# AutoML: Neural Architecture Search (NAS)

## Blackbox Optimization Methods

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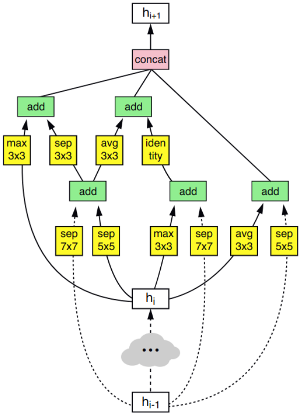
  - 2 categorical variables choosing between operations
  - 1 categorical variable choosing the combination method
  - Total number of hyperparameters for the cell: 5B (with B=5 by default)



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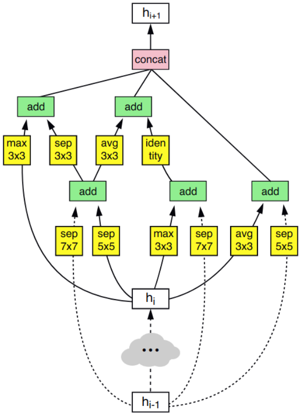


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- In general: one may require conditional hyperparameters
  - E.g., chain-structured search space
    - Top-level hyperparameter: number of layers L
    - Hyperparameters of layer k conditional on L $\geq$ k

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  - Initialize a population of $N$ random architectures
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- Mutations include adding, changing or removing a layer

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  - Joint optimization of a vision architecture with 238 hyperparameters [Bergstra et al. 2013]
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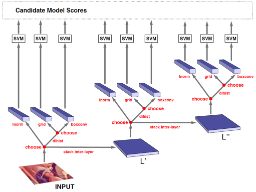

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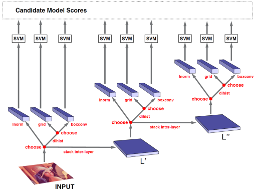

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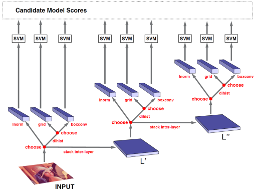


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  - In 2015, Auto-Net already had several successes in ML competitions
    - E.g., human action recognition:
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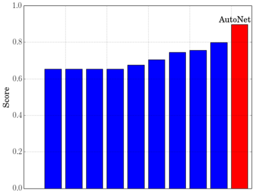

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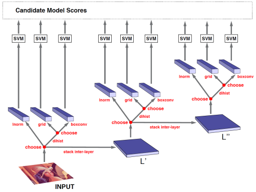
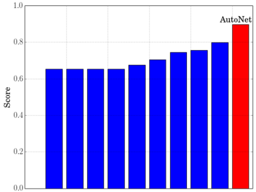
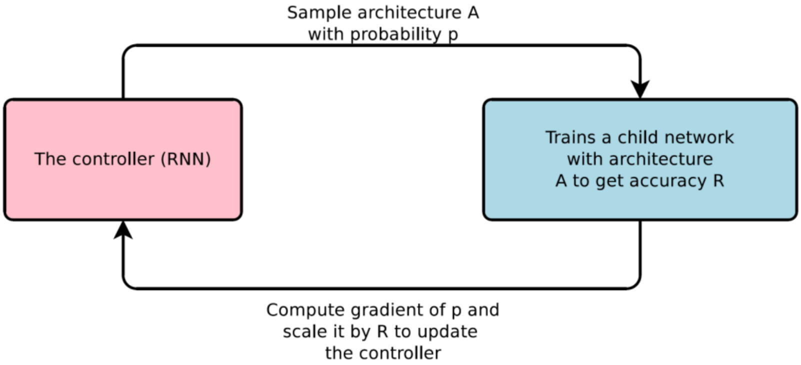
- With Gaussian processes:
  - Arc kernel [Swersky et al. 2013]



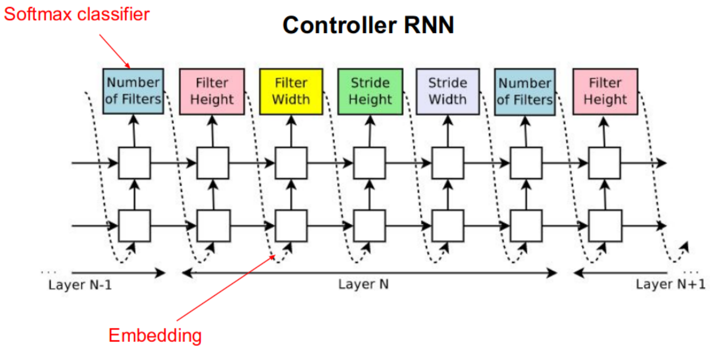



# Reinforcement Learning [Zoph and Le. 2016]




- Use RNN ("Controller") to generate a NN architecture piece-by-piece
- Train this NN ("Child Network") and evaluate it on a validation set
- Use Reinforcement Learning (RL) to update the parameters of the Controller RNN to optimize the performance of the child models

# Learning CNNs with RL [Zoph and Le. 2016]

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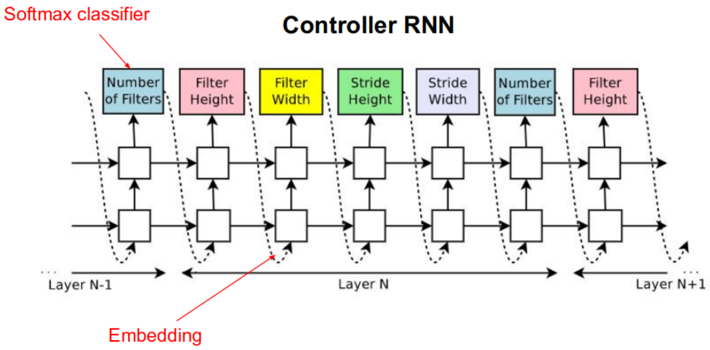


