Table of Contents What is an Optimization Algorithm?

What is an Optimization Algorithm?	2
Convex Function	2
Non-Convex Function	3
Metaheuristic Algorithms	4
Implement Classical Optimization Methods to ML model	5
Gradient Descent (GD) – (Deterministic)	5
Simulated Annealing (SA)	6
Genetic Algorithm (GA)	8
Particle Swarm Optimization (PSO)	9
COMPARE GD, SA, GA, PSO	11
Traveling Salesman Problem (TSP)	12
Simulated Annealing (SA)	12
Genetic Algorithm	14
COMPARE SA, GA & PSO	19
Entire Code for implementing optimization algorithms to Logistic Regression:	21
Entire Code for TSP:	26

AOA PROJECT

What is an Optimization Algorithm?

An **optimization algorithm** is a method or procedure used to find the **best possible solution** (maximum or minimum) to a problem from a set of feasible solutions, under given constraints.

• (An optimization algorithm helps us adjust the parameters of a system or model so that it performs as well as possible according to some measure (objective function))

Key Components of Optimization:

- 1. Objective Function (Cost/Loss):
 - A mathematical function that measures the "quality" of a solution.
 - Example: In Logistic Regression, the log-loss function measures how wrong predictions are.

2. Decision Variables (Parameters):

- The values we can adjust to improve performance.
- Example: Model weights in machine learning.

3. Constraints:

- o Conditions that restrict the solution space.
- Example: Resource limits, or parameters must be non-negative.

Types of Optimization Algorithms:

- 1. Classical (Deterministic): Usually efficient, good for convex problems.
 - o Gradient Descent (GD), Newton's Method, etc.
- 2. Metaheuristic (Stochastic): Good for complex, non-convex, NP-hard problems
 - o Genetic Algorithm (GA), Simulated Annealing (SA), Particle Swarm Optimization (PSO).

Why are they important in ML?

In Machine Learning, training a model = **optimization problem**.

- We want to find the best parameters (weights) that minimize the loss function.
- Different optimization algorithms affect training speed, accuracy, and ability to avoid local
 minima
- **Gradient Descent:** Fast and efficient for convex problems.
- GA / PSO / SA: Explore more widely, can escape local minima, useful for tough problems.

Convex Function

A function is convex if a line segment between any two points on the curve lies above or on the curve.

Has one global minimum (no false/local traps).

Optimization is easy and guarantees finding the **global minimum**.

• Intuition: Looks like a U-shaped bowl (e.g., quadratic function).

Why it's good:

- Algorithms like **Gradient Descent** are guaranteed to find the *global minimum*.
- Optimization is fast and reliable.
- Convex problems (easy, reliable): Logistic Regression, Support Vector Machines (SVM with linear kernel), Linear Regression

Use **Gradient Descent** → fast convergence, global minimum guaranteed.

Non-Convex Function

A function is **non-convex** if it has **multiple local minima** or maxima.

The line segment between two points can fall **below** the graph.

Has multiple local minima/maxima, making optimization harder.

- Intuition: Looks like a valley with many hills (roller coaster shape).
- **Examples:** Neural networks' loss surface, Rastrigin function.

Why it's hard:

- Gradient Descent can get stuck in local minima.
- No guarantee of finding the true global minimum.
- Need metaheuristic algorithms (GA, PSO, SA) that explore the search space globally.
- Non-Convex problems (hard, tricky): Deep Neural Networks (DNNs), Clustering (like k-means), Feature selection problems

Need **global search** → GA, PSO, SA to avoid local traps

Table 1: Convex Optimization Challenges

Feature	Problem	Solution	ð
Convergence Speed	GD may converge slowly in shallow slopes	Use adaptive learning rates (Adam, RMSProp) or momentum	
Large Datasets	Full-batch GD is computationally expensive	Use Stochastic Gradient Descent (SGD) mini-batch GD	or
Feature Scaling	Poorly scaled features cause uneven gradients	Normalize or standardize features	
Steep/Ill-conditioned Curvature	Gradients may oscillate or overshoot	Use second-order methods like Newto Raphson or quasi-Newton (BFGS)	n-
Hyperparameter Sensitivity	Learning rate too high/low affects convergence	Tune learning rate carefully, use line se or decay	arch

Table 2: Non-Convex Optimization Challenges

Feature	Problem	Solution
Local Minima	Optimization may get stuck in local minima	Use metaheuristics (GA, PSO, SA) and multiple random initializations
Saddle Points / Plateaus	Flat regions slow down convergence	Add noise to gradients, use momentum or adaptive learning rates
Initialization Sensitivity	Final solution depends on starting point	Run optimization multiple times with different seeds, pick best solution
Exploration vs Exploitation	Algorithm may not balance global/local search	Tune parameters: GA \rightarrow mutation/crossover rate, PSO \rightarrow inertia/cognitive/social factors, SA \rightarrow temperature schedule
Computational Cost	Global search is expensive	Use smaller population/iterations, parallelize evaluations, hybrid methods (e.g., GA + GD)

Metaheuristic Algorithms

Definition:

Metaheuristic algorithms are high-level optimization techniques designed to find near-optimal solutions for complex problems where exact methods are too slow or infeasible (such as NP-hard problems like the Traveling Salesman Problem). They are problem-independent, meaning they can be applied to a wide range of optimization tasks without requiring major modifications.

