Introduction to Evolutionary Algorithms

AI Interest Group

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About me

- Zach (Zichao) Wen | https://www.linkedin.com/in/zachwen/

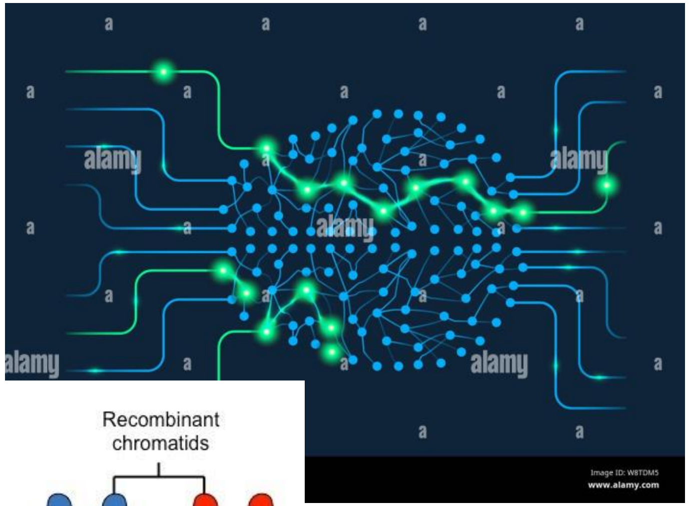
- Ph.D. in Applied Mathematics, University of Chinese Academy of Sciences, Beijing, China
- Instructor in Obstetrics and Gynecology, Washington University School of Medicine

- Expertise:
  - Applied Mathematics – math modeling, optimization, differential equations, simulation, eigenvalue problems
  - Biomedical imaging – electromyography, signal processing, multimodal data integration, spatiotemporal visualization
  - ML/AI – feature engineering, classification, a student of Dr. An's *AI application of Health Data Certificate*

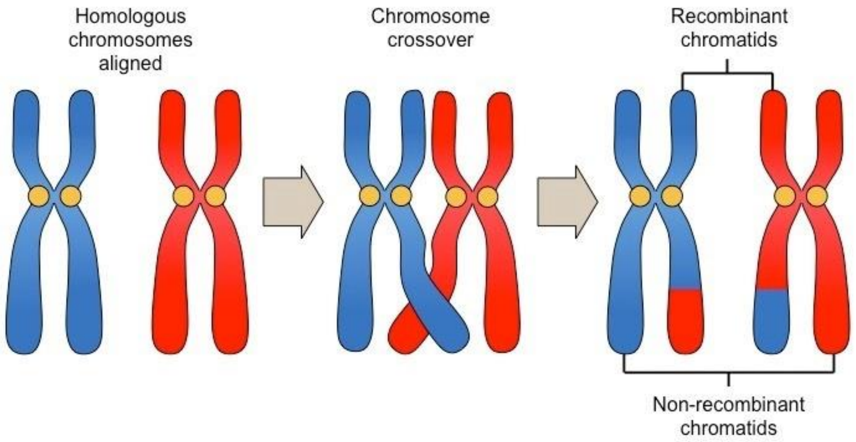
- Husband, and Father of 2 boys (4 and 2.5 years old)
- Lived in St. Louis for 7+ years
- Welcome to connect!

Bio-inspired Artificial Intelligence

- Neural networks (human brain)



- Evolutionary Algorithms
  - Genetic Algorithms (DNA)
  - Particle swarm optimization
  - Artificial immune systems
  - Ant colony optimization



Machine Learning Approaches

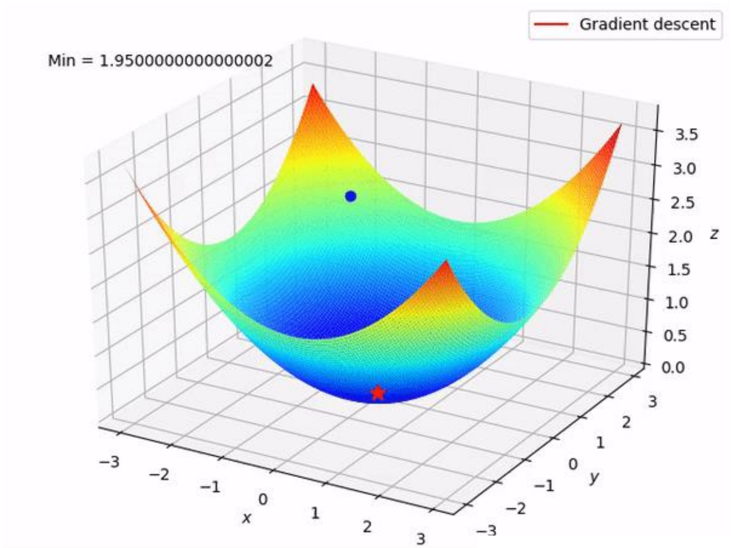
- Supervised Learning:
  - Uses **labeled Data** to train models to predict outcomes accurately
  - Commonly used for **classification** and **regression** tasks.

