OPTIMIZATION FOR AI

GLOBAL AND MULTI-OBJECTIVE OPTIMIZATION

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DIFFERENTIAL EVOLUTION, PARTICLE SWARM OPTIMISATION, AND ANT COLONY OPTIMISATION

DIFFERENTIAL EVOLUTION

DIFFERENTIAL EVOLUTION: IDEAS

- **Differential evolution** (DE) was invented in 1997 by Storn and Price
- Used for the solution of real-valued optimisation problems
- The approach is evolutionary, but different from GA for two main reasons:
  - The way new individuals are generated
  - The selection process

NOTATION

- The search space is $\mathbb{R}^m$ for some $m \in \mathbb{N}$
- We still have a population of solution consisting of n individuals
- The i^{th} individual is a vector $\mathbf{x}_i = (x_{i,1}, \ldots, x_{i,m}) \in \mathbb{R}^m$

DIFFERENTIAL MUTATION

- Select one candidate solution $\mathbf{x}_i$ from the current population
- Select three other vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ from the current population (in the original formulation $\mathbf{a}, \mathbf{b}, \mathbf{c}$, and $\mathbf{x}_i$ are all distinct)
- Compute the **"donor" vector** for $\mathbf{x}_i$ as $\mathbf{v}_i = a + F \cdot (b - c)$ where $F \in [0,2]$ is called the **mutation factor**

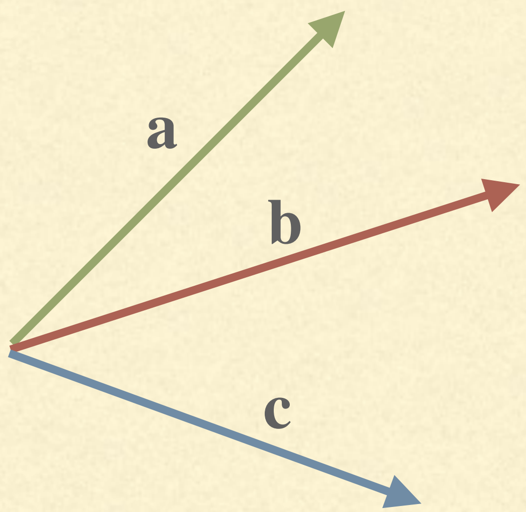
BINOMIAL CROSSOVER

- The solution $\mathbf{x}_i$ and the "donor" vector $\mathbf{v}_i$ are combined in a **"trial" vector $\mathbf{u}_i$**
- $\mathbf{u}_i$ is defined, for each coordinate $j \in \{1,\ldots,m\}$, as
$$u_{i,j} = \begin{cases} v_{i,j} & \text{if } \mathrm{rnd}_{i,j} \leq p_{\mathrm{CR}} \text{ or } I_{\mathrm{rnd}} = j \\ x_{i,j} & \text{otherwise} \end{cases}$$
- Where p_{CR} is the crossover probability, $I_{\mathrm{rnd}} \in \{1,\ldots,m\}$ is a randomly selected index, and $\mathrm{rnd}_{i,j}$ are random numbers in $[0,1]$

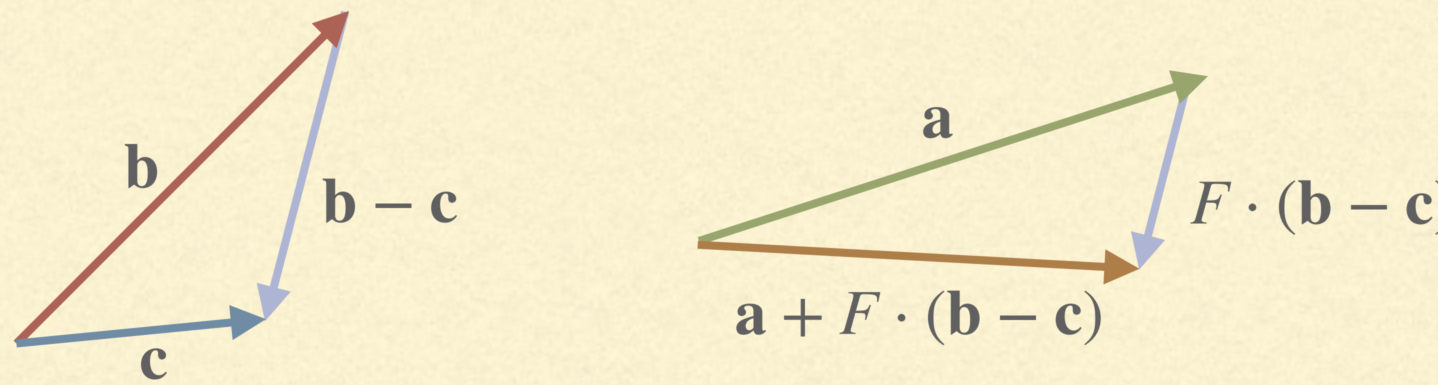
DE: SELECTION

- Given the parent $\mathbf{x}_i$ and the "trial" vector $\mathbf{u}_i$, selection is done by keeping only the individual with the best fitness:
  - $\mathbf{x}_i$ is kept if the $f(\mathbf{x}_i) < f(\mathbf{u}_i)$ (in a minimisation problem)
  - $\mathbf{u}_i$ replaces $\mathbf{x}_i$ otherwise
- This mutation/crossover/selection process is repeated for all individuals in the population to produce a new population of solutions

