Evolution of Neural Networks

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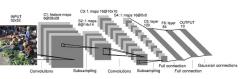
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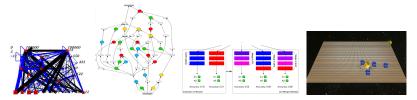
Why Use Neural Networks?





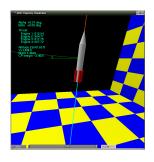
- ► Neural nets powerful in many statistical domains
 - ► E.g. vision, language, control, prediction, decision making
 - ▶ Where no good domain theory, but plenty of examples
- Good supervised training algorithms exist
 - ► Learn a nonlinear function that matches the examples
 - ► Utilize big datasets, big compute

Why Evolve Neural Networks?



- ▶ I. Original role (since 1990s): RL Tasks & especially POMDP
 - ► Both the structure and the weights evolved (no training)
 - Power from recurrency; behavior
- ▶ II. A new role (since 2016): Optimization of Deep Learning Nets
 - Architecture, hyperparameters, functions evolved; weights trained
 - ► Power from complexity
- ▶ **III.** A possible future role: Optimizing LLMs
 - Orchestration of multiple LLMs
 - Evolution of prompts & fine-tuning
- ▶ IV. A possible future role: Emergence of intelligence
 - ► Body/brain co-evolution; Competitive co-evolution
 - ► Evolution of memory, language, learning

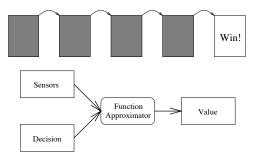
I. Reinforcement Learning / POMDP Tasks





- A sequence of decisions creates a sequence of states
 - States are only partially known
 - Optimal outputs are not known
 - ► We can only tell how well we are doing
- Exist in many important real-world domains
 - ► Robot/vehicle/traffic control
 - ► Computer/manufacturing/process optimization
 - ► Game playing; Artificial Life; Biological Behavior

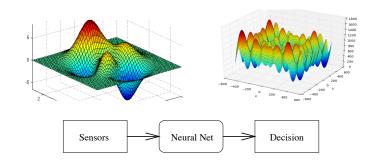
Value-Function Reinforcement Learning



- ► E.g. Q-learning, Temporal Differences
 - ► Generate targets through prediction errors
 - ► Learn when successive predictions differ
- ► Predictions represented as a value function
 - ► Values of alternatives at each state
- ► Difficult with large/continuous state and action spaces
- ▶ Difficult with hidden states

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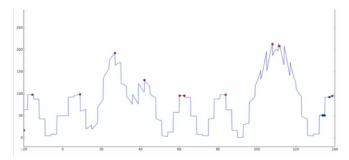
Policy-Search Reinforcement Learning



- ► E.g. REINFORCE, policy gradients
- ► The policy is optimized directly through hill climbing
- ► Works well in simple cases
 - ► Large/continuous states and actions possible
 - ► Hidden states (in POMDP) disambiguated through memory
 - Does not scale well

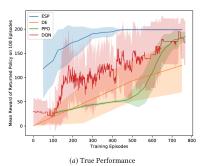
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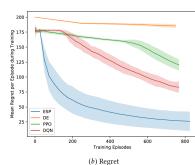
Neuroevolution Reinforcement Learning



- ► Takes advantage of population-based search
 - ► In essence, multiple interacting searches
 - ► Each discover building blocks that are combined
 - ► Extensive exploration possible
- ► Makes it possible to scale up:
 - ► to large spaces (e.g. 2²⁷⁰ states⁵⁶)
 - ► to high dimensionality (e.g. up to 1B¹²)
 - ► to deceptive landscapes (with e.g. multiobj and novelty ⁸⁴)

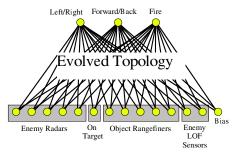
How Well Does It Work?