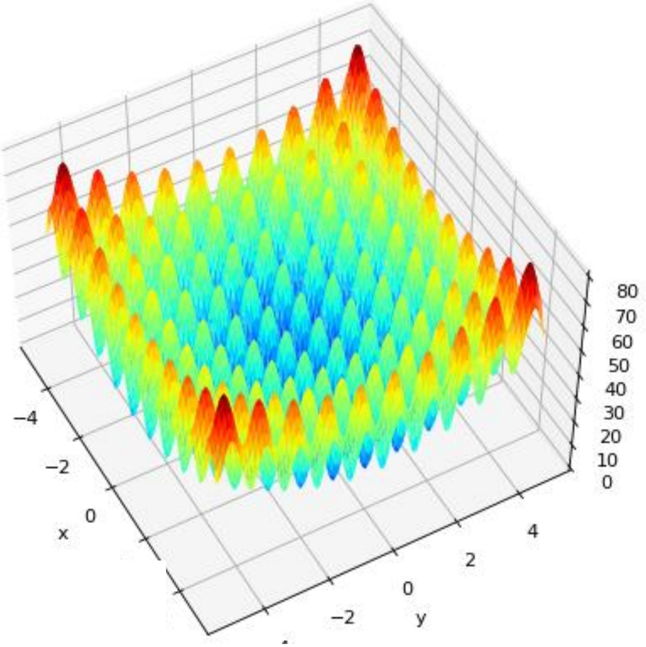
- Unsupervised Learning:
  - Focuses on identifying patterns, relationships, or structures in **unlabeled data**.
  - Used for **clustering**, **dimensionality reduction**, and **association**.

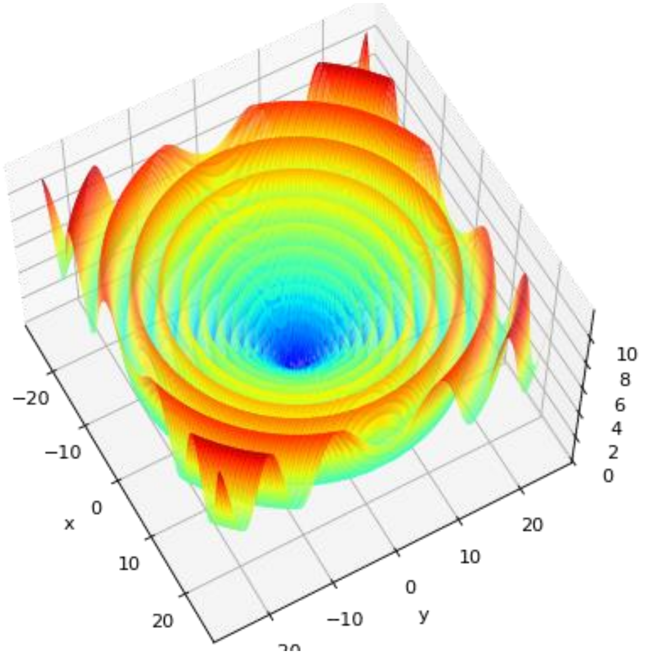
- Reinforcement Learning:
  - An agent learns through interaction to make decisions.
  - Ideal for **sequential decision-making problems** (game playing, robotics, and navigation).

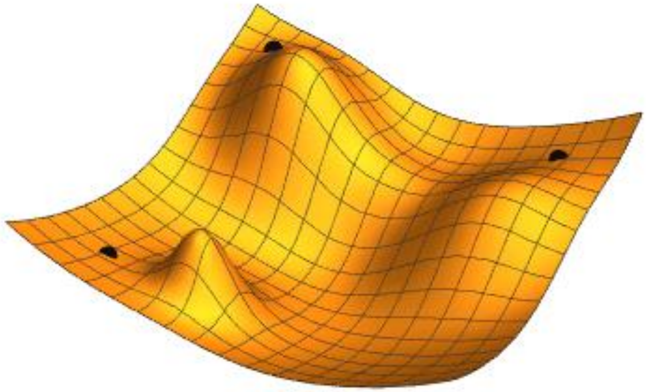
- Evolutionary Algorithms:
  - Uses mechanisms inspired by **biological evolution** to solve optimization problems.
  - Suitable for **complex optimization problems** (scheduling, design, and ML model optimization)

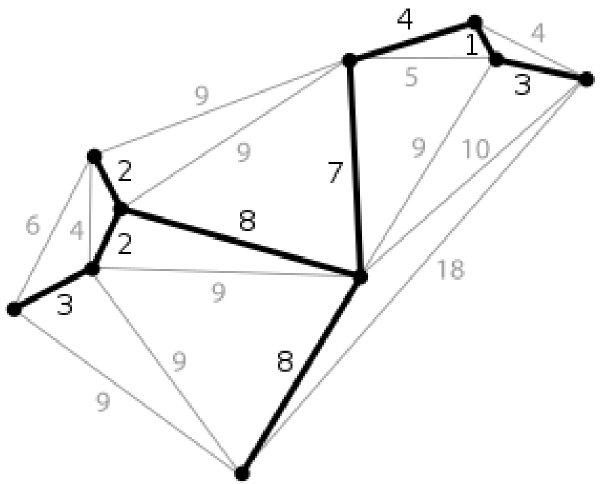
Optimization problems – gradient descent?





