Oboe: Collaborative Filtering for AutoML Model Selection

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What is AutoML?

an **Automated Machine Learning (AutoML) system**

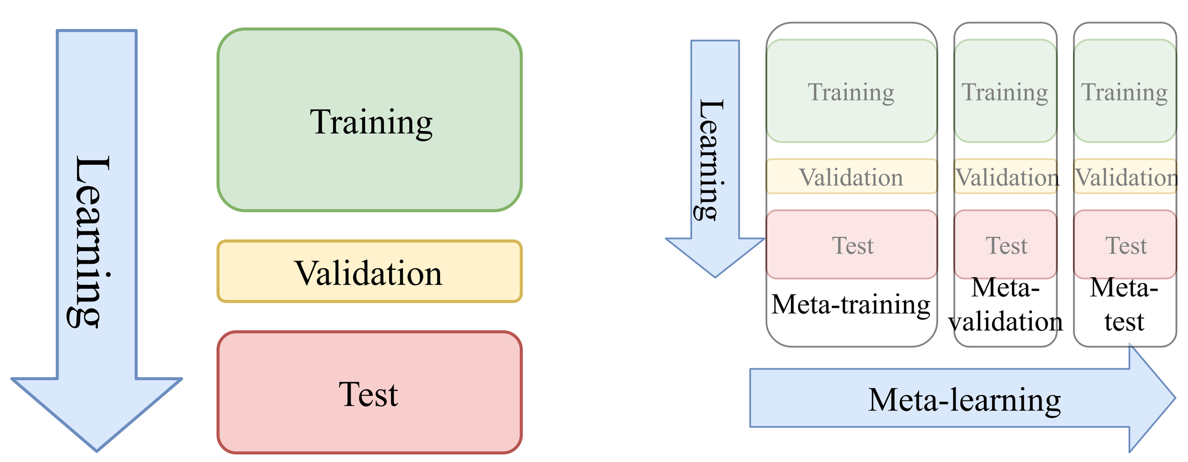
- chooses an algorithm together with hyperparameters
- to achieve the best performance on a (supervised learning) task
- without human intervention.

why AutoML?

- humans are expensive (especially data scientists!)
- computation is cheap
- too many models; can't try them all

to find a reasonable answer, fast, we need:

- *Information.* What meta-features predict model performance?
- *Speed.* What meta-features are worth computing?

