#### 36-755: Advanced statistics

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## 7.1 Recap: covariance matrix estimation

For A an  $m \times n$  matrix, take  $A = UDV^T$ . U, V orthonormal columns, D diagonal. Then:

$$\begin{split} \sigma_{max} &= \max_{x \in \mathbb{S}^{n-1}} ||Ax|| \text{ (largest singular value)} \\ &= \max_{\substack{x \in \mathbb{R}^n \\ x \neq 0}} \frac{||Ax||}{||x||} \\ &= \max_{\substack{x \in \mathbb{S}^{n-1} \\ y \in \mathbb{S}^{n-1}}} |y^T Ax| \end{split}$$

If A  $(n \times n)$  is symmetric,  $\sigma_{max}(A) = \max_{x \in \mathbb{S}^{n-1}} |x^T A x|$ .

If A  $(n \times n)$  is PSD,  $\sigma_{max}(A) = \max_{x \in \mathbb{S}^{n-1}} x^T A x$ , the largest eigenvalue of A.

For a generic A  $(m \times n)$ ,  $\sigma_{max}(A)$  also called the "operator norm".  $||A||_{op}$  is the  $L_{\infty}$  norm of its singular values.

 $|A||_F = \sqrt{\sum_{i,j} A_{ij}^2}$  is the "Frobenius" norm. It is the  $L_2$  norm over the singular values.

Nuclear norm of A:  $\sum_{i} \sigma_{i}$ , the  $L_{1}$  norm of the singular values.

## 7.2 Operator Norm

Take A, B to be  $m \times n$  matrices.. If  $||A - B||_{op} \to 0$  then  $|y^T A x - y^T B x| \to 0$  uniformly over  $x \in \mathbb{S}^{n-1}, y \in \mathbb{S}^{n-1}$ . And this implies  $\max_{i,j} |A_{ij} - B_{ij}| \to 0$ .

If  $\Sigma$  is the covariance matrix and  $\hat{\Sigma}$  an estimator of it (both PSD), then:

$$\begin{split} ||\Sigma - \hat{\Sigma}||_{op} &\to 0 \\ \Rightarrow \max_{v \in \mathbb{S}^{n-1}} |v^T \Sigma v - v^T \hat{\Sigma} v| &\to 0 \\ \Rightarrow \max_{v \in \mathbb{S}^{n-1}} |\mathbb{V}(v^T X) - \mathbb{V}(v^T \tilde{X})| &\to 0 \end{split}$$

Where  $X \sim (\mu, \Sigma)$  and  $\tilde{X} \sim (\tilde{\mu}, \hat{\Sigma})$ .

### 7.3 Weyl Inequality

A, B are  $m \times n$  with singular values:

$$\sigma_1(A) \ge \sigma_2(A) \ge \cdots \ge \sigma_{\min(n,m)}(A)$$
  
 $\sigma_1(B) \ge \sigma_2(B) \ge \cdots \ge \sigma_{\min(n,m)}(B)$ 

 $\Rightarrow \max_{k=1,\dots,min(m,n)} |\sigma_k(A) - \sigma_k(B)| \le ||A - B||_{op} = \sigma_{max}(A - B)$ 

Recall: a random vector  $X \in SG(\sigma^2)$  if:

$$\mathbb{E}(e^{\lambda v^T X}) \le e^{\frac{\lambda \sigma^2}{2}} \tag{7.1}$$

then  $X \in SG_d(\sigma^2)$  if its coordinates are independent  $SG(\sigma^2)$  or  $X \sim N_d(0, \Sigma)$  with  $\sigma^2 = ||\Sigma||_{op}$  because:

$$\mathbb{V}(v^T X) = v^T \Sigma v \Rightarrow \max_{v \in \mathbb{S}^{d-1}} (v^T \Sigma v) = ||\Sigma||_{op}$$
(7.2)

