Spectral Clustering

Much of this uses information from A Tutorial on Spectral Clustering by Ulrike von Luxburg and Proximity in Statistical Machine Learning by Michael Trosset.

The Ratio Cut Problem

Ratio Cut for $k = 2$

It can be shown that in the relaxed case for $k = 2$, minimizing:

$$W(k) = \sum_{i=1}^{k} (x_i - m_1)^2 + \sum_{i=k+1}^{n} (x_i - m_2)^2$$

where m_1 and m_2 are k-means centers, as perscribed by Luxburg results in the same clustering as by assigning clusters by minimizing

$$R(k) = \sum_{i=1}^{k} \left(x_i + \sqrt{\frac{n-k}{k}} \right)^2 + \sum_{i=k+1}^{n} \left(x_i - \sqrt{\frac{k}{n-k}} \right)^2$$

in $\mathbb{R}^1$ and where x_is are ordered, i.e., $x_i \leq \cdots \leq x_n$. We also constrain the problem to $\sum_i^n x_i = 0$ and $\sum_i^n x_i^2 = n$.

The k-means centers in $\mathbb{R}$ are

$$m_1 = \frac{1}{k} \sum_{i=1}^{k} x_i$$

$$m_2 = \frac{1}{n-k} \sum_{i=k+1}^{n} x_i$$

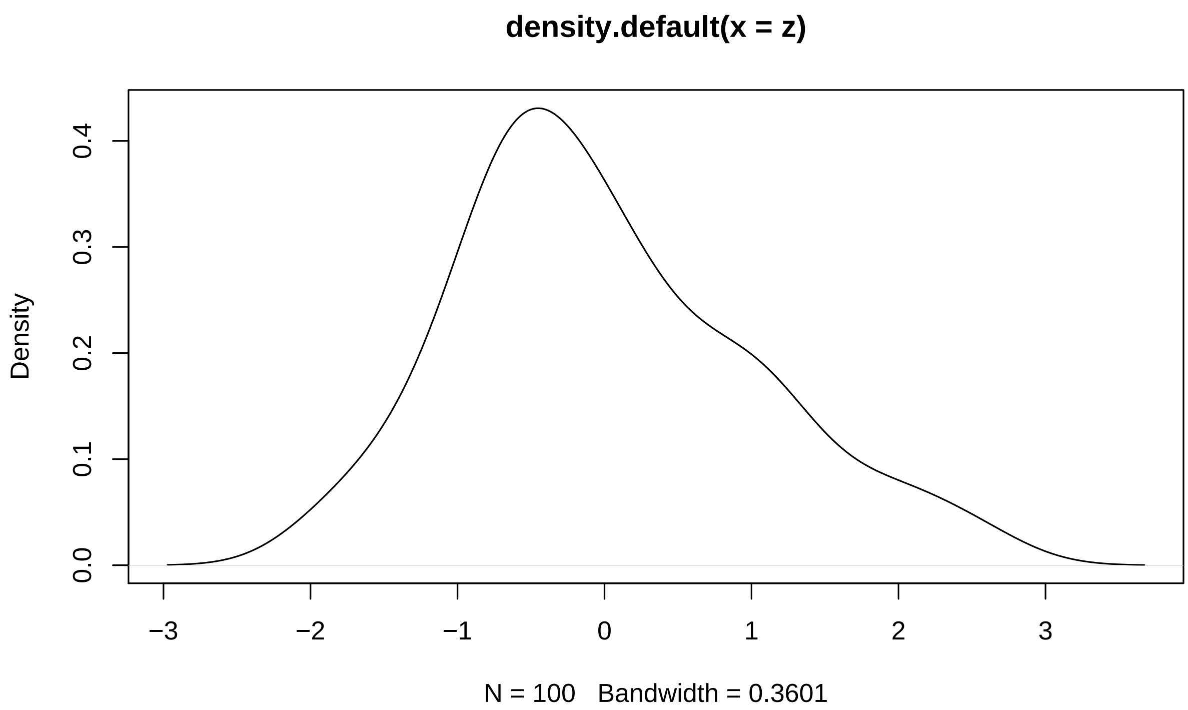
Note that m_1 and m_2 are functions of k.

