Automating Machine Learning

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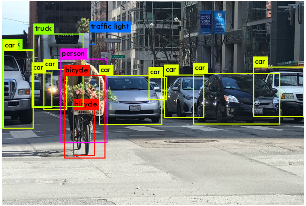
Based on joint work with Chengrun Yang (Cornell)

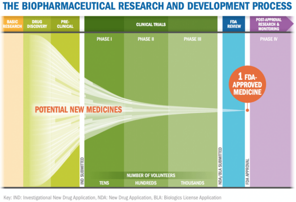
WIDS workshop, March 2021

Outline

So many machine learning problems. . .

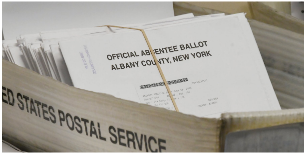


object detection



drug discovery

speech recognition



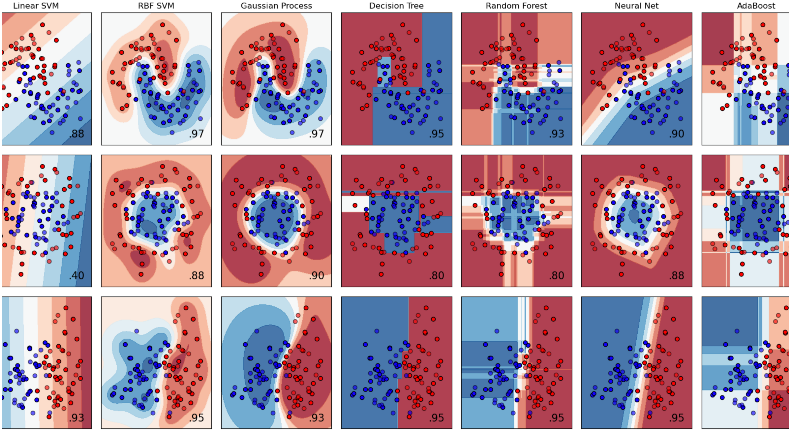
social science

. . . so little time

```
classifiers = [
    KNeighborsClassifier(3),
    SVC(kernel="linear", C=0.025),
    SVC(gamma=2, C=1),
    GaussianProcessClassifier(1.0 * RBF(1.0)),
    DecisionTreeClassifier(max_depth=5),
    RandomForestClassifier(max_depth=5, n_estimators=10, max_fe
    MLPClassifier(alpha=1, max_iter=1000),
    AdaBoostClassifier(),
    GaussianNB(),
    QuadraticDiscriminantAnalysis()]
```

source: `https://scikit-learn.org`

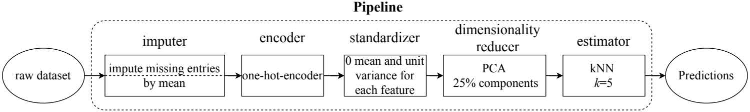
Different models perform differently



source: `https://scikit-learn.org`

Decisions, decisions...

a **pipeline**: a directed graph of learning components



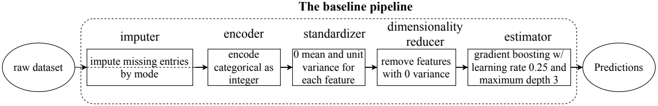
so many choices to make:

- data imputer: fill in missing values by median? ...
- encoder: one-hot encode? ...
- standardizer: rescale each feature? ...
- dimensionality reducer: PCA, or select by variance? ...
- estimator: use decision tree or logistic regression? ...
- hyperparameters: depth of decision tree?

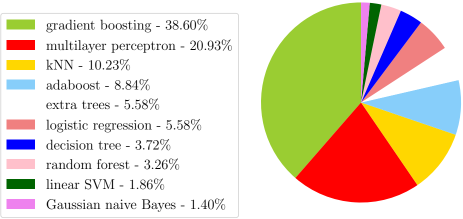
No Free Lunch

On 215 midsize OpenML classification datasets:

- The best-on-average pipeline (highest average ranking):



- The best estimator for each dataset:



source: [Yang et al.(2020)Yang, Fan, Wu, and Udell]

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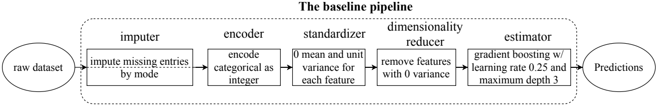

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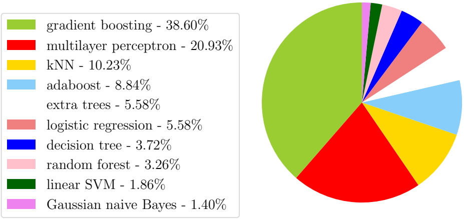

source: [Yang et al.(2020)Yang, Fan, Wu, and Udell]

Theorem (No free lunch [Wolpert(1996)])

There is no one model that works best for every problem.

