بسم الله الرحمن الرحیم

دانشگاه شهید بهشتی ۱۳۳۸
دانشکده فیزیک

مقدمات درس روشهای شبیه سازی در فیزیک (نظریه و محاسبات)

Preliminaries for Advanced topics in computational Physics and Optimization

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نیم سال اول، سال تحصیلی ۱۴۰۴-۱۴۰۳

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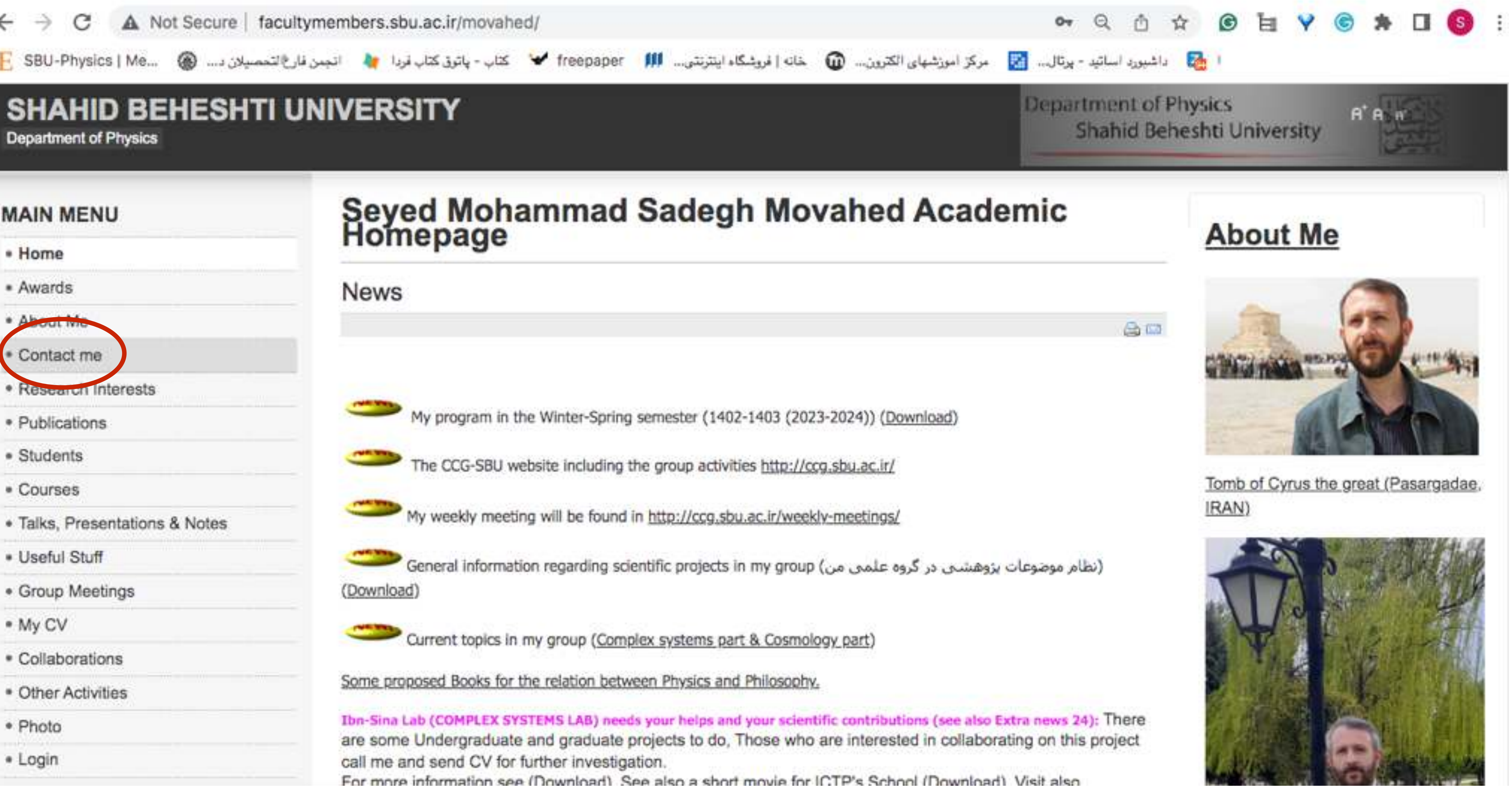
Computational Cosmology Group Of Shahid Beheshti University

