PCA redistribution of “energy”

Recall “amount of structure” is quantified as:

“sum of squares about the mean” = $\sum_{i=1}^{n} \left\| \underline{X}_i - \underline{\overline{X}} \right\|^2$

And insight comes from “decomposition” (ANOVA)

[toy graphic]

PCA redistribution of “energy” (cont.)

$$\sum_{i=1}^{n}\left\|\underline{X}_i-\overline{\underline{X}}\right\|^2=\sum_{i=1}^{n}\left(\underline{X}_i-\overline{\underline{X}}\right)^t\left(\underline{X}_i-\overline{\underline{X}}\right)=(n-1)tr\left(\tilde{X}^t\tilde{X}\right)$$

where: $$\tilde{X}=\frac{1}{\sqrt{n-1}}\left(\underline{X}_1-\overline{\underline{X}}\quad\cdots\quad\underline{X}_n-\overline{\underline{X}}\right)_{d\times n}$$

$$\sum_{i=1}^{n}\left\|\underline{X}_i-\overline{\underline{X}}\right\|^2=(n-1)tr\left(\tilde{X}\tilde{X}^t\right)=(n-1)tr\left(\hat{\Sigma}\right)$$

- “Energy is expressed in trace of covariance matrix”

PCA redistribution of "energy" (cont.)

$$\frac{1}{n-1}\sum_{i=1}^{n}\left\|\underline{X}_i-\underline{\overline{X}}\right\|^2=tr\left(BDB^t\right)=tr\left(BB^tD\right)=tr(D)=\sum_{j=1}^{d}\lambda_j$$

- Eigenvalues provide "atoms of SS decomposition"
- Useful Plots are:

  "Power Spectrum": λ_j vs. j

  "log Power Spectrum": $\log(\lambda_j)$ vs. j

  "Cumulative Power Spectrum": $\sum_{j'=1}^{j}\lambda_{j'}$ vs. j

Recall PCA graphic (get SS for free, but watch factors of $\sqrt{n-1}$)

Different Views of PCA

Recall 2-d graphic

1. Direction to maximize SS of 1-d projected data

2. Direction to minimize SS of residuals

   (same, by Pythagorean Theorem)

3. "Best fit line" to data in "orthogonal sense"

   (vs. "regression of Y on X" = vertical sense

   & "regression of X on Y" = horizontal sense)