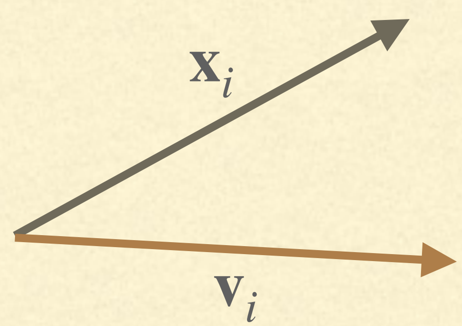
GRAPHICAL REPRESENTATION



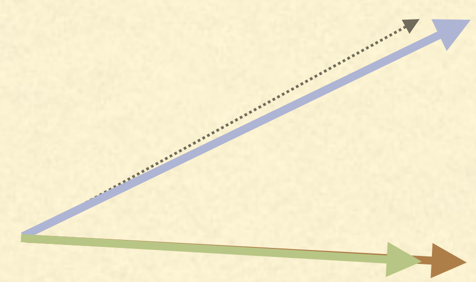
Extraction of three
vectors from the population



Computing the "donor vector"



Donor vector and $\mathbf{x}_i$



Possible trial vectors and the original vector $\mathbf{x}_i$

TAXONOMY

- The described scheme is sometimes called **DE/rand/1** with the meaning:
  - **DE**: self-explanatory
  - **rand**: the first vector of the differential mutation is selected uniformly at random across all the individuals
  - **1**: the donor vector is created using only one differential mutation

TAXONOMY

Best individual found so far

NAME	DIFFERENTIAL MUTATION
DE/best/1	$\mathbf{v}_i = \mathbf{x}_{\text{best}} + F \cdot (\mathbf{b} - \mathbf{c})$
DE/current-to-best/1	$\mathbf{v}_i = \mathbf{x}_i + F \cdot (\mathbf{x}_{\text{best}} - \mathbf{x}_i) + F \cdot (\mathbf{b} - \mathbf{c})$
DE/rand/2	$\mathbf{v}_i = \mathbf{a} + F \cdot (\mathbf{b} - \mathbf{c}) + F \cdot (\mathbf{d} - \mathbf{e})$
DE/rand-to-best/1	$\mathbf{v}_i = \mathbf{a} + F \cdot (\mathbf{x}_{\text{best}} - \mathbf{a}) + F \cdot (\mathbf{b} - \mathbf{c})$

ADAPTIVE DE (JADE)

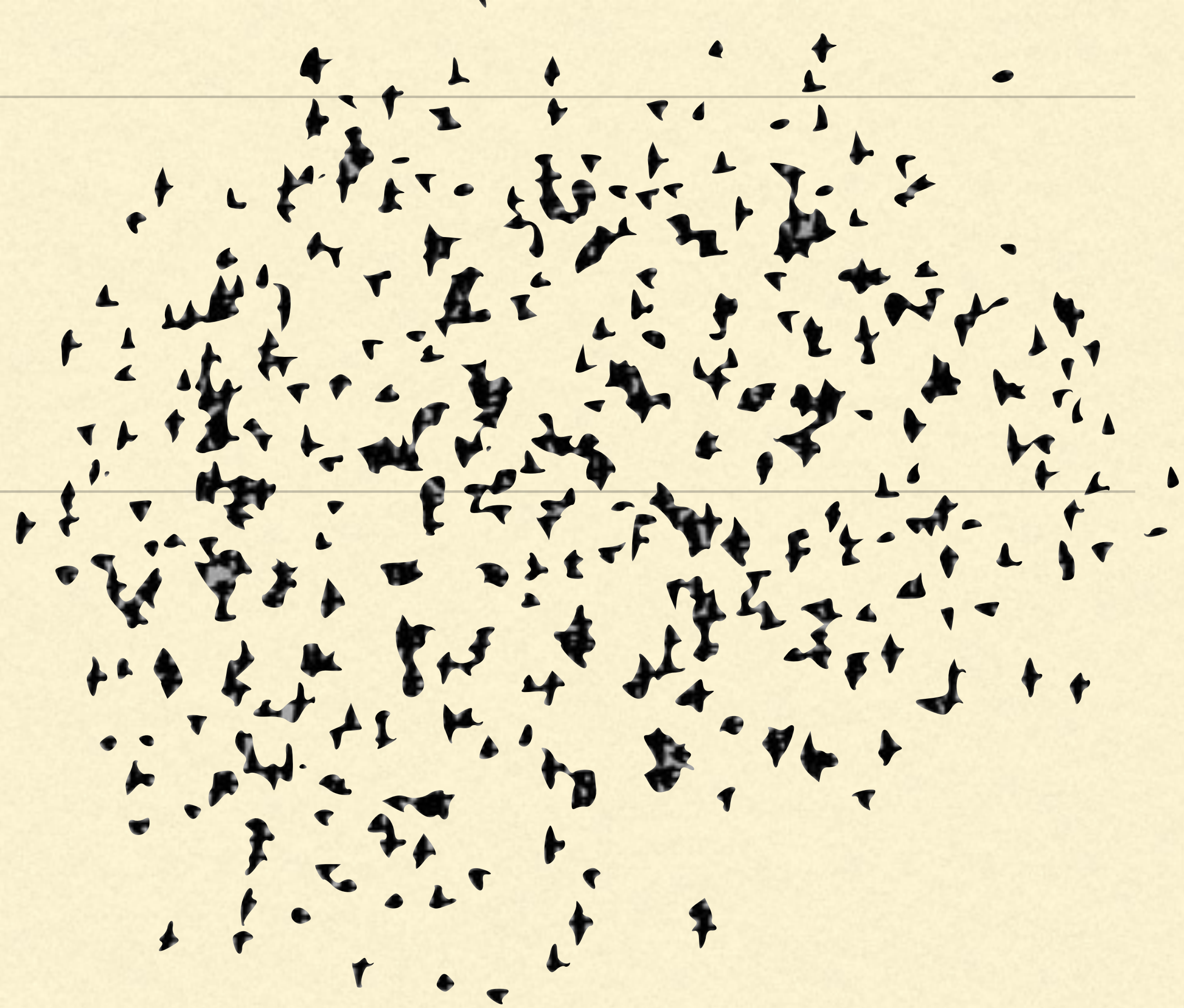
- Introduced in 2009 by Zhang and Sanderson
- New mutation strategy
- External archive of sub-optimal solutions
- Dynamic update of hyper-parameters
- See https://ieeexplore.ieee.org/abstract/document/5208221

