Lecture 07 - Real-valued optimisation

Optimisation CT5141

James McDermott

NUI Galway

OÉ Gaillimh
NUI Galway

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Overview

1. **Real-valued optimisation: big picture and applications**
2. Covariance Matrix Adaptation
3. Particle Swarm Optimisation

Real-valued optimisation

In real-valued optimisation we have a vector of real DVs. We already saw some black-box algorithms for this:

- In HC, LAHC, SA, GA, we can use `init`, `nbr` (and `crossover` for GA) suitable for real vectors.

LP and gradient descent

If a stronger algorithm is available, we won't use a black-box algorithm:

- Some applications with real DVs have linear objective and constraints, so we would use LP;
- In some applications with real DVs, we can find the gradient, so we would use gradient descent.

Black-box real-valued optimisation

But if we have to, we can use a metaheuristic for real optimisation.

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Now, a confession:
LAHC, SA and GA are not the best metaheuristics for this

- Covariance Matrix Adaptation
- Particle Swarm Optimisation

Black-box real-valued optimisation

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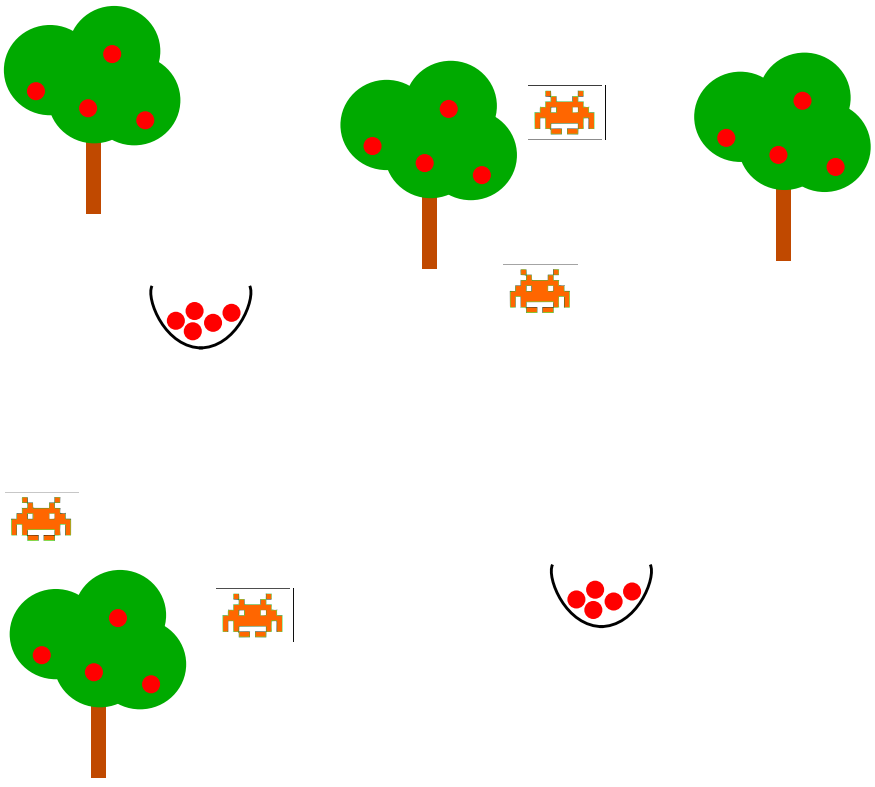
- Particle Swarm Optimisation

First let's consider applications.

Facility location



Large field with n fruit trees at locations t_i. Tree i has w_i fruit. We have a swarm of tiny flying robot fruit pickers. Each robot picks a fruit and flies to a bin. We can place m bins b_j each with unlimited capacity. Where in the field should we put them?

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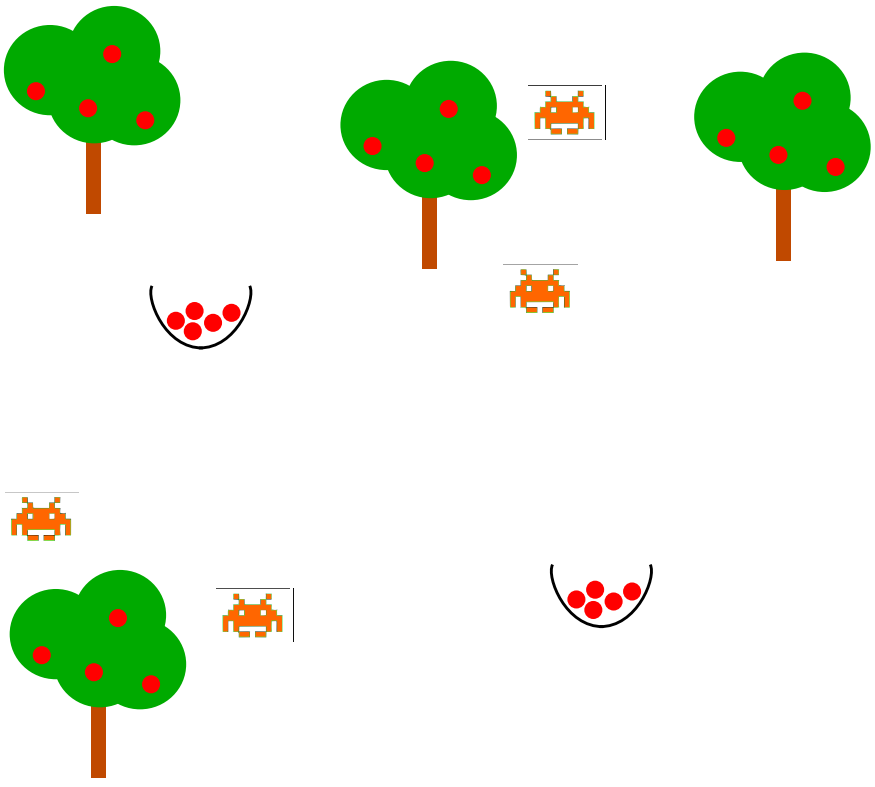

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Minimise $f(x_1, x_2, \ldots, x_{2m}) = \sum_i w_i \min_j(d(t_i, b_j))$

where d is Euclidean distance.

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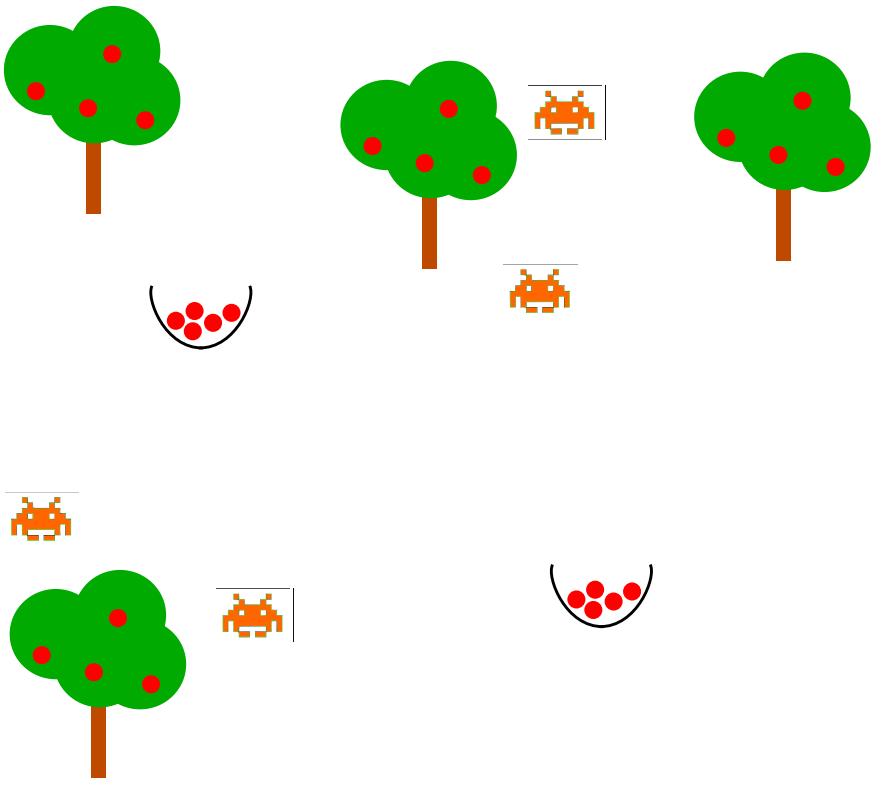

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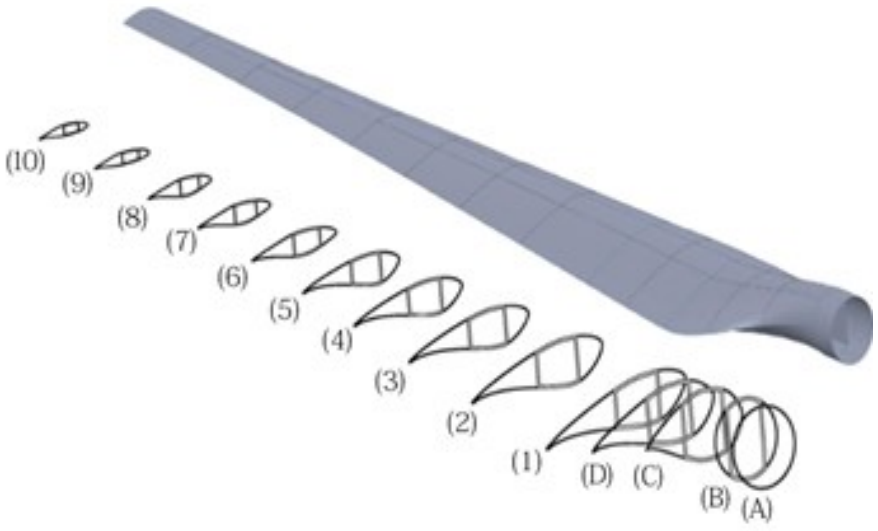
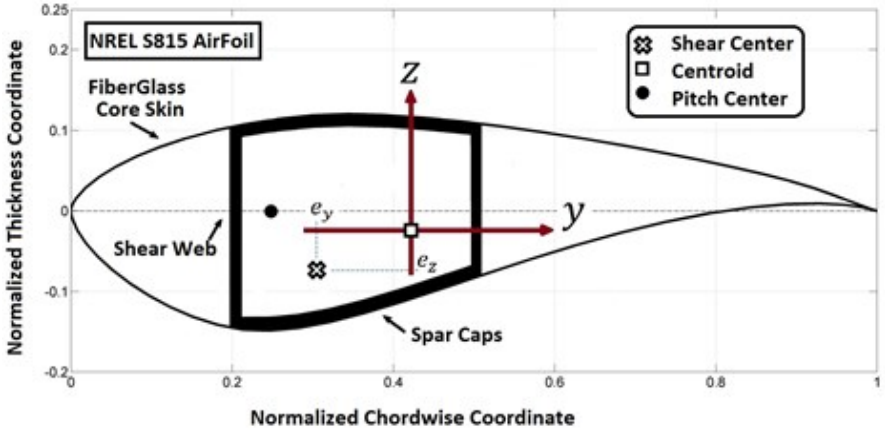
Exactly the same problem arises when choosing where to locate a supermarket to serve several cities.

Wind turbine engineering

In a wind turbine, what **shape** should the sails be?