COMPLEXLAB SHAHID BEHESHTI UNIVERSITY

Part 1
The website of course

وبسایت درس



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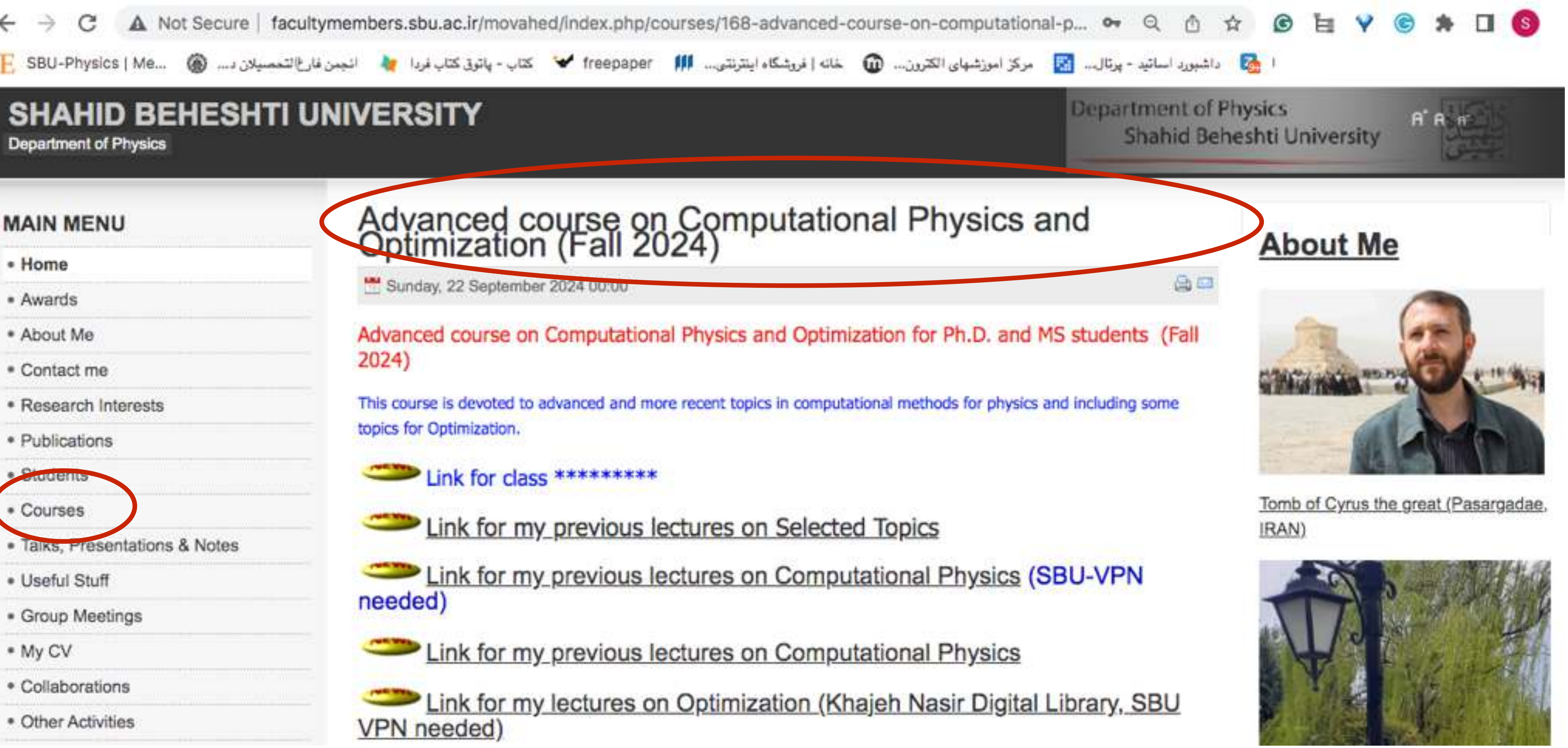
وبسایت درس



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Part 2
The Roadmap and Benefits

The timetable of Course
طرح درس و برنامه زمانبندی

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Some relevant references in my webpage
برخی از منابع مندرج در وبسایت درس

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Simulation and Data Sciences
شبیه سازی و علم داده

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Optimization: General view
بهینه سازی: نگاه کلی

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Generic examples

1) Common notion in everyday life
2) Shortest path
3) Euler-Lagrange differential equation
4) Variational approach to compute the upper limit of ground state of a typical system
5) Many physical systems are governed by minimization principle (Gravity, Thermodynamics, …)

Transformation into the optimization problems

1) Determination of the self affine properties of polymers in random media
2) Study of interfaces and elastic manifolds in disordered environments
3) Investigation of the low-temperature behavior of disordered magnets
4) Investigation of morphology of fox line in superconductors
5) Solution of Protein Folding
6) Calculation of ground state of electronic systems
7) Optimization of laser fibers
8) .
9) .
10) .

Canonical definition of Linear optimization

$$X = (x_1, x_2, ..., x_N)$$ a row vector

$$X \in R$$

$$\mathcal{H} \subset R$$ (cost function)