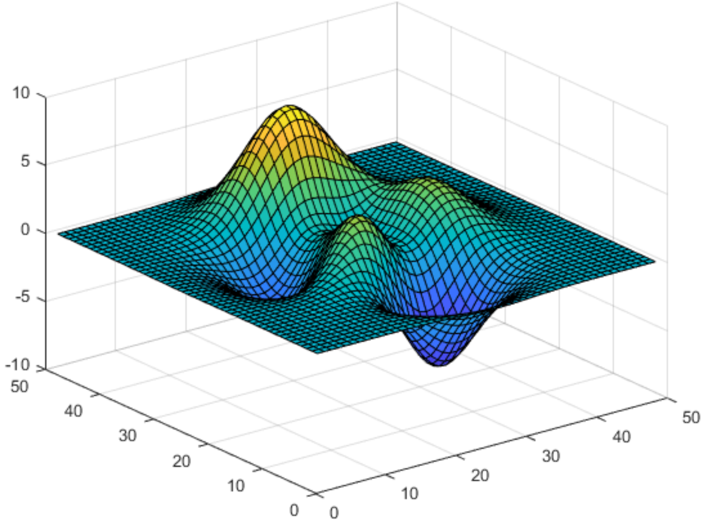


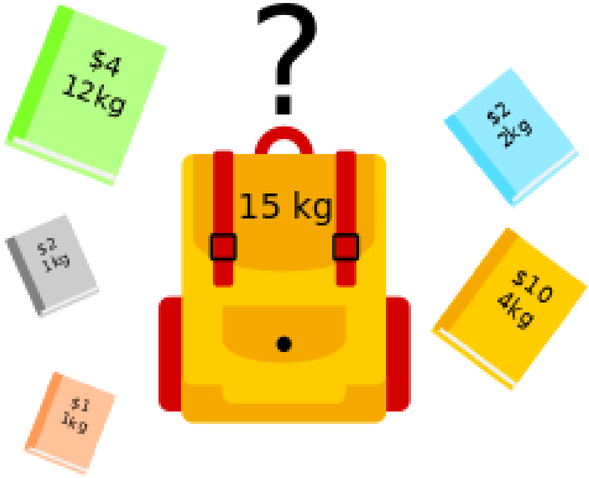




Optimization problems

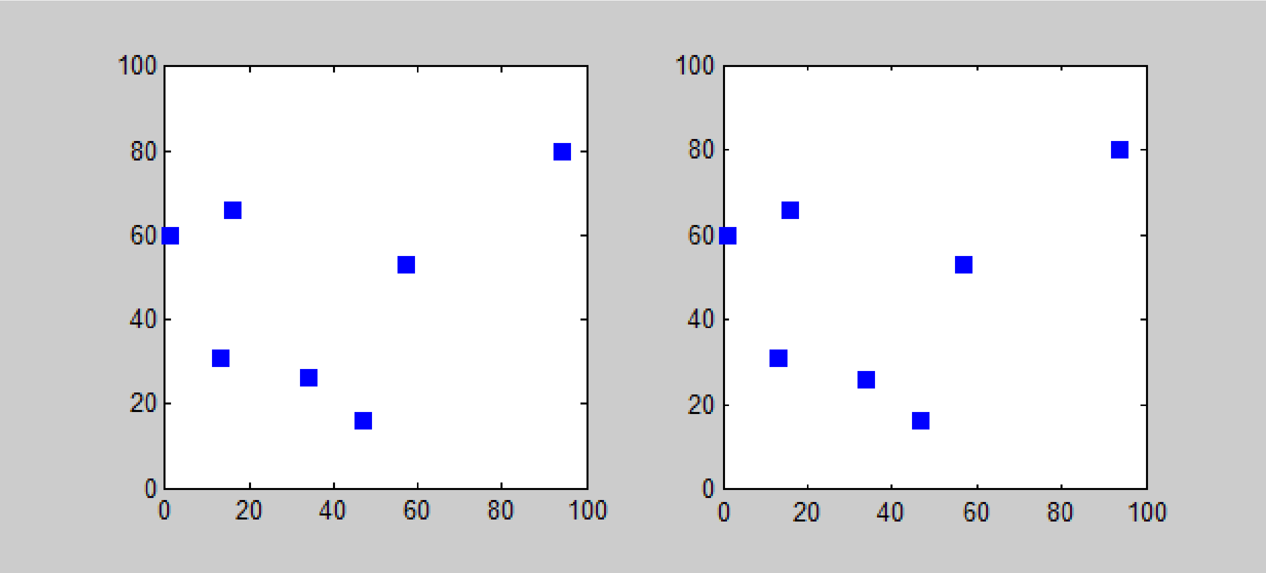
- Key Components
  - Objective Function y=f(x)
  - Variables x = (x1, x2, …, xn)
  - Constraints 0<x1<1; x2 in [0, 1]
  - Feasible Solution
  - Optimal Solution





- Types of Optimization problems
  - Linear vs Nonlinear
  - Continuous vs Discrete (Combinatorial)
    Knapsack problem; travelling salesman problem

- Solution methods
  - Analytical
  - Numerical (gradient descent)
  - (Meta)heuristic (greedy algorithms; EA)



Solution to a symmetric TSP with 7 cities using brute force search.
Note: Number of permutations: (7−1)!/2 = 360. O(n!).
Dynamic programming: O(n^2 * 2^n). NP-hard.

