Networked Life: Project

The project's goal is to introduce new algorithms and techniques to provide custom recommendations to users based on what other users liked. This should remind you of the Netflix chapter, where a linear regression is used to recommend movies to a user based on a large (sparse) matrix of ratings. The chapter tells you about this big dataset that Netflix made available for scientists to play with (with added benefits for Netflix of course!) We will be using parts of this dataset for the project, allowing you to use real data and learn a few tricks that data scientists have developed over the last few years.

The project is divided in three parts:

- First, you will expand on the homework given to you for chapter 4 by reusing the code you have written previously, applying it to the Netflix training dataset. You may need to perform a few additional steps to obtain the data in the right format, but you will be guided along the way.
- Second, you will review a few concepts of Bayesian inference that will come handy when developing another algorithm to predict a user's preferences: the restricted Boltzmann machines. We will give you some theory and it will be your job to fill in the gaps in our code.

As was explained in the Networked Life book, the teams competing in the Netflix prize were given the opportunity to test their algorithms against a hidden test set. We will do the same, hiding from you a part of the dataset, and rewarding teams that perform best against the test set. There is no unique way of implementing the best algorithm, and a lot of the work is "guessing" (smartly) which parameters to use and which combination of techniques works best. Along the way, there will be tests to make sure that you have implemented the base algorithms correctly, but we also encourage you to experiment and see for yourself. Due to the popularity of the Netflix contest, a whole universe of online articles flourished, detailing the techniques used to win the contest and explaining them in a very approachable way. You may find some of these during your research, which you can take inspiration from (and duly cite in your reports!)

The project is built in a way such that you can get an early start, as soon as chapter 4's homework is completed. The three parts will be equally demanding, so we do advise you to start at this point. Both Python and some good skills in machine learning (more broadly: data science) are great to have on your resumes if you are going to pursue any career in technology. We hope this project gives you more tools to convince your dream company that you are ready for the job!

1 Linear regression on the Netflix dataset

In the folder you have downloaded containing the project, you will find in the resources subfolder the training dataset, training.csv. The CSV file can be imported in your code using the getTrainingData function in the projectLib file. Similarly, we give a validation.csv file that can be loaded with the getValidationData function.

Both files have three columns: one for the movie ID, one for the user ID and one for the rating ID, in that order. For example, a row of 5,3,4 means that user 3 has given to movie 5 a rating of 4. Note that to make the scripts (a lot) simpler, we have reindexed movies and users so that movies are $0, 1, \ldots, M$ and users are $0, 1, \ldots, U$, where M is the total number of movies and U is the total number of users.

The training data set provided can be divided in two, one part, the training set, containing 80% of the data and the other, the validation set, with 20% of the data. In this project, we give you two CSV files containing the training set and the validation set. The training set has a rating for every movie and every user in the dataset, so you will not see any new user or new movie appear in either the validation set or the test set that we keep hidden!

Question 1.1. Using the solution you have worked out in the homework for chapter 4 or the one provided, run the parameter estimation param function to compute the estimator for the training set, without regularisation. Once this is done, use the predict function to compute the predicted rating of every (movie, user) pair of the training set. You now have the real rating from the dataset $r_{m,u}$ and the one predicted by your model $\hat{r}_{m,u}$. You can compute the RMSE to compare the two.

Question 1.2. As you have seen in Chapter 4, you can regularise this model so that it does not overfit, by adding a penalty to your biases. You should now complete the param_reg function with your previous homework implementation.

In section 3, you will learn how to tune the regularisation parameter λ to optimise the performance of your model on a validation set, a good proxy for the test set.

2 The hidden patterns: predicting the rating with Restricted Boltzmann Machines

2.1 Presentation of the model

Neural networks are all the rage when it comes to training estimators on very large datasets, due to their flexibility. Our previous model was biased in the sense that we give the shape of the function we use for our estimator (the average rating plus the biases). Neural networks on the other hand are relatively agnostic when it comes to which part of the function space to explore to find the best estimator, which works especially well when the dataset is very big.