PARTICLE SWARM OPTIMIZATION

PSO: IDEAS

- Particle Swarm Optimisation (PSO) is part of a family of bio-inspired optimisation methods called **swarm intelligence**
  - Individuals are simple agents with limited capabilities (i.e., no "intelligent" agents).
  - Any intelligent behaviour emerges from the interactions of the simple agents
- See: swarm of birds, colony of ants, colony of bees. Linked to the ideas of "superorganism"

PSO: IDEAS



- PSO, like the other method we will see, is based on the exchange of information among different individuals (**particles**) that are part of the population (**swarm**)
- It is inspired by the collective movement of a group of animals (e.g., flock of birds, school of fishes, swarm of bees, etc)

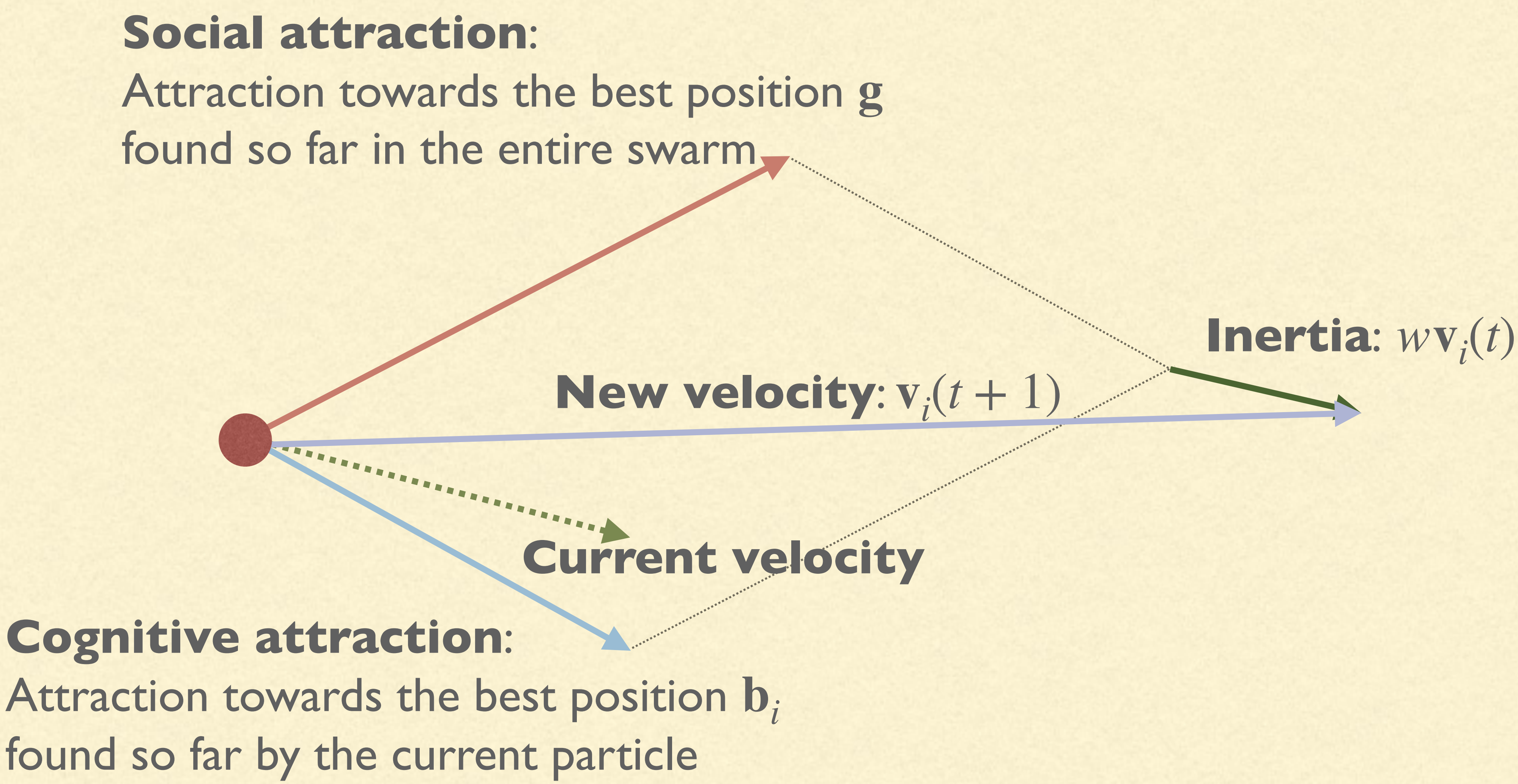
PSO: DEFINITION

- The search space is m-dimensional, usually $\mathbb{R}^m$
- The swarm is composed of n particles.
  - $\mathbf{x}_i(t)$ is the **position** of the i^{th} particle of the swarm at time t
