# GPs, GMRFs, and Splines, Oh My!

## Nonparametric modeling with correlated Gaussian effects

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# Why GPs?

- You don't have to assume functional forms
- No need for training data (i.e., cross-validation) for parameter estimation
- Works quite well at prediction
- Certain GPs are equivalent to a infinite node NN

# Why not GPs

- They are computationally burdensome (scales like $n^3$)
- Estimation can be numerically tricky
- There's actually not much software out there for complex data analysis using GPs (in the base form)

# The basics

# Multivariate normal distribution

$$x \sim N(m, V)$$

$m$ is the expected value (mean) of $x$

$V = [\sigma_{ij}]$ is the variance-covariance matrix

- $\sigma_{ii} = \text{var}(x_i)$
- $\sigma_{ij} = \text{cov}(x_i, x_j)$

$V$ has some mathy constraints such as nonnegative-definiteness, that is $a'Va \geq 0$ for any $a$.

# Some properties

$x \sim N(m, V)$

- $Ax \sim N(Am, AVA')$
- Decompose $V = M\Lambda M'$ where $\Lambda$ is diagonal $(\lambda_1 > \cdots > \lambda_n)$ if $\lambda_k$s are small for after some $p$, then $\tilde{V} = M\tilde{\Lambda}M'$ is a low rank approximation created by setting $\lambda_k = 0$ for $k > p$

# Bayesian inference

Bayes rule

$$p(x|y) = \frac{p(y|x)p(x)}{\int p(y|x)p(x)dx}$$

Typically,

- $x = \theta$ and represents a set of parameters
- $p(y|x)$ is a probability model interest
- $p(x)$ is the **prior** distribution of $x$ before data is collected
- $p(x|y)$ is the **posterior** distribution of $x$ after learning from y.

# Gaussian processes

# Gaussian processes (the mathy version)

GPs are prior distributions over functions

$$f(x) \sim \mathcal{GP}(m(x), k(x, x'))$$

characterized by
– $m(x) =$ mean function (usually constant or 0) and
– $k(x, x') =$ the covariance function

Gaussian process because for any $x_1, \ldots, x_n$
$[f(x_1), \ldots, f(x_n)] \sim N(0, K)$

# Covariance functions

Linear

$$k(x, x') = \xi x \cdot x'$$

Squared exponential

$$k(x, x') = \xi \exp\{-\theta(x - x')^2/2\}$$

Exponential

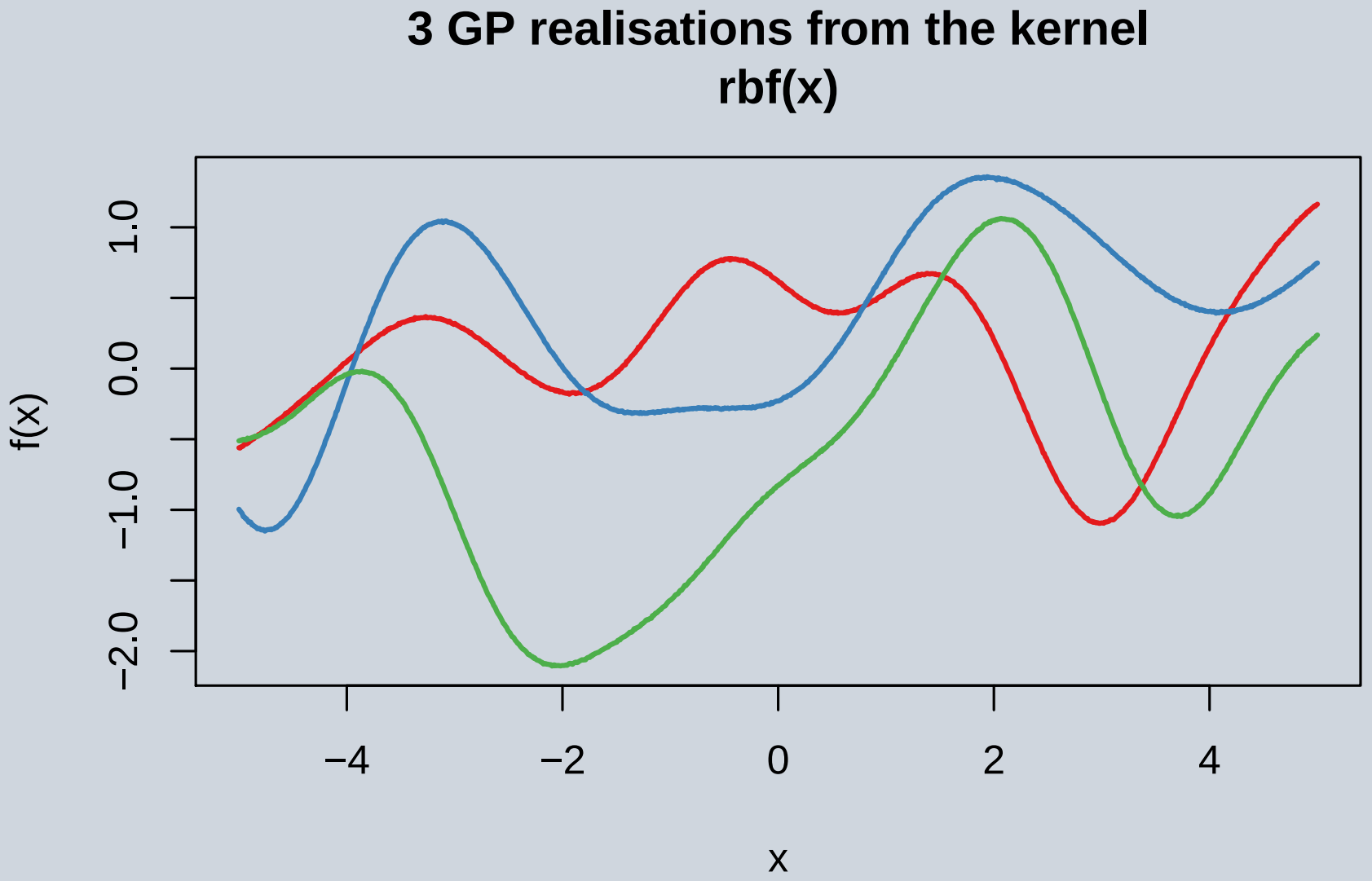
$$k(x, x') = \xi \exp\{-\theta(x - x')\}$$