Numerical results

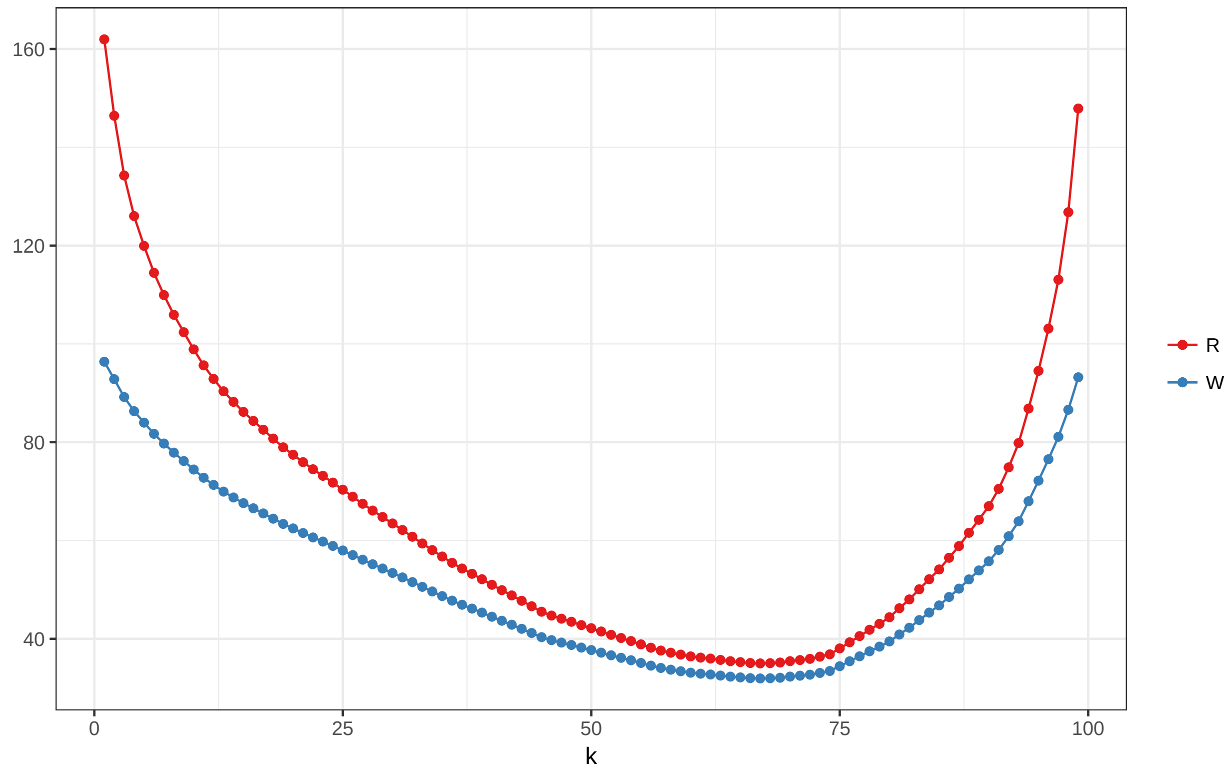
Using an arbitrary vector $\overrightarrow{x} \in \mathbb{R}^n$ such that $|\overrightarrow{x}|_1 = 0$ and $|\overrightarrow{x}|_2^2 = n$:

```
library(ggplot2)
import::from(magrittr, `%>%`)
theme_set(theme_bw())

normalize <- function(x) {
  y <- x - mean(x)
  z <- y / sqrt(mean(y ** 2))
  return(z)
}
```

