Chapter 6

Matrix Factorization Methods

Note: The reader may find it useful to review Section 3.2 before continuing.

This chapter covers one of the more popular RS methods, matrix factorization. The overall theme will be *low-rank approximation*: given a matrix M_1, find a matrix M_2 for which

$$rk(M_2) << rk(M_1) \tag{6.1}$$

and

$$M_2 \approx M_1 \tag{6.2}$$

This is important for *dimension reduction*. In RS, our ratings matrix may have hundreds of millions of rows and millions of columns, which presents both computational and overfitting problems.

To set the stage, we start with a more basic matrix operation, PCA.

6.1 An Approach to Approximate Rank: Principal Components Analysis

Suppose the matrix in (3.1) had been

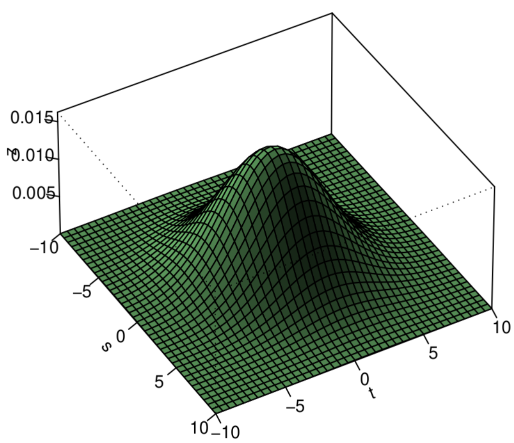
$$M = \begin{pmatrix} 1 & 5 & 1 & -2 \\ 8.02 & 2.99 & 2 & 8.2 \\ 9 & 8 & 3 & 6 \end{pmatrix} \tag{6.3}$$

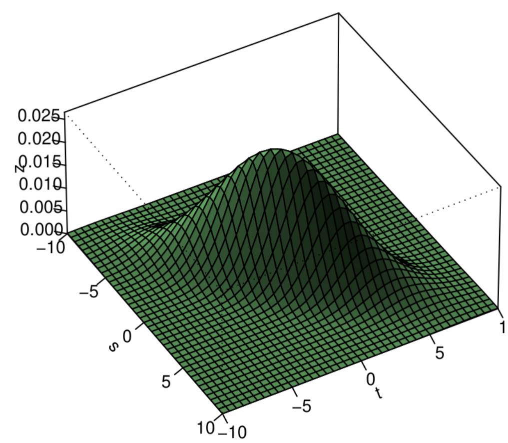
Intuitively, we still might say that the rank of M is "approximately" 2. So row 3 still seems redundant, Let's formalize that, leading to one of the most common techniques in statistics/machine learning.

The reason this is of interest is dimension reduction. We would like to reduce our feature set from p variables to s, with $s << p$, with the goal of avoiding overfitting.

6.1.1 Exploiting Correlations

Statistically, the issue is one of correlation. In (6.3), the third row is highly correlated with (the sum of) the first two rows. To explore the correlation idea further, recall our two graphs of bivariate normal densities from Section 4.4.2:





The two plots were for a low-correlation (0.2) distribution and a high-correlation (0.8) one. As we said at the time about the latter:

> The probability that $X_2 \approx X_1$ is high. So, to a large extent, there is only one variable here, X_1 (or other choices, e.g. X_2), not two.

In the case of correlation 0.2, the two variables are more separate. The probability that $X_2 \approx -X_1$ is lower here.

Note one more time, though, the approximate nature of the approach we are developing. There really *are* two variables even in that correlation 0.8 example. By using only one of them, **we are relinquishing some information. But with the need to avoid overfitting, use of the approximation may be a net win for us.**

Well then, how can we determine a set of near-redundant variables, so that we can consider omitting them from our analysis? Let's look at those graphs a little more closely.

Any *level set* in the above graphs, i.e. a curve one obtains by slicing the bells parallel to the (t_1, t_2) plane, can be shown to be an ellipse. As noted, the major axis of the ellipse will be the line $t_1 + t_2 = 0$. The minor axis will be the line perpendicular to that, $t_1 - t_2 = 0$. That suggests forming new variables,

$$W_1 = X_1 + X_2 \tag{6.4}$$

and

$$W_2 = X_1 - X_2 \tag{6.5}$$

In fact, taking

$$A = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{6.6}$$

in (4.21) shows that $\rho(W_1, W_2) = 0$.

Here is the point so far:

- The high value of $\rho(X_1, X_2)$ suggests that for this dataset, "one variable is enough." Thus we might consider using just X_1 rather than X_1 and X_2.
- Or, we might consider using W_1 for our one variable.

Now suppose we have p variables, $X_1, X_2, ..., X_p$, not just two. If our data is on people, these variables may be height, weight, age, blood glucose level, and so on, i.e. $X =$ (height, weight, age, blood glucose level,...)'.

X is different for each person, so it is a random vector. Let C denote the $p \times p$ covariance matrix of X.

