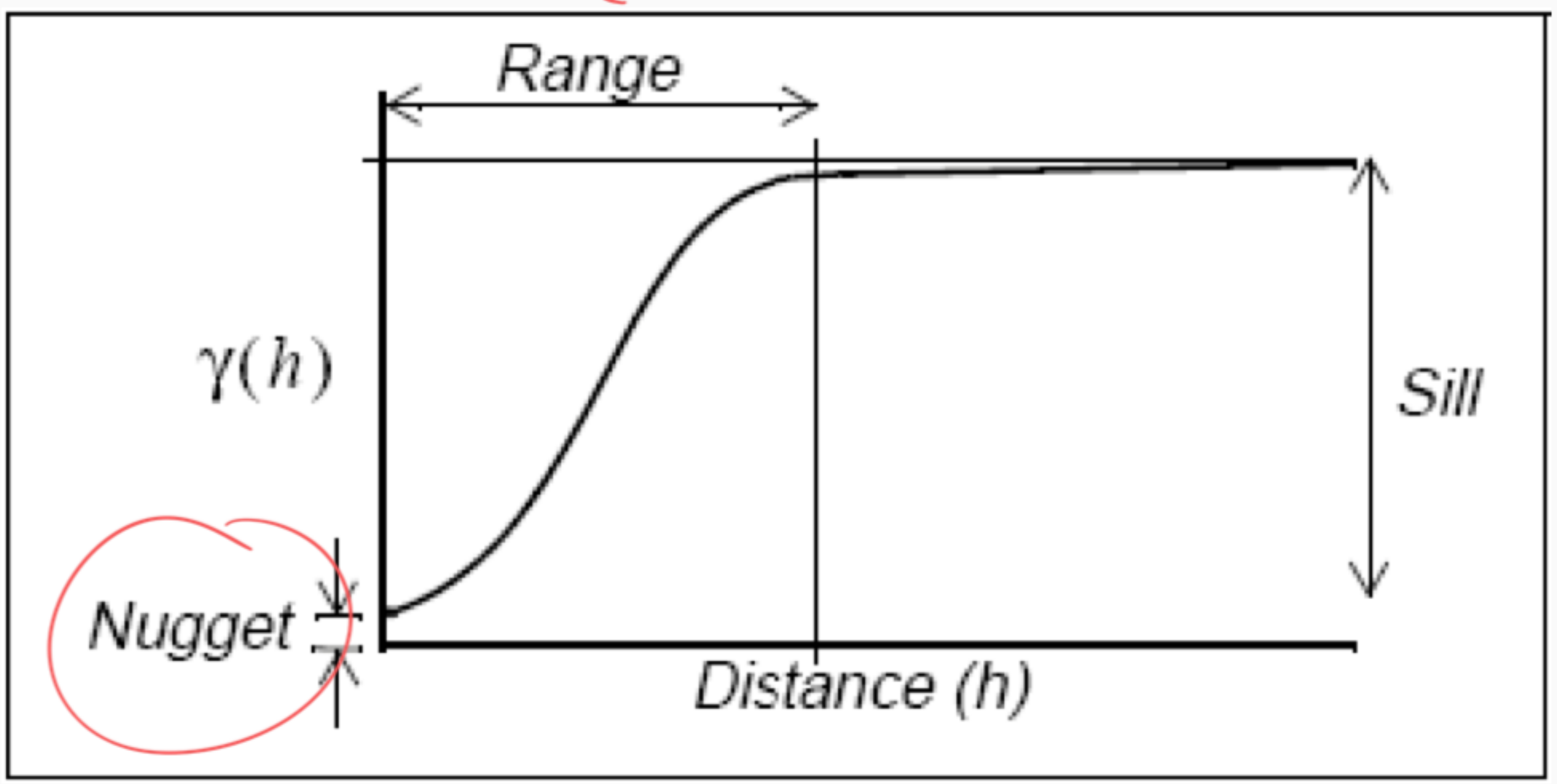


Variogram features

Nugget → σ_ν^2

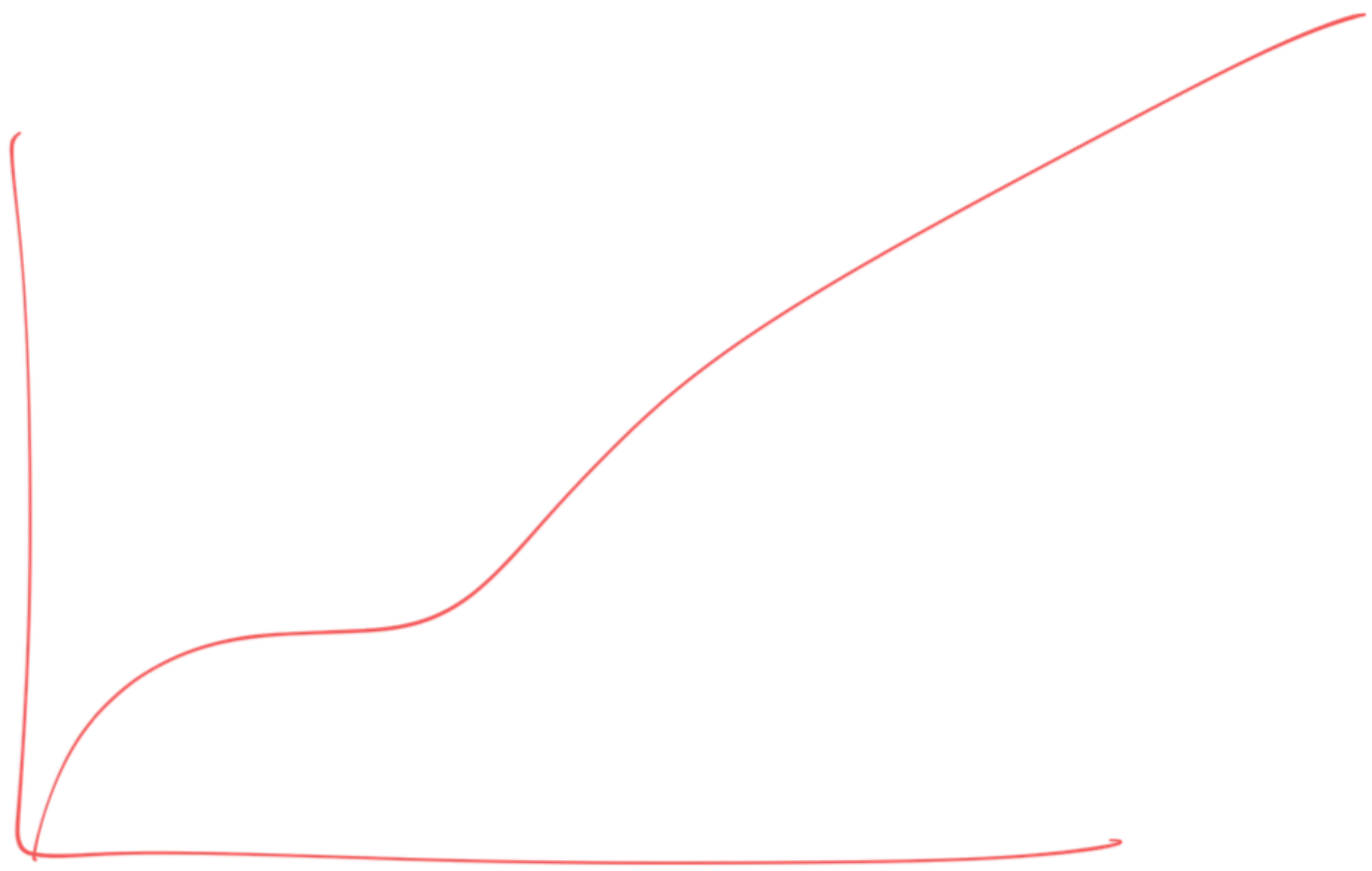
Sill → $\sigma_\nu^2 + \sigma^2$

Range $d = \frac{\sqrt{3}}{\ell}$ (sq