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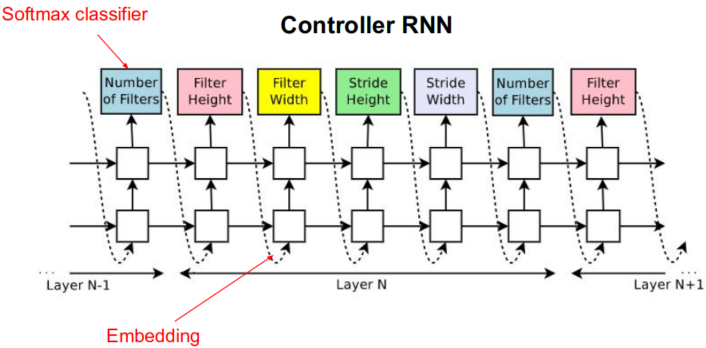
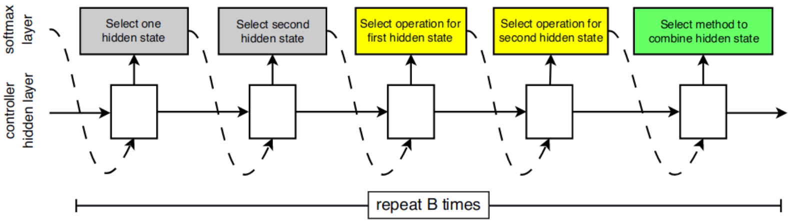


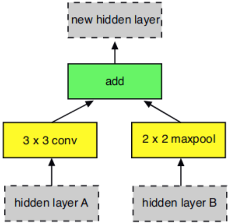

- For a fixed number of layers, select:
  - Filter width/height, stride width/height, number of filters
- Large computational demands (800 GPUs for 2 weeks, 12.800 architectures evaluated)
- State-of-the-art results for CIFAR-10 & Penn Treebank architecture

  $\rightarrow$ Brought NAS into the limelight

# Learning CNN cells with RL [Zoph et al. 2018]

- 2 types of cells: normal and reduction cells
- For each type of cell: $B$ blocks, each with 5 choices
  - Choose two previous feature maps (from this cell)
  - For each of these, choose an operation (3$\times$3 conv, max-pool, etc.)
  - Choose a merge operation to combine the two results (concat or add)



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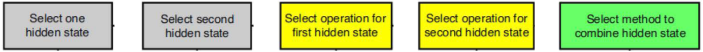
- Evolution simply tackles this as a HPO problem with $2\times5\times B$ variables:



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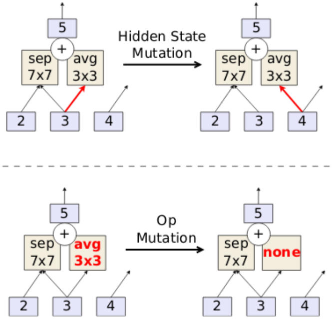


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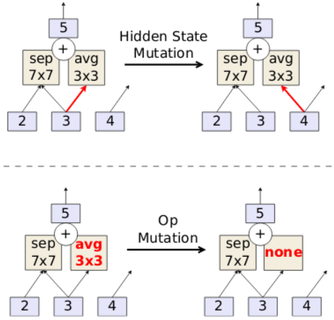


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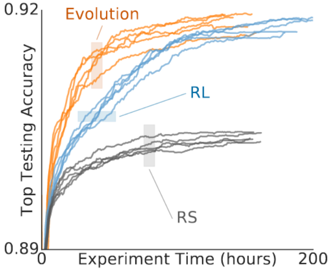


State-of-the-art performance in apples-to-apples comparison
→ AmoebaNet

# Bayesian Optimization (BO)

- Encode the architecture space by categorical hyperparameters (like regularized evolution)
- Strong performance with tree-based models
  - TPE [Bergstra et al. 2013]
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- BO is very competitive, has been shown to outperform RL [Ying et al. 2019]

# Current State of the Art: Differential Evolution

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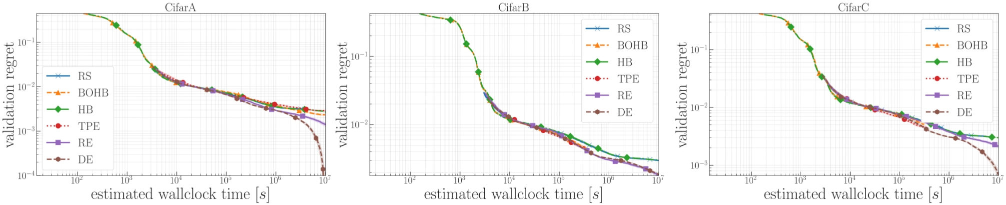
- Results:
  - Regularized evolution is very robust, typically amongst best of the methods discussed so far
  - Evolution variant of differential evolution is yet better; most efficient and robust method



# Questions to Answer for Yourself / Discuss with Friends

- Repetition:
  What are some pros and cons of using black-box optimizers for NAS?
- Repetition:
  How can NAS be modelled as a HPO problem?
- Discussion:
  Given enough resources, will blackbox NAS approaches always improve performance?
- Discussion:
  Why does discarding the oldest individual (rather than the worst) help in regularized/aging evolution?
- Transfer:
  How would you write NAS with the hierarchical search space as a HPO problem?