

High-Dimensional Statistics & Sparsity

UDRC Summer School

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Motivation

Hypothesis testing in high-dimensions



ProblemObserve a random vector $X \in \mathbb{R}^d$ $X \sim \mathbb{P}_0$ or $X \sim \mathbb{P}_1$?

False positive:

$$= \mathbb{P}(\text{decide } X \sim \mathbb{P}_1 \, \big| \, X \sim \mathbb{P}_0)$$

False negative: $\beta = \mathbb{P}(\text{decide } X \sim \mathbb{P}_0 \mid X \sim \mathbb{P}_1)$

 α



Decision Rule: Likelihood Ratio

 x_1, \ldots, x_n : i.i.d. realizations of X

For a given $\ T \geq 0$,

If
$$\frac{\mathbb{P}_1(x_1,\ldots,x_n)}{\mathbb{P}_0(x_1,\ldots,x_n)} > T$$

, then decide
$$\ X\sim \mathbb{P}_1$$

MAP rule / minimizes risk when

$$T = \frac{\mathbb{P}(X \sim \mathbb{P}_0)}{\mathbb{P}(X \sim \mathbb{P}_1)}$$

If
$$\frac{\mathbb{P}_1(x_1,\ldots,x_n)}{\mathbb{P}_0(x_1,\ldots,x_n)} \le T$$

, then decide
$$\ X \sim \mathbb{P}_0$$

$$\left| \begin{array}{c} \frac{\mathbb{P}_{1}(x_{1},\ldots,x_{n})}{\mathbb{P}_{0}(x_{1},\ldots,x_{n})} \right|$$
positive: $\alpha_{L} = \mathbb{P}(L(x_{1},\ldots,x_{n}) > T \mid X \sim \mathbb{P}_{0})$

False

False negative: β_L

$$= \mathbb{P}(L(x_1,\ldots,x_n) \le T \mid X \sim \mathbb{P}_1)$$





Neyman-Pearson Lemma

$$\alpha_L = \mathbb{P}(L(x_1, \dots, x_n) > T \mid X \sim \mathbb{P}_0)$$

$$\beta_L = \mathbb{P}(L(x_1, \dots, x_n) \le T \mid X \sim \mathbb{P}_1)$$



Neyman-Pearson Lemma

The likelihood ratio test is *optimal*:

If there is another (possibly random) decision rule $D(x_1,\ldots,x_n)$ such that

$$\mathbb{P}(D(x_1,\ldots,x_n) \text{ decides } X \sim \mathbb{P}_1 \mid X \sim \mathbb{P}_0) \leq \alpha_L,$$

then

$$\mathbb{P}(D(x_1,\ldots,x_n) \text{ decides } X \sim \mathbb{P}_0 | X \sim \mathbb{P}_1) \geq \beta_L.$$

And vice-versa.



Linear Discriminant Analysis

$$\mathbb{P}_{0} = \mathcal{N}(\mu_{0}, \Sigma_{0})$$

$$\mathbb{P}_{1} = \mathcal{N}(\mu_{1}, \Sigma_{1})$$

$$\mathbb{R}^{d}$$

$$X \sim \mathcal{N}(\mu, \Sigma) \implies f_{X}(x) = \frac{1}{(2\pi)^{\frac{d}{2}} |\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(x-\mu)^{\top} \Sigma^{-1}(x-\mu)\right)$$

Assume (to simplify): $\Sigma_0 = \Sigma_1 = \Sigma$ and n = 1 (one observation)

$$L(x) > T \quad \Longleftrightarrow \quad \Psi(x) := \left(x - \frac{\mu_0 + \mu_1}{2}\right)^\top \Sigma^{-1} \left(\mu_1 - \mu_0\right) > \log T$$



$$\Psi(x) := \left(x - \frac{\mu_0 + \mu_1}{2}\right)^\top \Sigma^{-1} \left(\mu_1 - \mu_0\right) > \log T$$

Probability of error (assuming \mathbb{P}_0 and \mathbb{P}_1 are equally likely)

$$\operatorname{Err}(\Psi) = \mathbb{P}(\Psi(X) > 0 \& \mathbb{P}_0 \operatorname{true}) + \mathbb{P}(\Psi(X) \leq 0 \& \mathbb{P}_1 \operatorname{true})$$
$$= \mathbb{P}(\Psi(X) > 0 \mid \mathbb{P}_0) \cdot \mathbb{P}(\mathbb{P}_0) + \mathbb{P}(\Psi(X) \leq 0 \mid \mathbb{P}_1) \cdot \mathbb{P}(\mathbb{P}_1)$$
$$= \frac{1}{2} \mathbb{P}(\Psi(X) > 0 \mid \mathbb{P}_0) + \frac{1}{2} \mathbb{P}(\Psi(X) \leq 0 \mid \mathbb{P}_1)$$