exp) $\quad d = \frac{3}{\ell}$ (exp)



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

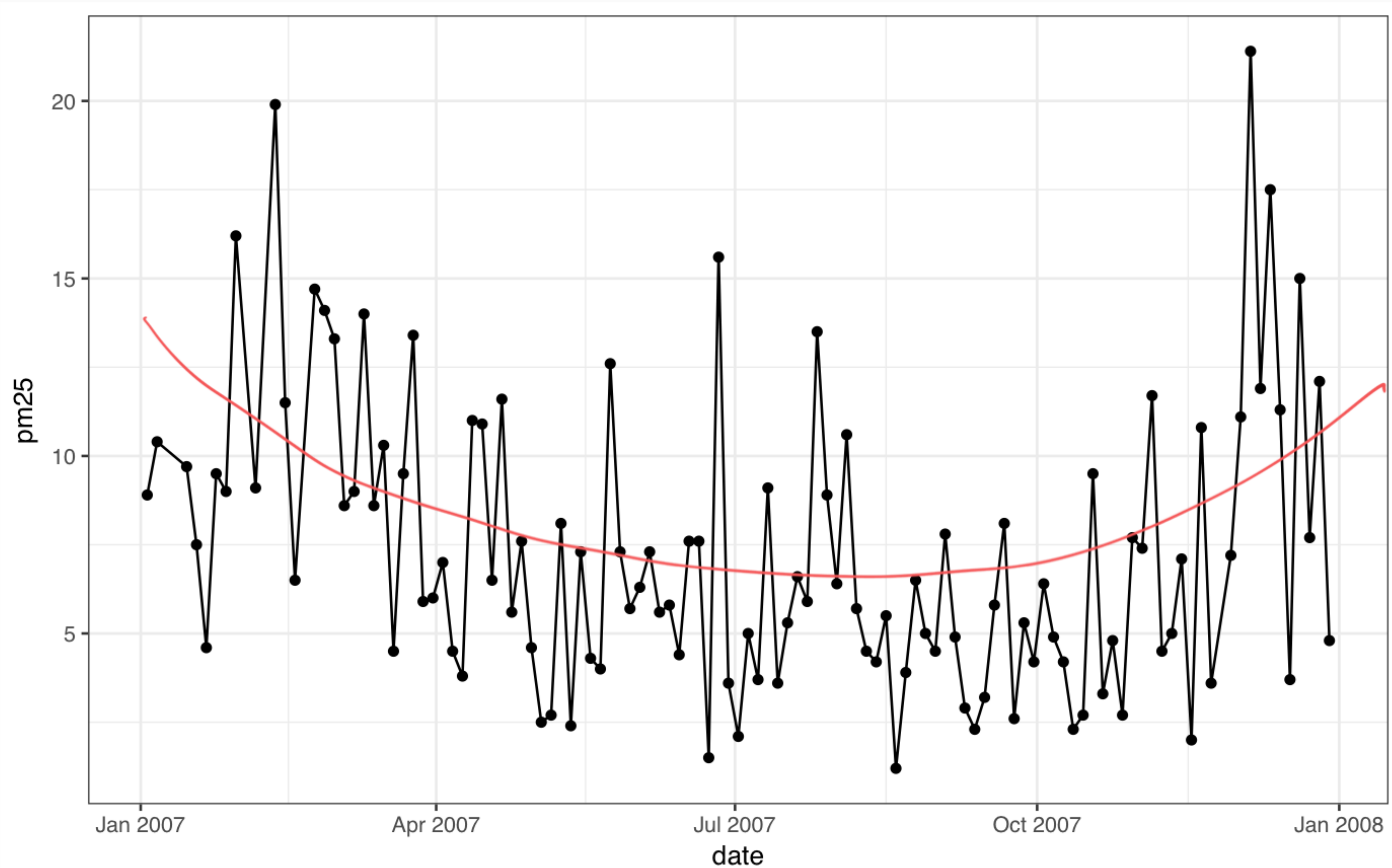
$w \sim GP(0, \Sigma)$ $\quad \nu \sim N(0, \sigma_\nu^2)$