Construct a valid function

$$f(x) = \int b(u - x)w(u)du$$

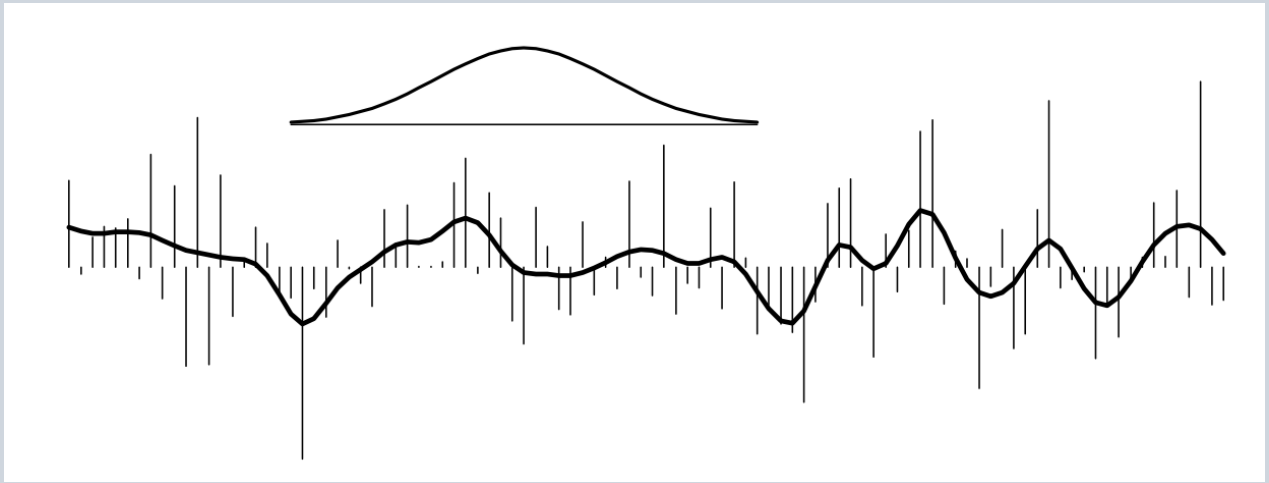
$$k(x, x') = \int b(u - x)b(x' - u)du$$

# Draws of a GP using squared-exponential



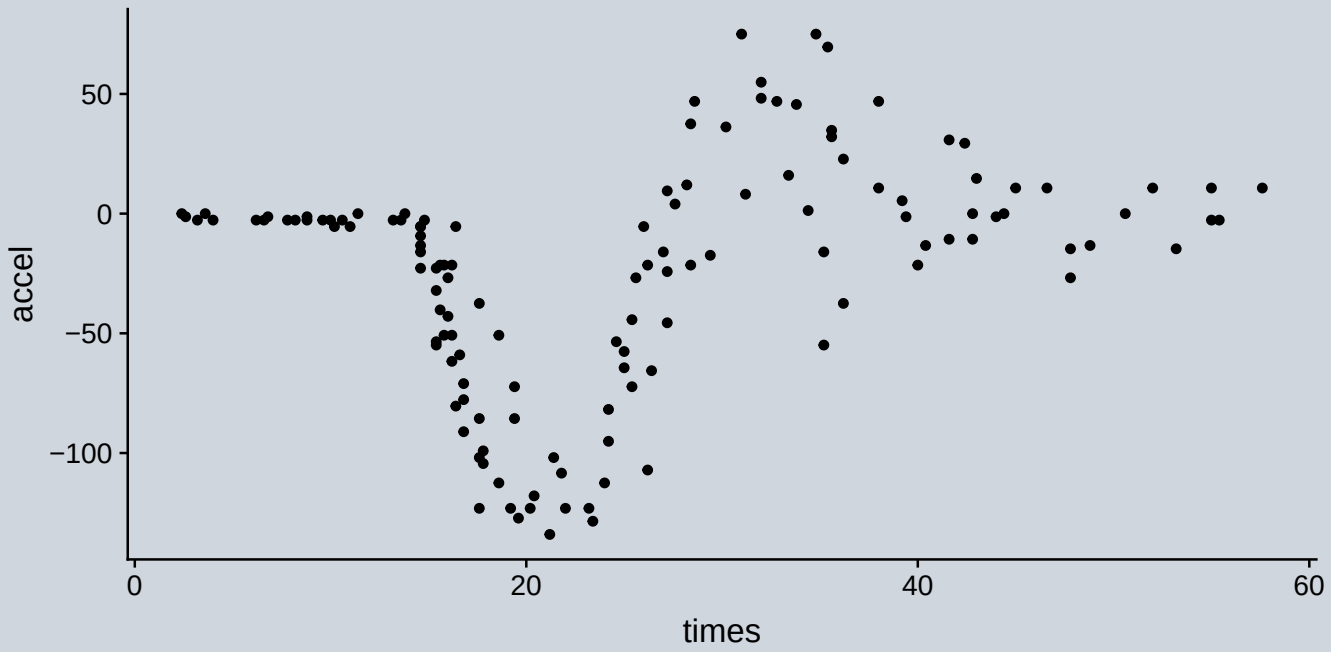
# Gaussian process regression (in practice)

- Gaussian processes are usually too burdensome to work with for real problems
- Process convolution provides a way out
- Set $f(x) = \sum b(u_k - x)w(u_k)$



# The motorcycle data

```
library(MASS); data(mcycle)
```

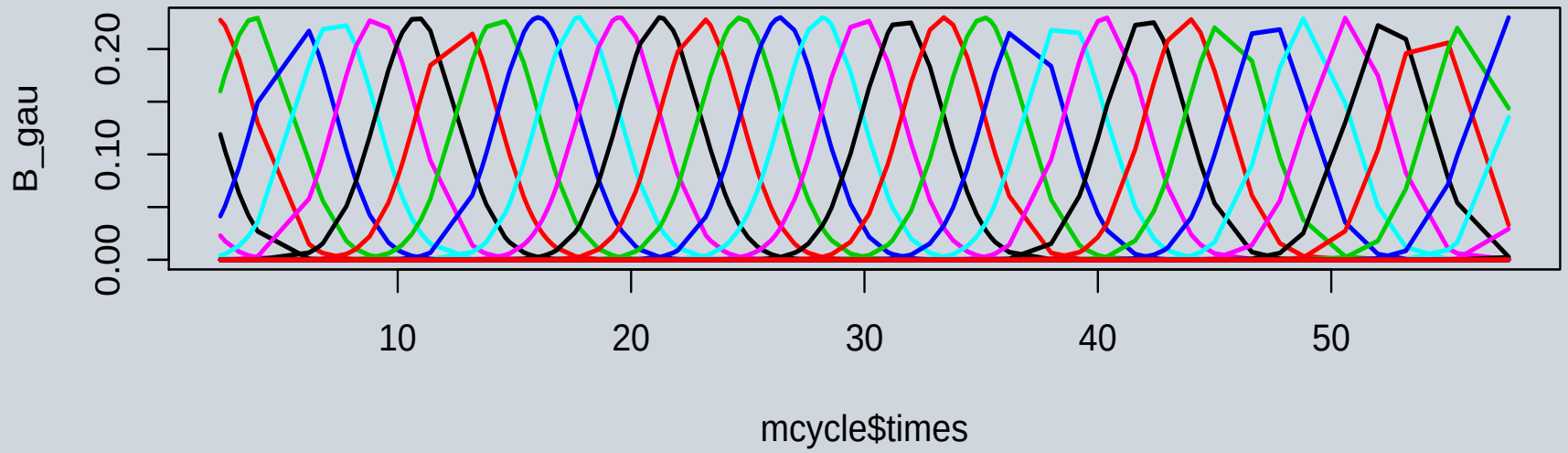



Model:

accel = f(times) + error

```r
u <- seq(-10, 75, length=50)
sd_fac <- 1

B_gau <- outer(
  mcycle$times,u,
  FUN=function(x,y,sd){dnorm(x,y,sd)},
  sd=sd_fac*diff(u[1:2])
)
```




$$\mathbf{f}(\mathbf{x}) = \mathbf{Bw};\ w(u_k) \sim N(0, \xi^2)$$

$$\mathbf{f}(\mathbf{x}) \sim N(\mathbf{0}, \xi^2 \mathbf{B}\mathbf{B}')$$

## Model

$$\mathbf{y} = \mathbf{B}\mathbf{w} + \boldsymbol{\epsilon}$$

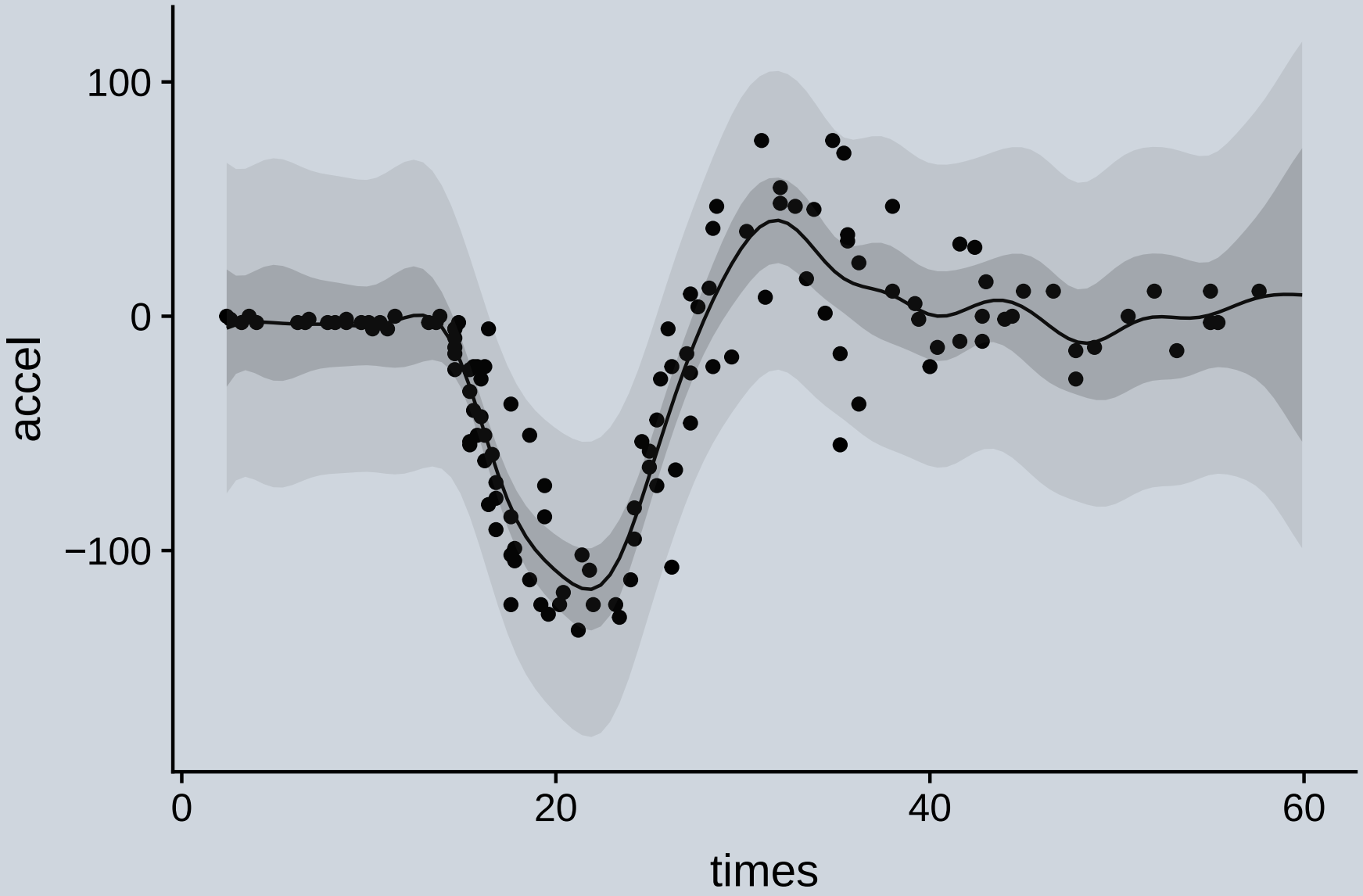
$$(n \times 1) = (N \times p)(p \times 1) + (n \times 1)$$

$$w_k \sim \text{i.i.d.} N(0, \xi^2) \text{ and } \epsilon_i \sim \text{i.i.d.} N(0, \sigma^2)$$