Several real-valued parameters:





Sheibani and Akbari

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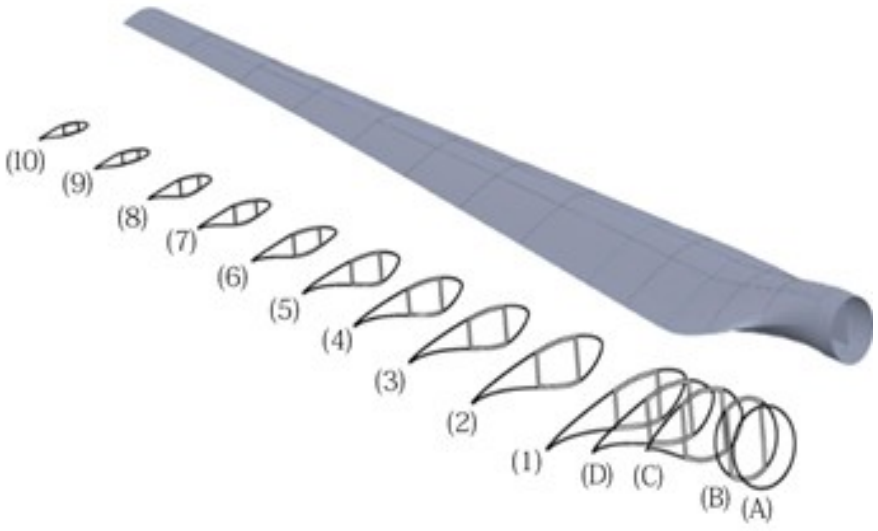
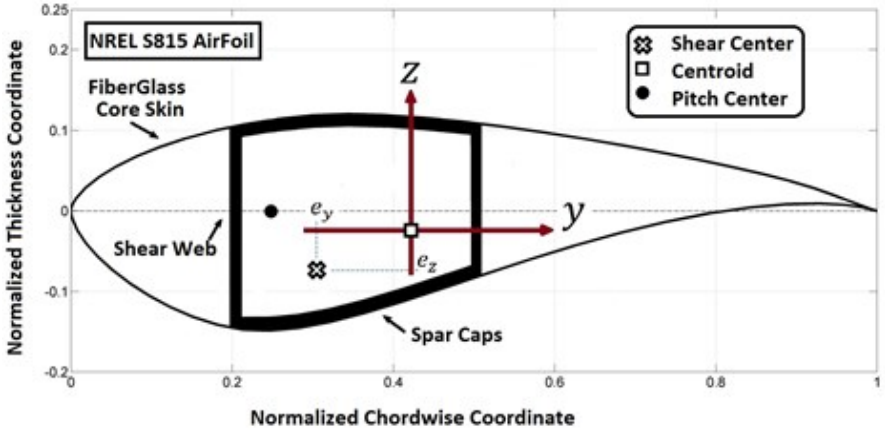
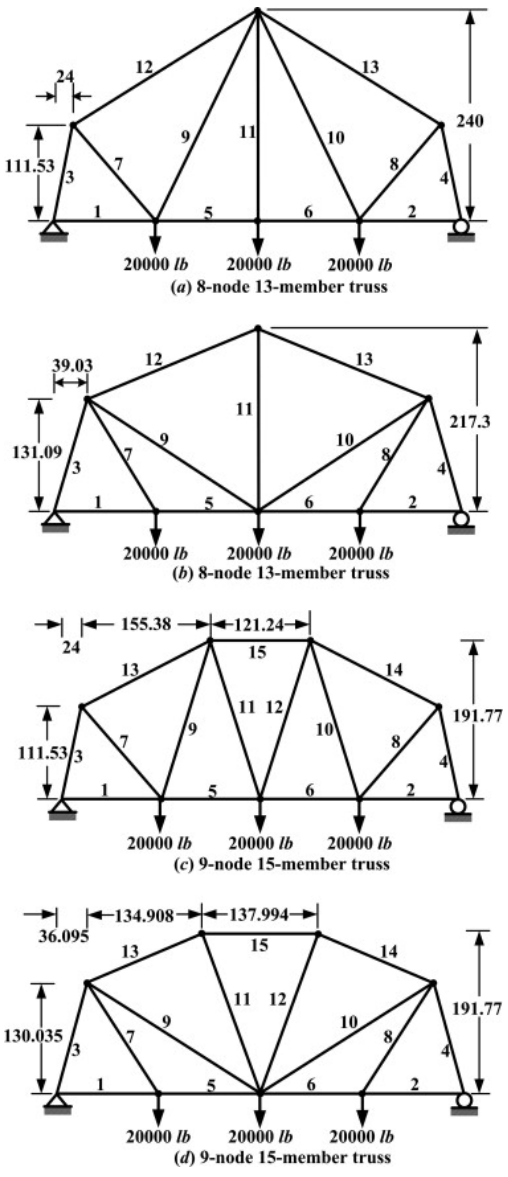




Sheibani and Akbari

We program a finite-element simulation to estimate the **annual energy production** for a given shape.

A-frame truss design



From Luh and Lin

- **Truss**: a 2D or 3D engineering design of beams or rods, attached at nodes – like in the attic of a house.
- Calculate behaviour under gravity, taking account of beam width/weight etc.
- Numerical parameters: node positions and beam widths.
- Objective: minimise weight, minimise deflection, prevent collapse.
- Simple example: https://pythonhosted.org/pyswarm/
- An interactive setting: https://www.polybridge2.com/

FM Synthesis

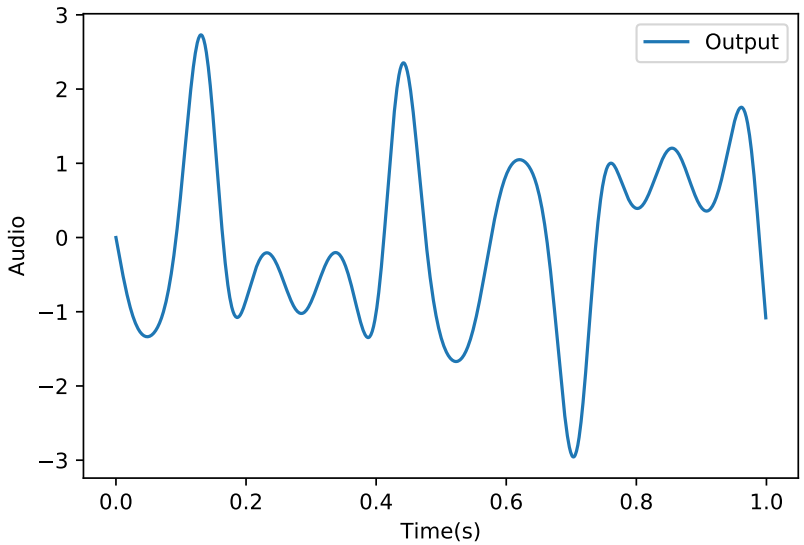
- Frequency-modulation synthesis is an approach to sound synthesis for music
- Invented by Chowning and popularised by Yamaha
- Common in 1980s synth music, e.g. Blade Runner
- Core idea: to take the sine of a sine, giving a sound spectrum with many frequencies.

FM Synthesis control problem

The output of an FM Synth at time t is:

$$\hat{y}(t) = a_1 \sin(\omega_1 t\theta) + a_2 \sin(\omega_2 t\theta + a_3 \sin(\omega_3 t\theta))$$

where $\theta = 2\pi/f_s$, and f_s is sampling frequency, e.g. 44.1kHz.

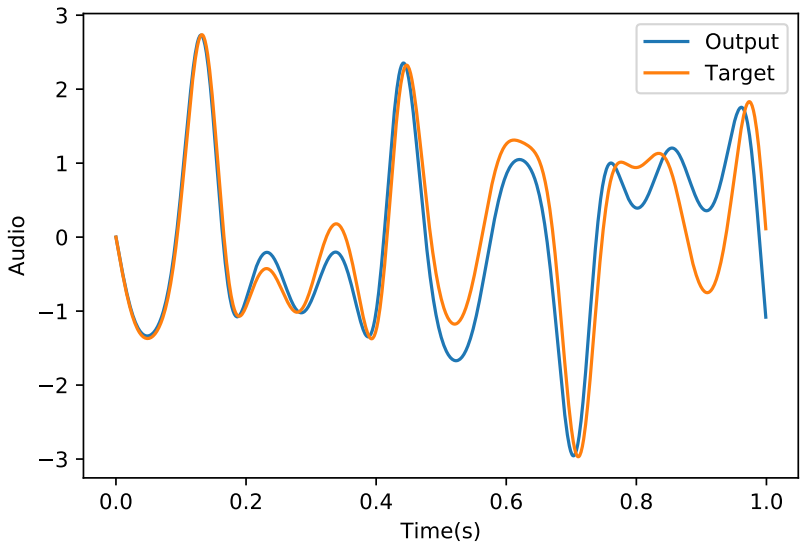


FM Synthesis control problem

We are given some target sound y which we wish to match using FM Synthesis. We **minimise**:

$$f(a_1, \omega_1, a_2, \omega_2, a_3, \omega_3) = \text{RMSE}(y, \hat{y}).$$

(The parameters are constrained, e.g. to $[-6.4, 6.35]$)



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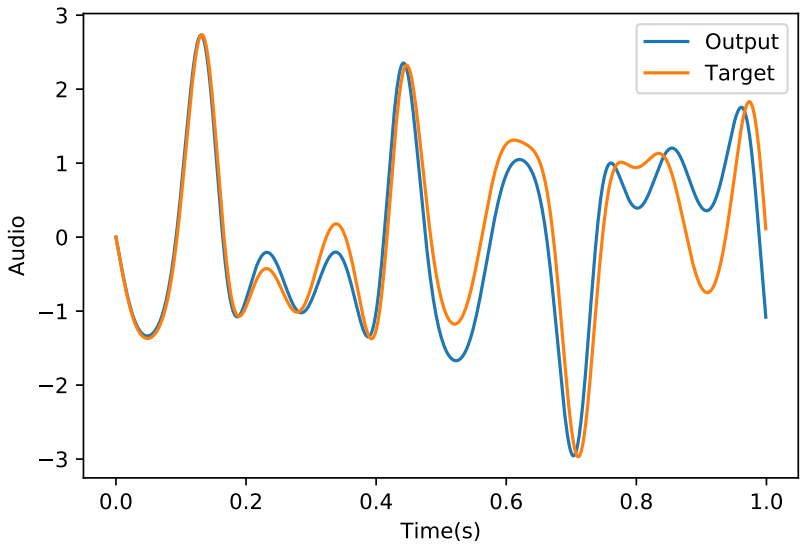

(Formulation from Das and Suganthan, 2011, in Blackboard.)

FM Synthesis control problem

(My PhD was in this area, but with a different type of synthesizer. E.g., I experimented with other objectives that work better than RMSE.)

Some more applications

Again see Das and Suganthan (2011) in Blackboard:

- Radar pulse code optimisation
- Antenna array
- Economic dispatch (like unit commitment)
- Spacecraft trajectory optimisation

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How does a GA work? Another view

- In a GA, the population implicitly represents our knowledge of f
- Think of the population as samples from a distribution
- We draw new samples using crossover and mutation
- These new samples are concentrated in high-fitness regions thanks to selection.

Genetic operators

- Mutation takes in **one** individual and returns a new one

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- Could we have 3-parent operators, or higher?
- These do exist, but are rarely used
- But taking a blend of **all parents at once** is quite common: it is called **Estimation of Distribution**.

Estimation of Distribution Algorithms

The **Estimation of Distribution Algorithm** (EDA):

1. Create an initial population
2. Discard the worst according to f
3. **Estimate** a statistical model of the remainder
4. **Draw samples** from the model to create new population
5. Go to 2.

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Think of this as a **crossover** which blends **all parents at once**.

