Math 504 HW12

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2

a

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

From$\sum_{j=1}^{K-4} \alpha_j b_j(x_i)$, 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 α 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 ρ 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 Ω 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 α:

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

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

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 <- t(Bpp) %*% Bpp * h
```

c

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

```
det(t(B) %*% B) == 0
```

```
## [1] TRUE
```

To show that $B^T B + \rho\Omega$ is invertible, first show that Ω is invertible. `det(Omega) =` ∞. The matrix determinant lemma (wiki) states that if A is an $n \times n$ invertible matrix, and U and V are $n \times m$ matrices, the $\det(A + UV^T) = \det(I_m + V^T A^{-1} U)\det(A)$. Applying to our data, we get $\det(\Omega + B^T B) = \det(I_{259} + B\Omega^{-1}B^T)\det(\Omega) \rightarrow \det(\rho\Omega + B^T B) = \det(I_{259} + B\rho^{-1}\Omega^{-1}B^T)\det(\rho\Omega)$. Since we know that $\det(\Omega)$ is very large (`R` outputs it as ∞), we simply need to show that $\det(I_{259} + B\Omega^{-1}B^T) \neq 0$:

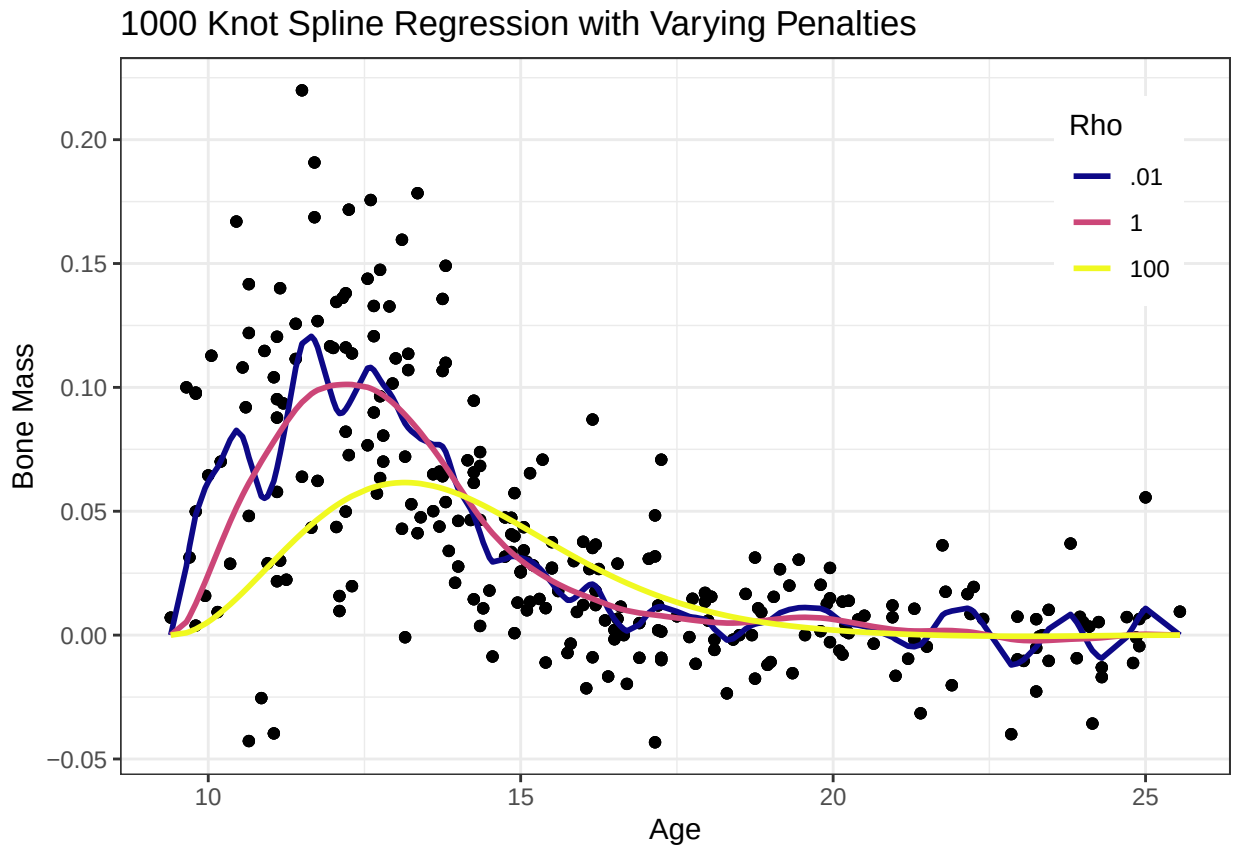
```
I259 <- diag(nrow = 259, ncol = 259)
det(I259 + B %*% solve(Omega) %*% t(B))
```

