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Recommender systems meet species distribution modelling

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Abstract

Recommender systems techniques can naturally lend themselves to species distribution modelling if biological species are treated as items and places where they occur are treated as users. In this setting recommendation scores can reflect which habitats are suited for which species. Recommendation scores can also be used for reconstructing relative abundances of species, and analysing their rises and declines over millions of years in the past. Analysis of such predictions can shed light on the effects of changing environments on the biosphere now and in the past, as well as help to make predictions for the future. The major potential advantage of the recommender systems treatment over many existing solutions is the large spatial and temporal scale at which such analysis can be done within a single model. A single model makes predictions easier to compare globally in space and over time. While algorithmic application of recommender systems techniques to species distribution modelling is relatively straightforward, model selection and evaluation is particularly challenging, as there is no possibility for online tests or on-demand sampling, since the past worlds are long gone. Explainability is paramount in these tasks. Here we highlight the main challenges and promising directions of evaluation of such modelling, which is still in early stages of development. We show how aggregated prediction statistics and constraints may help for reliable model selection and evaluation. We illustrate the approaches on a case study of the mammalian fossil record from Europe around 8-17 millions of years ago.

Keywords

matrix factorization, implicit feedback, species distribution modeling, NOW database

1. Introduction

Species distribution modelling is at the centre of ecology research and conservation applications [1, 2]. Typically, the computational task is to predict the probability of occurrence of biological species as a function of environmental conditions, as well as co-occurrence of species [3, 4]. Species distribution modelling is thriving for analysing the biodiversity on Earth today, and gaining popularity for analysing organismic evolution of the past [5, 6].

Most species distribution models in ecology focus on predicting the probabilities of occurrence for one species at a time, even if species co-occurrences are taken into account as inputs. Such models are primarily used for understanding habitats of individual species. Biodiversity management and conservation applications, however, require an integrative view over ecosys-

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tems. While multispecies distribution models, modelling several species at a time, are coming about [7, 8], their primary focus is still on modeling ecological niches across environmental gradients. This relies on high resolution climatic data, which realistically is not available for the record of distant past.

Collaborative filtering techniques of recommender systems can be used to model preferences of organisms for different habitats without explicitly characterizing those habitats. This approach would extract patterns of species co-occurrence and extrapolate them over large spatial and temporal scales. Modelling the dynamics of an ecosystem with a single model makes the predictions directly comparable across different species and different biodiversity spots. The inferred model then can be used:

1. for identifying species that would do well but are likely to be missing at sites;
2. for reconstructing relative population sizes from species lists (this is similar to predicting product ratings from transactional data);
3. for tracking co-occurrences and co-evolution over time and space, and for analyzing macroevolutionary processes.

Technical research in recommender systems for species distribution modeling is in early stages, but has already shown promising results [9].

2. Recommender systems for species distribution modelling

The recommender system task naturally lends itself to analysis of ecosystems if we consider species as items and sites where they occur as users. The relationship is not the other way around, because each user can consume only a limited number of products, but each product can be consumed by potentially infinite number of users. Similarly, each site can accommodate a limited number of species, but each species potentially can occur in an infinite number of sites. While both species and sites can potentially be described by features, here we consider the simplest scenario where only occurrence information is available. Thus, we are in the collaborative filtering task setting.

Data for such analysis of ecosystems can come from many sources. Many biodiversity databases maintain records of species diversity today, the majority of them aggregate data from many sources¹[10]. Fossil databases, describing ecosystems of the past, are also widely available [11]. There are also databases that aggregate biodiversity databases, for instance, GBIF². Some data may come from expert surveys, research expeditions or professional wildlife monitoring projects, another portion of data may come from citizen observations. Naturally, even within a single database data can be of varying quality, which is not unlike user data typically used for recommender systems. Most notably, the uncertainty of absences is higher than the uncertainty of presences. If a species has been not been reported at a place it is uncertain whether it does not occur there, or it just has not been encountered yet. This applies to species occurrence data at present as well as in the fossil record. Similarly, presence of a transaction in typical data for

¹https://en.wikipedia.org/wiki/List_of_biodiversity_databases

²<https://www.gbif.org/>

recommender systems signals that a user preferred a particular product, while absence of a transaction might mean either that the user did not like the product or has never come across it.

