AutoML: Neural Architecture Search (NAS)

Practical Recommendations for NAS and HPO

Bernd Bischl   Frank Hutter   Lars Kotthoff
Marius Lindauer   Joaquin Vanschoren

Maturity of the Fields of NAS and HPO

- Hyperparameter optimization is a mature field
  - Blackbox HPO has been researched for decades; there are many software packages
  - Multi-fidelity HPO has also become quite mature

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- Given a new dataset, HPO is crucial for good performance; NAS may not be necessary
  - The biggest gains typically come from tuning key hyperparameters (learning rate, etc)
  - Reusing a previous achitecture often yields competitive results

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    - + Auto-PyTorch Tabular [Zimmer, Lindauer & Hutter, 2020]
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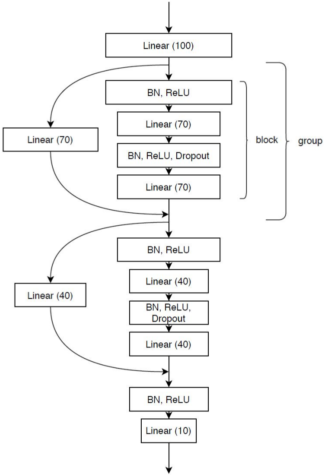
    - + If you don't have decent hyperparameters: first run HPO to get competitive

Case Study: NAS & HPO in Auto-PyTorch Tabular [Zimmer, Lindauer & Hutter, 2020]

- Joint Architecture Search and Hyperparameter Optimization



	Name	Range	log	type	cond.
Archi-tecture	network type	[ResNet, MLPNet]	-	cat	-
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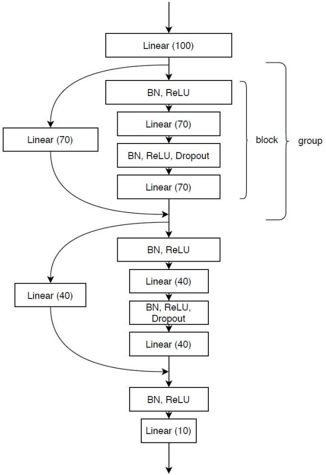

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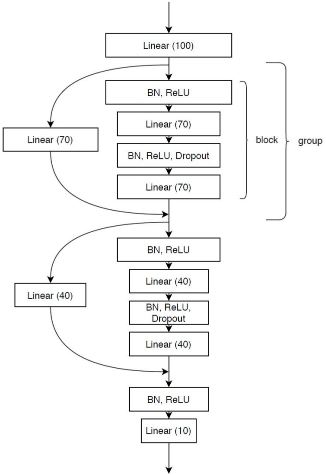

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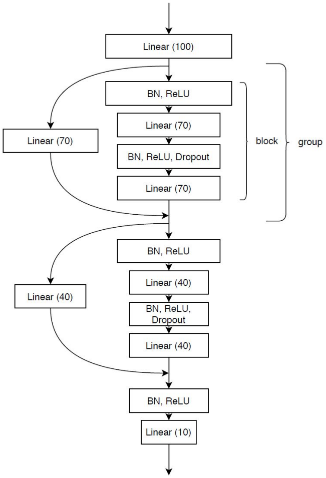

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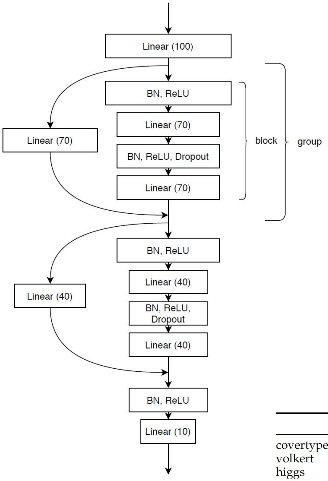

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	Auto-PyTorch	AutoGluon	AutoKeras	Auto-Sklearn	hyperopt-sklearn
covertype	**96.86 ± 0.41**	-	61.61 ± 3.52	-	-
volkert	**79.46 ± 0.43**	68.34 ± 0.10	44.25 ± 2.38	67.32 ± 0.46	-
higgs	**73.01 ± 0.09**	72.6 ± 0.00	71.25 ± 0.29	72.03 ± 0.33	-
car	**99.22 ± 0.02**	97.19 ± 0.35	93.39 ± 2.82	98.42 ± 0.62	98.95 ± 0.96
mfeat-factors	**99.10 ± 0.18**	98.03 ± 0.23	97.73 ± 0.23	98.64 ± 0.39	97.88 ± 38.48
apsfailure	99.32 ± 0.01	**99.5 ± 0.03**	-	99.43 ± 0.04	-
phoneme	**90.59 ± 0.13**	89.62 ± 0.06	86.76 ± 0.12	89.26 ± 0.14	89.79 ± 4.54
dibert	**99.04 ± 0.15**	98.17 ± 0.05	96.51 ± 0.62	98.14 ± 0.47	-

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  - Estimate depth from stereo images

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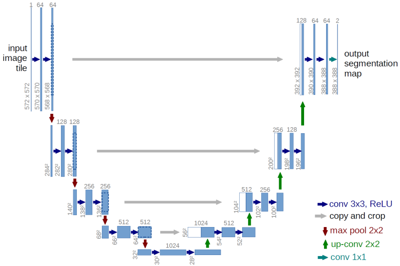

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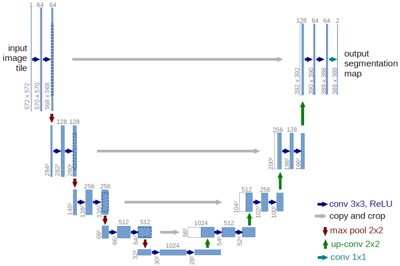
  - 3 cells: keeping spatial resolution, downsampling, and new upsampling cell that supports U-Net like skip connections



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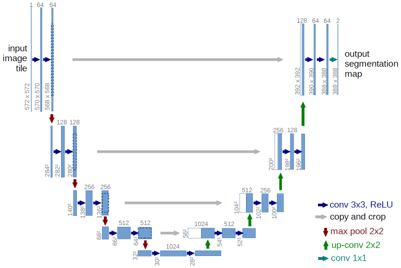
  - 3 cells: keeping spatial resolution, downsampling, and new upsampling cell that supports U-Net like skip connections
- Both NAS and HPO improved the state of the art [Saikat et al. 2019]:
  - End-point-error (EPE) on Sintel dataset: 2.36 $\rightarrow$ 2.14 (by DARTS)
  - Subsequent HPO: 2.14 $\rightarrow$ 1.94 (by BOHB)



Questions to Answer for Yourself / Discuss with Friends

- Repetition:
  If you want to use both HPO and NAS for your problem, how could you proceed?
- Discussion:
  Think of a problem of your particular interest. For that problem, which approach would you use to combine HPO and NAS, and why?