How Powerful are Performance Predictors in Neural Architecture Search?

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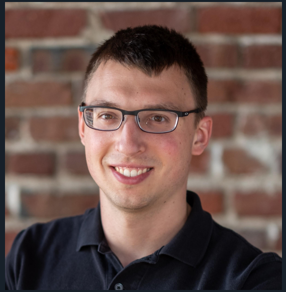

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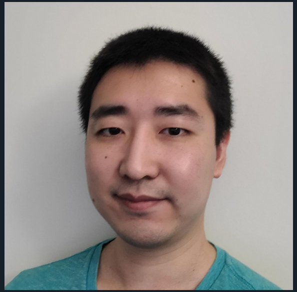

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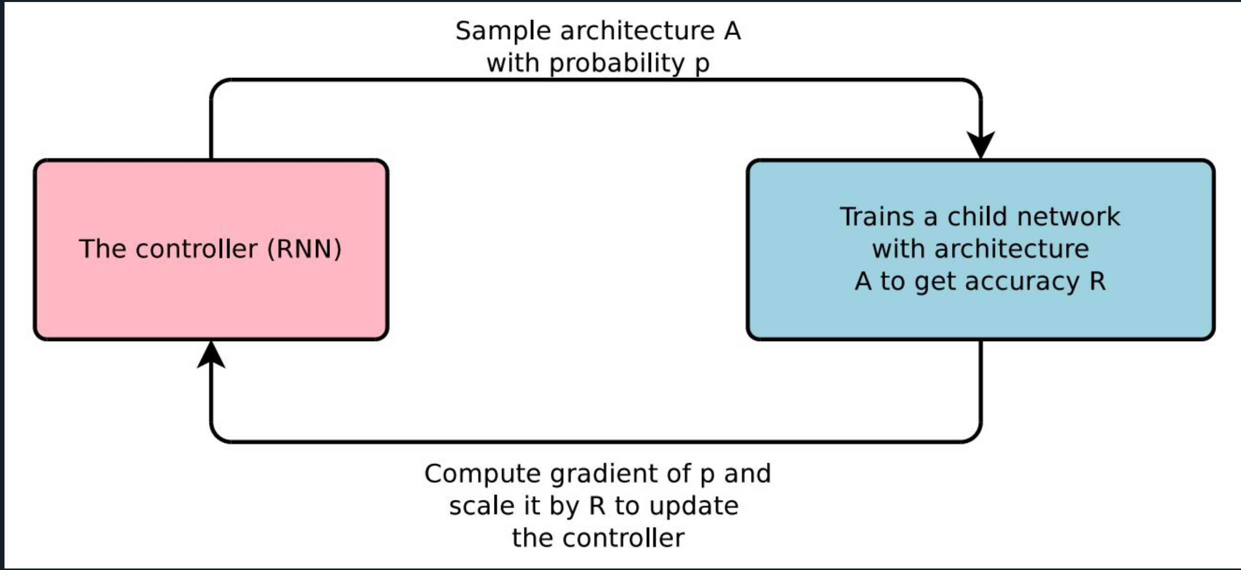
Slides (with hyperlinks): https://crwhite.ml

Performance prediction techniques

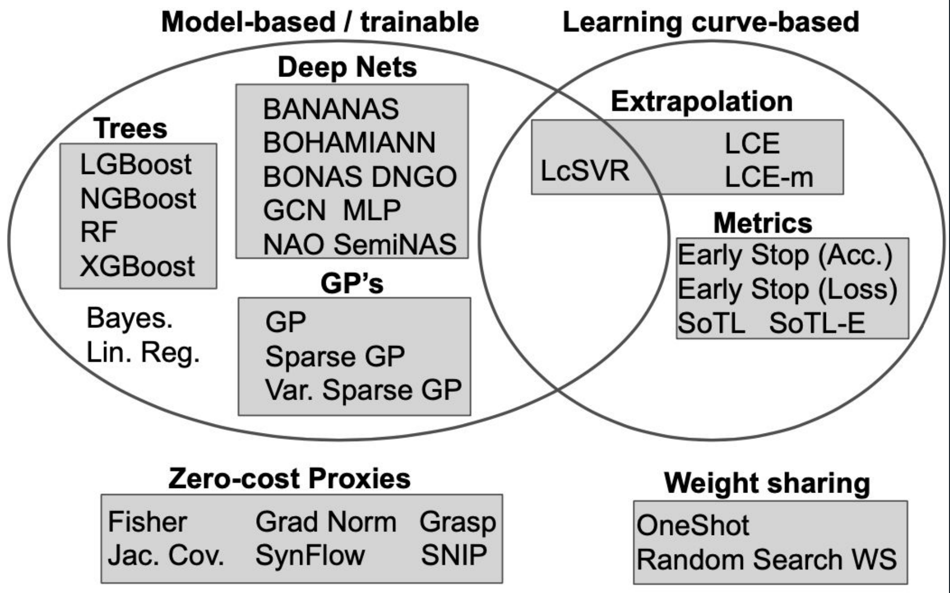
- Early NAS algos required fully training 1000s of architectures [Zoph and Le 2016]
- Recent algos use techniques to predict the final performance of architectures



Performance Predictors

A *performance predictor* is any technique which predicts the final accuracy or ranking of architectures, without fully training them

- ***Initialization:*** performs any necessary pre-computation
- ***Query:*** take any architecture as input, and output predicted accuracy
- (***Update:*** similar to initialization)



Outline

- Motivation
- Introduction to Performance Predictors
  - Model-based predictors
  - Learning curve based predictors
  - Zero-cost predictors
  - Weight sharing
- Experiments: 31 performance predictors
  - Stand-alone predictor experiments
  - OMNI
  - NAS experiments
- Conclusion

