

MS-E2112 Multivariate Statistical Analysis (5cr)

Lecture 4: Measures of Robustness, Robust Principal Component Analysis

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Robust Statistical Methods

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In statistics, robust methods are methods that perform well – or do not perform too poorly – in the presence of outlying observations.

Robust Statistical Methods, Example

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Mean vs median...

Measures of Robustness

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Let x denote a random variable or a random vector with a cumulative distribution function F_x , and let $X = \{x_1, x_2, \dots, x_n\}$, where x_1, x_2, \dots, x_n are n independent and identically distributed observations from the distribution F_x . Consider functional $Q(F_x)$ (or $Q(F_n)$). We wish to measure **robustness** of that functional.

Influence Function

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Influence Function

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Influence function measures the effect on functional Q when the underlying distribution deviates slightly from the assumed one.

$$IF(y, Q, F_x) = \lim_{0 < \varepsilon \rightarrow 0} \frac{Q((1 - \varepsilon)F_x + \varepsilon\delta_y) - Q(F_x)}{\varepsilon},$$

where δ_y is the cumulative distribution function having all its probability mass at y i.e.

$$\delta_y(t) = \begin{cases} 0, & t < y, \\ 1, & t \geq y. \end{cases}$$

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Influence function measures the effect of point-mass contamination, and thus it is considered as a measure of **local robustness**.

A functional with **bounded influence function** (with respect to for example L_2 norm) is considered as robust and desirable.

Example, Population Mean (Expected Value)

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$$\begin{aligned} IF(y, \mu, F_x) &= \lim_{0 < \varepsilon \rightarrow 0} \frac{\mu((1 - \varepsilon)F_x + \varepsilon\delta_y) - \mu(F_x)}{\varepsilon} \\ &= \lim_{0 < \varepsilon \rightarrow 0} \frac{E[(1 - \varepsilon)x + \varepsilon y] - E[x]}{\varepsilon} \\ &= \lim_{0 < \varepsilon \rightarrow 0} \frac{E[x - \varepsilon x + \varepsilon y] - E[x]}{\varepsilon} \\ &= \lim_{0 < \varepsilon \rightarrow 0} \frac{E[x] - \varepsilon E[x] + \varepsilon E[y] - E[x]}{\varepsilon} \\ &= \lim_{0 < \varepsilon \rightarrow 0} \frac{-\varepsilon E[x] + \varepsilon y}{\varepsilon} \\ &= \lim_{0 < \varepsilon \rightarrow 0} -E[x] + y = -E[x] + y = y - E[x] = y - \mu(F_x). \end{aligned}$$

This is not bounded with respect to y .

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Empirical influence function (also called the sensitivity curve) is a measure of the dependence of the estimator on the value of one of the points in the sample.

The empirical influence function can be seen as an estimate of the theoretical influence function.

Empirical Influence Function

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Let $X = \{x_1, x_2, \dots, x_n\}$, and let $X_y = \{x_1, x_2, \dots, x_n, y\}$. Now

$$\begin{aligned} IF_E(y, Q, F_n) &= \frac{Q((1 - \frac{1}{n+1})F_n + \frac{1}{n+1}\delta_y) - Q(F_n)}{\frac{1}{n+1}} \\ &= (n+1)(Q((1 - \frac{1}{n+1})F_n + \frac{1}{n+1}\delta_y) - Q(F_n)) \\ &= (n+1)(Q(X_y) - Q(X)). \end{aligned}$$

Example, Sample Mean

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$$\begin{aligned} IF_E(y, \hat{\mu}, F_n) &= (n+1)(\hat{\mu}(X_y) - \hat{\mu}(X)) \\ &= (n+1)\left(\frac{1}{n+1}\left(\sum_{i=1}^n x_i + y\right) - \frac{1}{n}\sum_{i=1}^n x_i\right) \\ &= \sum_{i=1}^n x_i + y - \frac{n+1}{n}\sum_{i=1}^n x_i \\ &= y - \left(\frac{n+1}{n} - 1\right)\sum_{i=1}^n x_i \\ &= y - \left(\frac{n+1-n}{n}\right)\sum_{i=1}^n x_i \\ &= y - \frac{1}{n}\sum_{i=1}^n x_i = y - \hat{\mu}(X). \end{aligned}$$

This is not bounded with respect to y . Note that the empirical influence function estimates the theoretical influence function.