Find $X \in R$ which minimizes or maximizes $\mathcal{H}$

Canonical definition of Linear optimization

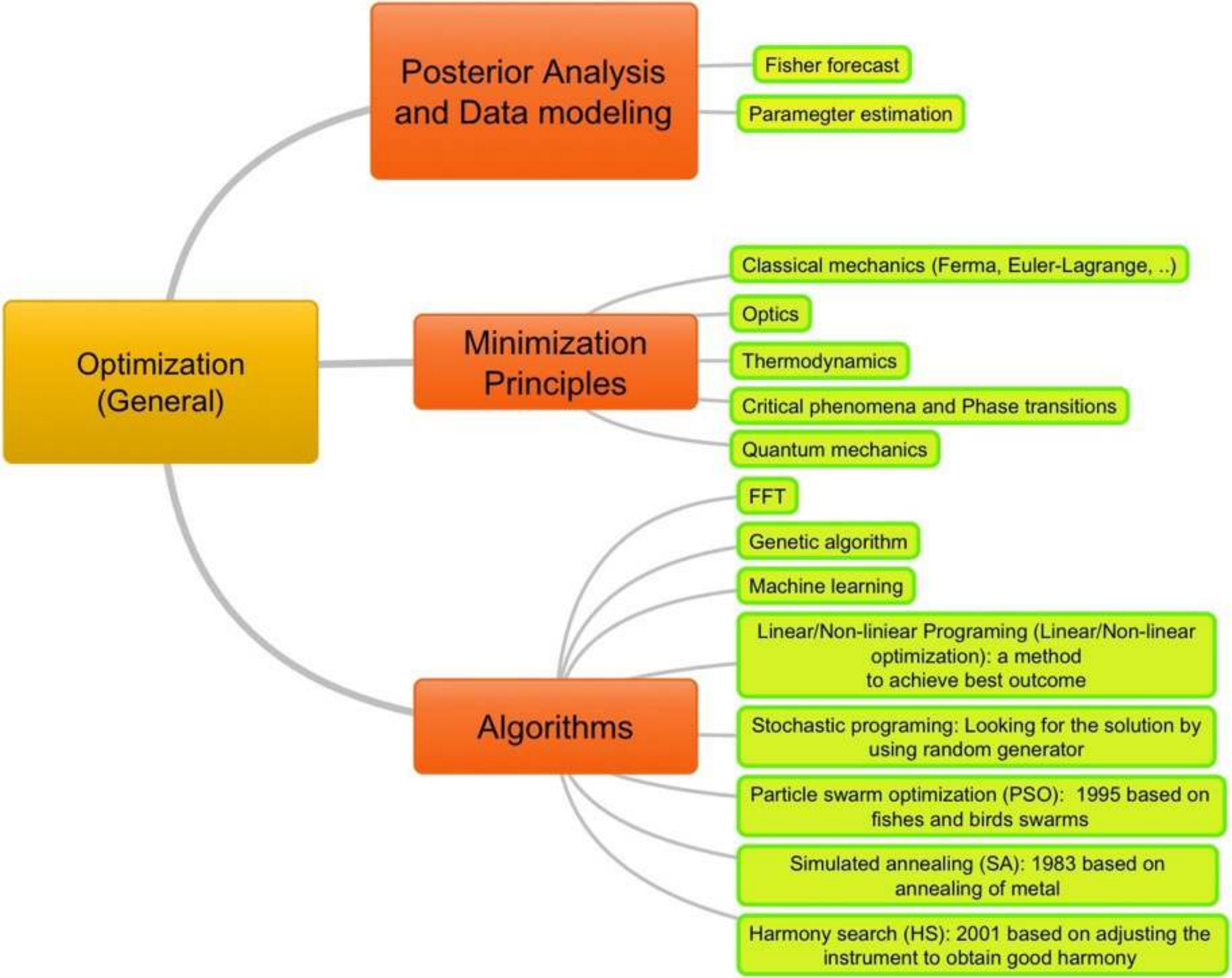
$$X = (x_1, x_2, ..., x_N)$$ a row vector

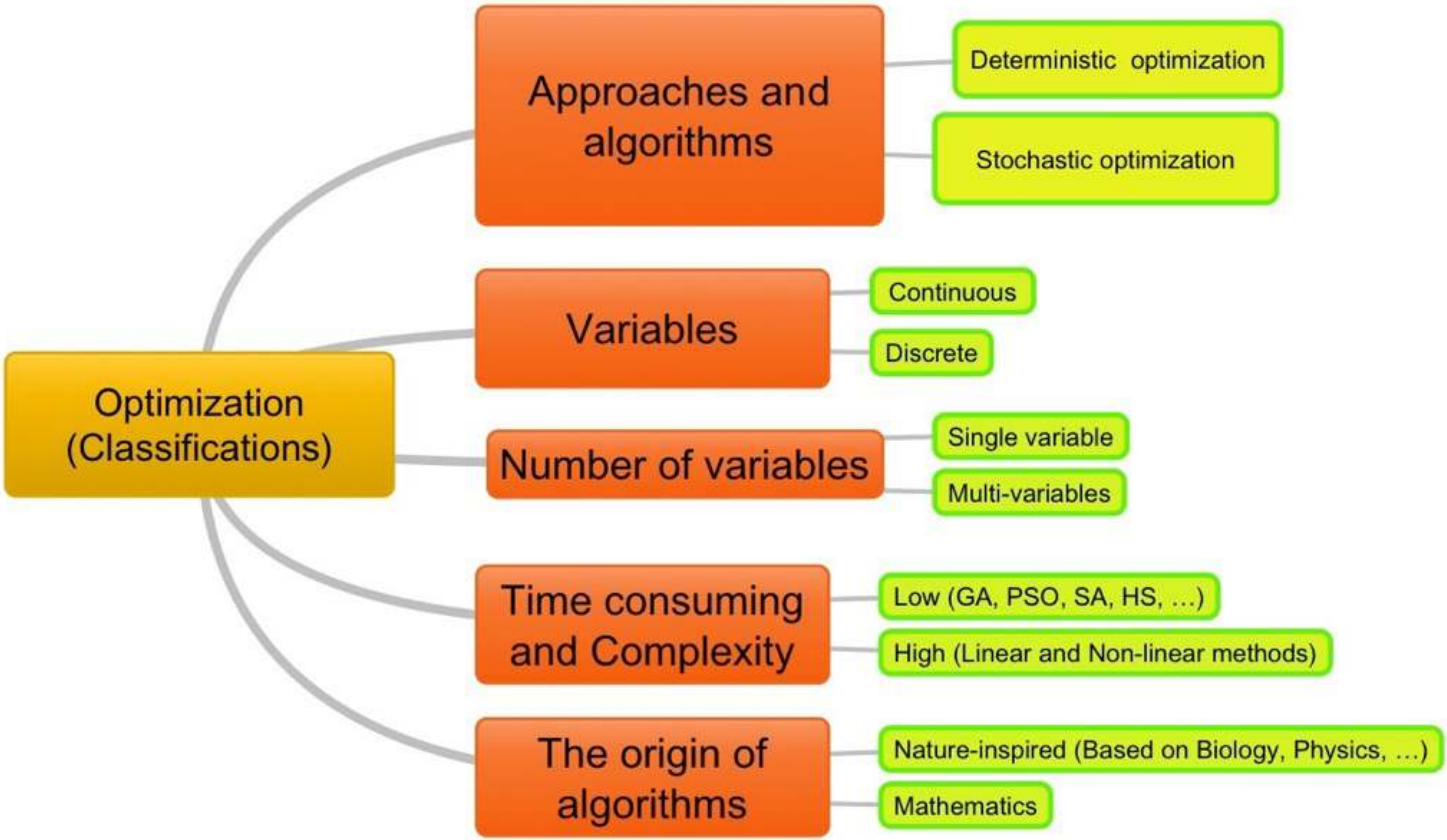
$$C^T X$$ To be minimized (cost function)

