## Probabilistic Matrix Factorization for Automated Machine Learning

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#### Abstract

In order to achieve state-of-the-art performance, modern machine learning techniques require careful data pre-processing and hyperparameter tuning. Moreover, given the ever increasing number of machine learning models being developed, model selection is becoming increasingly important. Automating the selection and tuning of machine learning pipelines consisting of data pre-processing methods and machine learning models, has long been one of the goals of the machine learning community. In this paper, we tackle this meta-learning task by combining ideas from collaborative filtering and Bayesian optimization. Using probabilistic matrix factorization techniques and acquisition functions from Bayesian optimization, we exploit experiments performed in hundreds of different datasets to guide the exploration of the space of possible pipelines. In our experiments, we show that our approach quickly identifies high-performing pipelines across a wide range of datasets, significantly outperforming the current state-of-the-art.

#### 1 Introduction

Machine learning models often depend on hyperparameters that require careful fine-tuning. For example, deep neural networks need to have a specific number of hidden layers of a determined size and an initial learning rate at the beginning of training. These hyperparameters can be learned by cross-validation (or holdout set performance) over a grid of values, or by randomly sampling the hyperparameter space [Bergstra & Bengio, 2012], but these approaches ignore any continuity in parameter space. More recently, *Bayesian optimization* has emerged as a promising alternative to these approaches [Srinivas et al., 2009, Hutter et al., 2011, Osborne et al., 2009, Bergstra et al., 2011, Snoek et al., 2012, Bergstra et al., 2013]. In Bayesian optimization, the loss (*e.g.* root mean square error) is modeled as a function of the hyperparameters. A regression model (usually a Gaussian process) and an acquisition function are then used to iteratively decide which hyperparameter setting should be evaluated next. More formally, the goal of Bayesian optimization is to find the vector of hyperparameters  $\theta$  that corresponds to

 $\arg\min_{\boldsymbol{\theta}} \mathscr{L}(\mathcal{M}(\mathbf{x};\boldsymbol{\theta}),\,\mathbf{y}),$ 

where  $\mathcal{M}(\mathbf{x} | \boldsymbol{\theta})$  are the predictions generated by a machine learning model  $\mathcal{M}$  (*e.g.* a DNN, random forest, etc.) with hyperparameters  $\boldsymbol{\theta}$  on some inputs  $\mathbf{x}$ ;  $\mathbf{y}$  are the targets/labels and  $\mathcal{L}$  is a loss function. Usually, the hyperparameters are a subset of  $\mathbb{R}^D$ , although in practice many hyperparameters can be discrete (*e.g.* the number of layers in a neural network) or categorical (*e.g.* the loss function to use in a gradient boosted regression tree).

Bayesian optimization techniques have been shown to be very effective in practice and sometimes identify better hyperparameters than human experts, leading to state-of-the-art performance in computer vision tasks Snoek et al. [2012]. One drawback of these techniques is that they are known



Figure 1: Two-dimensional embedding of 5,000 ML pipelines across 576 OpenML datasets. Each point corresponds to a pipeline and is colored by the AUROC obtained by that pipeline in one of the OpenML datasets (OpenML dataset id 943).

to suffer in high-dimensional hyperparameter spaces and often perform comparably to random search [Li et al., 2016]. This limitation has both been shown in practice [Li et al., 2016], as well as studied theoretically [Srinivas et al., 2009, Grünewälder et al., 2010] and is due to the necessity of sampling enough hyperparameter configurations to get a good estimate of the predictive posterior over a high-dimensional space. In practice, this is not an insurmountable obstacle to the fine-tuning of a handful of parameters in a single model, but it's increasingly becoming impractical as the focus of the community shifts from identifying individual parameters to identifying entire ML pipelines consisting of data pre-processing methods, machine learning models and their parameters [Feurer et al., 2015].

One way to address this problem is to take advantage of experiments performed on multiple related datasets. To this end, Swersky et al. [2013] have proposed a multi-task Bayesian optimization approach leveraging multiple related datasets in order to find the best hyperparameter setting for a new task. For instance, they suggested using a smaller dataset to tune the hyperparameters of a bigger dataset that is more expensive to evaluate. More recently, Feurer et al. [2015] used optimization "traces" from related dataset as initialization to warm-start the Bayesian optimization algorithm. In particular, they compute meta-features of both the dataset under examination as well as a variety of OpenML datasets. These meta-features include for example the number of classes or the number of samples in each dataset. They measure similarity between datasets by computing the L1 norm of the meta-features and use the optimization runs from the nearest datasets to warm-start the optimization.