- ► In the OpenAl Gym CartPole-v0 benchmark vs. PPO, DQN
 - ▶ NE converges faster, has lower variance, lower regret
 - ► NE is more efficient, reliable, and safer ¹⁸
- ► In a double-pole benchmark vs. Sarsa, Q-MLP, etc.
 - ► The only method that can find solutions to 1m, 0.1m, POMDP²³
- ► The fundamental difference is exploration
 - ► Evolution provides more exploration than gradients do ^{35,78,92}

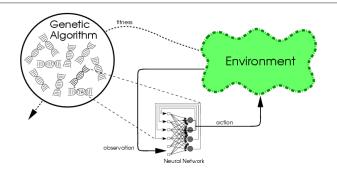
Neuroevolution for RL/POMDP



- ► Input variables describe the state observed through sensors
- ► Output variables describe actions
- Network between input and output:
 - ► Recurrent connections implement memory
 - ► Memory helps with POMDP

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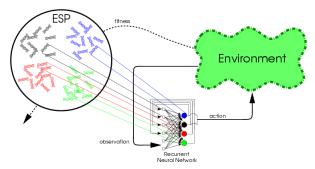
Basic Neuroevolution



- ► Evolving connection weights in a population of networks ^{62,79,103,104}
- ► Chromosomes are strings of connection weights (bits or real)
 - ► E.g. 10010110111001011111001
 - ► Usually fully connected, fixed, initially random topology
- ► A natural mapping between genotype and phenotype
 - ► GA and NN are a good match!

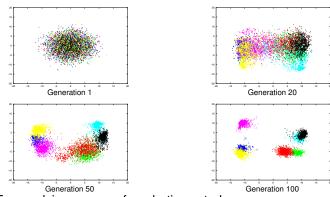
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Advanced NE 1: Evolving Partial Networks



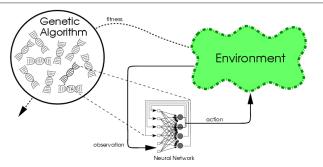
- ► Evolving individual neurons to cooperate in networks ^{1,63,66}
- ► E.g. Enforced Sub-Populations (ESP²¹)
 - ► Each (hidden) neuron in a separate subpopulation
 - ► Fully connected; weights of each neuron evolved
- ► Can be applied at the level of weights, and modules ²³

Why Is It a Good Idea?



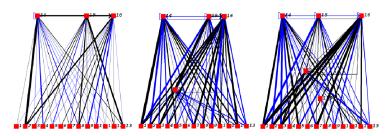
- ► E.g. evolving neurons for robotic control
 - ► Simulated Kheperas running a maze
- ► Subpopulations discover & optimize compatible subtasks
 - ► E.g. slow down with obstacle on front veer left with obstacle at right, etc.
- ► Each neuron part of 2-3 subtasks
 - ► Robust coding of behavior during search

Advanced NE 2: Evolutionary Strategies



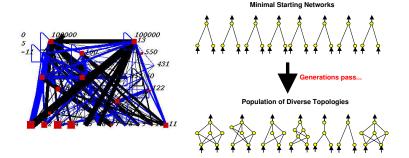
- ► Evolving complete networks with ES (CMA-ES³¹)
- ► Small populations, no crossover
- ► Instead, intelligent mutations
 - ► Adapt covariance matrix of mutation distribution
 - ► Take into account correlations between weights
- ► Why is it a good idea?
 - ▶ Discovers good weight combinations → CM

Advanced NE 3: Evolving Network Structure



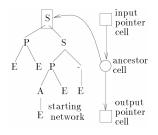
- ► Optimizing connection weights and network topology^{3,15,19,105}
- ► E.g. Neuroevolution of Augmenting Topologies (NEAT 86,89)
- ► Based on Complexification
- Of networks:
 - Mutations to add nodes and connections
- ▶ Of behavior:
 - Elaborates on earlier behaviors

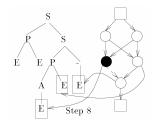
Why Is It a Good Idea?