In this project we use a much simpler version of a neural network, the Restricted Boltzmann Machine (RBM). Developed by Salakhutdinov et al. for use on the Netflix dataset, it is a two layer network as shown in figure 1. The bottom layer, which we call visible layer V or input layer, receives an input, typically a piece of data (such as the ratings). The top layer, also called hidden layer H, receives a non-linear transformation of the input. The non-linear part matters because this is what allows neural networks to explore a large space of functions to find the estimator. We will present the precise model in the next section.

The edges connecting the visible layer to the hidden one are given weights W. It is in fact the end goal of the learning procedure: to find the best weights W to represent our data. By representing our data, we mean that we want at the end of our training to have one very good RBM to work with. A good RBM is one that encodes the information contained in our dataset properly, i.e is able to pick out patterns from the ratings of the users. These patterns could be anything from "Users with an odd ID number like movies with an ID ending in a 2" or

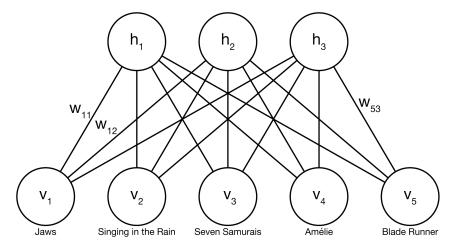


Figure 1: A restricted Boltzmann Machine with 5 visible units and 3 hidden units.

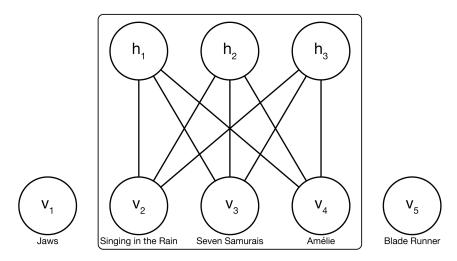


Figure 2: We only look at a part of the main RBM if the user has seen *Singing in the Rain*, *Seven Samurais* and *Amélie*, but not the other two. Only the weights inside the box will be updated when we compute the gradient for that user.

"Users who enjoyed movie i did not really like movie q", though the latter is definitely what a good RBM will find out. This good RBM corresponds to a particular choice of weights W. After training our model on the data, we get an estimator of W, similar to our previous estimation of the biases in the linear regression method.

We now explain how we will use the RBM model. Each visible unit will correspond to one unique movie. Each hidden unit will correspond to some "abstract" notion. The model is powerful because we do not need to specify what these abstract notions are. It may happen that the model will be able to separate sci-fi movies from action movies, simply by looking at the data and the associated ratings. One hidden unit may activate (more on this later) when the ratings fed to the visible layer are those of a sci-fi movie fan, and this may help predict the rating given to an unseen sci-fi movie by the same user.

The dataset we provide contains a smaller set of m movies. We call **the main RBM** one big RBM consisting of m visible units and a number F hidden units (which you can tune). Each user u has rated a subset M_u of movies. This user u will be associated with a part of the main RBM, consisting of all the hidden units and *only* the visible units corresponding to movies rated by this user. You can see some details on figure 2.

2.2 Preliminary work

We will start implementing a few functions to create the model. These functions will help us run operations that are common when using RBMs. Let $v_i, i \in V$ represent the value held by the *i*-th node of the visible layer. This value is binary, i.e it is equal to 0 or to 1. We denote a vector of inputs by $\mathbf{v} = (v_1, \ldots, v_n)$. Let $h_j, j \in H$ denote the value held by the *j*-th node of the hidden layer, also binary. The edge connecting v_i to h_j has a weight $W_{ij} \in \mathbb{R}$.

When the visible layer receives an input, this input is transformed and sent to the hidden layer, in the following way: the probability that h_j equals 1, or that h_j is on, given the visible input \mathbf{v} , is equal to

$$\mathbb{P}(h_j = 1 | \mathbf{v}) = \sigma\left(\sum_{i \in V} v_i W_{ij}\right), \text{ where } \sigma(x) = \frac{1}{1 + e^{-x}} . \tag{1}$$

In words, we do a weighted sum of the inputs and apply the σ function, also called *logistic* function, to obtain the probability. Observe that this function takes values from 0 to 1 and is highly non-linear.