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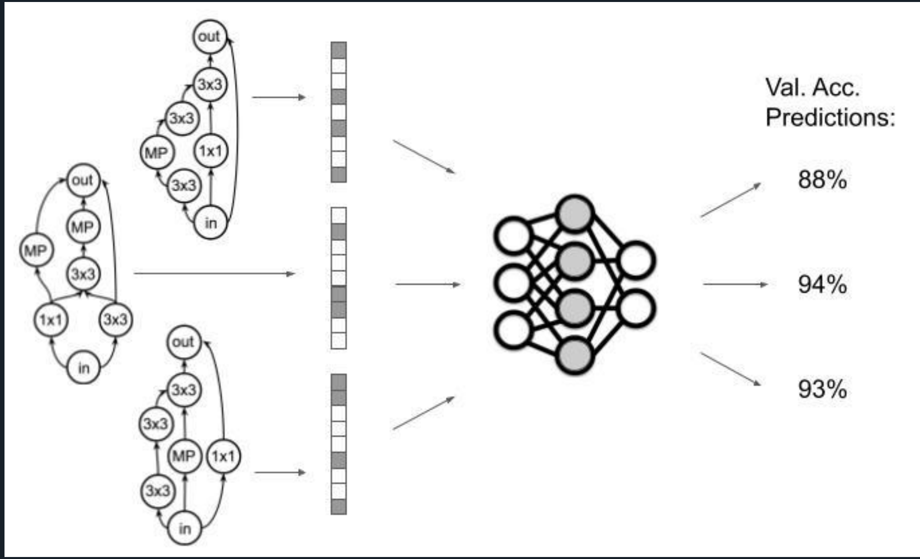
Model-Based Predictors

- Supervised learning - regression
  - X - the architecture encoding (e.g. one-hot adjacency matrix)
  - Y - validation accuracy of trained architecture



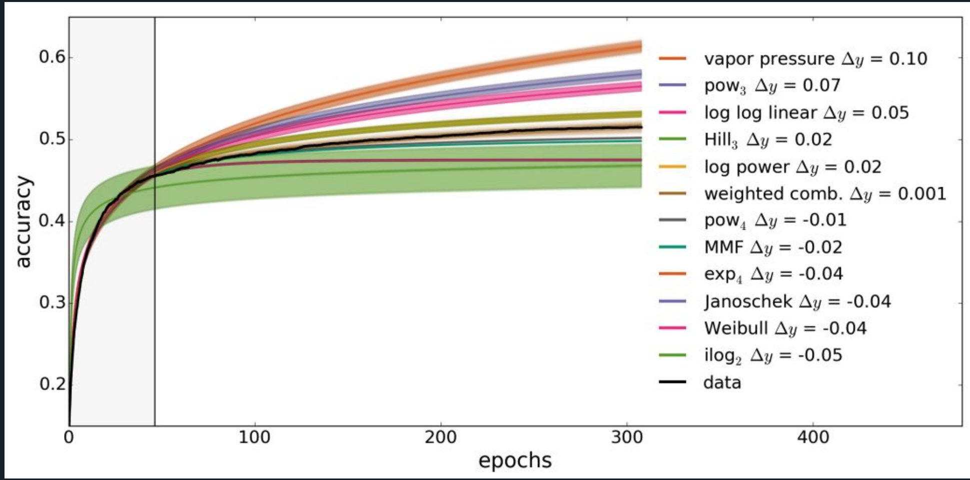
[White et al. 2019]

- Gaussian processes [Kandasamy et al. 2018], [Jin et al. 2018]
- Boosted trees [Luo et al. 2020], [Siems et al. 2020]
- GNNs [Shi et al. 2019], [Wen et al. 2019]
- Specialized encodings [White et al. 2019], [Ning et al. 2020]

High init time, **low query time**

Learning curve based predictors

- Learning curve extrapolation
  - Fit partial learning curve to parametric model [Domhan et al. 2015]
  - Bayesian NN [Klein et al. 2017]
- Training statistics
  - Early stopping (val acc) [Elsken et al. 2018]
  - Sum of training losses [Ru et al. 2020]



[Elsken et al. 2018]

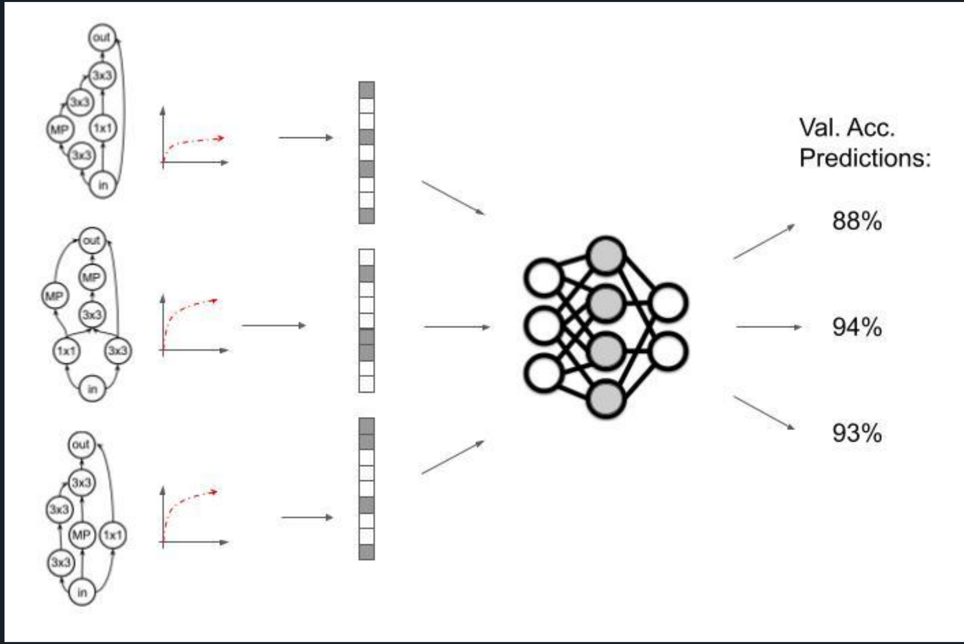
No init time, **high query time**

Hybrid model-based + LC predictors

Train a model, using partial learning curve + hyperparams, to predict final accuracy

- First and second derivatives as features, SVR [Baker et al. 2017]
- Full LC as features, Bayesian NN [Klein et al. 2017]