Note: In our data, we will have n people, each of which has a different value of the vector X. Our data is then a matrix (or data frame) of p columns, with the value of X for person i in column i. If we call the R function **cov()** on that matrix, we get $\widehat{C}$, the estimate of C.

We want to create a new 4-dimensional random vector $W = (W_1, W_2, W_3, W_4)'$, with each W_i being some linear combination of X_1, X_2, X_3 and X_4.

We can no longer visualize in higher dimensions, but one can show that the level sets will be p-dimensional ellipsoids. These now have p axes rather than just two, and we can define our W_i is such a way that

(a) The W_i are uncorrelated.

(b) They are ordered in terms of variance:

$$Var(W_1) \geq Var(W_2) \geq ... \geq Var(W_p) \tag{6.7}$$

Now we have a promising solution to our dimension reduction problem. In (b) above, we can choose to use just the first few of the W_i, omitting the ones with small variance since they are essentially constants, uninformative. And again, since the W_i will be uncorrelated, we are eliminating a source of possible redundancy among them; after all, we are doing dimension reduction, i.e. we wish to reduce the number of variables, so we don't want any redundant ones.

PCA won't be a perfect solution — there is no such thing — as might be the case if the relations between variables is nonmonotonic. A common example is age and income, with mean income given age tending to be a quadratic (or higher degree) polynomial relation. But PCA is a very common "go to" method for dimension reduction, and may work well even in (mildly) nonmonotonic settings.

Note too that although we've motivated things here with multivariate normal distributions, we haven't assumed it. We are merely talking about finding a set of uncorrelated variables that are linear functions of our original ones.

Now, how do we find these W_i?

6.1.2 Eigenanalysis

So, we are interested in finding new variables that are linear combinations of our original ones. Let's look at the first one. We want to choose u to maximize

$$Var(u'X) = u'Cu \tag{6.8}$$

where we have used (4.21) with $A = u'$.

Of course, this maximization problem doesn't make sense in the form stated, since we can just make u larger and larger to make $Var(u'X)$ large. We need a constraint, say norm 1, $u'u = 1$.

This calls for the method of *Lagrange multipliers.* We redefine that problem as maximizing

$$u'Cu - \omega(u'u - 1) \tag{6.9}$$

where ω is an artificial variable that enforces the constraint. Then

$$\frac{d}{du}[u'Cu - \omega(u'u - 1)] = 2Cu + 2\omega u \tag{6.10}$$

Setting this to 0, we have

$$0 = (C - \omega I)u \tag{6.11}$$

In other words,

$$Cu = \omega u \tag{6.12}$$

Aha! The vector u would have to be an eigenvector of C.

Let's call that vector u_1. Then what about the second linear combination, u_2? Again we would find u to maximize

$$Var(u'X) = u'Cu \tag{6.13}$$

with the constraintt

$$u'u = 1 \tag{6.14}$$

but now with the additional constraint that we want u_2 to be uncorrelated with u_1. Using (4.21), that means

$$u'u_1 = 0 \tag{6.15}$$

Using two-variable Lagrange, we would find that u_2 is also an eigenvector of C.

Say we have a sample of n observations on p variables, say p measurements on each of n people. The measurements are $X_1, ..., X_p$. For example, we might have $p = 3$, with $X_1,\ X_2,$ and X_3 being height, weight and age.

Let C denote the covariance matrix of $X_1, ..., X_p$. Note that since $Cov(X_i, X_j) = Cov(X_j, X_i)$, the matrix C is *symmetric*,

$$C' = C \tag{6.16}$$

Another way of looking at the above derivation:

It can be shown[1] that any symmetric matrix has real (not complex) eigenvalues, and that the corresponding eigenvectors $U_1, ..., U_p$ are *orthogonal*,

$$U_i' U_j = 0, \; i \neq j \tag{6.17}$$

We always take the U_i to have length 1: Just divide the vector by its length, so it now has length 1, and is still an eigenvector.

Let U denote the $p \times p$ matrix whose i^{th} column is U_i. Then from the orthogonality of the eigenvectors, we have

$$U'U = I \tag{6.18}$$

so

$$U^{-1} = U' \tag{6.19}$$

where Iis the $p \times p$ identity matrix. We also refer to U as *orthogonal*, for this property.

It also can be shown that

$$UCU' = D \tag{6.20}$$

where D is a diagonal matrix with the eigenvalues of C on the diagonal.

$X = (X_1, ..., X_p)'$ is a random vector, i.e. different for each person or other entity in the population. Now, form a new random vector from X:

$$W = UX \tag{6.21}$$

[1] Here and below, "can be shown" means that the assertion is proved in any standard textbook on linear algebra.

Let's find its covariance matrix, again using (4.21):

$$Cov(W) = UCU' = D \tag{6.22}$$

Aha! The components of this new random vector are uncorrelated! Just what we need. And that gives us PCA:

6.1.3 PCA

- Find the (sample) covariance matrix of X in our data.
- Diagonalize as above, yielding U and D.
- Reorder D so that the eigenvalues are in nonincreasing order. Reorder the rows of U accordingly.
- We are doing dimension reduction, reducing from p. Decide the new dimension s.
- Replace U by its first s rows.
- We've created a new random vector $W = UX$, with the new U. W will have length s, thus achieving dimension reduction.