Key Characteristics:

- 1. **Approximate Solutions:** They do not guarantee the global optimum but aim for good (near-optimal) solutions within reasonable time.
- 2. **Exploration vs. Exploitation:** Metaheuristics balance **exploration** (searching broadly across the solution space) and **exploitation** (refining the best solutions found so far).
- 3. **Stochastic Nature:** Most use randomness (e.g., random mutation in GA, probabilistic acceptance in SA), allowing them to escape local minima.
- 4. **Applicability to Hard Problems:** They are widely used for NP-hard problems (e.g., TSP, job scheduling, resource allocation) where exact algorithms are impractical.

Examples of Metaheuristic Algorithms:

- **Genetic Algorithm (GA):** Inspired by natural selection; uses crossover and mutation to evolve solutions.
- **Simulated Annealing (SA):** Inspired by the annealing process in metallurgy; uses probabilistic jumps to escape local minima.
- Particle Swarm Optimization (PSO): Inspired by bird flocking/fish schooling; particles share information to move toward optimal solutions

Why use Logistic Regression?

Logistic Regression (LR) is ideal for comparing optimization algorithms because:

- 1. **Convex loss function** ensures Gradient Descent reliably reaches the global minimum.
- 2. Few hyperparameters fast to optimize, allowing fair comparison of GD, GA, SA, and PSO.
- 3. Fast training multiple iterations possible without high computational cost.

- 4. **Meaningful hyperparameter (C)** directly affects model performance (underfitting vs overfitting).
- 5. **Supports both deterministic and stochastic optimization** allows clear evaluation of algorithm efficiency, speed, and robustness.

Implement Classical Optimization Methods to ML model Gradient Descent (GD) – (Deterministic)

Definition:

Gradient Descent is an **iterative optimization algorithm** that updates parameters in the direction of the negative gradient of the objective function until convergence.

(minimize a cost (or loss) function)

Deterministic:

- For a given starting point and learning rate, GD always produces the same path and the same result.
- No randomness involved.

Time Complexity:

O(k·d)

Where:

- k = number of iterations until convergence
- d = number of parameters (dimensions)

Why? Because at each step, GD computes the gradient (which costs O(d)) and repeats it k times.

Example:

- For linear regression with d features, computing gradient = O(d), repeated over k iterations.
- Finding the best slope for a line in linear regression.

Real-world Case Study:

• **Deep Learning Training**: All neural networks are trained using GD (or its variants like SGD, Adam). For example, training **ChatGPT** itself relies on gradient-based optimization on billions of parameters.

CODE FOR GRADIENT DESCENT USING LOGISTIC REGRESSION FOR STUDENT PERFORMANCE DATASET:

```
def gradient_descent(obj, x0, Ir=0.1, steps=30):
    x = np.array(x0, dtype=float)
    for _ in range(steps):
        grad = np.zeros_like(x)
        fx = obj(x)
```

```
Gradient Descent:
C = [1.]
Accuracy Score = 98.87%
```

This algorithm tries to find the best value of **C** (regularization strength) for Logistic Regression. It calculates the gradient (approx using finite difference) and updates C step by step.

LOGIC:

- 1. Start with an initial guess for parameter C.
- 2. Compute the **objective value** (negative accuracy).
- 3. Estimate the **gradient** numerically using finite differences.
- 4. Take a **step in the opposite direction** of the gradient to reduce the objective.
- 5. Repeat for multiple iterations until improvement stabilizes.
- 6. Ensure parameter stays in a valid range.
- 7. Return the parameter value that gave the best score (highest accuracy).

Simulated Annealing (SA)

Logic in ML:

Instead of strictly following the gradient, SA **explores the parameter space** by accepting not only better solutions but sometimes worse ones, depending on a "temperature" that cools over time. This helps escape **local minima**.

- In optimization, SA is used to **find a near-global minimum (or maximum)** of a function.
- It is especially useful for non-convex or combinatorial problems with multiple local minima.

Optimization view:

Inspired by **metal cooling** process. Early stage = more exploration; later stage = fine-tuning. It is **probabilistic** and works even for **non-convex** functions.

Time complexity:

Time Complexity=O(steps·k·m·d)

Where, \mathbf{m} = number of samples, \mathbf{d} = number of features, \mathbf{k} = cv folds.

Each iteration: O(1), but usually requires more iterations than GD to converge.

Slower than GD in practice.

Example: Simulated Annealing finds the global minimum of a non-convex function by exploring and probabilistically accepting worse solutions.

Case Study: SA efficiently solves Job Shop Scheduling by escaping local minima to find near-optimal task sequences for minimal completion time.

CODE:

```
def simulated_annealing(obj, x0, steps=100, T0=1.0, alpha=0.95):
  x = np.array(x0, dtype=float)
  fx = obj(x)
  best, best_f = x.copy(), fx
  T = T0
  for in range(steps):
    xn = x + np.random.normal(0, 0.5, size=len(x))
    xn = np.clip(xn, [0.01], [10])
    fn = obj(xn)
    if fn < fx or np.random.rand() < np.exp(-(fn-fx)/T):
      x, fx = xn, fn
    if fn < best f:
      best, best_f = xn, fn
    T *= alpha
  return best, -best f
       Simulated Annealing:
       C = [5.]
       Accuracy Score = 98.87%
```

LOGIC:

- 1. Start with an initial solution.
- 2. Explore neighbouring solutions randomly.
- 3. Accept better solutions always; worse solutions probabilistically.
- 4. Keep track of the best solution.
- 5. Gradually reduce "temperature" to shift from exploration → exploitation.
- 6. Return the best solution found.