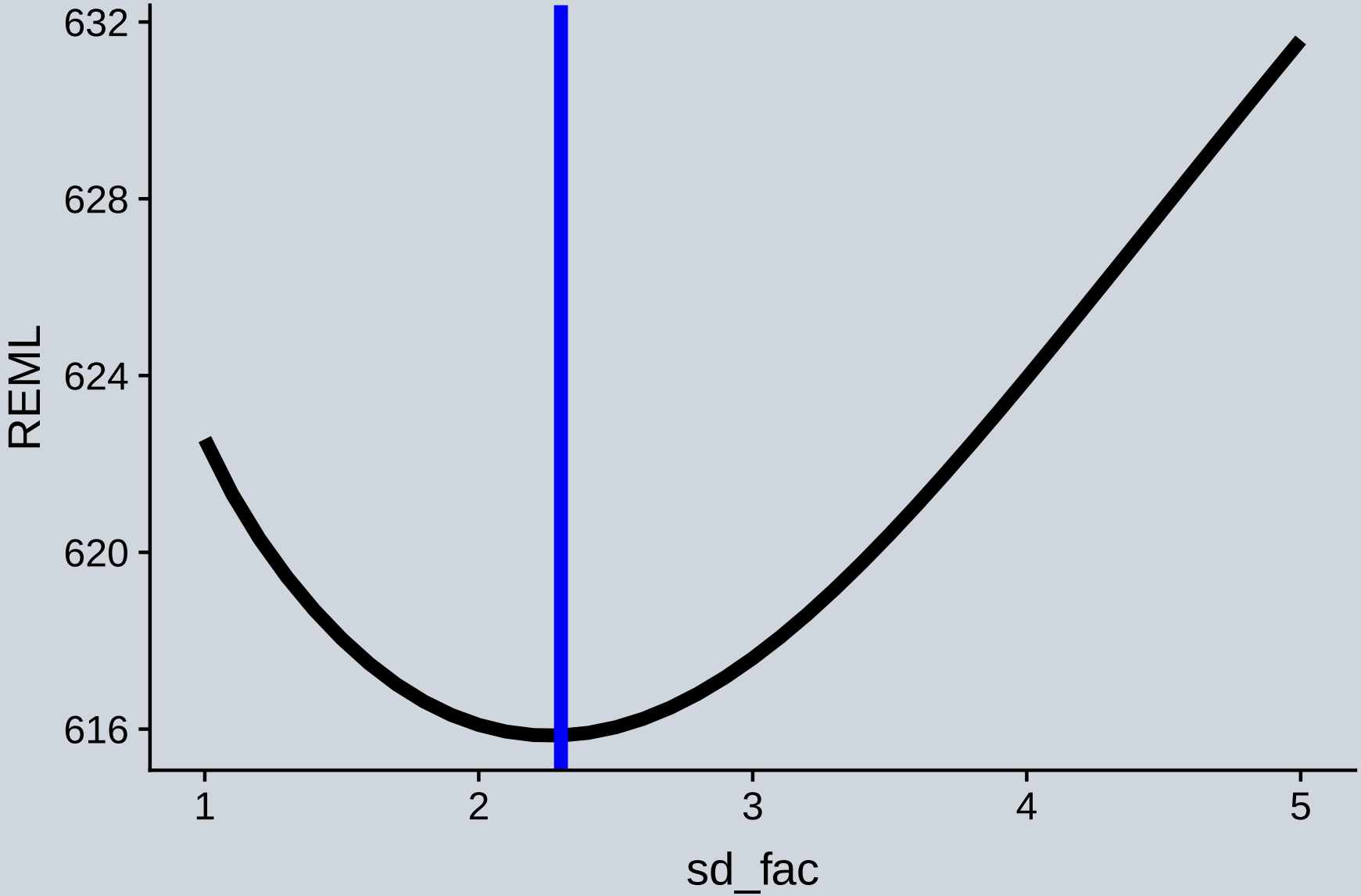
## mgcv syntax

```
fit_gau <- mgcv::gam(
  accel ~ times + B_gau,
  data=mcycle,
  paraPen=list(B_gau=list(S=diag(length(u)))),
  method="REML"
)
```

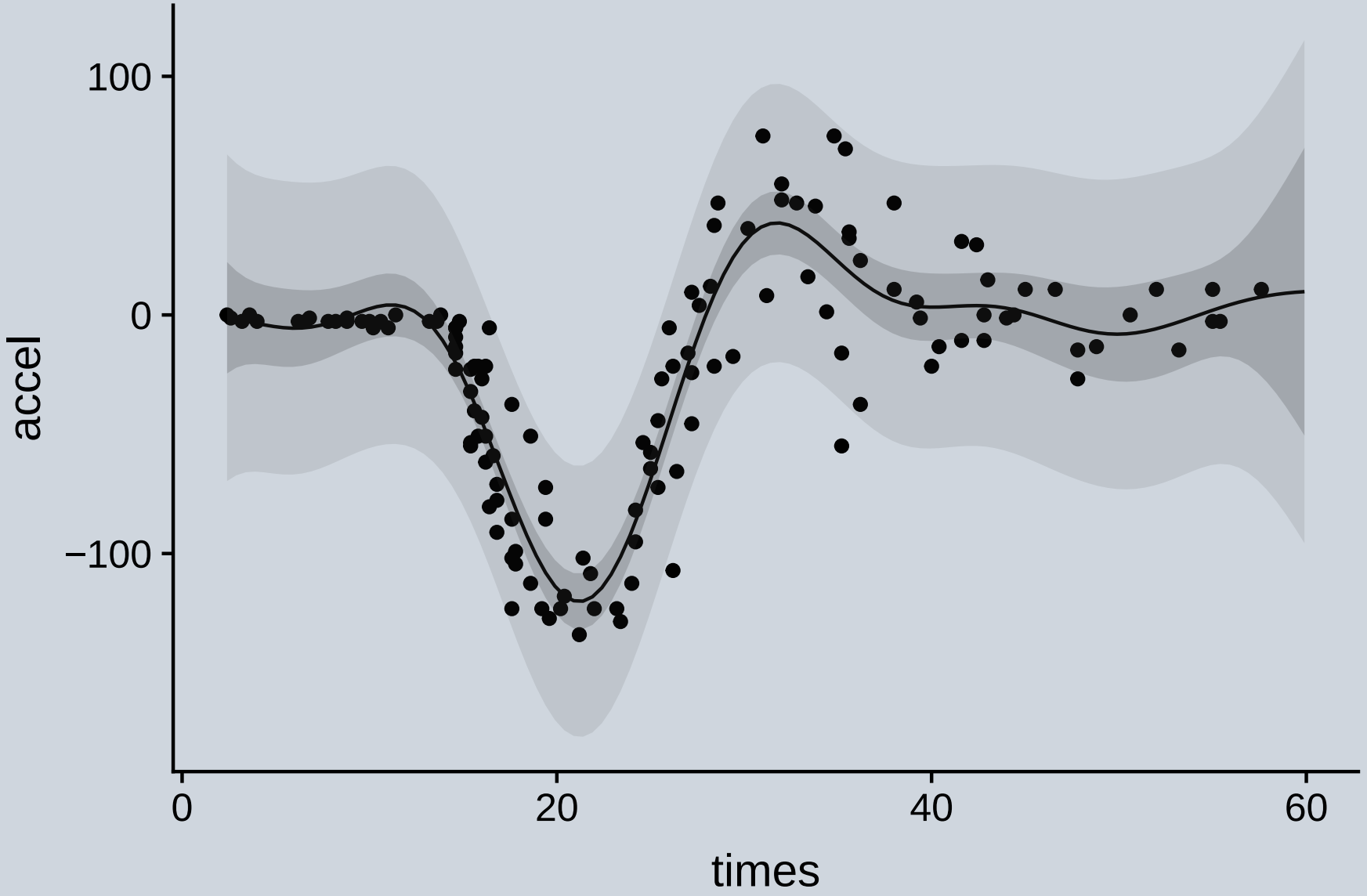
# Some prediction



# Choosing the optimal kernel



# Some better predictions?



# Ok, where's the Bayesian part?

- $\hat{f}(x)$ and $var(\hat{f}(x))$ are the Best Linear Unbiased Estimator
- The BLUP is equivalent to the mean and variance of $p(f|\xi, \mathbf{y})$, the posterior distribution of $f$ (conditioned on $\xi$)
- mgcv can approximate the variance of $p(f|\mathbf{y})$, the true posterior
- $p(f|\xi, \mathbf{y})$ is normal for normal response, approximate for non-normal (e.g., Poisson)