PM2.5 Example

FRN Data

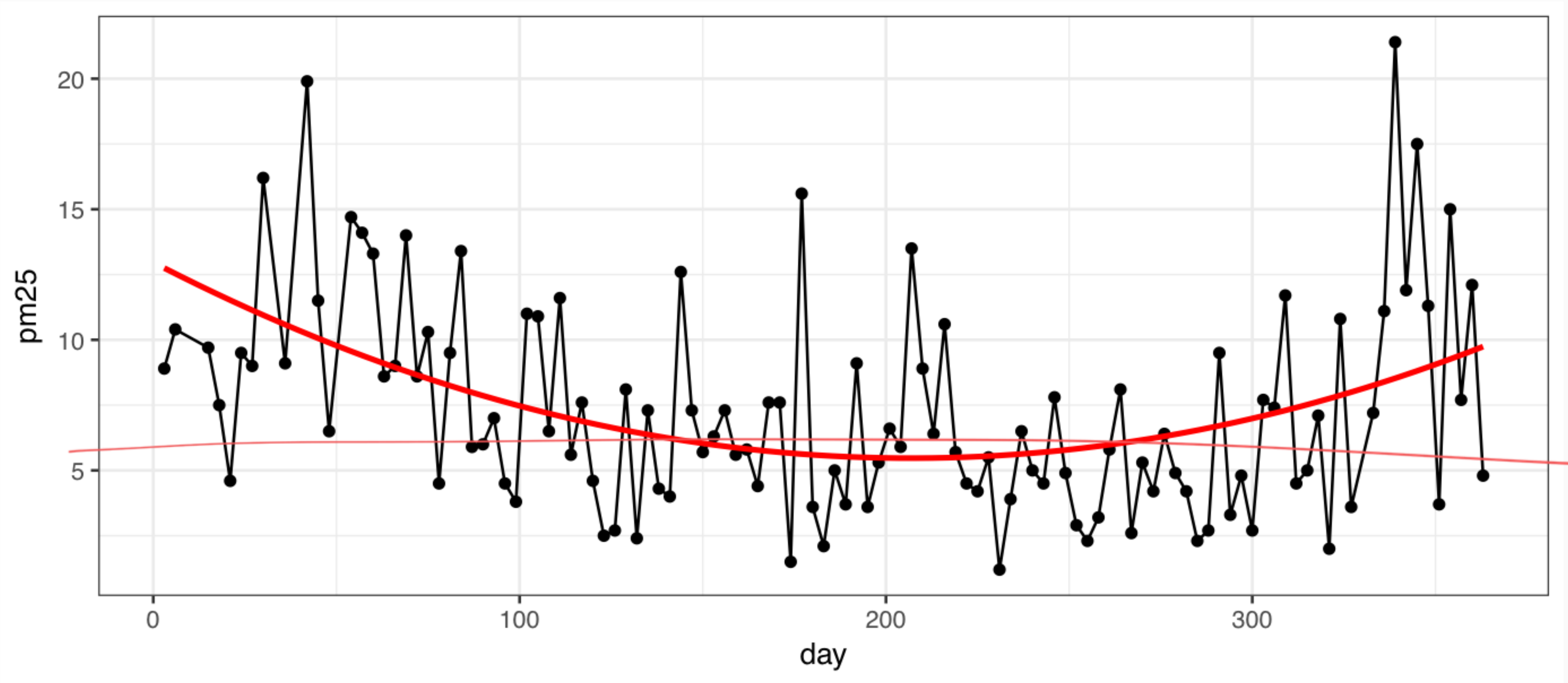
Measured PM2.5 data from an EPA monitoring station in Columbia, NJ.



FRN Data

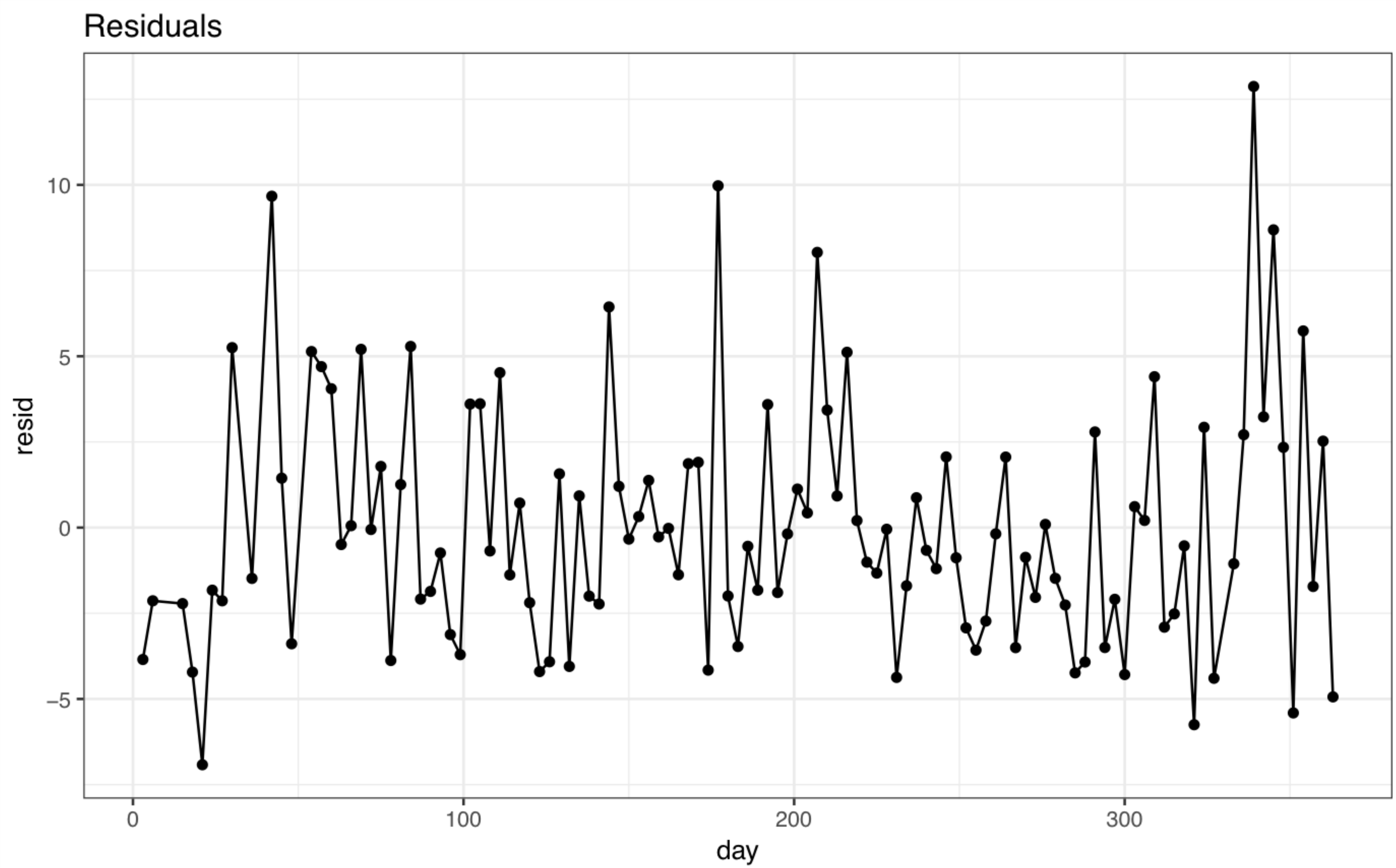
site	latitude	longitude	pm25	date	day
230031011	46.682	-68.016	8.9	2007-01-03	3
230031011	46.682	-68.016	10.4	2007-01-06	6
230031011	46.682	-68.016	9.7	2007-01-15	15
230031011	46.682	-68.016	7.5	2007-01-18	18
230031011	46.682	-68.016	4.6	2007-01-21	21
230031011	46.682	-68.016	9.5	2007-01-24	24
230031011	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