Racehorse Bloodlines

goal function
- Racehorse competition:
  - just run fast!
  - $50B to U.S. GDP

solution
- Champion horses (DNA!)

optimization
- Breeding history

initiation
  - Racehorse's origin from 3 horses
    - Byerley Turk (1680~1703 AD)
    - Darley Arabian (1700~1722 AD)
    - Godolphin Arabian (1724~1753)

selection
  - Select good horses (winners and relatives)

crossover
  - Breeding – female and male horses gens

mutation
  - Gen mutation naturally happens

reproduction
  - Next generation of horses

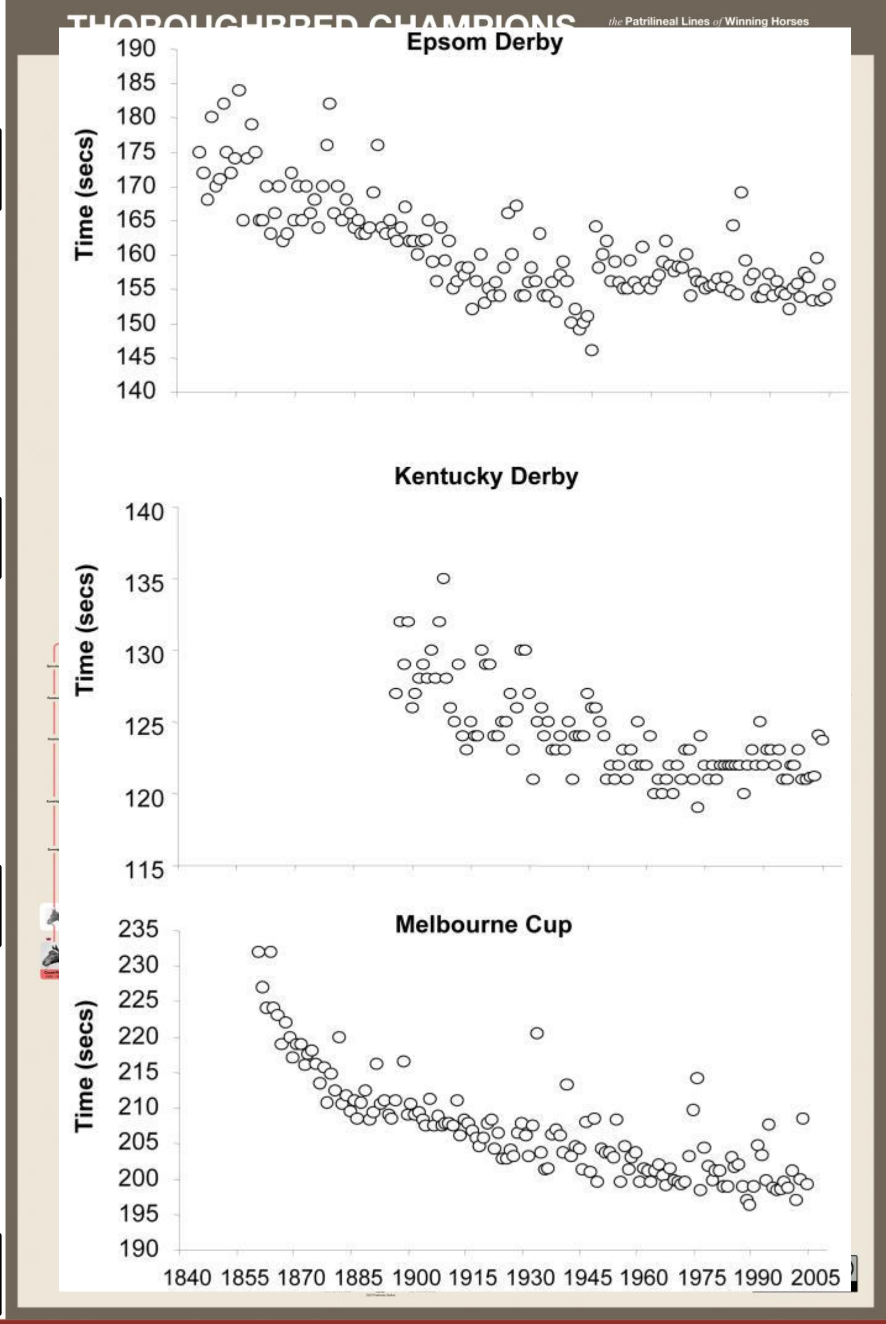
evaluation
  - Competitions

1700

1800

1900

2000



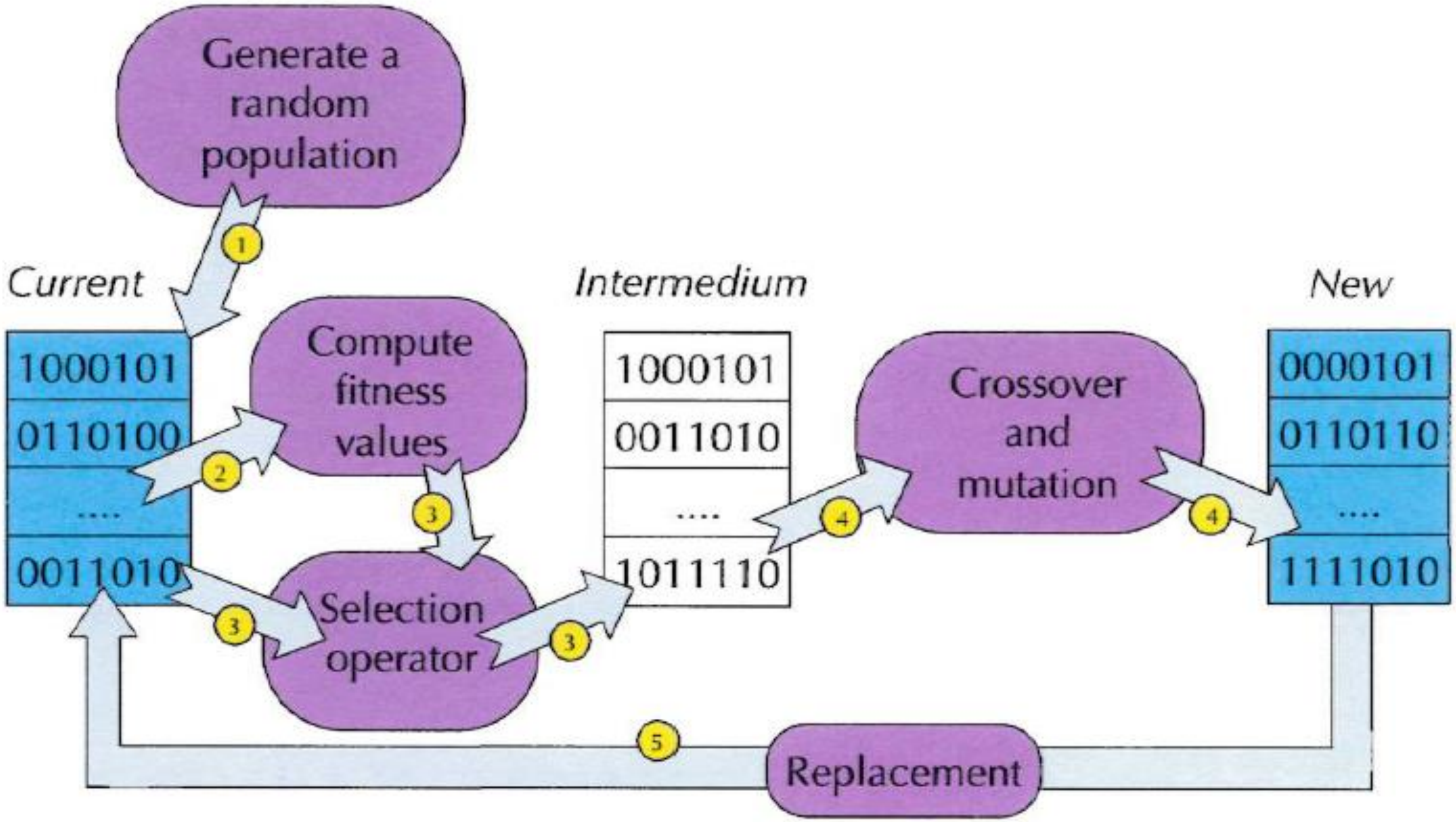
