A review of Principle Hessian Directions and some unexpected results

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Principle Hessian Directions (PHD, Li 1992) is a modern dimension reduction method and data visualization technique. PHD enables us to reduce high dimension data sets through the use of the dimension reduced model shown below

$$\boldsymbol{Y} = f(\boldsymbol{\beta}_1^T\boldsymbol{X}, \dots, \boldsymbol{\beta}_K^T\boldsymbol{X}, \varepsilon)$$

where $\boldsymbol{X} = [X_1, \dots, X_P]^T \sim N_P(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ and is independent of the error term $\boldsymbol{\varepsilon}$. The $\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_K$ are effective dimension reduction, or EDR, directions. PHD seeks to find these EDR directions. To find the EDR directions, the following matrix $\boldsymbol{H}$ is calculated

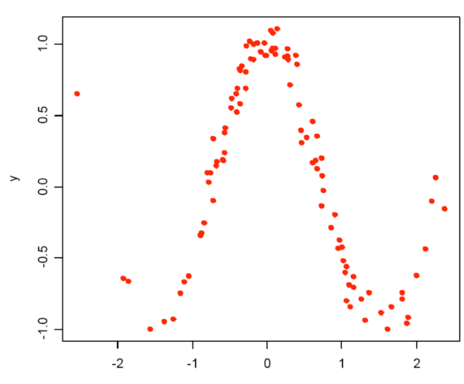
$$\boldsymbol{H} = E[(Y - E(Y))\Sigma^{-1}(\boldsymbol{X} - \boldsymbol{\mu})(\boldsymbol{X} - \boldsymbol{\mu})^T\Sigma^{-1}]$$

It is the eigenvectors of $\boldsymbol{H}$ corresponding to nonzero eigenvalues that are EDR directions.

As part of my project, I simulated the PHD process through a function I wrote in R. This function estimates the $\boldsymbol{H}$ matrix and returns the estimated EDR directions. All data used for these simulations was also generated in R. A unique aspect of the PHD method is that it does not require a defined function to work. For example, if we randomly generate 100 observations according to

$$\boldsymbol{Y} = \cos\left(2\boldsymbol{\beta}_1^T\boldsymbol{X}\right) + 0.1\varepsilon$$

we can input the data into the PHD function to estimate the EDR directions. Below is plot of the responses versus the $\widehat{\boldsymbol{\beta}}_1^T X_i$'s



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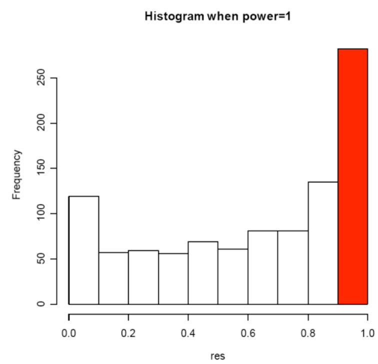
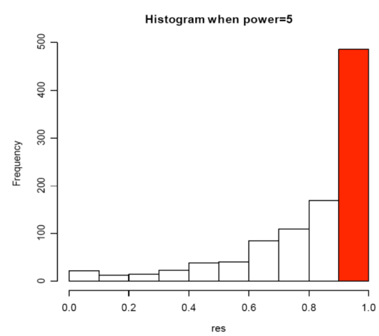
No consideration for a cosine model was entered into the PHD function, yet it was able to determine the shape of *f*.

An interesting feature of this method is that occasionally, it will work when it is not expected to. Examine the following ***Y*** model

$$\boldsymbol{Y} = X_1^C + \varepsilon$$

where *C* is odd. Taking the previous ***H*** matrix with $\boldsymbol{\mu} = 0, \Sigma^{-1} = I$ and $\boldsymbol{\beta_1} = [1,0,\dots,0]^T$ it can be shown ***H*** is expected to equal 0. Therefore, PHD is not expected to recover EDR directions. However, running the model through the PHD function reveals the method often works. The following histograms show frequency of the squared cosine of the angle between the true and estimated directions when *C=1* and *C=5* for 1000 simulations:





The red bar on each histogram indicates the trails that worked extremely when run through the PHD function, indicating the estimated direction was extremely close to the true direction. The first histogram indicates there is a general trend towards the method working well. The second histogram shows that as the power increases this trend becomes stronger. The reason this method works so well when we did not expect it to work at all is due to the high variability of the first diagonal component of ***H***. This high variability indicates the actual value of this component is unlikely to zero as expected and indicates this component is most likely to be the dominant component of ***H***, enabling PHD to find a good estimate of the EDR direction.

I found my project to be very rewarding while challenging. My topic was a relatively new area and one I had not previously studied, making my project demanding at times. Overall, I found the vacation program to be very enjoyable.

Reference

Li, K. C. (1992), "On Principle Hessian Directions for Data Visualization and Dimension Reduction: Another Application of Stein's Lemma," *Journal of the American Statistical Association*, 87, 1025-1039.

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