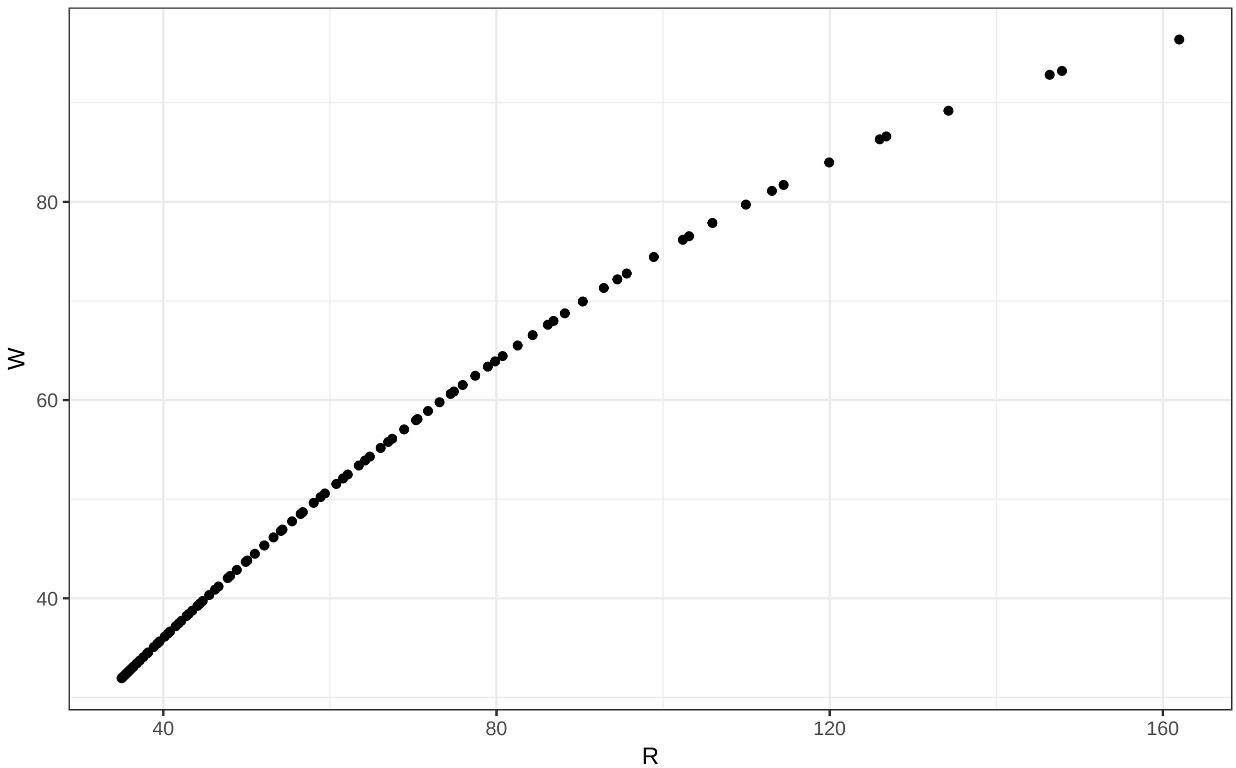
```r
k.means <- function(x) {
  x <- sort(x)
  n <- length(x)

  sapply(seq(n - 1), function(k) {
    m1 <- 1 / k * sum(x[seq(k)])
    m2 <- 1 / (n - k) * sum(x[seq(k + 1, n)])

    W <- sum((x[seq(k)] - m1)^2) + sum((x[seq(k + 1, n)] - m2)^2)
    return(W)
  })
}

ratio.cut <- function(x) {
  x <- sort(x)
  n <- length(x)

  sapply(seq(n - 1), function(k) {
    Ac <- sqrt((n - k) / k)
    A <- sqrt(k / (n - k))

    R <- sum((x[seq(k)] + Ac)^2) + sum((x[seq(k + 1, n)] - A)^2)
    return(R)
  })
}

# generate random data
n <- 100
k <- 4
x <- c(rnorm(n / k, -1),
       rnorm(n / k, 0),
       rnorm(n / k, 1),
       rnorm(n / k, 3))
z <- normalize(x)
plot(density(z))
```




```
# compute W and R
W <- k.means(z)
R <- ratio.cut(z)

# visualizations
k <- seq(n - 1)

ggplot() +
  geom_point(aes(x = k, y = W, colour = 'W')) +
  geom_line(aes(x = k, y = W, colour = 'W')) +
  geom_point(aes(x = k, y = R, colour = 'R')) +
  geom_line(aes(x = k, y = R, colour = 'R')) +
  scale_colour_brewer(palette = 'Set1') +
  labs(x = 'k', y = NULL, colour = NULL)
```




```r
ggplot() +
  geom_point(aes(x = R, y = W))
```