Simple real EDA

1. Create population using `init`
2. Evaluate and discard worst to give "parents" P
3. Create one vector representing the **mean**

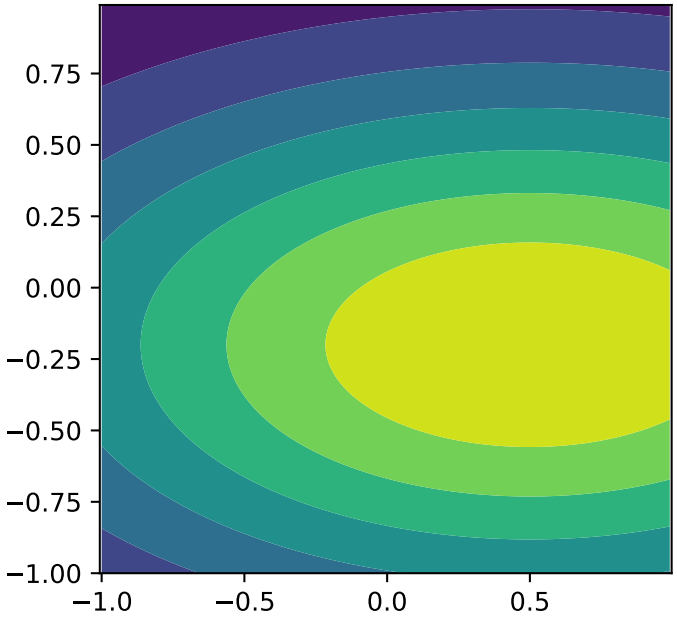
$$\mu \in \mathbb{R}^n : \mu_i = \frac{1}{|P|} \sum_{x \in P} x_i$$

and one representing the **standard deviation**

$$\sigma \in \mathbb{R}^n : \sigma_i = \sqrt{\frac{1}{|P|} \sum_{x \in P} (x_i - \mu_i)^2}$$

4. Draw new individuals x by sampling: $x_i \sim N(\mu_i, \sigma_i)$
5. Go to 2.

What will happen?



$$\mu = (0.5, -0.25), \sigma = (2.0, 0.5)$$

- μ_i will gradually move towards the best value for DV x_i
- But this is **independent** of the values at other i
- σ_i will gradually decrease (the distribution narrows).

Reminder: linkage

Linkage between DVs makes problems harder.

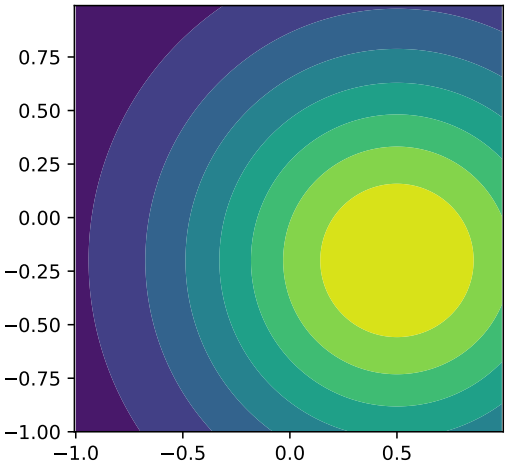
Other words for linkage:

- dependency
- epistasis
- synergy
- “more than the sum of its parts”.

Problem: our EDA is too simple

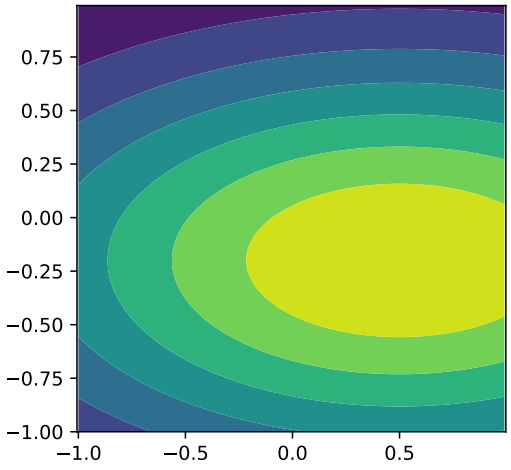
- All positions x_i are considered **independently**
- Cannot learn about linkage between two variables
- But the **covariance** between two variables would give that information
- (Covariance is just **correlation** in disguise)
- **Solution**: use a more complex distribution with covariance

Multivariate Normal: $N(\mu, \Sigma)$



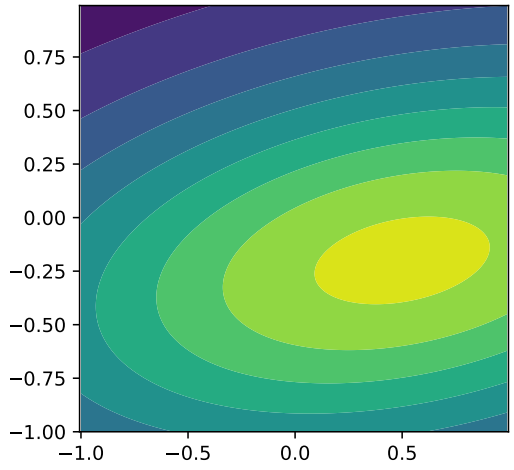
Spherical

$$\Sigma = \begin{bmatrix} 0.5 & 0.0 \\ 0.0 & 0.5 \end{bmatrix}$$



Diagonal

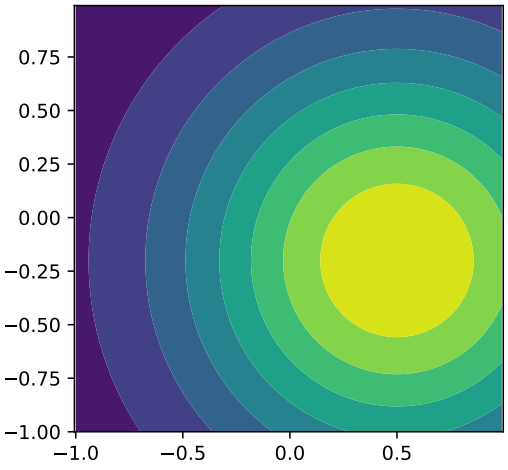
$$\Sigma = \begin{bmatrix} 2.0 & 0.0 \\ 0.0 & 0.5 \end{bmatrix}$$



Full

$$\Sigma = \begin{bmatrix} 2.0 & 0.3 \\ 0.3 & 0.5 \end{bmatrix}$$

Multivariate Normal: $N(\mu, \Sigma)$



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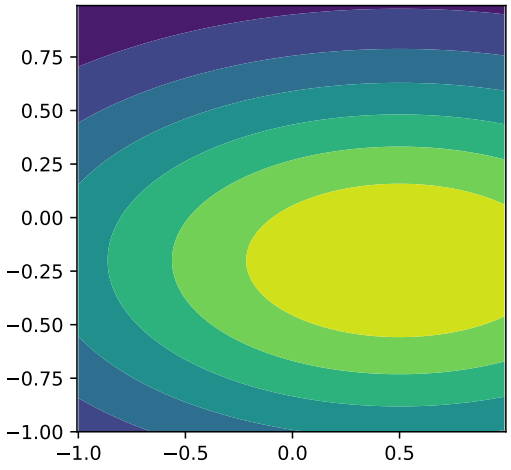

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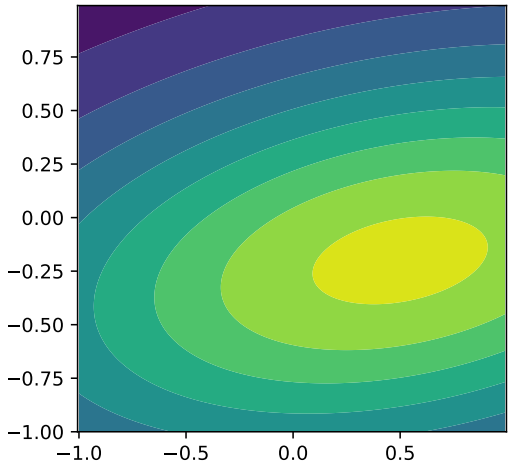


Full

$$\Sigma = \begin{bmatrix} 0.5 & 0.0 \\ 0.0 & 0.5 \end{bmatrix} \qquad \Sigma = \begin{bmatrix} 2.0 & 0.0 \\ 0.0 & 0.5 \end{bmatrix} \qquad \Sigma = \begin{bmatrix} 2.0 & 0.3 \\ 0.3 & 0.5 \end{bmatrix}$$

Don't get confused: **diagonal** means Σ is diagonal. The distribution is then **axis-aligned**. A **full** matrix is more flexible (still must be symmetric): distribution can be diagonal.

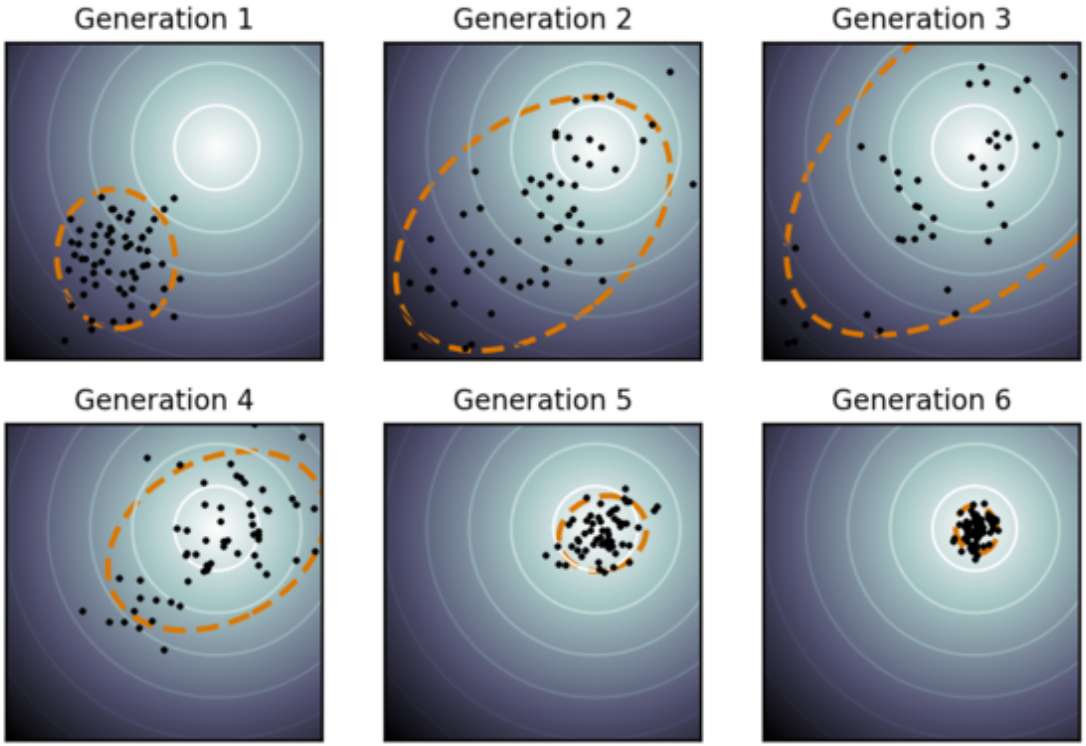
Covariance matrix

The covariance matrix Σ gives the **shape** of the distribution as shown.
In our simple EDA we had a **diagonal** Σ: no linkage.