Further challenges arise due to sparsity of data, especially that of the past ecosystems. Each fossil site presents only a tiny fraction of all species that have ever lived. Similarly, one user can realistically watch only a small fraction of movies that have ever been made. The total number of movies can vary from user to user as the number of species can vary from site to site.

Last but not least, synonymy is a challenge for modelling user preferences as it is for analysing the fossil record. Just as the same movie may appear under different titles in different contexts (or countries), the same species can appear under different names in different research communities. Recommender system techniques are generally equipped to be robust to these shared challenges and hopefully can lend their perspectives to species distribution modelling.

Sometimes information on abundances of species at sites might be available. This corresponds to availability of user ratings. Yet availability of relative abundances at large scales is rare. Typically, only lists of species that have occurred at sites are given. This corresponds to transactional user data without ratings. The latter setting calls for recommender systems solutions with implicit feedback [12, 13]. Such solutions may draw on the repetitiveness of a transaction or the certainty associated with a transaction in general. In the species modelling world certainty can be quantified via qualifiers associated with species identification. Fortunately, neither certainty nor presence-absence information has to be complete; recommender systems typically operate on incomplete information and such is the nature of information about species occurrences.

3. Evaluation challenges and evaluation criteria

Latent factor models [12, 14, 15, 16] largely dominate the collaborative filtering research for over a decade due to their simplicity and effectiveness. For our case study consider a weighted latent factor model (WFM) [12] for collaborative filtering with implicit feedback.

Let $\mathbf{D}_{m \times n}$ be a binary matrix of observed presence or absence of taxa at sites. WFM defines a confidence matrix as $\mathbf{C} = 1 + \alpha \mathbf{D}$, where α is a parameter that accounts for asymmetry of uncertainties about presence and absence. The higher α the more certainty is put on presences in contrast to absences.

WFM factorizes the occurrence matrix into two preference matrices taking into account confidences of the transactions $\mathbf{D} \xrightarrow{\mathbf{C}} \mathbf{X}_{m \times k} \times \mathbf{Y}_{n \times k}^T$. Here k is a parameter specifying the dimensionality of the projection.

WFM minimizes cost function $\min_{x^*, y^*} \sum_{u,i} c_{ui} (d_{ui} - X_u^T Y_i)^2 + \lambda (\sum_u \|X\|^2 + \sum_i \|Y_i\|^2)$. Here c and d are elements of matrices \mathbf{C} and \mathbf{D} (defined earlier), and X and Y are rows of matrices \mathbf{X} and \mathbf{Y} . λ a regularisation parameter.

All in all WFM requires setting four parameters: α , k , λ and the number of iterations for minimizing the cost function. Next we need to define quantitative evaluation criteria and a testing procedure for choosing the parameter values.

While many indirect evaluation approaches exist for recommender systems [17], usually the most reliable is online testing, where users are exposed to different recommender solutions at random. Yet, since species occurrence data is almost always exclusively observational, online

evaluation is not an option and we are left to evaluate the model fit based on the observational data used for modelling.

If we wanted the model to reconstruct the observational data as closely as possible, the best approach would be to set the number of internal dimensions k as high as possible and to set the regularisation parameter λ to zero. Such a model would memorise and reconstruct underlying data perfectly but it would not have predictive power, since it would overfit.

Cross-validation, that would normally be used in predictive modeling to avoid overfitting, is not an option since there is no easy way to hold out a separate testing set. Variants of cross-validation have been used for testing autoencoder-based collaborative filtering [18, 19]. They would leave out some users for testing, which is possible with autoencoders, since they have explicit inputs to the model and outputs. That does not straightforwardly apply to latent factor models, however.

For latent factor models we can do pseudo-cross-validation, where individual occurrences are nullified at random [16], and check which parameter settings best reproduce the nullified occurrences. Yet, this is not sufficient either. If we were simply to maximise this leave-one-out accuracy, the optimal solution would be to predict everything as ones, that is to predict all species to occur everywhere. Clearly, this is not an informative outcome either.

Ideally, we want the model not only to reproduce observed occurrences but also to identify the species that are most likely to be missing at sites, as well as flag potential misidentifications. Thus, predictions must be inaccurate with respect to the training data in order to produce meaningful predictions. Our approach [9] thus is to push the model (1) to predict more occurrences than in the original data while at the same time (2) reproduce the occurrences in the original data reasonably accurately.

