MSA220/MVE440 STATISTICAL LEARNING FOR BIG DATA LECTURE 11

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

- Past lectures: SVD, PCA, SOM
- Today: 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

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

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• We approximate the matrix by a sum over layers!

- SVD does explain matrices as best possible (in terms of L2 error)
- But difficult to interpret!
- Sparsity *can* help but that depends on the actual "true" sparsity of the data
- The sum of layers is also difficult to interpret since the loadings can be both positive and negative

- The 1st component is usually very close to an average
- E.g. average 16*16 digit image looks like a bunch of blurry superimposed digits
- To approximate a particular digit you add and subtract blurry versions of each digit correcting for "mistakes" in each layer

• The problem is that we insisted on an orthogonal transformation

- What is the idea of layer summation is our key feature?
- Each layer should add some information to the representation (not correct previous layers)

• NMF:

$$X = WH, W \ge 0 H \ge 0$$

- X is our $n \times p$ matrix where each row is an observation and each column a feature
- W is a $n \times r$ matrix, or *basis* which gives you the coordinates for each of the *n* observations in the lower-dimensional space....
- ... indexed by *H*: a $r \times p$ matrix of coefficients, or a *codebook*.

• NMF:

$X = WH, W \ge 0 H \ge 0$

- Example from the handwritten digits: Let's say we choose to approximate the data with rank ${\it K}$
- *H* will contain *K* images of the same size as each original digit, illuminating important pixels that summarize the data
- *W* is a matrix where each row *j* tells you how to combine the images in *H* to recreate the *j*th digit in the data set.

- Both SVD and NMF try to find a linear dimension reduction of the data to summarize the data well
- The difference lies in the assumed structure of the dimension reduction
- SVD creates orthogonal components (perhaps sparse)
- NMF creates component-wise non-negative coefficients and basis elements.
- NMF applied to non-negative data (but you can translate or run NMF separately on positive and negative data,....etc)

- Let's say we have found a rank K approximation
- We can approximate the *j*th observation by

$$\hat{X}_j \sum_{l=1}^{K} W_{jl} H_{l.}$$

- Since we have a non-negative contraint on *W* and *H* this consists of adding layers together, no corrections or subtractions.
- The result of the non-negative constraint is that the coefficients in *H* tend to be *sparse*!!!

- How do we obtain the NMF representation?
- Several algorithms exist
- First, just think about how the problem is written (with L2-loss there are other options here)

$$\min_{W,H} ||X - WH||^2 \quad W \ge 0, \quad H \ge 0$$

• This kind of looks like regression...

$$\min_{W,H} ||X - WH||^2 \quad W \ge 0, \quad H \ge 0$$

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- The above problem is NP hard
- We use starting values and iterative procedures
- Converges to stationary points

$$\min_{W,H} ||X - WH||^2 \quad W \ge 0, \quad H \ge 0$$

- The above problem is ill-posed
- Many solutions equally good.
- Careful about reading too much into explicit form of W and H

- Impose more structure on these: sparsity or other regularization
- Also tricky to choose the rank K application dependent

$$\min_{W,H} ||X - WH||^2 = \sum_{j=1}^{p} H'_j(W'W)H_j - 2H_j(W'X_j) + ||X_j||^2$$

- Turned into p separate non-negative LS problems
- These can be solved in several ways
- The problem is symmetric in W and H
- Two-block coordinate descent update H given W and W given H

• Let
$$F(W, H) = ||X - WH||^2$$

• First order optimality conditions

$$W \ge 0: \nabla_W F = WHH^t - XH^t \ge 0, W * \nabla_W F = 0$$
$$H \ge 0: \nabla_H F = W^t WH - W^t X \ge 0, H * \nabla - HF = 0$$

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where * is component-wise multiplication

- Multiplicative method (Lee and Seung, 1999)
- From the first order conditions we can obtain updates as

$$W * \frac{XH^{t}}{WHH^{t}}$$
$$H * \frac{W^{t}X}{W^{t}WH}$$

• It's just a gradient based update since

$$W * \frac{XH^{t}}{WHH^{t}} = W - \frac{W}{WHH^{t}} * \nabla_{W}F$$
$$H * \frac{W^{t}X}{W^{t}WH} = H - \frac{H}{W^{t}WH} * \nabla_{H}F$$

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- Alternating least squares
- Just iterate LS keeping W fixed and then H fixed
- negative elements are projected onto the nonnegative solution (set to 0)
- Fast and simple
- Tricky if we want to use more complicated regularizations, then most people use multiplicative updates

• ANNLS - slower but works well in practice

• How to start off the computation?

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- SVD solution
- Clustering solution for ${\boldsymbol W}$
- Random starts

- 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

- What's good and bad about SOMS?
- 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

- MDS: only use the pairwise distances so cheaper updates
- MDS: not restricted to 2-dim space

- We compute all the pairwise distances between objects *i* and *j*: *d_{ij}*
- We can be clever about using appropriate distances here depending on the variable types (daisy package in R)
- We want to find observations z_i in a low-dimensional space such that

$$\sum_{i \neq i'} (d_{ii'} - ||z_i - z_{i'}||)^2$$

is small.

- We can scale the mapping distance by $d_{ii'}$ which preserved small distances better
- We can also use rank-based mapping (called non-metric scaling) depending if subsets of data are very spread out.

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