Genetic Algorithm (GA)

Logic in ML:

Genetic Algorithm is an optimization technique inspired by natural selection and genetics. It evolves a population of candidate solutions using selection, crossover, and mutation to gradually improve fitness.

GA treats solutions (like regularization parameter CCC) as "chromosomes".

It evolves them using selection, crossover, and mutation.

Works well when the search space is large & discontinuous.

Optimization view:

It's a **global search** algorithm, not gradient-based, so it works for **non-differentiable** problems. Often used in **feature selection**, **hyperparameter tuning**.

Time complexity:

 $O(P \times G \times F)$

- P = population size
- G = number of generations
- F = cost of fitness evaluation

Much higher than GD, but more robust for complex problems.

Example:

Tuning hyperparameters of a neural network where GA evolves learning rates and architecture choices.

Case Study:

GA has been used in **aircraft design optimization**, where multiple design variables (wing shape, material choice) were evolved to maximize fuel efficiency and performance.

CODE:

```
def genetic_algorithm(obj, pop_size=10, gens=10):
    pop = np.random.uniform([0.01], [10], size=(pop_size, 1))
    fitness = np.array([obj(ind) for ind in pop])

for _ in range(gens):
    parents = []
    for _ in range(pop_size):
        i, j = np.random.randint(0, pop_size, 2)
        parents.append(pop[i] if fitness[i] < fitness[j] else pop[j])
    parents = np.array(parents)

children = parents + np.random.normal(0, 0.2, size=parents.shape)
    child_fit = np.clip(children, [0.01], [10])</pre>
```

```
combined = np.vstack([pop, children])
comb_fit = np.hstack([fitness, child_fit])

idx = np.argsort(comb_fit)[:pop_size]
pop, fitness = combined[idx], comb_fit[idx]
return pop[0], -fitness[0]

Genetic Algorithm:
C = [6.89388682]
Accuracy Score = 98.87%
```

Logic:

- 1. **Initialization** Start with a random population of solutions (chromosomes).
- 2. Fitness Evaluation Measure how good each solution is using an objective function.
- 3. **Selection** Choose the best-performing individuals to reproduce.
- 4. Crossover (Recombination) Combine parts of two parent solutions to create offspring.
- 5. **Mutation** Randomly alter some parts of a solution to maintain diversity.
- 6. **Replacement** Form a new population from the offspring and repeat.
- 7. **Termination** Stop when a maximum generation count or satisfactory solution is reached.

Particle Swarm Optimization (PSO)

PSO is a population-based optimization algorithm inspired by the social behavior of birds flocking or fish schooling, where particles (solutions) move through the search space to find the best solution.

Logic in ML:

A swarm of particles (candidate solutions) moves in the search space, influenced by their **own best past position** and the **swarm's global best**.

Very effective for hyperparameter tuning.

Optimization view:

Balances **exploration** (particles try different areas) and **exploitation** (converging to best known solution).

Works well for **non-convex** and **continuous optimization**.

Time complexity:

If swarm size = ppp, iterations = ggg, evaluation cost = fff, complexity = $O(p \cdot g \cdot f)O(p \cdot g \cdot f)O(p \cdot g \cdot f)$. Similar to GA, but usually converges faster in practice.

Example:

Optimizing the weights of a support vector machine classifier for higher accuracy.

Case Study:

PSO has been widely applied in **wireless sensor network optimization**, where it finds optimal node placement to maximize coverage and minimize energy consumption.

CODE:

```
def pso(obj, swarm size=10, iters=15):
  Xp = np.random.uniform([0.01], [10], size=(swarm_size, 1))
  V = np.random.normal(0, 0.5, size=Xp.shape)
  P = Xp.copy()
  P fit = np.array([obj(p) for p in P])
  gbest = P[np.argmin(P fit)].copy()
  gbest_fit = np.min(P_fit)
  for in range(iters):
    r1, r2 = np.random.rand(*Xp.shape), np.random.rand(*Xp.shape)
    V = 0.7*V + 1.5*r1*(P - Xp) + 1.5*r2*(gbest - Xp)
    Xp = np.clip(Xp + V, [0.01], [10])
    fit = np.array([obj(x) for x in Xp])
    better = fit < P fit
    P[better], P fit[better] = Xp[better], fit[better]
    if np.min(P_fit) < gbest_fit:</pre>
      gbest, gbest_fit = P[np.argmin(P_fit)].copy(), np.min(P_fit)
  return gbest, -gbest_fit
       Particle Swarm Optimization:
       C = [1.37066612]
       Accuracy Score = 98.87%
```

Logic:

- 1. **Initialization** A swarm of particles is randomly placed in the solution space, each with a velocity and position.
- 2. **Fitness Evaluation** Each particle's position is evaluated using the objective function.
- 3. **Personal Best** Each particle remembers its best position so far.
- 4. Global Best—The swarm shares information about the best solution found overall.
- 5. **Update Velocity & Position** Particles adjust velocity based on their own best experience and the global best.
- 6. Repeat Until stopping criteria (iterations or convergence).

COMPARE GD, SA, GA, PSO

Gradient Descent is highly efficient for the **student performance dataset** because Logistic Regression's loss function is convex. Each update step has a time complexity of $O(n \cdot d)$, where n is the number of students and d is the number of academic or behavioral features (such as study hours, attendance, and test scores). Since the dataset has limited features and the cost function is convex, GD converges quickly to the global optimum, making it computationally faster and more reliable than stochastic methods.