The first criterion – pushing the model to predict more positives than in the original data is easy to achieve by increasing α . However, at the same time it is important not to overshoot the carrying capacity of the environments. Species-area relationships are restrictive in a sense that environments can accommodate only a limited number of species [20], which is somewhat predictable from the climatic conditions [21]. While a movie recommender system could potentially keep recommending highly scored movies to the user for as long as the user keeps watching them, an informative species distribution model should recommend a finite number of species that can exist on a site, and this number will certainly vary from site to site. An evaluation criteria that can be used to control for the model realism from this perspective could be requiring that the total-number of recommended species does not exceed, say, 20% of the species that are already there.

The second criterion – keeping the occurrences in the original data accurately reconstructed should rely on a subset of data points for which we have high confidence of both positive occurrences and absences. Repetitive presences (if any of those are reported) can be considered as true positives. Absences out of the time range when the species is known to have been extinct (or has not originated yet) can be considered as true negatives. The latter requires a temporal information in the meta data and thus is primarily suitable for fossil data.

With these two targets in mind one can aim at maximising a conventional evaluation metric, for example, the area under curve (ROC), on a subset of the data that only includes true positives and true negatives and let the aggregated statistics of positive predictions over sites and species take care of not deviating too far from the carrying capacity limits.

4. A case study

Our case study shows an application of matrix factorisation with implicit feedback to reconstructing relative abundances of large plant eating mammals in Europe from about 17 to about 8 million years ago. This time range captures sites assigned to the European Land Mammal biozones from MN4 to MN12 [22], that include a major faunal turnover. Species occurrence data comes from a public fossil mammal database called NOW [23]. The database records sites where fossils have been found. Age information is assigned to sites, not to individual fossils. Each site has a list of species that have been found there. Some identifications of species may be uncertain, the database records uncertainty qualifiers. The database also records features that characterize each species, but we have not used this information in this study. We aggregated the data at the genus level rather than analyzing it at the species level. There is no difference from the algorithmic perspective, but this way the results are easier to interpret from the ecology perspective. Details of preprocessing can be found in [9]. The preprocessed dataset contains 104 genera (items), 351 sites (users) and 2616 occurrences (transactions). Sparsity is 93%. The preprocessed dataset used for this case study is available on GitHub³.

Following the principles outlined in the previous section we monitored the following quantitative performance measures:

1. \hat{P}_{all} mean prediction score over all the data (the prior probability over all the data is $P_{all} = 0.063$) [we want \hat{P}_{all} to be slightly higher than P_{all} , but not too much higher];
2. MAE_{all} mean absolute error over all the data [we want it to be small, but not zero];
3. $MAE_{animals}$ mean absolute error over the numbers of occurrences for the animals [we want it to be small, but not zero];
4. MAE_{sites} mean absolute error over how many animals each site hosts [this relates to the carrying capacity, we want the error to be small, but not zero];
5. AUC_{all} area under ROC on all training data [we want it to be close to one];
6. \hat{P}_{pos+} is mean prediction score over true positives) [ideally, we want $\hat{P}_{pos+} = 1$];
7. $sd(\hat{P}_{pos+})$ the standard deviation;
8. \hat{P}_{neg+} is mean prediction score over true negatives) [ideally, we want $\hat{P}_{neg+} = 0$];
9. $sd(\hat{P}_{neg+})$ the standard deviation;
10. AUC_{+} area under ROC on selected true positives and true negatives [we want it to be close to one];
11. $sd(AUC_{+})$ the standard deviation.

We tested around 200 parameter setting variants via a grid search in the 3-dimensional model parameter space (α, k, λ) . We kept the number of model fitting iterations fixed to 10. Instead of testing on all true positives and true negatives we randomly selected 10 of each and repeated 10 times for each model. This saved computational costs and sidestepped the challenge of class imbalance. We initialised the factor matrices by drawing random values from the normal distribution with zero mean and unit variance. It took a couple of minutes to fit one model using ad hoc implementation in R suite on a commodity laptop.