  - $\mathbf{v}_i^t$ is the **velocity** of the i^{th} particle of the swarm at time t
- At each (discrete) time step, the position of the particle is updated as $\mathbf{x}_i(t+1) = \mathbf{x}_i(t) + \mathbf{v}_i(t)$

PSO: DEFINITION

- The update of the velocity is more involved and keep track of three factors:
  - Inertia: the particle cannot change direction immediately
  - Social attraction: try to follow the swarm
  - Cognitive attraction: try to follow what the particle knows

VELOCITY COMPONENTS



Usually each component of the velocity
is bounded (in absolute value) between $[v_{\min}, v_{\max}]$

PSO: VELOCITY UPDATE

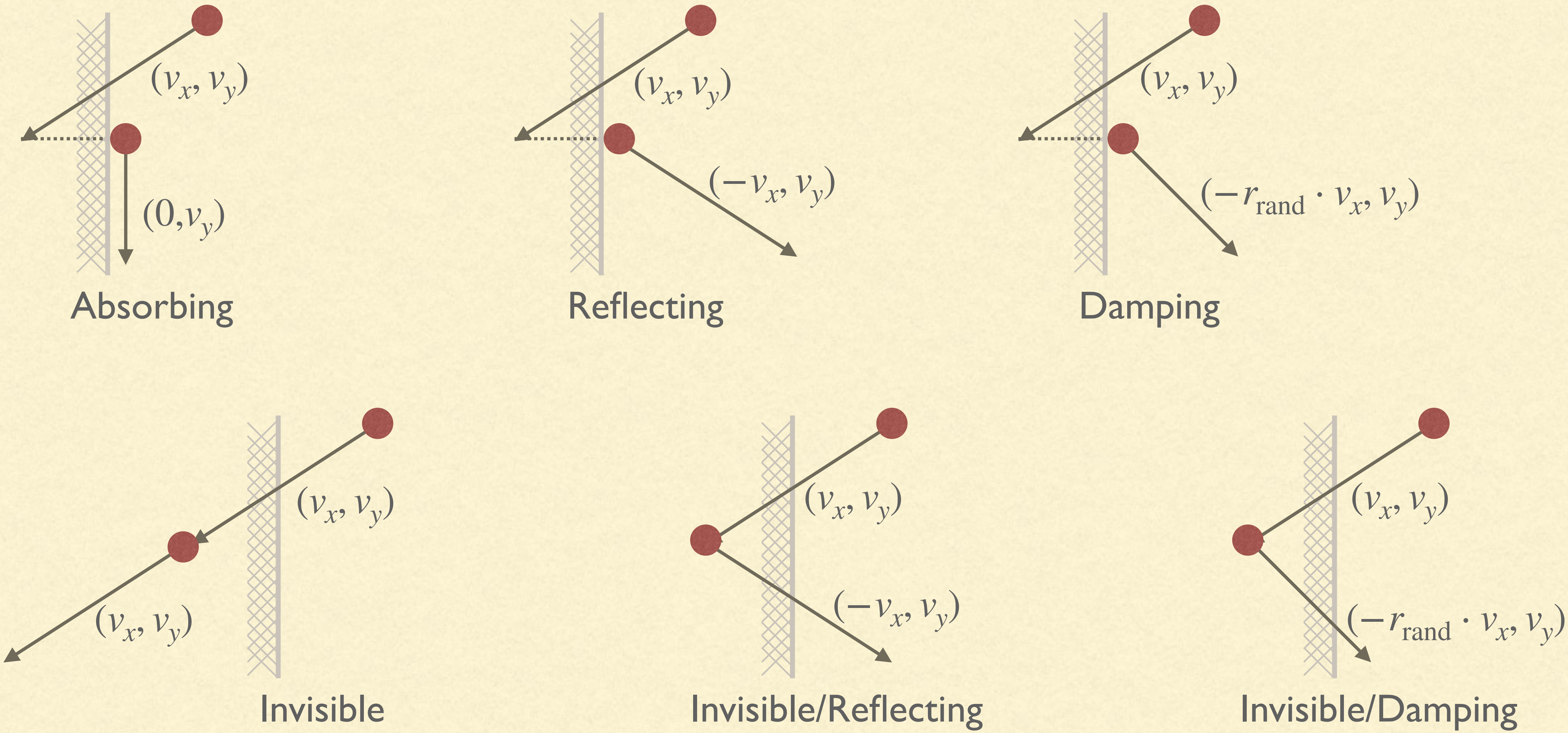
The formula for the velocity update is:
$\mathbf{v}_i(t+1) = w \cdot \mathbf{v}_i(t) + c_{\text{soc}} \cdot \mathbf{r}_1 \otimes (\mathbf{g} - \mathbf{x}_i(t)) + c_{\text{cog}} \cdot \mathbf{r}_2 \otimes (\mathbf{b}_i - \mathbf{x}_i(t))$