Question 2.1. In the rbm.py file, complete the functions sig. It should accept a vector of inputs and return another vector, where the logistic function has been applied to each component.

Hold on, our inputs are not binary! The rating from a user can be one of the five options $K = \{1, 2, 3, 4, 5\}$. One way to circumvent this difficulty is to encode each rating as a binary vector of size 5. All components of the vector are zero except the k-th component, if k is the rating given. So if a user gives a rating 3, that piece of data will be encoded by the vector (0,0,1,0,0). The formula to go from visible states to the hidden ones is very similar:

$$\mathbb{P}(h_j = 1 | \mathbf{v}) = \sigma \left(\sum_{k \in K} \sum_{i \in V} v_i^k W_{ij}^k \right) . \tag{2}$$

Each user will be associated to one part of the main RBM. Each visible unit in this smaller RBM will correspond to one movie. A visible unit receives a binary vector encoding one rating given by the user. So the RBM receives a list of binary vectors \mathbf{v} to work with. The weights w_{ij}^k are divided between five matrices, one for each k=1,2,3,4,5. You can represent it easily in Numpy, as a 3D array. Our weights array is of dimensions $|V| \times |H| \times |K|$ (respectively the number of visible units, the number of hidden units and the number of possible ratings). To get the matrix of weights for a particular k, you can simply write $\mathbb{W}[:,:,k]$. The first and second axes will correspond respectively to the users and the movies.

Question 2.2. Write a function to propagate the visible input (binary vectors of ratings) to the hidden layer, in visibleToHiddenVec, using equation 2.

RBMs are part of a family of generative models. Given inputs, we can use the estimated weights to compute the probabilites that hidden units will activate. But we can also go the other direction: if we know the values of the hidden units, then we can *generate* data. Say we have a vector of hidden units that encodes the preferences of a user that likes action movies, but not sci-fi. We could generate data that looks like the ratings of such a user, for example would assign 5 to *The Bourne Identity* but 2 to *Star Trek*.

How do we go from the hidden layer to the visible one then? The equation governing this transformation is known as *softmax*: we are going to be careful when deciding the ratings of a user with the current activations of the hidden layer, so we will return a probability distribution over the possible ratings, as such:

$$\mathbb{P}(v_i^k = 1|\mathbf{h}) = \frac{\exp\left(\sum_{j \in H} h_j W_{ij}^k\right)}{\sum_{l=1}^5 \exp\left(\sum_{j \in H} h_j W_{ij}^l\right)} . \tag{3}$$

Notice that summing over k when i is fixed, the probabilities add up to 1. A rating k will also have more probability assigned to it if $\sum_{j\in H} h_j W_{ij}^k$ is high, so you can see here the binding between predicted rating and the weights we are trying to learn.

Question 2.3. Implement the hiddenToVisible function, taking as input a binary vector of hidden units and the edge weights. (Hint: Numpy's tensordot method can come in handy to perform the $\sum_{j\in H} h_j W_{ij}^k$ part). (Hint 2: You can also make use of the softmax function given in the rbm file, that makes sure your implementation is numerically stable, i.e doesn't blow up for large input values).

2.3 Learning the weights

We move on to the next part of the problem: learning the weights. We use what is called a gradient ascent method. Finding the best weights to represent our data can be written as an optimisation problem: find the weights that maximise a certain function. We usually pick the log-likelihood, i.e we seek to find the weights that maximise the probability that our model would generate the data it has been trained on. Just like the linear regression case, we can regularise the model so that it does not fit too closely the training set and is able to generalise well, but we will not do that here (it is, however, an interesting extension to better your performance).

It would be too long to present every last detail of the gradient ascent, but here is the general idea: we want to move our weights in a direction where this log-likelihood function is greater. We first initialise our weights to some random value (done in getInitialWeights) and then perform some updates.