³<https://github.com/zliobaite/fossilrec>

Table 2 gives the scores. We can see that there is no clear winning variant, but we see some strong relationships. A higher number of internal dimensions gives more of positive predictions. The lower number of inner dimensions generally gives more tiled predictions. Higher regularisation (λ) generally, but not always gives fewer of positive predictions. Higher α generally gives higher mean absolute error, especially on animals. This parameter controls the asymmetry of uncertainties about presence and absence, high values emphasise presence over absence. In practice, it seems, that absences in the fossil record are more certain, then, for instance, absences in movie recommendations, thus there is no need for as high values of this parameter as recommended in the original WFM publication [12].

Our earlier experimentation with various cuts of the data from NOW database revealed that the parameter values are somewhat sensitive to the overall size of the training matrix, but not too sensitive. As compared to commercial applications of recommender systems, ecological analyses will have relatively small datasets. Our dataset in this case study has 104 genera (animals) and 351 sites, and the density of ones in the matrix is nearly 7%.

We conclude the case study by predicting relative abundances for one fossil site. We use a model with the following parameter settings: $\alpha = 10$, $k = 10$, $\lambda = 10$, and 10 iterations for model fitting.

In principle, we can use recommendation scores coming from the model for predicting relative abundances for all 351 sites, but we can only do quantitative evaluation on one site for which we have additional information on bone counts [24]. thus, we know in relative relatively how many of which animals were found there. Due to complex preservation processes [25] the bone counts do not necessarily reflect the relative numbers of animals that lived there many millions of years ago, but as the first approximation for evaluation these counts are fine. Generally, this information is rare in ecological data. Here we use this information only for evaluation purposes, not for model training.

The remaining question is how to convert recommendation scores into relative abundance percentages. We mapped preference scores to relative abundances at site j as:

$$\pi_{ij} = \frac{(p_{ij} - 0.5)}{\sum_{d_{ij} > 0} p_{ij}}, \quad (1)$$

where p_{ij} is the preference score for species i to occur at site j , coming from the model; d_{ij} is the presence-absence matrix, where $d_{ij} > 0$ means that we only sum taxa that are reported to be present at site j . The subtraction of 0.5 from the probability score is an arbitrary cutoff implying that preference scores below 0.5 signal absence. In this study we only analyse the relative abundances of animals that are present, but in principle, the recommender systems approach would allow the estimation of potential relative abundances of animals that are absent as well. The challenge is how to keep the total number of recommended animals contained and in line with the carrying capacity of the environment, as discussed earlier. This is an open question for further research.

Table 1 shows the results. We see that the order from the most abundant to the least abundant animals (genera) is not too far off, but the predictions for rare animals are quite too high.

Table 1

Predicting relative population sizes at fossil site Somosaguas Norte, Spain (14-16 million years old), the numbers of fragments found come from [24] .

Animal genus	# fragments found	% fragments found	recommendation score	% predicted
<i>Gomphotherium</i>	786	51%	0.88	31%
<i>Anchitherium</i>	484	31%	1.02	33%
<i>Prosantorhinus</i>	92	6%	0.40	<1%
<i>Tethytragus</i>	39	3%	0.65	10%
<i>Micromeryx</i>	34	2%	0.75	16%
<i>Heteroprox</i>	6	<1%	0.66	10%

5. Concluding remarks

Recommender systems approaches open new perspectives for analysing ecosystems and species distribution modelling. Reliable evaluation of such approaches is an open challenge. Here we outline several evaluation criteria that are based on domain knowledge about ecosystems. Hopefully similar solutions can potentially be useful in user modelling applications of recommender systems as well. Curious is to learn that the two settings are more similar than it may look from the first sight.

Our case study showed that an off-the-shelf matrix factorisation approach already works reasonably well for fossil species distribution modelling, but many methodological challenges remain. Open directions for future research include taking time and energy constraints into the models. As not all species are alive at all times, models could take constraints of species being alive into their optimisation criteria. As ecosystems vary in energy (for example, tropical forests produce much more edible biomass than semi-deserts), models could incorporate such constraints as well. In the product world this would correspond to one customer having much more purchasing power than another. At a larger scale, different epochs with different climates may be considered as different contexts, where context-aware recommender systems [26] can offer better treatment. Finally, there is a large potential for blending occurrence information with descriptive features of animals and sites, drawing on recent works in reconstructing past environments [27, 28, 29, 30, 31]. The ultimate purpose is to understand how the living world was in the past, when is it livable, and how it works in general.