Problem solved!

```
>>> import autosklearn.classification
>>> cls = autosklearn.classification.AutoSklearnClassifier()
>>> cls.fit(X_train, y_train)
>>> predictions = cls.predict(X_test)
```

```
dls = TabularDataLoaders.from_csv(path/'adult.csv', path=path, y_names="salary",
    cat_names = ['workclass', 'education', 'marital-status', 'occupation',
                 'relationship', 'race'],
    cont_names = ['age', 'fnlwgt', 'education-num'],
    procs = [Categorify, FillMissing, Normalize])

learn = tabular_learner(dls, metrics=accuracy)
learn.fit_one_cycle(2)
```

```
from flaml import AutoML
automl = AutoML()
automl.fit(X_train, y_train, task="classification")
```

```
# Run AutoML for 20 base models (limited to 1 hour max runtime by default)
aml = H2OAutoML(max_models=20, seed=1)
aml.train(x=x, y=y, training_frame=train)
```

```
from autogluon.tabular import TabularDataset, TabularPredictor
train_data = TabularDataset('https://autogluon.s3.amazonaws.com/datasets/Inc/train.csv')
test_data = TabularDataset('https://autogluon.s3.amazonaws.com/datasets/Inc/test.csv')
predictor = TabularPredictor(label='class').fit(train_data, time_limit=60)  # Fit models for 60s
leaderboard = predictor.leaderboard(test_data)
```

Definitions

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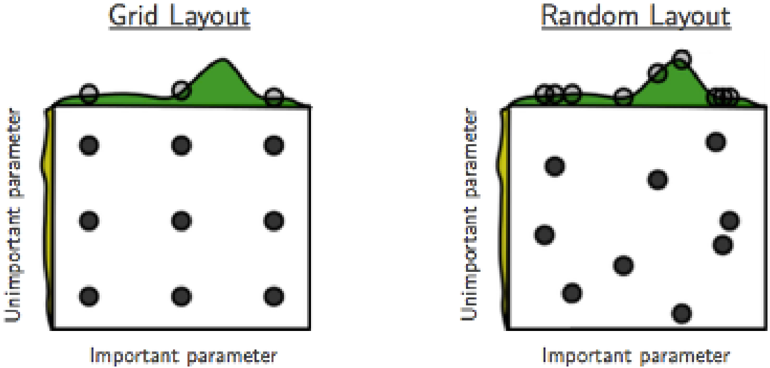
kinds of datasets: **tabular**, timeseries, image, text, video, genomics, . . .

Outline

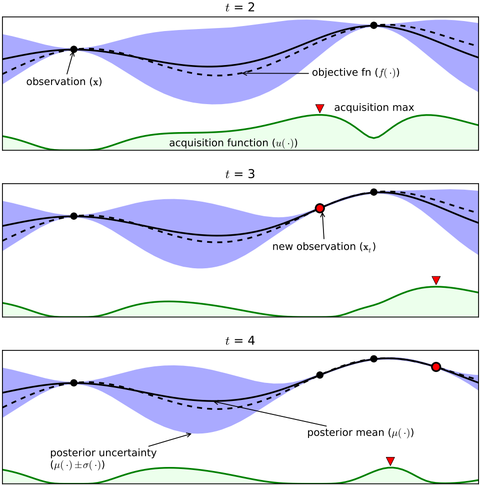
Grid search vs random search



source: Bergstra & Bengio 2012 [Bergstra and Bengio(2012)].

- grid search is more well-known
- random search samples more distinct values of each hyperparameter
- random search is more efficient when only some hyperparameters are important

Bayesian optimization (BO)

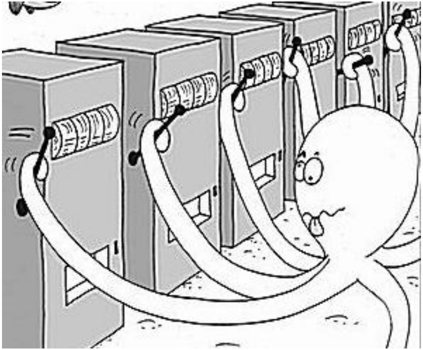


source: Brochu et al, 2010
[Brochu et al.(2010)Brochu, Cora, and De Freitas]

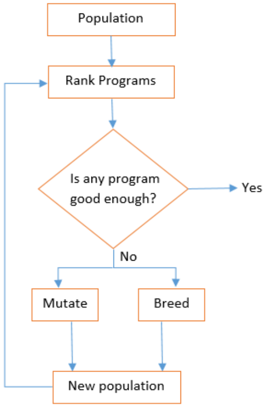
Multi-armed bandit

How long to spend evaluating each pipeline?