Covariance Matrix Adaptation

- In CMA, we model the population as a **multivariate normal**
- For each decision variable we have a **mean**
- We also have a **full covariance matrix**.
- (Think of the distribution as an ellipse, non-axis aligned)

CMA: illustration of a run



Wiki

In this picture, fitness is shown as grey-scale. The current population is modelled using a multivariate normal with full covariance. This distribution changes location **and shape** to model the population.

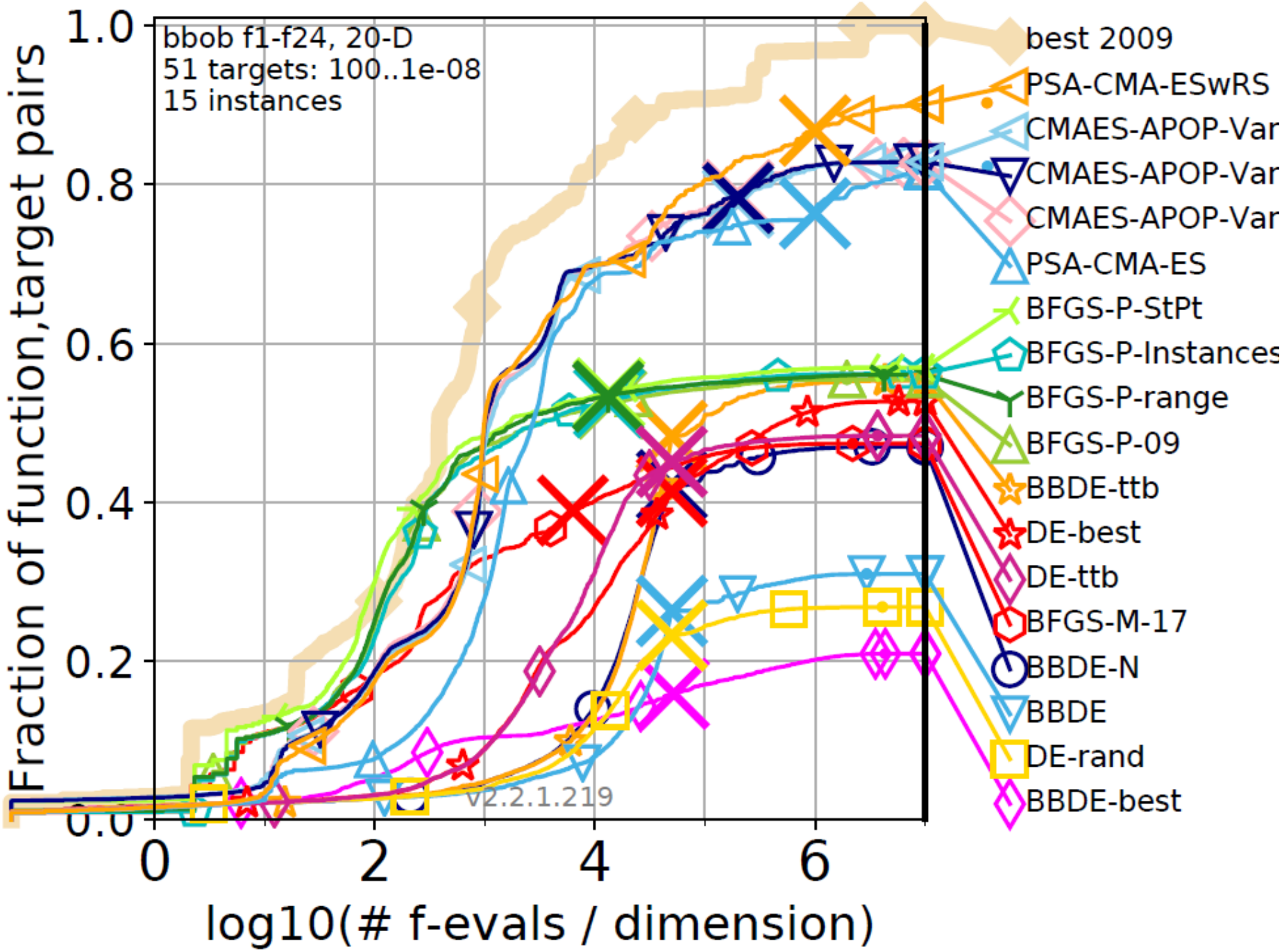
CMA

- Uses **standard** statistical methods to draw samples from the multivariate normal, giving the new population
- Also use some **sophisticated** methods to update the distribution based on new population at each step
- (i.e. don't just re-learn it from scratch)
- It also **self-adapts** many hyperparameters
- Further details are omitted and will not be examinable.

CMA: performance?

CMA and variants often win the “Black-box optimisation benchmarking” competition (BBOB)

See https://coco.gforge.inria.fr/.