- $\mathbf{r}_1$ and $\mathbf{r}_2$ are random vectors from $[0,1]^m$
and $\otimes$ denotes the Hadamard product
- $c_{\text{soc}} \in \mathbb{R}^+$ is the **social factor**
- $c_{\text{cog}} \in \mathbb{R}^+$ is the **cognitive factor**
- $w \in \mathbb{R}^+$ is the **inertia weight**

PSO: PARAMETERS

- $c_{\text{soc}} \in \mathbb{R}^+$ is the **social factor**, it modulates the attraction towards the global best (i.e., the best solution found so far by the entire swarm). Usually $c_{\text{soc}} = 1.49445$.
- $c_{\text{cog}} \in \mathbb{R}^+$ is the **cognitive factor**, it modulates the attraction towards the local best (i.e., the best solution found so far by the current particle). Usually $c_{\text{cog}} = 1.49445$.
- $w \in \mathbb{R}^+$ is the **inertia weight**, it is used to balance global and local search. It is usually decremented linearly from 0.9 to 0.4

BOUNDARY CONDITIONS



SELECTION OF PSO PARAMETERS

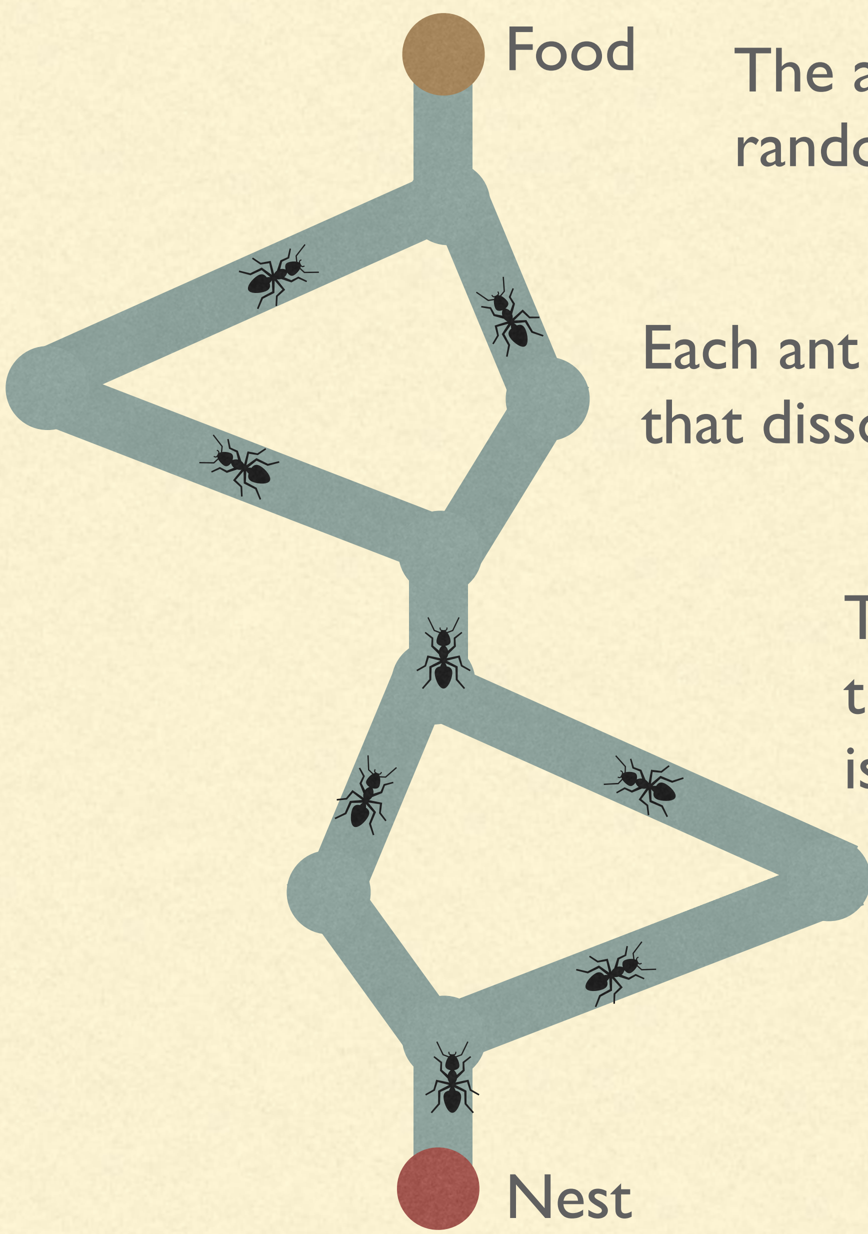
- The settings for PSO are problem-dependent. To optimise them there are three main approaches:
  - Differential investigation of the impacts of the different settings
  - "Good enough" defaults
  - Self-tuning PSO that automatically adjust the parameters

