

Class 8: PCA Mini project

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For example:

```
colMeans(mtcars)
```

| mpg | cyl | disp | hp | drat | wt | qsec |
|-----------|----------|------------|------------|----------|----------|-----------|
| 20.090625 | 6.187500 | 230.721875 | 146.687500 | 3.596563 | 3.217250 | 17.848750 |
| vs | am | gear | carb | | | |
| 0.437500 | 0.406250 | 3.687500 | 2.812500 | | | |

```
apply(mtcars, 2, sd)
```

| mpg | cyl | disp | hp | drat | wt |
|-----------|-----------|-------------|------------|-----------|-----------|
| 6.0269481 | 1.7859216 | 123.9386938 | 68.5628685 | 0.5346787 | 0.9784574 |
| qsec | vs | am | gear | carb | |
| 1.7869432 | 0.5040161 | 0.4989909 | 0.7378041 | 1.6152000 | |

```
x<- scale(mtcars)
```

```
x
```

| | mpg | cyl | disp | hp | drat |
|-------------------|-------------|------------|-------------|-------------|-------------|
| Mazda RX4 | 0.15088482 | -0.1049878 | -0.57061982 | -0.53509284 | 0.56751369 |
| Mazda RX4 Wag | 0.15088482 | -0.1049878 | -0.57061982 | -0.53509284 | 0.56751369 |
| Datsun 710 | 0.44954345 | -1.2248578 | -0.99018209 | -0.78304046 | 0.47399959 |
| Hornet 4 Drive | 0.21725341 | -0.1049878 | 0.22009369 | -0.53509284 | -0.96611753 |
| Hornet Sportabout | -0.23073453 | 1.0148821 | 1.04308123 | 0.41294217 | -0.83519779 |
| Valiant | -0.33028740 | -0.1049878 | -0.04616698 | -0.60801861 | -1.56460776 |
| Duster 360 | -0.96078893 | 1.0148821 | 1.04308123 | 1.43390296 | -0.72298087 |
| Merc 240D | 0.71501778 | -1.2248578 | -0.67793094 | -1.23518023 | 0.17475447 |

| | | | | | |
|---------------------|--------------|-------------|-------------|-------------|-------------|
| Merc 230 | 0.44954345 | -1.2248578 | -0.72553512 | -0.75387015 | 0.60491932 |
| Merc 280 | -0.14777380 | -0.1049878 | -0.50929918 | -0.34548584 | 0.60491932 |
| Merc 280C | -0.38006384 | -0.1049878 | -0.50929918 | -0.34548584 | 0.60491932 |
| Merc 450SE | -0.61235388 | 1.0148821 | 0.36371309 | 0.48586794 | -0.98482035 |
| Merc 450SL | -0.46302456 | 1.0148821 | 0.36371309 | 0.48586794 | -0.98482035 |
| Merc 450SLC | -0.81145962 | 1.0148821 | 0.36371309 | 0.48586794 | -0.98482035 |
| Cadillac Fleetwood | -1.60788262 | 1.0148821 | 1.94675381 | 0.85049680 | -1.24665983 |
| Lincoln Continental | -1.60788262 | 1.0148821 | 1.84993175 | 0.99634834 | -1.11574009 |
| Chrysler Imperial | -0.89442035 | 1.0148821 | 1.68856165 | 1.21512565 | -0.68557523 |
| Fiat 128 | 2.04238943 | -1.2248578 | -1.22658929 | -1.17683962 | 0.90416444 |
| Honda Civic | 1.71054652 | -1.2248578 | -1.25079481 | -1.38103178 | 2.49390411 |
| Toyota Corolla | 2.29127162 | -1.2248578 | -1.28790993 | -1.19142477 | 1.16600392 |
| Toyota Corona | 0.23384555 | -1.2248578 | -0.89255318 | -0.72469984 | 0.19345729 |
| Dodge Challenger | -0.76168319 | 1.0148821 | 0.70420401 | 0.04831332 | -1.56460776 |
| AMC Javelin | -0.81145962 | 1.0148821 | 0.59124494 | 0.04831332 | -0.83519779 |
| Camaro Z28 | -1.12671039 | 1.0148821 | 0.96239618 | 1.43390296 | 0.24956575 |
| Pontiac Firebird | -0.14777380 | 1.0148821 | 1.36582144 | 0.41294217 | -0.96611753 |
| Fiat X1-9 | 1.19619000 | -1.2248578 | -1.22416874 | -1.17683962 | 0.90416444 |
| Porsche 914-2 | 0.98049211 | -1.2248578 | -0.89093948 | -0.81221077 | 1.55876313 |
| Lotus Europa | 1.71054652 | -1.2248578 | -1.09426581 | -0.49133738 | 0.32437703 |
| Ford Pantera L | -0.71190675 | 1.0148821 | 0.97046468 | 1.71102089 | 1.16600392 |
| Ferrari Dino | -0.06481307 | -0.1049878 | -0.69164740 | 0.41294217 | 0.04383473 |
| Maserati Bora | -0.84464392 | 1.0148821 | 0.56703942 | 2.74656682 | -0.10578782 |
| Volvo 142E | 0.21725341 | -1.2248578 | -0.88529152 | -0.54967799 | 0.96027290 |
| | wt | qsec | vs | am | gear |
| Mazda RX4 | -0.610399567 | -0.77716515 | -0.8680278 | 1.1899014 | 0.4235542 |
| Mazda RX4 Wag | -0.349785269 | -0.46378082 | -0.8680278 | 1.1899014 | 0.4235542 |
| Datsun 710 | -0.917004624 | 0.42600682 | 1.1160357 | 1.1899014 | 0.4235542 |
| Hornet 4 Drive | -0.002299538 | 0.89048716 | 1.1160357 | -0.8141431 | -0.9318192 |
| Hornet Sportabout | 0.227654255 | -0.46378082 | -0.8680278 | -0.8141431 | -0.9318192 |
| Valiant | 0.248094592 | 1.32698675 | 1.1160357 | -0.8141431 | -0.9318192 |
| Duster 360 | 0.360516446 | -1.12412636 | -0.8680278 | -0.8141431 | -0.9318192 |
| Merc 240D | -0.027849959 | 1.20387148 | 1.1160357 | -0.8141431 | 0.4235542 |
| Merc 230 | -0.068730634 | 2.82675459 | 1.1160357 | -0.8141431 | 0.4235542 |
| Merc 280 | 0.227654255 | 0.25252621 | 1.1160357 | -0.8141431 | 0.4235542 |
| Merc 280C | 0.227654255 | 0.58829513 | 1.1160357 | -0.8141431 | 0.4235542 |
| Merc 450SE | 0.871524874 | -0.25112717 | -0.8680278 | -0.8141431 | -0.9318192 |
| Merc 450SL | 0.524039143 | -0.13920420 | -0.8680278 | -0.8141431 | -0.9318192 |
| Merc 450SLC | 0.575139986 | 0.08464175 | -0.8680278 | -0.8141431 | -0.9318192 |
| Cadillac Fleetwood | 2.077504765 | 0.07344945 | -0.8680278 | -0.8141431 | -0.9318192 |
| Lincoln Continental | 2.255335698 | -0.01608893 | -0.8680278 | -0.8141431 | -0.9318192 |
| Chrysler Imperial | 2.174596366 | -0.23993487 | -0.8680278 | -0.8141431 | -0.9318192 |
| Fiat 128 | -1.039646647 | 0.90727560 | 1.1160357 | 1.1899014 | 0.4235542 |