```
## [1] 7.181395e+13
```

Thus, since $\det(\Omega + B^T B) = \det(I_{259} + B\Omega^{-1}B^T)\det(\Omega) \neq 0 \Longrightarrow \Omega + B^T B$ is invertible, and if $\rho > 0$, then $\det(\rho\Omega + B^T B) \neq 0$ and $B^T B + \rho\Omega$ is invertible for $\rho > 0$

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 ρ (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.

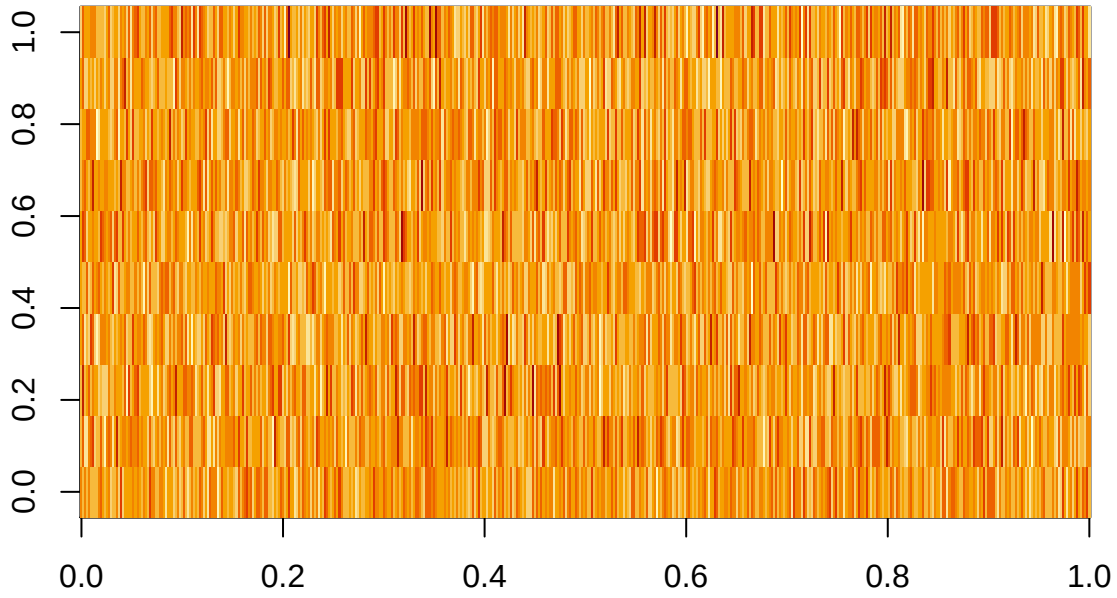
3

a

`signal.R`:

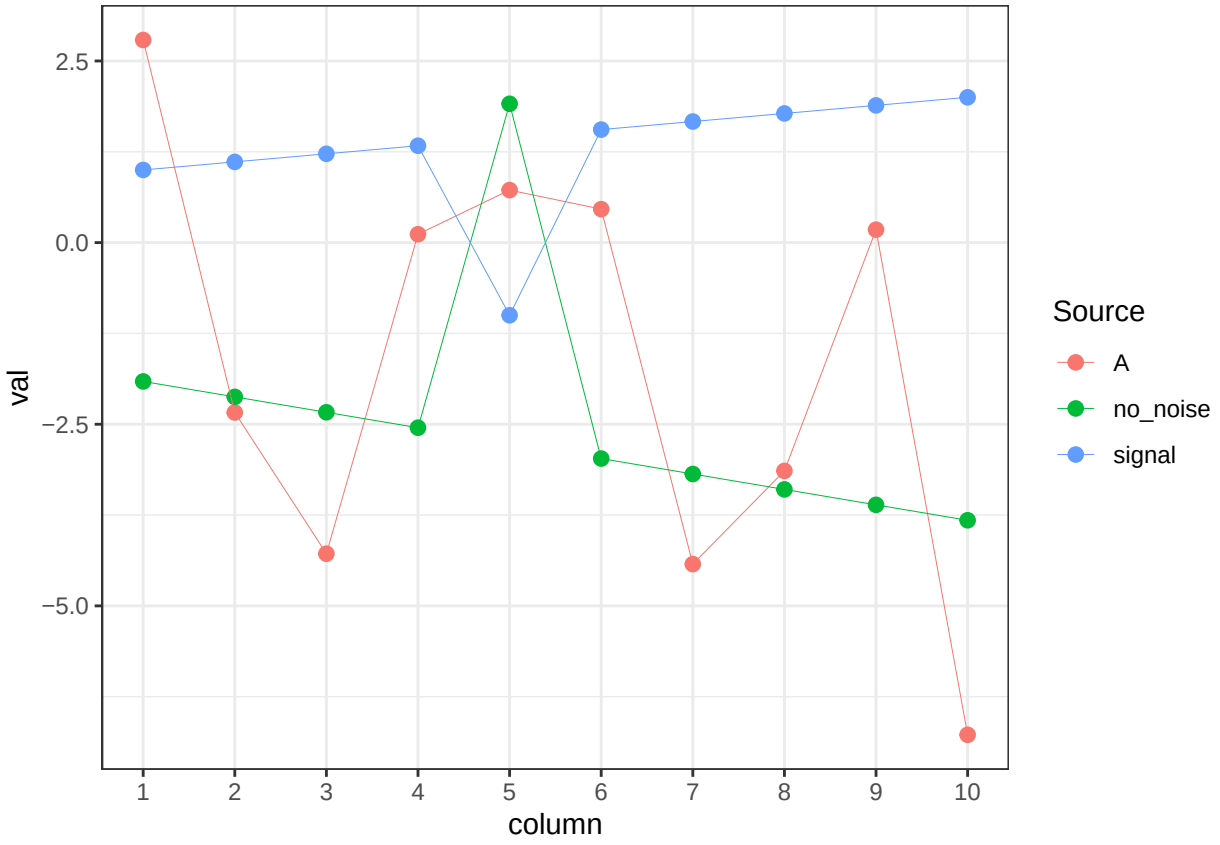
```
set.seed(1236)