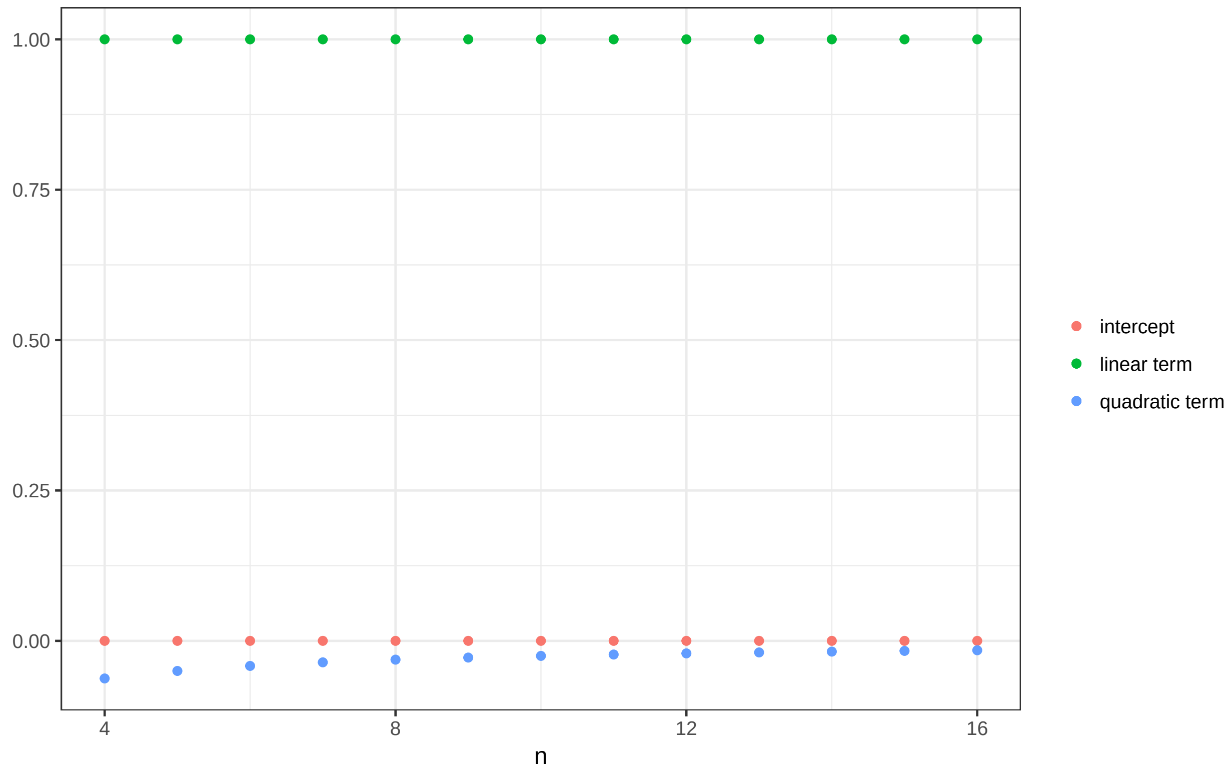
It appears that there is a definite relationship between W and R. Using quadratic regression:

```r
summary(lm(W ~ R + I(R ** 2)))
```

```

Call:
lm(formula = W ~ R + I(R^2))

Residuals:
       Min         1Q     Median         3Q        Max 
-3.250e-14 -4.566e-15  2.140e-16  4.333e-15  5.514e-14 

Coefficients:
              Estimate Std. Error    t value Pr(>|t|)    
(Intercept)  1.143e-14  6.116e-15  1.868e+00   0.0648 .  
R            1.000e+00  1.679e-16  5.958e+15   <2e-16 ***
I(R^2)      -2.500e-03  9.952e-19 -2.512e+15   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.035e-14 on 96 degrees of freedom
Multiple R-squared:      1, Adjusted R-squared:      1 
F-statistic: 1.416e+32 on 2 and 96 DF,  p-value: < 2.2e-16
```