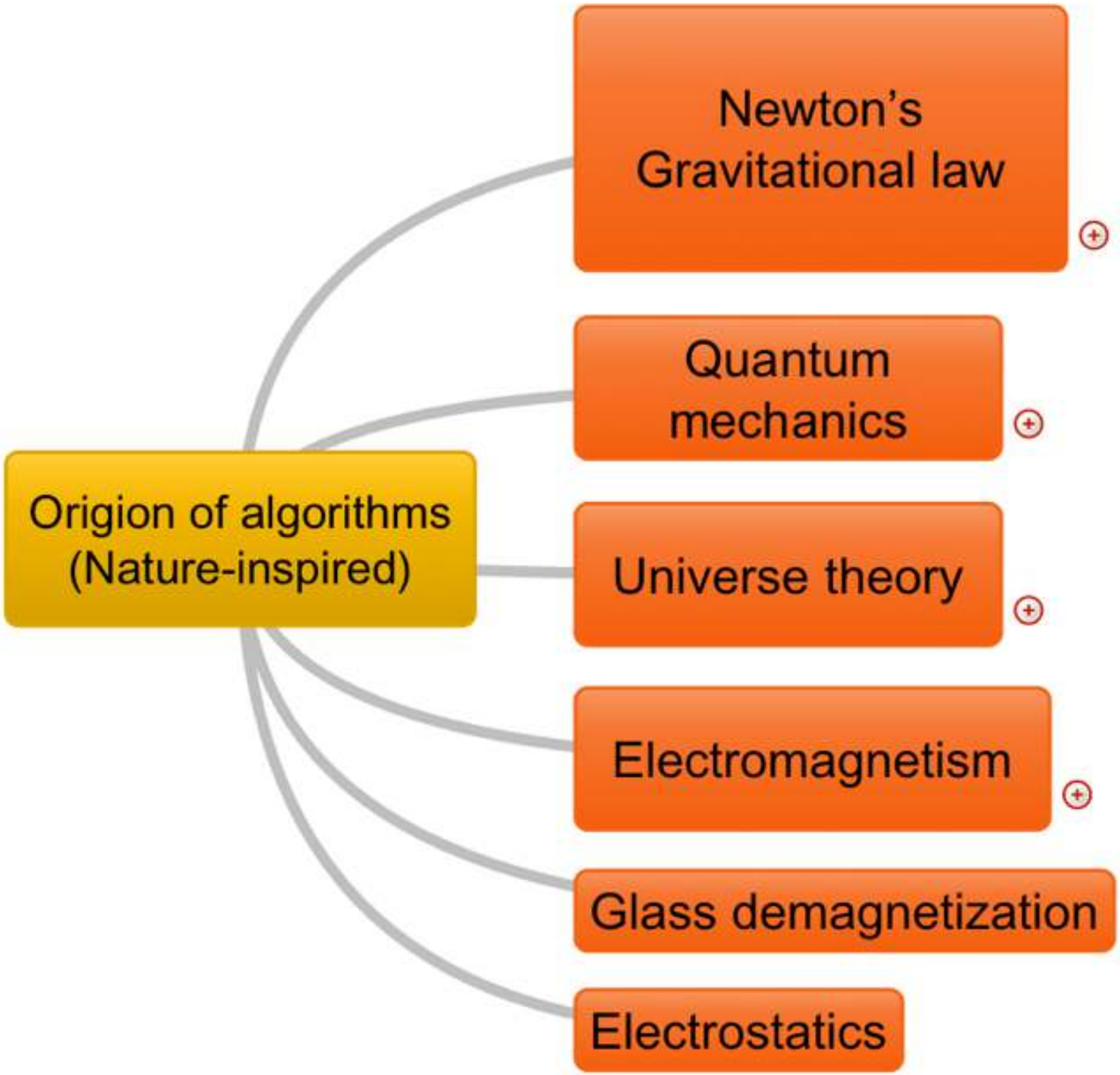
$$AX \leq B$$
$$X \geq 0$$
Constraints

Some keywords:

- Feasible region: A set of value of X which fulfills or satisfies all conditions;
- Robustness: Resilience against perturbation;
- Complexity: Time and algorithms