bbob f1-f24, 20-D
51 targets: 100..1e-08
15 instances
Fraction of function,target pairs
log10(# f-evals / dimension)
v2.2.1.219
best 2009
PSA-CMA-ESwRS
CMAES-APOP-Var
CMAES-APOP-Var
CMAES-APOP-Var
PSA-CMA-ES
BFGS-P-StPt
BFGS-P-Instances
BFGS-P-range
BFGS-P-09
BBDE-ttb
DE-best
DE-ttb
BFGS-M-17
BBDE-N
BBDE
DE-rand
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Using CMA in practice

```
$ pip install cma
```

```
import cma
 ...
# pass in initial mean and sigma - just a guess
es = cma.CMAEvolutionStrategy(mu0, sigma0,
                              {'bounds': (lb, ub)
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es.optimize(f, iterations=maxits / es.popsize)
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It chooses good hyperparameter values by itself :)

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Bio-inspired optimisation

- Evolutionary algorithms: inspired by Darwinian evolution
- **Particle swarm optimisation**: inspired by bird flocking behaviour
- Ant colony optimisation: inspired by ant foraging

Flocking

Murmuration: https://www.youtube.com/watch?v=eakKfY5aHmY

Flocking seagulls

Boids and Crowds

Reynolds' Boids website: http://www.red3d.com/cwr/boids/

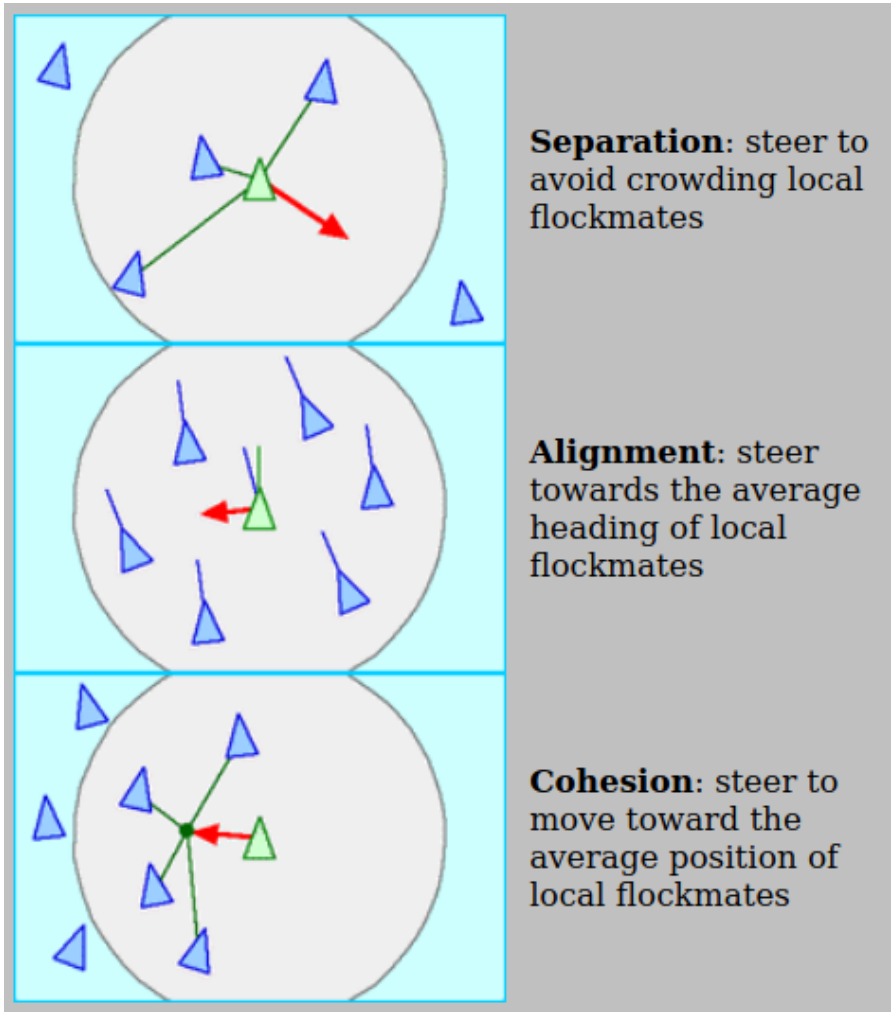
Reynolds' paper (SIGGRAPH 1987)

Boids video: https://www.youtube.com/watch?v=QbUPfMXXQIY