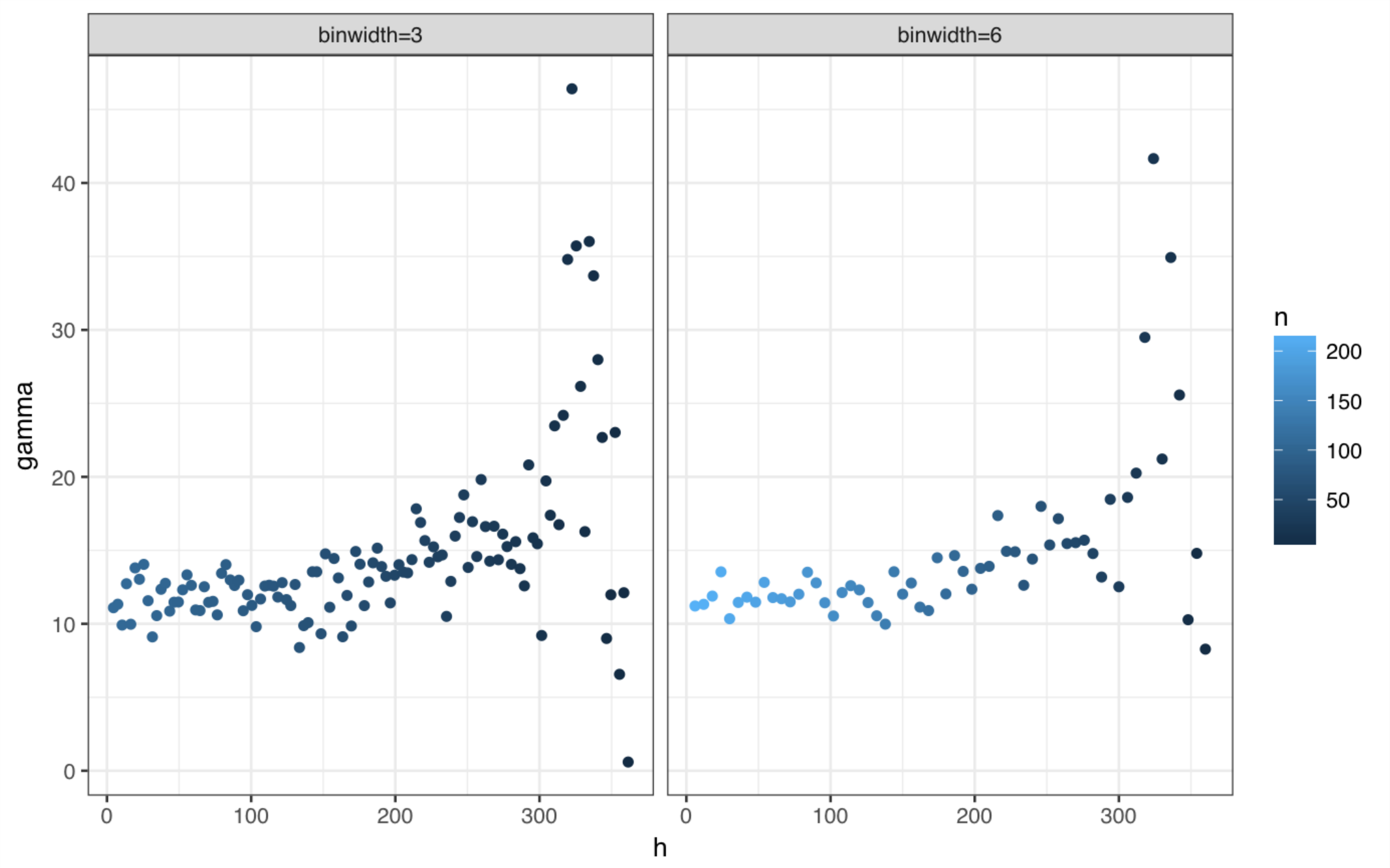



```
##
## Call:
## lm(formula = pm25 ~ day + I(day^2), data = pm25)
##
## Coefficients:
## (Intercept)          day     I(day^2)
##  12.9644351   -0.0724639    0.0001751
##
## Call:
## lm(formula = pm25 ~ day + I(day^2), data = pm25)
```

Detrended Residuals



Empirical Variogram



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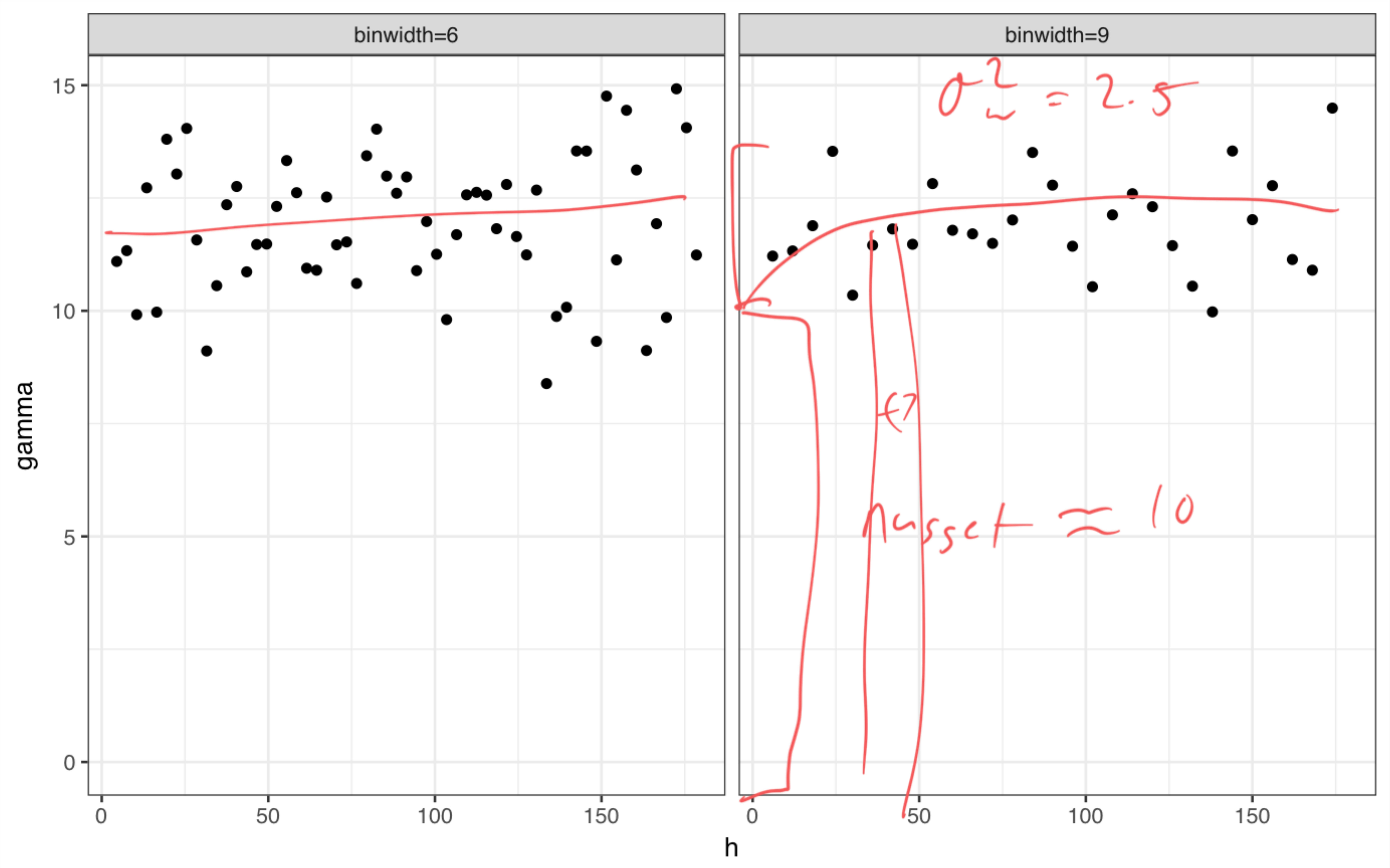

