# Math 504 HW12

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## 2

### a

$$\min_{\alpha} \sum_{i=1}^{N} |y_i - \sum_{j=1}^{K-4} \alpha_j b_j(x_i)|^2 + \rho \int_{x_{\min}}^{x_{\max}} \left( (\sum_{j=1}^{K-4} \alpha_j b_j(z))'' \right)^2 dz \tag{1}$$

Fromn$\sum_{j=1}^{K-4} \alpha_j b_j(x_i)$, we have $N \times K-4$ values from $b_j(x_i)$. Let each $b_j(x_i)$ be the $ij^{th}$ entry in the matrix $B$

Also, we can expand $\sum_{j=1}^{K-4} \alpha_j b_j(x_i)$ as $\alpha_1 b_1(x_i) + \alpha_2 b_2(x_i) + \cdots + \alpha_{K-4} b_{K-4}(x_i) = S(x_i)$. Thus, we can re-write

$$\sum_{i=1}^{N} |y_i - \sum_{j=1}^{K-4} \alpha_j b_j(x_i)|^2 = \sum_{i=1}^{N} |y_i - S(x_i)|^2 = ||y - B\alpha||^2$$

where $B$ is the $N \times K-4$ matrix as described above and $\alpha$ is $K-4$ column vector.

Next, look at $\rho \int_{x_{\min}}^{x_{\max}} \left( (\sum_{j=1}^{K-4} \alpha_j b_j(z))'' \right)^2 dz$. Since $\rho$ is a constant, we can ignore it for now. This leaves

$$\int_{x_{\min}}^{x_{\max}} \left( (\sum_{j=1}^{K-4} \alpha_j b_j''(z)) \right)^2 dz = \int_{x_{\min}}^{x_{\max}} \left( \left( \sum_{j=1}^{K-4} \alpha_j b_j''(z) \right) \left( \sum_{i=1}^{K-4} \alpha_i b_i''(z) \right) \right) dz =$$

$$\int_{x_{\min}}^{x_{\max}} \sum_{j=1}^{K-4} \sum_{i=1}^{K-4} \alpha_j \alpha_i b_j''(z) b_i''(z) dz = \sum_{j=1}^{K-4} \sum_{i=1}^{K-4} \alpha_j \alpha_i \left( \int_{x_{\min}}^{x_{\max}} b_j''(z) b_i''(z) dz \right)$$

Now define a $K-4$ square matrix $\Omega$ such that each $ji^{th}$ corresponds to $\int_{x_{\min}}^{x_{\max}} b_j''(z) b_i''(z) dz$. Then:

$$\sum_{j=1}^{K-4} \sum_{i=1}^{K-4} \alpha_j \alpha_i \left( \int_{x_{\min}}^{x_{\max}} b_j''(z) b_i''(z) dz \right) = \sum_{j=1}^{K-4} \sum_{i=1}^{K-4} \alpha_j \alpha_i \Omega_{ji} = \alpha^T \Omega \alpha$$

Putting this together, we get

$$\min_{\alpha} \sum_{i=1}^{N} |y_i - \sum_{j=1}^{K-4} \alpha_j b_j(x_i)|^2 + \rho \int_{x_{\min}}^{x_{\max}} \left( (\sum_{j=1}^{K-4} \alpha_j b_j(z))'' \right)^2 dz = \min_{\alpha} ||y - B\alpha||^2 + \rho \alpha^T \Omega \alpha \tag{2}$$

Solve for $\alpha$:

$$L(\alpha) = ||y - B\alpha||^2 + \rho \alpha^T \Omega \alpha = (y - B\alpha) \cdot (y - B\alpha) + \rho \alpha^T \Omega \alpha = y \cdot y - 2B\alpha \cdot y + B\alpha \cdot B\alpha + \rho \alpha^T \Omega \alpha \Rightarrow$$

$$\nabla_\alpha L(\alpha) = -2B^T y + 2B^T B\alpha + 2\rho\Omega\alpha = 0 \longrightarrow B^T B\alpha + \rho\Omega\alpha = B^T y \rightarrow$$
$$(B^T B + \rho\Omega)^{-1}(B^T B + \rho\Omega)\alpha = (B^T B + \rho\Omega)^{-1} B^T y \Rightarrow$$
$$\alpha = (B^T B + \rho\Omega)^{-1} B^T y$$

## b

```
bone_mass <- read_delim("BoneMassData.txt", delim = " ")
females <- bone_mass %>% filter(gender == "female")
K <- 1000
min_x <- min(females$age)
max_x <- max(females$age)
myknots = seq(min_x, max_x, length.out = 1002)[2:1001]

h <- (max_x - min_x) / 2500
mygrid <- seq(min_x, max_x, h)

B <- splineDesign(knots = myknots, x = females$age, outer.ok = T)
Bpp <- splineDesign(knots = myknots, x = mygrid, derivs = 2, outer.ok = T)

Omega <- matrix(0, nrow = K-4, ncol  = K-4)

test <- sum(Bpp[,10] * Bpp[,15] * h)

for(i in 1:(K-4)){
  for(j in 1:(K-4)){
    Omega[i,j] = sum(Bpp[,i] * Bpp[, j] * h)
  }
}
```

## c

Show that $B^T B$ is not invertible - simply show $\det B^T B = 0$:

```
det(t(B) %*% B)
```

```
## [1] 0
```