Use in movies: https://www.youtube.com/watch?v=042YjQ9aZNk

Boids rules

A **boid** is a “bird” (a point moving in 2D or 3D space) obeying three rules



Reynolds

Boids properties

- **Emergence**: “complex global behavior can arise from the interaction of simple local rules” (Reynolds)
- Some **ordered** behaviour
- Also some **chaotic** behaviour: small changes in initial conditions lead to large changes later
- A system **at the edge of chaos** (Langton).

Particle Swarm Optimisation

- PSO is “a population based stochastic optimization technique”
- “inspired by social behavior of bird flocking or fish schooling.”
- (from http://www.swarmintelligence.org/tutorials.php)
- Proposed by Eberhart and Kennedy (1995).

PSO and GA

Similarities:

- Population of randomly-initialised points
- Many iterations
- Each generation formed by variation of the previous

Differences:

- Think of each point as **moving**, not being replaced by a new one
- Points have **velocity**.

PSO algorithm

- We store the best point ever observed, called `gbest`

  All particles move towards `gbest`. This is "social influence". Think of a seagull observing **another** seagull finding food.

- Each particle stores the best point it has visited, called `pbest`

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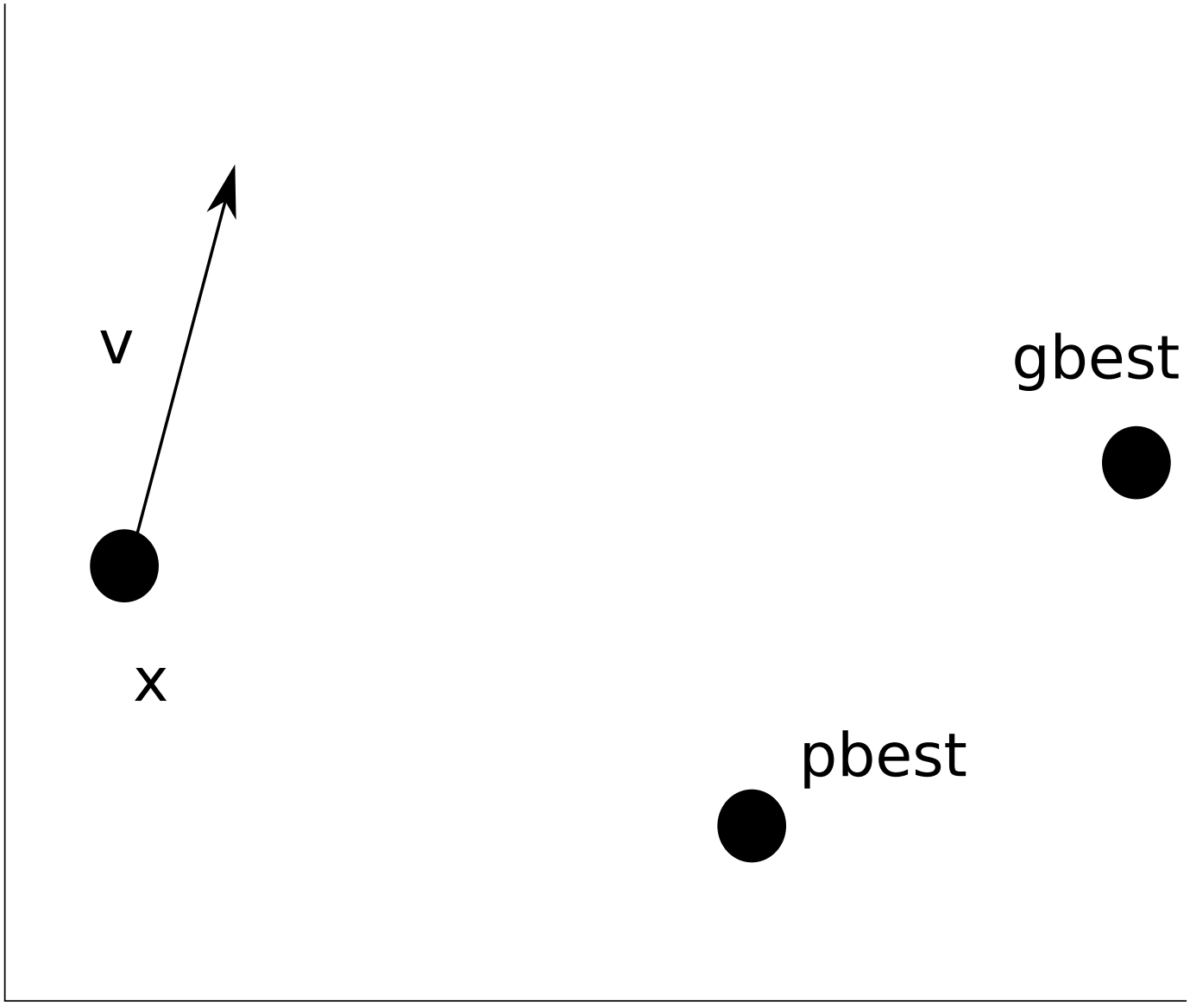