High init time, high query time

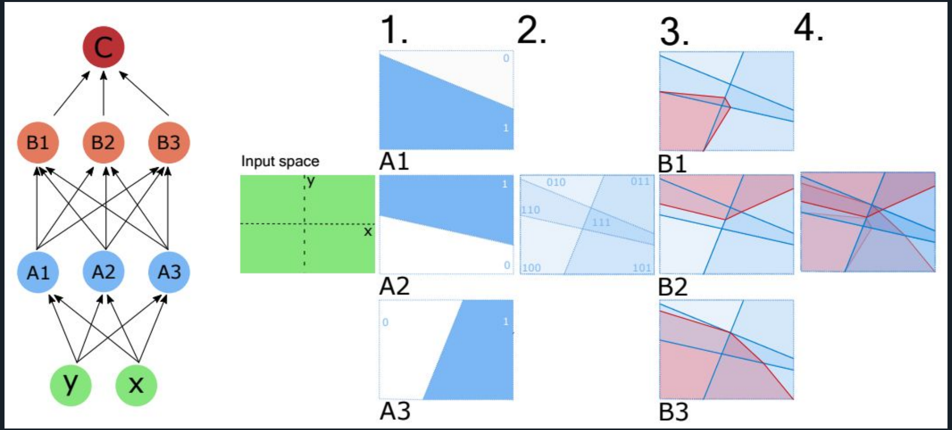


“Zero-cost” proxies

Compute a statistic of an architecture in 3-5 seconds

- Jacobian covariance [Mellor et al. 2020]
- Synaptic Flow [Abdelfattah et al. 2021]
    - SNIP [Lee et al. 2018]

Low init time, low query time



[Mellor et al. 2020]

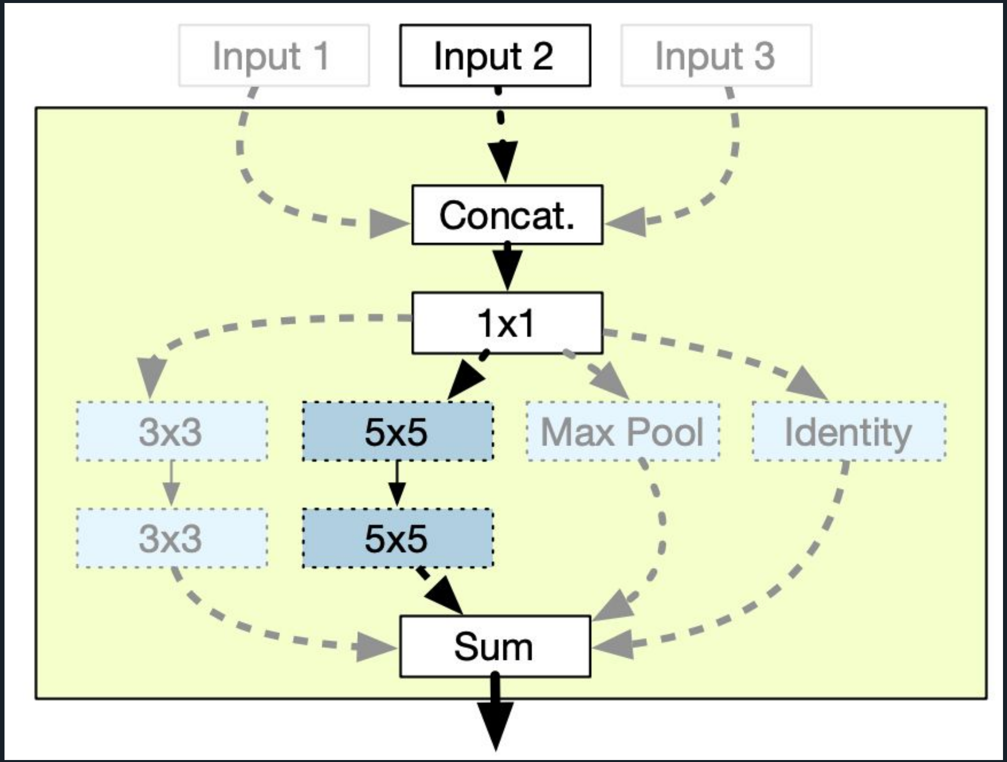
[Abdelfattah et al. 2021]

$$\texttt{snip} : \mathcal{S}_p(\theta) = \left| \frac{\partial \mathcal{L}}{\partial \theta} \odot \theta \right|, \qquad \texttt{grasp} : \mathcal{S}_p(\theta) = -(H \frac{\partial \mathcal{L}}{\partial \theta}) \odot \theta, \qquad \texttt{synflow} : \mathcal{S}_p(\theta) = \frac{\partial \mathcal{L}}{\partial \theta} \odot \theta$$

Weight Sharing

Train a set of shared weights that can be used by all architectures (the Supernetwork)

- OneShot [Bender et al. 2018]
- Random Search WS [Li & Talwalkar 2019]



[Bender et al. 2018]