| | | | | | |
|---------------------|--------------|-------------|------------|------------|------------|
| Honda Civic | -1.637526508 | 0.37564148 | 1.1160357 | 1.1899014 | 0.4235542 |
| Toyota Corolla | -1.412682800 | 1.14790999 | 1.1160357 | 1.1899014 | 0.4235542 |
| Toyota Corona | -0.768812180 | 1.20946763 | 1.1160357 | -0.8141431 | -0.9318192 |
| Dodge Challenger | 0.309415603 | -0.54772305 | -0.8680278 | -0.8141431 | -0.9318192 |
| AMC Javelin | 0.222544170 | -0.30708866 | -0.8680278 | -0.8141431 | -0.9318192 |
| Camaro Z28 | 0.636460997 | -1.36476075 | -0.8680278 | -0.8141431 | -0.9318192 |
| Pontiac Firebird | 0.641571082 | -0.44699237 | -0.8680278 | -0.8141431 | -0.9318192 |
| Fiat X1-9 | -1.310481114 | 0.58829513 | 1.1160357 | 1.1899014 | 0.4235542 |
| Porsche 914-2 | -1.100967659 | -0.64285758 | -0.8680278 | 1.1899014 | 1.7789276 |
| Lotus Europa | -1.741772228 | -0.53093460 | 1.1160357 | 1.1899014 | 1.7789276 |
| Ford Pantera L | -0.048290296 | -1.87401028 | -0.8680278 | 1.1899014 | 1.7789276 |
| Ferrari Dino | -0.457097039 | -1.31439542 | -0.8680278 | 1.1899014 | 1.7789276 |
| Maserati Bora | 0.360516446 | -1.81804880 | -0.8680278 | 1.1899014 | 1.7789276 |
| Volvo 142E | -0.446876870 | 0.42041067 | 1.1160357 | 1.1899014 | 0.4235542 |
| carb | | | | | |
| Mazda RX4 | 0.7352031 | | | | |
| Mazda RX4 Wag | 0.7352031 | | | | |
| Datsun 710 | -1.1221521 | | | | |
| Hornet 4 Drive | -1.1221521 | | | | |
| Hornet Sportabout | -0.5030337 | | | | |
| Valiant | -1.1221521 | | | | |
| Duster 360 | 0.7352031 | | | | |
| Merc 240D | -0.5030337 | | | | |
| Merc 230 | -0.5030337 | | | | |
| Merc 280 | 0.7352031 | | | | |
| Merc 280C | 0.7352031 | | | | |
| Merc 450SE | 0.1160847 | | | | |
| Merc 450SL | 0.1160847 | | | | |
| Merc 450SLC | 0.1160847 | | | | |
| Cadillac Fleetwood | 0.7352031 | | | | |
| Lincoln Continental | 0.7352031 | | | | |
| Chrysler Imperial | 0.7352031 | | | | |
| Fiat 128 | -1.1221521 | | | | |
| Honda Civic | -0.5030337 | | | | |
| Toyota Corolla | -1.1221521 | | | | |
| Toyota Corona | -1.1221521 | | | | |
| Dodge Challenger | -0.5030337 | | | | |
| AMC Javelin | -0.5030337 | | | | |
| Camaro Z28 | 0.7352031 | | | | |
| Pontiac Firebird | -0.5030337 | | | | |
| Fiat X1-9 | -1.1221521 | | | | |
| Porsche 914-2 | -0.5030337 | | | | |
| Lotus Europa | -0.5030337 | | | | |

```

Ford Pantera L      0.7352031
Ferrari Dino        1.9734398
Maserati Bora       3.2116766
Volvo 142E         -0.5030337
attr(,"scaled:center")
      mpg      cyl      disp      hp      drat      wt      qsec
20.090625  6.187500 230.721875 146.687500  3.596563  3.217250 17.848750
      vs      am      gear      carb
0.437500  0.406250  3.687500  2.812500
attr(,"scaled:scale")
      mpg      cyl      disp      hp      drat      wt
6.0269481  1.7859216 123.9386938 68.5628685  0.5346787  0.9784574
      qsec      vs      am      gear      carb
1.7869432  0.5040161  0.4989909  0.7378041  1.6152000

```

```
colMeans(x)
```

```

      mpg      cyl      disp      hp      drat
7.112366e-17 -1.474515e-17 -9.085614e-17  1.040834e-17 -2.918672e-16
      wt      qsec      vs      am      gear
4.682398e-17 5.299580e-16 6.938894e-18 4.510281e-17 -3.469447e-18
      carb
3.165870e-17

```

```
round(colMeans(x))
```

```

mpg  cyl disp  hp drat  wt qsec  vs  am gear carb
0    0    0    0  0    0    0    0  0    0    0

```

Key point: It is usually always a good idea to scale your data before to PCA

Breast Cancer Biopsy Analysis

```

#save input data file into project directory
fna.data <- "WisconsinCancer.csv"

#use read.csv() to read the data and save it in wisc.df
wisc.df <- read.csv(fna.data, row.names=1)
head(wisc.df)

```

| | diagnosis | radius_mean | texture_mean | perimeter_mean | area_mean |
|----------|-----------------|------------------------|------------------|---------------------|-------------------|
| 842302 | M | 17.99 | 10.38 | 122.80 | 1001.0 |
| 842517 | M | 20.57 | 17.77 | 132.90 | 1326.0 |
| 84300903 | M | 19.69 | 21.25 | 130.00 | 1203.0 |
| 84348301 | M | 11.42 | 20.38 | 77.58 | 386.1 |
| 84358402 | M | 20.29 | 14.34 | 135.10 | 1297.0 |
| 843786 | M | 12.45 | 15.70 | 82.57 | 477.1 |
| | smoothness_mean | compactness_mean | concavity_mean | concave.points_mean | |
| 842302 | 0.11840 | 0.27760 | 0.3001 | | 0.14710 |
| 842517 | 0.08474 | 0.07864 | 0.0869 | | 0.07017 |
| 84300903 | 0.10960 | 0.15990 | 0.1974 | | 0.12790 |
| 84348301 | 0.14250 | 0.28390 | 0.2414 | | 0.10520 |
| 84358402 | 0.10030 | 0.13280 | 0.1980 | | 0.10430 |
| 843786 | 0.12780 | 0.17000 | 0.1578 | | 0.08089 |
| | symmetry_mean | fractal_dimension_mean | radius_se | texture_se | perimeter_se |
| 842302 | 0.2419 | | 0.07871 | 1.0950 | 0.9053 |
| 842517 | 0.1812 | | 0.05667 | 0.5435 | 0.7339 |
| 84300903 | 0.2069 | | 0.05999 | 0.7456 | 0.7869 |
| 84348301 | 0.2597 | | 0.09744 | 0.4956 | 1.1560 |
| 84358402 | 0.1809 | | 0.05883 | 0.7572 | 0.7813 |
| 843786 | 0.2087 | | 0.07613 | 0.3345 | 0.8902 |
| | area_se | smoothness_se | compactness_se | concavity_se | concave.points_se |
| 842302 | 153.40 | 0.006399 | 0.04904 | 0.05373 | 0.01587 |
| 842517 | 74.08 | 0.005225 | 0.01308 | 0.01860 | 0.01340 |
| 84300903 | 94.03 | 0.006150 | 0.04006 | 0.03832 | 0.02058 |
| 84348301 | 27.23 | 0.009110 | 0.07458 | 0.05661 | 0.01867 |
| 84358402 | 94.44 | 0.011490 | 0.02461 | 0.05688 | 0.01885 |
| 843786 | 27.19 | 0.007510 | 0.03345 | 0.03672 | 0.01137 |
| | symmetry_se | fractal_dimension_se | radius_worst | texture_worst | |
| 842302 | 0.03003 | | 0.006193 | 25.38 | 17.33 |
| 842517 | 0.01389 | | 0.003532 | 24.99 | 23.41 |
| 84300903 | 0.02250 | | 0.004571 | 23.57 | 25.53 |
| 84348301 | 0.05963 | | 0.009208 | 14.91 | 26.50 |
| 84358402 | 0.01756 | | 0.005115 | 22.54 | 16.67 |
| 843786 | 0.02165 | | 0.005082 | 15.47 | 23.75 |
| | perimeter_worst | area_worst | smoothness_worst | compactness_worst | |
| 842302 | 184.60 | 2019.0 | 0.1622 | | 0.6656 |
| 842517 | 158.80 | 1956.0 | 0.1238 | | 0.1866 |
| 84300903 | 152.50 | 1709.0 | 0.1444 | | 0.4245 |
| 84348301 | 98.87 | 567.7 | 0.2098 | | 0.8663 |
| 84358402 | 152.20 | 1575.0 | 0.1374 | | 0.2050 |
| 843786 | 103.40 | 741.6 | 0.1791 | | 0.5249 |
| | concavity_worst | concave.points_worst | symmetry_worst | | |