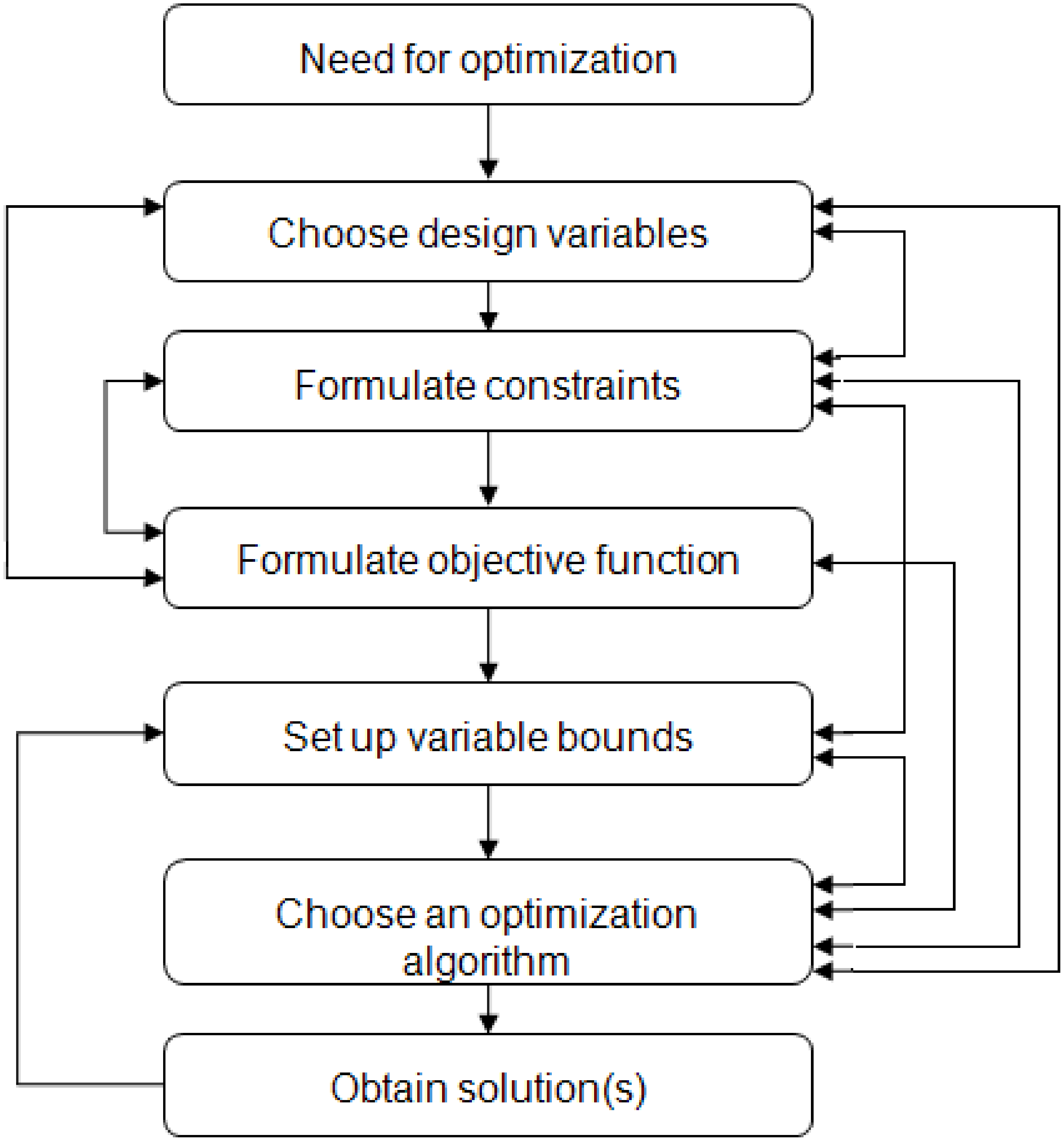

Posterior Analysis and Data modeling
Fisher forecast
Paramegter estimation
Optimization (General)
Minimization Principles
Classical mechanics (Ferma, Euler-Lagrange, ..)
Optics
Thermodynamics
Critical phenomena and Phase transitions
Quantum mechanics
Algorithms
FFT
Genetic algorithm
Machine learning
Linear/Non-liniear Programing (Linear/Non-linear optimization): a method to achieve best outcome
Stochastic programing: Looking for the solution by using random generator
Particle swarm optimization (PSO): 1995 based on fishes and birds swarms
Simulated annealing (SA): 1983 based on annealing of metal
Harmony search (HS): 2001 based on adjusting the instrument to obtain good harmony


Optimization (Classifications)
Approaches and algorithms
Deterministic optimization
Stochastic optimization
Variables
Continuous
Discrete
Number of variables
Single variable
Multi-variables
Time consuming and Complexity
Low (GA, PSO, SA, HS, …)
High (Linear and Non-linear methods)
The origin of algorithms
Nature-inspired (Based on Biology, Physics, …)
Mathematics



Biswas, Anupam, et al. "Physics-inspired optimization algorithms: a survey." Journal of Optimization 2013 (2013).

Optimization Flowchart



https://mech.iitm.ac.in/meiitm/

Optimization Flowchart

A) Design variables
- Model building
- Observable quantities
- Prior informations

Optimization Flowchart

B) Constraints

- Geometry and topology
- Boundary conditions (periodic boundary, ….)

Optimization Flowchart

C) Objective Function (cost function)

- Posterior and Likelihood
- Hamiltonian
- Entropy
- Thermodynamic Potential
- Nature-inspired functions