Medium init time, low query time

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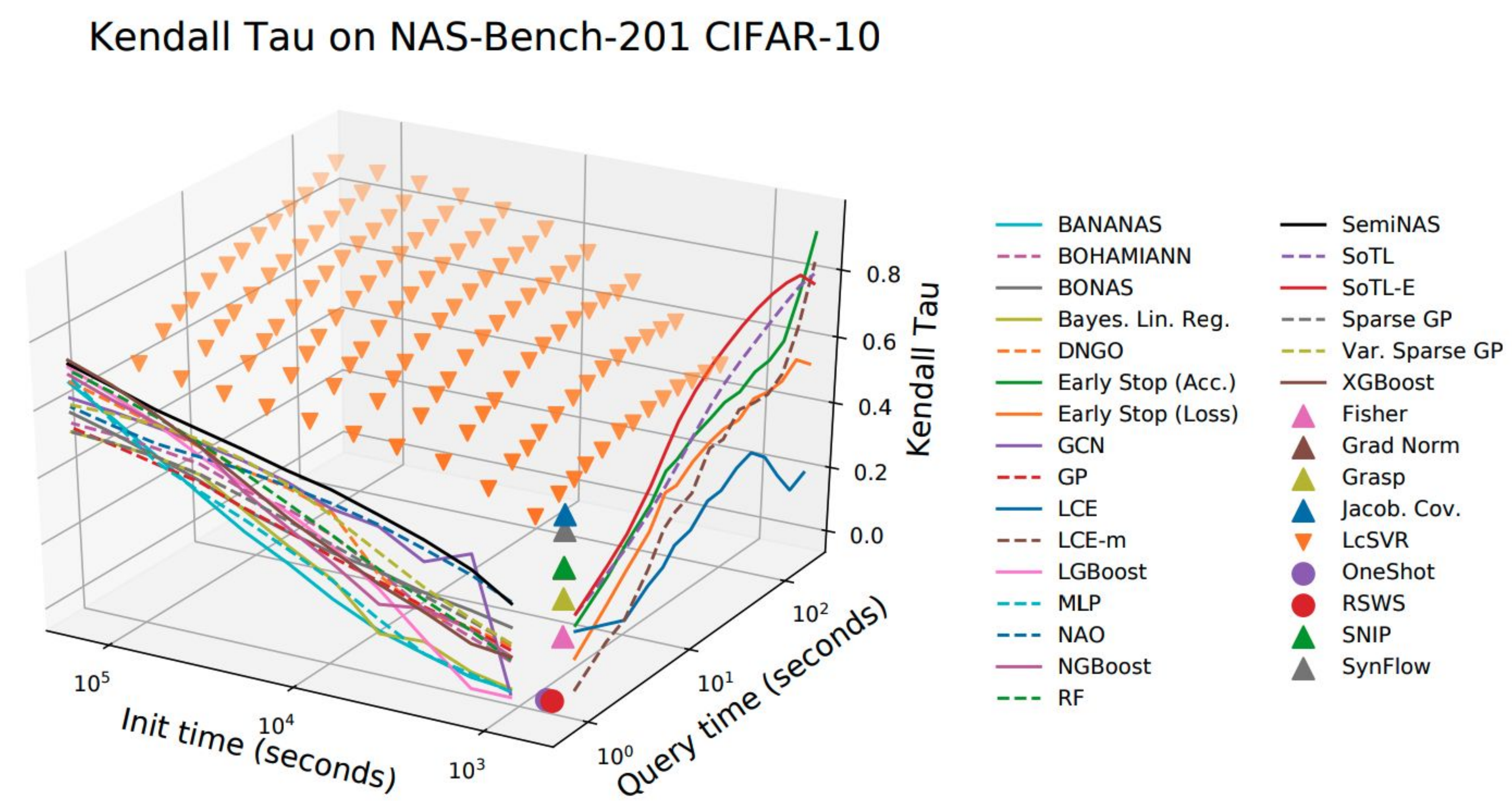
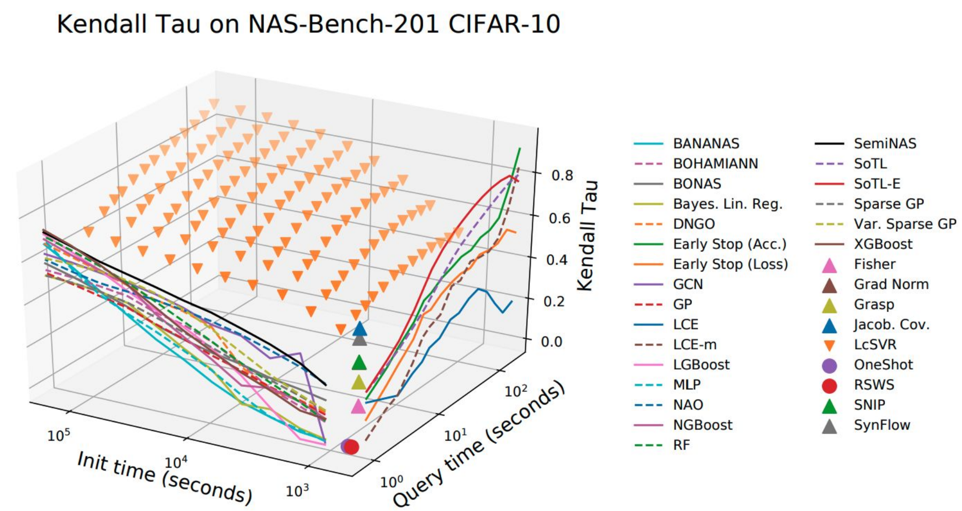
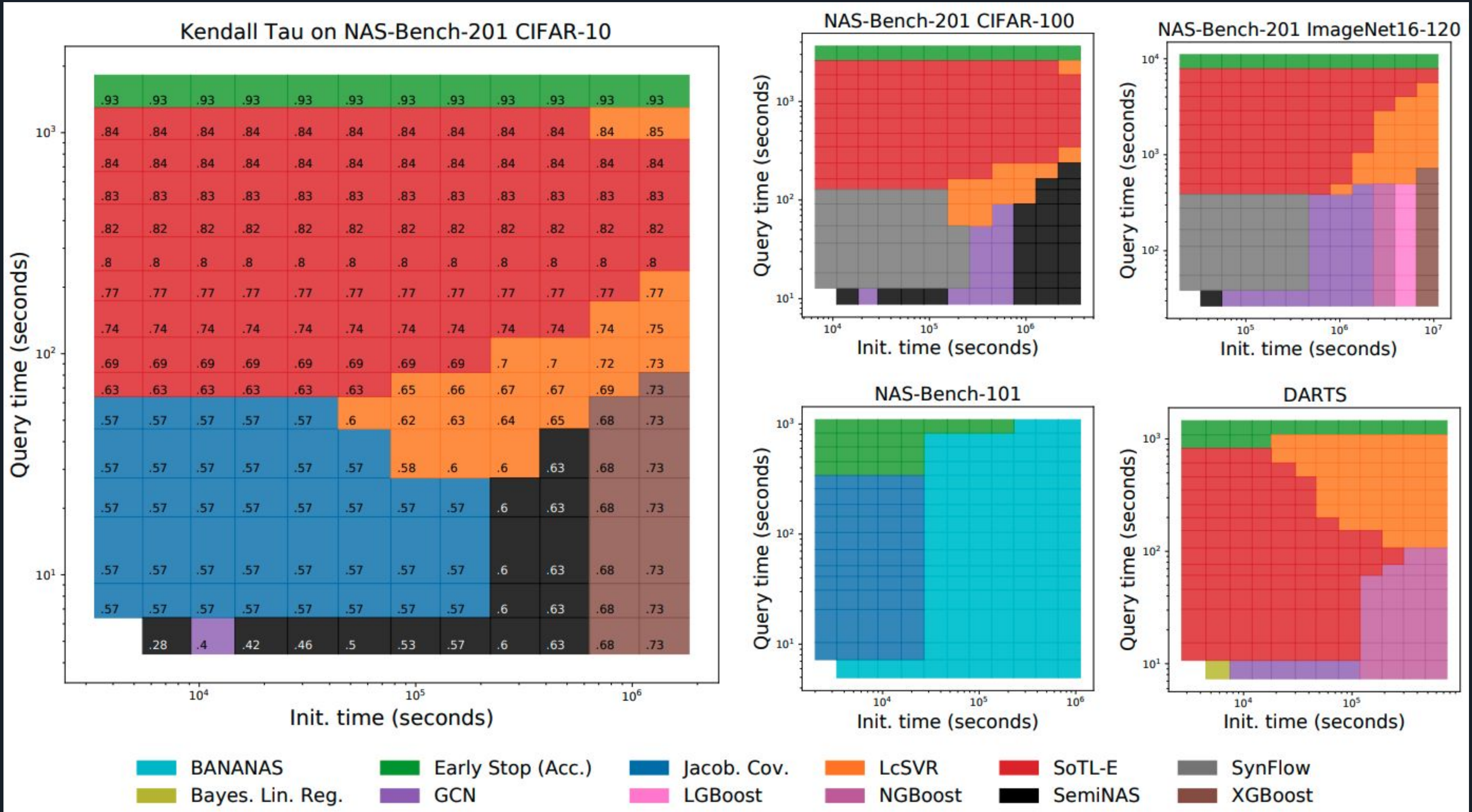