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Table 2

Performance evaluation of models with different parameter settings. 10 best results within each evaluation criterion are highlighted in bold.

α	k	λ	\hat{P} all	MAE all	MAE animals	MAE sites	AUC all	\hat{P}_{pos+}	sd (\hat{P}_{pos+})	\hat{P}_{neg+}	sd (\hat{P}_{neg+})	AUC_+	sd (AUC_+)
5	5	5	0.05	0.235	9.74	5.194	0.9894	0.598	0.087	0.225	0.046	0.86	0.085
5	5	10	0.208	0.183	18.635	5.316	0.9826	0.561	0.082	0.075	0.032	0.964	0.054
5	5	15	0.131	0.133	8.51	2.709	0.9929	0.514	0.072	0.036	0.026	0.97	0.031
5	5	20	0.134	0.128	7.692	2.792	0.9914	0.443	0.047	0.025	0.021	0.966	0.032
5	10	5	0.296	0.258	42.048	12.333	0.9624	0.53	0.176	0.068	0.136	0.891	0.09
5	10	10	0.202	0.172	15.385	4.148	0.989	0.533	0.085	0.097	0.041	0.94	0.069
5	10	15	0.138	0.124	7.865	2.353	0.9957	0.512	0.045	0.024	0.029	0.988	0.016
5	10	20	0.14	0.128	8.221	2.749	0.9918	0.464	0.102	0.026	0.021	0.976	0.039
5	15	5	0.276	0.234	34.356	10.031	0.9734	0.51	0.146	0.161	0.088	0.854	0.135
5	15	10	0.155	0.131	8.346	2.011	0.9978	0.477	0.076	0.092	0.018	0.904	0.075
5	15	15	0.141	0.122	7.76	2.134	0.9966	0.463	0.069	0.035	0.023	0.96	0.053
5	15	20	0.133	0.123	7.721	2.726	0.9931	0.499	0.091	0.032	0.015	0.988	0.016
5	20	5	0.217	0.187	21.327	6.148	0.9853	0.43	0.085	0.108	0.102	0.85	0.136
5	20	10	0.183	0.149	9.952	2.464	0.9959	0.527	0.072	0.095	0.024	0.937	0.036
5	20	15	0.144	0.122	7.731	2.04	0.9969	0.468	0.071	0.035	0.018	0.97	0.028
5	20	20	0.137	0.126	8	2.684	0.9925	0.425	0.04	0.039	0.026	0.951	0.045
10	10	10	0.225	0.195	24.904	6.986	0.9954	0.581	0.068	0.105	0.055	0.909	0.055
10	10	15	0.173	0.156	17.308	4.439	0.9984	0.56	0.088	0.037	0.013	0.97	0.024
10	10	20	0.168	0.15	15.837	3.969	0.9977	0.602	0.105	0.028	0.027	0.984	0.019
10	10	5	0.093	0.234	13.115	5.749	0.9986	0.618	0.099	0.1	0.096	0.914	0.069
10	15	10	0.195	0.167	16.212	4.467	0.9985	0.544	0.063	0.074	0.055	0.949	0.058
10	15	15	0.172	0.146	13.577	3.47	0.9992	0.529	0.078	0.036	0.026	0.966	0.033
10	15	20	0.164	0.142	13.577	3.35	0.9987	0.54	0.048	0.03	0.03	0.984	0.025
10	15	5	0.216	0.211	28.154	8.353	0.988	0.544	0.09	0.073	0.145	0.893	0.083
10	20	10	0.174	0.145	10.712	2.952	0.9996	0.49	0.091	0.052	0.032	0.95	0.064
10	20	15	0.168	0.138	11.567	2.932	0.9995	0.549	0.068	0.034	0.029	0.962	0.039
10	20	20	0.164	0.138	12.76	3.068	0.9989	0.551	0.075	0.033	0.022	0.989	0.018
10	20	5	0.266	0.227	32.212	9.544	0.9826	0.527	0.062	0.109	0.108	0.88	0.072
10	5	10	0.196	0.19	27.519	7.407	0.9961	0.631	0.086	0.042	0.035	0.962	0.048
10	5	15	0.204	0.188	25.308	6.627	0.9936	0.602	0.077	0.04	0.04	0.982	0.025