- ► NN search space is complex with nonlinear interactions
- ► Complexification keeps the search tractable
 - ► Start simple, add more sophistication
- ► Incremental discovery of complex solutions

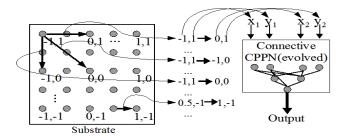
Advanced NE 4: Indirect Encodings (1)





- ► Instructions for constructing the network evolved
 - ► Instead of specifying each unit and connection 3,15,61,85,105
- ► E.g. Cellular Encoding (CE²⁷)
- ► Grammar tree describes construction
 - Seguential and parallel cell division
 - ► Changing thresholds, weights
 - ► A "developmental" process that results in a network

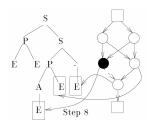
Indirect Encodings (2)

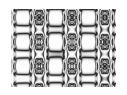


- ► Encode the networks as spatial patterns
- ► E.g. Hypercube-based NEAT (HyperNEAT 10)
- Evolve a neural network (CPPN) to generate spatial patterns
 - ▶ 2D CPPN: (x, y) input \rightarrow grayscale output
 - ► 4D CPPN: (x_1, y_1, x_2, y_2) input $\rightarrow w$ output
 - ► Connectivity and weights can be evolved indirectly
 - ► Works with very large networks (millions of connections)



Why Is It a Good Idea?

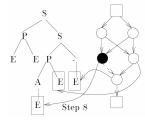


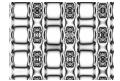


- ► Describes structure efficiently
 - ► Recurrency symbol in CE: XOR → parity
 - ► Repetition with variation in CPPNs
- ► Useful for evolving topology
 - ► E.g. large structured networks
 - ► E.g. repetition of motifs

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Future Opportunities





- ► Several possible directions
 - More general L-systems; developmental codings; embryogeny⁹⁰
 - ► Scaling up spatial coding ^{11,20}
 - ► Genetic Regulatory Networks⁷⁵
 - ► Evolution of symmetries 99
- ► Theory starting to emerge
 - Expressive Encodings⁵⁵: Simple GAs are universal probability approximators

Further NE Techniques

- ► Incremental and multiobjective evolution ^{22,82,98,104}
- ► Utilizing population culture ^{4,47,95}
- ► Utilizing evaluation history⁴⁶
- ► Evolving NN ensembles and modules ^{33,45,65,76,101}
- ► Evolving transfer functions and learning rules 8,77,91
- ► Bilevel optimization of NE⁴³
- ► Evolving LSTMs for strategic behavior ³⁹
- ► Extrapolation with Context+Skill modules 97
- ► Combining learning and evolution 7,16,47,64,87,95,102
- ► Evolving for novelty

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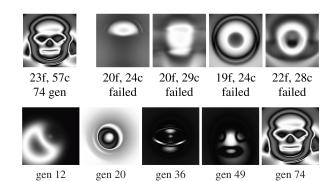
Evolving for Novelty



- ► Motivated by humans as fitness functions
- ► E.g. picbreeder.com, endlessforms.com⁸³
 - ► CPPNs evolved; Human users select parents
- ► No specific goal
 - Interesting solutions preferred
 - ► Similar to biological evolution?

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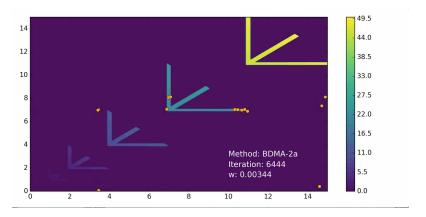
Novelty Search



- ► Evolutionary algorithms maximize a performance objective
 - ► But sometimes hard to achieve it step-by-step
- ► Novelty search rewards candidates that are simply different ^{37,88}
 - Stepping stones for constructing complexity

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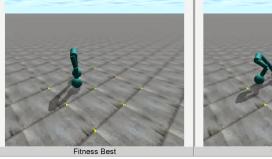
Novelty Search Demo (1)



- ► Illustration of stepping stones ^{49,50}
 - ► Nonzero fitness on "feet" only; stepwise increase
 - ► Top and right "toes" are stepping stones to next "foot"
 - ► Difficult for fitness based search; novelty can do it

► DEMO

Novelty Search Demo (2)





- ► Fitness-based evolution is rigid
 - ► Requires gradual progress
- ► Novelty-based evolution is more innovative, natural ^{37,88}
 - ► Allows building on stepping stones
- ► How to guide novelty search towards useful solutions?
 - ► Quality Diversity methods ^{17,67}

▶ DEMO

Neuroevolution Applications Control Pole-Balancing Satellite Asst. Robotics Games Othello NERO NERO Pole-Balancing Applications Rocket Rocket Unreal Unreal

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Example 1: Evolving Humanlike Behavior



- ► Botprize competition, 2007-2012
 - ► Turing Test for game bots (\$10,000 prize)
- ► Three players in Unreal Tournament 2004:
 - ► Human confederate: tries to win
 - Software bot: pretends to be human
 - Human judge: tries to tell them apart!