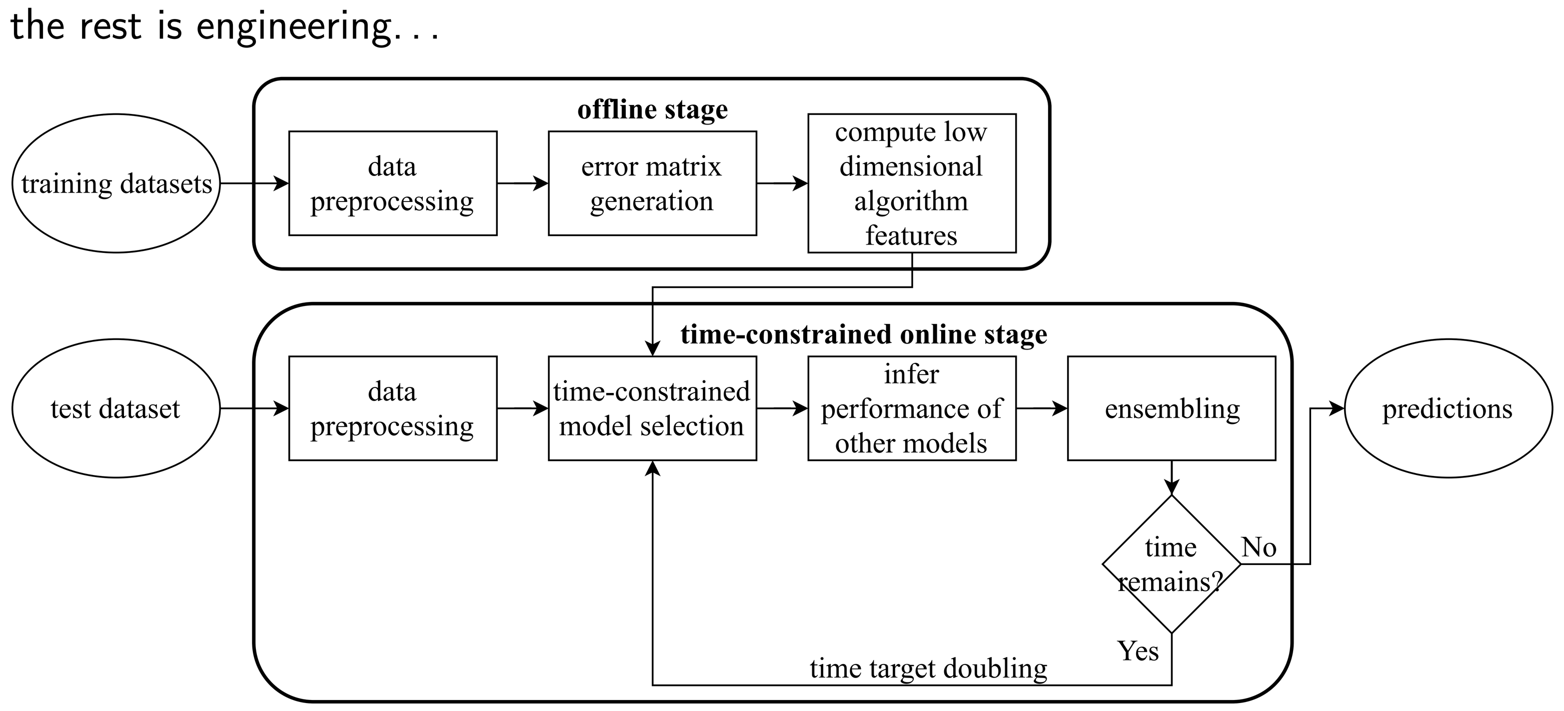


(a) Learning (b) Meta-learning

Our approach

main idea used by Oboe:

- algorithm performance is low rank
- rank decomposition gives best meta-features
- the rest is engineering. . .



c.f. previous SOTA in AutoML: auto-sklearn [2]

at train time (offline stage):

- compute meta-features of training datasets.
- determine best model(s) on training datasets (try them all and pick the best!)

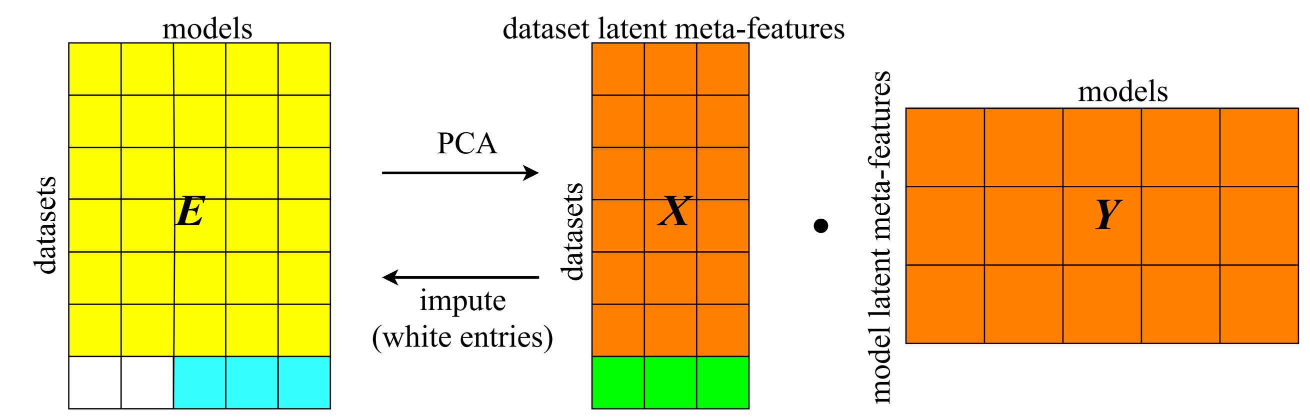
at test time (online stage):

- compute meta-features of test dataset.
- find *similar* datasets (w.r.t. meta-features)
- form ensemble using models that performed best on similar datasets
- tune hyperparameters

e.g., using Gaussian processes [2, 3, 5], bandit-based methods [6], sparse Boolean functions [4] , . . .