# Penalized splines

# Nonparametric regression modeling

$$y_i = f(x_i|\theta) + \epsilon_i$$

- The form of $f(\cdot|\beta)$ is unknown
- $\epsilon_i \sim N(0, \sigma)$

estimate $(\beta, \sigma)$ by minimizing **penalized likelihood**

$$\hat{\beta} = \underset{\beta}{\operatorname{argmax}} \left\{ \sum_i \log \mathcal{L}(y_i|\beta, \sigma) + J_\lambda(\beta) \right\}$$

where $J_\lambda$ is a penalty that keeps the parameters from overfitting (i.e., keeps the wiggliness down)

# Gaussian surface interpretation

There are many different types of penalized spline smoother: cubic, thin-plate, P-splines, B-splines, etc.

But they all look like this:

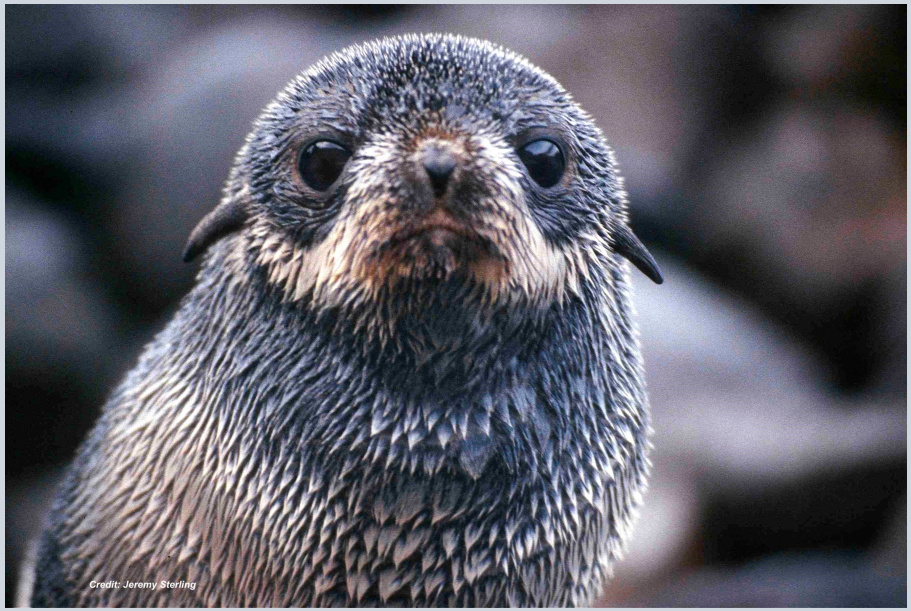
$f(x) = \sum_k^p \beta_k b_k(x)$

$J_\lambda(\beta) = -\lambda \frac{1}{2} \beta' \mathbf{S} \beta$

Looks familiar, hmmm.....