ANT COLONY OPTIMIZATION

ACO: IDEAS

- **Stigmergy** is a mechanism of *indirect coordination* mediated by the environment
    - Stigmergy can allow for complex behaviours without need of planning, control, or direct communication
    - Stigmergy allows the collaboration of very simple agents, lacking memory, intelligence, or even awareness of each other
- Standard example: *ants' pheromone trails*

STIGMERGY IN NATURE: THE DOUBLE BRIDGE EXPERIMENT

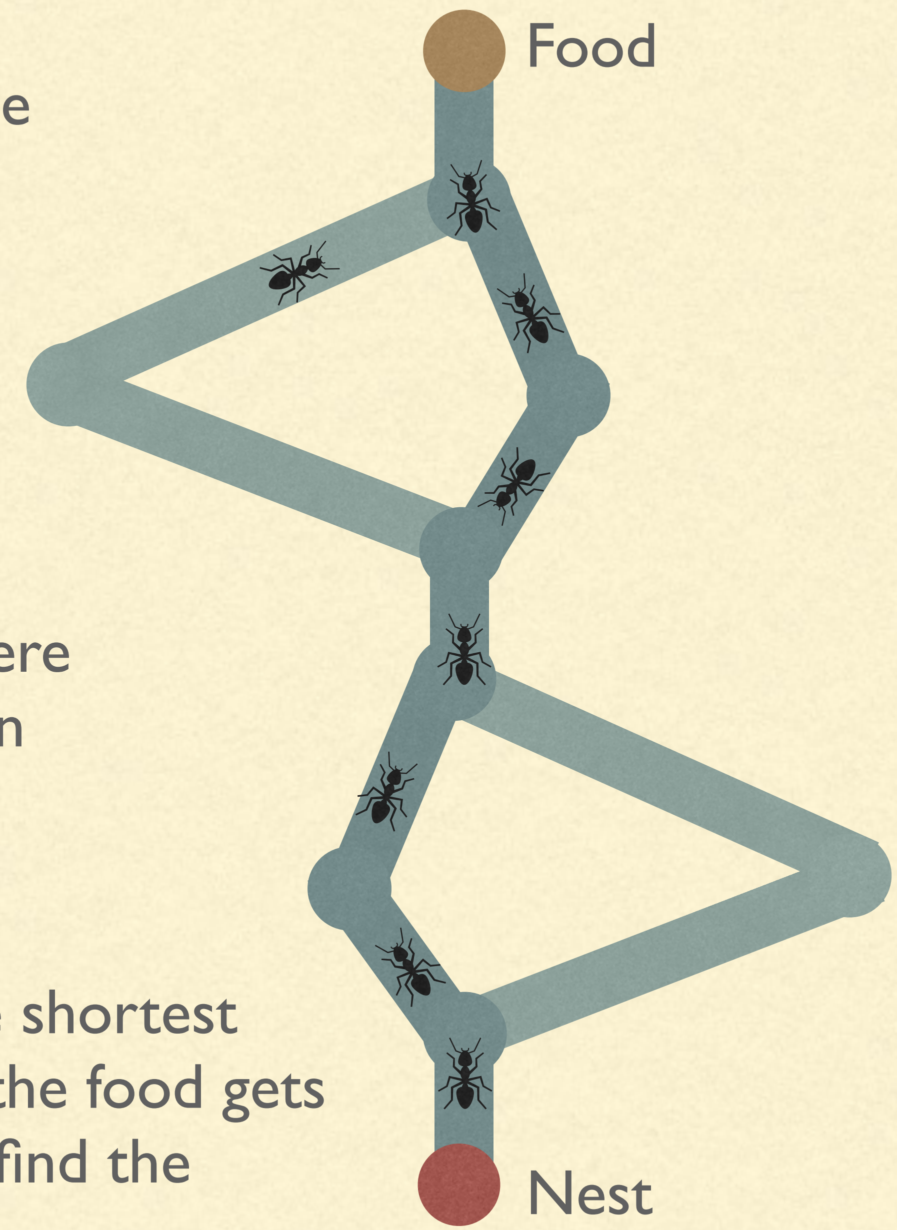


The ants initially explore the space randomly searching for food

Each ant leaves a pheromone trail that dissolves with time

The ants follow the trails where the pheromone concentration is higher

The pheromone trail on the shortest path between the nest and the food gets reinforced, allowing ants to find the shortest path to the food