So for example, denote the k^{th} value of X in our original dataset, i.e. column k, by $X^{(k)}$. The corresponding new vector is $W^{(k)} = UX^{(k)}$. When dealing with a new case $X^{(\text{new})}$ in the future, premultiply by U to get the W value.

6.1.4 Choosing the Number of Principal Components

The number of components we use, s, is a hyperparameter. So, how do we choose s?

First one must ask what the goal of PCA is in the given application. It might be simply descriptive; if we can reduce some complex set of variables down to a few while losing only a small amount of information, those remaining variables may give us insight into the underlying workings of the process being studied.

For this goal, the (rather) standard approach is "proportion of total variance"; s is chosen so that

$$\sum_{j=1}^{s} \lambda_j \tag{6.23}$$

is "most" of total variance (that total is the above expression with p instead of s), but even this is usually done informally.

In ML/RS settings, though, s is typically chosen by cross validation. Say we are predicting Y from $X = (X_1, ..., X_p)'$, using a linear model. We fit such a model, predicting Y from W_1 alone; then we predict Y from only W_1 and W_2, use then $s = 3$, then 4 and so on. In each case, we look at our prediction accuracy in our holdout set. In the end, we use the value of s that gives the best accuracy. The **qePCA()** function does this.

6.1.5 Software and UCI Repository Example

The most commonly used R function for PCA is **prcomp()**. As with many R functions, it has many optional arguments; we'll take the default values here.

For our example, let's use the Turkish Teaching Evaluation data, available from the UC Irvine Machine Learning Data Repository. It consists of 5820 student evaluations of university instructors. Each student evaluation consists of answers to 28 questions, each calling for a rating of 1-5, plus some other variables we won't consider here.

```
> turk <- read.csv('turkiye-student-evaluation.csv',header=T)
> head(turk)
  instr class nb.repeat attendance difficulty Q1 Q2 Q3 Q4
1     1     2         1          0          4  3  3  3  3
2     1     2         1          1          3  3  3  3  3
3     1     2         1          2          4  5  5  5  5
4     1     2         1          1          3  3  3  3  3
5     1     2         1          0          1  1  1  1  1
6     1     2         1          3          3  4  4  4  4
  Q5 Q6 Q7 Q8 Q9 Q10 Q11 Q12 Q13 Q14 Q15 Q16 Q17 Q18 Q19
1  3  3  3  3  3   3   3   3   3   3   3   3   3   3   3
2  3  3  3  3  3   3   3   3   3   3   3   3   3   3   3
3  5  5  5  5  5   5   5   5   5   5   5   5   5   5   5
4  3  3  3  3  3   3   3   3   3   3   3   3   3   3   3
5  1  1  1  1  1   1   1   1   1   1   1   1   1   1   1
6  4  4  4  4  4   4   4   4   4   4   4   4   4   4   4
  Q20 Q21 Q22 Q23 Q24 Q25 Q26 Q27 Q28
1   3   3   3   3   3   3   3   3   3
2   3   3   3   3   3   3   3   3   3
3   5   5   5   5   5   5   5   5   5
4   3   3   3   3   3   3   3   3   3
5   1   1   1   1   1   1   1   1   1
```

```
6   4   4   4   4   4   4   4   4   4
> tpca <- prcomp(turk[,-(1:5)]
```

Let's explore the output. First, the standard deviations of the new variables:

```
> tpca$sdev
 [1] 6.1294752 1.4366581 0.8169210 0.7663429 0.6881709
 [6] 0.6528149 0.5776757 0.5460676 0.5270327 0.4827412
[11] 0.4776421 0.4714887 0.4449105 0.4364215 0.4327540
[16] 0.4236855 0.4182859 0.4053242 0.3937768 0.3895587
[21] 0.3707312 0.3674430 0.3618074 0.3527829 0.3379096
[26] 0.3312691 0.2979928 0.2888057
> tmp <- cumsum(tpca$sdev^2)
> tmp / tmp[28]
 [1] 0.8219815 0.8671382 0.8817389 0.8945877 0.9049489
 [6] 0.9142727 0.9215737 0.9280977 0.9341747 0.9392732
[11] 0.9442646 0.9491282 0.9534589 0.9576259 0.9617232
[16] 0.9656506 0.9694785 0.9730729 0.9764653 0.9797855
[21] 0.9827925 0.9857464 0.9886104 0.9913333 0.9938314
[26] 0.9962324 0.9981752 1.0000000
```

This is striking. The first principal component (PC) already accounts for 82% of the total variance among all 28 questions. The first five PCs cover over 90%. This suggests that the designer of the evaluation survey could have written a much more concise survey instrument with almost the same utility.

