Lecture 13

Gaussian Process Models - Part 2

10/19/2018

Lecture 13

Gaussian Process Models - Part 2

10/19/2018

EDA and GPs

Variogram

When fitting a Gaussian process model, it is often difficult to fit the covariance parameters (hard to identify). Today we will discuss some EDA approaches for getting a sense of the values for the scale, range and nugget parameters.

When fitting a Gaussian process model, it is often difficult to fit the covariance parameters (hard to identify). Today we will discuss some EDA approaches for getting a sense of the values for the scale, range and nugget parameters.

σ^2 $\quad l$ $\quad \sigma_w^2$

From the spatial modeling literature the typical approach is to examine an *empirical variogram*, first we will define the *theoretical variogram* and its connection to the covariance.

Variogram

When fitting a Gaussian process model, it is often difficult to fit the covariance parameters (hard to identify). Today we will discuss some EDA approaches for getting a sense of the values for the scale, range and nugget parameters.

From the spatial modeling literature the typical approach is to examine an *empirical variogram*, first we will define the *theoretical variogram* and its connection to the covariance.

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.

Some Properties of the theoretical Variogram / Semivariogram

- are non-negative

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

Some Properties of the theoretical Variogram / Semivariogram

- are non-negative

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

- are equal to 0 at distance 0

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

Some Properties of the theoretical Variogram / Semivariogram

- are non-negative

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

- are equal to 0 at distance 0

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

- are symmetric

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

Some Properties of the theoretical Variogram / Semivariogram

- are non-negative

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

- are equal to 0 at distance 0

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

- are symmetric

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

- if observations are independent

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

Some Properties of the theoretical Variogram / Semivariogram

- are non-negative

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

- are equal to 0 at distance 0

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

- are symmetric

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

- if observations are independent

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

- if the process *is not* stationary

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

Some Properties of the theoretical Variogram / Semivariogram

- are non-negative

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

- are equal to 0 at distance 0

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

- are symmetric

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

- if observations are independent

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

- if the process *is not* stationary

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

- if the process *is* stationary

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

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:

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

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:

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

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.

$$\gamma(t_i, t_j) = \mathrm{Var}(Y_{t_i}) - \mathrm{Cov}(Y_{t_i}, Y_{t_j})$$

Stationarity

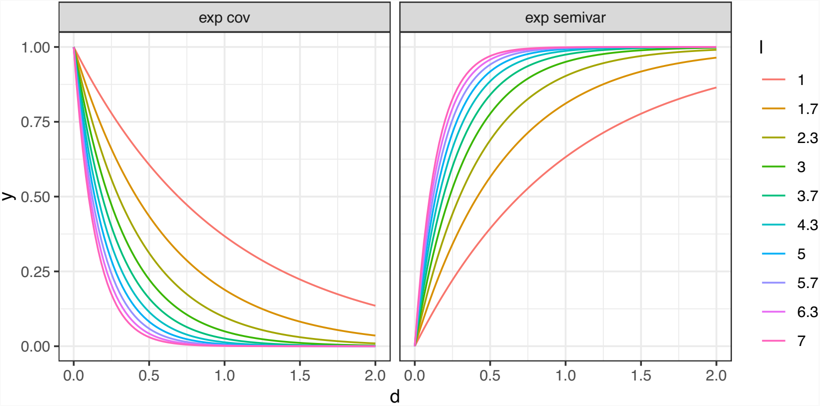
$$= \mathrm{Cov}(Y_{t_i}, Y_{t_i}) - \mathrm{Cov}(Y_{t_i}, Y_{t_j})$$

$$= \sigma^2 + \sigma_v^2 - \left(\sigma^2 e^{-(|t_i - t_j| \ell)^2} + \sigma_v^2 \mathbb{1}_{|t_i - t_j| = 0}\right)$$

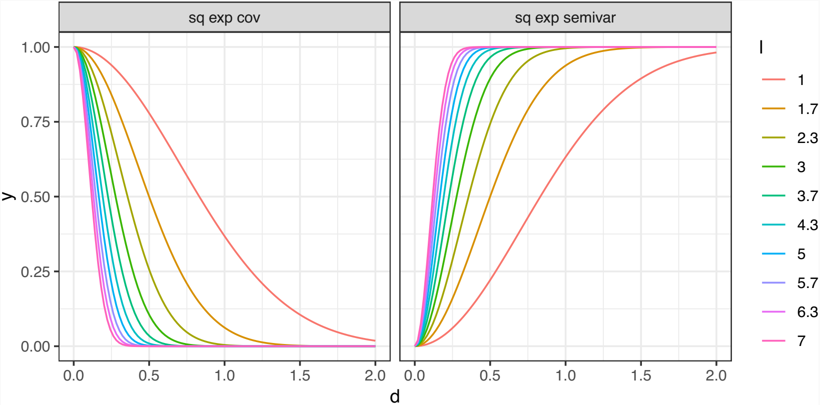
$$\mathrm{Cov}(Y_{t_i}, Y_{t_j}) = \sigma^2 e^{-\left(|t_i - t_j| \ell\right)^2} + \sigma_v^2 \mathbb{1}_{|t_i - t_j| = 0}$$