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Another very often used measure of robustness is the breakdown point. Whereas influence function measures local robustness, the **breakdown point** can be seen as a **measure of global robustness**.

Breakdown Point

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Let $X_n = \{x_1, x_2, \dots, x_n\}$, where x_1, x_2, \dots, x_n are n independent and identically distributed observations from the distribution F_X . Assume that $m < n$ and replace x_1, x_2, \dots, x_m with $x_1^*, x_2^*, \dots, x_m^*$. Let $X_n^* = \{x_1^*, x_2^*, \dots, x_m^*, x_{m+1}, \dots, x_n\}$.

Now, the maximum bias

$$\maxBias(m, X_n, Q) = \sup_{x_1^*, x_2^*, \dots, x_m^*} d(Q(X_n), Q(X_n^*)),$$

where $d(\cdot, \cdot)$ denotes some distance function (for example the Euclidean distance).

The finite sample breakdown point is now given by

$$BP(Q, n) = \min_m \left\{ \frac{m}{n} \mid \maxBias(m, X_n, Q) = \infty \right\},$$

and the (asymptotic) breakdown point

$$BP(Q) = \lim_{n \rightarrow \infty} BP(Q, n).$$

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A functional with **large breakdown point** is considered as robust. If $BP(Q) = \frac{1}{2}$, then Q is very robust (according to its breakdown point), and if $BP(Q) = 0$, then Q is very nonrobust. When the value is in between $\frac{1}{2}$ and 0, then it is a matter of taste ;-).

Example, Sample Mean

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Let $X_n = \{x_1, x_2, \dots, x_n\}$ a sample of n independent and identically distributed observations from some distribution F_X .

Let $\hat{\mu}(X_n) = \frac{1}{n} \sum_{i=1}^n x_i$ and let $\hat{\mu}(X_n^*) = \frac{1}{n} (\sum_{i=2}^n x_i + x_1^*)$. Let $d(\hat{\mu}(X_n), \hat{\mu}(X_n^*))$ be the Euclidean distance between $\hat{\mu}(X_n)$ and $\hat{\mu}(X_n^*)$. If now $x_1^* \rightarrow \infty$, then also $\hat{\mu}(X_n^*) \rightarrow \infty$ and consequently

$$\max_{x_1^*} d(\hat{\mu}(X_n), \hat{\mu}(X_n^*)) = \infty.$$

Contaminating just one data point is enough to make the Euclidean distance arbitrarily large. Thus the finite sample breakdown point

$$BP(\hat{\mu}, n) = \frac{1}{n}$$

and the (asymptotic) breakdown point of the sample mean is

$$BP(\hat{\mu}) = \lim_{n \rightarrow \infty} BP(\hat{\mu}, n) = \lim_{n \rightarrow \infty} \frac{1}{n} = 0.$$

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Example, Sample Median (1/4)

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Let $X_n = \{x_1, x_2, \dots, x_n\}$ be a sample of independent and identically distributed observations from some distribution F_X . Let $Med(X_n)$ be the sample median calculated from the original sample and let $Med(X_n^*)$ be the sample median calculated from the contaminated sample $X_n^* = \{x_1^*, x_2^*, \dots, x_m^*, x_{m+1}, \dots, x_n\}$. Let $d(Med(X_n), Med(X_n^*))$ be the Euclidean distance between $Med(X_n)$ and $Med(X_n^*)$.

Example, Sample Median (2/4)

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Assume first that n is even. When n is even, the sample median is the average of the two middle values of the ordered observations. Now, one has to contaminate at least half of the observations in order to make the sample median and consequently the Euclidean distance arbitrarily large. Thus, for even n , the number of contaminated observations m has to be at least $n/2$ for

$$\max Bias(m, X_n, Med) = \sup_{X_1^*, X_2^*, \dots, X_m^*} d(Med(X_n), Med(X_n^*)) = \infty$$

to hold, and the finite sample breakdown point is then

$$BP(Med, n) = \min_m \left\{ \frac{m}{n} \mid \max Bias(m, X_n, Med) = \infty \right\} = \frac{n/2}{n} = \frac{1}{2}.$$

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Example, Sample Median (3/4)