(using Gaussianity and manipulating...)

$$= \Phi\left(-\frac{\gamma}{2}\right) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{-\gamma/2} e^{-t^2/2} dt$$

classical error expression

$$\begin{split} \gamma = \sqrt{(\mu_0 - \mu_1)^\top \Sigma^{-1} (\mu_0 - \mu_1)} \\ \big| \quad \big| \quad \big| \\ \text{need to be estimated} \end{split}$$

 n_0 and n_1 samples

<u>High-dimensional regime</u>: n_0 and n_1 same order as d



Fisher Linear Discriminant

$$\Psi(x) = \left(x - \frac{\mu_0 + \mu_1}{2}\right)^\top \Sigma^{-1} (\mu_1 - \mu_0)$$

$$\gamma = \sqrt{(\mu_0 - \mu_1)^\top \Sigma^{-1} (\mu_0 - \mu_1)} \qquad \text{Err}(\Psi) = \Phi\left(-\frac{\gamma}{2}\right)$$

Unbiased estimators:

$$\widehat{\mu}_0 := \frac{1}{n_0} \sum_{i=1}^{n_0} x_i \qquad \qquad \widehat{\mu}_1 := \frac{1}{n_1} \sum_{i=1}^{n_1} y_i$$

$$\widehat{\Sigma} := \frac{1}{n_0 - 1} \sum_{i=1}^{n_0} (x_i - \widehat{\mu}_0) (x_i - \widehat{\mu}_0)^\top + \frac{1}{n_1 - 1} \sum_{i=1}^{n_1} (y_i - \widehat{\mu}_1) (y_i - \widehat{\mu}_1)^\top$$

Plug estimators into log-likelihood ratio:

$$\widehat{\Psi}(x) := \left(x - \frac{\widehat{\mu}_0 + \widehat{\mu}_1}{2}\right)^\top \widehat{\Sigma}^{-1} \left(\widehat{\mu}_1 - \widehat{\mu}_0\right)$$

Fisher linear discriminant function



Fisher Linear Discriminant

Assume $\mathbb{P}(\mathbb{P}_0) = \mathbb{P}(\mathbb{P}_1)$ $\Sigma = I_d$ d = 400 $n_0 = n_1 = 800$

Vary $\gamma = \|\mu_0 - \mu_1\|_2$ between 1 and 2 Test with $\widehat{\Psi}(x)$ over 5000 random trials



[Kolmogorov]	
$(d, n_0, n_1) \to \infty$	$\frac{d}{n_0}, \ \frac{d}{n_1} \to \alpha$
$\operatorname{Err}(\widehat{\Psi}) \xrightarrow{\operatorname{prob.}} \Phi\Big(-$	$-\frac{\gamma^2}{2\sqrt{\gamma^2+2lpha}}\Big)$



What can help in high-dimensions?

Structure e.g., <u>sparsity</u>

Suppose μ_0 and μ_1 are sparse: only have $s \ll d$ nonzero entries



Procedure: *hard-threshold* entries of estimates

$$\widehat{\mu}_0' = \frac{1}{n_0} \sum_{i=1}^{n_0} x_i \quad \longrightarrow \quad (\widehat{\mu}_0)_i = H_\lambda \left(\left(\widehat{\mu}_0' \right)_i \right)$$

(same for μ_1)

hard-thresholding operator

$$H_{\lambda}(x) := \begin{cases} x & , \text{ if } |x| > \lambda \\ 0 & , \text{ if } |x| \leq \lambda \end{cases}$$



Example

hard-thresholding operator

$$H_{\lambda}(x) := \begin{cases} x & , \text{ if } |x| > \lambda \\ 0 & , \text{ if } |x| \le \lambda \end{cases}$$

$$d = 400$$
 $n = 800$ $s = 5$ $\lambda = \sqrt{\frac{2\log d}{n}} = 0.1224$





Same Experiments

Assume $\mathbb{P}(\mathbb{P}_0) = \mathbb{P}(\mathbb{P}_1)$ $\Sigma = I_d$

Vary $\gamma = \|\mu_0 - \mu_1\|_2$ between 1 and 2

 $d = 400 \qquad \qquad n_0 = n_1 = 800$

Test with $\widehat{\Psi}(x)$ over 5000 random trials

$$s = 5$$
 $\lambda = \sqrt{\frac{2\log d}{n}}$



Sparsity makes problem low-dimensional



Outline

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Introduction to LASSO and other sparsity problems