| | | | |
|----------|--------|--------|--------|
| 842302 | 0.7119 | 0.2654 | 0.4601 |
| 842517 | 0.2416 | 0.1860 | 0.2750 |
| 84300903 | 0.4504 | 0.2430 | 0.3613 |
| 84348301 | 0.6869 | 0.2575 | 0.6638 |
| 84358402 | 0.4000 | 0.1625 | 0.2364 |
| 843786 | 0.5355 | 0.1741 | 0.3985 |

fractal_dimension_worst

| | |
|----------|---------|
| 842302 | 0.11890 |
| 842517 | 0.08902 |
| 84300903 | 0.08758 |
| 84348301 | 0.17300 |
| 84358402 | 0.07678 |
| 843786 | 0.12440 |

```
# We can use -1 here to remove the first column diagnosis
wisc.data <- wisc.df[,-1]
head(wisc.data)
```

| | radius_mean | texture_mean | perimeter_mean | area_mean | smoothness_mean |
|----------|-------------|--------------|----------------|-----------|-----------------|
| 842302 | 17.99 | 10.38 | 122.80 | 1001.0 | 0.11840 |
| 842517 | 20.57 | 17.77 | 132.90 | 1326.0 | 0.08474 |
| 84300903 | 19.69 | 21.25 | 130.00 | 1203.0 | 0.10960 |
| 84348301 | 11.42 | 20.38 | 77.58 | 386.1 | 0.14250 |
| 84358402 | 20.29 | 14.34 | 135.10 | 1297.0 | 0.10030 |
| 843786 | 12.45 | 15.70 | 82.57 | 477.1 | 0.12780 |

| | compactness_mean | concavity_mean | concave.points_mean | symmetry_mean |
|----------|------------------|----------------|---------------------|---------------|
| 842302 | 0.27760 | 0.3001 | 0.14710 | 0.2419 |
| 842517 | 0.07864 | 0.0869 | 0.07017 | 0.1812 |
| 84300903 | 0.15990 | 0.1974 | 0.12790 | 0.2069 |
| 84348301 | 0.28390 | 0.2414 | 0.10520 | 0.2597 |
| 84358402 | 0.13280 | 0.1980 | 0.10430 | 0.1809 |
| 843786 | 0.17000 | 0.1578 | 0.08089 | 0.2087 |

| | fractal_dimension_mean | radius_se | texture_se | perimeter_se | area_se |
|----------|------------------------|-----------|------------|--------------|---------|
| 842302 | 0.07871 | 1.0950 | 0.9053 | 8.589 | 153.40 |
| 842517 | 0.05667 | 0.5435 | 0.7339 | 3.398 | 74.08 |
| 84300903 | 0.05999 | 0.7456 | 0.7869 | 4.585 | 94.03 |
| 84348301 | 0.09744 | 0.4956 | 1.1560 | 3.445 | 27.23 |
| 84358402 | 0.05883 | 0.7572 | 0.7813 | 5.438 | 94.44 |
| 843786 | 0.07613 | 0.3345 | 0.8902 | 2.217 | 27.19 |

| | smoothness_se | compactness_se | concavity_se | concave.points_se |
|--------|---------------|----------------|--------------|-------------------|
| 842302 | 0.006399 | 0.04904 | 0.05373 | 0.01587 |
| 842517 | 0.005225 | 0.01308 | 0.01860 | 0.01340 |

| | | | | |
|---|----------|----------|---------|---------|
| 84300903 | 0.006150 | 0.04006 | 0.03832 | 0.02058 |
| 84348301 | 0.009110 | 0.07458 | 0.05661 | 0.01867 |
| 84358402 | 0.011490 | 0.02461 | 0.05688 | 0.01885 |
| 843786 | 0.007510 | 0.03345 | 0.03672 | 0.01137 |
| symmetry_se fractal_dimension_se radius_worst texture_worst | | | | |
| 842302 | 0.03003 | 0.006193 | 25.38 | 17.33 |
| 842517 | 0.01389 | 0.003532 | 24.99 | 23.41 |
| 84300903 | 0.02250 | 0.004571 | 23.57 | 25.53 |
| 84348301 | 0.05963 | 0.009208 | 14.91 | 26.50 |
| 84358402 | 0.01756 | 0.005115 | 22.54 | 16.67 |
| 843786 | 0.02165 | 0.005082 | 15.47 | 23.75 |
| perimeter_worst area_worst smoothness_worst compactness_worst | | | | |
| 842302 | 184.60 | 2019.0 | 0.1622 | 0.6656 |
| 842517 | 158.80 | 1956.0 | 0.1238 | 0.1866 |
| 84300903 | 152.50 | 1709.0 | 0.1444 | 0.4245 |
| 84348301 | 98.87 | 567.7 | 0.2098 | 0.8663 |
| 84358402 | 152.20 | 1575.0 | 0.1374 | 0.2050 |
| 843786 | 103.40 | 741.6 | 0.1791 | 0.5249 |
| concavity_worst concave.points_worst symmetry_worst | | | | |
| 842302 | 0.7119 | 0.2654 | 0.4601 | |
| 842517 | 0.2416 | 0.1860 | 0.2750 | |
| 84300903 | 0.4504 | 0.2430 | 0.3613 | |
| 84348301 | 0.6869 | 0.2575 | 0.6638 | |
| 84358402 | 0.4000 | 0.1625 | 0.2364 | |
| 843786 | 0.5355 | 0.1741 | 0.3985 | |
| fractal_dimension_worst | | | | |
| 842302 | 0.11890 | | | |
| 842517 | 0.08902 | | | |
| 84300903 | 0.08758 | | | |
| 84348301 | 0.17300 | | | |
| 84358402 | 0.07678 | | | |
| 843786 | 0.12440 | | | |

```
# Create diagnosis vector for later
diagnosis <- wisc.df[,1]
```

Remove this first ‘diagnosis’ column from the dataset as I don;t want to pass this to PCA etc.