- At each "generation", we update each particle's velocity v and then position x.

1. $v := wv + c_p$ `rand()` (`pbest` $-x$) $+ c_g$ `rand()` (`gbest`$-x$)
2. $x := x + v$

Adding vectors



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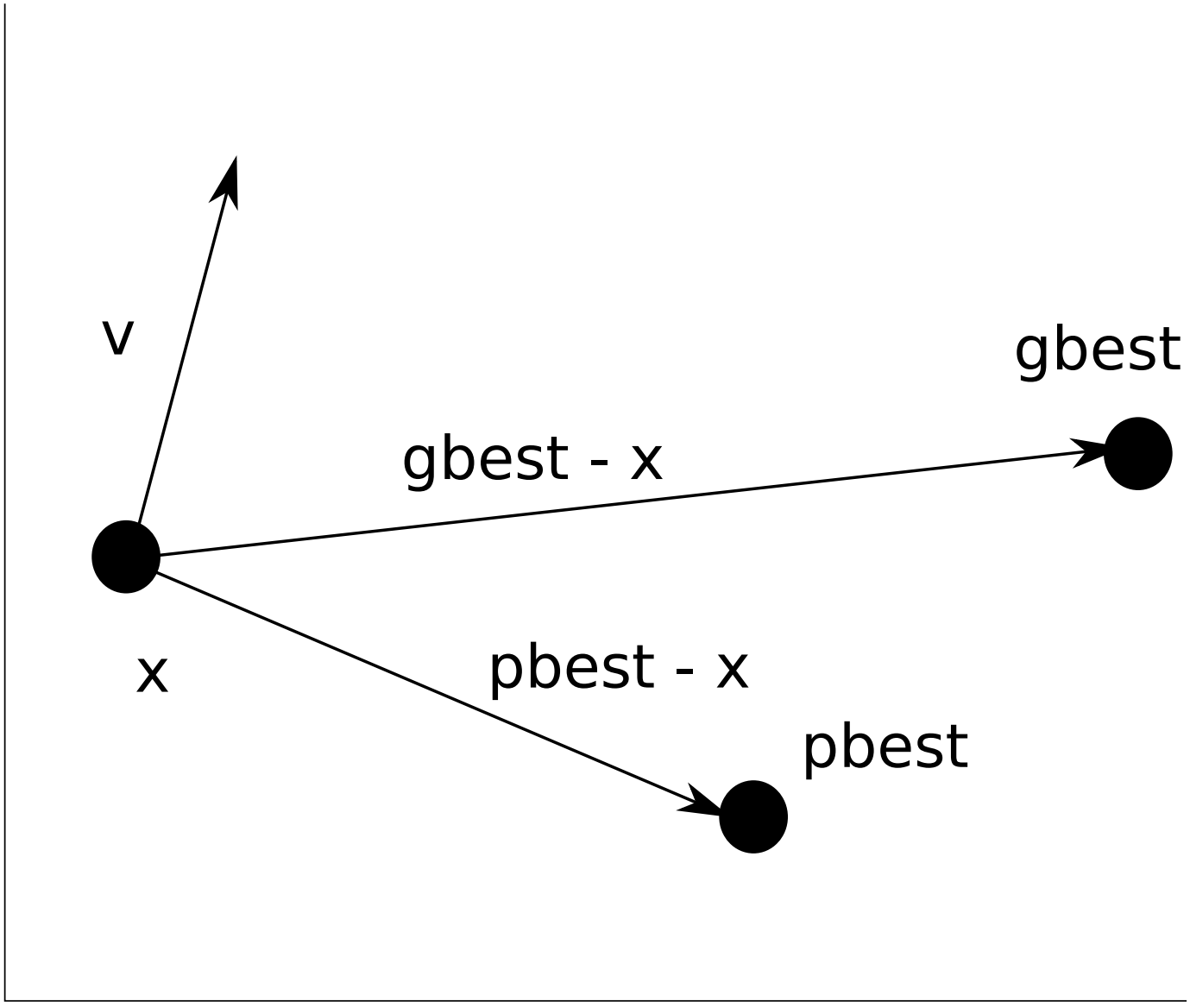

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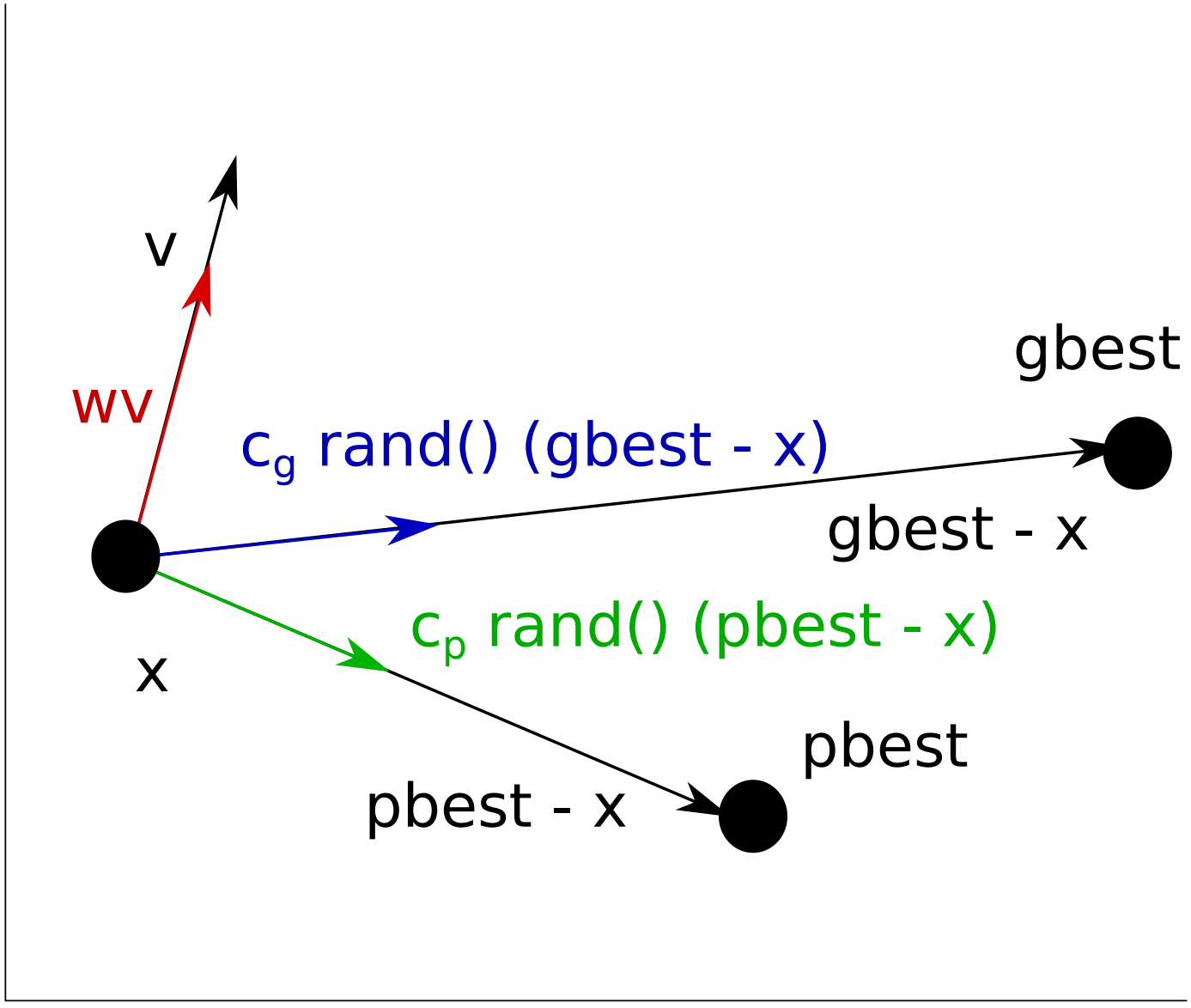

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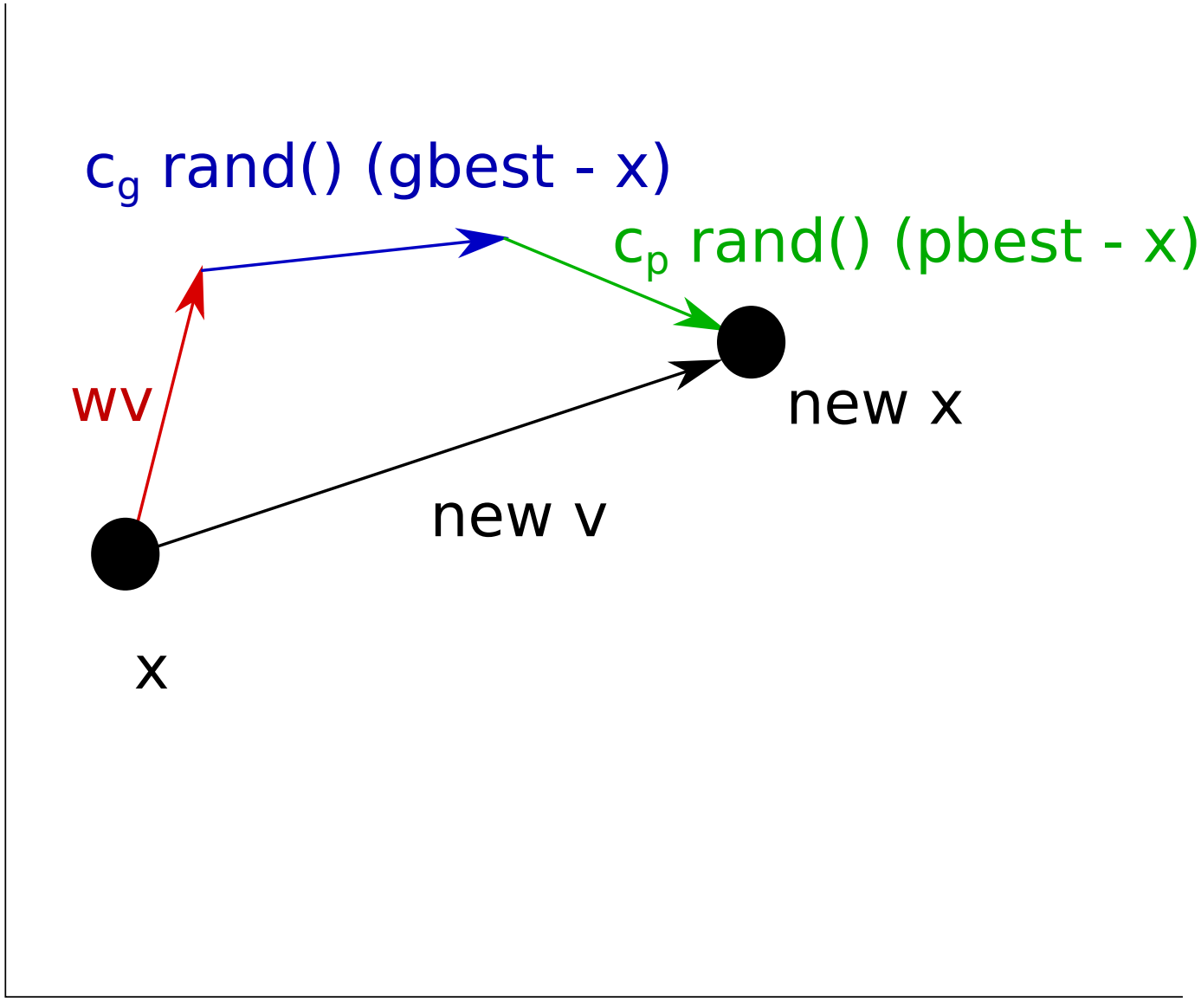

Control parameters

c_p and c_g control the strength of the two rules. Often $c_p = c_g = 2$.

Inertia

- w controls **inertia** (i.e. momentum)
- Large w: velocity more influential: exploration
- Small w: `gbest` and `pbest` more influential: exploitation
- Sometimes w is on an **schedule**, e.g. gradually reduce w from 0.9 to 0.4 over 1000 generations.

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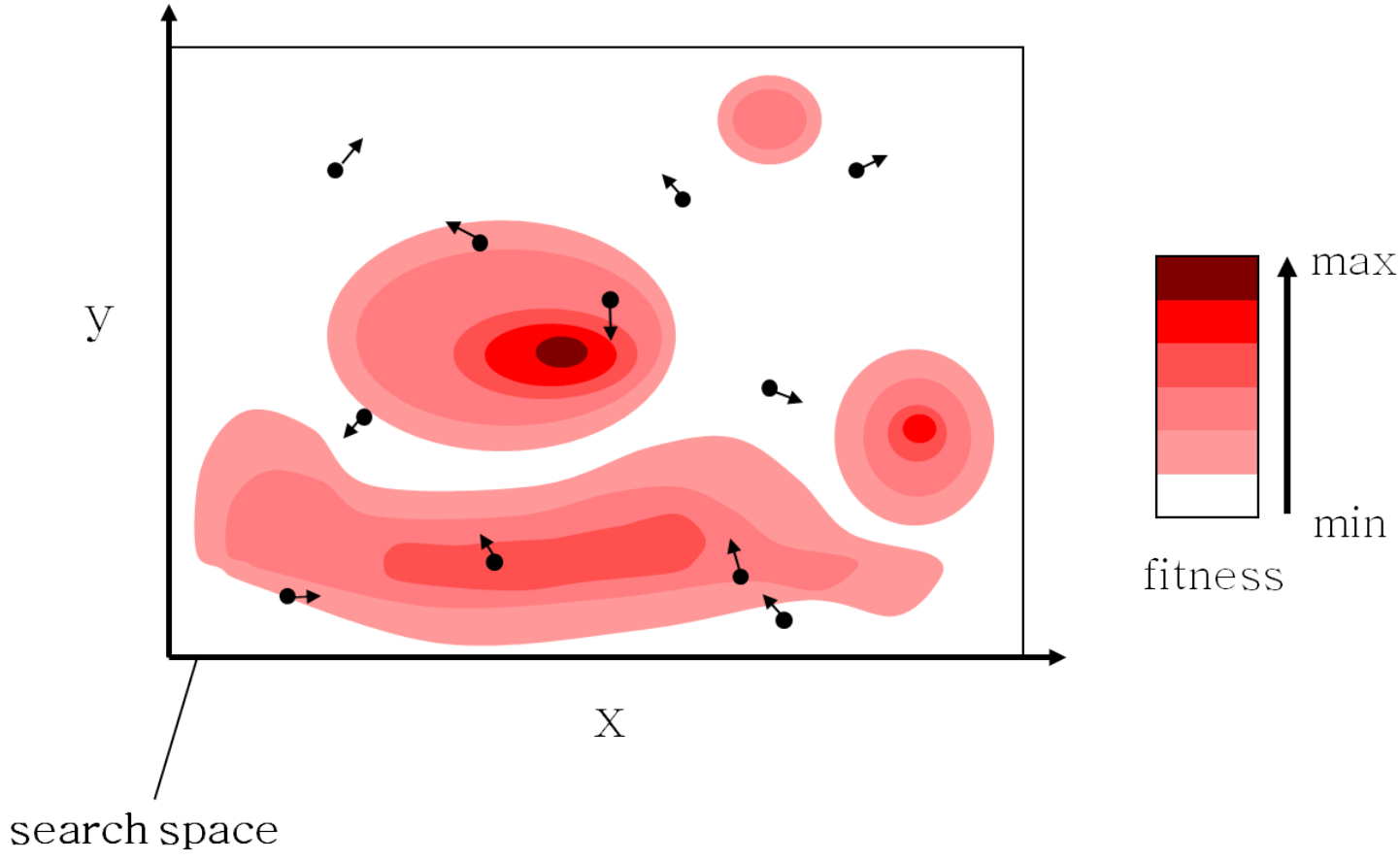
Gradually move from exploration to exploitation over time: just like SA

PSO animation

Wiki:

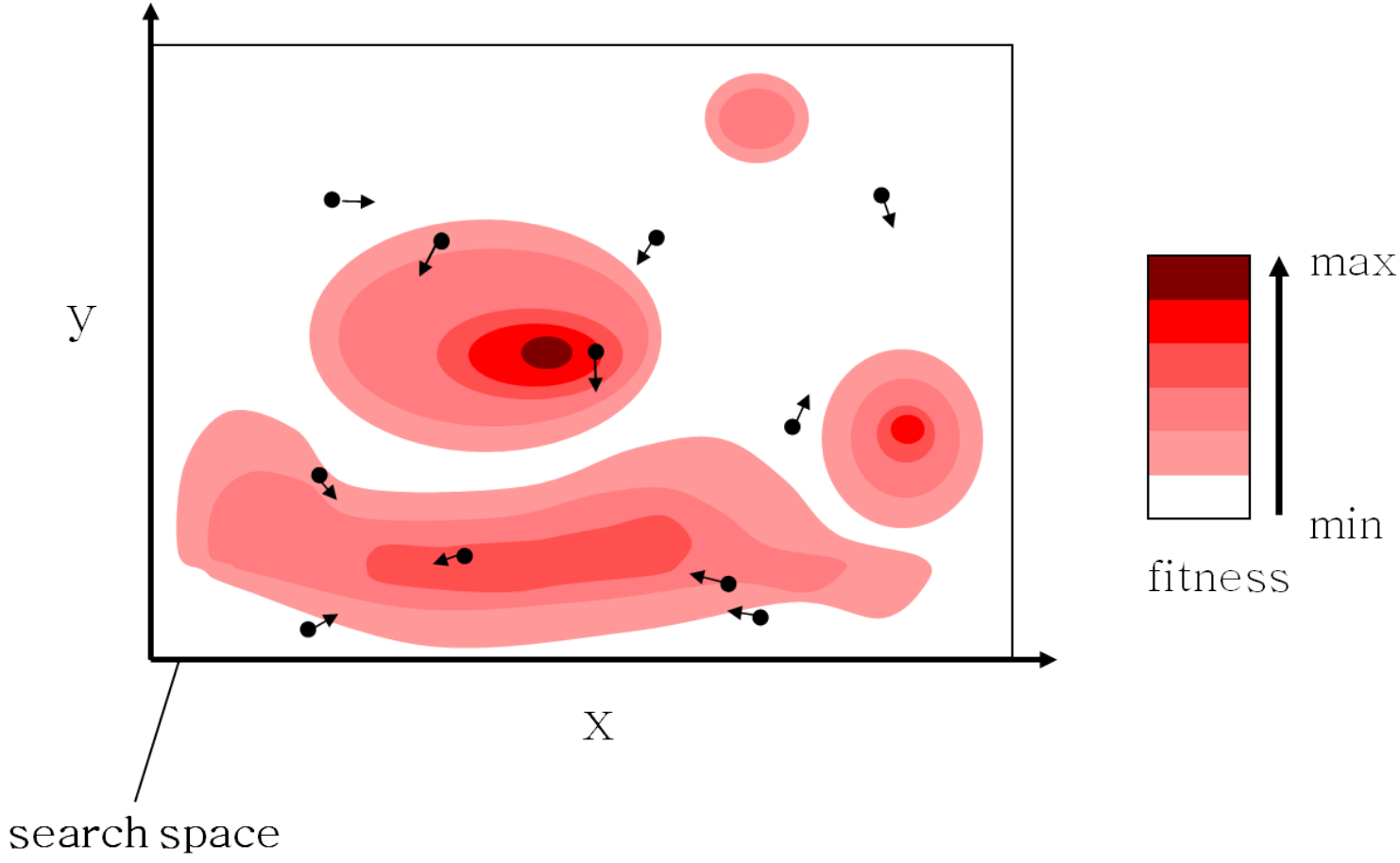
https://commons.wikimedia.org/wiki/File:ParticleSwarmArrowsAnimatio
gif

PSO AT WORK (MAX OPTIMIZATION PROBLEM)

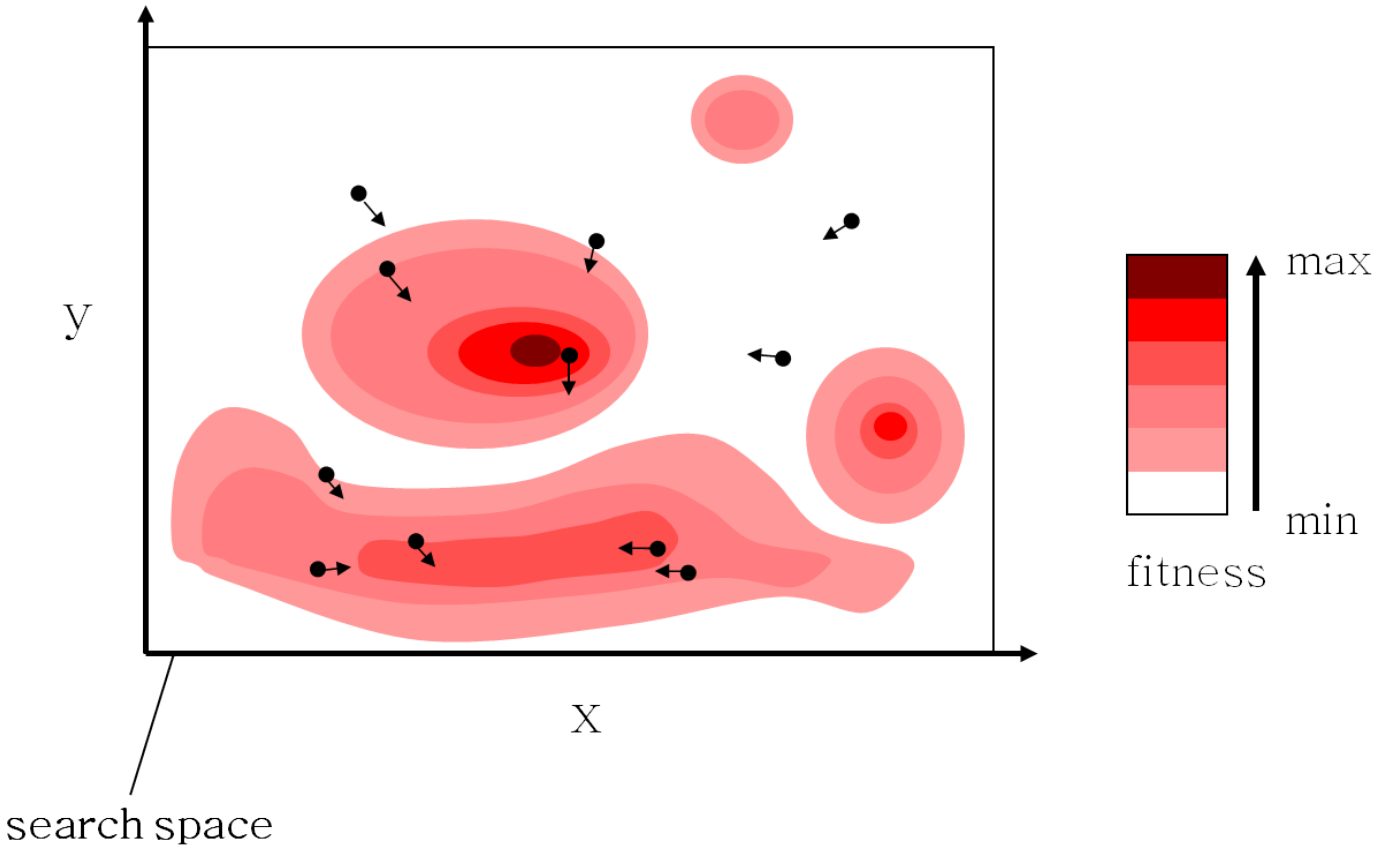


Example slides from Pinto et al.

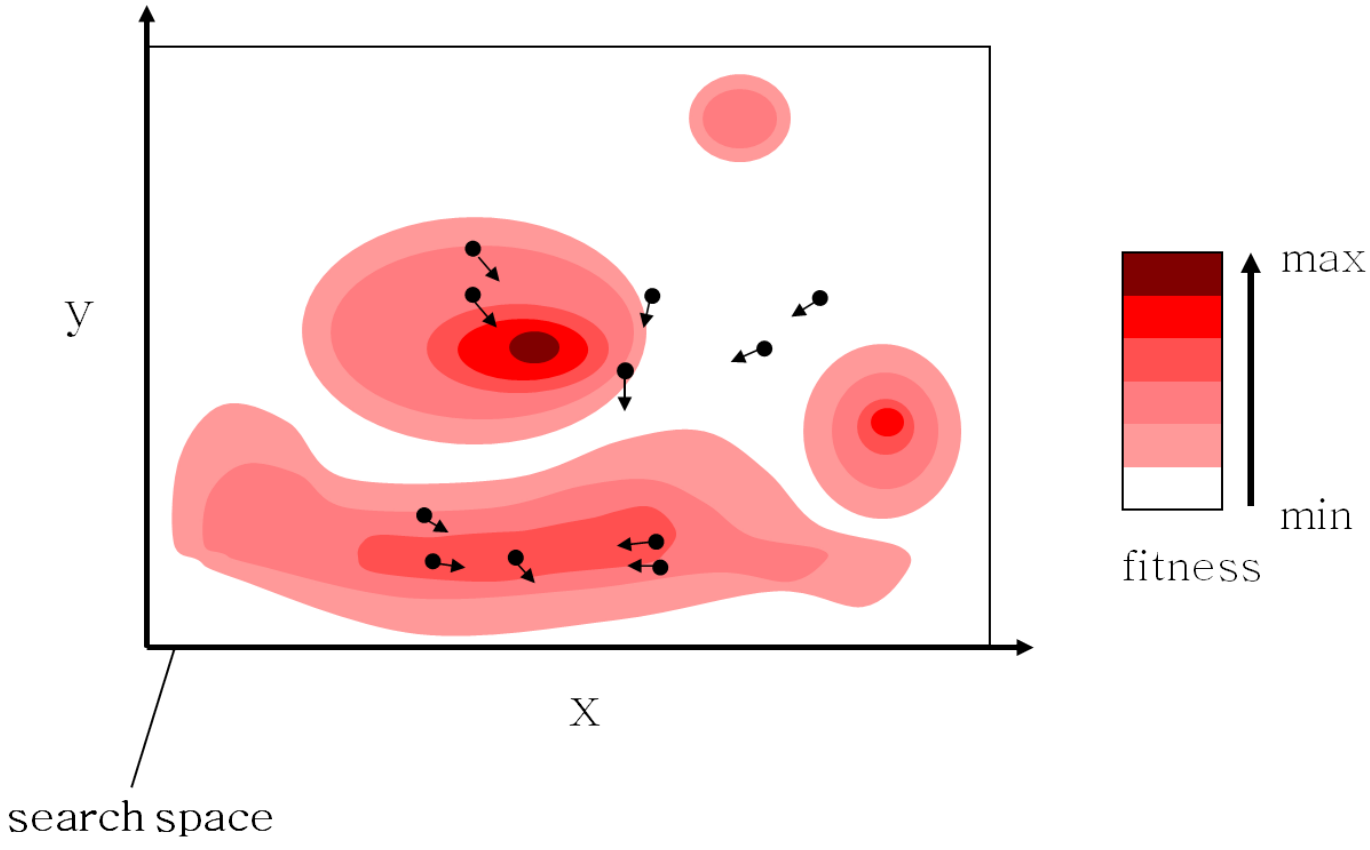
