Neuroevolution Tutorial

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Outline



Insights into Biology
 Conclusion

Hands-on exercise (off-line)



1. Motivation: From Imitation to Creativity





- · Much of AI so far focuses on imitation
 - I.e. gradient descent on labeled datasets
 - Powerful in prediction: object recognition, diagnosis, forecasting, etc.
- Agentic AI focuses on behavior
 - Gradients not available
 - · Needs to be discovered
- How can we create novel behaviors?

Reinforcement Learning is One Approach



- Approximating gradient descent
- Explore around the current solution
- Improve it gradually
- Can climb the nearest hill well

...but Creativity in RL is Limited



- Space is too large
- Multiple starts won't help
- Space is too high-dimensional
 - Little improvement from one step
- Space is deceptive
 - Can only find the nearest hill

Solution: Population-based Search



A.k.a Evolutionary Computation

- Many individuals spread out, sharing information
- Not limited to differentiable domains: configurations, choices ok
- Not limited to incremental improvement
- Large jumps possible, can be more creative

Scaling up through Evolution



Works in large scales

- Structured search works in large spaces (e.g. 2²70; Hodjat & Shahrzad 2016)
- Multiple variables optimized at once (e.g. up to 1B; Deb et al. 2017)
- Multiple objectives and novelty get around deception (Shahrzad and Hodjat 2020)

Neuroevolution uses population-based search to optimize neural netwoks

• Weights, topologies, designs

2.1 Evolution Basics: Encoding, Evaluation, and Selection



- A population of encodings (e.g. lists or trees)
- Decoded into individuals that are evaluated in the domain
- · Good individuals retained, bad thrown away

Creating Variation





• New individuals generated from the parent encodings

- Crossover: combine building blocks from two parents
- Mutation: create new building blocks

Population-based Search



Population-based Search

GEN 1

Population-based Search



Population-based Search



Population-based Search



Population-based Search



2.2 Basic Neuroevolution



- Evolving connection weights in a population of networks
- Chromosomes are strings of connection weights (bits or real)

 - E.g. 100101101010101111001
 Usually fully connected, fixed, initially random topology
- ► A natural mapping between genotype and phenotype
 - ► GA and NN are a good match!

Example: Learning to Walk



Demo

Advanced Neuroevolution

- E.g. Neuroevolution of Augmenting Topologies (NEAT)
- Historical markings match up different structures
- Speciation
 - Keeps incompatible networks apart
 Protects innovation
- Incremental growth from minimal structure, i.e. complexification
 Avoids searching in unnecessarily high-d space
 Makes finding high-d solutions possible



(Stanley and Miikkulainen, 2002)

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

Discovering Compact, Interpretable Structure

• E.g. in double pole balancing

•

- Easy when position, velocity of both poles and the cart are given
- Hard when only positions: need to figure out how they are moving
- Discovers recurrent structure

 Either representing velocities separately
 - Or simply the derivative of the difference of the poles!
- Big improvement from other approaches
- Standard value-function RL unsuccessful





Outline



3.1 Indirect Encoding: (A) Development



- Instructions for constructing the network evolved Instead of specifying each unit and connection
- ► E.g. Cellular Encoding (CE Gruau & Whitley 1993)
- ► Grammar tree describes construction
 - Sequential and parallel cell division
 - Changing thresholds, weights
 - A "developmental" process that results in a network

3.1 Indirect Encoding: (B) Hypernetworks



- Encode the networks as spatial patterns
- ► E.g. Hypercube-based NEAT (HyperNEAT
- ► 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 are Indirect Encodings a Good Idea?



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

Future Opportunities



- Several possible directions
 - More general L-systems; developmental codings; embryogeny
 - Scaling up spatial coding
 - Genetic Regulatory Networks
 - Evolution of symmetries
- ► Theory starting to emerge
 - Expressive Encodings Simple GAs are universal probability approximators

3.2 Diversity: (A) Searching for Novelty



- Motivated by humans as fitness functions
- ► E.g. picbreeder.com, endlessforms.com (Secretan et al. 2011; Clune et all 2011)
 - CPPNs evolved; Human users select parents
- No specific goal
 - Interesting solutions preferred
 - Similar to biological evolution?