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Assume now that n is odd. When n is odd, the sample median is the middle value of the ordered observations. Now, one has to contaminate at least $(n+1)/2$ observations in order to make the sample median and consequently the Euclidean distance arbitrarily large. Thus, for odd n , the number of contaminated observations m has to be at least $(n+1)/2$ for

$$\max_{\text{Bias}}(m, X_n, \text{Med}) = \sup_{x_1^*, x_2^*, \dots, x_m^*} d(\text{Med}(X_n), \text{Med}(X_n^*)) = \infty$$

to hold, and the finite sample breakdown point is then

$$BP(\text{Med}, n) = \min_m \left\{ \frac{m}{n} \mid \max_{\text{Bias}}(m, X_n, \text{Med}) = \infty \right\} = \frac{(n+1)/2}{n} = \frac{n+1}{2n}.$$

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Example, Sample Median (4/4)

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If n is even, the (asymptotic) breakdown point

$$BP(\text{Med}) = \lim_{n \rightarrow \infty} BP(\text{Med}, n) = \lim_{n \rightarrow \infty} \frac{1}{2} = \frac{1}{2}.$$

If n is odd, the (asymptotic) breakdown point

$$\begin{aligned} BP(\text{Med}) &= \lim_{n \rightarrow \infty} BP(\text{Med}, n) = \lim_{n \rightarrow \infty} \frac{n+1}{2n} \\ &= \lim_{n \rightarrow \infty} \left(\frac{n}{2n} + \frac{1}{2n} \right) = \lim_{n \rightarrow \infty} \left(\frac{1}{2} + \frac{1}{2n} \right) = \frac{1}{2}. \end{aligned}$$

Thus, the (asymptotic) breakdown point of sample median is $1/2$.

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Breakdown Point, Some Remarks

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- The applied distance does not have to be Euclidean.
- Sometimes $\max Bias(m, X_n, Q) = \infty$ is not seen as the only "breaking down" case. For example Scatter = 0 can be seen as breaking down too.
- For matrices, breaking down is sometimes considered to be equal to the largest eigenvalue approaching ∞ .
- It does not make much sense to try construct estimators that have breakdown point larger than $1/2$.

Robust PCA

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If the data can be assumed to arise from elliptical distribution, then principal component analysis can be robustified by replacing the sample covariance matrix with some robust scatter estimate. The reason for that is that, under elliptical distribution, all scatter estimates do estimate the same population quantity (up to the scale). Note that in general (without ellipticity assumption) this does not hold!

Minimum Covariance Determinant (MCD) Method

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The determinant (volume) of a covariance matrix, can be seen as a measure of total variation of the data, and it is then called the generalized variance. Data points that are far away from the data cloud increase the volume of the covariance matrix.

Minimum Covariance Determinant (MCD) Method

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Minimum Covariance Determinant (MCD) method is a well-known method for robustifying the estimation of the covariance matrix, and the mean vector, under the assumption of multivariate ellipticity.

MCD method is based on considering all subsets containing $p\%$ (usually 50%) of the original observations, and estimating the covariance matrix, and the mean vector, on the data of the subset associated with the smallest covariance matrix **determinant**. This is equivalent to finding the sub-sample with the smallest multivariate spread. The MCD sample covariance matrix, and the MCD sample mean vector, are then defined as the sample covariance matrix (up to the scale), and the sample mean vector, computed over this sub-sample.

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Note that, as $\det(AB) = \det(A)\det(B)$ for all square matrices and as the point mass probability of continuous distributions is 0, MCD should be affine equivariant under continuous distributions. However, the fast versions of the algorithm are not necessarily affine equivariant. Some error might occur due to "smart" sub-sampling.

Under the ellipticity assumption, PCA can be performed using the MCD scatter estimate instead of the traditional sample covariance matrix. MCD estimates are very robust, and thus as a consequence, robust PCA is obtained.

Note that MCD is not the only possible robust scatter estimate - there exists several robust scatter estimates that all estimate the same population quantity (up to the scale) under the assumption of multivariate ellipticity.

Words of Warning

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Some Words of Warning

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- It is possible that a functional Q has bounded influence function, but its breakdown point is 0!
- Robust PCA, based on some robust scatter matrix, can be performed under the assumption of multivariate ellipticity. If the ellipticity assumption does not hold, instead of estimating the PCA transformation matrix Γ , one may be estimating some other population quantity.

Next Week

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Next week we will talk about bivariate correspondence analysis (CA).

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References II

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References III

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