Machine learning is full of tricks to make the gradient ascent more accurate and faster. One of them is the *mini-batch* training. In the linear regression, we have used the full dataset at once to get our estimator. On the other hand, in online training, where we may not have the whole data but a stream that keeps growing, we update our estimator with every incoming piece of data. Mini-batch is between the two: we sample from a big dataset a smaller batch (the size can be tuned) and update our current estimator with this new data.

How do we get the gradient then? This formula is derived from the computed $\mathbb{P}(h_j = 1|\mathbf{v})$ and the data v_i^k itself, by simple multiplication:

$$\nabla W_{i,j}^k = \mathbb{P}(h_j = 1 | \mathbf{v}) \cdot v_i^k .$$

But what Hinton and peers found out is that if we only update the gradient this way, we do too much learning. So we effectively make the model unlearn by doing another pass, a procedure called contrastive divergence. Here is the full recipe:

Learning

- We start with the data $\mathbf{v} = v_i^k$ for a particular user.
- Compute $\mathbb{P}(h_i = 1|\mathbf{v})$ with visibleToHiddenVec.
- Call positive gradient $PG = \mathbb{P}(h_i = 1|\mathbf{v}) \cdot v_i^k$ (computed by probProduct).

• Unlearning

- Sample the states of the hidden units according to $\mathbb{P}(h_j = 1 | \mathbf{v})$.
- Use hiddenToVisible to compute "negative" data $\overline{\mathbf{v}}$.
- Essentially repeat the steps of the Learning part, this time with "negative" data, i.e compute $\mathbb{P}(h_j = 1|\overline{\mathbf{v}})$ and call "negative" gradient $NG = \mathbb{P}(h_j = 1|\overline{\mathbf{v}}) \cdot \overline{v}_i^k$.

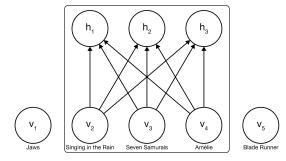


Figure 3: Visible input flows up in the network.

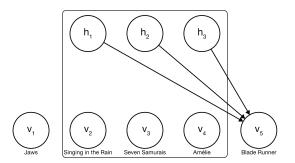


Figure 4: Hidden activations flow down to give a distribution over the ratings.

• Synthesis We now update the weights W as such

$$W \leftarrow W + \frac{\epsilon}{\# \text{users}} \cdot (PG - NG)$$
.

where ϵ is a small learning rate (usually set to 0.1) and we divide by the number of users to obtain an average.

2.4 Predicting the ratings

We sum up the work we have done up until now.

- We have implemented some functions to represent the data (ratings) as binary vectors.
- We then worked on how to go from the visible layer to the hidden one and vice-versa.
- We gave the description of a simple gradient descent algorithm in section 2.3 to learn the best estimator of the weights. This is essentially done in the mainRBM.py file.

We have everything we need to perform the prediction! In fact, we have done most of the hard work required to implement this part. Assume we now would like to predict a movie q for user u. We can get the binary matrix of visible inputs \mathbf{v} for that user and use our visibleToHiddenVec function to propagate the values to the hidden units (seen in Figure 3). Once we have these hidden activations (by using the sampleHidden function), we can go in the reverse direction, just like we do in the unlearning part of the gradient ascent algorithm. We take the vector p of hidden activations and use our hiddenToVisible function to get the "negative data". We can do this to reconstruct the movie we want to predict the rating of, such as $Blade\ Runner$ in Figure 4. In fact we can do this for movies that are part of the training set, allowing us to compute its RMSE.

Question 2.4. Implement the function getPredictedDistribution to get the predicted distribution over the ratings for a movie, using the description given in the previous paragraph and the comments in the function stub to be found in rbm.py.

The negative data gives us a distribution over the possible ratings the user might attribute to this unseen movie. It is now up to us to decide what we are going to do with the distribution. We are given two options to decide the predicted rating we want to return:

• Predict the rating with the highest score We can return the rating that is the most weighted by the distribution $\overline{v_q}$.