Covariance vs Semivariogram - Exponential

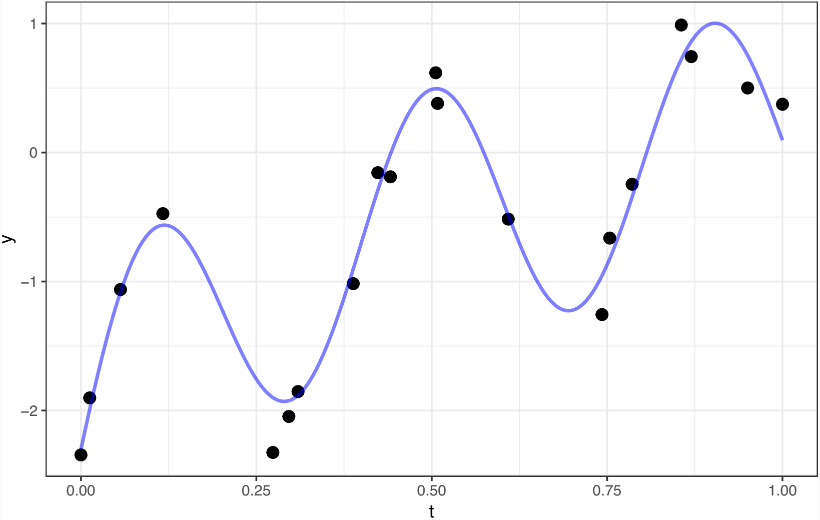
$\sigma_{\sim}^2 = 0$



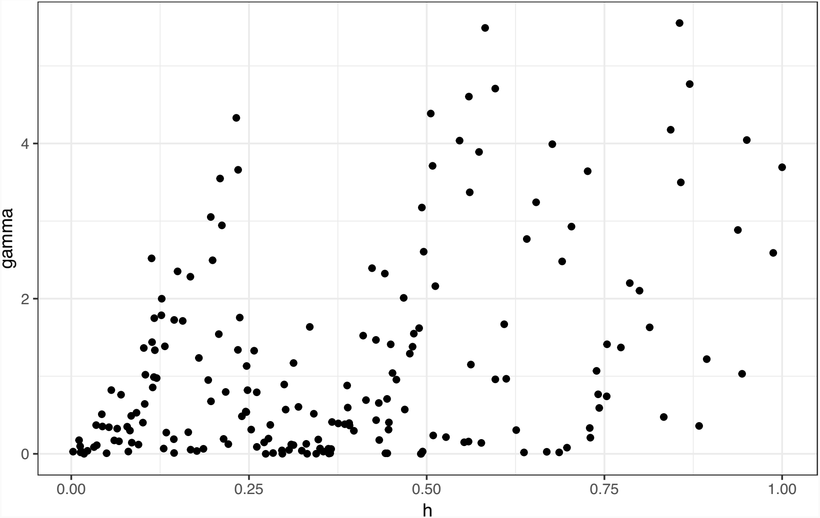
Covariance vs Semivariogram - Square Exponential