Gaussian graphical model selection

Matrix completion



A Crime Problem

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1	40	74	11	31	20	478
2	32	72	11	43	18	494
3	57	70	18	16	16	643
4	31	71	11	25	19	341
5	67	72	9	29	24	773
6	25	68	8	32	15	603
7	34	68	12	24	14	484
8	33	62	13	28	11	546
9	36	69	7	25	12	424
:	:	:	÷	÷	:	÷
50	66	67	26	18	16	940

<u>Goal:</u> Predict *# crimes / million* based on the other indicators



Linear Regression

Linear/affine model

d = 5 predictors

n=50 samples

$$y_{i} \simeq x_{0} + \sum_{j=1}^{d} a_{ij}x_{j} \quad i = 1, \dots, n \iff$$

$$| offset | coefficient to be determined table entry (crime rate)$$





Find coefficients: *least-squares*



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Linear Regression

$$\underset{\overline{x}}{\operatorname{minimize}} \quad \frac{1}{2} \left\| y - \overline{A} \overline{x} \right\|_2^2$$

$$\overline{x}_{\rm LS}^{\star} = \left(\overline{A}^{\top}\overline{A}\right)^{-1}\overline{A}\,y$$

	489.6486	offset
	10.9807	police funding / resident (\$/year)
	-6.0885	% of 25+ year-olds with 4+ years of high-school
	5.4803	% of 16-19 year-olds not in high-school
	0.3770	% of 18-24 year-olds in college
	5.5005	% of 25+ year-olds with 4+ years of college

Problems with least-squares

little interpretabilityall coefficients contribute to predictionsmall bias, large variancezeroing coefficients can improve mean-squared error



LASSO

least absolute selection and shrikange operator

Coefficient value



In reality, we solved ...

$$\min_{x_0, x} \frac{1}{2n} \|y - x_0 \mathbf{1}_n - Ax\|_2^2 + \lambda \|x\|_1$$

$$\| \\ \| \\ \text{necessary because } \frac{1}{n} \sum_{i=1}^n y_i \neq 0$$



L1-Norm Induces Sparsity

minimize
$$\frac{1}{2n} \|y - Ax\|_{2}^{2} + \lambda \|x\|_{1}$$

LASSO (aka Basis Pursuit Denoising)

$$igcap_{}$$
 for some $\, au\,$ depending on $\,\lambda$

$$\begin{array}{ll} \underset{x}{\text{minimize}} & \left\| y - Ax \right\|_{2}^{2} \\ \text{subject to} & \|x\|_{1} \leq \tau \end{array}$$

$$\ensuremath{\Uparrow}$$
 for some $\,\sigma\,$ depending on $\,\tau\,$

$$\begin{array}{ll} \underset{x}{\text{minimize}} & \|x\|_{1} \\ \text{subject to} & \left\|y - Ax\right\|_{2} \leq \sigma \end{array}$$

Constrained LASSO

Relaxed Basis Pursuit

Basis Pursuit when $\sigma = 0$



L1-Norm Induces Sparsity

$$\widehat{x} \in \underset{x}{\operatorname{arg\,min}} \|x\|_{1} \\ \text{s.t.} \|y - Ax\|_{2} \leq \sigma$$

Assume $\sigma = 0$:

$$y = Ax$$
 has solutions $\widetilde{x} + \operatorname{null}(A)$
 $y = A\widetilde{x} \Big| \quad \Big| \{d : Ad = 0\}$

Assume $\sigma > 0$: margin around $\tilde{x} + \operatorname{null}(A)$

What about the L2-norm?

$$\widehat{x}_{2} \in \underset{x}{\operatorname{arg\,min}} \|x\|_{2}^{2}$$
s.t.
$$\|y - Ax\|_{2} \leq \sigma$$





Example: Compressed Sensing





Application: Image Reconstruction



 $256 \times 496 \qquad \implies \quad z^{\star} \in \mathbb{R}^{126976}$

not sparse

Natural images have sparse representations

$$z^{\star} = \Psi x^{\star}$$

sparse or near-sparse *dictionary* (wavelet, DCT, gradient space)





Application: Image Reconstruction

Suppose we observe *only 50%* of pixels



Solve $\widehat{x} = \arg \min \|x\|_1$ x $y = \Phi \Psi x$ s.t. wavelet observed indices



PSNR: 21.31 dB



Application: Image Reconstruction



Solve $\widehat{x} = \arg \min \|x\|_1$ xs.t. $y = \Phi \Psi x$ wavelet partial DFT

each entry of y has info from entire image



 \widehat{x}

PSNR: 24.93 dB



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Gaussian graphical model selection