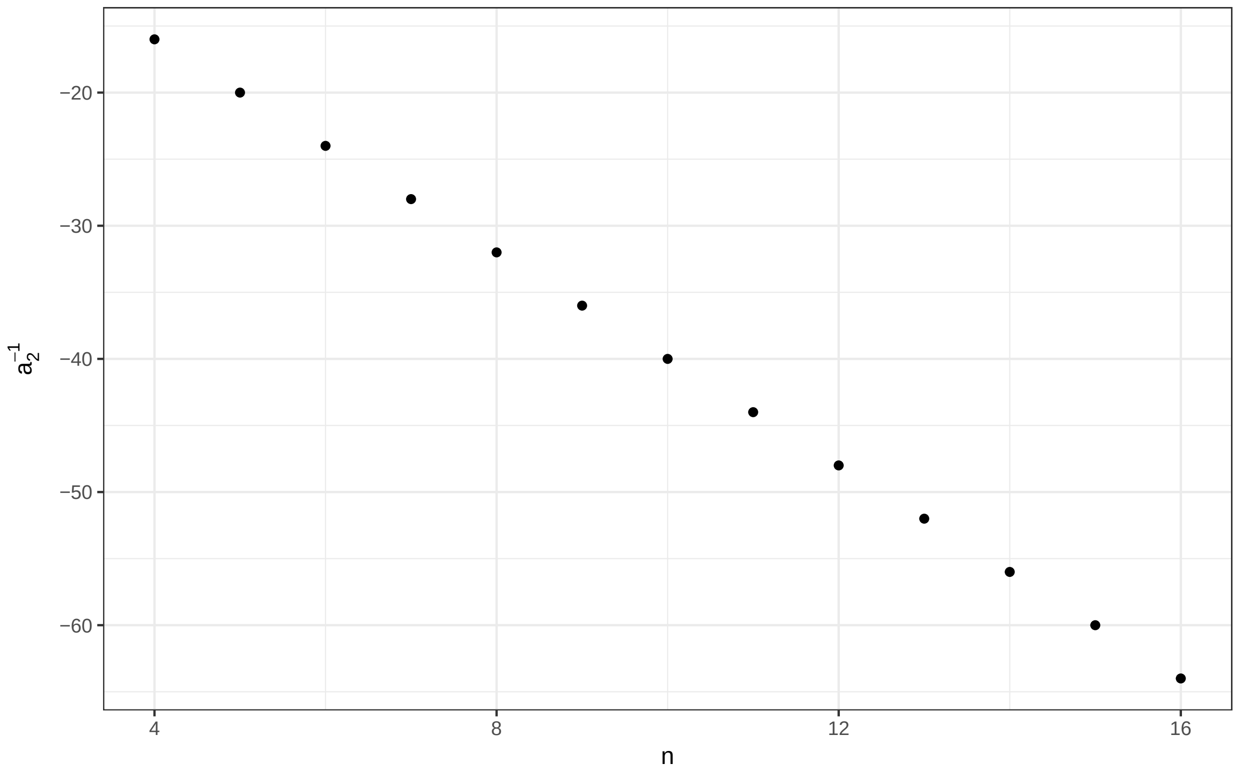
… we get a perfect fit. We can try several values of the data size n:

```r
N <- 2 ** 4  # number of obs to try
coefs.df <- lapply(seq(4, N), function(n) {
  x <- normalize(rnorm(n))  # generate data

  # compute results
  W <- k.means(x)
  R <- ratio.cut(x)

  # compute coefs for quadratic equation
  quad.coefs <- lm(W ~ R + I(R ** 2))$coefficients
  a0 <- quad.coefs['(Intercept)']
  a1 <- quad.coefs['R']
  a2 <- quad.coefs['I(R^2)']

  # compile into data frame
  dplyr::data_frame(n, a0, a1, a2)
}) %>%
  dplyr::bind_rows()

ggplot(coefs.df) +
  geom_point(aes(x = n, y = a0, colour = 'intercept')) +
  geom_point(aes(x = n, y = a1, colour = 'linear term')) +
  geom_point(aes(x = n, y = a2, colour = 'quadratic term')) +
  labs(colour = NULL, y = NULL)
```



The intercept term stays at 0 and the linear term stays at 1. Looking closer at the quadratic term:

```
ggplot(coefs.df) +
  geom_point(aes(x = n, y = a2 ** -1)) +
  labs(y = expression(a[2]^-1))
```



Then we arrive at the result $W = R - \frac{1}{4n}R^2$.

Analytic result

We can show:

$$W(k) = R(k) - \frac{(R(k))^2}{4n}$$

or $W(R) = R - \frac{1}{4n}R^2$. This function is strictly increasing for $R(k) \leq 2n$. Expanding $R(k)$, we get:

$$R(k) = 2n + 2\sqrt{\frac{n-k}{k}}\sum_{i=1}^{k} x_i - 2\sqrt{\frac{k}{n-k}}\sum_{i=k+1}^{n} x_i$$

It can be shown that $R(k)$ is maximized at the endpoints.

Note that since $\sum_i^n x_i = 0$, $\sum_i^{k<n} x_i \leq 0$, $x_n \geq 0$, and $x_i \leq 0$.

k can range from 1 to $n-1$. If $k = n-1$, we get $R(n-1) = 2n + 2\sqrt{\frac{1}{k}}\sum_i^{n-1} x_i - 2\sqrt{n-1}x_n$. The second term is ≤ 0 and the third term is ≥ 0, so we get $R \leq 2n$. On the other hand, if $k = 1$, $R(1) = 2n + 2\sqrt{n-1}x_1 - \frac{2}{\sqrt{n-1}}\sum_{i=2}^{n} x_i = 2n + 2\sqrt{n-1}x_1 - \frac{2}{\sqrt{n-1}}(-x_1) = 2n + x_1\big(2\sqrt{n-1} + \frac{2}{\sqrt{n-1}}\big) \leq 2n$.