Now keep in mind that each PC here is essentially a "super-question" capturing student opinion via a weighted sum of the original 28 questions. Let's look at the first two PCs' weights:

```
> tpca$rotation[,1]
        Q1         Q2         Q3         Q4         Q5
-0.1787291 -0.1869604 -0.1821853 -0.1841701 -0.1902141
        Q6         Q7         Q8         Q9        Q10
-0.1870812 -0.1878324 -0.1867865 -0.1823915 -0.1923626
       Q11        Q12        Q13        Q14        Q15
-0.1866948 -0.1862382 -0.1922729 -0.1911814 -0.1902380
       Q16        Q17        Q18        Q19        Q20
-0.1962885 -0.1808833 -0.1935788 -0.1927359 -0.1931985
       Q21        Q22        Q23        Q24        Q25
-0.1911060 -0.1908591 -0.1948393 -0.1931334 -0.1888957
       Q26        Q27        Q28
-0.1908694 -0.1897555 -0.1886699
```

```
> tpca$rotation[,2]
         Q1          Q2          Q3          Q4          Q5
 0.35645673  0.23223504  0.11551155  0.24533527  0.20717759
         Q6          Q7          Q8          Q9         Q10
 0.20075314  0.24290761  0.24901577  0.12919618  0.18911720
        Q11         Q12         Q13         Q14         Q15
 0.11051480  0.21203229 -0.10616030 -0.15629705 -0.15533847
        Q16         Q17         Q18         Q19         Q20
-0.04865706 -0.26259518 -0.12905840 -0.15363392 -0.19670071
        Q21         Q22         Q23         Q24         Q25
-0.22007368 -0.22347198 -0.10278122 -0.06210583 -0.20787213
        Q26         Q27         Q28
-0.12045026 -0.07204024 -0.21401477
```

The first PC turned out to place approximately equal weights on all 28 questions. The second PC, though, placed its heaviest weight on Q1, with substantially varying weights on the other questions.

While we are here, let's check that the columns of U are orthogonal.

```
> t(tpca$rotation[,1]) %*% tpca$rotation[,2]
              [,1]
[1,] -2.012279e-16
```

Yes, 0 (with roundoff error). As an exercise in matrix partitioning, the reader should run

```
t(tpca$rotation) %*% tpca$rotation
```

then check that it produces the identity matrix I, then ponder why this should be the case.

6.1.6 More on the PC Coefficients

There is more to consider.

Do the PC coefficients have any interpretation? The answer is probably no for ordinary people, but for the *domain experts*, very possibly yes. In the teaching evaluation example above, a specialist in survey design or teaching methods may well be able to interpret the dominance of Q1 in the second PC. A method called *factor analysis*, an extension of PCA, is popular in social science research.

For the rest of us, PCA is just a handy way to do dimension reduction.

But there is geometric terminology that will be helpful, as follows. Let's look at the **mlb** dataset from the **regtools** package. This is data on Major League baseball players.

```
             Name Team       Position Height Weight   Age
1   Adam_Donachie  BAL        Catcher     74    180 22.99
2       Paul_Bako  BAL        Catcher     74    215 34.69
3 Ramon_Hernandez  BAL        Catcher     72    210 30.78
4    Kevin_Millar  BAL  First_Baseman     72    210 35.43
5     Chris_Gomez  BAL  First_Baseman     73    188 35.71
6   Brian_Roberts  BAL Second_Baseman     69    176 29.39
  PosCategory
1     Catcher
2     Catcher
3     Catcher
4   Infielder
5   Infielder
6   Infielder
```

Let's apply PCA:

```
> hw <- as.matrix(mlb[,4:5])
> pcout <- prcomp(hw)
> pcout$rotation
               PC1         PC2
Height -0.05948695  0.99822908
Weight -0.99822908 -0.05948695
```

If we were to plot **hw**, we would put **hw[1,]** at the point (74,180) on our graph. Recall from high school math that 74 and 180 are called the *coordinates* of **hw2[1,]**, with respect to our "H axis" and "W axis."

But in doing PCA, we are creating new axes, PC1 and PC2, which are rotated versions of the H and W axes. (Hence the naming of the U matrix as "rotation" in the **prcomp()** return value.) Let's find the coordinates of **hw[1,]** with respect to the new axes:

```
> hw[1,] %*% pcout$rotation
           PC1     PC2
[1,] -184.0833 63.1613
```

So (74,180) has become (-184.1,63.2) under the new coordinate system. Let's see what the angle of rotation is. We can do that by seeing where a point on the H axis rotates to.

```
> pc10 <- c(1,0) %*% pcout$rotation
> pc10
             PC1       PC2
[1,] -0.05948695 0.9982291
```

```
> (atan(pc10[2] / pc10[1])) * 180/pi
[1] -86.58964
```

Almost 90 degrees clockwise.

6.1.7 Scaling

Some analysts prefer to *scale* the data before applying PCA. For each column, we would subtract the column mean and divide by the column standard deviation. The column would now have mean 0.0 and variance 1.0.

The rationale for doing this is that if PCA is applied to the original data, variables with large variance will dominate. And then units would play a role; e.g. a distance variable would have more impact if it were measured in kilometers than miles.