Matrix completion

Gaussian Graphical Model Selection

 $X = (X_1, X_2, \dots, X_d) \sim \mathcal{N}(0_d, \Sigma^{\star})$

<u>Problem</u>: given *n* idd observations of *X*, denoted $X^{(1)}, \ldots, X^{(n)}$, estimate Σ^{\star}

Assumption: most pairs of coordinates (X_i, X_j) are conditionally independent

$$\Downarrow$$
 precision matrix $\Theta^{\star} := (\Sigma^{\star})^{-1}$ is *sparse*





 X_4

 X_5

 X_3

 X_6

 X_2

 X_1

Gaussian Graphical Model Selection

$$X = (X_1, X_2, \dots, X_d) \sim \mathcal{N}(0_d, \Sigma^{\star})$$

$$\mathsf{pdf}: \quad f_X(x;\,\Theta^\star) = \frac{\sqrt{\det\,\Theta^\star}}{(2\pi)^{\frac{d}{2}}} \exp\left(-\frac{1}{2}x^\top\Theta^\star x\right)$$

Maximum likelihood estimator of $\, \Theta^{\star} \,$

$$\widehat{\Theta}_{\mathrm{ML}} = \underset{\Theta}{\mathrm{arg\,max}} \log \prod_{i=1}^{n} f\left(x^{(1)}, \dots, x^{(n)}; \Theta\right)$$

$$= \underset{\Theta}{\operatorname{arg\,min} - \log\,\det\,\Theta + \operatorname{tr}\left(\Theta\,\widehat{\Sigma}_n\right)} \\ = \widehat{\Sigma}_n^{-1}$$

sample covariance matrix

$$\widehat{\Sigma}_n := \frac{1}{n} \sum_{i=1}^n x^{(i)} x^{(i)^{\top}}$$

(assuming it is invertible \implies n > d)



Graphical LASSO

Maximum likelihood estimator

$$\widehat{\Theta}_{\mathrm{ML}}^{\star} = \underset{\Theta}{\operatorname{arg\,min}} - \log \, \det \, \Theta + \operatorname{tr} \left(\Theta \, \widehat{\Sigma}_n \right)$$



Assumption: most pairs of coordinates (X_i, X_j) are conditionally independent

Graphical LASSO

$$\widehat{\Theta}_{\mathrm{GL}} = \underset{\Theta}{\operatorname{arg\,min}} - \log\,\det\Theta + \operatorname{tr}\left(\Theta\,\widehat{\Sigma}_n\right) + \lambda \|\Theta\|_{1,\mathrm{off}} - d \\ \left|\sum_{\substack{i\neq j \\ i\neq j}} |\Theta|_{i\neq j}\right| = \left| \begin{array}{c} \star & \star & 0 & 0 & \star \\ \star & \star & \star & 0 & \star & \star \\ 0 & \star & \star & \star & \star & 0 \\ 0 & 0 & \star & \star & \star & \star & 0 \\ 0 & \star & \star & \star & \star & \star & \star \\ \star & \star & 0 & 0 & \star & \star \end{array} \right|$$

 $\left|\sum_{i \neq j} |\Theta_{ij}|\right|$ applies L1-norm only to off-diagonal entries

sensible estimators even for non-Gaussian RVs



Price of stock of *6 companies* at beginning of each week of 2011 (Jan-Jun)

Week	Alcoa	${f American}\ {f Express}$	Boeing	Bank of America	Caterpillar	Cisco Systems	_
1	14.67	43.30	66.15	10.59	100.25	14.94	_
2	15.29	43.73	69.26	10.89	101.30	15.14	
3	15.82	43.86	69.42	11.18	102.59	16.04	
4	15.87	43.86	70.29	11.47	102.72	16.41	
5	15.92	43.96	70.86	11.87	103.42	16.59	
6	15.95	44.13	71.17	11.89	103.56	16.82	
7	15.96	44.20	71.43	12.28	104.86	16.88	
8	16.18	44.75	71.52	12.32	105.58	16.93	
9	16.19	44.94	71.60	12.36	105.87	17.01	
÷	:	÷	÷	÷	÷	:	
24	17.42	50.74	79.31	14.77	96.93	21.22	
25	18.06	51.39	80.35	15.08	99.62	22.11	
	\widetilde{X}_1	\widetilde{X}_2	\widetilde{X}_3	\widetilde{X}_4	\widetilde{X}_5	\widetilde{X}_6	
remove mean	Ļ	Ļ	Ļ	Ļ	Ļ	Ļ	d =
	X_1	X_2	X_3	X_4	X_5	X_6	n =