- Budget: training examples or training time
- Estimate performance of each pipeline with small budget
- Allocate budget to promising pipelines



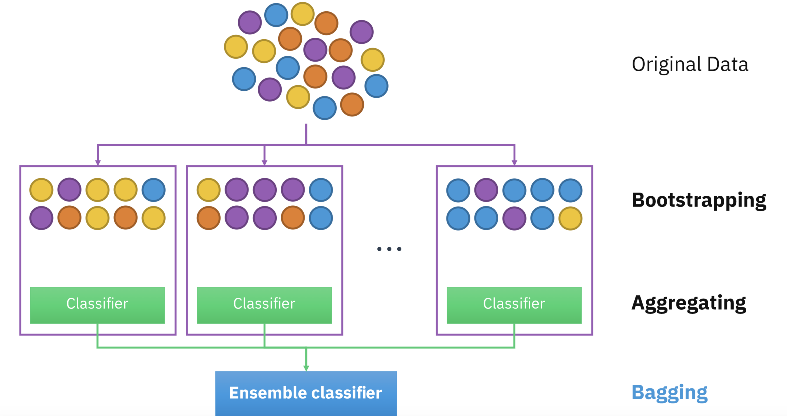
Genetic programming



"Survival of the fittest": Automatically explore numerous possible pipelines to find the best for the given dataset

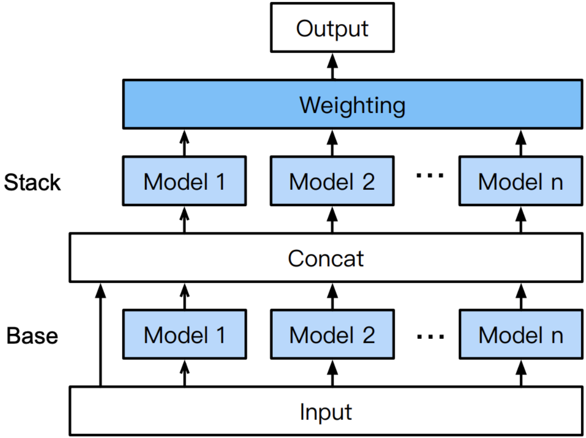
source: dotnetlovers.com

Ensemble



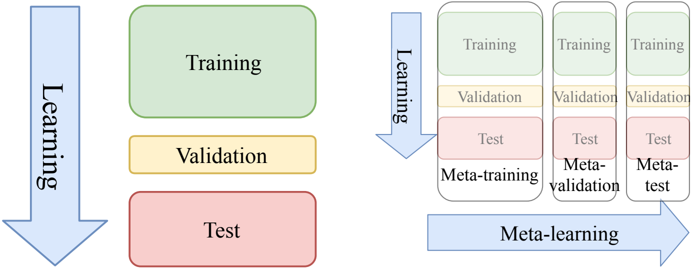
source: By Sirakorn - Own work, CC BY-SA 4.0,
https://commons.wikimedia.org/w/index.php?curid=85888768

Stacking



source: AutoGluon Tabular
[Erickson et al.(2020)Erickson, Mueller, Shirkov, Zhang, Larroy, Li, and Smola]

Metalearning



Learning

Metalearning

- learning splits datasets
- metalearning splits learning instances:
  - same model, different datasets ("sets of datasets")
    e.g., stock market data on different days
  - different models, same dataset
    e.g., performance of ridge regression at different λ's

source: OBOE [Yang et al.(2019)Yang, Akimoto, Kim, and Udell]

OBOE: low rank autoML

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$$A \approx XY$$

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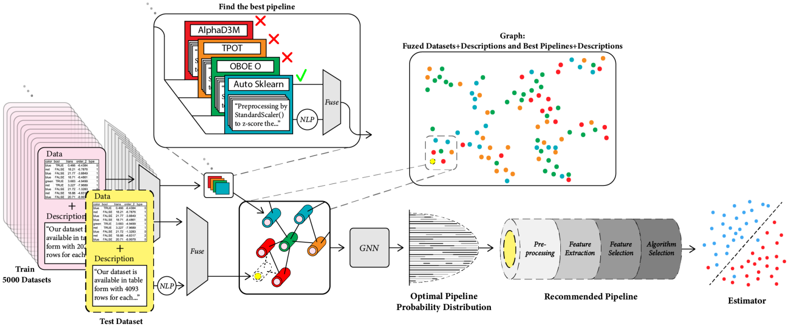
- rows $x_i \in \mathbf{R}^k$ of X are *dataset metafeatures*
- columns $y_j \in \mathbf{R}^k$ of Y are *model metafeatures*
- $x_i y_j \approx A_{ij}$ are *predicted model performance*

source: OBOE [Yang et al.(2019)Yang, Akimoto, Kim, and Udell]

Metalearning with NLP and GNNs



source: Real-time AutoML
[Drori et al.(2020)Drori, Liu, Ma, Deykin, Kates, and Udell]

Outline

AutoML systems

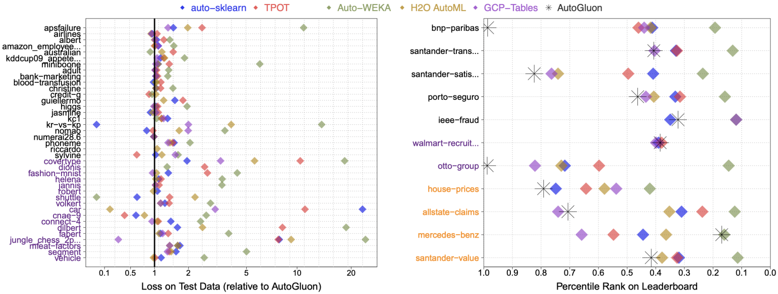
Optimizing over scikit-learn style models:

- **Auto-WEKA** [Thornton et al.(2013)Thornton, Hutter, Hoos, and Leyton-Brown]: BO on conditional search space
- **auto-sklearn** [Feurer et al.(2015)Feurer, Klein, Eggensperger, Springenberg, Blum meta-learning + BO
- **TPOT** [Olson et al.(2016)Olson, Urbanowicz, Andrews, Lavender, Kidd, ar genetic programming
- **Hyperband** [Li et al.(2018)Li, Jamieson, DeSalvo, Rostamizadeh, and Talwalkar multi-armed bandit
- **PMF** [Fusi et al.(2018)Fusi, Sheth, and Elibol]: matrix factorization + BO
- **Oboe** [Yang et al.(2019)Yang, Akimoto, Kim, and Udell]: matrix factorization + experiment design

Neural architecture search (NAS)

- **Google NAS** [Zoph and Le(2016)]: reinforcement learning
- **NASBOT** [Kandasamy et al.(2018)Kandasamy, Neiswanger, Schneider, Poczo
  BO + optimal transport
- **Auto-Keras** [Jin et al.(2019)Jin, Song, and Hu]: BO + network morphism
- **AutoML-Zero** [Real et al.(2020)Real, Liang, So, and Le]: genetic programming
- ...

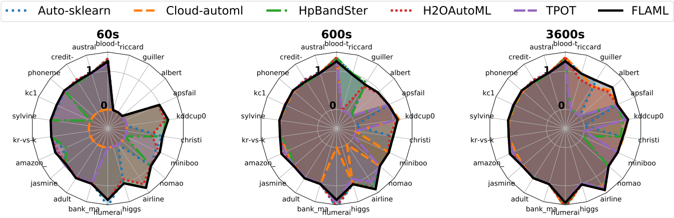
Lots of good options!



(A) AutoML Benchmark (1h) **(B)** Kaggle Benchmark (4h)

source: AutoGluon Tabular
[Erickson et al.(2020)Erickson, Mueller, Shirkov, Zhang, Larroy, Li, and Smola]

Fast and slow options



Binary classification datasets ordered by size counter clockwise, from smallest (blood-transfusion) to largest (riccardo). Metric: AUC.

source: FLAML [Wang et al.(2020)Wang, Wu, Weimer, and Zhu]

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- interpretability: can we find good, interpretable models? when is interpretability necessary?
- feature engineering
- overfitting
- cost:
  e.g., Google RL-based NAS [Zoph and Le(2016)]: 1k GPU days
  ($>$ \$70k on AWS)

Summary

- AutoML automatically picks a good ML pipeline for your problem
- lots of easy-to-use packages
- lots of interesting ideas

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