PSO AT WORK



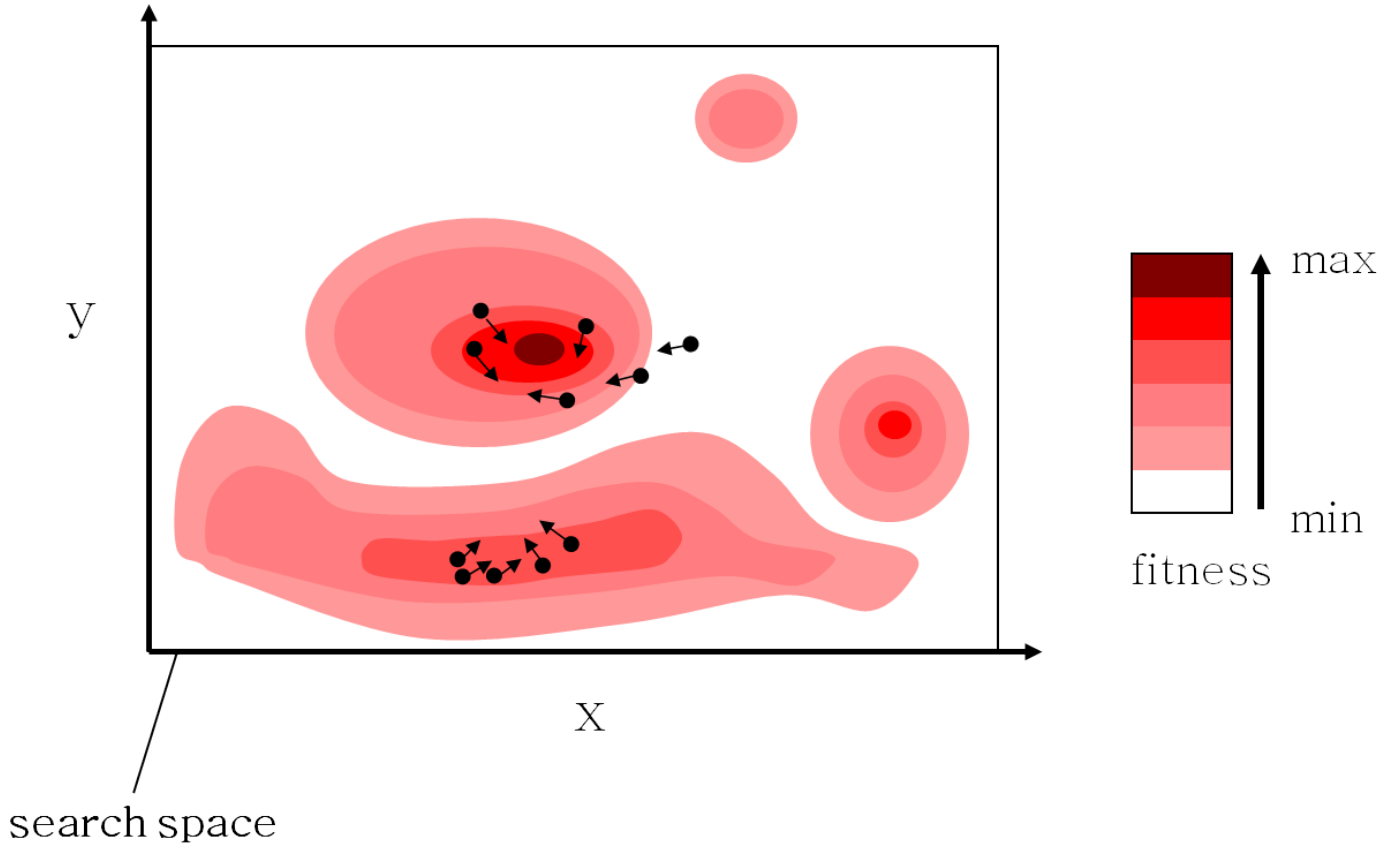
PSO AT WORK



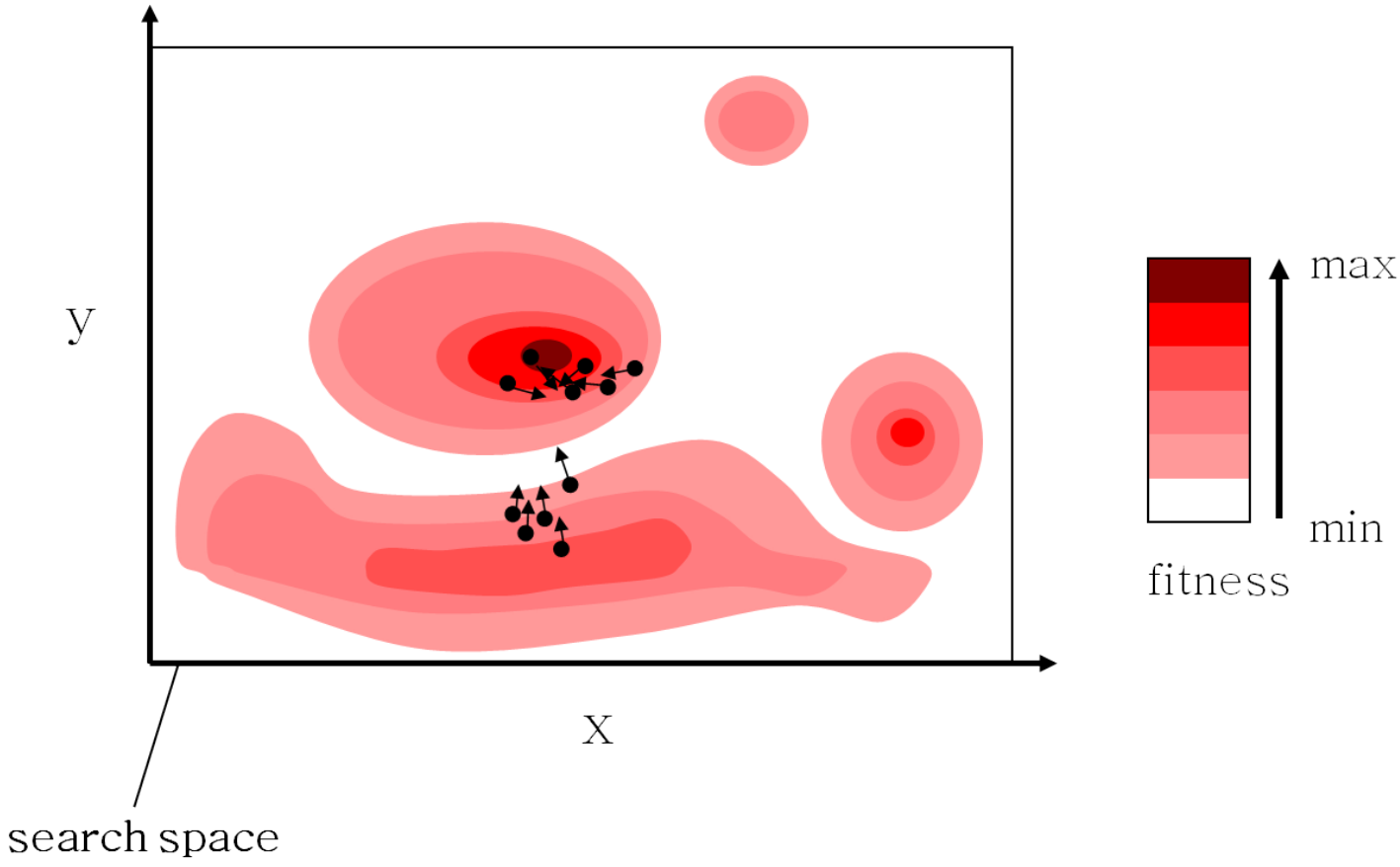
PSO AT WORK



PSO AT WORK



PSO AT WORK



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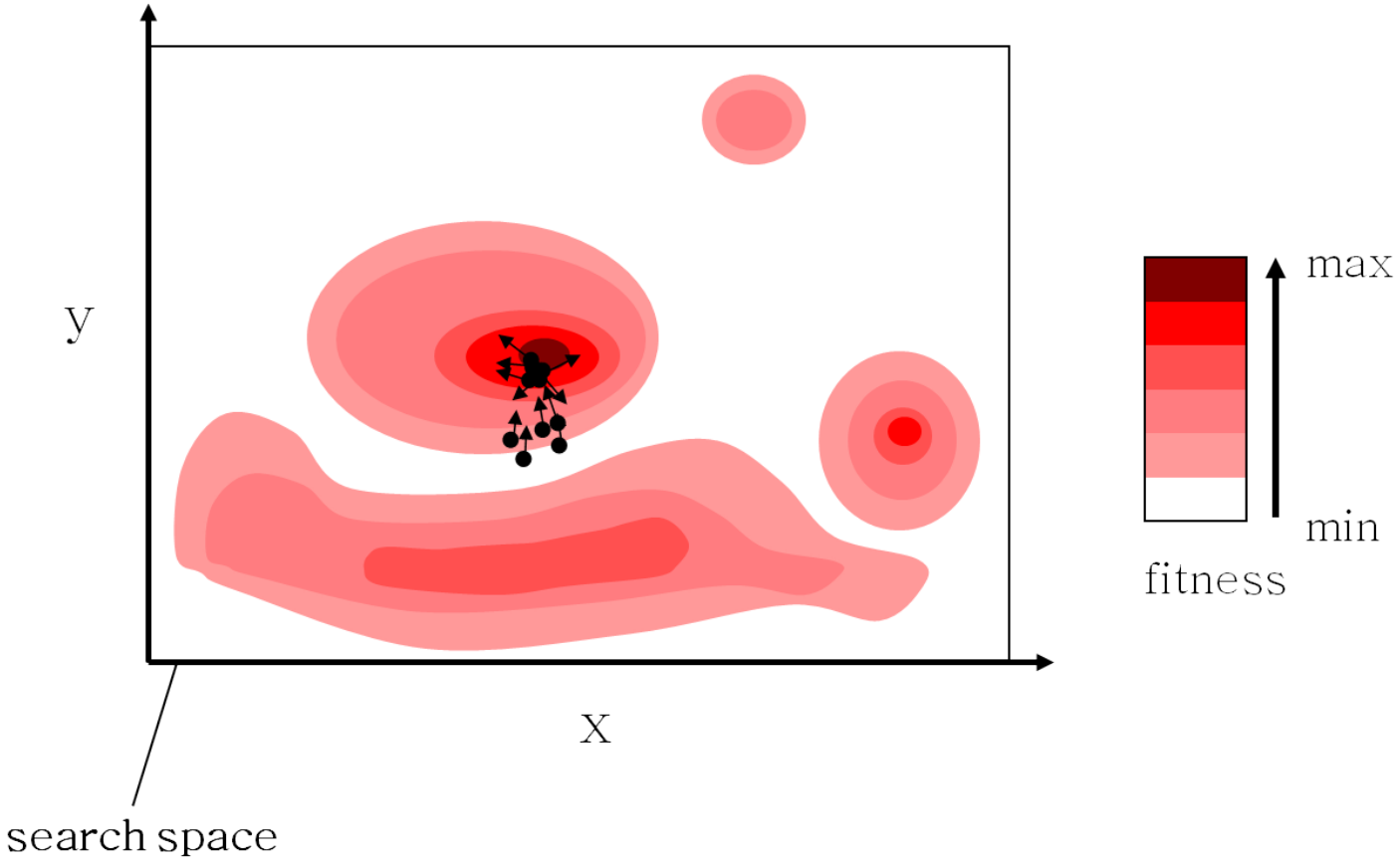
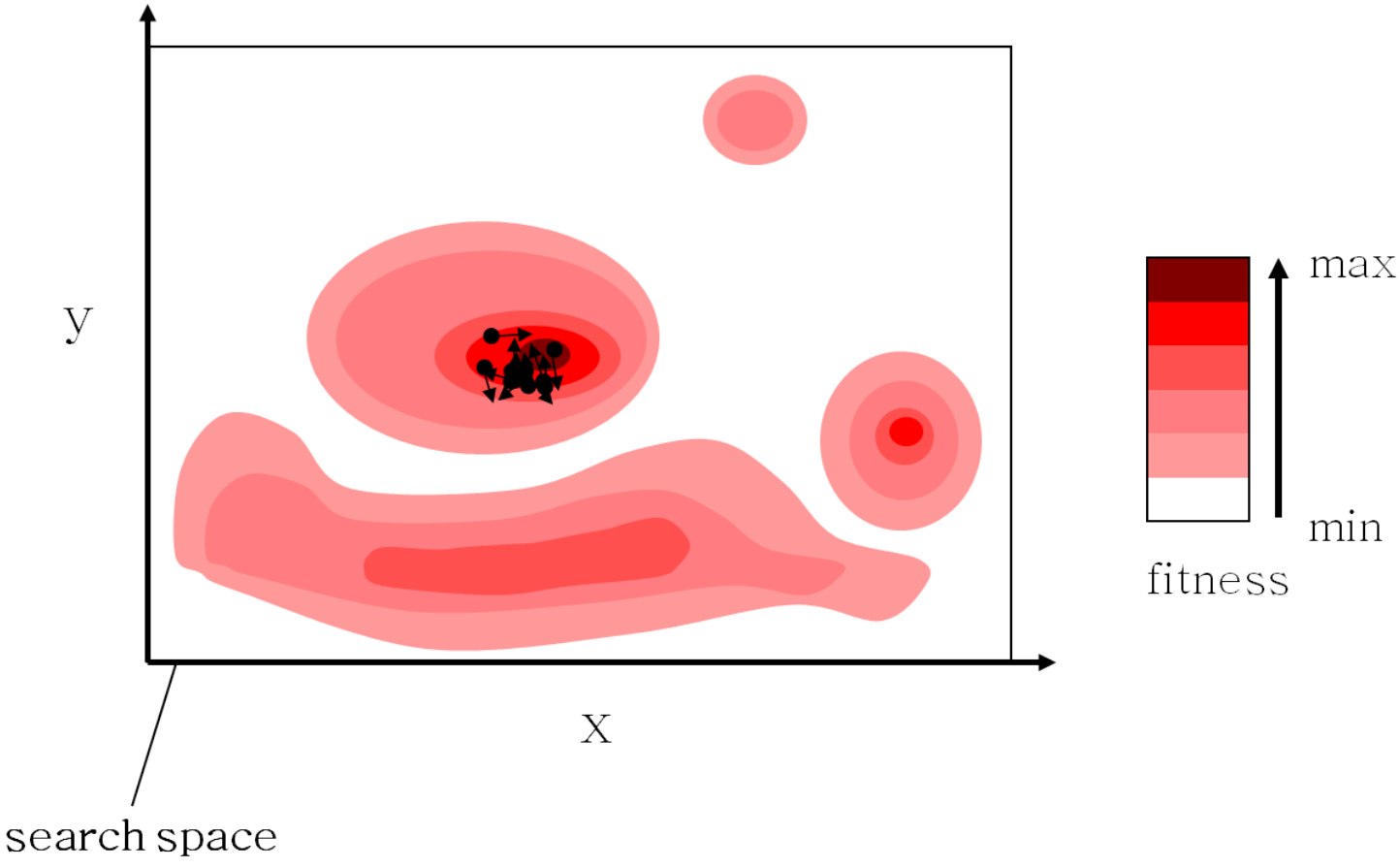


PSO AT WORK



(These images are from Di Caro, credited there to Pinto, I can’t find Pinto!)

Why does it work?

Velocity tends to help because a particle sometimes just “flies past” local optima.

`gbest` means there is **information-sharing** among particles.

Using a PSO in practice

We can program PSO without too much difficulty. But there are some nice libraries, e.g.:

- PySwarms https://github.com/ljvmiranda921/pyswarms
- DEAP https://deap.readthedocs.io/en/master/examples/pso_basic.html

Real-valued optimisation: summary

- Real-valued **GA**
- **CMA** is not really bio-inspired
  - Multivariate normal with full covariance matrix
  - Smart hyperparameters
  - Wins competitions.
- **PSO** is another large branch of bio-inspired computing
  - Inspired by flocking behaviour, not evolution
  - Steer towards personal best and global best
  - But often grouped together with EC.

Overview

1. Real-valued optimisation: big picture and applications
2. Covariance Matrix Adaptation
3. Particle Swarm Optimisation