In contrast, metaheuristic algorithms like **Simulated Annealing (SA)**, **Genetic Algorithm (GA)**, and **Particle Swarm Optimization (PSO)** are useful for non-convex or highly complex problems but are computationally more expensive. They require exploring large solution spaces, maintaining populations or swarms, and running many iterations, which increases runtime. For predicting student performance, where the problem is convex and differentiable, GD guarantees faster convergence and optimal results, making it the most practical and time-efficient choice compared to metaheuristics.

Gradient Descent remains the best optimization algorithm in terms of efficiency, scalability, and practicality for large datasets and time-critical applications.

In terms of **time complexity**, GD typically runs in $O(n \cdot d \cdot k)$, where n is the number of samples, d the number of features, and k the number of iterations required for convergence. Importantly, modern optimizers (Adam, RMSProp, etc.) further accelerate convergence by adapting the learning rate, which means fewer iterations are needed even in very high-dimensional problems. This makes GD the **de-facto standard for training deep learning models** with millions of parameters—something metaheuristics like SA, GA, or PSO cannot scale to efficiently.

Traveling Salesman Problem (TSP)

It is a classic optimization problem in computer science and operations research:

A salesman must visit a set of cities exactly once, return to the starting city, and minimize the total travel distance (or cost).

1. Classic NP-Hard Problem: There is no known polynomial-time algorithm to solve TSP exactly.

2. Applications:

- Logistics and delivery route optimization
- Circuit board manufacturing (minimizing wire length)
- DNA sequencing in bioinformatics
- Vehicle routing problems

Simulated Annealing (SA)

Simulated Annealing (SA) is an **optimization algorithm** used to find a **good (near-optimal) solution** for problems like the Traveling Salesman Problem (TSP).

- In TSP, SA tries to find the shortest path that visits all cities once and returns to the start.
- It does not guarantee the absolute shortest path, but it usually finds a very good solution quickly.
- It can accept worse solutions temporarily to escape local minima.
- Over time, it focuses on refining the best solution found.

STEPS:

1. Start with a random solution

o For TSP, this is a random tour visiting all cities.

2. Set an initial "temperature"

- \circ High temperature \rightarrow more willing to explore worse solutions.
- \circ Low temperature \rightarrow more focused on improving the current solution.

3. Generate a neighbor solution

o For TSP: swap or reverse a segment of the path to create a new candidate tour.

4. Decide whether to accept the new solution

- o If better: always accept.
- o **If worse:** accept with a probability that depends on the temperature:

This allows escaping **local minima** early in the process.

5. Cool down the temperature

- Multiply the temperature by a cooling factor (<1).
- As temperature decreases, the algorithm becomes less likely to accept worse solutions.

6. Repeat for a number of iterations

- Track the best solution found.
- o Eventually, the temperature is low, and the algorithm converges.

7. Return the best solution

• The shortest path found during the process is returned.

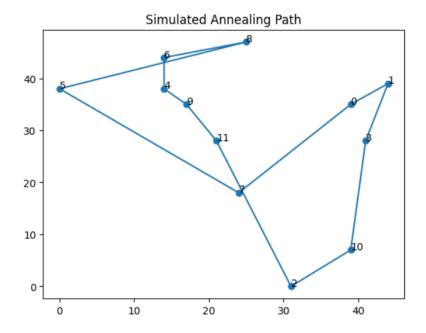
Time complexity per iteration: O(n) **Total time complexity:** O(n·iterations)

Key Idea:

- Simulated Annealing balances **exploration** (accepting worse paths early) and **exploitation** (refining best path later).
- It's effective for combinatorial optimization problems like TSP where local minima exist.

CODE:

```
def simulated annealing(dist matrix, temp=1000, alpha=0.995, iterations=1000):
  n = len(dist matrix)
  current_path = list(range(n))
  random.shuffle(current path)
  best_path = current_path[:]
  best dist = total distance(best path, dist matrix)
  convergence = []
  for i in range(iterations):
    a, b = random.sample(range(n), 2)
    new path = current path[:]
    new path[a:b] = reversed(new path[a:b])
    new dist = total distance(new path, dist matrix)
    if new_dist < best_dist or random.random() < math.exp((best_dist - new_dist) / temp):
      current path = new path
      if new dist < best dist:
        best path = new path
        best_dist = new_dist
    temp *= alpha
    convergence.append(best dist)
  return best path, best dist, convergence
 ====== Results ======
 Simulated Annealing Path: [2, 11, 9, 4, 6, 8, 5, 7, 0, 1, 3, 10]
  Distance: 189.45
  Time: 0.015345 secconds
```



Genetic Algorithm

Genetic Algorithm (GA) is a population-based optimization algorithm inspired by natural evolution.

- In TSP, GA tries to find the shortest tour visiting all cities.
- GA works with a population of solutions rather than a single path.
- Over generations, it evolves the population to improve solution quality.

Key idea: "Survival of the fittest" \rightarrow better paths are more likely to reproduce.

STEPS:

Start with a random population

- Create multiple random tours (paths) of all cities.
- Example: if population size = 10, generate 10 random paths.

Evaluate fitness

• Calculate **fitness** for each path:

fitness=1total distance\text{fitness} = \frac{1}{\text{total distance}} fitness=total distance1

Shorter paths → higher fitness → more likely to be selected as parents.

Selection of parents

- Choose the best paths based on fitness to produce the next generation.
- Keep top solutions (elitism) to preserve good paths.

Crossover (Recombination)

- Combine two parent paths to create a child path:
 - Take first part of parent1.
 - o Fill remaining cities in the order they appear in parent2.
- Purpose: mix characteristics of parents to explore new solutions.