Find the meta-features that best predict performance

given: m training datasets, n machine learning models
measure: error of each model on each dataset
form: $m \times n$ error matrix E (yellow)
find: $X \in \mathbf{R}^{m\times k}$, $Y \in \mathbf{R}^{k\times n}$ (orange) for which



interpretation:

- rows $x_i \in \mathbf{R}^k$ of X are *dataset meta-features*
- columns $y_j \in \mathbf{R}^k$ of Y are *model meta-features*
- $x_i y_j \approx E_{ij}$ are *predicted model performance*

prefix property: SVD on error matrix gives optimal k-dimensional meta-features for every k

AutoML = linear algebra

at test time (online stage)

- new test dataset = new row of E (blue and white)
- run some algorithms on new dataset (blue blocks, observed)
- estimate dataset latent meta-features $\hat{x}$ (green blocks) using least squares
- estimate model performance (white blocks) as $\hat{e} = \hat{x}Y$
- select models with best predicted performance to use in ensemble

Test time: which models to run?

choose fast, informative models (blue blocks)

- predict runtime $\hat{t}_j$ of model j on test dataset (predictors = # data points, # features)
- Use (D-optimal) **experiment design** to choose fast, informative models. Solve

$$\begin{aligned} \underset{v_j}{\text{minimize}} \quad & \log\det\left(\sum_{j=1}^{n} v_j y_j y_j^T\right)^{-1} \\ \text{subject to} \quad & \sum_{j=1}^{n} v_j \hat{t}_j \leq \tau \\ & v_j \in [0,1] \quad \forall j \in [n]. \end{aligned}$$

- Value v_i is large for fast, informative models. Run those! (blue blocks) (must run at least k models to fit k-dimensional latent meta-features)

Put it in a loop

given time budget τ for learning on new dataset
initialize rank $k = k_0$, time target $t = \tau_0 < \tau/2$
while time remains

- choose k fast, informative models using experiment design
- run those models on the dataset and use to infer performance of other models
- create ensemble using models with predicted best performance
- double time budget t, increase rank k

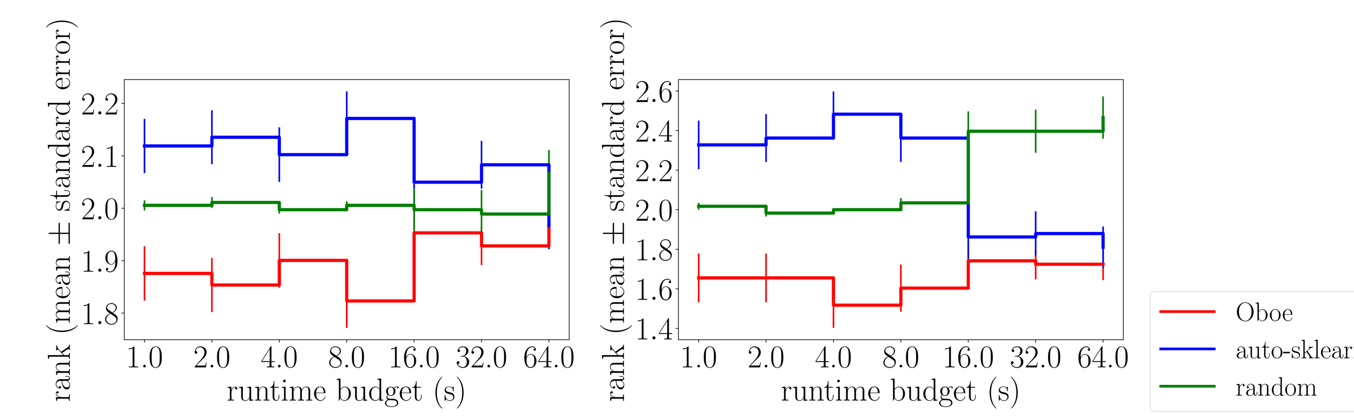
It works!

Experimental setup.

- Datasets: OpenML [8] and UCI [1] with 150–10,000 data points and no missing entries.
- error matrix
  - 418 OpenML datasets by 219 models
  - Metric: balanced error rate
- Candidate algorithms from Python scikit-learn: Adaboost, decision tree, extra trees, random forest, gradient boosting, Gaussian naive Bayes, kNN, logistic regression, multilayer perceptron, perceptron, kernel SVM, linear SVM

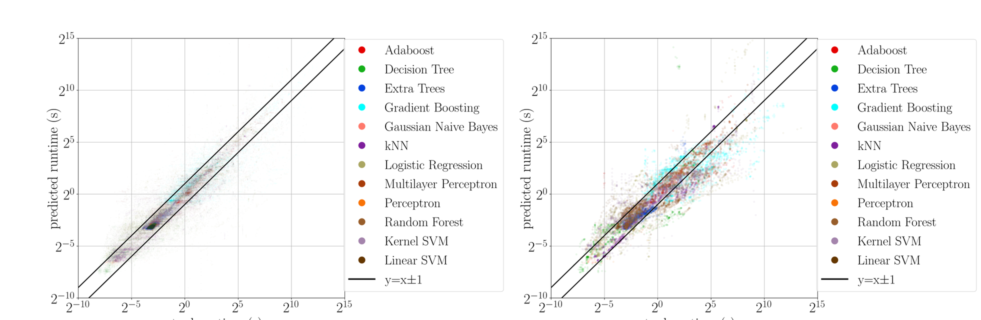
Numerical results

- Oboe achieves SOTA performance

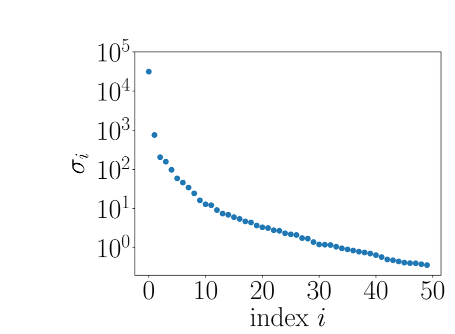


(a) Ranking on OpenML datasets (meta-LOOCV) as a function of time. (b) Ranking on UCI datasets (meta-test) as a function of time.

- Modeling assumptions are warranted

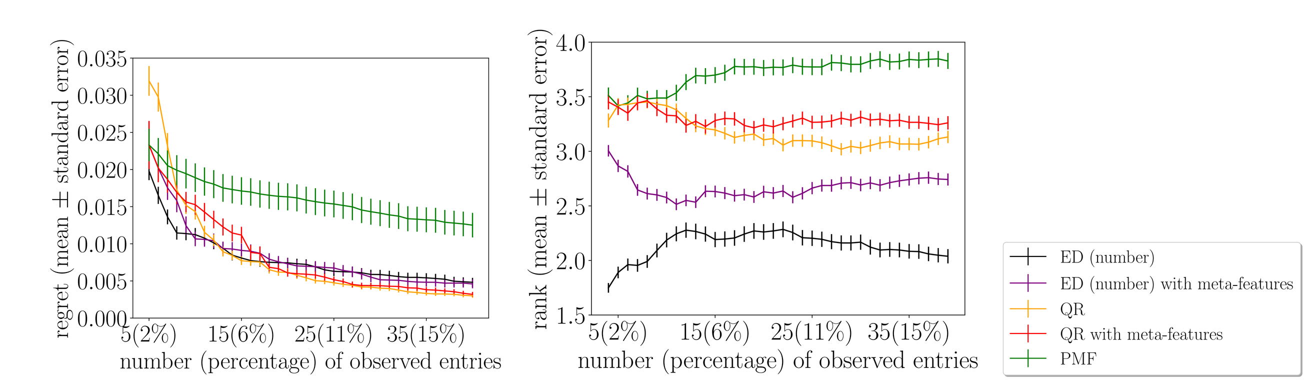


(a) Meta-LOOCV runtime prediction performance on 418 OpenML classification datasets with number of points 150–10,000. (b) Meta-test runtime prediction performance on 72 subsampled OpenML classification datasets with original number of points 10,000–200,000.



Error matrix E is (apx) low rank [7]

- Experiment design selects most informative models



Comparison of sampling schemes (QR or ED) in Oboe and PMF. "QR" denotes QR decomposition with column pivoting; "ED (number)" denotes experiment design with number of observed entries constrained. The left plot shows the regret of each AutoML method as a function of number of entries; the right shows the ranking of each AutoML method in the regret plot (1 is best and 5 is worst).

Thanks!

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