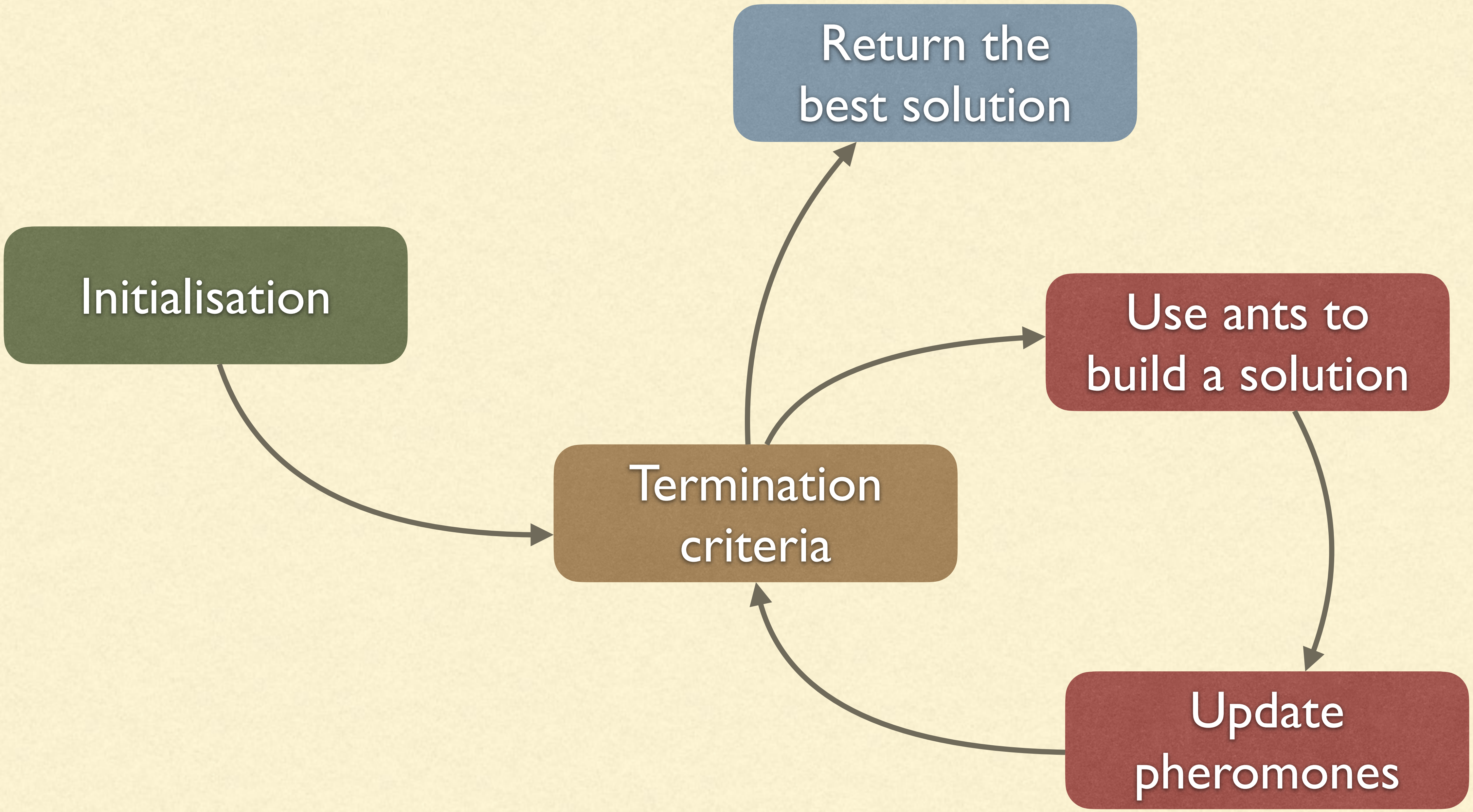
STIGMERGIC SYSTEM

- A **Stigmergic system** has three main characteristics:
  - A **global environment** that is only partially perceivable by the agents
  - A **set of agents** that populate the environment with no single agent having complete knowledge of the system's state
  - **Complexity** emerging from the interaction of the previous to aspects that cannot be predicted or reduced to their simpler components