• Predict the rating with the expectation We can also return the expected value of the distribution $\overline{v_q}$ as the predicted rating.

As an example, suppose we have $\overline{v_q} = (0.1, 0.2, 0.4, 0.3, 0.0)$, i.e the score of rating 1 is 0.1, the score of rating 2 is 0.2 etc. Our first method would return 3 as predicted rating, since 3 has the highest score. Our second method would return

$$0.1 \times 1 + 0.2 \times 2 + 0.4 \times 3 + 0.3 \times 4 + 0.0 \times 5 = 2.9$$

Question 2.5. Implement the two functions predictRatingMax and predictRatingExp, described above.

You can test which of the two functions gives you the better RMSE.

2.5 Some extensions

To make your algorithm better, we encourage you to tweak it using the tips we give below. They are not explicitly detailed but we add a number of stars next to indicate the difficulty of implementing them, (*) being easier and (***) harder. You may find additional resources online to help you with the implementation. This implementation can only add some extra points to your grade, but it is not required.

- Momentum (*) An easy addition to the existing code, momentum will give some inertia to the gradient updates, limiting the risk that your gradient starts oscillating.
- Adaptive learning rates (**) This method progressively reduces the learning rate, as your algorithm zeroes in on the best estimator of the weights.
- Early stopping (*) With the momentum and other tricks, your RMSE is susceptible to increase from one iteration to the next. Early stopping simply means keeping in memory the best weights found so far, e.g if your RMSE at epoch 950 is better than the one at the end of your training, you would use the weights obtained at epoch 950.
- Regularisation (**) Following the same principle used in the linear regression, you can add a penalty to your cost function if your weights grow too large. Hint: you can modify how the grad variable is set.
- Mini batch (**) In the linear regression, we have used the full dataset at once to get our estimator. On the other hand, in online training, where we may not have the whole data but a stream that keeps growing, we update our estimator with every incoming piece of data. Mini-batch is between the two: we sample from a big dataset a smaller batch (the size can be tuned) and update our current estimator with this new data. In practice, you will compute the gradient for a few users, add these up and then update your weights with this computed gradient.
- Biases (***) The method described above is not exactly complete. We would usually add biases to the visible and hidden units, and estimate their value just like we would for the weights, using learning. The model with biases is described in the Salakhutdinov et al. paper, and parts of it are implemented in the associated code¹, though you will need to adapt it for the case of visible units receiving binary vectors as inputs. This is the hardest extension but an essential one to give your algorithm a big performance boost.

¹Paper and code can be found in the project folder, as hintonrbm.py and hintonrbm.py

3 Testing out your algorithms

After finishing up the two previous sections, you should have two algorithms to predict the rating that a user would give to unrated movies. One makes use of linear regression to compute biases per user and per movie, while the other is adapted from neural networks and uses latent factors to predict the rating. Both algorithms can be tuned to work better by using *cross-validation*.

In the resources of the project you will find a validation dataset, which you can get by calling the getValidationSet. It is important to train your model on the training set, to see how well it performs on previously unseen data contained in the validation set.

Why would you want to do this? In both methods, you have *hyperparameters* that you can change to make the algorithm more performant. Let us recapitulate them here:

• Linear regression

- The regularisation parameter λ This parameter controls the penalty given to weights in the objective function. A higher λ will penalise large biases, making your algorithm less likely to overfit (but with the cost of higher variance).

• Restricted Boltzmann Machines

- The number of hidden units F This parameter controls how many hidden units appear in your main RBM. The higher it is, the more likely it is that your model with overfit.
- The learning rate ϵ Gradient ascent needs a learning rate controlling how much the gradient is allowed to change from one iteration to the next. A higher learning rate will make your algorithm converge faster to a better value, but a value that is too high can also derail it and provoke oscillations. Here is an idea on how to tune it: at the end of every batch, when you update your weights, compute the RMSE on the training set. If it is steadily decreasing, you are on the right track and maybe you can increase your learning rate a bit. If it seems to oscillate, or increases, you have to decrease your learning rate.
- **Extensions** The extensions will add a lot more parameters to optimise: the momentum δ , the regularisation parameter λ , the mini-batch size B...