Model

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

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$$y(d) = \mu(d) + w(d) + w$$

where

$$\mu(d) = \beta 0 + \beta_1 d + \beta_2 d^2$$
$$w(d) \sim \mathcal{GP}(0, \Sigma)$$
$$w \sim \mathcal{N}(0, \sigma_w^2)$$

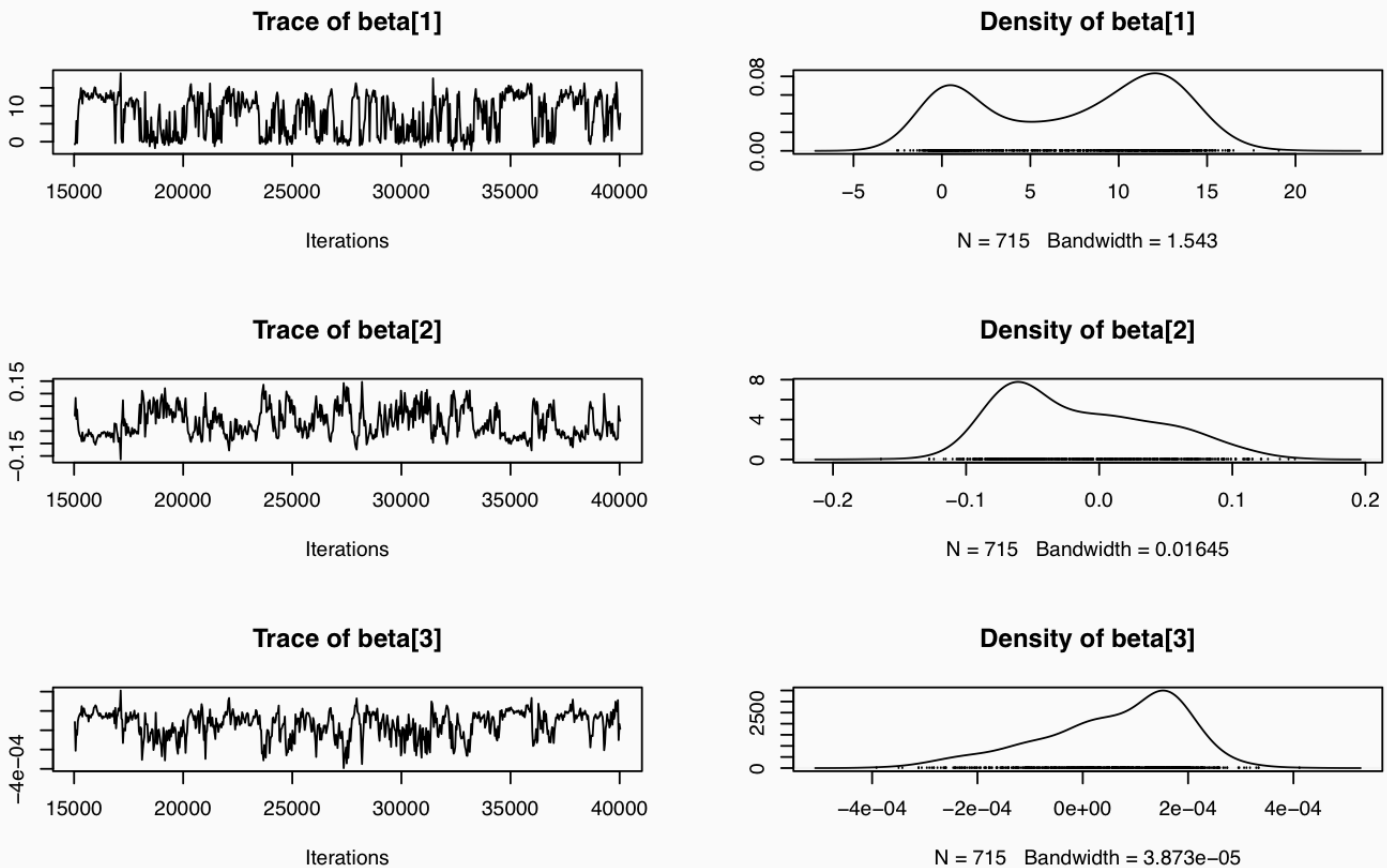
$$y(d) \sim GP\left(\mu(d), \Sigma + \sigma_w^2 I\right)$$