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Evolving an Unreal Bot

Alife



- ▶ Wandering, unstuck etc. based on scripts & learning from humans
- ► Evolve effective fighting behavior⁸¹
- ► Persistent gap: 30% vs. 80% human
 - ► Evolving to win results in unnatural behaviors
 - ► Human judges do not understand their expertise

After Five Years, Success!!!

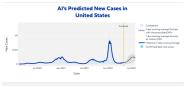


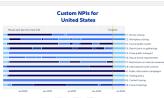
- ► Human-like behavior with resource limitations (speed, accuracy...
 - ► Best bot better than 50% of the humans
 - ► Two teams human 50% of the time
- ► Fascinating challenges remain:
 - ► Judges can still differentiate in seconds
 - ► Judges lay cognitive, high-level traps
 - ► Team competition: collaboration as well

► DEMO

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Example 2: Optimizing COVID-19 NPIs





Train a NN to predict COVID-19 cases

- Based on number of cases in different countries over time
- And non-pharmaceutical interventions (NPIs) over time

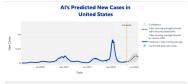
Using the predictive model as a surrogate, evolve a NN to recommend NPIs

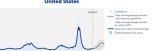
- · Resulting in smallest number of cases
- · With minimal economic cost

Not just what will happen, but what we should do about it!

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COVID-19 Predictions and Prescriptions







Retrained daily since May 2020⁵⁸

- Based on data from Oxford University ²⁸
- Adapting to the different stages of the pandemic
- Generalizing from experiences across the world

Recommendations about two weeks in advance, e.g.

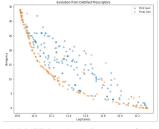
- May 2020: Focus on schools and workplaces (i.e. indoors)
- Sept 2020: Focus on gatherings, travel restrictions
- March 2021: Delta surge: India lockdown
- Dec 2021: Missed omicron surge; everywhere at once
- March 2022: Masking to avoid a second omicron surge

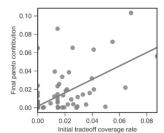
Interactive demo:

· https://evolution.ml/demos/npidashboard

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Using Neuroevolution to Leverage Human Insight





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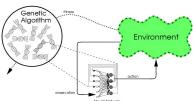
XPRIZE Pandemic Response Challenge 2021

· 169 expert-designed prescriptors

Distill into neural networks and evolve further 48 · Improve upon expert-designed entries

Improve upon evolution from scratch

Can realize latent potential hidden in poor entries Technology to bring the community effort together Part I Conclusion: Neuroevolution RL



- · A powerful way to train networks when gradients not available
 - E.g. recurrency in POMDP domains
- · Many evolutionary techniques are a good match with NE
 - · Partial solutions, CMA, Complexification, Indirect, Novelty, Constrained
- · Can discover surprising, believable, effective solutions

II. Optimization of Deep Learning Systems



Deep learning systems operate at a much larger scale

- 10⁶ 10¹² parameters
- Overparameterized; trained by gradient descent

A new problem: How to configure such systems?

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Configuring Complex Systems



A new general approach to engineering

- ► Humans design just the framework
- ► Machines optimize the details

Programming by optimization³⁰

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Configuring Deep Learning with Evolution



(A) Fundamental: Neural Architecture Search

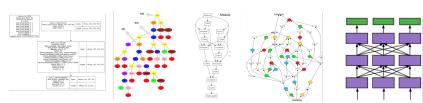
- Optimizing structure and hyperparameters
- Takes advantage of exploration in EC

(B) Extended: Data and training

- Loss functions, activation functions, data augmentation, initialization, learning algorithm
- Takes advantage of flexibility of EC