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25

6



$$\widehat{\Theta}_{\rm ML} = \widehat{\Sigma}_n^{-1} = \begin{bmatrix} 60.82 & 4.85 & -6.21 & -21.34 & -0.07 & -4.81 \\ 4.85 & 7.34 & -1.22 & -5.50 & 0.37 & -4.78 \\ -6.21 & -1.22 & 3.03 & 2.08 & -0.08 & -2.69 \\ -21.34 & -5.50 & 2.08 & 14.31 & -0.42 & 1.69 \\ -0.07 & 0.37 & -0.08 & -0.42 & 0.06 & 0.07 \\ -4.81 & -4.78 & -2.69 & 1.69 & 0.07 & 11.38 \end{bmatrix}$$





$$\widehat{\Theta}_{\text{GL}} = \underset{\Theta}{\operatorname{arg\,min}} - \log \, \det \, \Theta + \operatorname{tr} \left(\Theta \, \widehat{\Sigma}_n \right) + \lambda \left\| \Theta \right\|_{1, \text{off-d}} \quad \text{graphical LASSO}$$
$$(\widehat{\Theta}_{\text{GL}})_{ij} \left| \leq 10^{-3} \quad \Longrightarrow \quad \text{we assume no correlation, i.e., no edge} \quad (i, j)$$

Number of edges















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Matrix Completion

Suppose someone gave you \$1M for *completing* a table like this...



Key insight: only a few factors may explain users' tastes (genre, actors, ads, ...)





Singular value decomposition: any real $m \times n$ matrix can be decomposed as

$$A = U\Sigma V^{\top} = \underbrace{\begin{bmatrix} \begin{vmatrix} & & & & & \\ u_1 & \cdots & u_k \\ & & & \\ \end{vmatrix}}_{m \times k} \underbrace{\begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_k \end{bmatrix}}_{k \times k} \underbrace{\begin{bmatrix} - & v_1^{\top} & - \\ \vdots \\ - & v_k^{\top} & - \end{bmatrix}}_{k \times n}_{orthogonal}$$

$$= \underbrace{\begin{bmatrix} u_1 & \cdots & u_k \\ u_{k+1} & \cdots & u_m' \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_k \\ 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots &$$

 $m \times k \quad k \times n$







Our problem

minimize $\operatorname{rank}(X)$ nonconvex $X \in \mathbb{R}^{m \times n}$ subject to $X_{ij} = a_{ij}, \quad (i,j) \in \mathcal{O}$ observed entries relax nuclear norm $\underset{X \in \mathbb{R}^{m \times n}}{\text{minimize}} \quad \left\| (\sigma_1(X), \sigma_2(X), \dots, \sigma_r(X)) \right\|_1 = \|X\|_{\star}$ subject to $X_{ij} = a_{ij}, \quad (i,j) \in \mathcal{O}$ minimize $||X||_{\star}$ $X \in \mathbb{R}^{m \times n}$

subject to $\operatorname{tr}(XM_l) = a_l$, $l = 1, \dots, p$

movies



Example Result

Theorem [Chandrasekaran et al. 12']

 $X^{\star} \in \mathbb{R}^{m \times n}$ unknown, but rank k

iid entries $\mathcal{N}(0,1)$ $a_l = \operatorname{tr}(XM_l), \ l = 1, \dots, p$ measurements

$$p \ge 3k (m+n-k) + 1 \qquad \Longrightarrow \qquad X^{\star} = \underset{X}{\operatorname{argmin}} \quad \|X\|_{\star} \qquad \text{w.h.p.}$$

s.t. $\operatorname{tr}(XM_l) = a_l, \quad l = 1, \dots, p$



Experiments

 X^{\star} : 30 × 30

$$\operatorname{rank}(X^{\star}) = 3$$

 $\begin{array}{ll} \underset{X \in \mathbb{R}^{m \times n}}{\text{minimize}} & \|X\|_{\star} \\ \text{subject to} & \operatorname{tr}(XM_l) = a_l \,, \quad l = 1, \dots, p \\ \\ & & \\$

Sucess rate (20 trials)



Conclusions

- Structure is key in *high-dimensional* problems
- Sparsity encodes several types of structure
- Several applications (and theory)



- LASSO, basis pursuit, ... improve *interpretability* and (often) *performance*
- Didn't cover: optimization theory and *algorithms*









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Code & presentation

https://github.com/joaofcmota/udrc-summerschool

http://jmota.eps.hw.ac.uk/documents/Mota21-HighDimensionalStatsAndSparsity-UDRC.pdf