JAGS Model

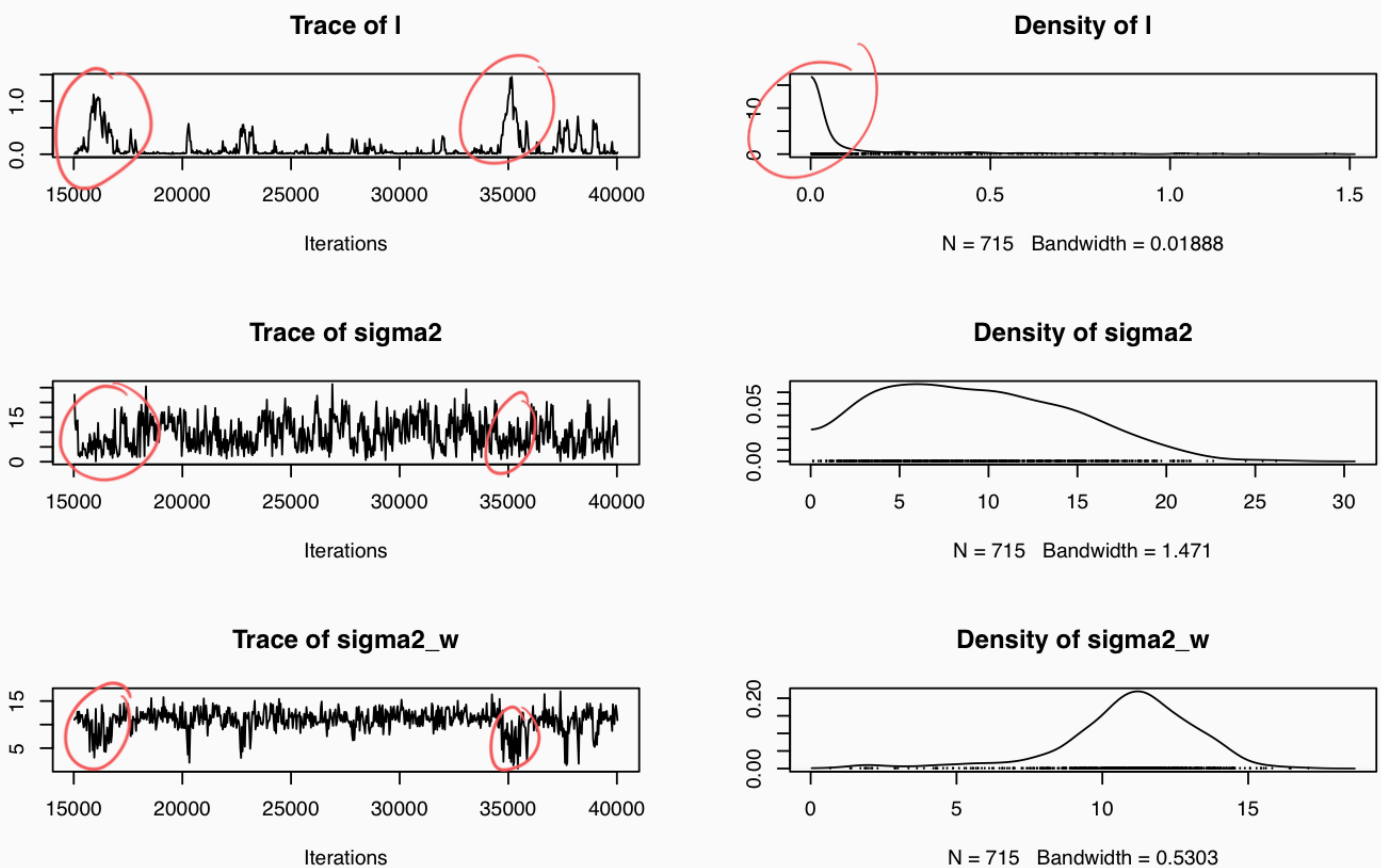
```
## model{
##   y ~ dmnorm(mu, inverse(Sigma))
##
##   for (i in 1:N) {
##     mu[i] <- beta[1]+ beta[2] * x[i] + beta[3] * x[i]^2
##   }
##
##   for (i in 1:(N-1)) {
##     for (j in (i+1):N) {
##       Sigma[i,j] <- sigma2 * exp(- pow(l*d[i,j],2))
##       Sigma[j,i] <- Sigma[i,j]
##     }
##   }
##
##   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,)
## }
```

Sq Exp

Posterior - Betas



Posterior - Covariance Parameters



Posterior

```
## # A tibble: 6 × 5
##      param     post_mean      post_med    post_lower   post_upper
## *    <chr>         <dbl>         <dbl>         <dbl>        <dbl>
## 1  beta[1]  7.283488e+00  8.667009e+00 -0.7461648059 1.503065e+01
## 2  beta[2] -1.627421e-02 -2.817415e-02 -0.0988863015 1.026401e-01
## 3  beta[3]  5.858818e-05  8.569993e-05 -0.0002481874 2.567976e-04
## 4        l  1.277712e-01  2.433287e-02  0.0060909947 8.443888e-01
## 5   sigma2  9.379213e+00  9.016621e+00  1.5643832453 1.979094e+01
## 6 sigma2_w  1.088809e+01  1.116626e+01  4.2665826402 1.448447e+01
```