The Essence of Evolutionary Algorithms

- Individuals and Genomes
- Population
- Fitness Function
- Selection
- Genetic Operators
  - Mutation
  - Crossover (Recombination)
- Generation
- Termination Criteria

- Niching Methods (maintain diversity)
- Elitism (keep the best individuals from the current generation)

Genetic Algorithm Process

*Slide adapted from Luis Martí for the graduate course Advanced Evolutionary Computation: Theory and Practice.



Genetic Algorithm Process

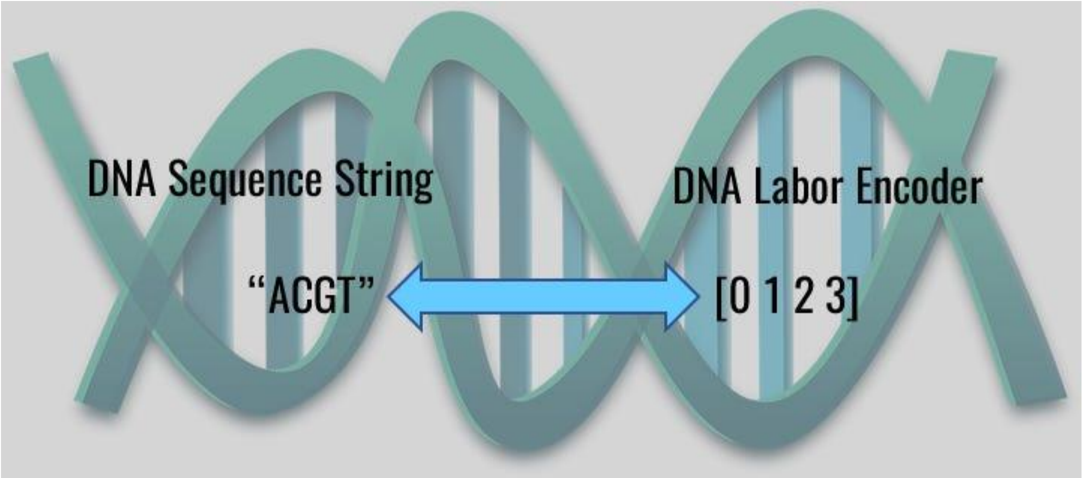
*Slide adapted from Luis Martí for the graduate course Advanced Evolutionary Computation: Theory and Practice.