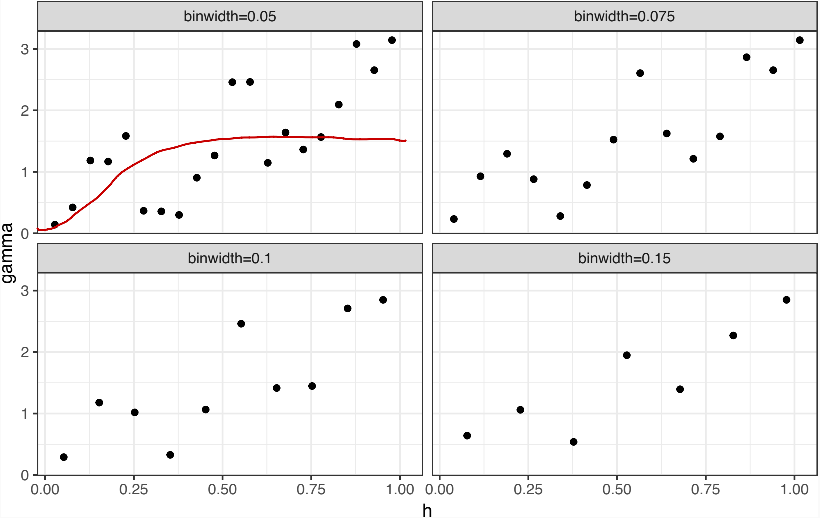
From last time



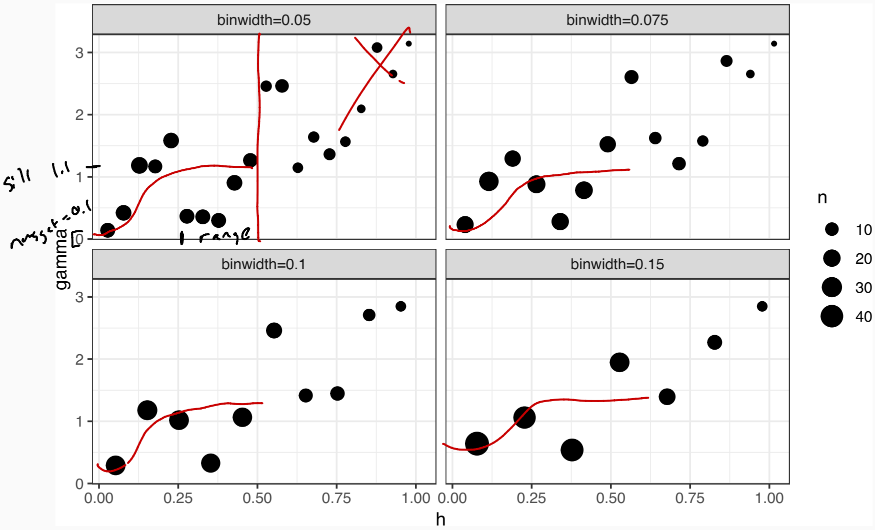
Empirical semivariogram - no bins / cloud



Empirical semivariogram (binned)



Empirical semivariogram (binned + n)



Theoretical vs empirical semivariogram

After fitting the model last time we came up with a posterior median of $\sigma^2 = 1.73$, $l = 7.01$, and $?^2_w = 0.13 for a square exponential covariance.

Theoretical vs empirical semivariogram

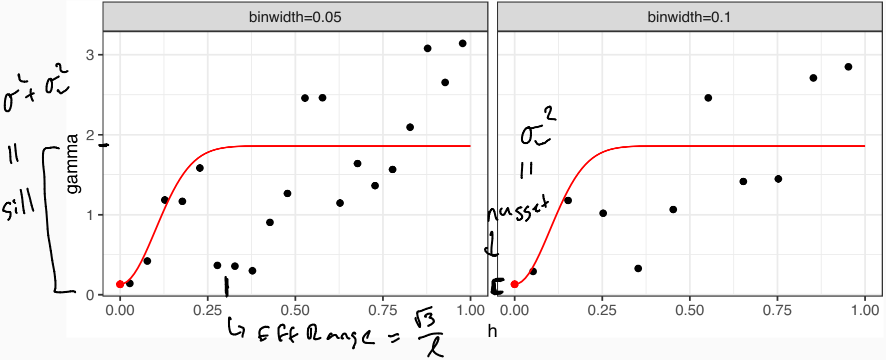
After fitting the model last time we came up with a posterior median of $\sigma^2 = 1.73, l = 7.01$, and $?^2_w = 0.13 for a square exponential covariance.

$$
\begin{aligned}
Cov(h) &= \sigma^2 \exp\big(-(h\,l)^2\big) + \sigma^2_w \mathbf{1}_{h=0} \\
\gamma(h) &= \sigma^2 + \sigma^2_w - \sigma^2 \exp\big(-(h\,l)^2\big) \\
&= 1.73 + 0.13 - 1.73 \exp\big(-(7.01\,h)^2\big)
\end{aligned}
$$

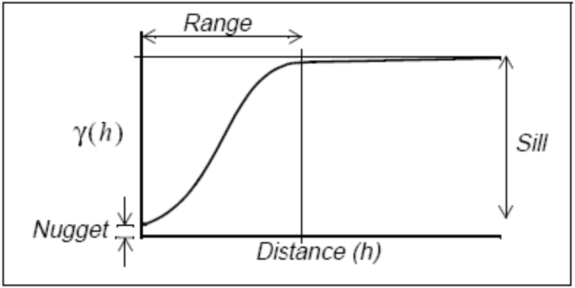
Theoretical vs empirical semivariogram

After fitting the model last time we came up with a posterior median of $\sigma^2 = 1.73$, $l = 7.01$, and $[?]^2_w = 0.13 for a square exponential covariance.

$$
\begin{aligned}
Cov(h) &= \sigma^2 \exp\left(-(h\,l)^2\right) + \sigma^2_w \mathbf{1}_{h=0} \\
\gamma(h) &= \sigma^2 + \sigma^2_w - \sigma^2 \exp\left(-(h\,l)^2\right) \\
&= 1.73 + 0.13 - 1.73 \exp\left(-(7.01\,h)^2\right)
\end{aligned}
$$