The problem is that if you train your model to be extremely performant (i.e give very good predictions) on the training set itself, you run the risk of *overfitting*. Overfitting happens when your model estimates very precisely ratings from your training set, but is incapable of generalising to a different dataset. By computing the RMSE on the validation set, you make predictions over data that your model *has not seen*, and thus you are able to control whether your model overfits. Overfitting typically happens when at first, both the training RMSE and the validation RMSE decrease, and after a while your validation RMSE starts increasing again, while training RMSE keeps going down. We are logging both values at every epoch of the gradient ascent for you to control, but you could go beyond and plot these curves to have a visual idea of what is going on.

Coming back to the hyperparameters, you should then be tuning their values such that your model avoids both underfitting and overfitting. Underfitting is harder to control for, but happens when your model is not trained enough. If at the end of your training, both validation and training RMSEs keep decreasing consistently, you may want to increase your number of epochs or, e.g, increase your number of hidden units.

3.1 Apply your model on the test data

Perhaps the most important part of the project: we are keeping from you a test set where real ratings appears. These ratings are taken from the same set of users and movies you have trained your model on, so you do not need to worry about how to treat these new cases. Once you believe that your hyperparameters have been optimised correctly (i.e, after repeated testing against a validation set), you will be able to try out your model on the hidden test.

To do so, you will predict a rating for *all* movies and for *all* users. The result should be a text file of less than 1MB, obtained by calling numpy.savetxt on a user/movie matrix. We give in the mainRBM.py file an example of how to achieve this, though you will have to write the function predictForUser yourself.

When you produce the text file, name it in the following format:

<name of the team>+v<version number>.txt. You will be given 4 different tries, so if your
team name is networkedliferules, you may send us 4 files, networkedliferules+v1.txt,
networkedliferules+v2.txt etc. After receiving one of your files, we will compute the RMSE
obtained on the test set and give you its value.

To encourage you to start early, we add the following restriction: you will only be able to submit one package of predictions per week. You will find the schedule of the five weeks of submissions below. At the end of each week, the current best RMSE (over all previous weeks) will be broadcasted to the class, for you to know which is the current goal to beat. Also, each week, the team with the best outstanding RMSE over the test set will get a bonus of 2 points.

Here is now the schedule:

Week number	Dates
1	Monday, March 27 - Sunday, April 2 (11:59PM)
2	Monday, April 3 - Sunday, April 9 (11:59PM)
3	Monday, April 10 - Sunday, April 16 (11:59PM)
4	Monday, April 17 - Sunday, April 23 (11:59PM)

The Sunday evening deadlines are strict: if you send us the predicted ratings at 00:02AM on the Monday morning of week 2, the RMSE will be counted towards week 2, and not week 1. We will release the best RMSE on Monday evening after computing it for your different submissions.

Finally, the team submitting the best RMSE of the project will obtain a 5 points bonus.

3.2 Other requirements

You are also required to submit two things:

- The source code of your implementation. You are able to modify the signature of the provided functions as long as you properly document why. On the other hand, you are not allowed to use machine learning libraries such as Theano or Scikit, though you can (and should) use Numpy. We will also test your code on a few key functions, though you are free to experiment with the extensions proposed earlier.
- A project report figuring some details of your implementations and, e.g, plots showing the
 evolution of your RMSE as the training occurs or how the extensions have improved your
 results.

References

- [1] Introduction to restricted boltzmann machines. http://blog.echen.me/2011/07/18/introduction-to-restricted-boltzmann-machines/. Accessed: 2017-01-17.
- [2] G. Louppe. Collaborative filtering: Scalable approaches using restricted Boltzmann machines. PhD thesis, Université de Liège, Belgique, 2010.
- [3] R. Salakhutdinov, A. Mnih, and G. Hinton. Restricted boltzmann machines for collaborative filtering. In *Proceedings of the 24th international conference on Machine learning*, pages 791–798. ACM, 2007.