Kendall Tau on NAS-Bench-201 CIFAR-10
Kendall Tau
0.0
0.2
0.4
0.6
0.8
Init time (seconds)
10^5
10^4
10^3
Query time (seconds)
10^0
10^1
10^2
BANANAS
BOHAMIANN
BONAS
Bayes. Lin. Reg.
DNGO
Early Stop (Acc.)
Early Stop (Loss)
GCN
GP
LCE
LCE-m
LGBoost
MLP
NAO
NGBoost
RF
SemiNAS
SoTL
SoTL-E
Sparse GP
Var. Sparse GP
XGBoost
Fisher
Grad Norm
Grasp
Jacob. Cov.
LcSVR
OneShot
RSWS
SNIP
SynFlow

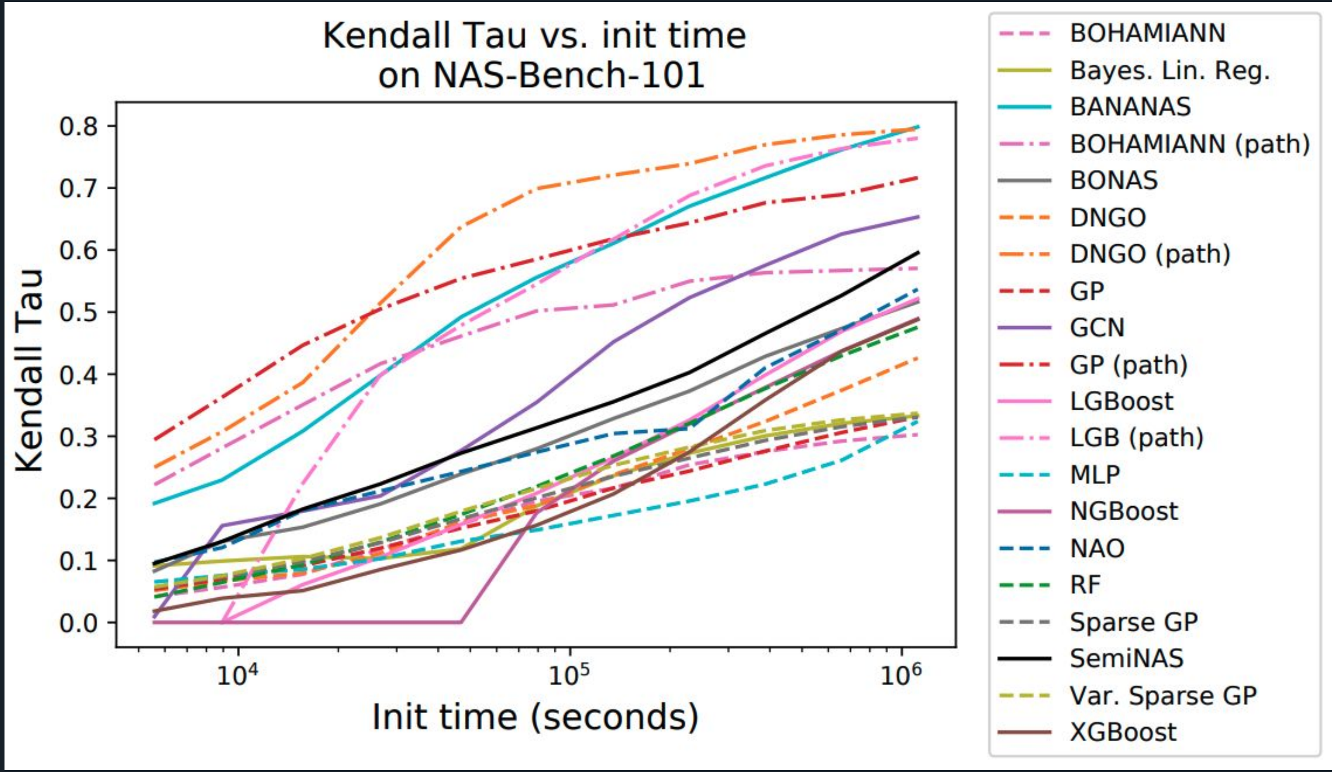
Notes on experiments

- Three axes of comparison: initialization time, query time, correlation / rank correlation metrics
- Official implementation whenever possible
- Train/test data drawn u.a.r.
- Light hyperparameter tuning
  - Levels the playing field
  - Cross-validation is often used during NAS