Exploratory data analysis

- **Q1.** How many observations are in this dataset?

```
31(diagnosis included)
```

```
ncol(wisc.df)
```

```
[1] 31
```

- **Q2.** How many of the observations have a malignant diagnosis?

```
212
```

```
table(wisc.df$diagnosis)
```

```
    B    M  
357 212
```

- **Q3.** How many variables/features in the data are suffixed with `_mean`?

```
grep("_mean", colnames(wisc.df), value = 1)
```

```
[1] "radius_mean"          "texture_mean"          "perimeter_mean"  
[4] "area_mean"            "smoothness_mean"       "compactness_mean"  
[7] "concavity_mean"       "concave.points_mean"   "symmetry_mean"  
[10] "fractal_dimension_mean"
```

Performing PCA

```
# Check column means and standard deviations  
colMeans(wisc.data)
```

| | | |
|------------------------|----------------------|-------------------|
| radius_mean | texture_mean | perimeter_mean |
| 1.412729e+01 | 1.928965e+01 | 9.196903e+01 |
| area_mean | smoothness_mean | compactness_mean |
| 6.548891e+02 | 9.636028e-02 | 1.043410e-01 |
| concavity_mean | concave.points_mean | symmetry_mean |
| 8.879932e-02 | 4.891915e-02 | 1.811619e-01 |
| fractal_dimension_mean | radius_se | texture_se |
| 6.279761e-02 | 4.051721e-01 | 1.216853e+00 |
| perimeter_se | area_se | smoothness_se |
| 2.866059e+00 | 4.033708e+01 | 7.040979e-03 |
| compactness_se | concavity_se | concave.points_se |
| 2.547814e-02 | 3.189372e-02 | 1.179614e-02 |
| symmetry_se | fractal_dimension_se | radius_worst |

| | | |
|----------------------|-------------------|-------------------------|
| 2.054230e-02 | 3.794904e-03 | 1.626919e+01 |
| texture_worst | perimeter_worst | area_worst |
| 2.567722e+01 | 1.072612e+02 | 8.805831e+02 |
| smoothness_worst | compactness_worst | concavity_worst |
| 1.323686e-01 | 2.542650e-01 | 2.721885e-01 |
| concave.points_worst | symmetry_worst | fractal_dimension_worst |
| 1.146062e-01 | 2.900756e-01 | 8.394582e-02 |

```
apply(wisc.data, 2, sd)
```

| | | |
|------------------------|----------------------|-------------------------|
| radius_mean | texture_mean | perimeter_mean |
| 3.524049e+00 | 4.301036e+00 | 2.429898e+01 |
| area_mean | smoothness_mean | compactness_mean |
| 3.519141e+02 | 1.406413e-02 | 5.281276e-02 |
| concavity_mean | concave.points_mean | symmetry_mean |
| 7.971981e-02 | 3.880284e-02 | 2.741428e-02 |
| fractal_dimension_mean | radius_se | texture_se |
| 7.060363e-03 | 2.773127e-01 | 5.516484e-01 |
| perimeter_se | area_se | smoothness_se |
| 2.021855e+00 | 4.549101e+01 | 3.002518e-03 |
| compactness_se | concavity_se | concave.points_se |
| 1.790818e-02 | 3.018606e-02 | 6.170285e-03 |
| symmetry_se | fractal_dimension_se | radius_worst |
| 8.266372e-03 | 2.646071e-03 | 4.833242e+00 |
| texture_worst | perimeter_worst | area_worst |
| 6.146258e+00 | 3.360254e+01 | 5.693570e+02 |
| smoothness_worst | compactness_worst | concavity_worst |
| 2.283243e-02 | 1.573365e-01 | 2.086243e-01 |
| concave.points_worst | symmetry_worst | fractal_dimension_worst |
| 6.573234e-02 | 6.186747e-02 | 1.806127e-02 |

```
wisc.pr <- prcomp(wisc.data, scale= TRUE)
```

See what is in our PCA result object:

```
summary(wisc.pr)
```

Importance of components:

| | PC1 | PC2 | PC3 | PC4 | PC5 | PC6 | PC7 |
|--------------------|--------|--------|---------|---------|---------|---------|---------|
| Standard deviation | 3.6444 | 2.3857 | 1.67867 | 1.40735 | 1.28403 | 1.09880 | 0.82172 |

| | | | | | | | |
|------------------------|---------|---------|---------|---------|---------|---------|---------|
| Proportion of Variance | 0.4427 | 0.1897 | 0.09393 | 0.06602 | 0.05496 | 0.04025 | 0.02251 |
| Cumulative Proportion | 0.4427 | 0.6324 | 0.72636 | 0.79239 | 0.84734 | 0.88759 | 0.91010 |
| | PC8 | PC9 | PC10 | PC11 | PC12 | PC13 | PC14 |
| Standard deviation | 0.69037 | 0.6457 | 0.59219 | 0.5421 | 0.51104 | 0.49128 | 0.39624 |
| Proportion of Variance | 0.01589 | 0.0139 | 0.01169 | 0.0098 | 0.00871 | 0.00805 | 0.00523 |
| Cumulative Proportion | 0.92598 | 0.9399 | 0.95157 | 0.9614 | 0.97007 | 0.97812 | 0.98335 |
| | PC15 | PC16 | PC17 | PC18 | PC19 | PC20 | PC21 |
| Standard deviation | 0.30681 | 0.28260 | 0.24372 | 0.22939 | 0.22244 | 0.17652 | 0.1731 |
| Proportion of Variance | 0.00314 | 0.00266 | 0.00198 | 0.00175 | 0.00165 | 0.00104 | 0.0010 |
| Cumulative Proportion | 0.98649 | 0.98915 | 0.99113 | 0.99288 | 0.99453 | 0.99557 | 0.9966 |
| | PC22 | PC23 | PC24 | PC25 | PC26 | PC27 | PC28 |
| Standard deviation | 0.16565 | 0.15602 | 0.1344 | 0.12442 | 0.09043 | 0.08307 | 0.03987 |
| Proportion of Variance | 0.00091 | 0.00081 | 0.0006 | 0.00052 | 0.00027 | 0.00023 | 0.00005 |
| Cumulative Proportion | 0.99749 | 0.99830 | 0.9989 | 0.99942 | 0.99969 | 0.99992 | 0.99997 |
| | PC29 | PC30 | | | | | |
| Standard deviation | 0.02736 | 0.01153 | | | | | |
| Proportion of Variance | 0.00002 | 0.00000 | | | | | |
| Cumulative Proportion | 1.00000 | 1.00000 | | | | | |

- **Q4.** From your results, what proportion of the original variance is captured by the first principal components (PC1)?

0.4427

- **Q5.** How many principal components (PCs) are required to describe at least 70% of the original variance in the data?

In order to get <70% of the original variance in the data, the cumulative poportion have to be grater than 0.7, which means 3 PCs is required according to the summary().

- **Q6.** How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

In order to get <90% of the original variance in the data, the cumulative poportion have to be grater than 0.9, which means 7 PCs is required according to the summary().

Interpreting PCA results

Main PC score plot, PC1 vs. PC2

```
attributes(wisc.pr)
```

```
$names
[1] "sdev"      "rotation" "center"    "scale"     "x"

$class
[1] "prcomp"
```

```
wisc.pr$center
```

| | | |
|------------------------|----------------------|-------------------------|
| radius_mean | texture_mean | perimeter_mean |
| 1.412729e+01 | 1.928965e+01 | 9.196903e+01 |
| area_mean | smoothness_mean | compactness_mean |
| 6.548891e+02 | 9.636028e-02 | 1.043410e-01 |
| concavity_mean | concave.points_mean | symmetry_mean |
| 8.879932e-02 | 4.891915e-02 | 1.811619e-01 |
| fractal_dimension_mean | radius_se | texture_se |
| 6.279761e-02 | 4.051721e-01 | 1.216853e+00 |
| perimeter_se | area_se | smoothness_se |
| 2.866059e+00 | 4.033708e+01 | 7.040979e-03 |
| compactness_se | concavity_se | concave.points_se |
| 2.547814e-02 | 3.189372e-02 | 1.179614e-02 |
| symmetry_se | fractal_dimension_se | radius_worst |
| 2.054230e-02 | 3.794904e-03 | 1.626919e+01 |
| texture_worst | perimeter_worst | area_worst |
| 2.567722e+01 | 1.072612e+02 | 8.805831e+02 |
| smoothness_worst | compactness_worst | concavity_worst |
| 1.323686e-01 | 2.542650e-01 | 2.721885e-01 |
| concave.points_worst | symmetry_worst | fractal_dimension_worst |
| 1.146062e-01 | 2.900756e-01 | 8.394582e-02 |