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Evolutionary NAS



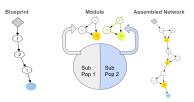
Evolution is a natural fit:

- Population-based search covers the space
- Crossover between structures discovers principles

Moreover,

- Can build on Neuroevolution work since the 1990s: partial solutions, complexification, indirect encoding, novelty search
- Applies to continuous values; discrete choices; graph structures; combinations
- Can evolve hyperparameters; nodes; modules; topologies; multiple tasks

E.G. NAS with CoDeepNEAT



Evolution at three levels 59

- Module subpopulations optimize building blocks
- Blueprint population optimizes their combinations
- Hyperparameter evolution optimizes their instantiation

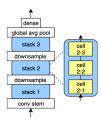
Fitness of the complete network drives evolution

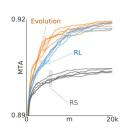
- Candidates need to be evaluated through training
- Expensive; use partial training, surrogates...

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Making NAS Evaluations Practical







Population-based training (DeepMind, Cognizant)32,40

Continual training and evolution

NAS benchmarks created to help evaluate (Google, Baidu, Freiburg)^{13,106,107}

• Collections of known architecture evaluations, surrogates Scaling and regularization (Google, Uber)^{73,92}

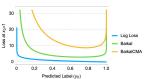
• State-of-the art at the time in CIFAR-10, CIFAR-100, ImageNet

Specialized crossover operators (Cognizant)⁶⁸

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Optimizing Other Aspects of Deep Learning Design







Optimizing activation functions and loss functions (Cognizant)^{5,6,24,25,26,40}

Regularization and refinement

Designing machine learning algorithms with GP (Google)44,74

- Adapts to different task types
- Discovering new layer types

Coevolution of multiple aspects of network design?

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Evolutionary AutoML

Current AutoML: Mostly hyperparameter optimization Future Evolutionary AutoML: Many design aspects

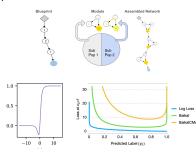
Performance

1. Improve state of the art With sufficient compute

Applicability

- 2. Improve over naïve baseline Service makes broadly available
- 3. Minimize network resources
 Train and run networks faster
- 4. Extend small datasets

 Multitasking with related datasets



1 & 2 in Evolving Age-Estimation Networks

Parameter	Possible Values	Type	Class
Algorithm	[adam, rmsprop]	Enum	Opt
Initial Learning Rate (LR)	[1e-5, 1e-3]	Float	Opt
Momentum	[0.7, 0.99]	Float	Opt
(Weight Decay) / LR [26]	[1e-7, 1e-3]	Float	Opt
Patience (Epochs)	[1, 20]	Int	Opt
SWA Epochs [21]	[1, 20]	Int	Opt
Rotation Range (Degrees)	[1, 60]	Int	Aug
Width Shift Range	[0.01, 0.3]	Float	Aug
Height Shift Range	[0.01, 0.3]	Float	Aug
Shear Range	[0.01, 0.3]	Float	Aug
Zoom Range	[0.01, 0.3]	Float	Aug
Horizontal Flip	{True, False}	Bool	Aug
Vertical Flip	{True, False}	Bool	Aug
Cutout Probability [7]	[0.01, 0.999]	Float	Aug
Cutout Max Proportion [7]	[0.05, 0.5]	Float	Aug
Pretrained Base Model	Keras App. [5]	Enum	Arch
Base Model Output Blocks	{B0, B1, B2, B3}	Subset	Arch
Loss function λ in Eq. 5	[0, 1]	Float	Arch



Estimate age from a facial image

Evolving multiple design aspects⁶⁰

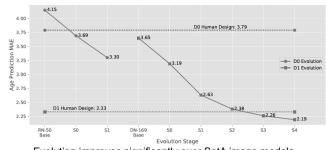
- Learning, data augmentation hyperparameters
- · Seeded architecture search
- Loss-function optimization: Combination of MAE and CE

Also

- · Population-based training
- · Ensembling of evolved solutions

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Age-Estimation Results



- D0 stages: ResNet-50, DenseNet-121
- D1 stages:
 DenseNet-169,
 DenseNet-201,
 more epochs.
 EfficientNet-B6,
 ensembling
- Human optimization of ResNet-50 (D0), EfficientNet-B6 (D1)