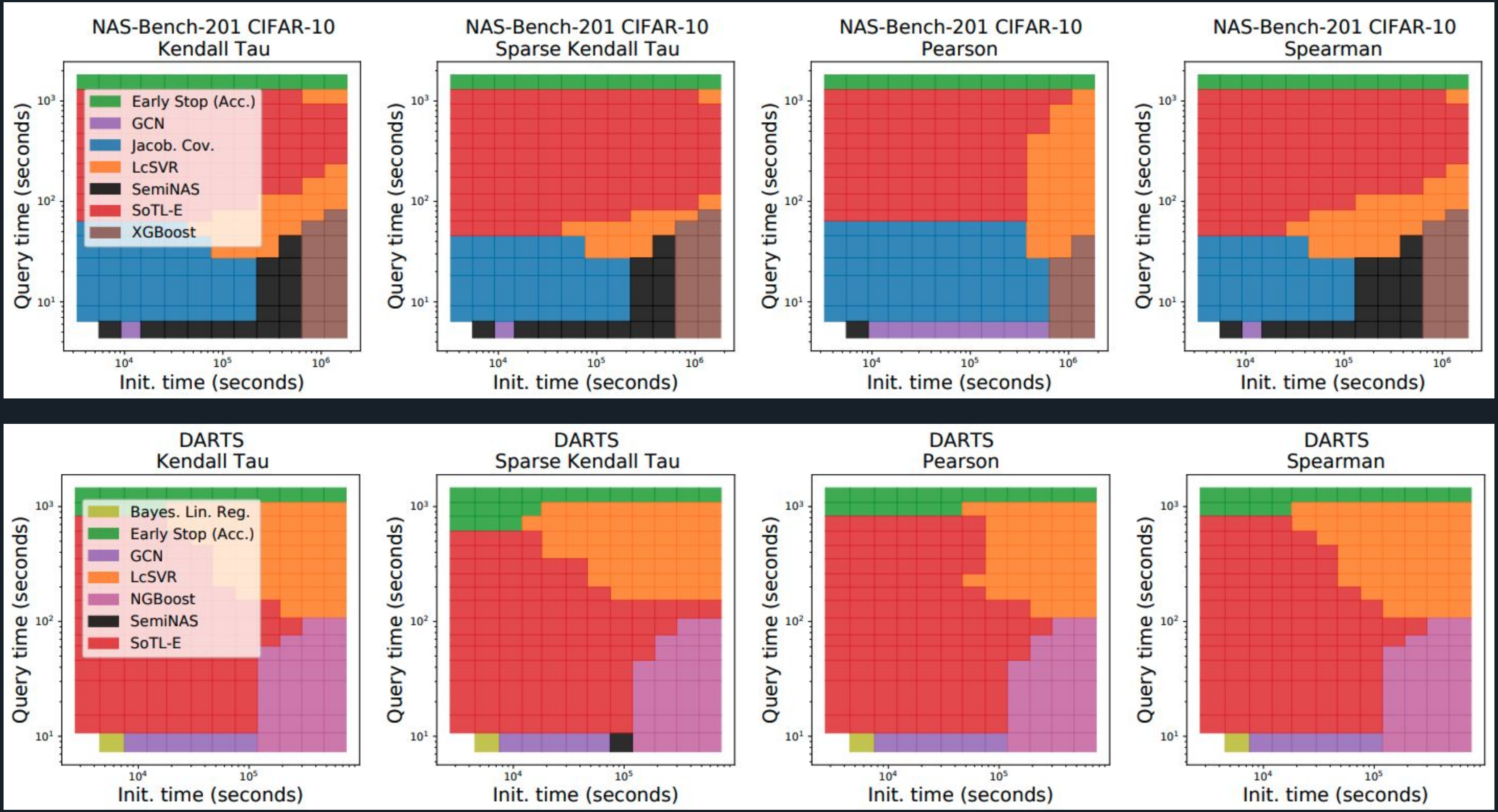



Kendall Tau on NAS-Bench-201 CIFAR-10
NAS-Bench-201 CIFAR-100
NAS-Bench-201 ImageNet16-120
NAS-Bench-101
DARTS
Query time (seconds)
Init. time (seconds)
BANANAS
Bayes. Lin. Reg.
Early Stop (Acc.)
GCN
Jacob. Cov.
LGBoost
LcSVR
NGBoost
SoTL-E
SemiNAS
SynFlow
XGBoost

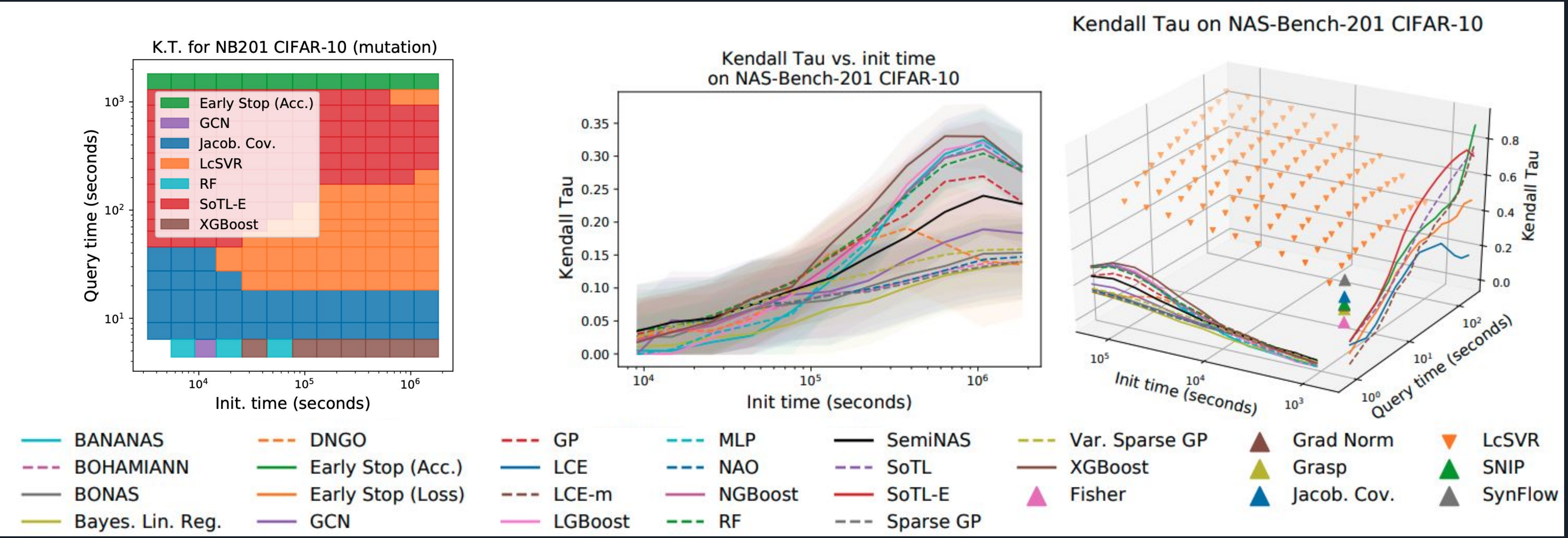
NAS-Bench-101: a more complex search space