Expanding $W(k)$, we get:

$$W(k) = \sum_{i=1}^{k} x_i^2 - 2m_1\sum_{i=1}^{k} x_i + km_1^2 + \sum_{i=k+1}^{n} x_i^2 - 2m_2\sum_{i=k+1}^{n} x_i + m_2^2(n-k)$$

$$
\begin{aligned}
&= n - \frac{2}{k}\left(\sum_{i=1}^{k} x_i\right)^2 + \frac{1}{k}\left(\sum_{i=1}^{k} x_i\right)^2 - \frac{2}{n-k}\left(\sum_{i=k+1}^{n} x_i\right)^2 + \frac{1}{n-k}\left(\sum_{i=k+1}^{n} x_i\right)^2 \\
&= n - \frac{1}{k}\left(\sum_{i=1}^{k} x_i\right)^2 - \frac{1}{n-k}\left(\sum_{i=k+1}^{n} x_i\right)^2 \\
&= n - km_1^2 - (n-k)m_2^2
\end{aligned}
$$

Since $\sum_i^n x_i = 0$, $km_1 + (n-k)m_2 = 0$, or, $-nm_2 = k(m_1 - m_2)$. Then

$$
\begin{aligned}
W(k) &= n - km_1^2 - (n-k)m_2^2 \\
&= n - km_1^2 - nm_2^2 + km_2^2 \\
&= n - km_1^2 + (nm_2)m_2 + km_2^2 \\
&= n - km_1 + k(m_1 - m_2)m_2 + km_2 2 \\
&= n + k(-m_1^2 + m_1 m_2 - m_2^2 + m_2^2) \\
&= n + km_1(m_2 - m_1)
\end{aligned}
$$

Using the relationship $-nm_2 = k(m_1 - m_2) \implies m_2 - m_1 = \frac{nm_2}{k}$ from before, we can again rewrite $W(k)$:

$$
\begin{aligned}
W(k) &= n - (n-k)m_2 \frac{nm_2}{k} \\
&= n \frac{(n-k)n}{k} m_2^2
\end{aligned}
$$

And we use the same relationship again: $m_2 - m_1 = \frac{n}{k} m_2 \implies m_2 = (m_2 - m_1)\frac{k}{n}$.

Then we can finally write $W(k)$ as:

$$
W(k) = n - \frac{(n-k)n}{k} \frac{k^2}{n^2} (m_1 - m_2)^2
$$

$$
\boxed{W(k) = n - \frac{(n-k)k}{n} (m_1 - m_2)^2}
$$

On the other hand, if we expand $R(k)$:

$$
\begin{aligned}
R(k) &= \sum_1^k x_i^2 + 2\sqrt{\frac{n-k}{k}} \sum_1^k x_i + n - k + \sum_{k+1}^n x_i^2 - 2\sqrt{\frac{k}{n-k}} \sum_{k+1}^n x_i + k \\
&= 2n + 2\sqrt{k(n-k)}m_1 - 2\sqrt{k(n-k)}m_2
\end{aligned}
$$

If we expand and simplify $-\frac{(R(k))^2}{4n}$, we get:

$$
-\frac{(R(k))^2}{4n} = -n - \frac{k(n-k)}{n} m_1^2 - \frac{k(n-k)}{n} m_2^2 - 2m_1\sqrt{k(n-k)} + 2m_2\sqrt{k(n-k)} + \frac{2k(n-k)}{n} m_1 m_2
$$

Then noting that some terms cancel each other out, $R(k) - \frac{(R(k))^2}{4n}$:

$$
\begin{aligned}
n - \frac{k(n-k}{n}m_1^2 - \frac{k(n-k)}{n}m_2^2 + 2\frac{k(n-k)}{n}m_1m_2 \\
= n - \frac{k(n-k)}{n}(m_1^2 + m_2^2 - 2m_1m_2) \\
\boxed{= n - \frac{k(n-k)}{n}(m_1 - m_2)^2}
\end{aligned}
$$

Which is exactly the same as our expression for $W(k)$.

$k > 2$

When $k > 2$, the methods as prescribed by Luxburg involve embedding the graph to $\mathbb{R}^k$ and then performing k-means clustering. In this case, we cannot perform the same sort of analysis since there is no way to "order" the x_i's.