$\mathbf{f(x)} \sim N(\mathbf{0}, \lambda^{-1} \mathbf{B S^{-} B'})$

# Modeling northern fur seal pup migration

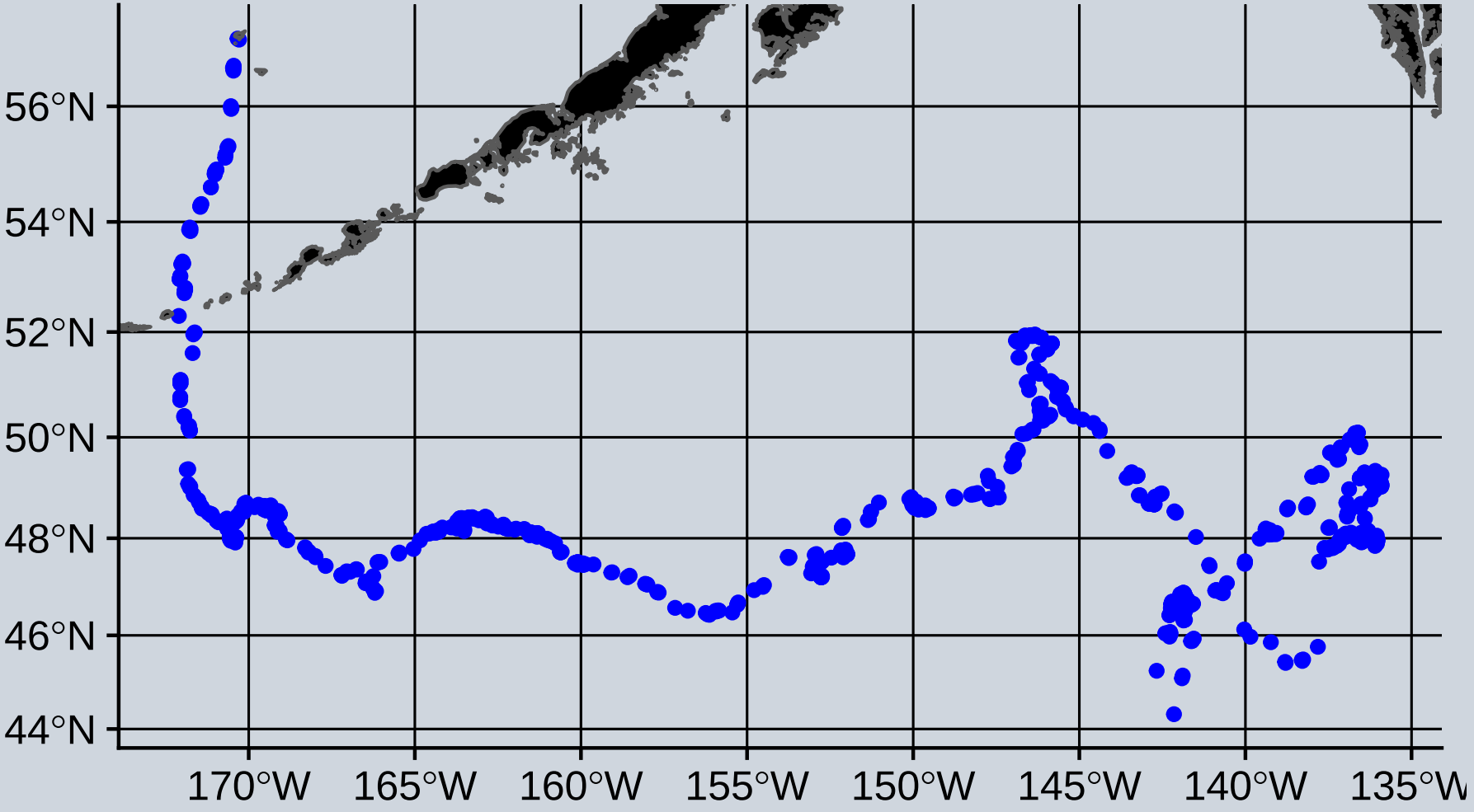


# The data: pup 355

```
library(crawl); data("northernFurSeal")
head(northernFurSeal)
```

```
##                   GMT     long    lat loc_class
## 1 2005-11-10 14:52:00 -170.292 57.109         3
## 2 2005-11-10 14:59:00 -170.336 57.126         1
## 3 2005-11-11 01:17:00 -170.452 56.679         2
## 4 2005-11-11 02:02:00 -170.474 56.645         1
## 5 2005-11-11 02:28:00 -170.454 56.632         1
## 6 2005-11-11 03:53:00 -170.460 56.597         1
```

# The data: pup 355



# Stack data for fitting

```
head(nfs_stack)
hour      loc quality coord
1 314342.9 4420274       3     X
2 314343.0 4415376       1     X
3 314353.3 4402463       2     X
4 314354.0 4400014       1     X
5 314354.5 4402241       1     X
6 314355.9 4401573       1     X
>
```

Notice the coords are projected now

# Model location error

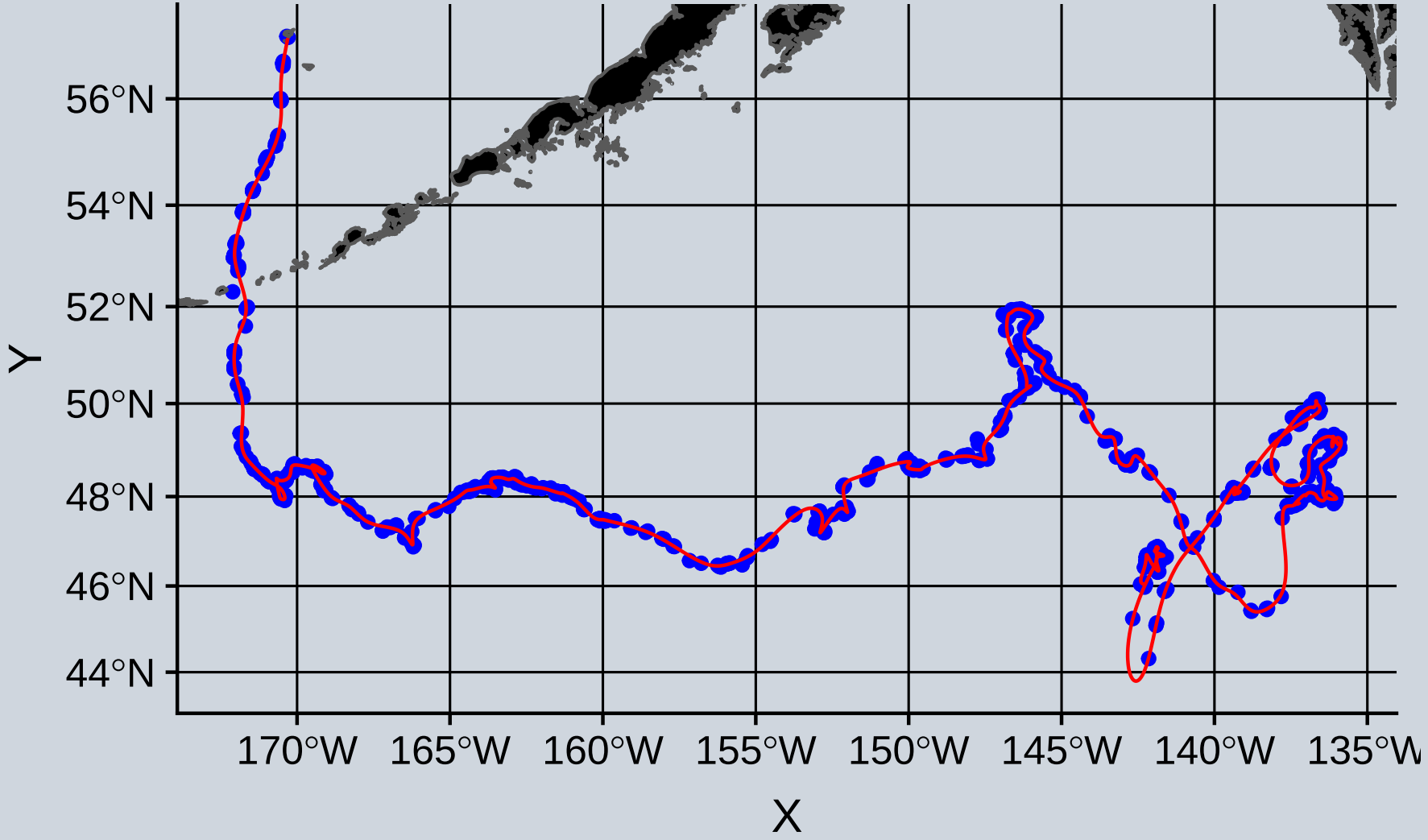
$var(\epsilon) = \exp(2\gamma_g v)$ where '$g$' indexes a group and '$v$' is a covariate

```
## define Argos error variance form
nfs_stack$ones <- 1
# necessary to trick the variance function
fix <- c('3'=log(150), '1'=log(500), '2'=log(250))
var_func <- varExp(
fixed = fix,
form = formula(~ones|quality)
)
```