Scaling does solve this problem, but its propriety is questionable. Consider a setting with two features, A and B, independent, with variances 500 and 2, respectively, and with mean 100 for both. Let A' and B' denote these features after centering and scaling.

As noted, PCA is all about removing features with small variance, as they are essentially constant. If we work with A and B, we would of course use only A. But if we work with A' and B', we would use both of them, as they both have variance 1.0.

So, dealing with the disparate-variance problem (e.g. miles vs. kilometers) shouldn't generally be solved by ordinary scaling, i.e. by dividing by the standard deviation. An alternative is to divide each column by its mean. This addresses the miles-vs.-kilometers problem, and makes sense in that a variance is large or small in relation to its mean.

6.2 SVD

The *Singular Value Decomposition* (SVD) is a generalization of PCA. It has many applications, but will be especially valuable for us in RS, as it can factor our ratings matrix into the product of a user matrix and an item matrix.

6.2.1 The Decomposition

Let A be any matrix, not necesarily square. In fact, it is nonsquare in typical applications, RS being a case in point. Let n and m denote the numbers of rows and columns of A. Then there exist matrices U, D and V such that

$$A = UDV' \tag{6.24}$$

where:

- The dimensions of U, D and V are $n \times n$, $n \times m$ and $m \times m$.
- U and V are orthogonal matrices, so that $UU' = I$ and $V'V = I$.
- D is a diagonal matrix in the sense that $D_{ij} = 0$ whenever $i \neq j$. The diagonal elements are the *singular values*. Let d_i denote the i^{th} diagonal element in D, $i = 1, 2, ..., \min(n, m)$. One can construct the matrices so that the singular values are nonnegative.

By permuting the rows and columns of A, e.g. in MovieLens, permuting the order of the users, and that of the movies, we can arrange things so that the singular values appear in descending order. We'll assume that here.

Let u_i and v_i denote the i^{th} row in U and V, respectively. By expanding the multiplication in (6.24), we have

$$A = \sum_{i=1}^{\min(n,m)} d_i u_i v_i' \tag{6.25}$$

6.2.2 Low-Rank Approximation

Equation (6.25) then suggests how to accomplish dimension reduction. Remember, the d_i are decreasing.[2] The last few may be really tiny, so we can delete those terms, just as we deleted the principal components with small variances.

Say we retain the first r terms, with $r < \min(n, m)$. That is equivalent to

- Retaining the $r \times r$ "northwest corner" of D.
- Retaining the first r columns of U.
- Retaining the first r columns of V.

[2]Technically, nonincreasing, but typically there are no cases of equality.

Result:

- The new U, D and V will now be of dimensions $n \times r$, $r \times r$ and $m \times r$.
- The new product UDV' will still have dimensions $n \times m$, the same as A. But, whereas we had

$$A = UDV' \tag{6.26}$$

before, we now have

$$A \approx UDV' \tag{6.27}$$

- The new UDV' will have rank r, hence the term *low-rank approximation*. In fact, it can be shown to be the best rank-r approximation to A, in the sense that the Frobenius norm (Section 3.3) of the difference is minimized:

$$UDV' = \arg\min_{Q} \|A - Q\|_F \tag{6.28}$$

over all $n \times m$ matrices Q having rank r.

6.2.3 Back to RS

Since D is a diagonal matrix with nonnegative diagonal entries, it has a square root, which we will denote as $D^{0.5}$—to obtain the square root matrix, take the square of each diagonal value. Then

$$A \approx (UD^{0.5})(D^{0.5}V') \tag{6.29}$$

So to obtain our desired factorization $A \approx WH$, we simply set

$$W = UD^{0.5}, \ H = D^{0.5}V' \tag{6.30}$$

In our RS context, the ratings matrix A has missing values. How can we find U, D and V?

If the proportion of missing values is low, as in our House Voting data, we can apply SVD to the intact rows of A, then treat the remaining rows as new cases to be predicted (Section 6.3.5 below).

Otherwise, the answer is that numeric methods exist to find the approximate SVD, based on the non-NA elements of A. They involve optimization of certain complicated quantities, using a nonlinear optimization technique. One such technique is *Stochastic Gradient Descent* (SGD), an iterative workhorse method in machine learning. It essentially sets derivatives to 0 and solves, but with various refinements. Of course, U, D and V will then turn out to be different from what they would be if A were intact.

6.3 General Issues with Matrix Factorization Methods

There are many refinements of the SVD approach described above, and indeed many other ways to achieve approximate factorization. We'll discuss other methods, later in this chapter.

In all methods, we have

$$A \approx WH \tag{6.31}$$

where W is of dimensions $n \times r$, H is of dimensions $r \times m$, and both matrices are of rank r. There are several issues to discuss.

6.3.1 Bias, Variance and Overfitting

There are nr numbers in W, and rm in H. Treating our data as a sample from a conceptual population—e.g. all moviegoers and all movies—estimating only $r(n+m)$ values is much better than estimating the much larger nm ones.