Similar to what was done in Feurer et al. [2015], our goal in this paper is not only to tune the hyperparameters of a given model, but also to identify which model to use and how to pre-process the data. We do so by leveraging experiments performed in datasets already analyzed  $\mathcal{D} = \{\mathcal{D}_1, \dots, \mathcal{D}_D\}$  to solve the optimization problem

$$\arg\min_{\mathcal{M}, \mathcal{P}, \theta_m, \theta_p} \mathscr{L}(\mathcal{M}(\mathcal{P}(\mathbf{x}; \boldsymbol{\theta}_p); \boldsymbol{\theta}_m), \mathbf{y}),$$

where  $\mathcal{M}$  is the ML model with hyperparameters  $\theta_m$  and  $\mathcal{P}$  is the pre-processing method with hyperparameters  $\theta_p$ . In the rest of the paper, we refer to the combination of pre-processing method, machine learning model and their hyperparameters as a *machine learning pipeline*. Some of the dimensions in ML pipeline space are continuous, some are discrete, some are categorical (e.g. the "model" dimension can be a choice between a random forest or a DNN), and some are conditioned on another dimension (e.g. "the number of trees" dimension in a random forest). The mixture of discrete, continuous and conditional dimensions in ML pipelines make modeling continuity in this space particularly challenging. For this reason, unlike previous work, we consider "instantiations" of pipelines, meaning that we fix the set of pipelines ahead of training. For example, an instantiated pipeline can consist in computing the top 5 principal components of the input data and then applying a random forest with 1000 trees. We show that the problem of predicting the performance of ML pipelines on a new dataset can be cast as a collaborative filtering problem that can be solved with probabilistic matrix factorization techniques. The approach we follow in the rest of this paper, based on Gaussian process latent variable models [Lawrence & Urtasun, 2009, Lawrence, 2005], embeds different pipelines in a latent space based on their performance across different datasets. For example, Figure 1 shows the first two dimensions of the latent space of ML pipelines identified by our model on OpenML [Vanschoren et al., 2013] datasets. Each dot corresponds to an ML pipeline and is colored depending on the AUROC (in the rest of the paper simply called AUC) achieved on a holdout set for a given OpenML dataset. Since our probabilistic approach produces a full predictive posterior distribution over the performance of the ML pipelines considered, we can use it in conjunction with acquisition functions commonly used in Bayesian optimization to guide the exploration of the ML pipeline space. Through extensive experiments, we show that our method significantly outperforms the current state-of-the-art in automated machine learning in the vast majority of datasets we considered.

#### 2 AutoML as probabilistic matrix factorization

One of the main problems with current automated machine learning (AutoML) techniques (other than the two mentioned in the introduction) is that they treat each new dataset as a completely new problem, with no transfer of information from experiments performed on datasets analyzed previously. In this paper, we develop a method that can draw information from *all* of the datasets for which experiments are available, whether they are immediately related (*e.g.* a smaller version of the current dataset) or not. The idea behind our approach is that if two datasets have similar (*i.e.* correlated) results for a few pipelines, it's likely that the remaining pipelines will produce results that are similar as well. This is somewhat reminiscent of a collaborative filtering problem for movie recommendation, where if two users liked the same movies in the past, it's more likely that they will like similar ones in the future.

More formally, given N machine learning pipelines and D datasets, we train each pipeline on part of each dataset and we evaluate it on an holdout set. This gives us a matrix  $\mathbf{Y} \in \mathbb{R}^{N \times D}$  summarizing the performance of each pipeline in each dataset. In the rest of the paper, we will assume that  $\mathbf{Y}$  is a matrix of AUCs and that we want to maximize the AUC for a new dataset, but our approach can be used with any loss function (*e.g.* RMSEs, accuracies, etc.). For most applications, we expect  $\mathbf{Y}$  to be very sparse, since it can be impractical to run and evaluate all pipelines on all datasets. Having observed the performance of different pipelines on different datasets, the task of predicting the performance of any of them on a new dataset can be cast as a matrix factorization problem.