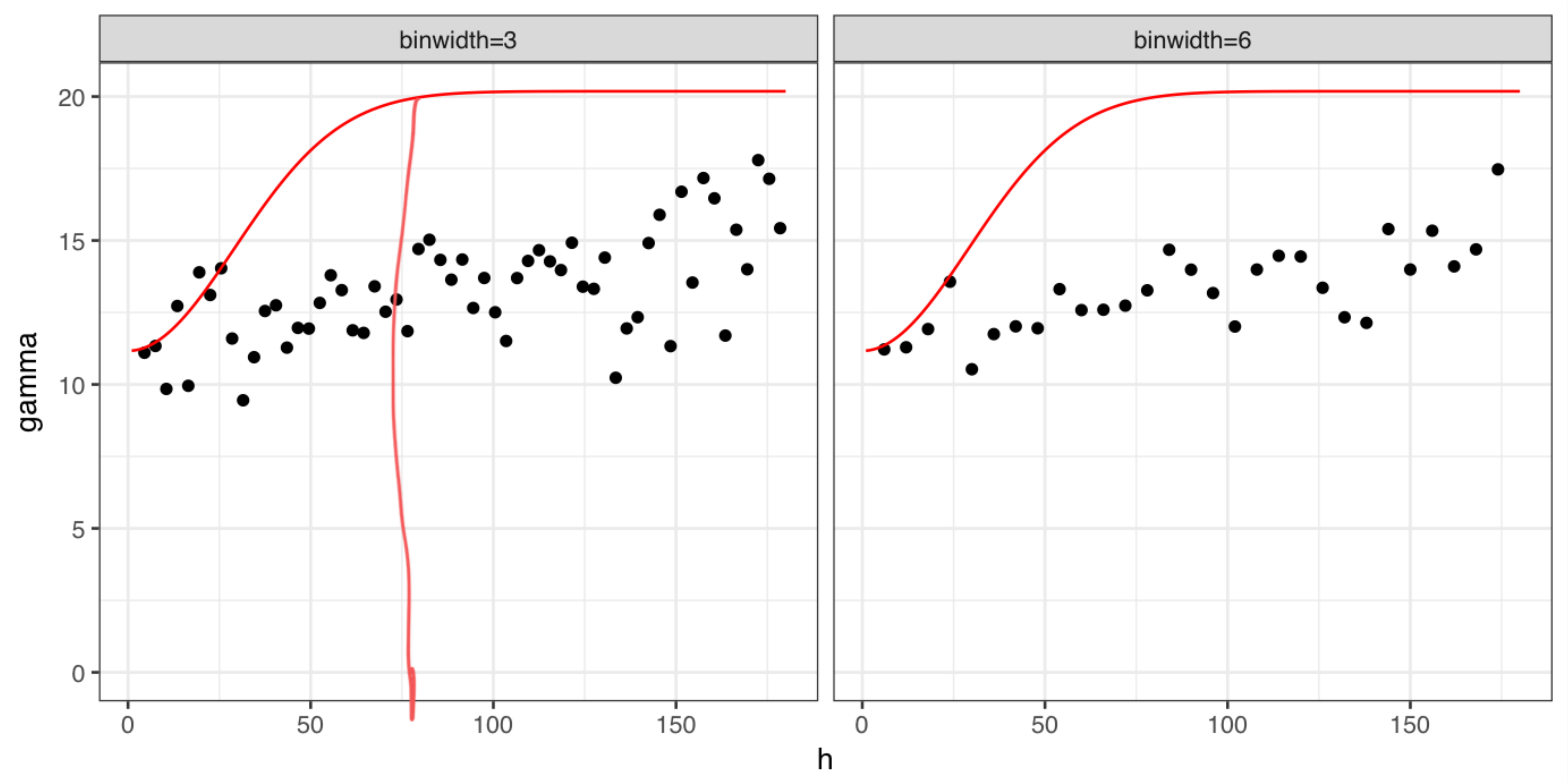
Fitted Variogram

$$Cov(h) = \sigma^2 e^{(-\ell^2 h^2)} + \sigma_v^2 1_{h=0}$$

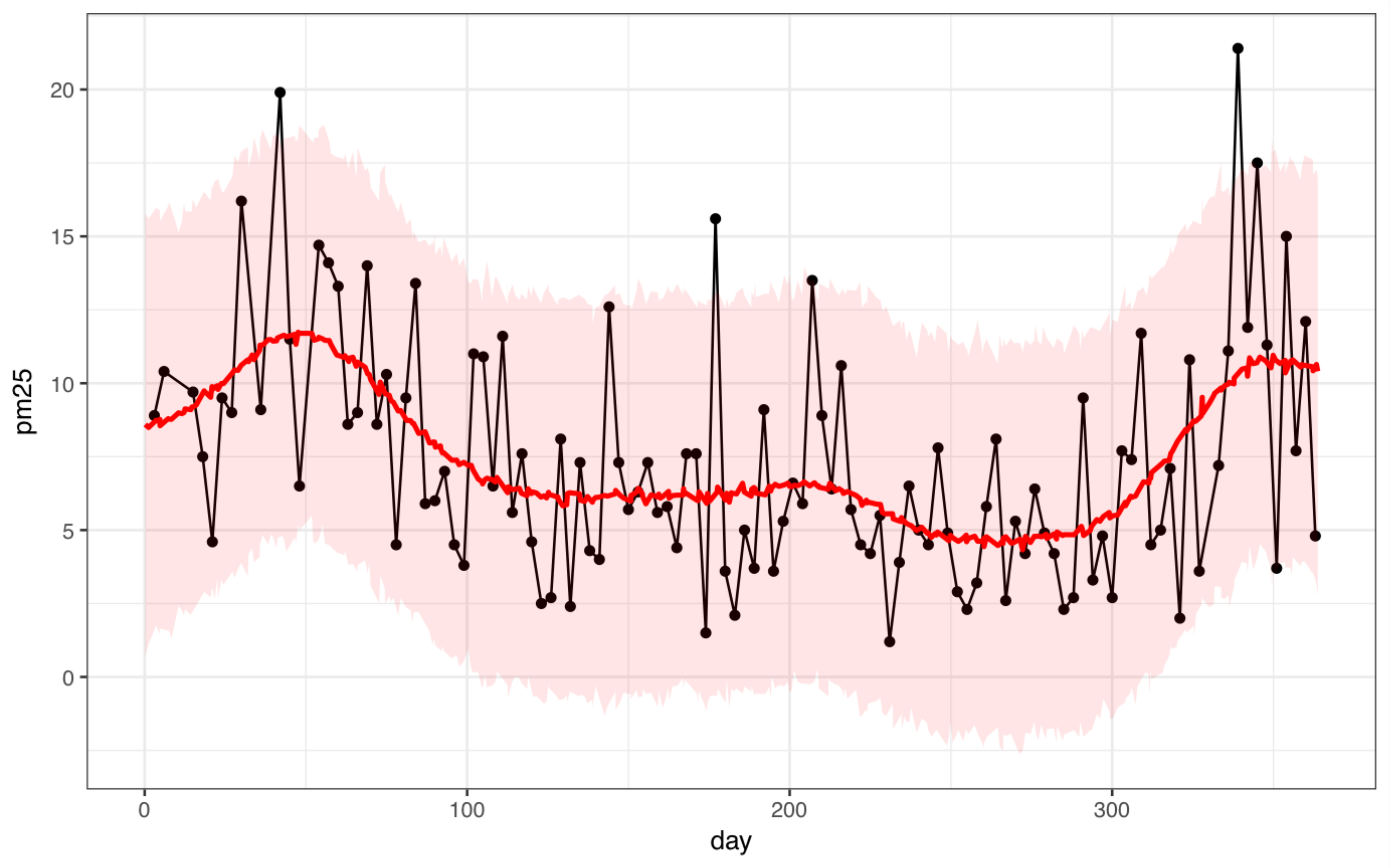
$$\gamma(h) = Cov(0) - Cov(h)$$

$$= \sigma^2 + \sigma_v^2 - \sigma^2 e^{-\ell^2 h^2} - \sigma_v 1_{h=0}$$

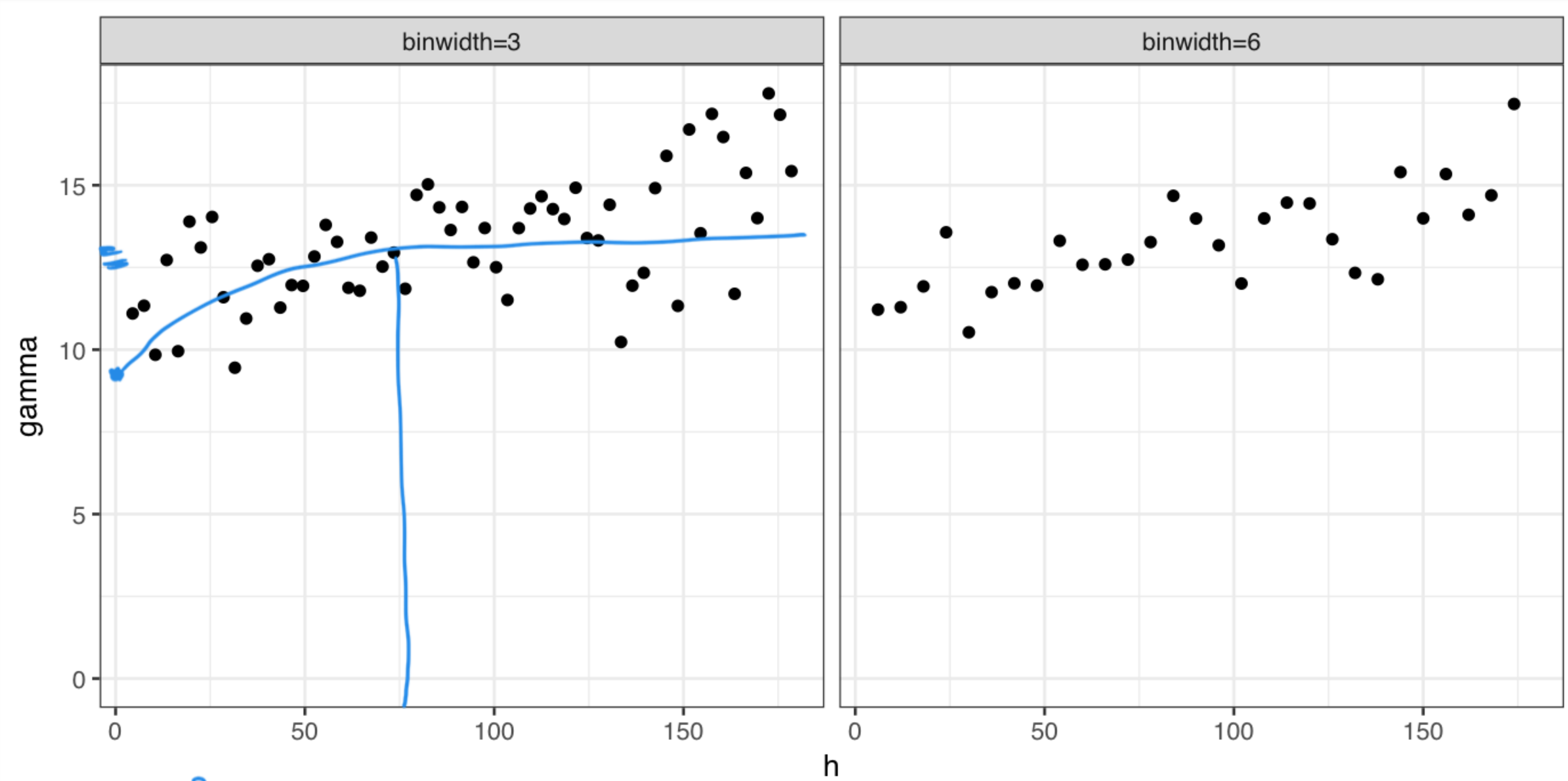