But this depends on r, which is our tuning parameter/hyperparameter for this method. We have a classical tradeoff:

As r grows, the variance increases, due to estimating more parameters, but the bias decrases. As usual, typically r is chosen by cross-validation.

6.3.2 Regularization

To some analysts, "If it's random, then shrink it." Matrix factorization is no exception. In the context here, that means shrinking both W and H, and we choose them to minimize

$$\|A - WH\|_F + \gamma_1 \|W\|_F^2 + \gamma_2 \|H\|_F^2 \tag{6.32}$$

6.3.3 "Bias" Removal

In machine learning circles, the term *bias* as a second, unrelated meaning beyond the "bias-variance tradeoff" context. This second meaning refers to the β_0 term in (5.4). Recall that if we have no covariates, i.e. $p = 0$ in that equation, β_0 reduces to EY, the unconditional mean of Y.

We will discuss covariates shortly, but for now the point is that it is customary to *center* the A ratings matrix by subtracting means. Let m, $m_{i.}$, and $m_{.j}$ denote the overall mean rating, the mean for user i and the mean for item j, respectively. Then the recommended approach is to first make the adjustment

$$A_{ij} \leftarrow A_{ij} - (m_{i.} + m_{.j} - m) \tag{6.33}$$

Then the factorizaiton is performed, and finally the adjustment is "undone":

$$A_{ij} \leftarrow A_{ij} + (m_{i.} + m_{.j} - m) \tag{6.34}$$

What is going on here? First, the expression

$$m_{i.} + m_{.j} - m \tag{6.35}$$

is motivated by the equivalent

$$m + (m_{i.} - m) + (m_{.j} - m) \tag{6.36}$$

which models the ratings as

overall mean + effect due to user i + effect due to item j

(Readers who are familiar with the *analysis of variance* should recognize this.) The idea is then to do our matrix factorization on the *residual*, i.e. what is "left over" after prediction by the model (6.36).

6.3.4 Dealing with Covariates

Why stop with just removing "biases"? We can go a step further and account for user or item covariates.

The easiest approach to handling covariates is again to subtract (and later add back) residuals, in this case those arising from a linear or other regression model. One would first put the data in (user ID, iterm ID, rating) format, then run **lm()** or whatever. Each element of A is then adjusted by subtracting the predicted value for that element. One would then perform matrix factorization to fill in the ratings matrix, then finally add the predicted values back to the result.

Another way would be to append user covariates as new columns in the A matrix, or item covariates as new rows.

6.3.5 Predicting New Cases

One drawback of matrix factorization methods is that there generally is no direct method to handle new users or new items not in the original data. One must compute the entire factorization all over again. This may not be too problematic, though, as most numerical methods are easy to update, rather than fitting from scratch.

One solution is to use a k-Nearest Neighbors analysis on the completed matrix. For a new case with ratings for a set of items, find the k rows closest to the new case, and average their ratings.

6.4 Interpretation of W and H

One of the big advantages of matrix factorization methods is interpretability.

For any matrix Q, let $Q_{i\cdot}$, $Q_{\cdot j}$, and Q_{ij} denote row i, column j, and element (i, j), respectively. Note the key relation, using the material in Section 3.2:

$$(WH)_{i\cdot} = \sum_{m=1}^{k} W_{im} H_{m\cdot} \tag{6.37}$$

In other words, in (6.37), we see that:

- The entire vector of predicted ratings by user i can be expressed as a linear combination of the rows of H.
- The rows of H can thus be thought of as synthetic "users" who are representative of users in general. H_{rs} is the rating that synthetic user r gives item s.

Of course, interchanging the roles of rows and columns above, we have that the columns of W serve as an approximate basis for the columns of A. In other words, the latter become synthetic, representative items, e.g. representative movies in the MovieLens data.

6.5 Alternating Least Squares (ALS)

Again, a general approach to finding W and H is to minimize the Frobenius norm of the approximation error:

$$W, H = \arg\min_{w,h} \|A - wh\|_F \tag{6.38}$$

Of course, minimizing that quantity is equivalent to minimizing its square, setting up a leasts-squares approach that we'll describe here. So, we wish to minimize

$$W, H = \arg\min_{w,h} \|A - wh\|_F^2 \tag{6.39}$$

As noted, we could use SGD for this. But the old saying, "Easier said than done" applies. SGD works really well for minimization of *convex* functions. Roughly, convexity means that a function is concave-up in one dimension (i.e. the function has one argument), "bowl-shaped" in two dimensions (two arguments), and the un-visualizable equivalent in multiple dimensions. Unfortunately, the function

$$f(w, h) = \|A - wh\|_F^2 \tag{6.40}$$

which has $nr + rm$ arguments, is not convex. It generally will have multiple local minima, causing possible convergence problems.

6.5.1 A Non-SGD Approach, ALS

For fixed h, the function $f(w, h)$ *is* convex. In fact, we will see below that it's our old friend from the linear model, which not only has a unique minimum but in fact has a close-form solution for the minimum! Indeed, we can use R's **lm()** function to obtain the solution. The same is true if we fix w and allow h to vary.