**Theorem 7.1** If  $X_1, \dots, X_n \stackrel{iid}{\sim} (0, \Sigma)$  in  $\mathbb{R}^d$  and  $\in SG(\sigma^2)$ , then, setting

$$\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^{n} X_i X_i^T \tag{7.3}$$

there exists a constant c > 0 such that:

$$\mathbb{P}(||\Sigma - \hat{\Sigma}||_{op} \le \sigma^2 C \min\{\sqrt{\frac{d + \log(2/\delta)}{n}}, \frac{d + \log(2/\delta)}{n}\}) \ge 1 - \delta$$
(7.4)

for  $\delta \in (0,1)$ 

This implies that if  $\Sigma = I, \sigma^2 = 1$  then:

$$||\hat{\Sigma} - I||_{op} \le \sqrt{\frac{d}{n}} + \frac{d}{n} \tag{7.5}$$

with high probability

Consistency requires d = o(n). Unless you make sparsity assumptions on  $\Sigma$  you must have d grow slowly with n.

**Proof:** The proof uses a discretization argument. Operator norm is the max over an infinite set, so we need to discretize. Take  $X \in SG(\sigma^2), X - E(X^2) \in SE(\nu^2, \alpha), \nu = \alpha = 16\sigma^2$ .

We also need the discretization lemma:

**Lemma 7.2** Let A  $(n \times n)$  symmetric (will eventually be  $\Sigma - \hat{\Sigma}$ ) and  $\mathcal{N}_{\epsilon}$  be an  $\epsilon$ -net of  $\mathbb{S}^{n-1}$ . Then

$$||A||_{op} = \max_{x \in \mathbb{S}^{n-1}} |x^T A x| \le (1 - 2\epsilon)^{-1} \max_{y \in \mathcal{N}_{\epsilon}} (y^T A y)$$
 (7.6)

**Proof:** Let  $x^* \in \mathbb{S}^{n-1}$  st  $||A||_{op} = |x^{*T}Ax^*|$ . Let  $y \in \mathcal{N}_{\epsilon}$  st  $||x^* - y|| \le \epsilon$ . Then:

$$\begin{array}{lll} |x^TAx^*-y^TAy| & = & |x^TA(x^*-y)+y^TA(x^*-y)| \text{ by symmetry} \\ & \leq & |x^TA(x^*-y)|+|y^TA(x^*-y)| \\ & \leq & ||x^*||A(x^*-y)|+||y||||A(x^*-y)| \\ & \leq & 2||A||_{op}||x^*-y|| \\ & \leq & 2\epsilon||A||_{op} \end{array}$$

Where the second to last inequality follows from  $||Az|| \leq ||A||_{op}||z||$ .

This gives:

$$|y^T A y| \ge |x^{*T} A x^*| - 2\epsilon ||A||_{op}$$
 (7.7)

$$\Rightarrow ||A||_{op} \leq \frac{1}{1 - 2\epsilon} |y^T A y| \tag{7.8}$$

$$\leq \frac{1}{1 - 2\epsilon} \max_{y \in \mathbb{S}^{n-1}} |y^T A y| \tag{7.9}$$

Now set  $A = \hat{\Sigma} - \Sigma$  ( $d \times d$  and symmetric) and consider  $\mathcal{N}_{\frac{1}{4}}$  a 1/4 - net of  $\mathbb{S}^{d-1}$ , then:

$$||\hat{\Sigma} - \Sigma||_{op} = ||A||_{op} \le 2 \max_{i} |v_i^T A v_i|$$
 (7.10)

where  $\{v_i, \dots, v_n\} = \mathcal{N}_{\frac{1}{4}}$ . Note that  $|\mathcal{N}_{\frac{1}{4}}| \leq 9^d$  because it is a volume calculation. So,  $\forall t > 0$ :

$$\begin{split} \mathbb{P}(||\hat{\Sigma} - \Sigma||_{op} \geq t) & \leq & \mathbb{P}(\max_{i} |v_{i}^{T}(\hat{\Sigma} - \Sigma)v_{i}| \geq t/2) \\ & \leq & \sum_{i \leq 9^{d}} \mathbb{P}(|v_{i}^{T}(\hat{\Sigma} - \Sigma)v_{i}| \geq t/2) \end{split}$$