Optimization Flowchart

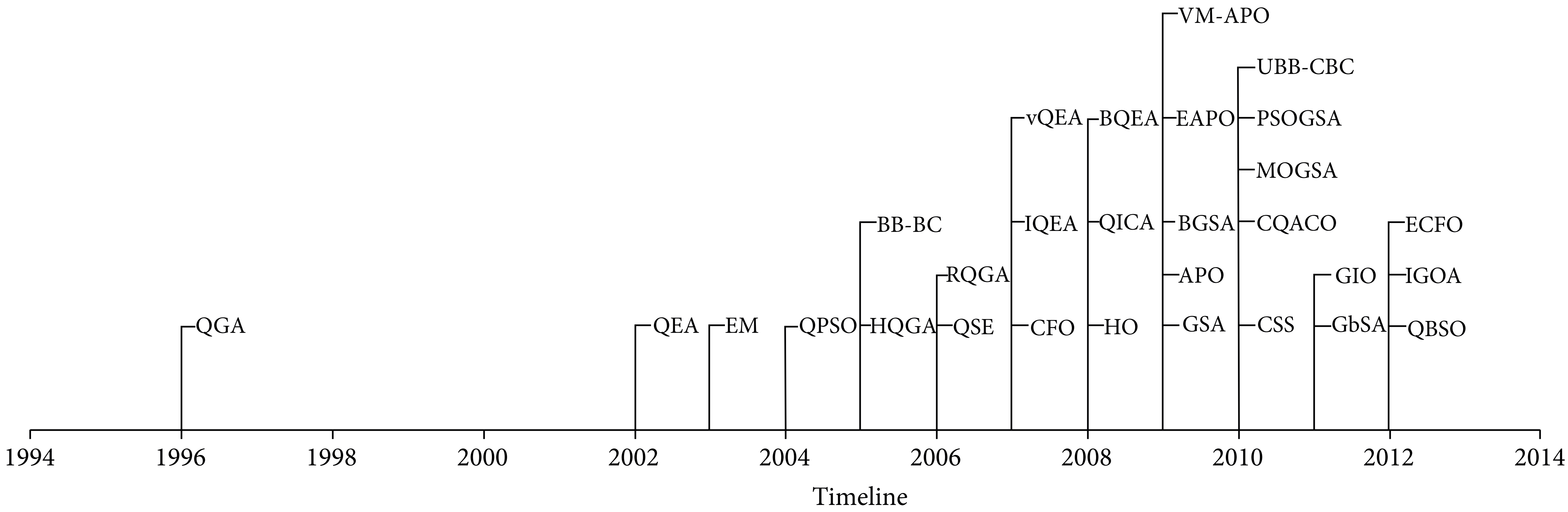
D) Variable bounds

- Variable domains coming from theories or experiments

Optimization Flowchart

E) Optimization Algorithms

Physics-inspired algorithms



Biswas, Anupam, et al. "Physics-inspired optimization algorithms: a survey." Journal of Optimization 2013 (2013).

Physics-inspired algorithms

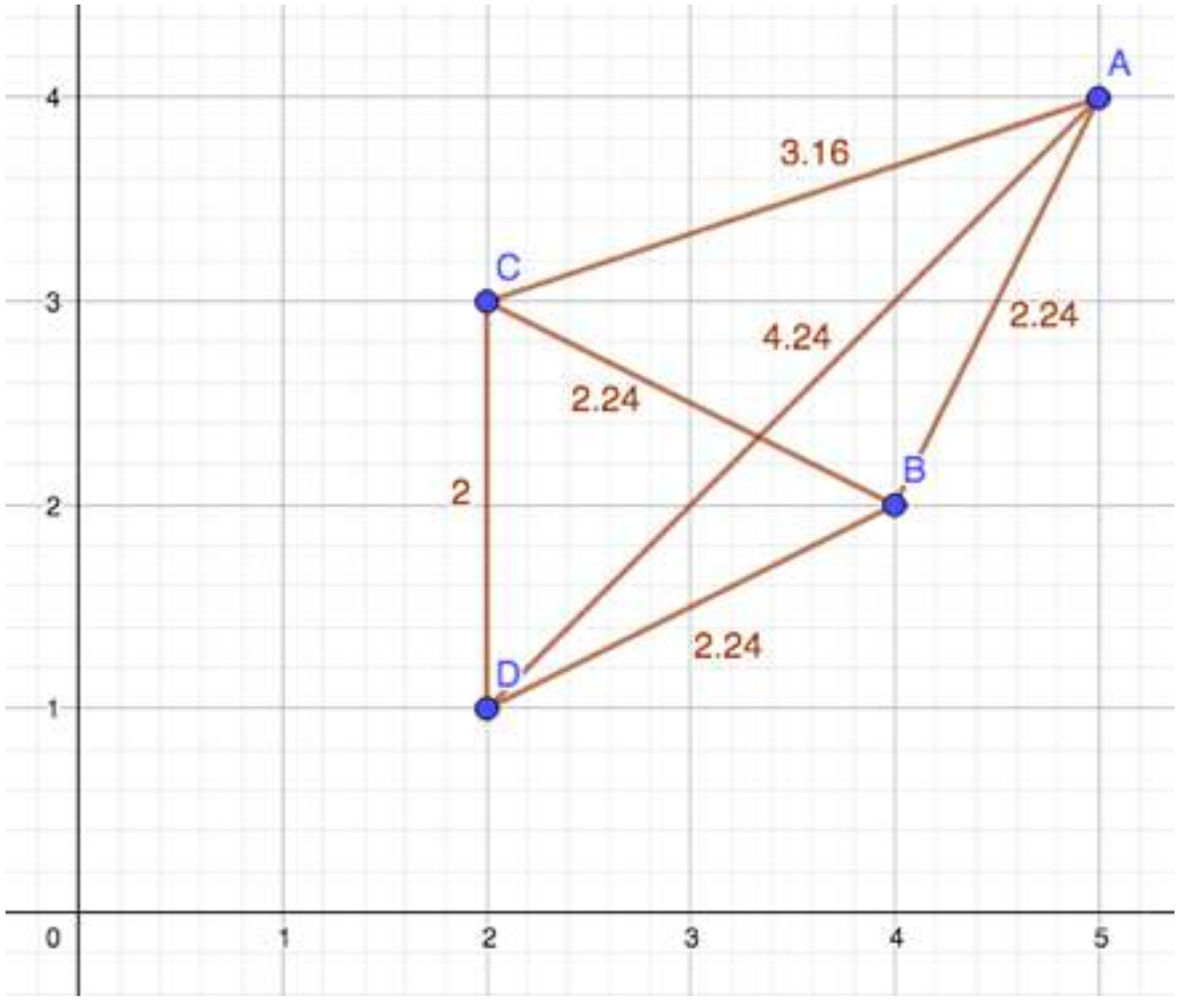
ACO: Ant colony optimization
APO: Artificial physics optimization
BB-BC: Big bang-big crunch
BFO: Bacterial forging optimization
BGSA: Binary gravitational search algorithm
BIS: Biological immune system
BQEA: Binary Quantum-inspired evolutionary algorithm
CFO: Central force optimization
CQACO: Continuous quantum ant colony optimization
CSS: Charged system search
EAPO: Extended artificial physics optimization
ECFO: Extended central force optimization
EM: Electromagnetism-like heuristic
GA: Genetic Algorithm
GbSA: Galaxy-based search algorithm
GIO: Gravitational interaction optimization
GSA: Gravitational search algorithm
HO: Hysteretic optimization
HQGA: Hybrid quantum-inspired genetic algorithm
HS: Harmony search
IGOA: Immune gravitation inspired optimization algorithm
IQEA: Improved quantum evolutionary algorithm
LP: Linear programming
MOGSA: Multiobjective gravitational search algorithm
NLP: Nonlinear programming
PSO: Particle swarm optimization
PSOGSA: PSO gravitational search algorithm
QBSO: Quantum-inspired bacterial swarming optimization
QEA: Quantum-inspired evolutionary algorithm
QGA: Quantum-inspired genetic algorithm
QGO: Quantum genetic optimization
QICA: Quantum-inspired immune clonal algorithm
QPSO: Quantum-behaved particle swarm optimization
QSE: Quantum swarm evolutionary algorithm
RQGA: Reduced quantum genetic algorithm
SA: Simulated annealing
TSP: Travelling salesman problem
UBB-CBC: Unified big bang-chaotic big crunch
VM-APO: Vector model of artificial physics optimization
vQEA: Versatile quantum-inspired evolutionary algorithm.