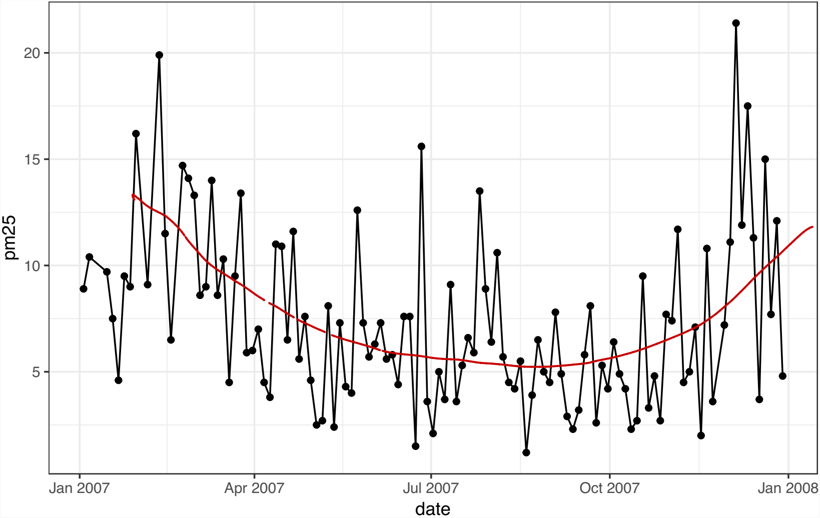


Variogram features



PM2.5 Example

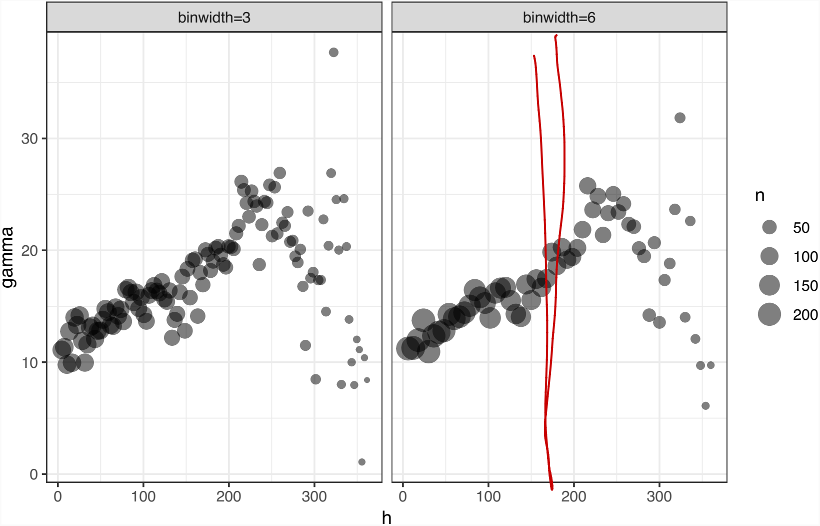
Measured PM2.5 data from an EPA monitoring station in Columbia, NJ.