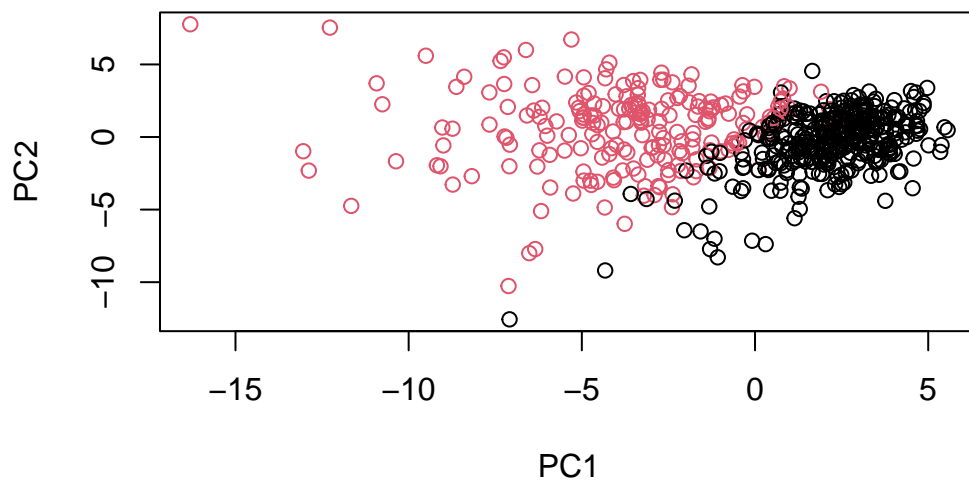
```
head(wisc.pr$x)
```

| | PC1 | PC2 | PC3 | PC4 | PC5 | PC6 |
|----------|------------|-------------|-------------|------------|------------|-------------|
| 842302 | -9.184755 | -1.946870 | -1.1221788 | 3.6305364 | 1.1940595 | 1.41018364 |
| 842517 | -2.385703 | 3.764859 | -0.5288274 | 1.1172808 | -0.6212284 | 0.02863116 |
| 84300903 | -5.728855 | 1.074229 | -0.5512625 | 0.9112808 | 0.1769302 | 0.54097615 |
| 84348301 | -7.116691 | -10.266556 | -3.2299475 | 0.1524129 | 2.9582754 | 3.05073750 |
| 84358402 | -3.931842 | 1.946359 | 1.3885450 | 2.9380542 | -0.5462667 | -1.22541641 |
| 843786 | -2.378155 | -3.946456 | -2.9322967 | 0.9402096 | 1.0551135 | -0.45064213 |
| | PC7 | PC8 | PC9 | PC10 | PC11 | PC12 |
| 842302 | 2.15747152 | 0.39805698 | -0.15698023 | -0.8766305 | -0.2627243 | -0.8582593 |
| 842517 | 0.01334635 | -0.24077660 | -0.71127897 | 1.1060218 | -0.8124048 | 0.1577838 |

| | | | | | | |
|----------|---------------|--------------|---------------|--------------|-------------|------------|
| 84300903 | -0.66757908 | -0.09728813 | 0.02404449 | 0.4538760 | 0.6050715 | 0.1242777 |
| 84348301 | 1.42865363 | -1.05863376 | -1.40420412 | -1.1159933 | 1.1505012 | 1.0104267 |
| 84358402 | -0.93538950 | -0.63581661 | -0.26357355 | 0.3773724 | -0.6507870 | -0.1104183 |
| 843786 | 0.49001396 | 0.16529843 | -0.13335576 | -0.5299649 | -0.1096698 | 0.0813699 |
| | PC13 | PC14 | PC15 | PC16 | PC17 | |
| 842302 | 0.10329677 | -0.690196797 | 0.601264078 | 0.74446075 | -0.26523740 | |
| 842517 | -0.94269981 | -0.652900844 | -0.008966977 | -0.64823831 | -0.01719707 | |
| 84300903 | -0.41026561 | 0.016665095 | -0.482994760 | 0.32482472 | 0.19075064 | |
| 84348301 | -0.93245070 | -0.486988399 | 0.168699395 | 0.05132509 | 0.48220960 | |
| 84358402 | 0.38760691 | -0.538706543 | -0.310046684 | -0.15247165 | 0.13302526 | |
| 843786 | -0.02625135 | 0.003133944 | -0.178447576 | -0.01270566 | 0.19671335 | |
| | PC18 | PC19 | PC20 | PC21 | PC22 | |
| 842302 | -0.54907956 | 0.1336499 | 0.34526111 | 0.096430045 | -0.06878939 | |
| 842517 | 0.31801756 | -0.2473470 | -0.11403274 | -0.077259494 | 0.09449530 | |
| 84300903 | -0.08789759 | -0.3922812 | -0.20435242 | 0.310793246 | 0.06025601 | |
| 84348301 | -0.03584323 | -0.0267241 | -0.46432511 | 0.433811661 | 0.20308706 | |
| 84358402 | -0.01869779 | 0.4610302 | 0.06543782 | -0.116442469 | 0.01763433 | |
| 843786 | -0.29727706 | -0.1297265 | -0.07117453 | -0.002400178 | 0.10108043 | |
| | PC23 | PC24 | PC25 | PC26 | PC27 | |
| 842302 | 0.08444429 | 0.175102213 | 0.150887294 | -0.201326305 | -0.25236294 | |
| 842517 | -0.21752666 | -0.011280193 | 0.170360355 | -0.041092627 | 0.18111081 | |
| 84300903 | -0.07422581 | -0.102671419 | -0.171007656 | 0.004731249 | 0.04952586 | |
| 84348301 | -0.12399554 | -0.153294780 | -0.077427574 | -0.274982822 | 0.18330078 | |
| 84358402 | 0.13933105 | 0.005327110 | -0.003059371 | 0.039219780 | 0.03213957 | |
| 843786 | 0.03344819 | -0.002837749 | -0.122282765 | -0.030272333 | -0.08438081 | |
| | PC28 | PC29 | PC30 | | | |
| 842302 | -0.0338846387 | 0.045607590 | 0.0471277407 | | | |
| 842517 | 0.0325955021 | -0.005682424 | 0.0018662342 | | | |
| 84300903 | 0.0469844833 | 0.003143131 | -0.0007498749 | | | |
| 84348301 | 0.0424469831 | -0.069233868 | 0.0199198881 | | | |
| 84358402 | -0.0347556386 | 0.005033481 | -0.0211951203 | | | |
| 843786 | 0.0007296587 | -0.019703996 | -0.0034564331 | | | |

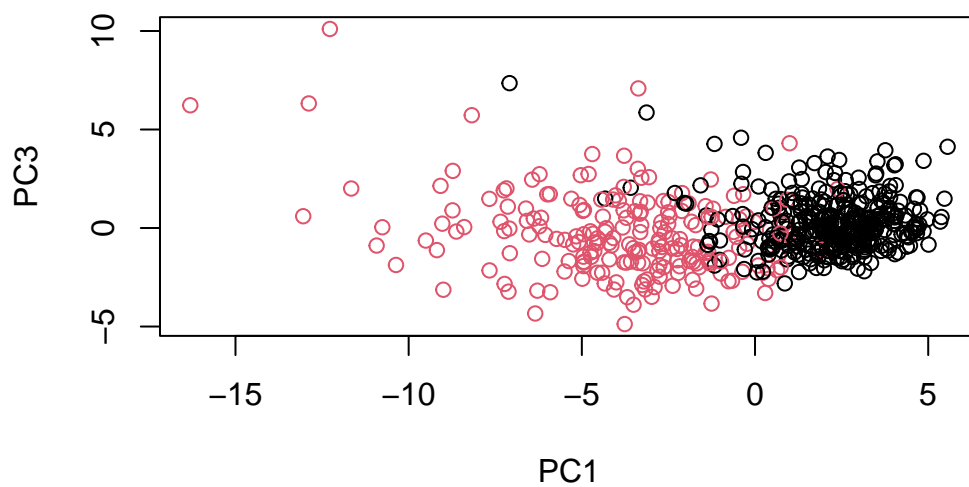
- **Q7.** What stands out to you about this plot? Is it easy or difficult to understand? Why?

```
biplot(wisc.pr)
```

- **Q8.** Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

```
plot(wisc.pr$x[,1], wisc.pr$x[,3], col=as.factor(diagnosis), xlab = "PC1", ylab = "PC3")
```

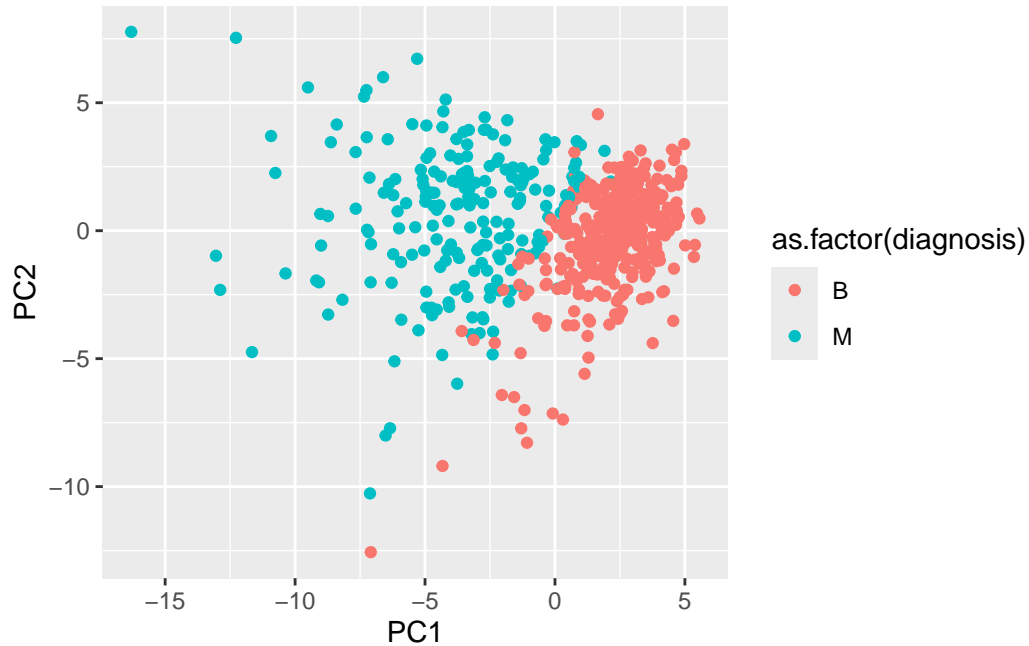


```
# Create a data.frame for ggplot
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis

# Load the ggplot2 package
library(ggplot2)
```

Warning: package 'ggplot2' was built under R version 4.3.3

```
# Make a scatter plot colored by diagnosis
ggplot(df) +
  aes(PC1, PC2, col= as.factor(diagnosis)) +
  geom_point()+
  labs(x="PC1", y="PC2")
```



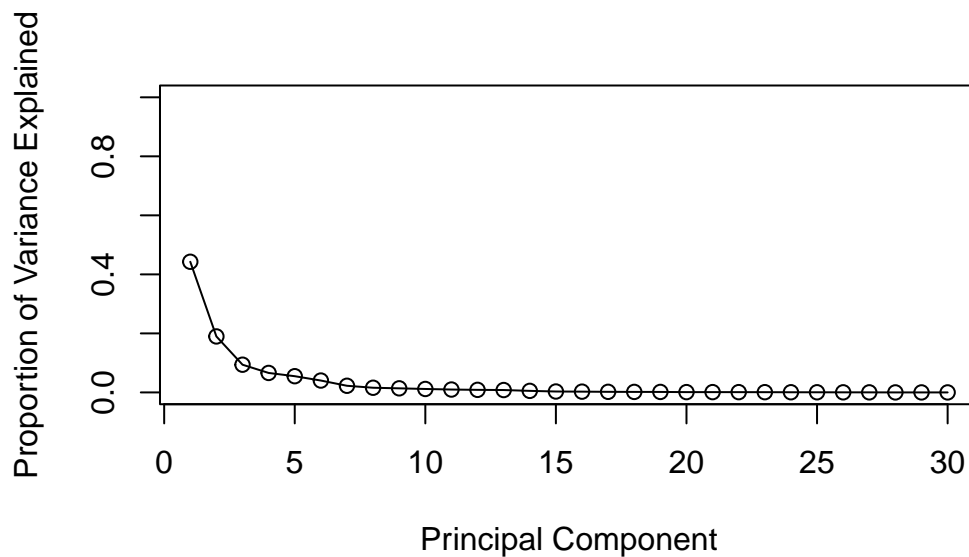
Variance explained

```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

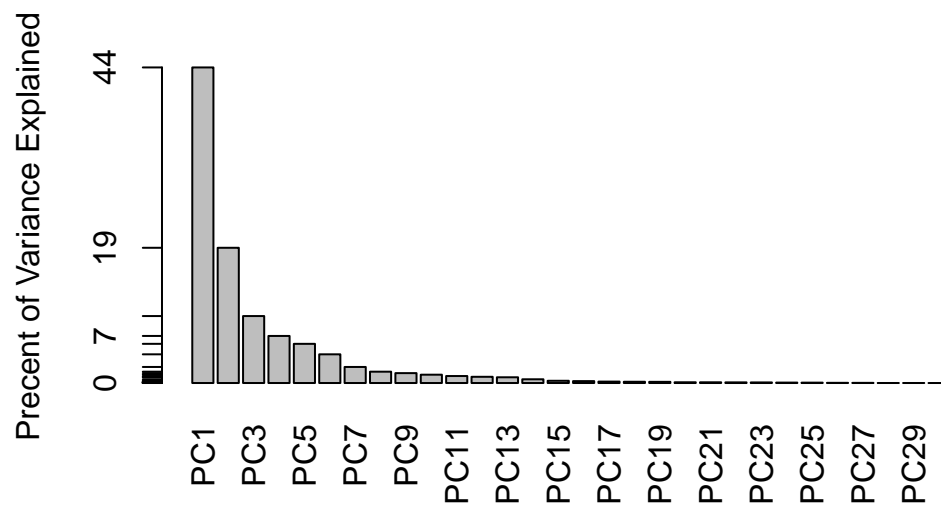
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# Variance explained by each principal component: pve
pve <- pr.var/sum(pr.var)

# Plot variance explained for each principal component
plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```



```
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
       names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```

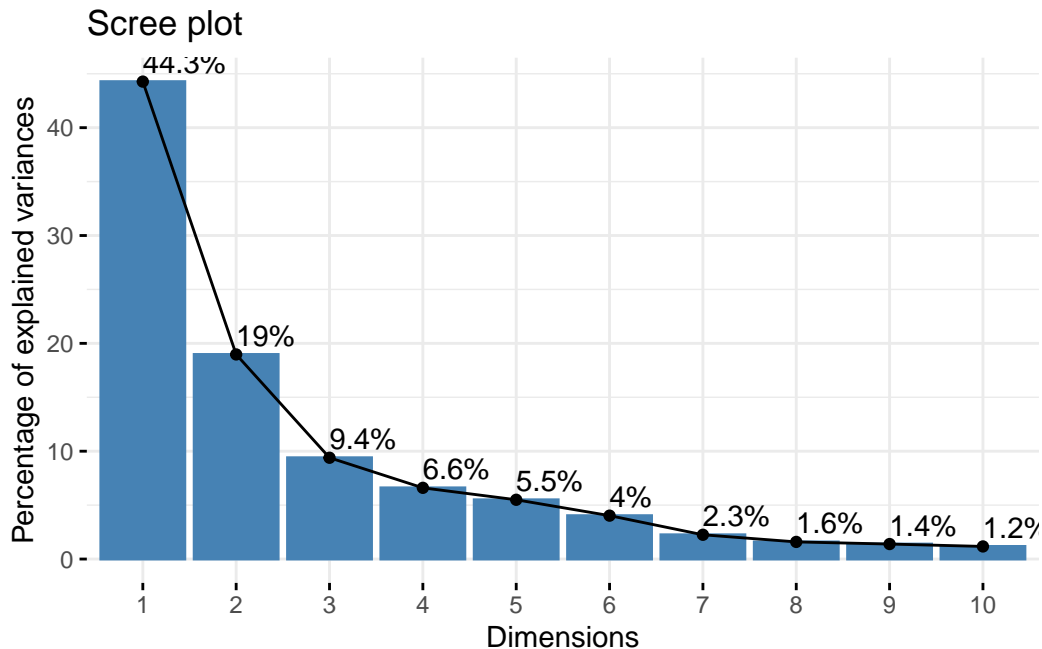



```
## ggplot based graph
#install.packages("factoextra")
library(factoextra)
```

Warning: package 'factoextra' was built under R version 4.3.3

Welcome! Want to learn more? See two factoextra-related books at <https://goo.gl/ve3WBa>

```
fviz_eig(wisc.pr, addlabels = TRUE)
```



- **Q9.** For the first principal component, what is the component of the loading vector (i.e. `wisc.pr$rotation[,1]`) for the feature `concave.points_mean`?

```
wisc.pr$rotation["concave.points_mean", 1]
```

```
[1] -0.2608538
```

- **Q10.** What is the minimum number of principal components required to explain 80% of the variance of the data?

5 PCs

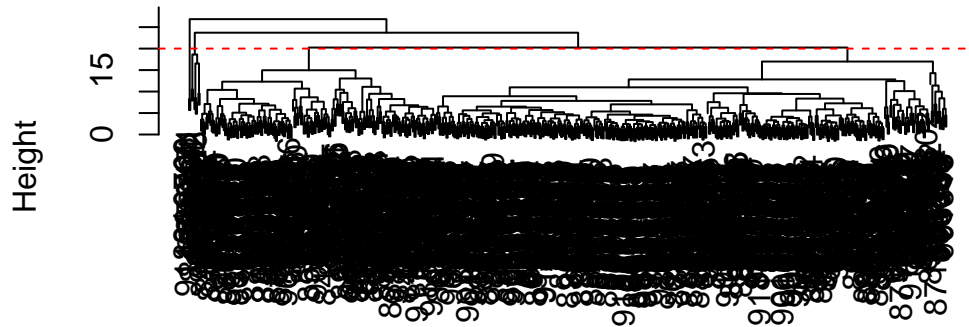
Hierarchical clustering

```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
wisc.hclust <- hclust(data.dist, method = "complete")
```

- **Q11.** Using the `plot()` and `abline()` functions, what is the height at which the clustering model has 4 clusters?

```
plot(wisc.hclust)
abline(h=20, col="red", lty=2)
```

Cluster Dendrogram



```
data.dist
hclust (*, "complete")
```

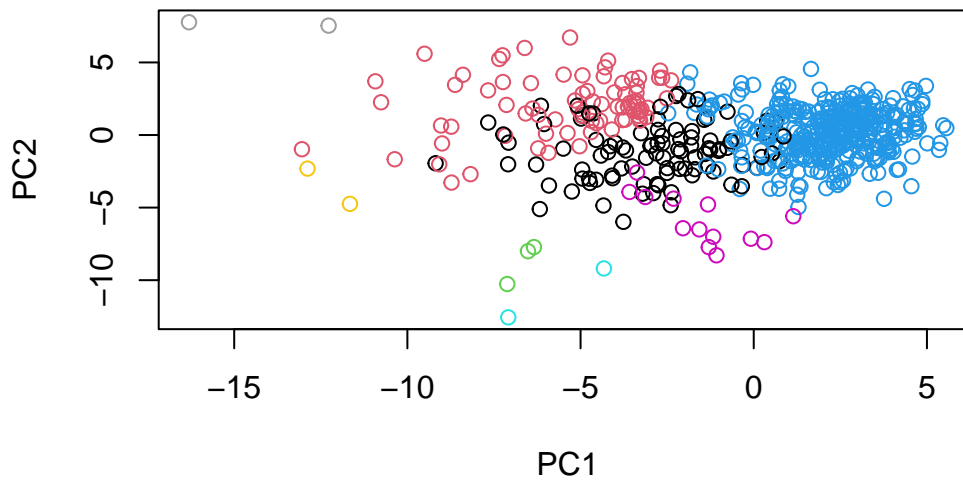
```
table(wisc.hclust.clusters, diagnosis)
```

```
wisc.hclust.clusters <- cutree(wisc.hclust, k=4)
table(wisc.hclust.clusters, diagnosis)
```

| | diagnosis | |
|----------------------|-----------|-----|
| wisc.hclust.clusters | B | M |
| 1 | 12 | 165 |
| 2 | 2 | 5 |
| 3 | 343 | 40 |
| 4 | 0 | 2 |

- **Q12.** Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

```
wisc.hclust.clusters <- cutree(wisc.hclust, k=8)
plot( wisc.pr$x[,1:2] , col = wisc.hclust.clusters,
xlab = "PC1", ylab = "PC2")
```



- **Q13.** Which method gives your favorite results for the same `data.dist` dataset? Explain your reasoning.

```
wisc.hclust_complete <- hclust(data.dist, method = "complete")
wisc.hclust_single <- hclust(data.dist, method = "single")
wisc.hclust_avg <- hclust(data.dist, method = "average")
wisc.hclust_ward <- hclust(data.dist, method = "ward.D2")
```

```
wisc.hclust.clusters <- cutree(wisc.hclust_complete, k=4)
table(wisc.hclust.clusters, diagnosis)
```

```
      diagnosis
wisc.hclust.clusters  B  M
1      12 165
2       2   5
3     343  40
4       0   2
```

```
wisc.hclust.clusters <- cutree(wisc.hclust_single, k=4)
table(wisc.hclust.clusters, diagnosis)
```

```
      diagnosis
wisc.hclust.clusters  B  M
1     356 209
```

| | | |
|---|---|---|
| 2 | 1 | 0 |
| 3 | 0 | 2 |
| 4 | 0 | 1 |

```
wisc.hclust.clusters <- cutree(wisc.hclust_avg, k=4)
table(wisc.hclust.clusters, diagnosis)
```

| | diagnosis | |
|----------------------|-----------|-----|
| wisc.hclust.clusters | B | M |
| 1 | 355 | 209 |
| 2 | 2 | 0 |
| 3 | 0 | 1 |
| 4 | 0 | 2 |