Specifically, we are seeking a low rank decomposition such that  $\mathbf{Y} \approx \mathbf{XW}$ , where  $\mathbf{X} \in \mathbb{R}^{N \times Q}$  and  $\mathbf{W} \in \mathbb{R}^{Q \times D}$ , where Q is the dimensionality of the latent space. As done in Lawrence & Urtasun [2009] and Salakhutdinov & Mnih [2008], we consider the probabilistic version of this task, known as *probabilistic matrix factorization* 

$$p(\mathbf{Y} | \mathbf{X}, \mathbf{W}, \sigma^2) = \prod_{i=1}^{N} \mathcal{N}(\mathbf{y}_i | \mathbf{x}_i \mathbf{W}, \sigma^2 \mathbb{I}),$$
(1)

where  $\mathbf{x}_i$  is a row of the latent variables  $\mathbf{X}$  and  $\mathbf{y}_i$  is a vector of measured performances for pipeline *i*. In this setting both  $\mathbf{X}$  and  $\mathbf{W}$  are unknown and must be inferred.

#### 2.1 Non-linear matrix factorization with Gaussian Process priors

The probabilistic matrix factorization approach just introduced assumes that the entries of Y are linearly related to the latent variables. In nonlinear probabilistic matrix factorization [Lawrence & Urtasun, 2009], the elements of Y are given by a *nonlinear function* of the latent variables,

 $y_{n,d} = f_d(\mathbf{x}_n) + \epsilon$ , where  $\epsilon$  is independent Gaussian noise. This gives a likelihood of the form

$$p\left(\mathbf{Y} \mid \mathbf{X}, \mathbf{f}, \sigma^2\right) = \prod_{n=1}^{N} \prod_{d=1}^{D} \mathcal{N}\left(y_{n,d} \mid f_d\left(\mathbf{x}_n\right), \sigma^2\right),$$
(2)

Following Lawrence & Urtasun [2009], we place a Gaussian Process prior over  $f_d(\mathbf{x}_n)$  so that any vector  $\mathbf{f}$  is governed by a joint Gaussian density,  $p(\mathbf{f}|\mathbf{X}) = \mathcal{N}(\mathbf{f}|\mathbf{0}, \mathbf{K})$ , where  $\mathbf{K}$  is a covariance matrix, and the elements  $\mathbf{K}_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j)$  encode the degree of correlation between two samples as a function of the latent variables. If we use the covariance function  $k(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^\top \mathbf{x}_j$ , which is a prior corresponding to linear functions, we recover a model equivalent to (1). Alternatively, we can choose a prior over non-linear functions, such as a squared exponential covariance function with automatic relevance determination (ARD, one length-scale per dimension),

$$k\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right) = \alpha \exp\left(-\frac{\gamma_{q}}{2} ||\mathbf{x}_{i} - \mathbf{x}_{j}||^{2}\right),\tag{3}$$

where  $\alpha$  is a variance (or amplitude) parameter and  $\gamma_q$  are length-scales. The squared exponential covariance function is infinitely differentiable and hence is a prior over very smooth functions. In practice, such a strong smoothness assumption can be unrealistic and is the reason why the Matern class of kernels is sometimes preferred [Williams & Rasmussen, 2006]. In the rest of this paper we use the squared exponential kernel and leave the investigation of the performance of Matern kernels to future work.

After specifying a GP prior, we can get the marginal likelihood by integrating out the function f under the prior

$$p(\mathbf{Y} | \mathbf{X}, \boldsymbol{\theta}, \sigma^2) = \int p(\mathbf{Y} | \mathbf{X}, \mathbf{f}) \, p(\mathbf{f} | \mathbf{X}) \, d\mathbf{f}$$
(4)

$$=\prod_{d=1}^{D} \mathcal{N}(\mathbf{y}_{:,d} \,|\, \mathbf{0}, \, \mathbf{K}(\mathbf{X}, \mathbf{X}) + \sigma^2 \mathbb{I}), \tag{5}$$

where  $\boldsymbol{\theta} = \{\alpha, \gamma_1, \dots, \gamma_q\}.$ 

#### 2.2 Inference with missing data

As we mentioned before, we expect  $\mathbf{Y}$  to be a sparse matrix, so we need to be able to perform inference with missing data. Given that the marginal likelihood in equation 5 follows a multivariate Gaussian distribution, marginalizing over missing values is straightforward and simply requires "dropping" the missing observations from the mean and covariance. More formally, we define an indexing function  $e(d) : \mathbb{N} \to \mathbb{N}^m$  that given a dataset index d returns the list of m pipelines that have been evaluated on d. We can then rewrite equation 5 as

$$p(\mathbf{Y} | \mathbf{X}, \boldsymbol{\theta}, \sigma^2) = \prod_{d=1}^{D} \mathcal{N}(\mathbf{y}_{e(d), d} | \mathbf{0}, \mathbf{C}_d),$$
(6)

where  $\mathbf{C}_{\mathbf{d}} = \mathbf{K}(\mathbf{X}_{e(d)}, \mathbf{X}_{e(d)}) + \sigma^2 \mathbb{I}$ .