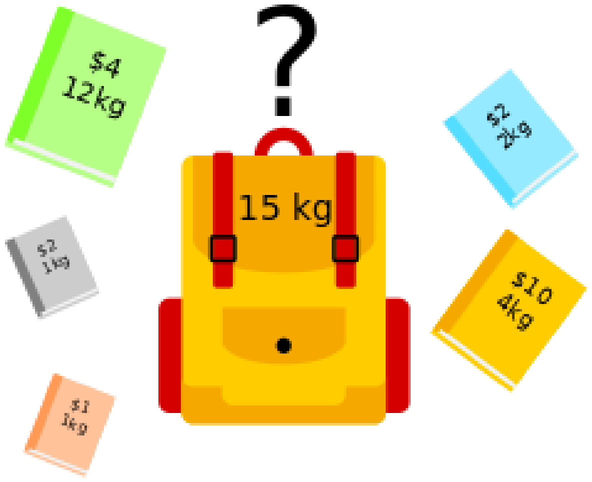
- Modeling the problem
  - Information encoding
  - Create a fitness function

- Algorithm configuration
  - Selection
  - Crossover
  - Mutation
  - Parameters
    - population size
    - Probability of crossover
    - Probability of mutation

Information Encoding

- The Basics of Encoding
- Common Encoding Strategies
  - Binary encoding
  - Integer encoding
  - Real-number encoding
- Data structure
  - List (vector)
  - Set (order does not matter; **knapsack problem**)
  - Graph
- Ready for genetic operations (selection, crossover, mutation)





Selection

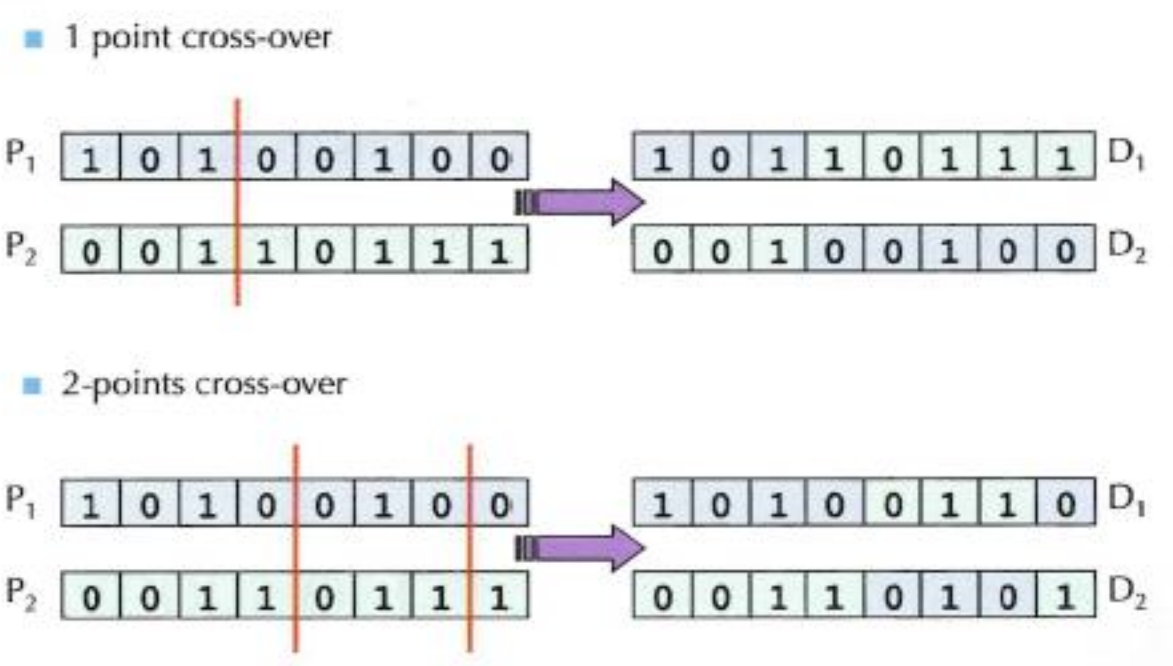
- What's selection all about – choose best candidates
- Goal – lead us to the optimal answer

- Fitness evaluation – every individual gets a fitness score
- Selection methods
  - Roulette Wheel Selection
  - Tournament Selection
  - Rank Selection
- Keep parent generation or not
  - Elitism (keep the best solution)

Crossover

*Slide adapted from Luis Martí for the graduate course Advanced Evolutionary Computation: Theory and Practice.