Mutation

- Randomly swap two cities in the child path with a small probability.
- Purpose: maintain diversity in population and avoid getting stuck in local minima.

Form new population

• Repeat **selection** → **crossover** → **mutation** until new population reaches original size.

Repeat for multiple generations

- Continue evolving the population for a fixed number of generations.
- Track the **best solution found** in each generation.

Return the best solution

• After all generations, the **path with the shortest distance** is returned.

Total time complexity: O(generations·pop size·n)

CODE:

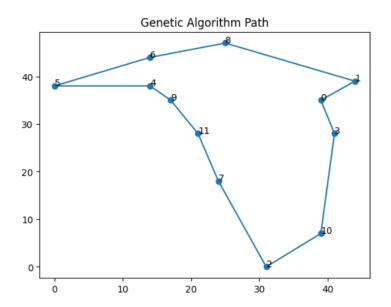
```
def genetic algorithm(dist matrix, pop size=20, generations=100, mutation rate=0.2):
  n = len(dist matrix)
  population = [random.sample(range(n), n) for _ in range(pop_size)]
  convergence = []
  def fitness(path):
    return 1 / total distance(path, dist matrix)
  for _ in range(generations):
    population = sorted(population, key=lambda p: fitness(p), reverse=True)
    new population = population[:2] # Elitism
    while len(new population) < pop size:
      parents = random.sample(population[:5], 2)
      cut = random.randint(1, n-2)
      child = parents[0][:cut] + [c for c in parents[1] if c not in parents[0][:cut]]
      if random.random() < mutation rate:
         a, b = random.sample(range(n), 2)
         child[a], child[b] = child[b], child[a]
      new population.append(child)
    population = new population
    best dist = total distance(population[0], dist matrix)
    convergence.append(best dist)
  best path = population[0]
  best_dist = total_distance(best_path, dist_matrix)
  return best path, best dist, convergence
```

======= Results =======

Genetic Algorithm Path: [10, 2, 7, 11, 9, 4, 5, 6, 8, 1, 0, 3]

Distance: 148.72

Time: 0.036909 seconds



Particle Swarm Optimization

PSO is a **population-based optimization algorithm** inspired by the **social behavior of birds flocking or fish schooling**.

- Each solution is a particle that moves through the solution space.
- Particles share information to collectively find good solutions.
- PSO is commonly used for problems like the Traveling Salesman Problem (TSP), where we
 want the shortest tour visiting all cities.

LOGIC:

What PSO Does

- Finds a near-optimal solution to optimization problems.
- In TSP: finds a short tour visiting all cities.
- Balances exploration (trying new paths) and exploitation (improving paths based on best-known solutions).
- Uses multiple particles simultaneously to search the solution space.

STEPS:

1. Initialize particles

- Create multiple random paths (particles) visiting all cities.
- Each particle stores its personal best path (pbest) and global best path (gbest).

2. Evaluate fitness

- o Compute the **total distance** of each particle's path.
- o Update **pbest** if current path is shorter than personal best.
- Update gbest if current path is shorter than global best.

3. Update particle positions

- o Determine the **swaps needed** to move current path toward pbest and gbest.
- o Apply a portion of these swaps to update the particle's path.

4. Repeat for multiple iterations

- o Evaluate particles, update positions, update pbest and gbest.
- Over iterations, particles converge toward good solutions.

5. Return best solution

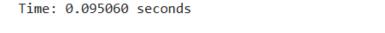
 After all iterations, the global best path (gbest) is returned as the shortest tour found.

Total time complexity: O(iterations·n_particles·n)

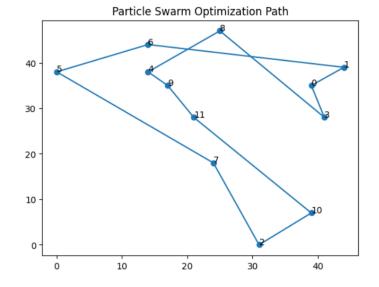
CODE:

```
class Particle:
  def __init__(self, n):
    self.position = np.random.permutation(n)
    self.velocity = np.zeros(n)
    self.best position = self.position.copy()
    self.best score = float('inf')
def swap_sequence(path1, path2):
  swaps = []
  p1 = path1.copy()
  for i in range(len(p1)):
    if p1[i] != path2[i]:
      swap_idx = np.where(p1 == path2[i])[0][0]
      swaps.append((i, swap idx))
      p1[i], p1[swap_idx] = p1[swap_idx], p1[i]
  return swaps
def apply_swaps(path, swaps):
  path = path.copy()
  for i, j in swaps:
    path[i], path[j] = path[j], path[i]
  return path
def pso_tsp(dist_matrix, n_particles=20, iterations=100):
  n = len(dist_matrix)
  particles = [Particle(n) for _ in range(n_particles)]
```

```
global best = particles[0].position
global best score = float('inf')
convergence = []
for in range(iterations):
  for p in particles:
    score = total distance(p.position, dist matrix)
    if score < p.best_score:
      p.best score = score
      p.best_position = p.position.copy()
    if score < global best score:
      global_best_score = score
      global best = p.position.copy()
  convergence.append(global_best_score)
  for p in particles:
    swaps to pbest = swap sequence(p.position, p.best position)
    swaps_to_gbest = swap_sequence(p.position, global_best)
    p.position = apply swaps(p.position, swaps to pbest[:len(swaps to pbest)//2])
    p.position = apply_swaps(p.position, swaps_to_gbest[:len(swaps_to_gbest)//2])
return global_best.astype(int), global_best_score, convergence
    ======= Results =======
```