# the "signal" that make up the rows of our matrix, with noise added.
sig <- seq(1,2,length.out = 10)
sig[5] <- -1


# each row of A will have the form: q*signal + noise
nsamples <- 500
A <- matrix(NA, ncol=10, nrow=nsamples)
```

```r
no_noise_A <- matrix(NA, ncol=10, nrow=nsamples)
q <- runif(nsamples, min=-3, max=3)
for (i in 1:nsamples) {
  noise <- rnorm(10, mean=0, sd=5)
  A[i,] <- q[i]*sig + noise
  no_noise_A[i,] <- q[i]*sig
}

write.table(no_noise_A, file="no_noise_A.txt", row.names = F, col.names = F)
write.table(A, file="A.txt", row.names = F, col.names = F)
write.table(q, file="q.txt", row.names=F, col.names=F)

image(A)
```




```r
plot_data <- data.frame(
  column = seq(1,10,1),
  A = A[1,],
  no_noise = no_noise_A[1,],
  signal = sig
) %>%
  pivot_longer(cols = 2:4, names_to = "Source", values_to = "val")


ggplot(data = plot_data, aes(x = column, y = val)) +
  geom_point(aes(col = Source), size = 2.25) +
```

```
  geom_line(aes(col = Source), size = .125) +
  scale_x_continuous(breaks = seq(1,10,1), minor_breaks = NULL) +
  theme_bw()
```



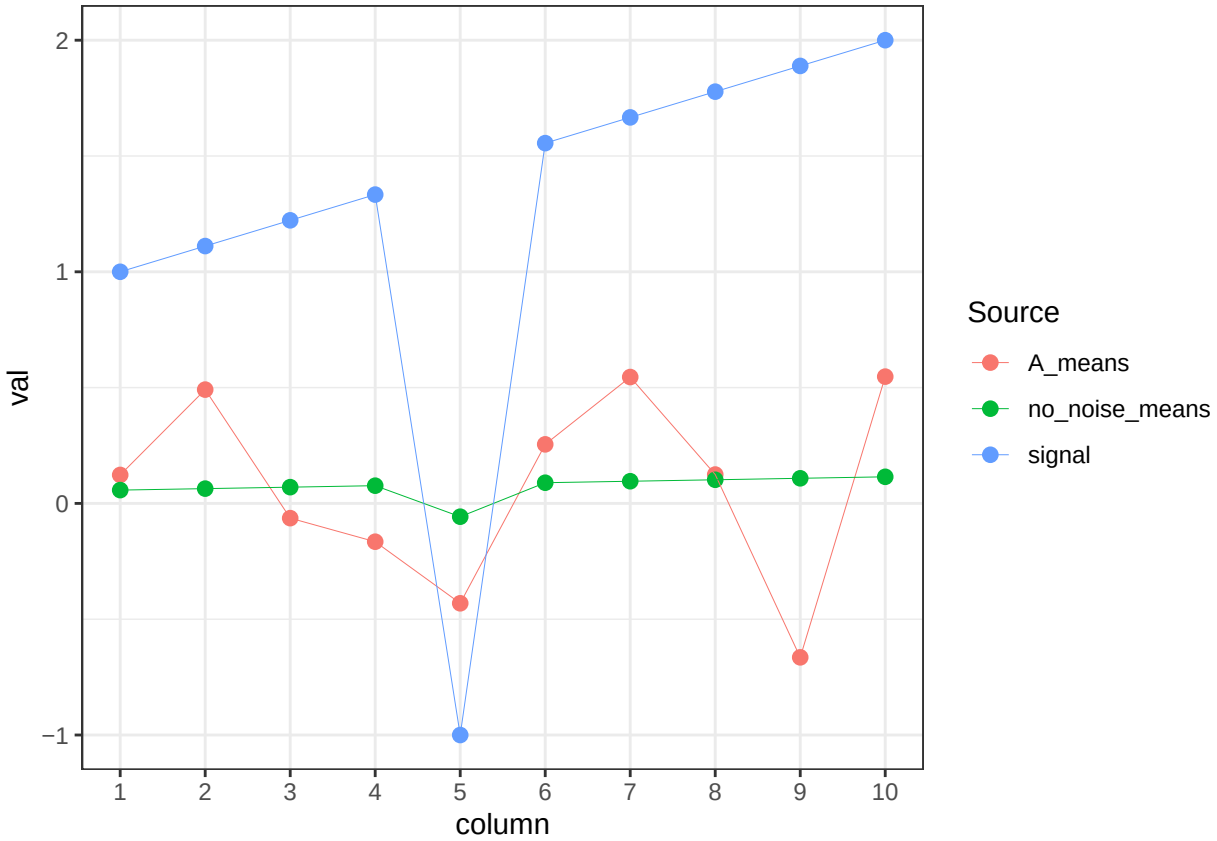
You can't derive the signal just using one observation of A and `no_noise_A`, as at a single row observation level the noise is too strong and causes A to not follow a tight enough window to derive the noise. As the first row of `no_noise_A` is derived from multiplying $q_1 = -1.911$ times the signal, we would expect to be able to derive the signal by dividing the first row by -1.911, but doing so with A does not give a result remniscient of our signal:

-1.4594568, 1.2235123, 2.2406375, -0.0602157, -0.3782986, -0.2410538, 2.3155057, 1.6442113, -0.093381, 3.5449524

Can we find the signal in A using the column means though?

```
col_means_A <- colMeans(A)
col_no_noise_A <- colMeans(no_noise_A)
plot_data_2 <- data.frame(
  column = seq(1,10,1),
  A_means = col_means_A,
  no_noise_means = col_no_noise_A,
  signal = sig
) %>%
  pivot_longer(cols = 2:4, names_to = "Source", values_to = "val")

ggplot(data = plot_data_2, aes(x = column, y = val)) +
  geom_point(aes(col = Source), size = 2.25) +
```