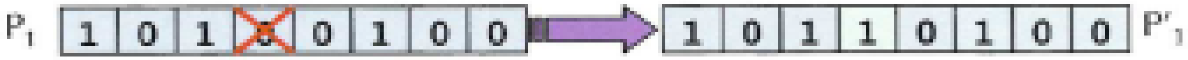
- Create Offspring
- Crossover methods
  - 1-point
  - Multi-point
  - Uniform crossover
- The goal – gambling on new combinations
- Diversity is the key

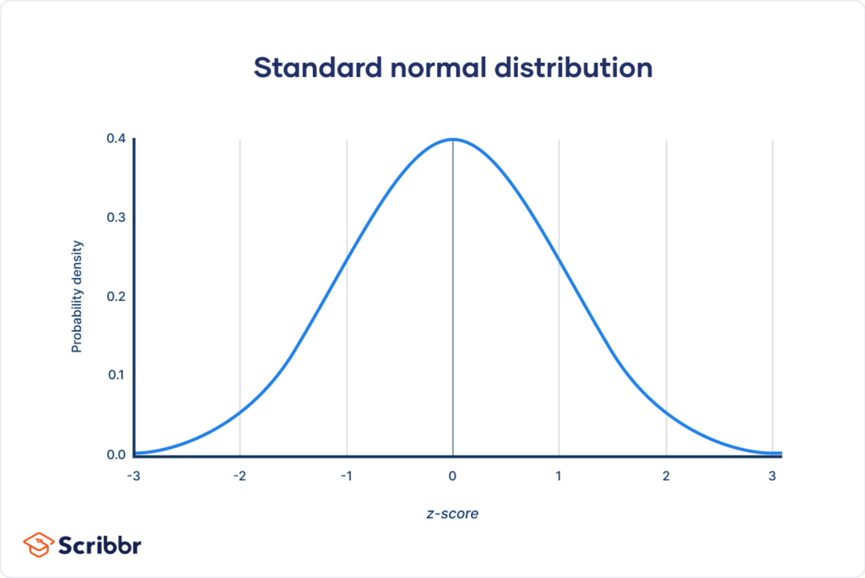


Mutation

*Slide adapted from Luis Martí for the graduate course Advanced Evolutionary Computation: Theory and Practice.

- Introduce randomness to avoid getting stuck
- Change a little bit, at a low probability
- Keeps the genetic pool diverse
- Mutation strategies
  - Bit Flip in Binary Encoding
  - Random tweaking in real-number encoding
  - Swapping in Integer or Permutation Encoding
- The balance
  - Tuning parameters (strategies, probability)





Evolutionary Strategies Tunning

*Slide adapted from Luis Martí for the graduate course Advanced Evolutionary Computation: Theory and Practice.

- Encoding
- Crossover
- Mutation
- Parent selection
- Survivor selection
  - (μ, λ) Strategy:
    λ offspring from μ parents
    select among λ offspring only
  - (μ + λ) Strategy:
    consider both the parents and the offspring when selecting the next generation

NN vs EA – why does NN get more attention in AI?

Neural Network		**Evolutionary Algorithms**
• Human brain	analogy	• Biological evolution
• Loss function	opt. funct.	• Fitness function
• Numerical vectors/tensors	encoding	• Categorical/numerical vectors
• Backpropagation	update	• Evolution (reproduction)
• Gradient descent	convergence	• Clone + Selection + Crossover
• Stochastic gradient descent	variation	• Mutation
• Data	Input	• Environment – f(x) & constraints
• A model to fit the data	Result	• An optimal solution
• Learn from data	Strategy	• Survive in the environment

Data-driven

Model

Understanding the Spotlight on Neural Networks

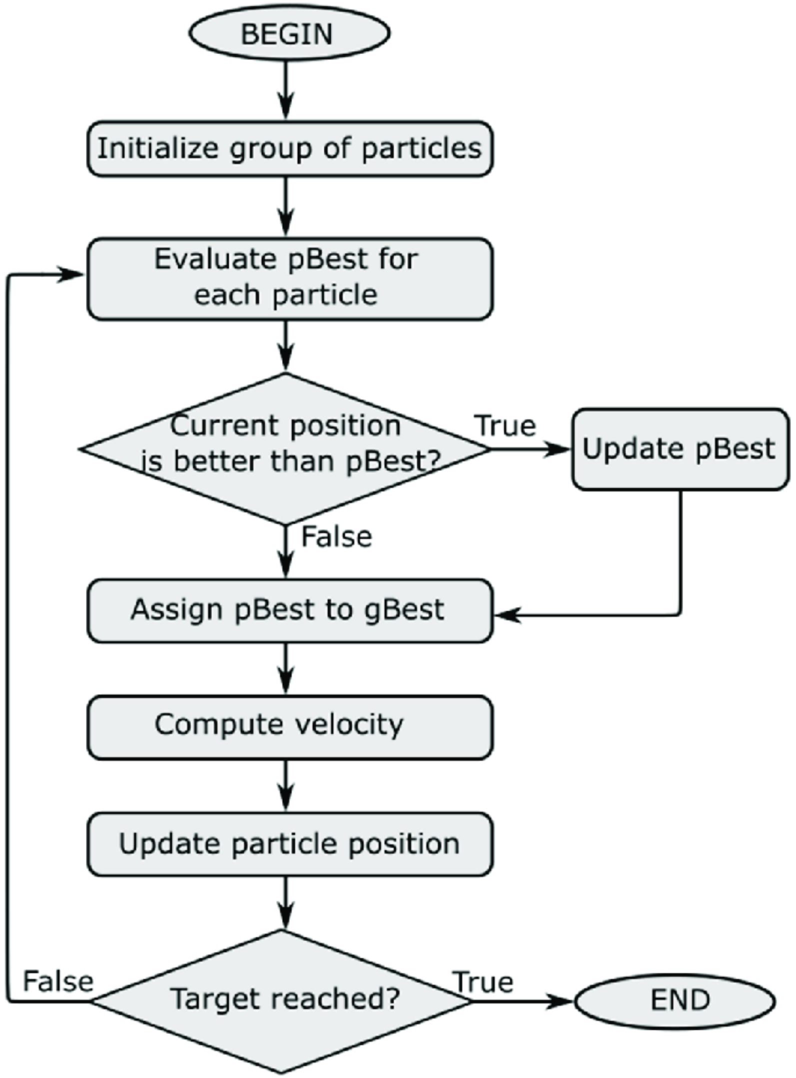
- Neural Networks: The Center of Attention
  - Versatility and Power
  - Breakthroughs and Media Coverage
  - Business and Investment