for a fixed  $v \in \mathbb{S}^{d-1}$ ,

$$v^{T}(\hat{\Sigma} - \Sigma)v = \frac{1}{n} \sum_{j=1}^{n} (v^{T}X_{i})^{2} - v^{T}\Sigma v$$
Note:  $v^{T}\hat{\Sigma}v = v^{T}(\frac{1}{n} \sum_{j=1}^{n} X_{i}X_{i}^{T})v = \frac{1}{n} \sum_{j=1}^{n} v^{T}X_{i}X_{i}^{T}v = \frac{1}{n} \sum_{j=1}^{n} (v^{T}X_{i})^{2}$ 

$$= \frac{1}{n} \sum_{j=1}^{n} [Z_{i}^{2} - \mathbb{E}(Z_{i}^{2})]$$

where  $Z_i = v^T X_i, \Sigma = \mathbb{E}(XX^T)$  We know  $Z_i^2 - \mathbb{E}(Z_i^2) \in SE(\nu^2, \alpha), Z_i iid$ . For each  $v_i \in \mathcal{N}_{\frac{1}{4}}$ , by Bernstein:

$$\mathbb{P}(|v_i(\hat{\Sigma} - \Sigma)v_i| \ge t/2) \le 2exp\{-\frac{n}{2}min\{(\frac{t}{32\sigma^2})^2, \frac{t}{32\sigma^2}\}\}(*)$$
(7.11)

Then:

$$\mathbb{P}(\frac{||\hat{\Sigma} - \Sigma||}{\sigma^2} \ge t) \le 2 \cdot 9^d \cdot (*)$$
set:  $\le \delta$ 

$$\Rightarrow \frac{t}{32} \ge \sigma \min\{\frac{2}{n}dlog(9) + \frac{2}{n}log(2/\delta), \sqrt{\frac{2}{n}dlog(9) + \frac{2}{n}log(2/\delta)}\}$$

# 7.4 (Sparse) Linear Models

Setup:  $Y = X\beta^* + \epsilon$ , with  $\epsilon_1, \dots, \epsilon_n$  independent  $SG(\sigma^2)$ 

Generally, X is considered fixed [Buja15].

There are 2 settings we are interested in where d grows with n (or even d > n).

- Prediction
- Estimation

### 7.4.1 Prediction

Prediction or mean estimation. Suppose we observe a new batch of data  $\tilde{Y}$  and want to estimate  $\beta^*$  with  $\hat{\beta}$  and we would like to predict Y as follows:

minimize: 
$$\frac{1}{n}\mathbb{E}[||\tilde{Y} - X\hat{\beta}||^2]$$
 (7.12)

this is the same as minimizing  $\frac{1}{n}\mathbb{E}[||X(\beta^* - \hat{\beta})||^2] + \mathbb{E}[||\epsilon||^2]$ . So we minimize  $\frac{1}{n}\mathbb{E}[MSE(X\hat{\beta})]$ :

$$MSE(X\hat{\beta}) = ||X\beta^* - X\hat{\beta}||^2, \hat{\beta} = f(Y)$$

$$(7.13)$$

### 7.4.2 Parameter estimation

minimize  $\mathbb{E}[||\beta^* - \hat{\beta}||^2]$ 

Prediction is simpler, because parameter estimation requires the true model

## 7.5 Least Squares in High Dimensions

Usual:  $\hat{\beta}^{LS} = (X^T X)^{-1} X^T Y$  if  $(X^T X)^{-1}$  exists. But  $\hat{\beta}^{LS}$  is not defined if d > n or X is rank deficient (linearly dependent).

Still, you can find a solution to:

$$\min_{\beta \in \mathbb{R}^d} ||Y - X\beta||^2 \tag{7.14}$$

The function  $\beta \to ||Y - X\beta||^2$  is convex.

To find its minimum, we set the gradient to zero:

$$\Rightarrow X^T X \beta = X^T Y \tag{7.15}$$

Any  $\beta$  satisfying this will be a minimum.

If  $(X^TX)^{-1}$  does not exist, we have infinitely many solutionss. But if all we want is  $X\beta$  (rather than  $\beta$ ) we can take any such solution.

## References

[Buja15] A. Buja, R. Berk, L. Brown, E. George, E. Pitkin, M. Traskin, L. Zhao and K. Zhang "Models as Approximations—A Conspiracy of Random Regressors and Model Deviation Against Classical Inference in Regression," *Submitted to Statistical Science*, 2015.