```
  geom_line(aes(col = Source), size = .125) +
  scale_x_continuous(breaks = seq(1,10,1), minor_breaks = NULL) +
  theme_bw()
```

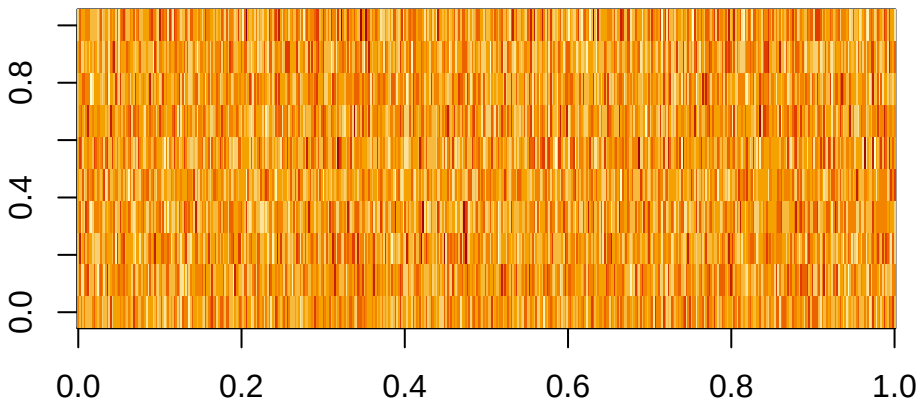


By taking the column means we can see the muted signal in `no_noise_A`, however the signal in A is still suppressed by the random noise added to the matrix generation.

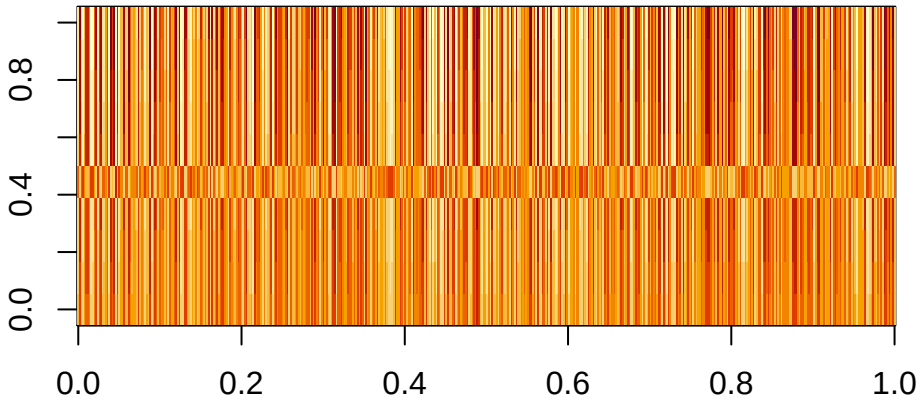
b

While Singular Value Decomposition says an $m \times n$ matrix A, $m > n$ can be expressed as $A = USV^T$, where U is an $m \times m$ matrix composed of the eigenvectors of AA^T, when using `R`'s `svd` function, it returns U as an $m \times n$ matrix. This is because the eigenvalues beyond the n^{th} eigenvector are pretty much 0, so the added information from the corresponding eigenvectors is minimal, and we can instead shorten our SVD to $A \approx U'SV^T$, where U' is the $m \times n$ matrix generated by `R`'s `svd` function. Additinally, S dfnow becomes an $n \times n$ diagonal matrix instead of an $m \times n$ diagonal matrix.

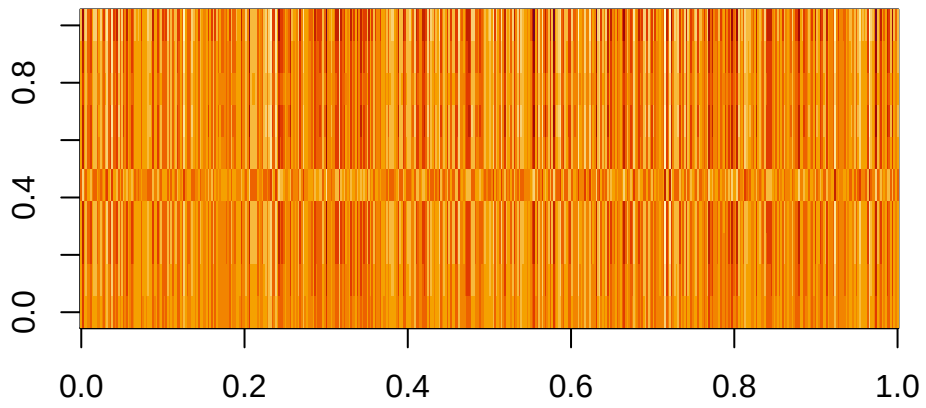
```
svd_A <- svd(A)
U <- svd_A$u
V <- svd_A$v
S <- diag(svd_A$d)

A_1 <- S[1,1] * U[,1] %*% t(V[,1])

image(A)
```




```
image(no_noise_A)
```



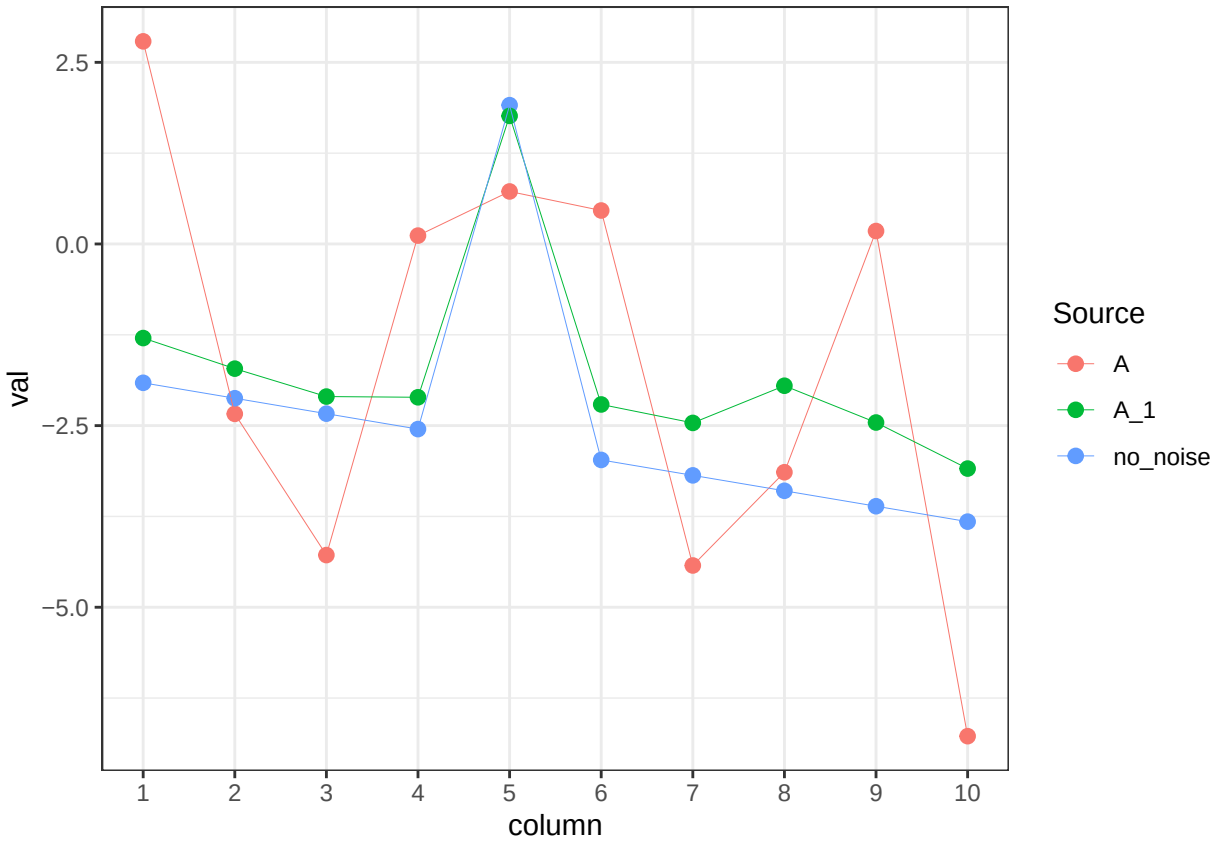

```
image(A_1)
```



We see that the first singular values remove most of the noise from A, as A_1 looks much closer to `no_noise_A` than A, and in particular we are able to see the clear negative value from the signal at the fifth signal entry.

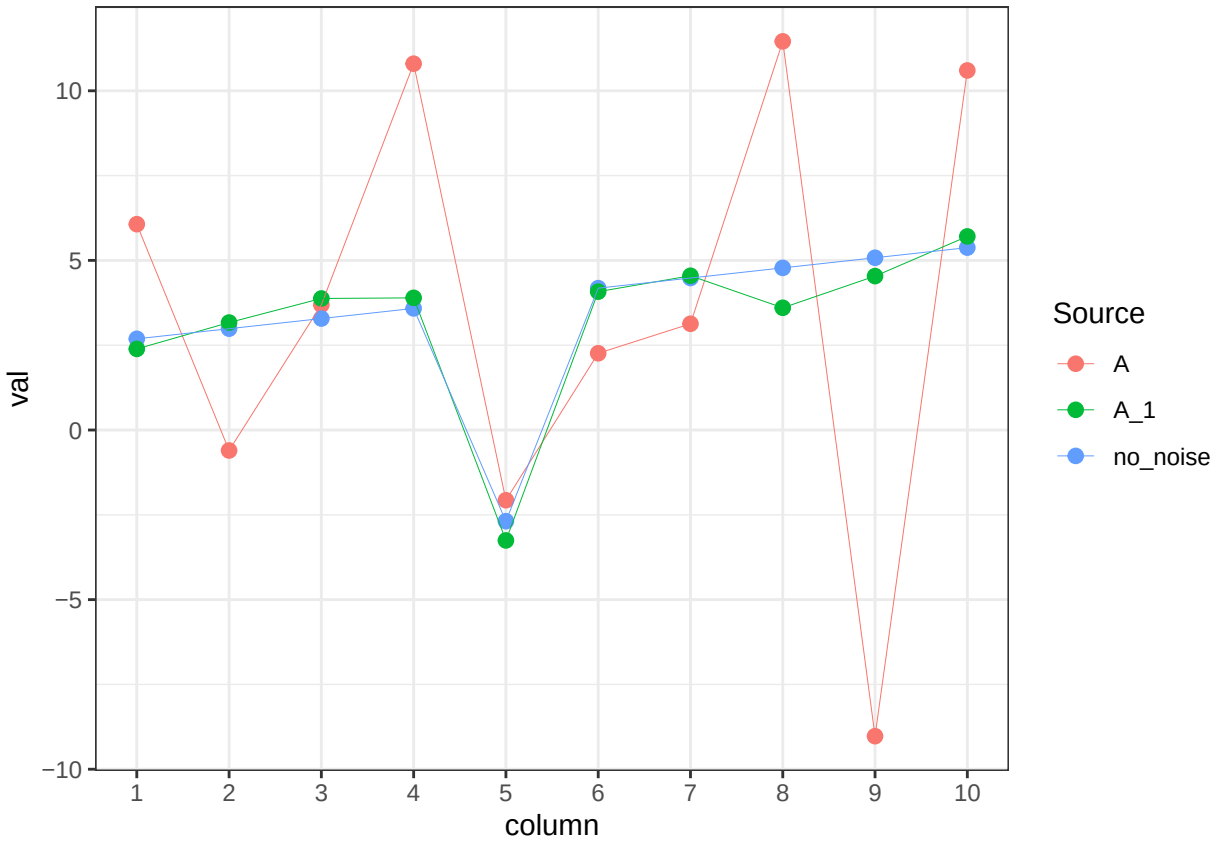
Compare first rows of A, A_1, `no_noise_A`:

```
plot_data <- data.frame(
  column = seq(1,10,1),
  A = A[1,],
  no_noise = no_noise_A[1,],
  A_1 = A_1[1,]
) %>%
  pivot_longer(cols = 2:4, names_to = "Source", values_to = "val")


ggplot(data = plot_data, aes(x = column, y = val)) +
  geom_point(aes(col = Source), size = 2.25) +
  geom_line(aes(col = Source), size = .125) +
  scale_x_continuous(breaks = seq(1,10,1), minor_breaks = NULL) +
  theme_bw()
```



We see that the first row of A_1 closely matches that of `no_noise_A`, suggesting that the first singular values do a good job of filtering out most of the noise in A and capture much of the signal. Now pick a row at random and see if we are able to make a similar observation.

```
sample_row <- sample(c(1:500), 1)
plot_data <- data.frame(
  column = seq(1,10,1),
  A = A[sample_row,],
  no_noise = no_noise_A[sample_row,],
  A_1 = A_1[sample_row,]
) %>%
  pivot_longer(cols = 2:4, names_to = "Source", values_to = "val")


ggplot(data = plot_data, aes(x = column, y = val)) +
  geom_point(aes(col = Source), size = 2.25) +
  geom_line(aes(col = Source), size = .125) +
  scale_x_continuous(breaks = seq(1,10,1), minor_breaks = NULL) +
  theme_bw()
```



While still not perfect, row 453 still closely follows the pattern of `no_noise_A`, this time tracking `no_noise_A` even more closely than in the first row. It is pretty evident that $v^{(1)}$, s_1, and $u^{(1)}$ filter out most of the noise in A and capture most of the relationship between q and sig