MSA220/MVE440 STATISTICAL LEARNING FOR BIG DATA LECTURE 10

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With big data we often need to find efficient data representations of a smaller dimension for both visualization and computation.

- SVD, PCA
- SOM
- And upcoming lectures MDS, NMF

SVD (singular value decomposition) is a workhorse that underpins much of the modeling we do!

- Data matrix X of dimension $n \times p$
- Before you do anything, you want to center and scale the columns of X!!!
- Otherwise the scale of individual variables dominate the representation and visualization is weird without centering
- We want to approximate the observations x_i in X by a lower-rank model
- Find the lower-rank model V_q to minimize the L2 error

$$\sum_{i=1}^N ||x_i - V_q \lambda_i||^2$$

where V_q is a $p \times q$ has orthogonal columns and λ_i is the variable specific coefficient

• If we knew V_q we can easily solve for λ in the problem below

$$\sum_{i=1}^{N} ||x_i - V_q \lambda_i||^2$$

•
$$\lambda_i = V_q^T x_i$$

• Now given λ we want to find V_q :

$$\sum_{i=1}^{N} ||x_i - V_q V_q^{\mathsf{T}} x_i||^2$$

- $V_q V_q^T = H_q$ is a projection matrix that maps x_i onto the space spanned by columns in V_q (this btw looks a lot like regression, yes?)
- The solution to the problem is the svd of $X = UDV^T$ where V_q is the first q columns of V

SVD

- $X = UDV^T$ where U is a $n \times p$ matrix, D is a diagonal $p \times p$ matrix and V is a $p \times p$ matrix where $U^T U = I$, $V^T V = I$
- We can also write VX = UD
- UD are called the principal components
- *VX* is the rotation *V* applied to the data *X* to project it onto the principal component space.
- The entries of each column in V are called *loadings* and tell you how much each original variable contribute to the make-up of the new dimension in PC space
- The leading components in V correspond to the largest values of D

SVD

• Another way of looking at SVD is building a structure from orthogonal components. To see this write

$$X = UDV^{T} = \sum_{j=1}^{P} d_j u_j v_j^{T}$$

where u_j is a $n \times 1$ vector and v_j^T is a $1 \times p$ vector.

- Each produce $u_j v_j^T$ construct a $n \times p$ matrix representation of X
- Scaled by d_j they represent approximation of X in orthogonal directions.
- The first component is the best rank 1 approximation of X

SVD

• Best rank q approximation

$$X_q = \sum_{j=1}^q d_j u_j v_j^T$$

with approximation error

$$||X - X_q||^2 = ||\sum_{j=q+1}^p d_j u_j v_j^T||^2 = \sum_{j=q+1}^p d_j^2$$

SVD AND REGRESSION

Least squares modeling

$$\min_{\beta} ||Y - X\beta||^2$$

- The LS solution $\beta = (X'X)^{-1}X'Y$
- If we plug in $X = UDV^T$ in the above expression we get

$$\beta = (VDU'UDV')^{-1}VDU'Y =$$

 $= (VD^{2}V')^{-1}VDU'Y = VD^{-2}V'VDU'Y = VD^{-1}U'Y$

- The expression $VD^{-1}U'$ is called the *pseudo-inverse* of X
- Notice then that the regression coefficients are really obtained through SVD
- Fitted values $\hat{y} = X\hat{\beta} = UDV'VD^{-1}U'Y = U(U'Y)$
- U is the ortogonal basis the spans the columns of X and regression projects onto these components

- In classification with LDA we sphered the data using U
- We classified using the manahalobis distance

$$c(x) = rgmin_c (x-\mu_c)' \Sigma^{-1} (x-\mu_c)$$

- We could write $X'X/n = \hat{\Sigma} = (VD^2V')/n$
- And so we can write

$$c(x) = \arg\min_{c} (V'(x - \mu_{c}))' D^{-2} (V'(x - \mu_{c}))$$

• Since the matrix *D* is diagonal, the sphered data is much easier to work with - just look at one "variable" at a time in this space