But $B^T B + \rho\Omega$ is invertible for $\rho > 0$ (show $\det \neq 0$):

```
rho = 3e-06
det(t(B)%*%B + rho * Omega)
```

```
## [1] 6.719545e+19
```

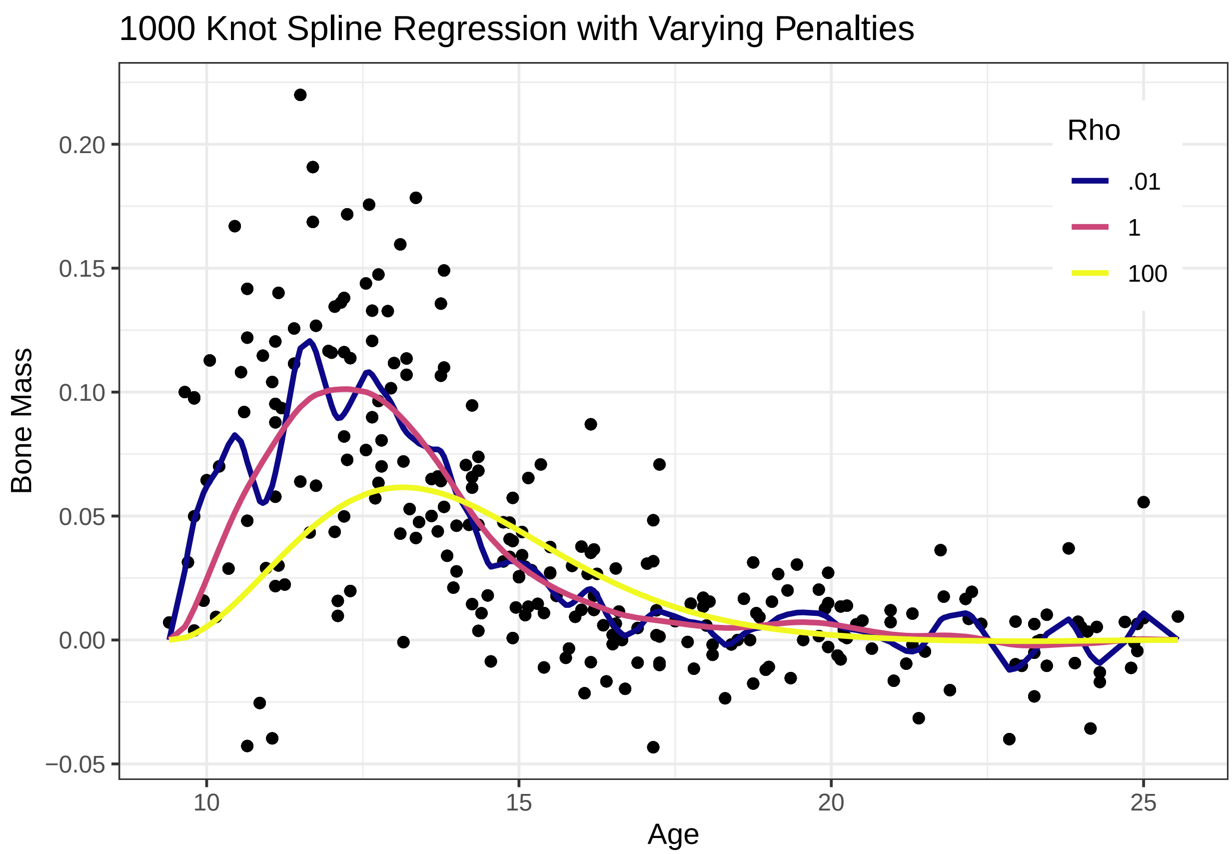
## d

```r
solveAlpha <- function(rho, b = B, omega = Omega, y = females$spnbmd){
  alpha <- solve(t(b) %*% b + rho * omega) %*% t(b) %*% y
  return(alpha)
}
alpha.01 <- solveAlpha(rho = 0.01)
alpha1 <- solveAlpha(rho = 1)
alpha100 <- solveAlpha(rho = 100)

spline_plot_data <- data.frame(x = females$age, boneMass = females$spnbmd,
                               `.01` =  B %*% alpha.01,
                               `1` = B %*% alpha1,
                               `100` = B %*% alpha100)

spline_test <- spline_plot_data %>%
  pivot_longer(cols = 3:5,
               names_to = "Rho",
               values_to = "S_x") %>%
  mutate(Rho = str_extract(Rho, "\\.[:digit:]+|[:digit:]+"))

ggplot(data = spline_test, aes(x = x)) +
  geom_point(aes(y = boneMass)) +
  geom_line(aes(y = S_x, color = Rho), size = 1) +
  scale_color_viridis(discrete = T, option = "C") +
  theme_bw() +
  labs(title = "1000 Knot Spline Regression with Varying Penalties",
       x = "Age",
       y = "Bone Mass") +
  theme(legend.position = c(0.9,0.8))
```




So we see that using too small of a $\rho$ (blue-ish purple line) causes the regression to be overfit, with the regression line oscillating heavily in small intervals. A spline with a modest penalty of $\rho = 1$ (magenta line), causes the spline regression to look similar to the one computed with two knots on our previous HW. It has a higher rise with the spike in data around ages 11-13 than a higher penalty, but it doesn't have heavy swings the way a lower penalty did. Meanwhile a highly penalized regression with $\rho = 100$ (yellow line), the regression had smaller moves with the data, and perhaps penalized too much. It seems to have too small of a rise with the data from 11-13, and then too slow to drop with the data after age 15.