Evolution improves significantly over SotA image models

· Fit the design to the task

Optimizes better than humans can

Many more parameters simultaneously

Performance exceeds that of humans: 2.19 vs. 3-4 years

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3. Minimize Network Resources

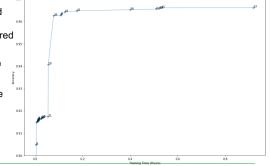
Evolution adds complexity only if needed

- Favors minimal solutions
- Over evolution a range of sizes explored
- Approximation of the Pareto front

Small networks found that perform well 41

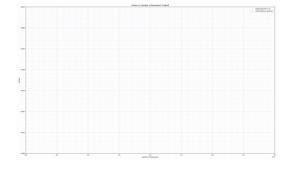
- · Minimization with little cost
- E.g. 0.38% drop with 1/12th of the size

Could we optimize for size directly?



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Multiobjective Minimization



- Animation: Pareto front by generation for single-objective (green) vs. multi-objective (blue)
- Single-objective focuses on improving *largest networks*
- Multi-objective focuses on improving the entire curve
- Result: Multi-objective finds much smaller models for the majority of performance values³⁶
- Evolution can find solutions that fit design constraints

4. Extend Small Datasets



Recognize handwritten characters in a given alphabet

Not enough samples to learn well

· A common problem in deep learning

Could we learn from multiple alphabets at once?

- More generalizable embeddings 42,52,53
- Can learn each task better

Evolve architecture to combine multiple tasks

· Network architecture can have a large effect

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· A good domain for NAS

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Multitasking Benchmarks

State-of-the-art in two ML benchmarks:

- Omniglot multialphabet character recognition 42
 - Improved state-of-the-art 31%
 - · Demo: evolution.ml/demos/omnidraw
- CelebA multiattribute face classification 51
 - Improved state-of-the-art 0.75%
 - · Demo: evolution.ml/demos/celebmatch

Improves learning in each task

· Even when little data available

Extend small datasets with multiple tasks









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Part II Conclusion: Optimizing Deep Learning Designs



- Deep learning designs are too complex for humans to optimize
- Evolutionary techniques are a good fit
 - · Large, structured space; continuous, discrete, and structured
- Can be applied to multiple aspects of the design
 - · How to utilize their interactions?
 - How to evaluate candidates efficiently?

III. Future: Neuroevolution through Large Language Models

11101111 LM prompt 11110111 (Parents) 10100111 LM output 11111111

(Children)

x^2 + 2.1*x sin x^2 + 7 3*sin x + 6.6 $x^2 \sin x + 6$ $\cos x^2 + 2.1*x$ the moon is bad the moon is boring the moon is cold the moon is zen

Better evolution through LLMs?

- Evolution through large models (ELM)³
- Language model crossover (LMX)54

10110111

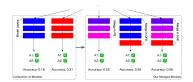
Level generation for Mario (MarioGPT) 93

E.g. Evolutionary prompting for NAS (EvoPrompting)

- · Existing architectures as prompts; generate new
- · Tune the prompts based on performance

fitness: fitness: -540 -1150

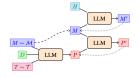
Future: Neuroevolution of Large Language Models



Better LLMs through evolution?

Model merging: combine multiple fine-tuned LLMs to one

- E.g. Japanese LLM with Math ² Evolving prompts: Promptbreeder
- Evolving mutation prompts to improve task prompts ¹⁴
 Evolving multi-LLM interactions
- E.g. roles for collaborative problem solving 29





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IV. Emergence of Intelligence





Evolved Virtual Creatures

- · Neuroevolution of intelligent behavior
- · Useful e.g. for video games

Can such experiments lead to insights in biology?