- Path encoding performs very well


NAS-Bench-201 CIFAR-10
Kendall Tau
NAS-Bench-201 CIFAR-10
Sparse Kendall Tau
NAS-Bench-201 CIFAR-10
Pearson
NAS-Bench-201 CIFAR-10
Spearman
Early Stop (Acc.)
GCN
Jacob. Cov.
LcSVR
SemiNAS
SoTL-E
XGBoost
Query time (seconds)
Init. time (seconds)
DARTS
Kendall Tau
DARTS
Sparse Kendall Tau
DARTS
Pearson
DARTS
Spearman
Bayes. Lin. Reg.
Early Stop (Acc.)
GCN
LcSVR
NGBoost
SemiNAS
SoTL-E
Query time (seconds)
Init. time (seconds)

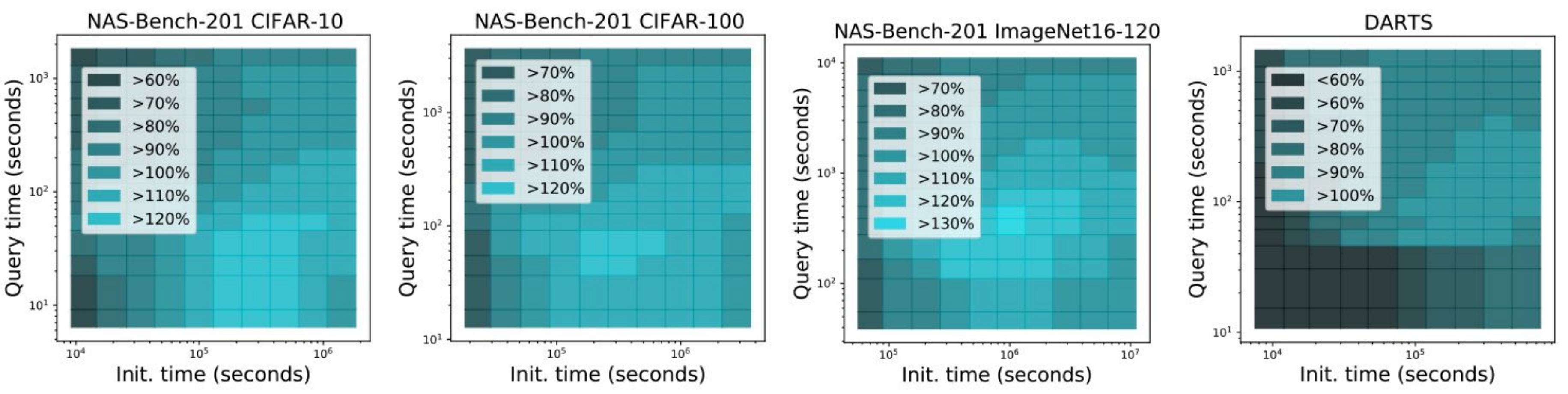
Mutation-based train/test sets



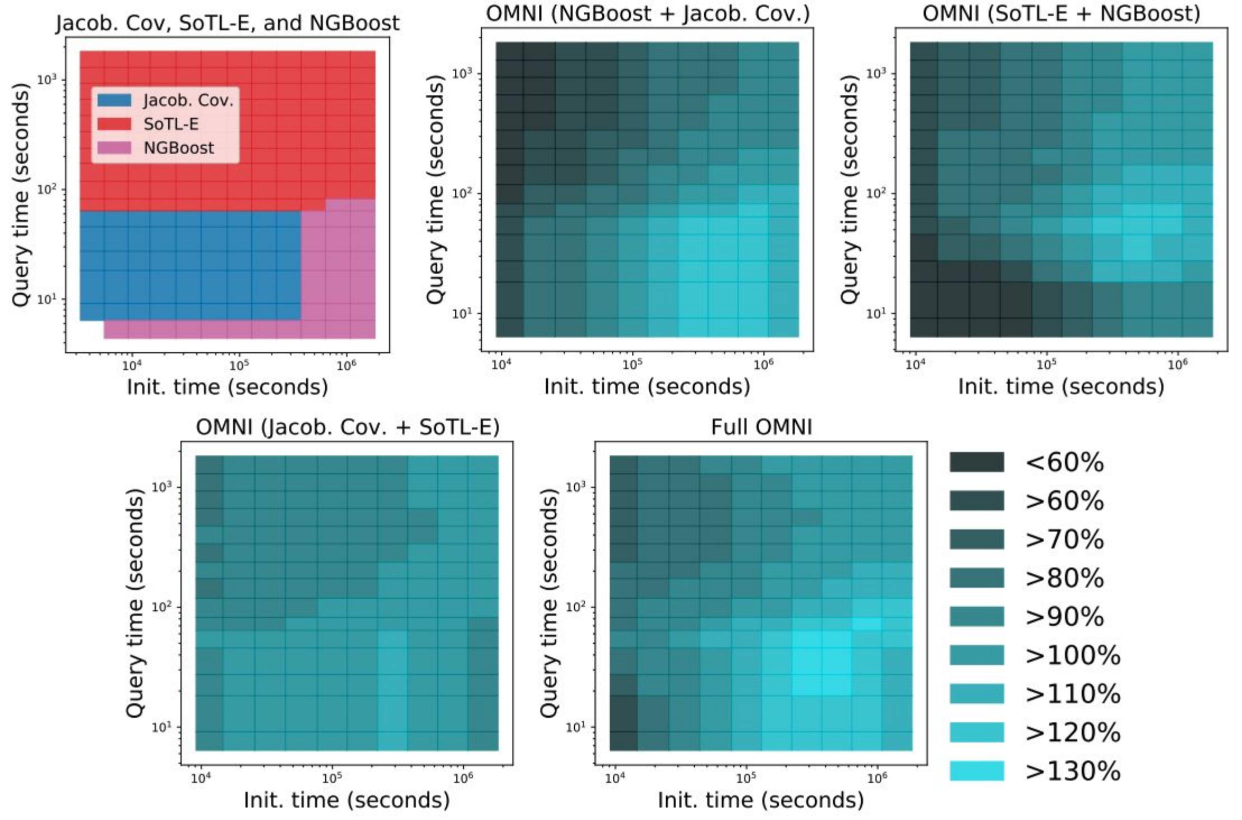
- Model-based predictors perform worse. Trees are comparatively better

OMNI: The Omnipotent Predictor

- Combine best predictors from three families: SoTL + Jacob. Cov + NGBoost
- Consistent performance almost everywhere
- 20% improvement in most-competitive bottom row