As done in Lawrence & Urtasun [2009], we infer the parameters  $\theta, \sigma$  and latent variables X by minimizing the log-likelihood using stochastic gradient descent. We do so by presenting the entries  $\mathbf{Y}_{e(d),d}$  one at a time and updating  $\mathbf{X}_{e(d)}$ ,  $\theta$  and  $\sigma$  for each dataset d. The negative log-likelihood of the model can be written as

$$\mathbf{L} = \sum_{d=1}^{D} -\text{const.} - \frac{N_d}{2} \log |\mathbf{C}_d| - \frac{1}{2} (\mathbf{y}_{e(d),d}^{\top} \mathbf{C}_d^{-1} \mathbf{y}_{e(d),d}),$$
(7)

where  $N_d$  is the number of pipelines evaluated for dataset d. For every dataset j we update the global parameters  $\theta$  as well as the latent variables  $\mathbf{X}_{e(d)}$  by evaluating at the t-th iteration:

$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^t - \eta \frac{\partial \mathbf{L}}{\partial \boldsymbol{\theta}} \tag{8}$$

$$\mathbf{X}_{e(d)}^{t+1} = \mathbf{X}_{e(d)}^{t} - \eta \frac{\partial \mathbf{L}}{\partial \mathbf{X}_{e(d)}},\tag{9}$$

where  $\eta$  is a learning rate parameter. In the rest of the paper, we will use a global  $\eta$  for all parameters, but it's also possible to specify a different learning rate per parameter (*i.e.*  $\eta$  is a vector) and, for example, use RMSprop [Tieleman & Hinton, 2012] to tune the learning rate at each iteration.

#### 2.3 Predictions

Predictions from the model can be easily computed by following the standard derivations for Gaussian Process [Williams & Rasmussen, 2006] regression. The predicted performance  $y_{m,j}^*$  of pipeline m for a new dataset j is given by

$$p(y_{m,d}^* | \mathbf{X}, \boldsymbol{\theta}, \sigma) = \mathcal{N}(y_{m,d}^* | \mu_{m,d}, v_{m,d})$$

$$\mu_{m,d} = \mathbf{k}_{e(d),m}^\top \mathbf{C}_d^{-1} \mathbf{y}_{e(d),d}$$

$$v_{m,d} = k_{m,m} + \sigma^2 - \mathbf{k}_{e(d),m}^\top \mathbf{C}_d^{-1} \mathbf{k}_{e(d),m},$$
(10)

remembering that  $\mathbf{C}_d = \mathbf{K}(\mathbf{X}_{e(d)}, \mathbf{X}_{e(d)}) + \sigma^2 \mathbb{I}$  and defining  $\mathbf{k}_{e(d),m} = \mathbf{K}(\mathbf{X}_{e(d)}, \mathbf{X}_m)$  and  $k_{m,m} = \mathbf{K}(\mathbf{X}_m, \mathbf{X}_m)$ .

The computational complexity for generating these predictions is largely determined by the number of pipelines already evaluated for a test dataset and is again due to the inversion of a  $N_j \times N_j$  matrix. This is not particularly onerous because the typical number of evaluations is likely to be in the hundreds, given the cost of training each pipeline and the risk of overfitting to the validation set if too many pipelines are evaluated.