Biswas, Anupam, et al. "Physics-inspired optimization algorithms: a survey." Journal of Optimization 2013 (2013).

Examples

1) Traveling Salesman Problem (TSP)

$$
\begin{aligned}
X &= (x_1, x_2, ..., x_N) \\
&= \{1, 2, 3, ..., N\} \\
\mathcal{H}(X) &= \sum_{i=1}^{N} d(x_i, x_{i+1}) \\
x_{N+1} &= x_1 \\
X &\rightarrow \hat{P}[1, 2, 3, ..., N]
\end{aligned}
$$

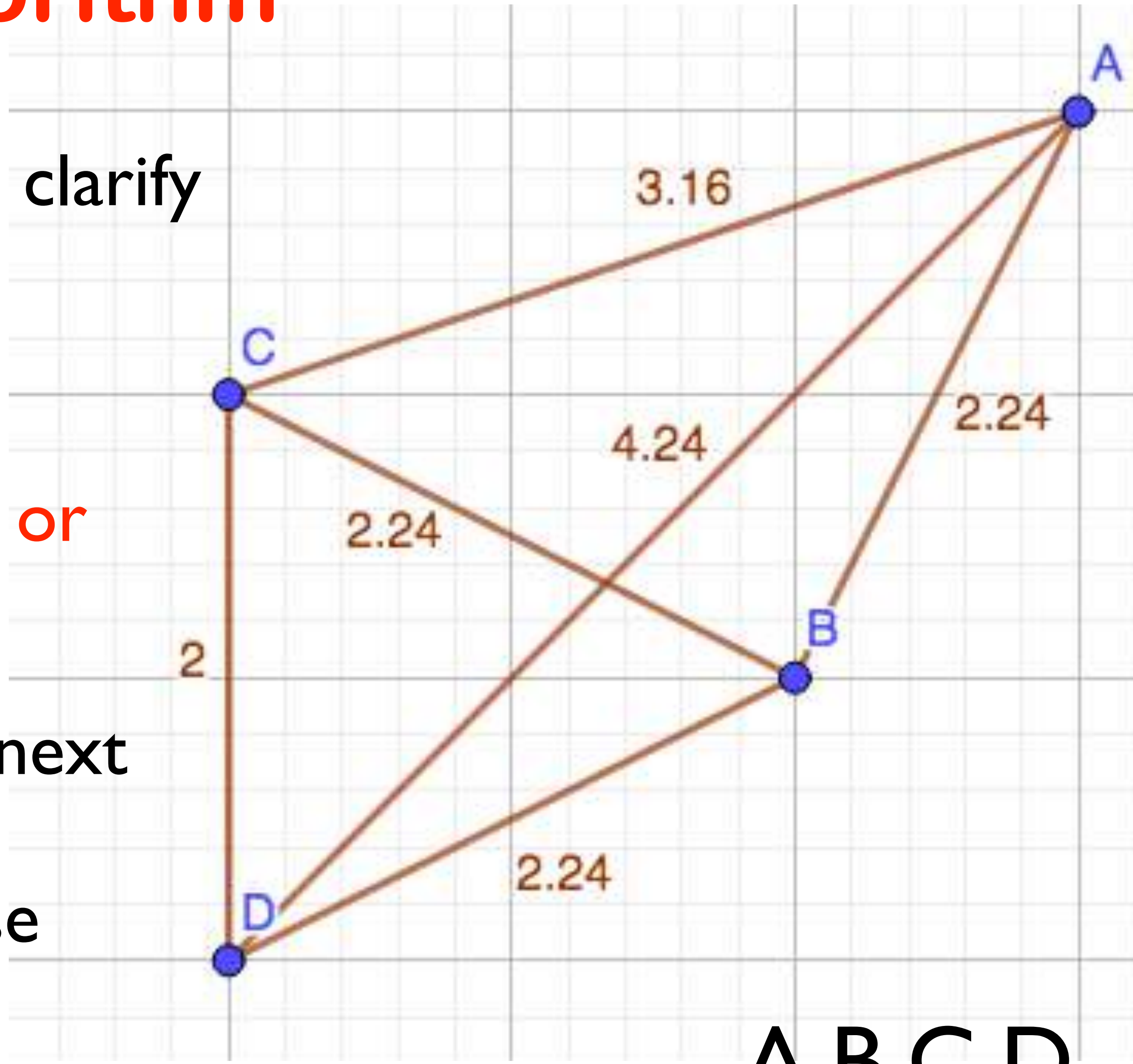


TSP Algorithm

1) Set the labels of each city to zero to clarify the times of visit
2) Starting from an arbitrary city
3) Traveling to another unvisited city

This can be done either in deterministic or stochastic approaches

1) For each given starting point select next unvisited destination randomly
2) Check the conditions of our purpose



A,B,C,D
A,B,D,C
C,D,B,A
D,C,B,A

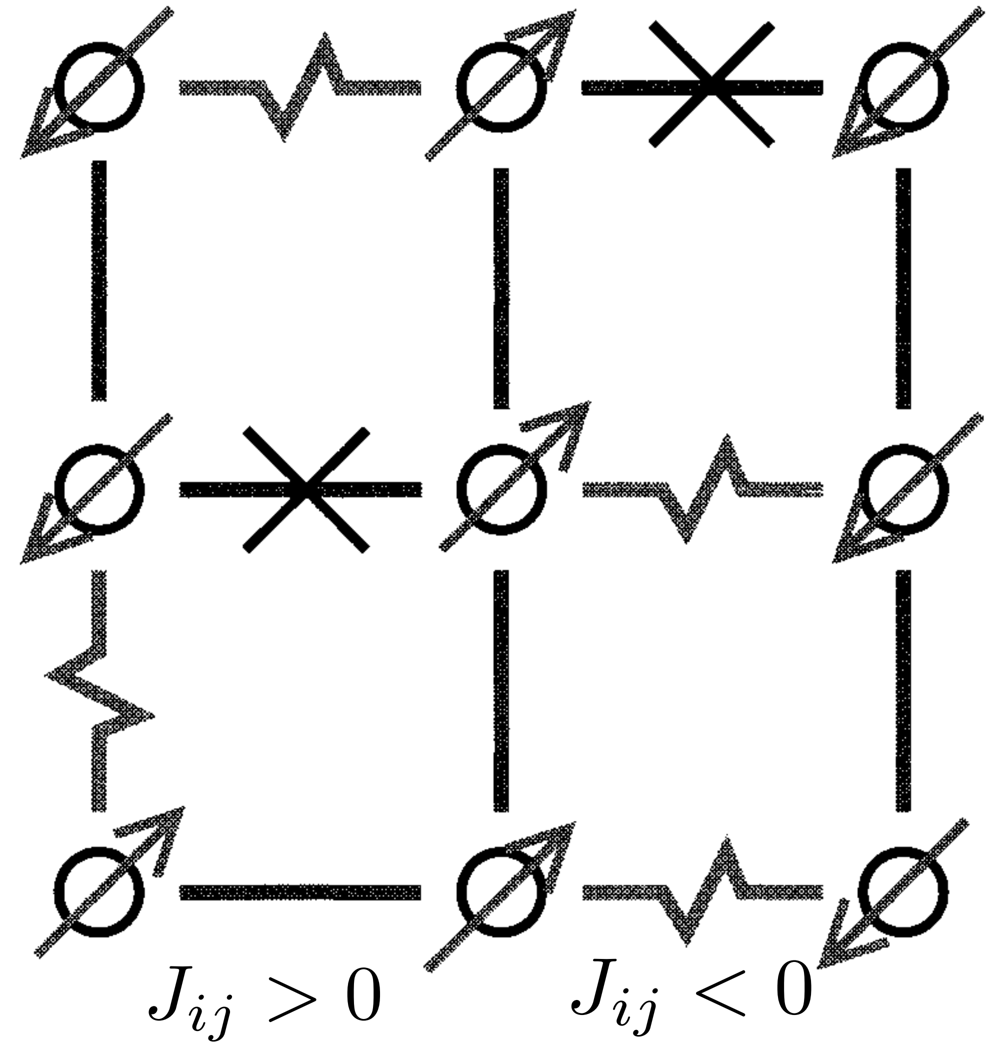
Exercise: Try to solve TSP according to following conditions:

- Visit twice C-City
- Visit necessarily C before D

Examples

2) Ising Spin Glasses

$$
\begin{aligned}
X &= (\sigma_1, \sigma_2, ..., \sigma_N) \\
&= \{1, 2, 3, ..., N\} \\
X &= \{-1, +1\} \\
\mathcal{H}(X) &= -\sum_{\langle i,j \rangle = 1}^{N} J_{ij} \sigma_i \sigma_j \\
\sigma_i &= \pm 1, \quad \sigma_i \mathbin{/\!/} \sigma_{i+1} \quad \mathrm{for J_{ij}} > 0 \\
\sigma_i &= \pm 1, \quad \sigma_i \not\mathbin{/\!/} \sigma_{i+1} \quad \mathrm{for J_{ij}} < 0
\end{aligned}
$$



Ferromagnetic and anti-Ferromagnetic

frustrated states

Terminal shell

Number Representation

Error estimation and propagation

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دانشکده فیزیک

از توجه شما سپاسگزارم

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