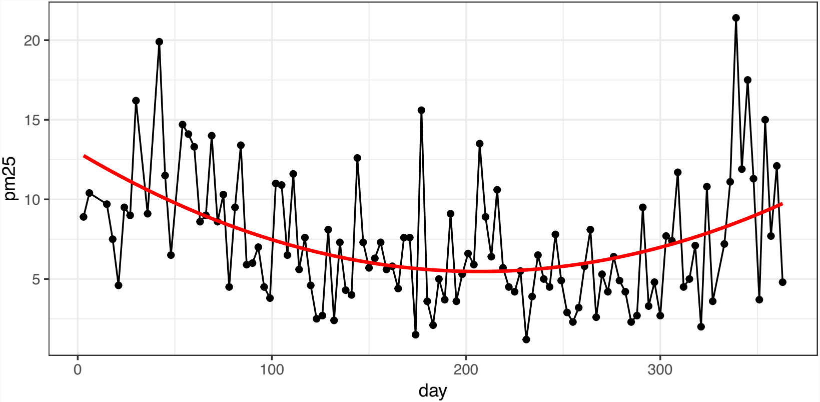
FRN Data

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

Empirical Variogram

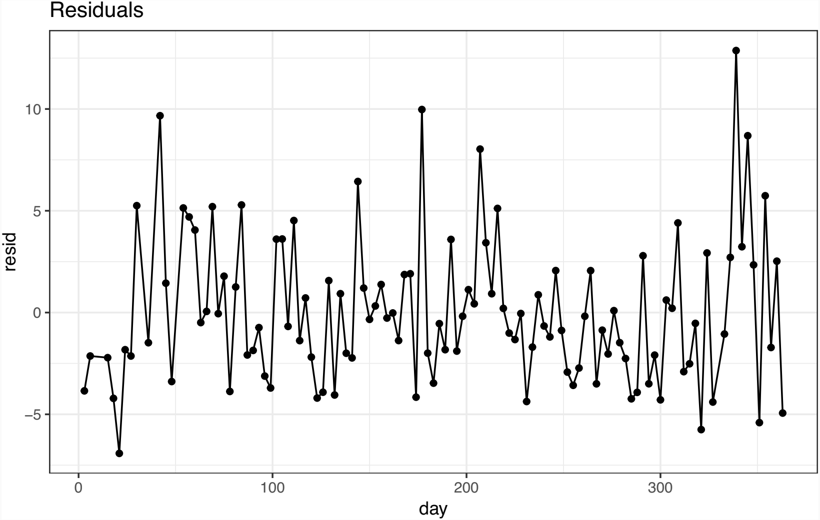


Mean Model

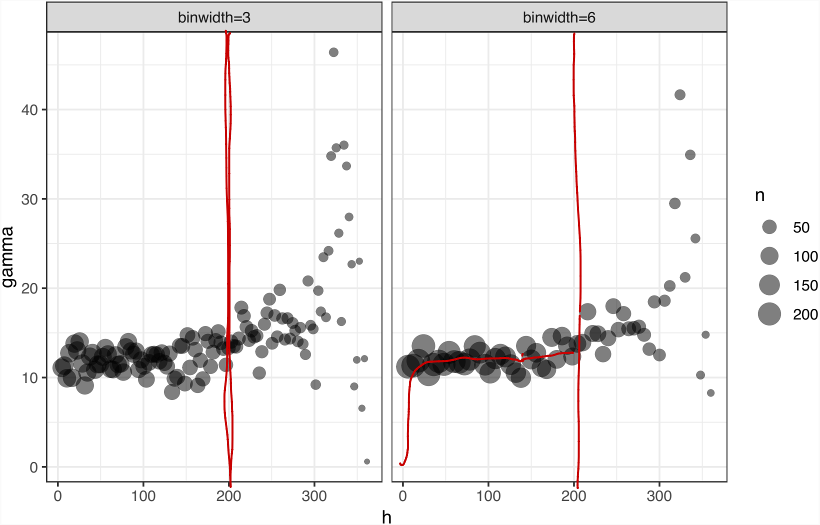



```
##
## Call:
## lm(formula = pm25 ~ day + I(day^2), data = pm25)
##
## Coefficients:
## (Intercept)          day     I(day^2)
##  12.9644351   -0.0724639    0.0001751
##
```

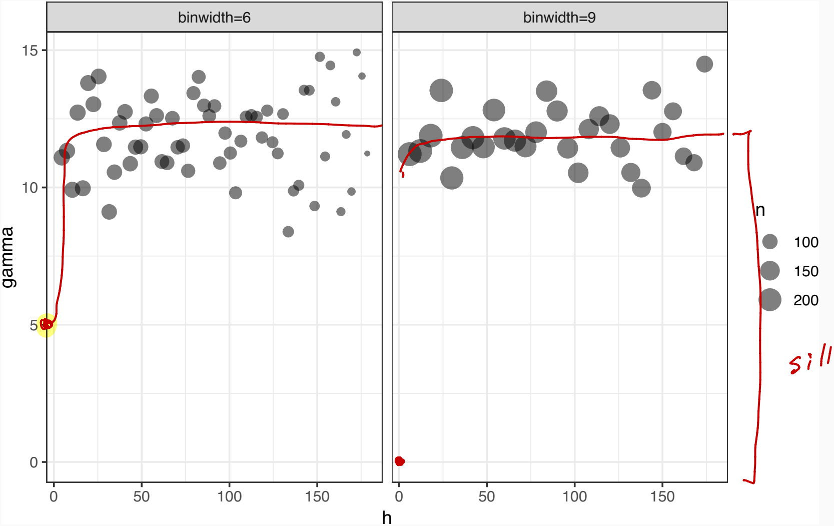
Detrended Residuals



Empirical Variogram - Residuals



Zoomed Empirical Variogram - Residuals



Model

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

Model

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

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

where

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

$$\{\boldsymbol{\Sigma}\}_{ij} = Cov(t_i, t_j) = \sigma^2 \exp(-(|t_i - t_j|\,l)^2)$$

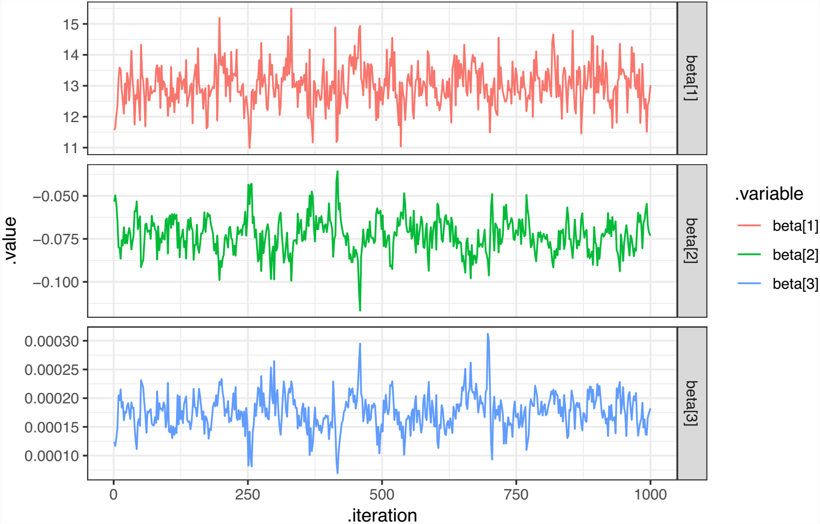
JAGS Model

```
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(coef[i], 2.5, 1)
  }
  sigma2_w ~ dnorm(5, 1/25) T(0,)
  sigma2   ~ dnorm(12.5, 1/25) T(0,)
  l        ~ dt(0, 2.5, 1) T(0,)
}"
```