#### 2.4 Acquisition functions

The model described so far can be used to predict the expected performance of each ML pipeline as a function of the pipelines already evaluated, but does not yet give any guidance as to which pipeline should be tried next. A simple approach to pick the next pipeline to evaluate is to iteratively pick the maximum predicted performance

arg max 
$$(\mu_{m,d})$$
,

but such a utility function, also known as acquisition function, would discard information about the uncertainty of the predictions. One of the most used acquisition functions is the expected improvement (EI) [Močkus, 1975], which given by the expectation of the improvement function

$$\begin{split} I(y_{m,d}^*, y_{best}) &\triangleq (y_{m,d}^* - y_{best}) \mathbb{I}(y_{m,d}^* > y_{best}) \\ & \\ \mathbb{EI}_{m,d} \triangleq \mathbb{E}[I(y_{m,d}^*, y_{best})], \end{split}$$

where  $y_{best}$  is the best result observed. Since  $y_{m,j}^*$  is Gaussian distributed (see Equation 10), this expectation can be computed analytically

$$\mathtt{EI}_{m,d} = v_{m,d} \left[ \gamma_{m,d} \Phi(\gamma_{m,d} + \mathcal{N}(\gamma_{m,d} \mid 0, 1)) \right]$$

where  $\Phi$  is the cumulative distribution function of the standard normal and  $\gamma_{m,j}$  is defined as

$$\gamma_{m,d} = \frac{\mu_{m,d} - y_{best} - \xi}{v_{m,d}}$$

where  $\xi$  is a free parameter to encourage exploration. After computing the expected improvement for each pipeline, the next pipeline to evaluate is simply given by

arg max 
$$(EI_{m,d})$$

The expected improvement is just one of many possible acquisition functions, and different problems may require different acquisition functions. See [Shahriari et al., 2016] for a review.

#### **3** Experiments

In this section, we compare our method to a series of baselines as well as to auto-sklearn [Feurer et al., 2015], the current state-of-the-art approach. We ran all of the experiments on 576 OpenML [Vanschoren et al., 2013] datasets, selected by filtering for binary and multi-class classification problems with no more than 10,000 samples and no missing values.



Figure 2: Average rank of all the approaches we considered as a function of the number of iterations. For each dataset, the methods are ranked based on AUC obtained on a validation set at each iteration. The ranks are then averaged across datasets. Lower is better. The shaded areas represent the standard error for each method.

#### 3.1 Generation of training data

We generated training data for our method by splitting each OpenML dataset in 80% training data, 10% validation data and 10% test data, running 20,000 ML pipelines on each dataset and measuring the AUC on the validation set. We generated the pipelines by sampling a combination of pre-processors  $\mathcal{P} = \{P^1, P^2, ..., P^n\}$ , machine learning models  $\mathcal{M} = \{M^1, M^2, ..., M^m\}$ , and their corresponding hyperparameters  $\Theta_P = \{\theta_P^1, ..., \theta_P^n\}$  and  $\Theta_M = \{\theta_M^1, ..., \theta_M^m\}$  from the entries in Supplementary Table 1. All of the models and pre-processing methods we considered were implemented in scikit-learn [Pedregosa et al., 2011]. We sampled the parameter space by using functions provided in the auto-sklearn library Feuer et al. [2015]. Similar to what was done in [Feuere et al., 2015], we limited the maximum training time of each individual model within a pipeline to 30 seconds and its memory consumption to 16GB. Because of network failures and cluster running out of memory, the resulting matrix **Y** was not fully sampled and had roughly 30% missing entries. As pointed out in the previous section, this is not a problem for our method, since it can easily handle sparse data.

#### 3.2 Parameter settings

We trained our model (described in section 2) on 527 of the datasets and we evaluated its performance on the remaining 49, picked at random. We set the number of latent dimensions Q = 20, the initial learning rate to  $\eta = 1e^{-6}$ , the momentum to  $\omega = 0.9$  and we initialized the latent space using PCA. Finally, we configured the acquisition function with  $\xi = 0.01$ . All of these parameters were tuned on an independent holdout set of 10 OpenML datasets with a random subset of 5,000 pipelines.

#### 3.3 Results

We compared the following models:

- **Random**. For each test dataset, we performed a random search by sampling each pipeline to be evaluated from the set of 20,000 at random without replacement.
- L1. For all the datasets in the training set, we computed meta-features as done in Feurer et al. [2015]. The set of meta-features includes, for example, the number of samples, number of classes, skewness and entropy of the labels (a full list is given as supplementary material in Feurer et al. [2015]). At test time, we computed the L1 distance between the meta-features of the training datasets and the test dataset. Finally, we took the closest training dataset



Figure 3: Difference between the maximum AUC observed on the test set and the AUC obtained by each method at each iteration. Lower is better. The shaded areas represent the standard error for each method.

in L1 space and we evaluated the pipelines ordered by performance (in this case, AUC) achieved in the training dataset. The idea behind this strawman method is that the ordering of pipelines in terms of loss function should be similar across related datasets. In all our experiments, we use this method to pick the first pipeline. We then use our method and acquisition function to select subsequent pipelines.