- X = UDV' = RV' where R = UD
- We can write the ridge-regression estimate as

$$\beta_r = (X'X + \lambda I)^{-1}X'y = V(R'R + \lambda I)^{-1}R'y$$

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- So β_r is $V\theta$ where θ is the ridge-regression on R instead of X
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- SVD is a component in many methods as you saw above
- We can also use it for data exploration
- We plot the principal components XV = UD for the leading components and since these preserve most of the information in X we get a dense summary of the data
- Excellent for finding groups in the data
- The loadings in V tells you in which variable set the information about X resides
- If PC1 and PC2 separates groups in the data, check which variables contribute to these (loadings in the 1st columns of V)

- Like in regression, it is not always easy to see which variables contribute to the PCs
- We can look for large factor loadings....
- OR we can adapt SVD to generate sparse V where only few variables do contribute

- A couple of different variants of sparse SVD have been proposed
- ScotLASS (Joliffe et al), sparse PCA (Witten et al) and sparse SVD (Zou et al) are a few
- They add an L1 penalty to the factor loadings, but how the problem then is solved is different

SPARSE SVD

- We want to find a sparse SVD
- Let's for now assume we have X = UDV' and call the principal components Z = UD and the loadings are in V
- Let's look at the *i*th PC $Z_i = U_i D_{ii}$
- Ridge-penalty

$$\min_{\beta} ||Z_i - X\beta||^2 + \lambda ||\beta||^2$$

• Solve the ridge-problem

$$\beta_r = (X'X + \lambda I)^{-1} X' U_i D_{ii} = V (D^2 + \lambda I)^{-1} V' V D U' U_i D_{ii} =$$
$$= V (D^2 + \lambda I) D U' U_i D_{ii} = V_i \frac{D_{ii}^2}{D_{ii}^2 + 1}$$

• Which means that $V_i = \beta_r / ||\beta_r||$

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• Recall the elastic net formulation

$$||Y - X\beta||^2 + (1 - \alpha)\lambda||\beta||^2 + \alpha\lambda||\beta||$$

- Now we add the L1 penalty to the above to get sparse loadings
- Of course, in this formulation we needed to already have the SVD iterative method.

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${\rm sparse}~{\rm SVD}$

• Alternatively, write the whole problem as follows

$$\sum_{i=1}^{N} ||x_i - AB^T x_i||^2$$

where A'A = I and $B \propto V$ and elastic net penalty on B

- B = A and $\lambda = 0$ this is just the standard PCA problem min $||X - AA^T X||^2$
- We will solve for A with B fixed and v.v.
- Given A, we solve for B using elastic net

$$\min_{B} ||X - XBA^{T}||^{2} + pen(B) = ||XA*||^{2} + ||XA - XB||^{2} + pen(B)$$

where A* orthornormal to A.

This is just a bunch of independent elastic-net problems!!

• B given A

$$\min_{A} ||X - (XB)A^T||^2$$

• B given A

$$\min_{A} ||X - (XB)A^T||^2$$

- That is, find the rotation A to make the data sets X and XB as similar as possible
- This is also solved by an SVD
- Let $SVD(X'(XB)) = UDV^T$ then $A = UV^T$ is the best rotation.
- And not we iterate until convergence

- PMA package and nsprcomp package
- Difficult to choose how much to penalize
- but good for visualization and exploration

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- We can visualize large data set by looking at the leading principal components
- SOM self-organizing maps is a very different way of looking at data
- We construct an artificial lower dimensional space where to explore the data

Self-organizing maps

- We construct a rectangular grid of prototypes m_j
- The prototypes live in the higher p-dim space but are parameterized by grid-points in a (usually) 2-dim space
- We can initialize with m_j in the two-dimensional space from the leading PC - i.e. draw up a rectangular grid in the PC1-PC2 plot and let m_j be the grid-coordinate points.
- We're now going to update the prototypes to better summarize the data, which corresponds to bending the PC plane to be able to map it to a rectangular grid.
- For each observation *x_i* we find the closest (euclidean distance) prototype *m_i*
- For all neighbors (on the grid) m_k of m_j we move them toward x_i (in p-space):

$$m_k = m_k + \alpha (x_i - m_k)$$

• α is the learning rate

- We can be a bit more clever with the updating, taking neighborhood distance into account
- We can also use *supervised* techniques, where some variables (dimensions) matter more in the distance calculation and other distance metrics can be used (more appropriate for categorical data).
- PRO: simple to use and interpret and customize (distance metrics to use)
- CON: need to revisit data points in update so problem with big n. May not be sufficient to visualize data in 2 dimensions when p is large

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