ANT COLONY OPTIMIZATION

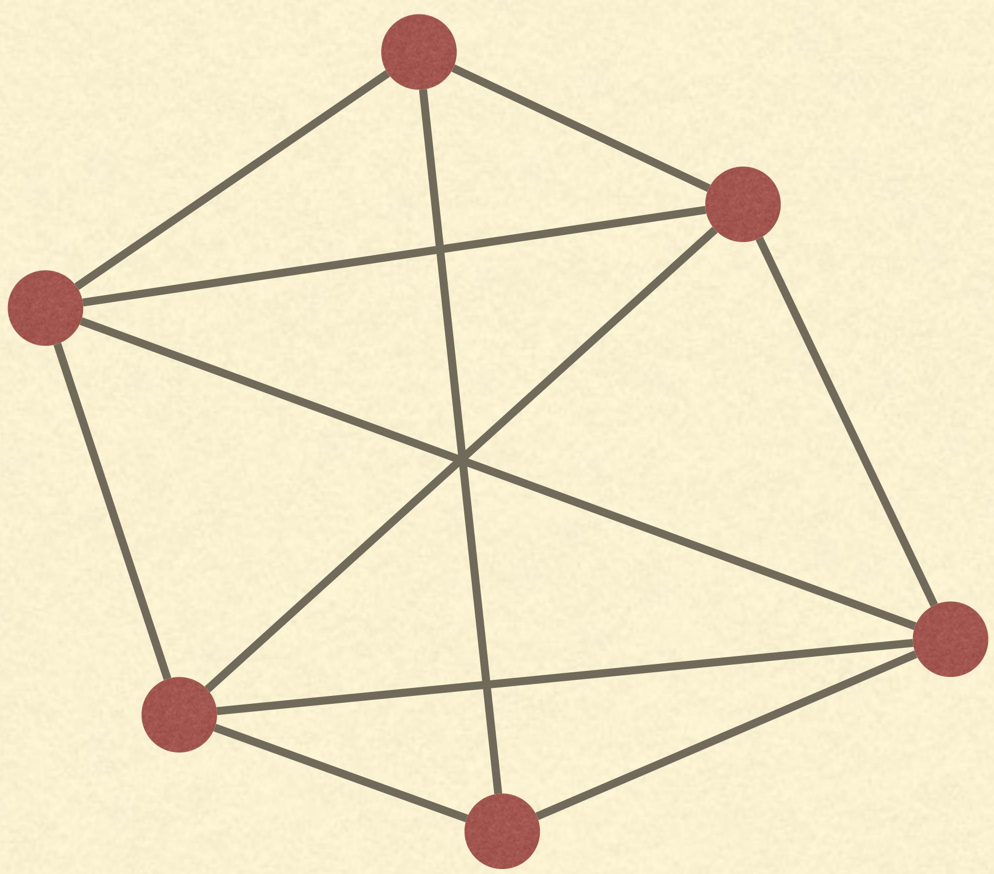
- **Ant Colony Optimization (ACO)** is inspired by the collective behaviour of ants and usually employed to solve problems on graphs
- ACO relies on stigmergy and simulated pheromone trails:
  - Pheromone left by ants in the search space evaporate over time
  - Pheromone traces guide the behaviour of the ants and, unless reinforced, evaporate over time
  - Ants are *stochastic solution building procedures* exploiting both simulated pheromone and available heuristic information about the problem being solved

ANT COLONY OPTIMIZATION



ACO FOR THE TSP

- We have a complete graph G of m nodes, representing m cities
- The edge between nodes i and j has weight/length $d_{i,j}$
- We want fo find the Hamiltonian circuit in G that minimises the sum of the weights of all the edges in the circuit (i.e., the shortest Hamiltonian circuit)



CONSTRUCTION OF THE SOLUTIONS

- $\tau_{i,j}(t)$ is the amount of pheromones on the edge (i, j) at time t
- $\eta_{i,j} = \dfrac{1}{d_{i,j}}$ is the heuristic information that we have on each edge
- $\mathcal{N}_i^k$ is the set of cities that the ant k has yet to visit when it is in city i
- An ant in city i will select which is the next city to visit according to a probability distribution based on some *heuristic information* and on the *amount of pheromones*.

CONSTRUCTION OF THE SOLUTIONS

- Each ant will start on a city and visit all cities selecting city j as the next one (in $\mathcal{N}_i^k$) with probability
- $p_{i,j}^k(t) = \dfrac{(\tau_{i,j}(t))^\alpha(\eta_{i,j})^\beta}{\sum_{\ell \in \mathcal{N}_i^k}(\tau_{i,\ell}(t))^\alpha(\eta_{i,\ell})^\beta}$
- Where α and β are parameters controlling how important are the pheromones and the heuristic information, respectively

UPDATE OF THE PHEROMONES

- Let L_k be the length of the solution found by ant k (for $k \in \{1,\ldots,n\}$)
- We define $\Delta\tau_{i,j}^{k}$ as $\dfrac{1}{L_k}$ if (i,j) is part of the solution of ant k and 0 otherwise
- Then we update the pheromone trails as
$$\tau_{i,j}(t+1) = (1-\rho)\tau_{i,j}(t) + \sum_{k=1}^{n} \Delta\tau_{i,j}^{k}$$
- Where $\rho \in [0,1]$ is a parameter used to decide how fast the pheromones evaporates

EFFECT OF THE UPDATE

- Edges that are part of better solutions (shortest length) receive more pheromones
- Edges that are part of more solutions receives more pheromones
- More pheromones make the edge more desirable
- If an edge is more desirable its probability of being selected increases