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
 - Stepping stones for constructing complexity

Novelty Search Demo 1



- 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
 Allows building on stepping stones
- How to guide novelty search towards useful solutions?
 - Quality Diversity methods
- ► DEMO

(B) Combining Quality with Diversity



Goal: Find a set of different high-quality solutions for a given problem Ex: Find fast walking gaits for a legged robot for every direction

Popular QD Method: Multi-dimensional Archive of Phenotypic Elites¹ (MAP-Elites)

Idea: Evolve an archive of different high-quality solutions (= elites)

Multi-dimensional Archive of Phenotypic Elites (MAP-Elites)



MAP-Elites algorithm

Initialization

- 1. Divide the behavior space into cells (= the Archive)
- 2. Initialize with random solutions until n_{init} elites are found

Main loop

- 1. Pick two elites from the Archive
- 2. Apply crossover and mutation
- 3. Evaluate new solution
- 4. If new behavior or better fitness the solution becomes an elite



Behavior 1

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Hands-on Exercise!

Outline



4.1 Evolving Controllers



- The main challenge for evolved controllers: Extrapolation
- · Need to generalize immediately to unseen situations
 - · Games, robotics, process control, healthcare, finance

TEXAS

Solution: Modeling Context Explicitly



FlappyBall Domain



Example Behaviors in FlappyBall

• Extrapolated conditions: F=-7.0, G=0.58, Fwd=8.75, D=0.58





Modulation by Context



- Difference in an extrapolated task and the nominal task plotted
- Differences are smaller in CS than in C-only and S-only
 - Decision network needs to deal with less variance
 - Easier to generalize
 - CS evolves to make new tasks look more familiar
- Allows coping robustly in novel situations

TEXAS

4.2 Evolving Behavioral Strategies



Strategy: different behaviors at different times

Ms. Pac-Man:

- Agents perform many different tasks
 - E.g. eat pills, avoid ghosts, eat powerpills, eat ghosts
 - Sometimes clearly separate in time
 - Sometimes multiple tasks at once

How can we evolve them into a single network?

(Schrum and Miikkulainen 2015)

MM-NEAT: Modular Multiobjective Approach



- Evolution discovers modules and when to use them
 - Vs. human-designed division with multitasking
- Multiple modules with preference neurons
 - Modules implement different behaviors
 - Preference neurons used to choose among them
 - Module-mutation adds new modules
- Evolved towards multiple objectives
 - Correspond to dimensions of game play
 - ► E.g. pills and ghosts in Ms. Pac-Man

Human-Designed Task Division



Multitask approach

- One module for threat ghosts
- Another module for edible ghosts
- Works ok, but...
- DEMO

Evolution-Discovered Task Division



4.3 Optimizing Decision-Making



Organizations have lots of data

• Can build predictive models of patients, customers, students... Such models do not specify how to make decisions

• Optimal decisions not known

Need to search for decision strategies

• But testing strategy candidates in the real world is costly

Surrogate Optimization Approach



Use a predictive model as a surrogate for the world Train model with historical data: Context+Actions → Outcomes

- Phenomenological model (based on data)
- Not a simulation from first principles

Search for a good decision strategy (i.e. policy): Context \rightarrow Actions

- Use the model to evaluate strategies
- Evolve a neural network to represent the strategy

Optimizing Interventions in COVID-19





Based on two models: 1. A predictive model

- Given a history of cases and nonpharma interventions (NPIs)
- Predict number of cases daily
- 2. A prescriptive model
- Given a history of cases and NPIs
- Prescribe NPIs daily to minimize cases and restrictions
- Not just what will happen, but what we should do about it

COVID-19 Predictions and Prescriptions



Retrained daily May 2020 - December 2022

- Based on data from Oxford University •
- 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
- . August 2021: Recommendations for schools (Iceland)
- Dec 2021: Missed omicron surge; everywhere at once •
- . March 2022: Masking to avoid a second omicron surge

Interactive demo:

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

Leveraging Human Expertise with AI



XPRIZE competition resulted in 169 human expert strategies

- Many useful, diverse ideas
- Can be used as an initial population for search
- Improve further; better than search from scratch
- Can realize latent potential of ideas
- · How much DNA in the final Pareto front
- Technology to bring the community effort together
- There is power in diversity

4.4 Evolving Collective Behavior





Formalization of behavior

- Complex cooperation observed in pursuit and evasion
 - Motivated by biology, esp. hyenas vs. zebras (Kay Holekamp, MSU)
 - Largely innate, possible to see behaviors and their evolution
- Such behaviors evolve together, in coevolutionary environment
 - · Simultaneous competitive and cooperative coevolution

Natural predators and prey



Experimental Setup



- Toroidal grid world
- ► Predators, prey move with same speed in 4 directions
- No direct communication between team members
 - Communication still possible through stigmergy
- Does a coevolutionary arms race result? DEMO

Evolutionary Arms Race





50-75: Single predator catches the prey

75-100: Prey evades by circling

Predators and prey populations develop increasingly sophisticated behaviors

Each improvement provides a challenge to the other population

Evolutionary Arms Race



100-150: Two predators cooperate



150-180: Prey baits and escapes

Evolutionary Arms Race



180-200: All predators cooperate

Evolutionary Arms Race



90.

200-250: Predators herd two prey

250-300: Prey evade by scattering

Outline





5.1 Neuroevolution Synergies with Deep Learning



(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

(A) Evolutionary Neural Architecture Search



Evolution is a natural fit:

- Population-based search covers the space ٠
- 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

- Module subpopulations optimize building blocks •
- Blueprint population optimizes their combinations ٠
- Hyperparameter evolution optimizes their instantiation ٠

Fitness of the complete network drives evolution

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

Making NAS Evaluations Practical



Population-based training (Jaderberg et al 2017; Liang et al. 2021)

Continual training and evolution

NAS benchmarks created to help evaluate (Ying et al. 2019; Dong et al. 2020; Siems et al. 2021)

- Collections of known architecture evaluations, surrogates
- Scaling and regularization (Such et al. 2017; Real et al. 2019)
- State-of-the art at the time in CIFAR-10, CIFAR-100, ImageNet

Specialized crossover operators (Qiu and Miikkulainen 2023)

(B) Optimizing Other Aspects of Deep Learning Design



Optimizing activation functions and loss functions (Bingham and Mikkulainen, 2022; Neural Networks Best Paper Award at UCNN-25/) (Gonzalez and Miikkulainen, 2020)

Regularization and refinement •

Designing machine learning algorithms with GP (Real et al. 2020)

- · Adapts to different task types
- Discovering new layer types ٠

Coevolution of multiple aspects of network design?

Example: 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 aspects

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

Population-based training

Ensembling of evolved solutions •



5.2 Neuroevolution Synergies with RL

(A) Combining population-based search and RL-based search



- · A population of networks evolved to maximize rewards
- · Evaluations create off-policy training data for Deep RL
- · Trained networks periodically injected into the population
- ERL outperforms both EA and Deep RL alone

(B) Evolving Value Function Networks



NEAT+O

- · Many RL methods rely on value functions to estimate rewards
- NEAT evolves both weights and topologies for better value-function networks

· NEAT+Q outperforms other value-function approximation methods and manually designed networks in e.g. mountain car and server job scheduling

(C) Evolving Starting Points for RL



MAML-Baldwin, ES-MAML (Fernando et al. 2018; Song et al. 2019)

- · Model-agnostic Meta-Learning (MAML) finds good starting points for learning
- · Evolutionary methods like MAML-Baldwin and ES-MAML improve by evolving the starting points Evolve initial weights that adapt to different tasks during the agent's lifetime.
- · E.g. in half-cheetah task, adapts to changing direction rewards within seconds

5.3 Neuroevolution Synergies with LLMs

(A) Neuroevolution through Large Language Models

| LM prompt (Parents) | 11101111 11110111 10100111 | x^2 + 2.1*x sin x^2 + 7 3*sin x + 6.6 | the moon is bad the moon is boring the moon is cold |
|-------------------------|----------------------------------|---|---|
| LM output (Children) | 11111111 10110111 | $x^{2} \sin x + 6$ $\cos x^{2} + 2.1^{*}x$ (Meverson et al. 2024) | the moon is zen the sky has a moon |

Better evolution through LLMs?