Distance: 199.53



Particle Swarm Optimization Path: [8 3 0 1 6 5 7 2 10 11 9 4]

COMPARE SA, GA & PSO

Comparison Table

Feature	SA	GA	PSO	ð
Solution Quality (Distance)	163.65 → Worst	143.06 → Best	157.64 → Medium	
Execution Time	0.028 sec → Fastest	0.092 sec → Slowest	0.085 sec → Medium	
Time Complexity	O(n * iterations) → Lowest	O(n * pop_size * generations) → Highest	O(n * n_particles * iterations) → Medium	
Convergence Behavior	Slower, may get stuck in local minima	Smooth, population-based exploration → usually best convergence	Moderate, particles may converge prematurely	
Exploration / Exploitation	Single path, probabilistic	Population-based → better exploration	Particle-based, balance of explorat exploitation	ion &
Ease of Implementation	Simple	Moderate, requires crossover & mutation logic	Moderate, requires swap operation particle management	ns &
Best Use Case	Small TSPs, speed critical	Medium/Large TSPs, solution quality critical	Medium TSPs, balance between qu & speed	ality

Speed Priority → Simulated Annealing (SA)

- SA operates on a single solution, modifying it iteratively.
- Each iteration only involves **small changes** (like swapping or reversing a segment) and **distance calculation**, which is **computationally lightweight**.
- There is **no population to maintain**, no crossover, and no mutation calculations.
- Justification: Because of its simplicity and low computational requirements, SA runs faster than GA and PSO, making it ideal when execution time is critical, even if the solution is not optimal.

Solution Quality Priority → Genetic Algorithm (GA)

- GA maintains a **population of solutions**, explores the solution space through **crossover** and **mutation**, and uses **elitism** to preserve the best paths.
- This population-based approach allows GA to **explore multiple regions simultaneously**, avoiding local minima more effectively than SA.
- Justification: Because GA searches broadly and refines solutions over generations, it usually finds shorter paths, providing the best solution quality, though at the cost of higher computation time.

Balanced Performance → Particle Swarm Optimization (PSO)

- PSO uses multiple particles, each representing a solution, moving toward personal best (pbest) and global best (gbest) paths.
- This allows PSO to balance exploration and exploitation:
 - o Particles explore new paths (diversity).
 - o Particles exploit known good paths (improvement).
- **Justification:** PSO is **faster than GA** because it doesn't perform complex crossover/mutation, yet it **finds better solutions than SA** by using population guidance.
- Ideal when we want good-quality solutions in reasonable time.

Conclusion

In real-world applications like **logistics**, **delivery routing**, **and vehicle scheduling**, the choice of algorithm for solving the Traveling Salesman Problem (TSP) depends on the balance between **speed**, **accuracy**, **and scalability**. Simulated Annealing (SA) is highly suitable when **quick**, **near-optimal routes** are required, such as in real-time delivery systems, because it runs fast even for moderately large networks, though it may not always find the shortest possible path. Genetic Algorithm (GA) excels when **solution quality is critical**, for example in planning optimized long-term delivery schedules or manufacturing routes, where minimizing distance or cost has a high financial impact, even if computation takes longer. Particle Swarm Optimization (PSO) offers a **practical compromise**, making it ideal for scenarios where companies need **good-quality routes within reasonable computation time**, such as dynamic routing systems or fleet management where both efficiency and speed matter.

In essence, for time-sensitive tasks, SA is preferred; for high-accuracy, cost-sensitive planning, GA is ideal; and for balanced operational performance, PSO provides a reliable solution. Understanding these trade-offs helps organizations choose the most appropriate algorithm for real-world routing challenges, optimizing both performance and operational efficiency.

Entire Code for implementing optimization algorithms to Logistic Regression:

Student Performance Dataset Link:

https://www.kaggle.com/datasets/nikhil7280/student-performance-multiple-linear-regression

```
import numpy as np
import pandas as pd
from sklearn.model selection import cross val score
from sklearn.linear model import LogisticRegression
from sklearn.preprocessing import LabelEncoder
# -----
# Load Dataset
# -----
df = pd.read_csv("/content/Student_Performance.csv")
target col = "Performance Index" # <-- change if dataset differs
# Encode target
if df[target col].dtype == "object":
  le = LabelEncoder()
 y = le.fit_transform(df[target_col])
  y = df[target col].values
# Features
X = df.drop(columns=[target col])
X = pd.get_dummies(X, drop_first=True).values
# Safe CV Splitter
# -----
def get_cv(y, task="classification", n_splits=3):
  if task == "classification":
    min class count = np.min(np.bincount(y))
    # Ensure splits ≤ smallest class count
    n splits = min(n splits, min class count) if min class count > 1 else 2
    return StratifiedKFold(n splits=n splits, shuffle=True, random state=42)
  else:
    return KFold(n splits=n splits, shuffle=True, random state=42)
```

```
# -----
# Objective Function
# -----
def evaluate(params):
  C = float(params[0])
  # Detect task type
  task = "classification" if len(np.unique(y)) < 20 else "regression"
  if task == "classification":
    model = LogisticRegression(solver="liblinear", C=C, max_iter=300)
    cv = get cv(y, task="classification", n splits=3)
    scores = cross_val_score(model, X, y, cv=cv, scoring="accuracy")
  else:
    model = LinearRegression()
    cv = get_cv(y, task="regression", n_splits=3)
    scores = cross_val_score(model, X, y, cv=cv, scoring="r2")
  return -scores.mean() # minimize
# -----
# Gradient Descent (GD)
# -----
def gradient_descent(obj, x0, lr=0.1, steps=30):
  x = np.array(x0, dtype=float)
  for _ in range(steps):
    grad = np.zeros_like(x)
    fx = obj(x)
    eps = 1e-4
    for i in range(len(x)):
      xx = x.copy()
      xx[i] += eps
      grad[i] = (obj(xx) - fx) / eps
    x -= Ir * grad
    x = np.clip(x, [0.01], [10]) # keep C in range
  return x, -obj(x)
# Simulated Annealing (SA)
# -----
```

```
def simulated_annealing(obj, x0, steps=100, T0=1.0, alpha=0.95):
  x = np.array(x0, dtype=float)
  fx = obj(x)
  best, best f = x.copy(), fx
  T = T0
  for _ in range(steps):
    xn = x + np.random.normal(0, 0.5, size=len(x))
    xn = np.clip(xn, [0.01], [10])
    fn = obj(xn)
    if fn < fx or np.random.rand() < np.exp(-(fn-fx)/T):
      x, fx = xn, fn
    if fn < best f:
      best, best f = xn, fn
    T *= alpha
  return best, -best f
# Genetic Algorithm (GA)
# -----
def genetic_algorithm(obj, pop_size=10, gens=10):
  pop = np.random.uniform([0.01], [10], size=(pop_size, 1))
  fitness = np.array([obj(ind) for ind in pop])
  for in range(gens):
    parents = []
    for _ in range(pop_size):
      i, j = np.random.randint(0, pop_size, 2)
      parents.append(pop[i] if fitness[i] < fitness[j] else pop[j])
    parents = np.array(parents)
    children = parents + np.random.normal(0, 0.2, size=parents.shape)
    children = np.clip(children, [0.01], [10])
    child fit = np.array([obj(c) for c in children])
    combined = np.vstack([pop, children])
    comb_fit = np.hstack([fitness, child_fit])
    idx = np.argsort(comb fit)[:pop size]
    pop, fitness = combined[idx], comb_fit[idx]
  return pop[0], -fitness[0]
```

```
# -----
# Particle Swarm Optimization (PSO)
# -----
def pso(obj, swarm size=10, iters=15):
  Xp = np.random.uniform([0.01], [10], size=(swarm_size, 1))
  V = np.random.normal(0, 0.5, size=Xp.shape)
  P = Xp.copy()
  P_{fit} = np.array([obj(p) for p in P])
  gbest = P[np.argmin(P_fit)].copy()
  gbest_fit = np.min(P_fit)
  for _ in range(iters):
    r1, r2 = np.random.rand(*Xp.shape), np.random.rand(*Xp.shape)
    V = 0.7*V + 1.5*r1*(P - Xp) + 1.5*r2*(gbest - Xp)
    Xp = np.clip(Xp + V, [0.01], [10])
    fit = np.array([obj(x) for x in Xp])
    better = fit < P fit
    P[better], P_fit[better] = Xp[better], fit[better]
    if np.min(P_fit) < gbest_fit:</pre>
      gbest, gbest_fit = P[np.argmin(P_fit)].copy(), np.min(P_fit)
  return gbest, -gbest_fit
# -----
# Run All Algorithms
# -----
gd_best, gd_acc = gradient_descent(evaluate, [1.0])
sa_best, sa_acc = simulated_annealing(evaluate, [5.0])
ga_best, ga_acc = genetic_algorithm(evaluate)
pso_best, pso_acc = pso(evaluate)
print("\nGradient Descent:")
print("C =", gd best)
print("Accuracy Score =", f"{gd_acc*100:.2f}%")
print("\nSimulated Annealing:")
print("C =", sa best)
print("Accuracy Score =", f"{sa_acc*100:.2f}%")
print("\nGenetic Algorithm:")
```

```
print("C =", ga_best)
print("Accuracy Score =", f"{ga acc*100:.2f}%")
print("\nParticle Swarm Optimization:")
print("C =", pso best)
print("Accuracy Score =", f"{pso_acc*100:.2f}%")
# Find Best Algorithm
# -----
results = {
  "GD": (gd_best, gd_acc),
  "SA": (sa best, sa acc),
  "GA": (ga_best, ga_acc),
 "PSO": (pso_best, pso_acc)
}
best algo = max(results.items(), key=lambda x: x[1][1])
print("\nBest Algorithm =", best_algo[0])
print("Best C =", best_algo[1][0])
print("Best Score =", best_algo[1][1])
```

OUTPUT:

```
Gradient Descent:

C = [1.]

Accuracy Score = 98.87%

Simulated Annealing:

C = [5.]

Accuracy Score = 98.87%

Genetic Algorithm:

C = [6.89388682]

Accuracy Score = 98.87%

Particle Swarm Optimization:

C = [1.37066612]

Accuracy Score = 98.87%

Best Algorithm = GD

Best C = [1.]

Best Score = 0.9887193722045957
```

