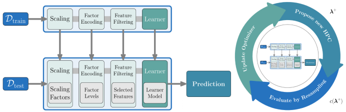
Introduction to Machine Learning

Hyperparameter Tuning
Pipelines and AutoML

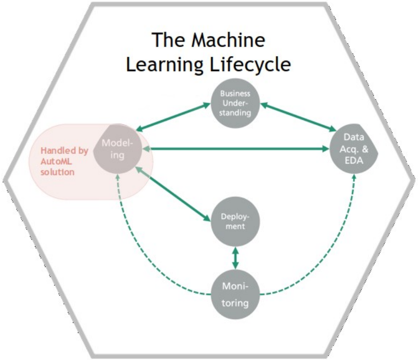


Learning goals

- Pipelines as connected steps of learnable operations
- Sequential pipeline
- Pipelines and DAGs

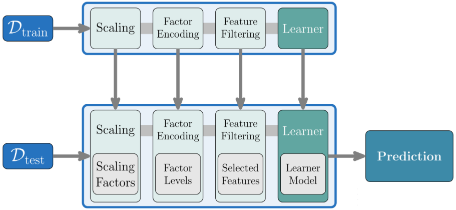
CASE FOR AUTOML

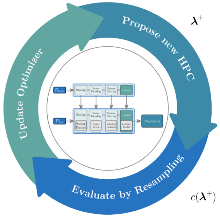
- More and more tasks are approached via data driven methods.
- Data scientists often rely on trial-and-error.
- The process is especially tedious for similar, recurring tasks.
- Not the entire machine learning lifecycle can be automated.



PIPELINES AND AUTOML

- ML typically has several data transformation steps before model fit
- If steps are in succession, data flows through sequential pipeline
- NB: Each node has a train and predict step and learns params
- And usually has HPs

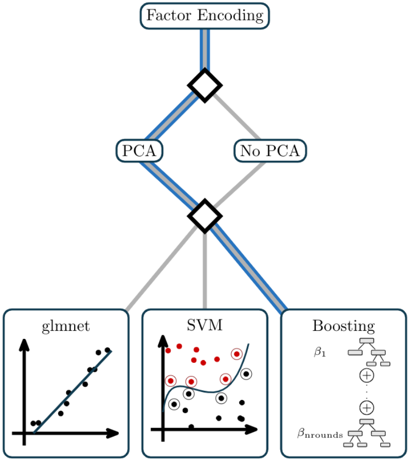




Pipelines are required to embed full model building into CV to avoid overfitting and biased evaluation!

PIPELINES AND AUTOML

- Further flexibility by representing pipeline as DAG
- Single source accepts $\mathcal{D}_{\text{train}}$, single sink returns predictions
- Each node represents a preprocessing operation, a learner, a postprocessing operation or controls data flow
- Can be used to implement ensembles, operator selection, . . .



PIPELINES AND AUTOML

- HPs of pipeline are the joint set of all HPs of its contained nodes: $\tilde{\mathbf{\Lambda}} = \tilde{\mathbf{\Lambda}}_{\text{op},1} \times \cdots \times \tilde{\mathbf{\Lambda}}_{\text{op},k} \times \tilde{\mathbf{\Lambda}}_{\mathcal{I}}$
- HP space of a DAG is more complex: Depending on branching / selection different nodes and HPs are active $\rightarrow$ **hierarchical search space**

Search Space $\tilde{\Lambda}$

Name	Type	Bounds/Values	Trafo
`encoding`	C	one-hot, impact	
◇ `pca`	C	PCA, no PCA	
◇ `learner`	C	glmnet, SVM, Boosting	
`if learner = glmnet`			
`s`	R	$[-12, 12]$	2^x
`alpha`	R	$[0, 1]$	–
`if learner = SVM`			
`cost`	R	$[-12, 12]$	2^x
`gamma`	R	$[-12, 12]$	2^x
`if learner = Boosting`			
`eta`	R	$[-4, 0]$	10^x
`nrounds`	I	$\{1, \ldots, 5000\}$	–
`max_depth`	I	$\{1, \ldots, 20\}$	–

A graph that includes many preprocessing steps and learner types can be flexible enough to work on a large number of data sets

Combining such graph with an efficient tuner is key in AutoML

AUTOML – CHALLENGES

- Most efficient approach?
- How to integrate human a-priori knowledge?
- How can we best (computationally) transfer “experience” into AutoML? Warmstarts, learned search spaces, etc.
- Multi-Objective goals, including model intepretability
- AutoML as a process is too much of a black-box, hurts adoption.