10	5	20	0.187	0.176	20.856	5.444	0.9937	0.662	0.066	0.02	0.031	0.988	0.012
10	5	5	0.188	0.206	30.423	8.444	0.9959	0.665	0.093	0.085	0.077	0.961	0.036
20	5	5	0.238	0.254	49.625	14.51	0.997	0.737	0.05	0.007	0.064	0.983	0.03
20	5	10	0.236	0.242	47.375	13.798	0.997	0.744	0.072	0.03	0.045	0.992	0.012
20	5	15	0.237	0.234	45.279	13.063	0.9971	0.721	0.061	0.084	0.063	0.953	0.039
20	5	20	0.235	0.224	42.904	12.251	0.9965	0.721	0.075	0.045	0.036	0.98	0.034
20	10	5	0.185	0.209	29.856	8.823	0.9992	0.676	0.074	0.015	0.063	0.976	0.029
20	10	10	0.196	0.2	30.673	9.037	0.9995	0.669	0.071	0.044	0.051	0.942	0.053
20	10	15	0.196	0.193	29.058	8.484	0.9994	0.643	0.081	0.032	0.048	0.955	0.057
20	10	20	0.2	0.186	28.471	8.225	0.9993	0.678	0.061	0.036	0.054	0.989	0.02
20	15	5	0.16	0.181	19.423	5.761	0.9998	0.53	0.099	0.02	0.059	0.942	0.064
20	15	10	0.197	0.181	22.154	6.547	0.9997	0.541	0.097	0.014	0.046	0.952	0.044
20	15	15	0.178	0.167	20.106	5.895	0.9997	0.57	0.071	0.038	0.035	0.956	0.034
20	15	20	0.183	0.166	20.904	6.023	0.9997	0.613	0.108	0.033	0.032	0.964	0.039
20	20	5	0.198	0.182	18.625	5.519	0.9994	0.504	0.07	0.029	0.06	0.936	0.054
20	20	10	0.196	0.17	16.442	4.86	0.9996	0.569	0.087	0.083	0.048	0.921	0.098
20	20	15	0.169	0.15	14.894	4.396	0.9999	0.498	0.09	0.019	0.047	0.928	0.055
20	20	20	0.176	0.152	16.885	4.889	0.9999	0.584	0.099	0.043	0.027	0.976	0.035
30	5	5	0.264	0.283	62.096	18.376	0.9976	0.743	0.06	0.053	0.044	0.965	0.033
30	5	10	0.262	0.274	59.952	17.718	0.9973	0.774	0.1	0.021	0.079	0.982	0.036
30	5	15	0.265	0.267	57.769	17.031	0.9975	0.749	0.094	0.082	0.061	0.979	0.031
30	5	20	0.264	0.261	58.471	17.217	0.9975	0.746	0.104	0.084	0.06	0.969	0.038
30	10	5	0.2	0.226	36.481	10.809	0.9992	0.667	0.139	0.008	0.037	0.942	0.076
30	10	10	0.204	0.22	35.904	10.638	0.9995	0.66	0.078	0.055	0.064	0.934	0.057
30	10	15	0.213	0.215	37.038	10.957	0.9996	0.689	0.053	0.04	0.051	0.964	0.039
30	10	20	0.218	0.21	36.76	10.846	0.9994	0.67	0.104	0.037	0.059	0.95	0.089
30	15	5	0.166	0.194	21.683	6.442	0.9997	0.592	0.05	-0.006	0.043	0.96	0.053
30	15	10	0.176	0.187	23.375	6.926	0.9999	0.57	0.115	0.023	0.058	0.934	0.069
30	15	15	0.186	0.184	24.625	7.291	0.9999	0.621	0.093	0.029	0.038	0.953	0.064
30	15	20	0.196	0.182	25.75	7.607	0.9999	0.6	0.106	0.043	0.046	0.923	0.073
30	20	5	0.14	0.169	13.269	3.932	1	0.497	0.095	0.036	0.043	0.882	0.07
30	20	10	0.171	0.166	15.971	4.732	1	0.517	0.091	0.005	0.038	0.938	0.073
30	20	15	0.173	0.163	17.769	5.265	1	0.529	0.106	0.028	0.05	0.941	0.066
30	20	20	0.182	0.162	19.846	5.869	0.9999	0.579	0.068	0.027	0.045	0.976	0.029