- Average. We computed the average performance of each pipeline across all datasets in the training set and evaluated them in order starting from the one with the highest AUC.
- **auto-sklearn** [Feurer et al., 2015]. We ran auto-sklearn for 1.5 hours per dataset and set to optimize AUC on a holdout set. We disabled the automated ensembling of models in order to obtain a fair comparison to the other non-ensembling methods.
- PMF. The model described in this paper.

This set of alternative methods includes baselines that completely ignore any experience gained in the analysis of previous datasets (*i.e.* "random"), methods that incorporate such information in a basic way (*i.e.*, "average", "L1") and methods that integrate such information and exploit traditional Bayesian Optimization techniques (*i.e.* "auto-sklearn").

Figure 2 shows the average rank for each method as a function of the number of iterations (*i.e.* the number of pipelines evaluated). Starting from the first few iterations, our approach consistently achieves the best average rank. L1 performs well in the first few iterations, but its performance resembles random search as more pipelines are evaluated. Surprisingly, auto-sklearn performed worse than random in our datasets. To further investigate this issue, we ran auto-sklearn using the default parameters settings (which performs ensembling of models). With these settings, auto-sklearn considers a larger set of pre-processing algorithms and models than our method. The results are shown in supplementary figures 1 and 2.

Rank plots such as Figure 2 are useful to understand the relative performance of a set of models, but they don't give any information about the magnitude of the difference in performance. For this reason, we measured the difference between the maximum AUC obtained by any pipeline in each dataset and the AUC obtained by the pipeline selected at each iteration. Given the range of possible AUCs in our test datasets, this metric has very high variance, but we still found it informative. The results summarized in Figure 3 show that our method still outperforms all the others. Random search is the second best method especially in the last few iterations, although we expect its performance to deteriorate as more and more pipelines are considered (*i.e.* considering 100,000 pipelines instead of our 20,000), because of the increase in the size of the search space.



Figure 4: (a) Root mean square error between predicted and observed AUCs in the test set as a function of the number of iterations. Lower is better. RMSE is averaged across all 49 datasets. (b) Posterior predictive standard deviation as a function of the number of iterations and averaged across all 49 datasets. Shaded area shows two standard errors around the mean.

Next, we investigated how quickly our model is able to improve its predictions as more pipelines are evaluated. Figure 4a shows the root mean square error computed on a test set of 1000 pipelines across 49 test datasets as a function of the number of evaluations. Figure 4b shows the uncertainty of the model (specifically, the posterior standard deviation) as a function of the number of evaluations. Overall, Figure 4 a and b support that as more evaluations are performed, the model becomes less uncertain and the accuracy of the predictions increases.

#### 4 Discussion

We have presented a new approach to automatically build predictive ML pipelines for a given dataset, automating the selection of data pre-processing method and machine learning model as well as the tuning of their hyperparameters. Our approach combines techniques from collaborative filtering and ideas from Bayesian optimization to intelligently explore the space of ML pipelines, exploiting experiments performed in previous datasets. We have benchmarked our approach against the state-of-the-art in 49 OpenML datasets with different sample sizes, number of features and number of classes. Overall, our results show that our approach outperforms both the state-of-the-art as well as a set of strong baselines.

One potential concern with our method is that it requires sampling (*i.e.* instantiating pipelines) from a potentially high-dimensional space and thus could require exponentially many samples in order to explore all areas of this space. We have found this not to be a problem for three reasons. First, many of the dimensions in the space of pipelines are conditioned on the choice of other dimensions. For example, the number of trees or depth of a random forest are parameters that are only relevant if a random forest is chosen in the "model" dimension. This reduces the effective search space significantly. Second, in our model we treat every pipeline as an additional sample, so increasing the sampling density also results in an increase in sample size (and similarly, adding a dataset also increases the effective sample size). Finally, very dense sampling of the pipeline space is only needed if the performance is very sensitive to small parameter changes, something that we haven't observed in practice. If this is a concern, we advise using our approach in conjunction with traditional Bayesian optimization methods (such as Snoek et al. [2012]) to further fine-tune the parameters.