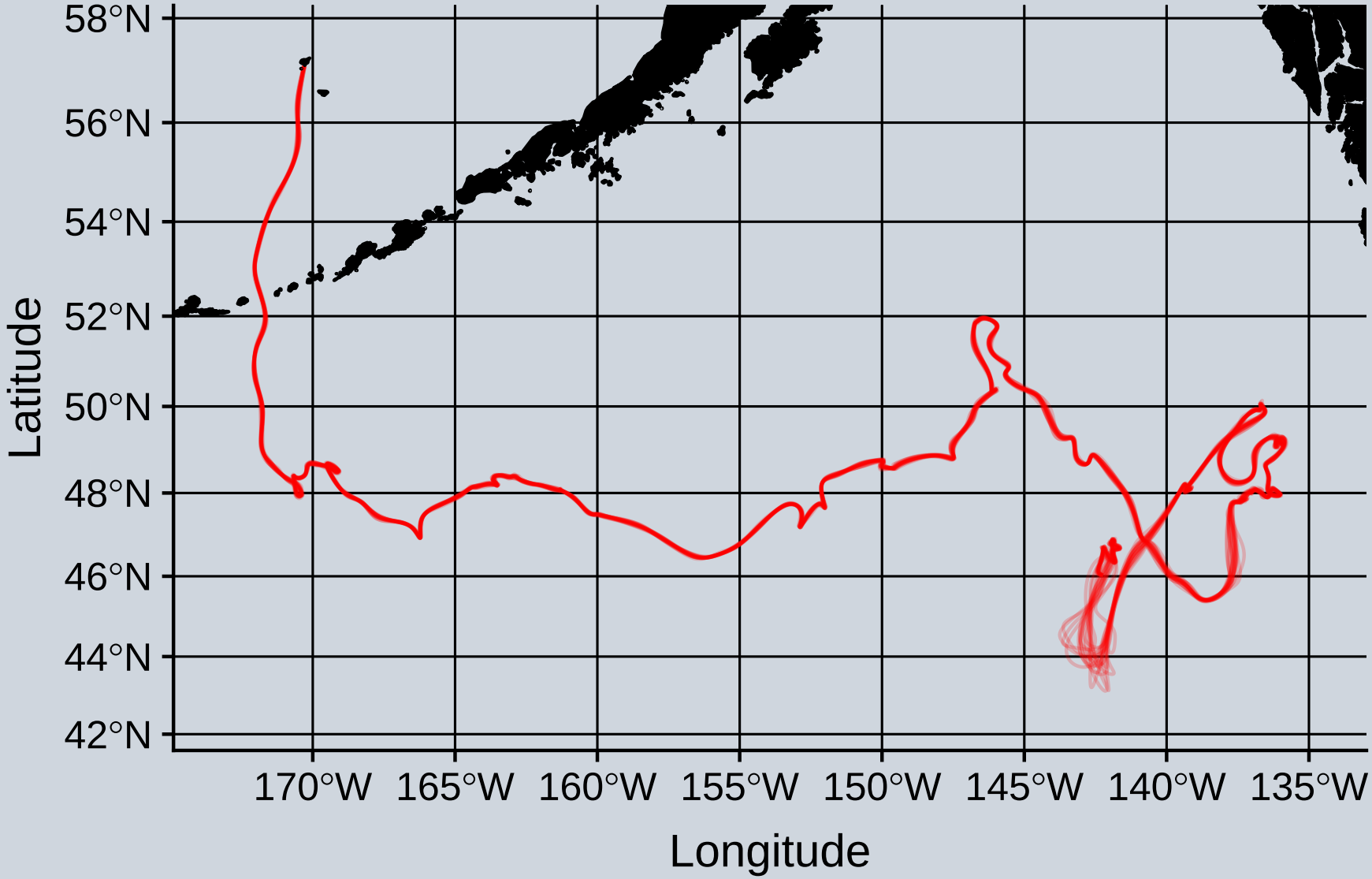
# Fit model and sample from posterior paths

```
fit = mgcv::gamm(
  loc ~ 0 + coord +
    s(hour,by=coord, k=200, bs=c("ps","ps")),
  weights = var_func,
  data=nfs_stack, method="REML")
### Make some simulated paths
B = predict(
  fit[["gam"]],newdata=newdata, type="lpmatrix")
beta = coef(fit$gam)
V = vcov(fit$gam, unconditional = T)
beta_smp = t(rmvnorm(20, beta, V))
paths <- foreach(i=1:20)%do%{
  p <- B %*% beta_smp[,i] %>%
    matrix(., nrow=nrow(newdata)/2, ncol=2)
  p
}
```

# Predicted path



# Path posterior samples



# Markov random fields

# Modeling functions discretely

- $f(x)$ only makes sense for, fixed $x_1, \ldots, x_k$
- Because we only have a few neighbors, lets model each location conditioned on it's neighbors