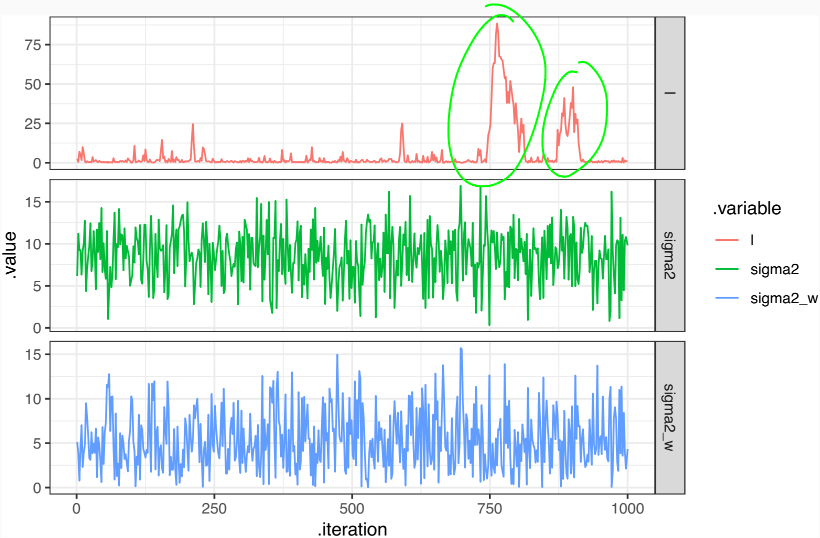
Y

115x1

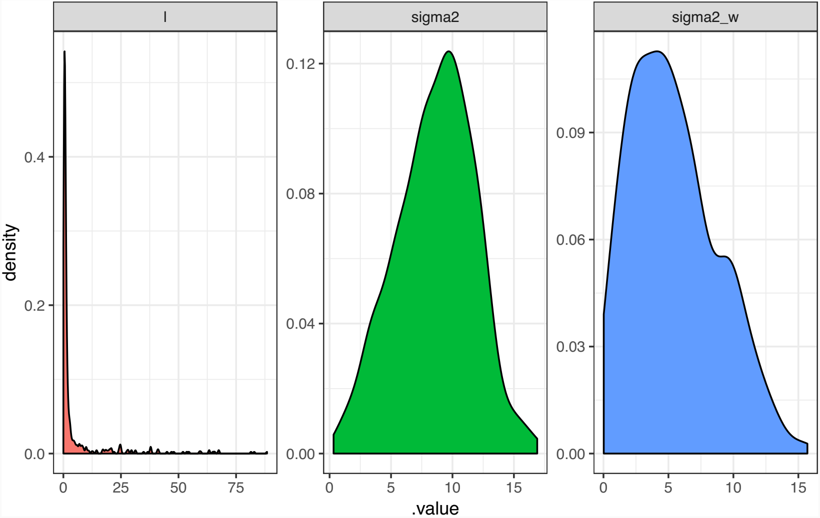
Posterior - Betas



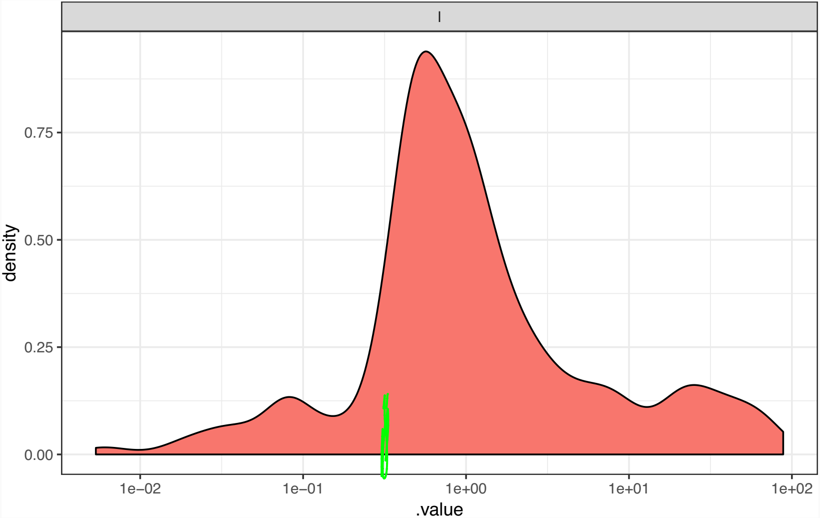
Posterior - Covariance Parameters



Posterior - Covariance Parameters



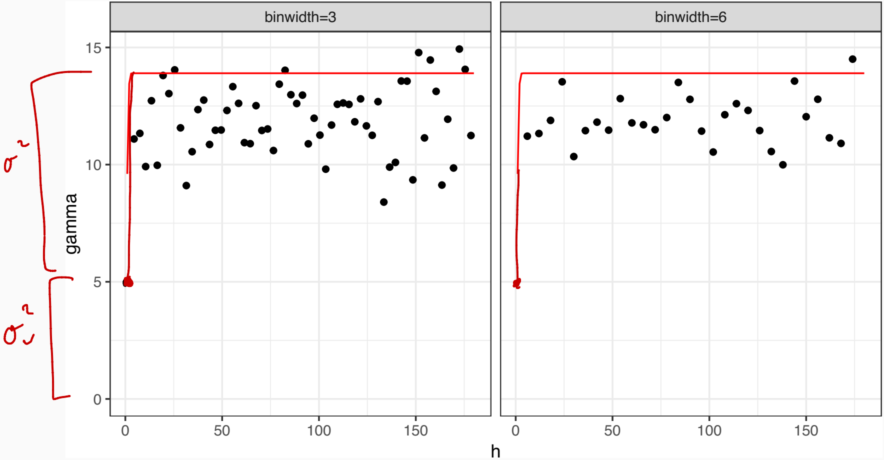
Posterior - Covariance Parameters - l