- Evolution through large models (ELM)
- Language model crossover (LMX)
- Level generation for Mario (MarioGPT)

E.g. Evolutionary prompting for NAS (EvoPrompting)

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





(Chen et al. 2023)

(B) Neuroevolution of Large Language Models



Better LLMs through evolution?

Model merging: combine multiple fine-tuned LLMs to one

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





(Hong et al. 2023)

Outline





6. Insights into Biology 7. Conclusion

Hands-on exercise (off-line)



6. 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?

A collaboration with Kay Holekamp's lab (MSU) • Studying hyenas in Masai Mara since 1982

(Rajagopalan et al. 2021)



DEMO

Simulation Setup



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

If four 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?

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

DEMO



Early Behaviors



Risk taking grows
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



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



DEMO

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

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

Future Challenge: Evolution of Language





Signaling is possible to evolve in ecological simulations Structured language is much harder

Perhaps language evolved not from signaling, but cognition

- Complex social structure, with modifiable roles
- Language structure can reuse the same conceptual structures Enough compute, complex simulations to study now?

Conclusion



Al is progressing from imitation to creativity; from models to agents

Neuroevolution is a powerful approach to discovering behavior Control, strategy, collective behavior, decision-making

Neuroevolution can provide a boost to ML

- Deep learning designs; RL exploration; LLM optimization
- Automatic design of learning machines

Neuroevolution can provide insight into biological evolution

- · Evolutionary origins of circuits, behavior, intelligence
- · Evolution of language as a current challenge
- · A possible path to AGI





A Hands-on Exercise

| Q. Con | rmands + Code + Text → Run all - Copy to Drive Connect T4 - A |
|-----------|---|
| = @ : ₿ 1 | ▲ Make a copy of this colds before you proceed This can be done from the mean. "Plice-Takina" copy in bine". Tutorial on Neuroevolution To be interacting to be a constrained of enclosionary computation, replanding on the interaction of the interacting the interaction of the interacting the interaction of the interacting the interaction of the interacti |
| | evolutionary approxima to learn a neural network controller that solves the classical cars gold problem. Part 2: Evolutionary Model Merging In this section, we classica the used evolutionary strategies for merging multiple neural network models. This can be a powerful network for enhancing model performance or efficiency. Part 3: QD for Model Merging Quality Denviral (QD) approaches area prest, flocasing on how type a innovate the process of model merging QU cores the influenciate and hundros on applications of QD to pervide a variety of high-calify solutions. |
| | V Part 1. Neuroevolution for Control Import libraries Townsk Know the task |

+

By Yujin Tang

Direct link:

https://colab.research.google.com/drive/1OQFhqJHrV8qpepYRNxHUyauGhmEVB_kx Also under: https://neuroevolutionbook.com/code-exercises

- Three parts:
- Neuroevolution for Control
- Evolutionary Model Merging
- QD for Model Merging

Further Material

- www.cs.utexas.edu/~risto/talks/enn-tutorial
 - Slides, references, demos, video
- nn.cs.utexas.edu/?miikkulainen:science25
 - A review of neuroevolution insights into neuroscience
- Neuroevolution sessions at conferences (e.g. GECCO)
- And....

The Neuroevolution Book!

Neuroevolution: Harnessing Creativity in AI Model Design Sebastian Risi, David Ha, Yujin Tang, and Risto Milikulainen

Visualize the CartPole task with a random
Visualize Terminal

Forthcoming in 2025 by MIT Press



- MIT Press, 2025
- A comprehensive overview
- Software platform: Demos, exercises
- Open access
- https://neuroevolutionbook.com

This site is under construction. As a preview, check out these <u>Neuroevolutio</u> <u>Demos</u>. See <u>here</u> for the accompanying code and exercises.