Entire Code for TSP:

```
import numpy as np
import random
import math
import matplotlib.pyplot as plt
import time
#TSP Setup
# -----
n cities = 12 # Increase number of cities for meaningful comparison
cities = np.random.randint(0, 50, size=(n_cities, 2))
def distance matrix(cities):
  n = len(cities)
 dist = np.zeros((n, n))
  for i in range(n):
    for j in range(n):
      dist[i, j] = np.linalg.norm(cities[i]-cities[j])
  return dist
dist_matrix = distance_matrix(cities)
def total_distance(path, dist_matrix):
  return sum(dist matrix[path[i-1], path[i]] for i in range(len(path)))
# -----
# Simulated Annealing
def simulated annealing(dist matrix, temp=1000, alpha=0.995, iterations=1000):
  n = len(dist_matrix)
  current_path = list(range(n))
  random.shuffle(current_path)
  best_path = current_path[:]
  best_dist = total_distance(best_path, dist_matrix)
  convergence = []
  for i in range(iterations):
    a, b = random.sample(range(n), 2)
    new_path = current_path[:]
```

```
new path[a:b] = reversed(new path[a:b])
    new dist = total distance(new path, dist matrix)
    if new_dist < best_dist or random.random() < math.exp((best_dist - new_dist) / temp):
      current path = new path
      if new dist < best dist:
        best path = new path
        best dist = new dist
    temp *= alpha
    convergence.append(best dist)
  return best path, best dist, convergence
# -----
# Genetic Algorithm
# -----
def genetic algorithm(dist matrix, pop size=20, generations=100, mutation rate=0.2):
  n = len(dist_matrix)
  population = [random.sample(range(n), n) for in range(pop size)]
  convergence = []
  def fitness(path):
    return 1 / total_distance(path, dist_matrix)
  for in range(generations):
    population = sorted(population, key=lambda p: fitness(p), reverse=True)
    new population = population[:2] # Elitism
    while len(new population) < pop size:
      parents = random.sample(population[:5], 2)
      cut = random.randint(1, n-2)
      child = parents[0][:cut] + [c for c in parents[1] if c not in parents[0][:cut]]
      if random.random() < mutation rate:
        a, b = random.sample(range(n), 2)
        child[a], child[b] = child[b], child[a]
      new population.append(child)
    population = new population
    best dist = total distance(population[0], dist matrix)
    convergence.append(best dist)
  best_path = population[0]
  best dist = total distance(best path, dist matrix)
  return best_path, best_dist, convergence
```

```
# -----
# Particle Swarm Optimization
# -----
class Particle:
  def init (self, n):
    self.position = np.random.permutation(n)
    self.velocity = np.zeros(n)
    self.best position = self.position.copy()
    self.best score = float('inf')
def swap_sequence(path1, path2):
  swaps = []
  p1 = path1.copy()
  for i in range(len(p1)):
    if p1[i] != path2[i]:
      swap_idx = np.where(p1 == path2[i])[0][0]
      swaps.append((i, swap idx))
      p1[i], p1[swap_idx] = p1[swap_idx], p1[i]
  return swaps
def apply_swaps(path, swaps):
  path = path.copy()
  for i, j in swaps:
    path[i], path[j] = path[j], path[i]
  return path
def pso_tsp(dist_matrix, n_particles=20, iterations=100):
  n = len(dist matrix)
  particles = [Particle(n) for _ in range(n_particles)]
  global_best = particles[0].position
  global_best_score = float('inf')
  convergence = []
  for _ in range(iterations):
    for p in particles:
      score = total_distance(p.position, dist_matrix)
      if score < p.best score:
         p.best_score = score
         p.best position = p.position.copy()
      if score < global_best_score:
```

```
global best score = score
        global best = p.position.copy()
    convergence.append(global_best_score)
    for p in particles:
      swaps to pbest = swap sequence(p.position, p.best position)
      swaps to gbest = swap sequence(p.position, global best)
      p.position = apply_swaps(p.position, swaps_to_pbest[:len(swaps_to_pbest)//2])
      p.position = apply_swaps(p.position, swaps_to_gbest[:len(swaps_to_gbest)//2])
  return global best.astype(int), global best score, convergence
# -----
# Run All Algorithms with timing
# -----
start = time.time()
sa_path, sa_dist, sa_conv = simulated_annealing(dist_matrix)
sa time = time.time() - start
start = time.time()
ga_path, ga_dist, ga_conv = genetic_algorithm(dist_matrix)
ga_time = time.time() - start
start = time.time()
pso path, pso dist, pso conv = pso tsp(dist matrix)
pso time = time.time() - start
print("====== Results ======\n")
print(f"Simulated Annealing Path:\n {sa path}\n Distance: {sa dist:.2f}\n Time: {sa time:.6f}
secconds\n")
print("======= Results ======\n")
print(f"Genetic Algorithm Path:\n {ga_path}\n Distance: {ga_dist:.2f}\n Time: {ga_time:.6f}
seconds\n")
print("======= Results ======\n")
print(f"Particle Swarm Optimization Path:\n {pso_path}\n Distance: {pso_dist:.2f}\n Time:
{pso time:.6f} seconds\n")
# Plot Paths
# -----
def plot_path(cities, path, title):
```

```
path = list(map(int, path))
  path coords = cities[path + [path[0]]]
  plt.plot(path_coords[:,0], path_coords[:,1], 'o-', label=title)
  for i, (x, y) in enumerate(cities):
    plt.text(x, y, str(i))
  plt.title(title)
  plt.show()
plot path(cities, sa path, "Simulated Annealing Path")
plot_path(cities, ga_path, "Genetic Algorithm Path")
plot_path(cities, pso_path, "Particle Swarm Optimization Path")
# Plot Convergence
# -----
plt.plot(sa conv, label="SA")
plt.plot(ga_conv, label="GA")
plt.plot(pso conv, label="PSO")
plt.xlabel("Iteration")
plt.ylabel("Best Distance")
plt.title("Convergence Comparison")
plt.legend()
plt.show()
```

OUTPUT:

