

PCP — <LOD Penalty - Boston data

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Data

- 20 air pollution species
- 2,478 days (~6.7 years)

```
# Read air pollution data
mixture <- readMat("./Data/mixtures_data.mat")

mixture_data <- as.data.frame(mixture) %>% as_tibble() %>%
  select(Al, As, Ba, bc, Br, Ca, Cl,
         Cr, Cu, Fe, K, Mn, Ni, Pb, S, Se, Si,
         Ti, V, Zn) %>%
  drop_na()

mixture_data

## # A tibble: 2,478 x 20
##       Al      As      Ba      bc      Br      Ca      Cl      Cr      Cu      Fe
##   <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1 0.0194 0      0      0.682 2.00e-3 0.0231 0.0027 5.00e-4 0.0054 0.026
## 2 0.0263 0.00120 0.0206 0.372 1.51e-2 0.0428 0.0239 9.00e-4 0.0056 0.0686
## 3 0.0281 0      0.0099 0.418 0      0.0332 0.0044 5.00e-4 0.0026 0.0369
## 4 0.0117 0.0005 0.0076 0.361 1.80e-3 0.0167 0.0022 0      0.0033 0.0211
## 5 0.0102 0.0019 0.0022 0.359 6.00e-4 0.0145 0.0034 8.00e-4 0.003 0.0346
## 6 0.0387 0.0008 0.0256 1.09 0      0.0261 0.0043 4.00e-4 0.0033 0.103
## 7 0.0217 0.0019 0.0037 0.552 0      0.0214 0.0018 6.00e-4 0.0037 0.0651
## 8 0.0118 0      0.0026 0.641 8.00e-4 0.0154 0.0022 8.00e-4 0.0035 0.047
## 9 0.0376 0.0015 0.0157 1.01 1.60e-3 0.0326 0.0079 1.50e-3 0.009 0.137
## 10 0.0401 0      0.0295 0.791 4.00e-4 0.0254 0.0019 0      0.0049 0.0546
## # ... with 2,468 more rows, and 10 more variables: K <dbl>, Mn <dbl>, Ni <dbl>,
## #   Pb <dbl>, S <dbl>, Se <dbl>, Si <dbl>, Ti <dbl>, V <dbl>, Zn <dbl>

summary(mixture_data)

##       Al              As              Ba              bc
## Min.   :0.00000   Min.   :0.0000000   Min.   :0.000000   Min.   :0.0539
## 1st Qu.:0.02950   1st Qu.:0.0000000   1st Qu.:0.000700   1st Qu.:0.3802
## Median :0.04195   Median :0.0003000   Median :0.006600   Median :0.5734
```

##	Mean	:0.04803	Mean	:0.0005764	Mean	:0.008541	Mean	:0.6480
##	3rd Qu.	:0.05958	3rd Qu.	:0.0010000	3rd Qu.	:0.013200	3rd Qu.	:0.8354
##	Max.	:0.37540	Max.	:0.0073000	Max.	:0.210600	Max.	:2.9620
##	Br		Ca		Cl		Cr	
##	Min.	:0.0000000	Min.	:0.00040	Min.	:0.0000	Min.	:0.0000000
##	1st Qu.	:0.0000000	1st Qu.	:0.01953	1st Qu.	:0.0013	1st Qu.	:0.0001000
##	Median	:0.0002000	Median	:0.02645	Median	:0.0024	Median	:0.0004000
##	Mean	:0.0008227	Mean	:0.02887	Mean	:0.0163	Mean	:0.0004283
##	3rd Qu.	:0.0013000	3rd Qu.	:0.03537	3rd Qu.	:0.0051	3rd Qu.	:0.0007000
##	Max.	:0.0151000	Max.	:0.11810	Max.	:1.6739	Max.	:0.0040000
##	Cu		Fe		K		Mn	
##	Min.	:0.0000000	Min.	:0.00250	Min.	:0.00040	Min.	:0.0000000
##	1st Qu.	:0.001500	1st Qu.	:0.03800	1st Qu.	:0.02340	1st Qu.	:0.0000000
##	Median	:0.003000	Median	:0.05370	Median	:0.03260	Median	:0.0000000
##	Mean	:0.003319	Mean	:0.05925	Mean	:0.04120	Mean	:0.0004234
##	3rd Qu.	:0.004700	3rd Qu.	:0.07408	3rd Qu.	:0.04578	3rd Qu.	:0.0003000
##	Max.	:0.099800	Max.	:0.30470	Max.	:3.58110	Max.	:0.0105000
##	Ni		Pb		S		Se	
##	Min.	:0.0000000	Min.	:0.0000000	Min.	:0.0008	Min.	:0.0000000
##	1st Qu.	:0.000625	1st Qu.	:0.003200	1st Qu.	:0.4545	1st Qu.	:0.0000000
##	Median	:0.001500	Median	:0.005000	Median	:0.7238	Median	:0.0000000
##	Mean	:0.002125	Mean	:0.005378	Mean	:0.9675	Mean	:0.0001374
##	3rd Qu.	:0.002775	3rd Qu.	:0.007200	3rd Qu.	:1.1676	3rd Qu.	:0.0000000
##	Max.	:0.022900	Max.	:0.037700	Max.	:6.6640	Max.	:0.0074000
##	Si		Ti		V		Zn	
##	Min.	:0.00190	Min.	:0.0000000	Min.	:0.0000000	Min.	:0.000000
##	1st Qu.	:0.03673	1st Qu.	:0.001900	1st Qu.	:0.000900	1st Qu.	:0.00510
##	Median	:0.05740	Median	:0.002800	Median	:0.001900	Median	:0.00810
##	Mean	:0.06806	Mean	:0.003292	Mean	:0.002677	Mean	:0.01008
##	3rd Qu.	:0.08555	3rd Qu.	:0.004300	3rd Qu.	:0.003400	3rd Qu.	:0.01238
##	Max.	:0.41810	Max.	:0.076600	Max.	:0.051000	Max.	:0.15710

Relative error

Overall

Low rank and sparse

Values $>$ and $<$ LOD

Resulting SVD solutions

Loading vectors vs. original data

Loading vectors vs. solution w/ no $<$ LOD

Score vectors vs. original data

Score vectors vs. solution w/ no $<$ LOD