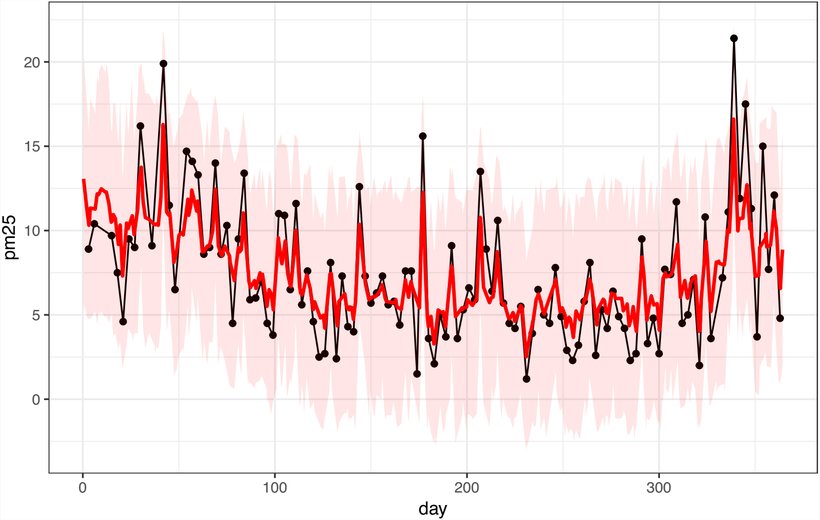
Posterior

.variable	post_mean	post_med	post_lower	post_upper
beta[1]	12.98786	12.96919	11.52626	14.56714
beta[2]	-0.07289	-0.07286	-0.09259	-0.05316
beta[3]	0.00018	0.00018	0.00011	0.00023
l	5.41433	0.86915	0.03329	52.39913
sigma2	8.87498	9.14124	2.26513	14.62043
sigma2_w	5.25459	4.75810	0.22093	12.52645