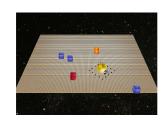
Collaboration with Kay Holekamp's lab (MSU)

Studying hyenas in Masai Mara since 1982

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Evaluating Biological Hypotheses





In simulation 69,70,71,72

· Manipulate constraints, observe outcomes, analyze trajectory of discovery

Computational support for hypotheses

- Reward structure: Emergence of cooperation in hunting
- · Lethality of conflicts: Emergence of a hierarchical society
- · Signaling in mate selection vs. hunting: Origins of communication

Example: Evolution of Intelligent Coordinated Behavior

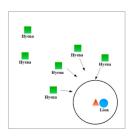
Stealing a kill from lions

- Succeeds in an otherwise impossible task (sometimes)
- More sophisticated than other hyena behaviors
- Highly rewarding compared to normal hunting
- · Largely genetically determined
- A breakthrough in evolution of intelligence?



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Simulation Setup



Lion at a kill, with an interaction circle around it ⁶⁹
Ten hyenas chosen and placed randomly in the field

If 4 or more hyenas enter the circle simultaneously, they get the kill

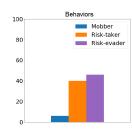
Otherwise they die

Does mobbing behavior evolve?

· What are the stepping stones for it?

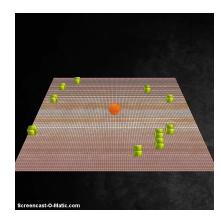
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Initial Behaviors



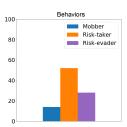
Risk evasion is common

- Never reach the circle; Medium fitness Risk taking is common
- Charge the circle; Frequent low fitness
- Occasional high fitness by accident



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Early Behaviors



Risk taking grows

55

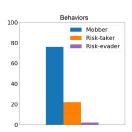
 As long as it is successful often enough Risk evasion also persists

Evasion at the circle starts to emerge

Is mostly detrimental, but an important stepping stone

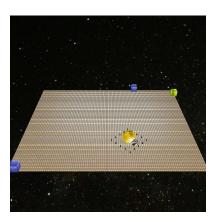
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Later Behaviors

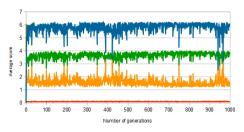


Mobbing emerges

- · Not just coincidence of risk takers
- Hyenas wait until there's enough of them Risk-evaders evolve into latecomers
 Simple risk-taking and risk-evasion still exist



These Behaviors Persist in Prolonged Evolution



Risk taking and risk evasion never go away completely

- They serve a role in maintaining the mobbing behavior
- · If mobbing starts to get lost, it can be reintroduced

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Insight into Real-life Behaviors



These behaviors are observed in real-life hyenas as well

A computational explanation of why they are there:

- · Stepping stones in discovery
- Safeguards in maintaining

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Constructing Intelligent Systems

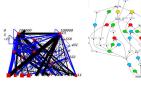


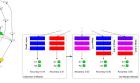
- Believable, complex behavior in embedded environments
 - Open-ended "arms race" ⁷²
- Similar to self-play e.g. in AlphaGo Zero
 - · Complexity beyond human ability to design it
- If we can build open-ended environments, we should be able to build more complex solutions
 - Co-evolve environments and behaviors? (e.g. POET, DET, EUREQA DET)
 - Evolution of memory, learning, language

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Challenge: Establish major transitions⁵⁷

Conclusion







Neuroevolution is a powerful approach for POMDPs

- Discovers surprising, believable, effective behavior
- Games, robotics, control, alife, decision-making...

Makes complex DL architectures possible

- Structure, components, hyperparameters, etc. fit to the task
- Automatic design of learning machines

A possible future focus: Emergence of intelligence

- Body/brain co-evolution; Competitive co-evolution
- Evolution of memory, language, learning; AGI

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Further Material

- Neuroevolution sessions at GECCO!
- www.cs.utexas.edu/users/risto/talks/enn-tutorial
 - Slides and references
 - Demos
 - A step-by-step neuroevolution exercise (evolving behavior in the NERO game)
- nn.cs.utexas.edu/?miikkulainen:encyclopedia20-ne
 - A short summary of neuroevolution
- www.nature.com/articles/s42256-018-0006-z
 - Nature Machine Intelligence survey on neuroevolution
- Risi, Ha, Tang, and Miikkulainen (2024): <u>Neuroevolution.</u> New York: Springer
 - Forthcoming textbook/monograph in Fall 2024
 - Extensive online excercises

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