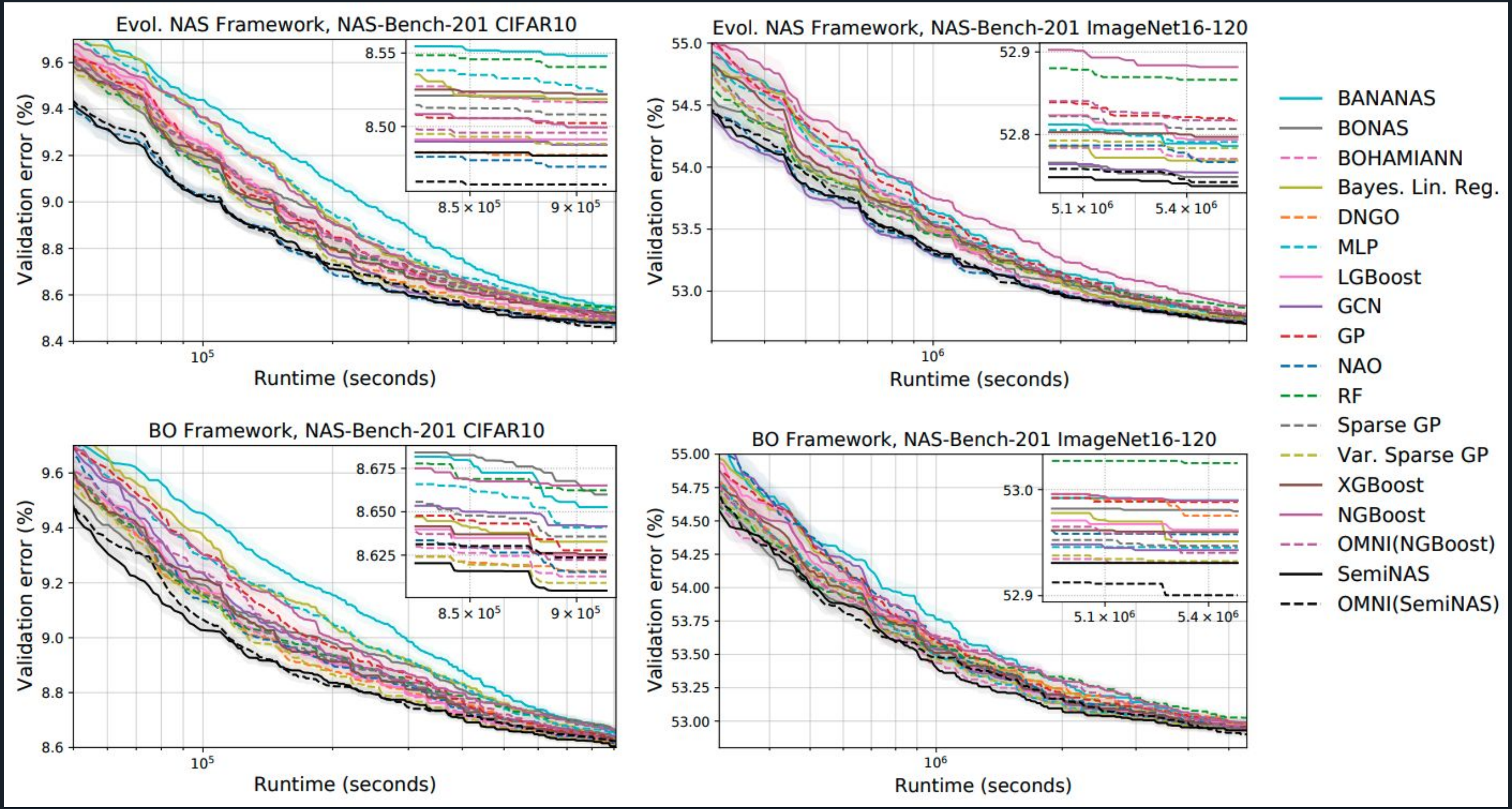


OMNI Ablation



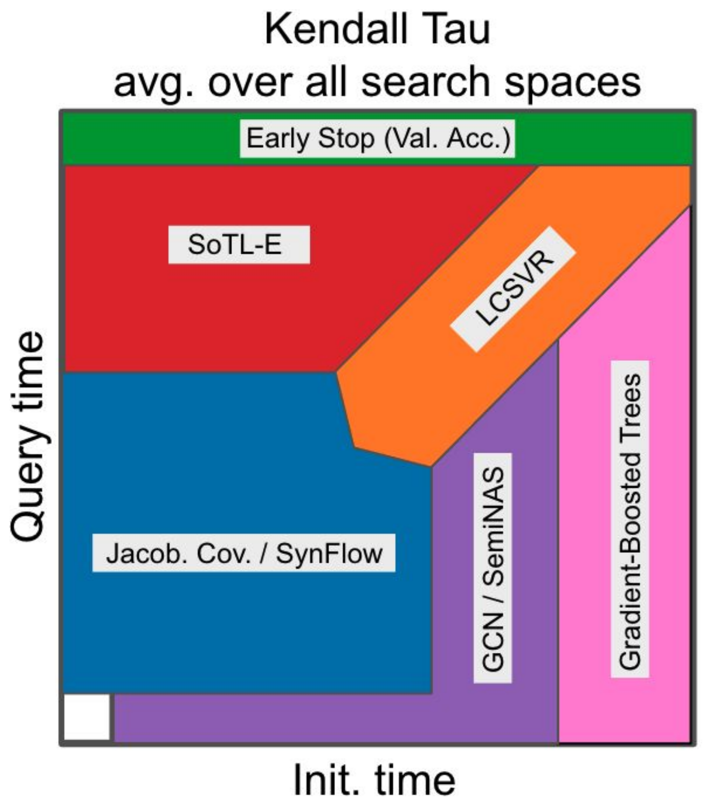
- Jacob. Cov + SoTL-E is consistent
- NGBoost needed for top performance in lower middle/right

NAS Experiments



So… How powerful are performance predictors?

- Largely the same trends across all experiments
- Combining predictors works the best
- Complex search spaces: specialized encodings (e.g. path encoding)



Conclusions & Future Work

- First large-scale study of performance predictors
- Four families, 31 total performance predictors
- OMNI achieves the best performance

Future work

- Zero-cost predictors that work on larger search spaces
- More sophisticated combinations of predictors + integration in NAS

Code: https://github.com/automl/NASLib

Full paper: https://arxiv.org/abs/2104.01177

Thanks!

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