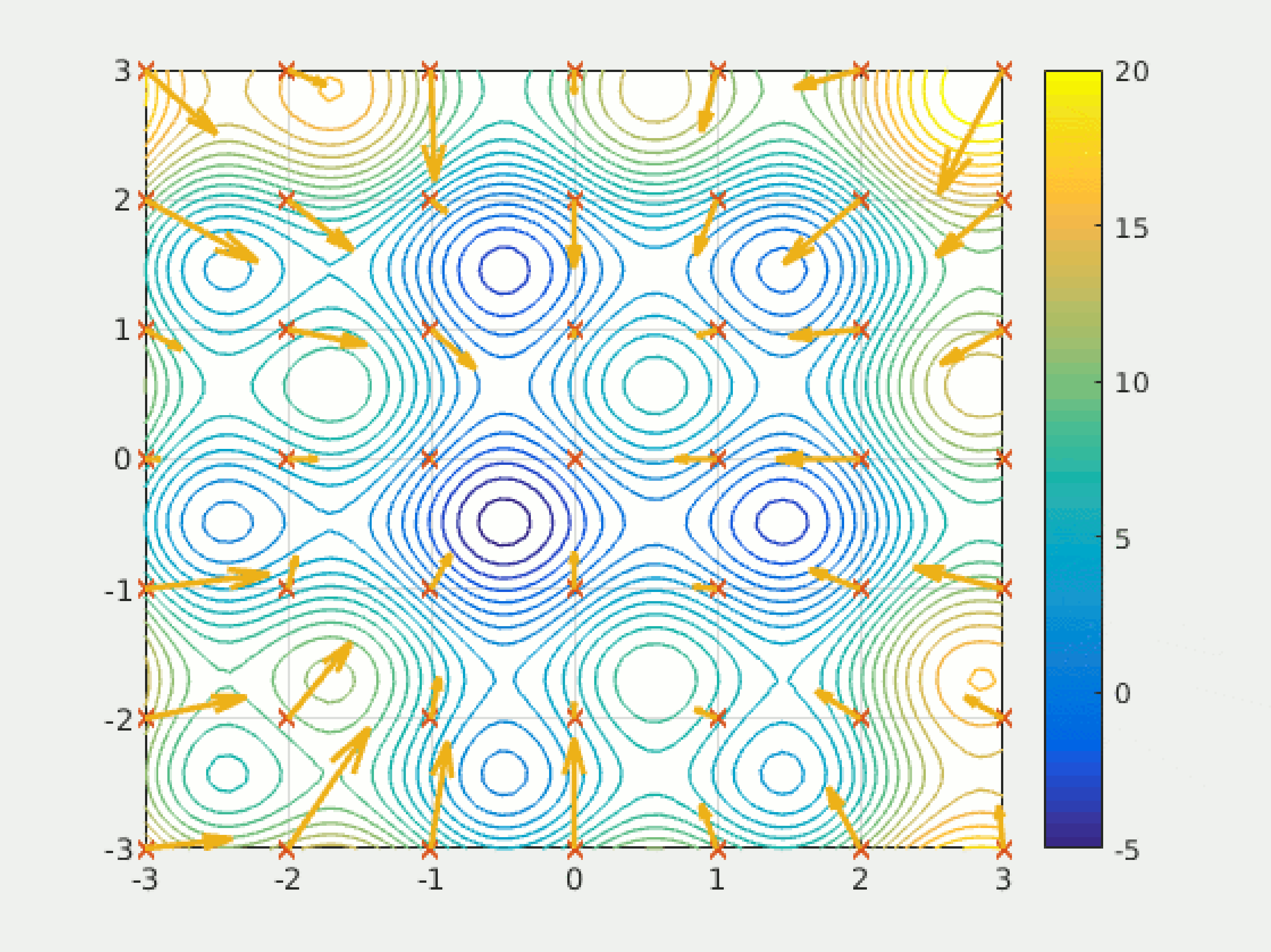
- Where Do Evolutionary Algorithms Stand?
  - A Complementary Relationship

Further reading

- Advanced Evolutionary Computation: Theory and Practice (Luis Martí)
  http://lmarti.com/aec-2014
  https://nbviewer.org/github/lmarti/evolutionary-computation-course/tree/master/
- DEAP github:
  https://github.com/DEAP/deap
- Genetic Programming

Particle Swarm Optimization





DEAP hands-on

- About DEAP
- Example: 1-max problem
- Example: 0-1 knapsack problem
- Example: optimization with PSO