Empirical + Fitted Variogram



Fitted Model + Predictions

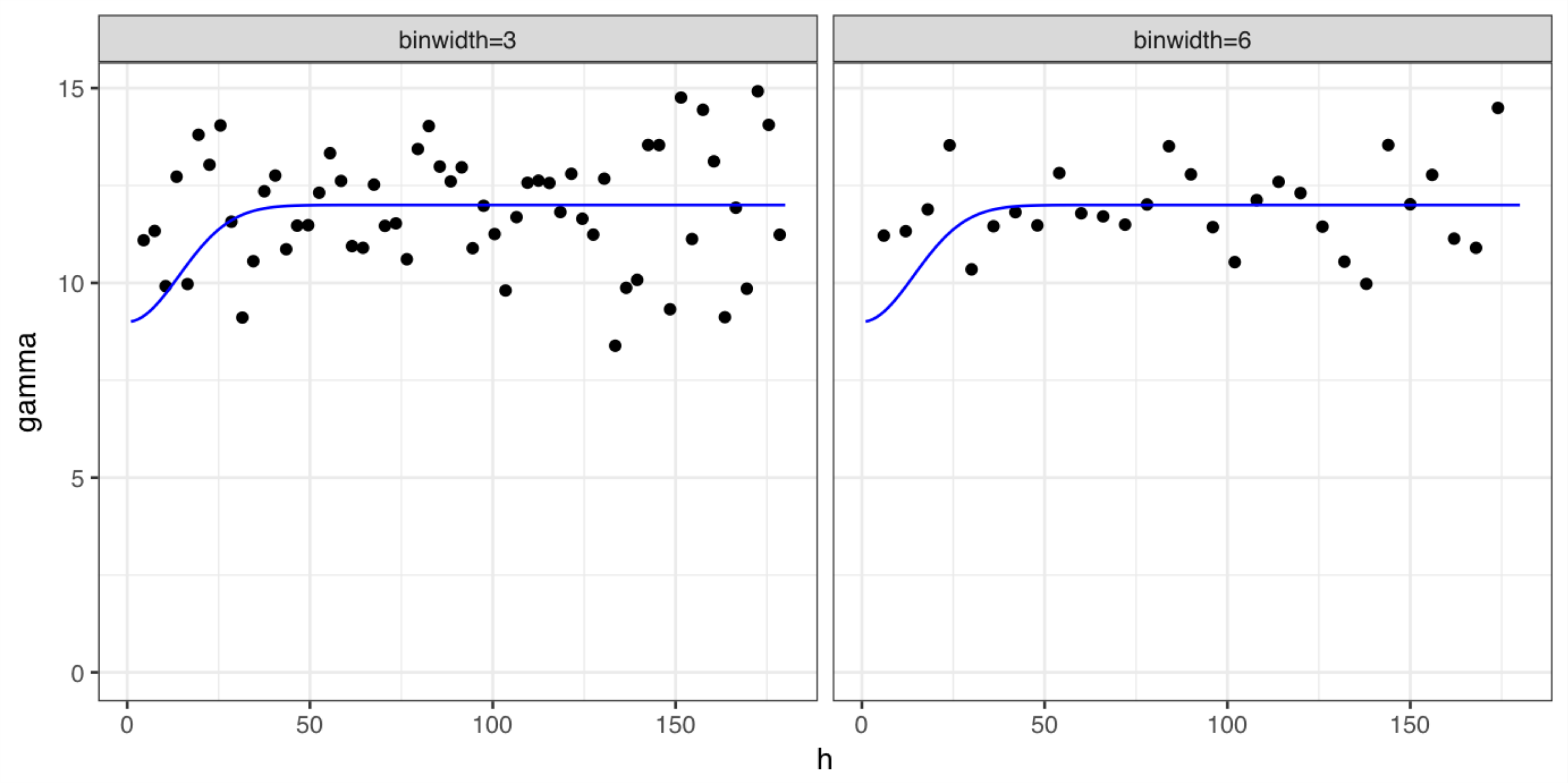


Empirical Variogram (again)



$\sigma_\nu^2 = 9$ $\quad$ sill $= 12$ $\quad$ $\Rightarrow \sigma^2 = 3$ $\quad$ $l = 0.05$

Empirical Variogram Model



Empirical Variogram Model + Predictions