We are currently investigating several extensions of this work. First, we would like to include more pipeline- and dataset-specific information in our model. As discussed in section 2, the only data taken into account by our model is the performance of each method in each dataset. Similarity between different pipelines is induced by having correlated performance across multiple datasets, and ignores potentially relevant metadata about both datasets and pipelines, such as the sample size or number of classes. We are currently working on including such information by extending our model with both a kernel including model information and a kernel including dataset information. Second, we are interested in using acquisition functions that include a factor representing the computational

cost of running a given pipeline [Snoek et al., 2012]. The machine learning models we used for our experiments were constrained not to exceed a certain runtime, but this could be impractical in real applications. Finally, we are planning to experiment with different probabilistic matrix factorization models based on variational autoencoders.

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# Supplementary material for "Probabilistic Matrix Factorization for Automated Machine Learning"

ML / PP Algorithm	Parameter	Range
Polynomial Features	degree	[2, 3]
Polynomial Features	interaction_only	{False, True}
Polynomial Features	include_bias	{True, False}
Principal Component Analysis	keep_variance	[0.5, 0.9999]
Principal Component Analysis	whiten	{False, True}
Linear Discriminant Analysis	shrinkage	{None, auto, manual}
Linear Discriminant Analysis	n_components	[1, 250]
Linear Discriminant Analysis	tol	[1e-05, 0.1]
Linear Discriminant Analysis	shrinkage_factor	[0.0, 1.0]
Extreme Gradient Boosting	max_depth	[1, 10]
Extreme Gradient Boosting	learning_rate	[0.01, 1.0]
Extreme Gradient Boosting	n_estimators	[50, 500]
Extreme Gradient Boosting	subsample	[0.01, 1.0]
Extreme Gradient Boosting	min_child_weight	[1, 20]
Quadratic Discriminant Analysis	reg_param	[0.0, 10.0]
Extra Trees	criterion	{gini, entropy}
Extra Trees	max_features	[0.5, 5.0]
Extra Trees	min_samples_split	[2, 20]
Extra Trees	min_samples_leaf	[1, 20]
Extra Trees	bootstrap	{True, False}
Decision Tree	criterion	{gini, entropy}
Decision Tree	max_depth	[0.0, 2.0]
Decision Tree	min_samples_split	[2, 20]
Decision Tree	min_samples_leaf	[1, 20]
Gradient Boosted Decision Trees	learning_rate	[0.01, 1.0]
Gradient Boosted Decision Trees	n_estimators	[50, 500]
Gradient Boosted Decision Trees	max_depth	[1, 10]
Gradient Boosted Decision Trees	min_samples_split	[2, 20]
Gradient Boosted Decision Trees	min_samples_leaf	[1, 20]
Gradient Boosted Decision Trees	subsample	[0.01, 1.0]
Gradient Boosted Decision Trees	max_features	[0.5, 5.0]
K Neighbors	n_neighbors	[1, 100]
K Neighbors	weights	{uniform, distance}

K Neighbors	p	{1, 2}
Multinomial Naive Bayes	alpha	[0.01, 100.0]
Multinomial Naive Bayes	fit_prior	{True, False}
Support Vector Machine	С	[0.03125, 32768.0]
Support Vector Machine	kernel	{rbf, poly, sigmoid}
Support Vector Machine	gamma	[3.05176e-05, 8.0]
Support Vector Machine	shrinking	{True, False}
Support Vector Machine	tol	[1e-05, 0.1]
Support Vector Machine	coef0	[-1.0, 1.0]
Support Vector Machine	degree	[1, 5]
Random Forest	criterion	{gini, entropy}
Random Forest	max_features	[0.5, 5.0]
Random Forest	min_samples_split	[2, 20]
Random Forest	min_samples_leaf	[1, 20]
Random Forest	bootstrap	{True, False}
Bernoulli Naive Bayes	alpha	[0.01, 100.0]
Bernoulli Naive Bayes	fit_prior	{True, False}

Table S1: List of preprocessing methods, ML models/algorithms and parameters considered.

# 1 Results using auto-sklearn with default parameters



Figure S1: Average rank of all the approaches we considered as a function of the number of iterations. For each datasets, the methods are ranked based on AUC obtained on a validation set at each iteration. The ranks are then averaged across datasets. Lower is better. The shaded areas represent the standard error for each method.



Figure S2: Difference between the maximum AUC observed on the test set and the AUC obtained by each method at each iteration. Lower is better. The shaded areas represent the standard error for each method.

## 2 Reproducing our auto-sklearn results

The raw data and code we used to run all of the auto-sklearn experiments is available here: https://github.com/elibol/amle