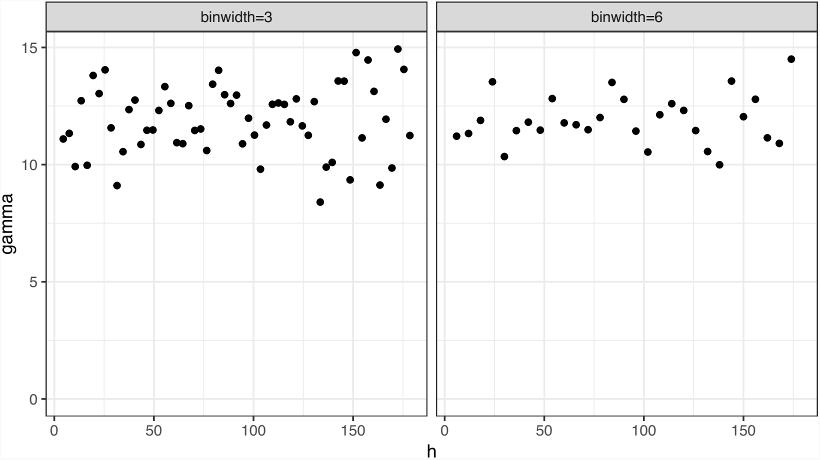
Empirical + Fitted Variogram – Post mod



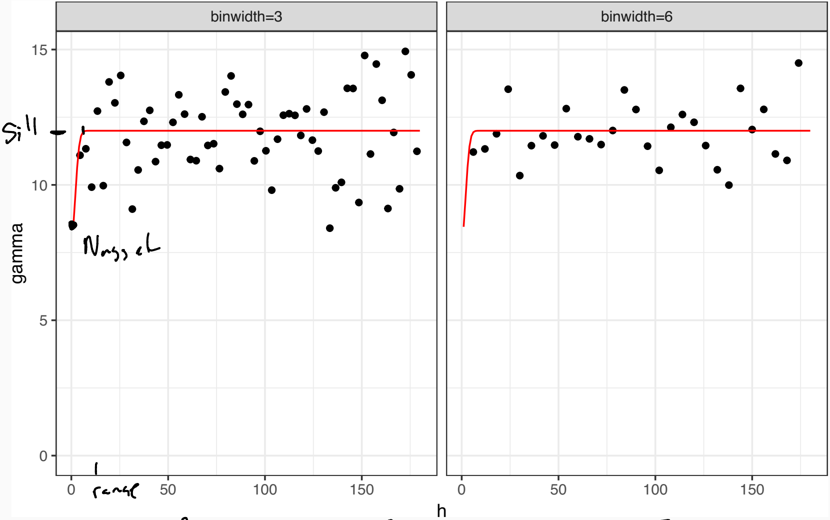
Fitted Model + Predictions – Plug in



Empirical Variogram Model

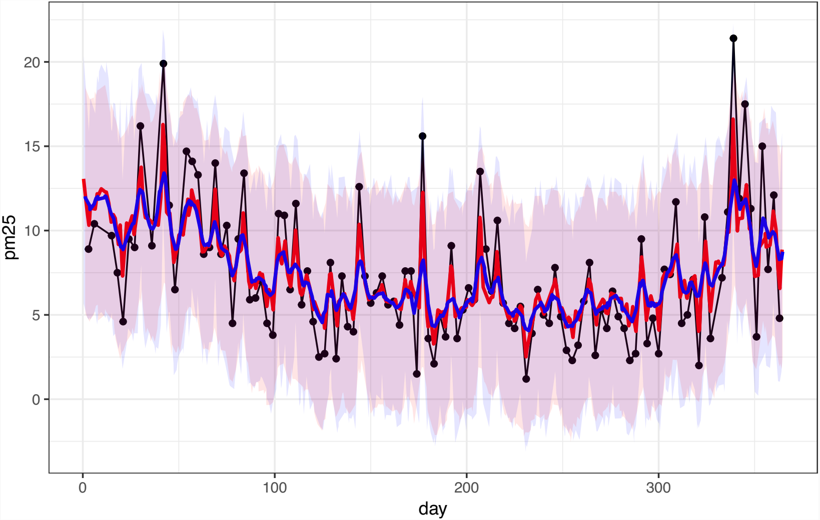


Fit



$$\sigma_w^2 = 7.5 \qquad \sigma^2 = 4.5 \qquad \ell = \frac{\sqrt{3}}{5}$$

Predictions



Full Posterior Predictive Distribution

Plug in Prediction

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

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

where $l^{(m)}, \ldots, {\beta_2}^{(m)}$, etc. are the posterior median of that parameter.

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

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

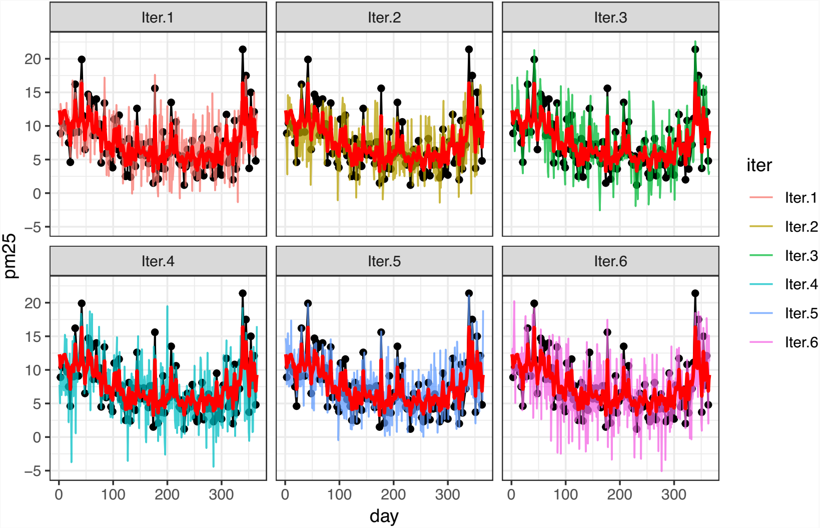
where $l^{(m)}, \ldots, {\beta_2}^{(m)}$, etc. are the posterior median of that parameter.

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