The *alternating least squares* approach to minimizing (6.40) exploits the fact that $f(w, h)$ is separately convex in w and h, holding one of them fixed. The algorithm is then

(1) Set an initial guess w_0 for the solution. (We won't need an initial guess for h.)

(2) Minimize $f(w_0, h)$ with respect to h, yielding our next guess, h_1.

(3) Minimize $f(w, h_1)$ with respect to w, yielding our next guess, w_1.

(4) Minimize $f(w_1, h)$ with respect to h, yielding our next guess, h_2.

(5) Repeat until convergence.

Here is more detail: In step (2) above, first write

$$f(w_0, h) = \sum_{j=1}^{n} \|A_{\cdot j} - w_0 \ h_{\cdot j}\|_F^2 \tag{6.41}$$

where $h_{0 \cdot j}$ means column j of h_0. If we can find h to minimize the j term in (6.41) for each j, then we will have minimized (6.41), achieving our goal.

But luckily this is exactly the structure we had in minimizing (5.11):

- The matrix A there is our w_0 here, known.
- The vector D there is our $A_{\cdot j}$ here, known.
- The vector b there is our $h_{\cdot j}$ here, unknown and to be solved for.

So we have

$$(h_1)_{\cdot j} = (w_0' w_0)^{-1} w_0' A_{\cdot j} \tag{6.42}$$

And again, via matrix partitioning,

$$(h_1) = (w_0' w_0)^{-1} w_0' A \tag{6.43}$$

for each j. In R code,

```
> h[,j] <- lm(a[,j] ~ w0 - 1)$coef
```

The -1 specifies that we do not want a constant term in the model, i.e. no 1s column..

On the other hand, what about step (3)?. We could take transposes,

$$A' = h'w' \tag{6.44}$$

and then just interchange the roles of w and h above. Here a call to **lm()** gives us a column of w', thus a row of w, and we do this for all rows.

6.5.2 Back to Recommender Systems: Dealing with the Missing Values

In our recommender systems setting, of course, much of A is missing. But we can easily adapt to that. Roughly speaking, in (6.41), do these replacements:

- replace $A_{\cdot j}$ by the known portion of $A_{\cdot j}$
- replace w_0 by the corresponding rows of w_0

Then proceed as before.

6.5.3 Convergence and Uniqueness Issues

There are no panaceas for applications considered here. Every solution has potential problems. I like to call this the Pillow Theorem — pound down on one fluffy part and another part pops up.

One issue with finding W and H by minimizing (6.38) is uniqueness — there might not be a unique pair (W, H) that minimizes (6.38). In fact, one can see this immediately: Doubling W while halving H leaves the product WH unchanged. Of course, the product is all that really counts, but in turn, this may result in convergence problems. Software documentation (see below) recommends running the computation multiple times; it will use a different seed for the random initial values each time.

Actually, the Alternating Least Squares method used here is considered by some to have better convergence properties, since the solution at each iteration is unique. This may come at the expense of slower convergence.

6.6 Nonnegative Matrix Factorization (NMF)

In most RS applications, the ratings are nonnegative. So, we might require that W and H be nonnegative.

6.6.1 Computation

In ALS, for instance, we might just truncate to 0 any elements in w_i and h_i that stray into negative territory.

Another popular approach is *multiplicative update*, due to Lee and Seung. Here are the update formulas for W given H and *vice versa*:

$$W \leftarrow W \circ \frac{AH'}{WHH'} \tag{6.45}$$

$$H \leftarrow H \circ \frac{W'A}{W'WH} \tag{6.46}$$

where $Q \circ R$ and $\frac{Q}{R}$ represent elementwise multiplication and division with conformable matrices Q and R, and the juxtaposition QR means ordinary matrix multiplication.

6.6.2 Why Nonnegative?

NMF makes sense since the ratings are nonnegative, and also there is hope that the resulting W and H are more likely to be sparse.

A second motivation is as follows: Matrix factorization methods have also been applied to image and text classification. Consider a facial image recognition case, say. There is hope that the nonzero elements of $W_{\cdot 1}$, say, correspond to eyes, $W_{\cdot 2}$ correspond to noses, and so on with other parts of the face. We are then "summing" to form a complete face. This may enable effective *parts-based recognition*, with helpful interpretations.

In our recommender systems setting, this parts-based effect, NMF would give us crisper distinction among the various synthetic users. This may reveal clusters of user behavior, which could be quite helpful to the analyst.

6.7 Software

Given that matrix factorization plays a major role in RS and many other applications, it's not surprising that many libraries have been developed for it.