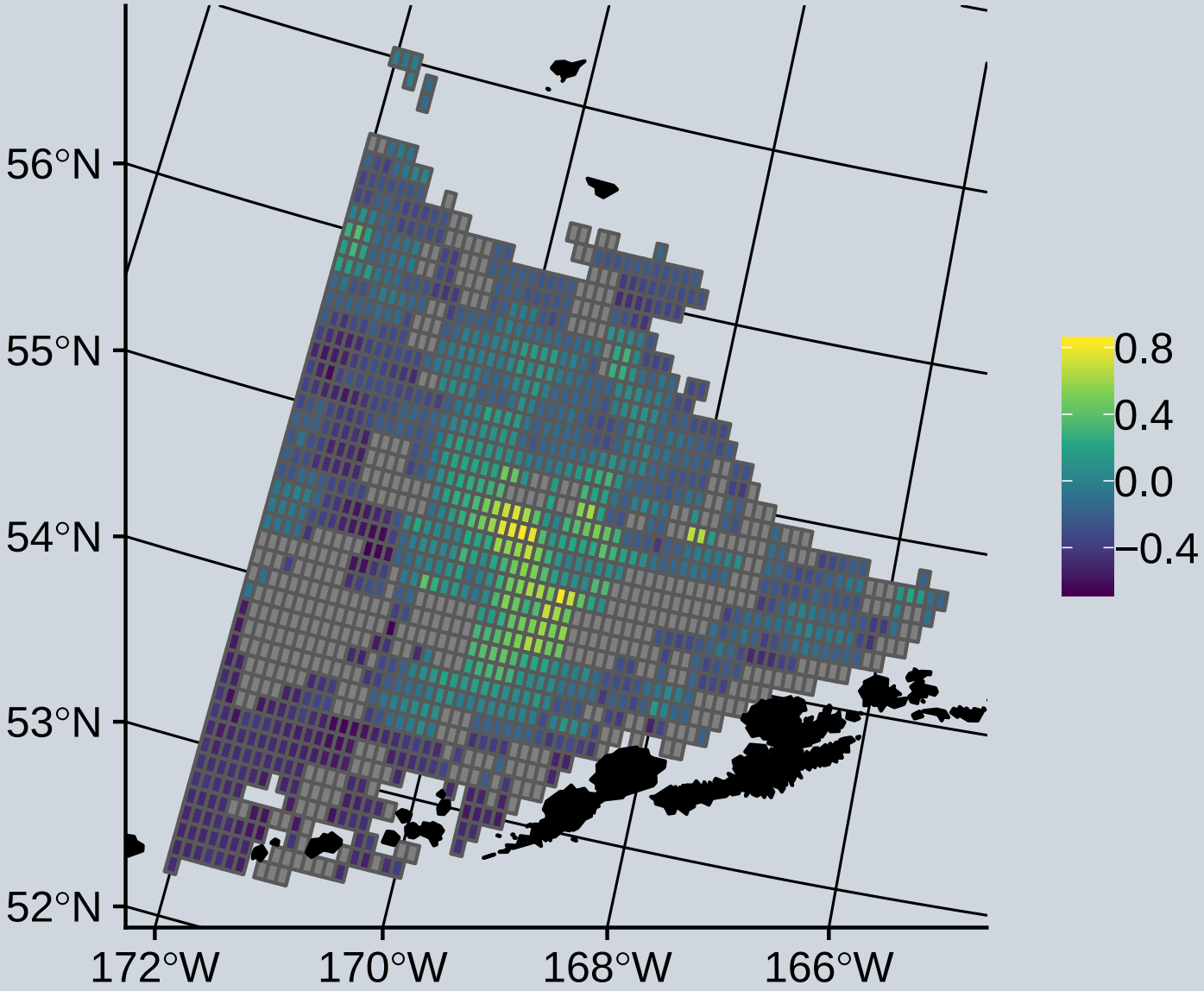
$$f(x_i) \sim N(\bar{f}_i, \xi^2/n_i)$$

- $\bar{f}_i$ mean $f(x_j)$ for all $x_i$ neighbors
- $n_i =$ number of neighbors of $x_i$
- This is known as the Intrinsic Conditionally Auto(R)egressive model, ICAR

# Markov random fields

- MRFs are based on the previous type of neighborhood structure
- Just like GPs, there are many different versions, ICAR is just a very common example
- Models are built on the precision matrix (inverse on the covariance matrix)
- Thus they can be very computationally efficient because there is no need to invert the covariance matrix in the likelihood

# Remote sensed CHl data

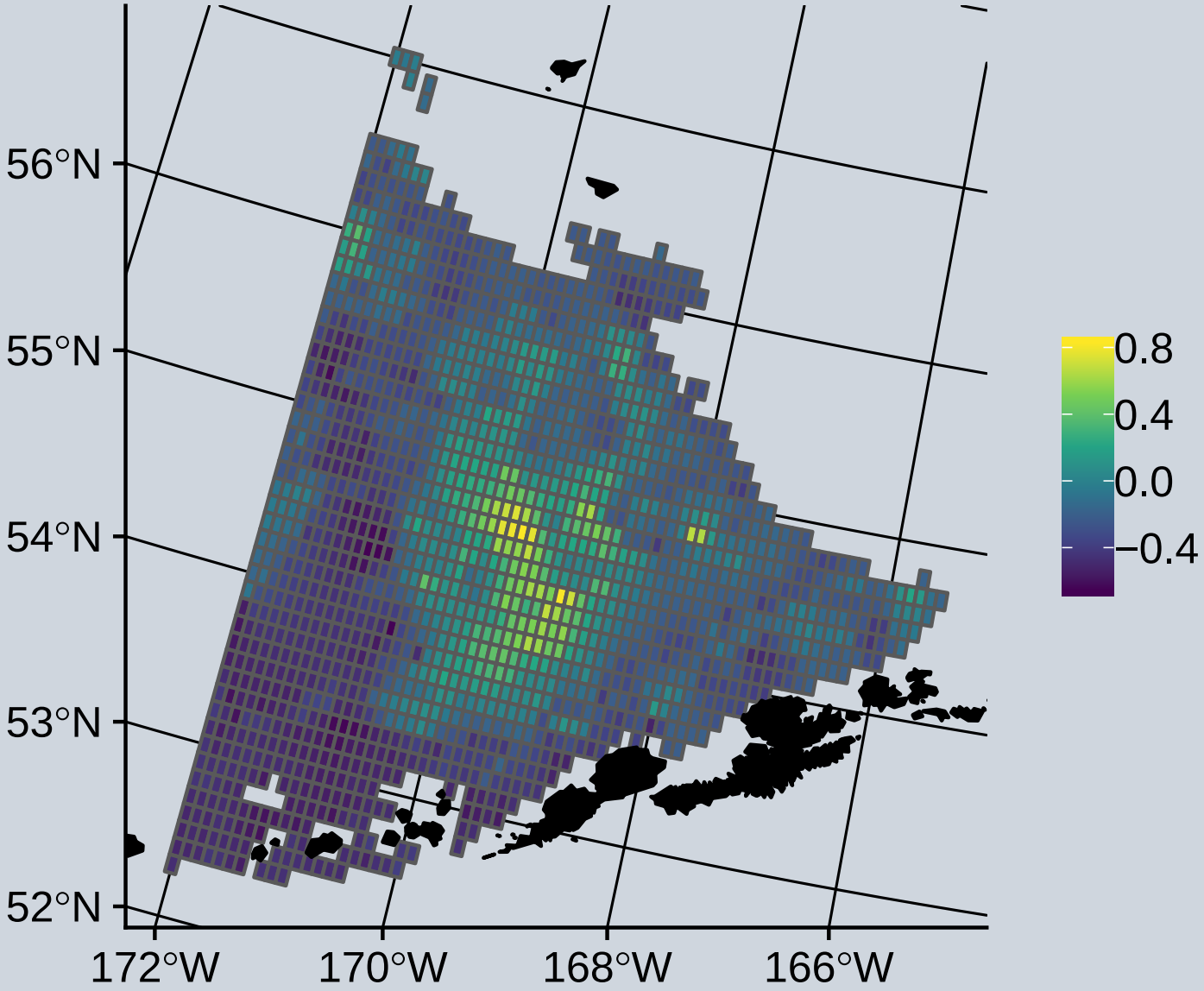


# mgcv, not the best choice for MRFs

```
nb <- chl %>% spdep::poly2nb() %>%
  `names<-`(chl$cell) %>% `class<-`("list")

chl <- chl %>%
  mutate(
    cell = factor(cell),
    weight = ifelse(is.na(log10chl), 0, 1),
    log10chl = ifelse(is.na(log10chl),
                      mean(log10chl, na.rm=T), log10chl)
  )
### Fit a GMRF model
fit <- mgcv::gam(log10chl ~ s(cell, bs="mrf",xt=list(nb=nb)),
                 data=chl, weights=weight)
### Predict missing values
chl <- bind_cols(chl, predict(fit, se.fit=T) %>%
                   as.data.frame())
```

# CHI prediction




The End