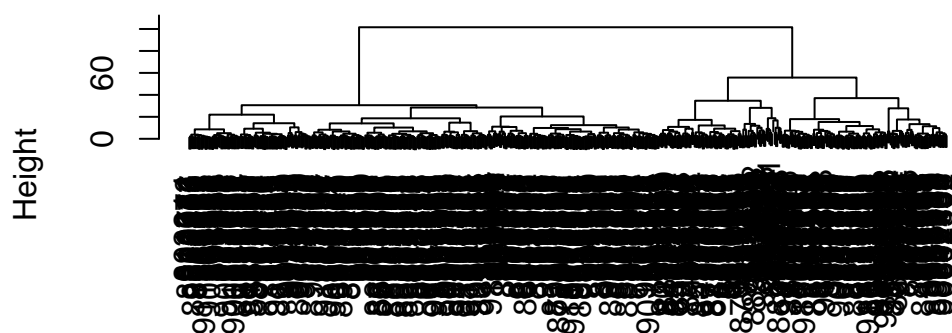
```
wisc.hclust.clusters <- cutree(wisc.hclust_ward, k=4)
table(wisc.hclust.clusters, diagnosis)
```

| | diagnosis | |
|----------------------|-----------|-----|
| wisc.hclust.clusters | B | M |
| 1 | 0 | 115 |
| 2 | 6 | 48 |
| 3 | 337 | 48 |
| 4 | 14 | 1 |

I like the ward.D2 method because I think it distributes the clusters in the most average way, which ensures each cluster would have enough data points.

```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[, 1:7]), method = "ward.D2")
plot(wisc.pr.hclust)
```

Cluster Dendrogram



```
dist(wisc.pr$x[, 1:7])
hclust (*, "ward.D2")
```

```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

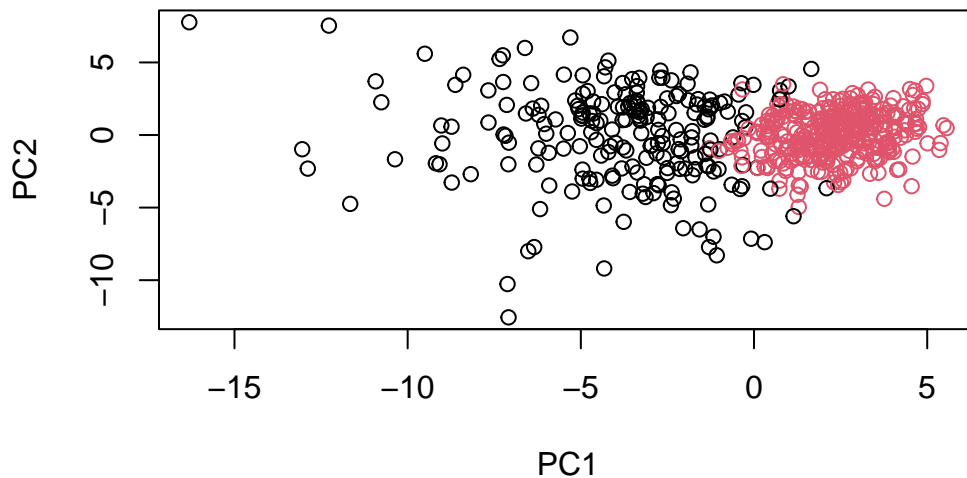
```
grps
  1  2
216 353
```

```
table(grps, diagnosis)
```

```
      diagnosis
grps   B    M
  1  28 188
  2 329  24
```

•

```
plot(wisc.pr$x[,1:2], col=grps)
```



- **Q15.** How well does the newly created model with four clusters separate out the two diagnoses?

```
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
# Compare to actual diagnoses
table(wisc.pr.hclust.clusters, diagnosis)
```

```
          diagnosis
wisc.pr.hclust.clusters  B  M
1          28 188
2         329  24
```

- **Q16.** How well do the k-means and hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses? Again, use the `table()` function to compare the output of each model (`wisc.km$cluster` and `wisc.hclust.clusters`) with the vector containing the actual diagnoses.

```
wisc.km <- kmeans(wisc.data, centers= 2, nstart= 20)
table(wisc.km$cluster, diagnosis)
```

```
diagnosis
  B  M
1 356 82
2   1 130
```

```
table(cutree(wisc.hclust, k=4), diagnosis)
```

```
diagnosis
  B  M
1 12 165
2   2   5
3 343  40
4   0   2
```

- **Q17.** Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity?

Specificity: Hierarchical clustering

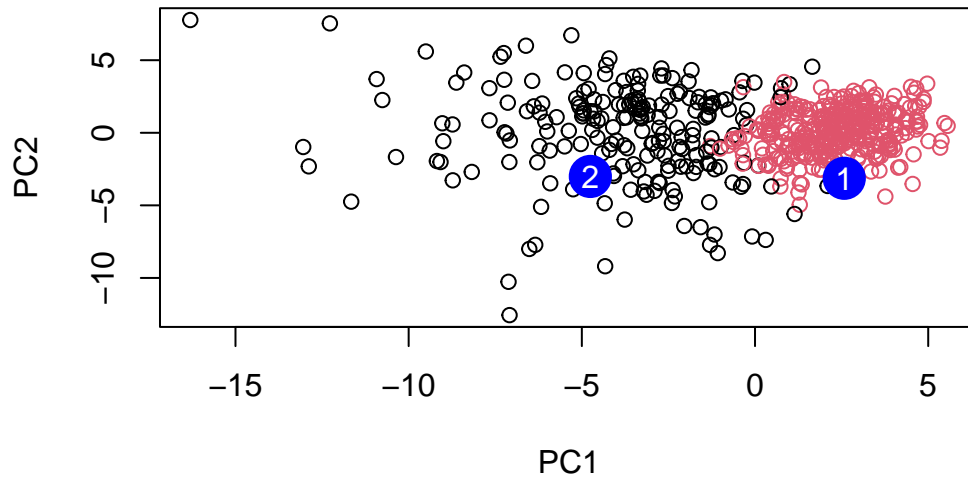
Sensitivity: Kmean

```
#url <- "new_samples.csv"
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
npc <- predict(wisc.pr, newdata=new)
npc
```

```
      PC1      PC2      PC3      PC4      PC5      PC6      PC7
[1,]  2.576616 -3.135913  1.3990492 -0.7631950  2.781648 -0.8150185 -0.3959098
[2,] -4.754928 -3.009033 -0.1660946 -0.6052952 -1.140698 -1.2189945  0.8193031
      PC8      PC9      PC10      PC11      PC12      PC13      PC14
[1,] -0.2307350  0.1029569 -0.9272861  0.3411457  0.375921  0.1610764  1.187882
[2,] -0.3307423  0.5281896 -0.4855301  0.7173233 -1.185917  0.5893856  0.303029
      PC15      PC16      PC17      PC18      PC19      PC20
[1,]  0.3216974 -0.1743616 -0.07875393 -0.11207028 -0.08802955 -0.2495216
[2,]  0.1299153  0.1448061 -0.40509706  0.06565549  0.25591230 -0.4289500
      PC21      PC22      PC23      PC24      PC25      PC26
[1,]  0.1228233  0.09358453  0.08347651  0.1223396  0.02124121  0.078884581
[2,] -0.1224776  0.01732146  0.06316631 -0.2338618 -0.20755948 -0.009833238
      PC27      PC28      PC29      PC30
[1,]  0.220199544 -0.02946023 -0.015620933  0.005269029
[2,] -0.001134152  0.09638361  0.002795349 -0.019015820
```



```
plot(wisc.pr$x[,1:2], col=as.factor(grps))
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], c(1,2), col="white")
```



- **Q18.** Which of these new patients should we prioritize for follow up based on your results?

Patient 1