6.7.1 The svd() Function

This is a general (i.e. not RS-specific) function to perform SVD. The function is part of base-R, and does not handle missing values. Here is an example:

```
> m
     [,1] [,2] [,3] [,4]
[1,]   15   18    5   11
```

```
[2,]    1   16   26    4
[3,]    5   12   13    5
> z <- svd(m)
> z
$d
[1] 40.9655903 18.1306964  0.3134599

$u
          [,1]        [,2]       [,3]
[1,] 0.5361629  0.80414164 -0.2566818
[2,] 0.7045689 -0.59380206 -0.3885637
[3,] 0.4648785 -0.02748343  0.8849478

$v
          [,1]       [,2]       [,3]
[1,] 0.2702611  0.6249570  0.5932112
[2,] 0.6469473  0.2561355 -0.6952051
[3,] 0.6601400 -0.6494748  0.3772584
[4,] 0.2695057  0.3492934  0.1498884
> z$u %*% diag(z$d) %*% t(z$v)
     [,1] [,2] [,3] [,4]
[1,]   15   18    5   11
[2,]    1   16   26    4
[3,]    5   12   13    5
```

6.7.2 The recosystem Package

The **recosystem** package does matrix factorization specifically for recommender systems, i.e. specifically for settings in which the matrix A has many missing values. It's written by experts in numerical matrix factorization, and features a number of useful options.

The **recosystem** authors recognized that RS systems tend to be large, with many rows and columns in a ratings matrix. Accordingly, the package does the following:

- It takes its input in the usual (user ID, item ID, rating) format, not the ratings matrix, which could be huge.
- As an option, it will stores the resulting W and H matrices as disk files, rather than writing them to memory.

The package uses R's R6 class system. This is transparent if one uses the wrapper **rectools::trainReco()**, but let's take a close look, calling the function directly.

Below is a **recosystem** session using the small MovieLens data, in the **ml100** data frame we've analyzed before.

Let's suppose we've decided on rank $k = 20$.

```
> library(recosystem)

> r <- Reco()
> class(r)
[1] "RecoSys"
attr(,"package")
[1] "recosystem"
# all action will take place within this R6 class instance; typically the
# output of a function will be stored back as a new component in r

# need to create an object of class 'DataSource', specifying which
# columns are user IDs, item IDs and ratings; here we will have the data
# in memory; see below
> ml.dm <- data_memory(ml100[,1],ml100[,2],ml100[,3],index1=TRUE)

# do the factorization, with rank 20; use NMF not SGD
> r$train(ml.dm,opts=list(dim=20,nmf=TRUE))
iter      tr_rmse          obj
   0       2.0381   5.0056e+05
   1       1.0296   1.7402e+05
   2       0.9529   1.6028e+05
   3       0.9449   1.5868e+05
   4       0.9418   1.5811e+05
   5       0.9397   1.5774e+05
   6       0.9382   1.5749e+05
   7       0.9371   1.5729e+05
   8       0.9362   1.5713e+05
   9       0.9355   1.5701e+05
  10       0.9348   1.5690e+05
  11       0.9343   1.5681e+05
  12       0.9338   1.5673e+05
  13       0.9334   1.5666e+05
  14       0.9330   1.5660e+05
  15       0.9327   1.5654e+05
```

```
  16        0.9324   1.5649e+05
  17        0.9321   1.5645e+05
  18        0.9318   1.5641e+05
  19        0.9316   1.5637e+05
# training went for 20 iterations; RMSE is the square root
# of MSPE
# for large data, write to disk; here we store in memory
> result <- r$output(out_memory(),out_memory())
> str(result)
List of 2
 $ P: num [1:943, 1:20] 0.676 0.677 0.574 0.836 0.574 ...
 $ Q: num [1:1682, 1:20] 0.712 0.614 0.568 0.645 0.612 ...
# P and Q are W and H'
> w <- result$P
> h <- t(result$Q)
# let's try a prediction, with a known rating; we can do the
# matrix multiply ourselves if we wish
> head(ml)
   V1  V2 V3        V4
1 196 242  3 881250949
2 186 302  3 891717742
3  22 377  1 878887116
...
> w[22,] %*% h[,377]
         [,1]
[1,] 2.196976
# there is a predict() method, not shown here
```

Various options are available, such as regularization parameters.

6.8 The softImpute Package

In the literature on missing values, we often sees the term *impute*, which is a fancy form of "guess." Hence the name of this package.

The package works directly on the ratings matrix A. If that matrix is too large for memory, there is an option to use the Spark system, which has an R interface **sparkr**. Spark is a highly complex system which may be difficult to install. We do not pursue that here.

The user has a choice of ALS or SVD, default value of ALS, though in both cases the algorithms used are refinements of what we see here.

Again, let's use MovieLens as an example:

```
> mlm <- rectools::buildMatrix(ml100[,-4],NAval=NA)
> library(softImpute)
> z <- softImpute(mlm,rank.max=10)  # rank 10
> mlmest <- z$u %*% diag(z$d) %*% t(z$v)
# try a known rating
> head(ml100)
   V1  V2 V3        V4
1 196 242  3 881250949
2 186 302  3 891717742
3  22 377  1 878887116
4 244  51  2 880606923
5 166 346  1 886397596
6 298 474  4 884182806
> mlm[22,377]
[1] 1
> mlmest[22,377]
[1] 1.156759
```