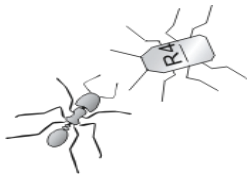
Evolutionary Strategies



Evolutionary Strategies (ES)

Rechenberg, 1973

Genetic representation = Vector of *n* real-valued numbers

Population = fixed size

μ = number of selected parents

λ = number of individuals in the population

Selection = truncated rank selection

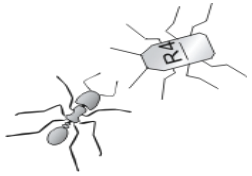
Two variants:

(μ, λ) = selected parents are replaced by their offspring

($\mu + \lambda$) = selected parents coexist with their offspring

Mutation = perturbations of all genes with normal probability density function

Crossover = not used

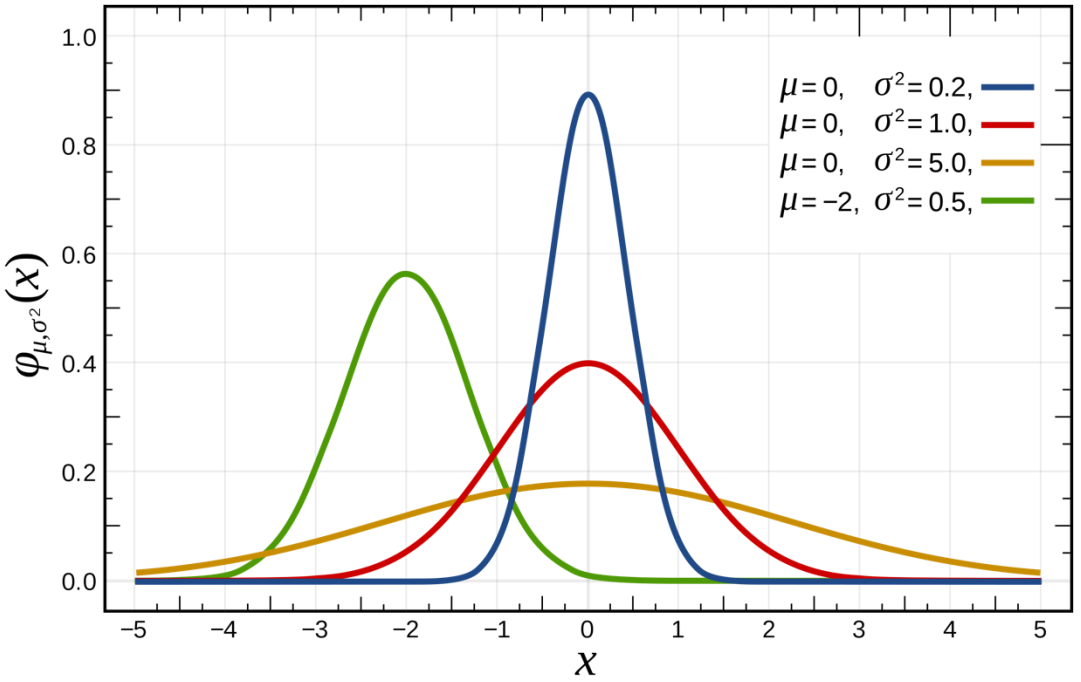


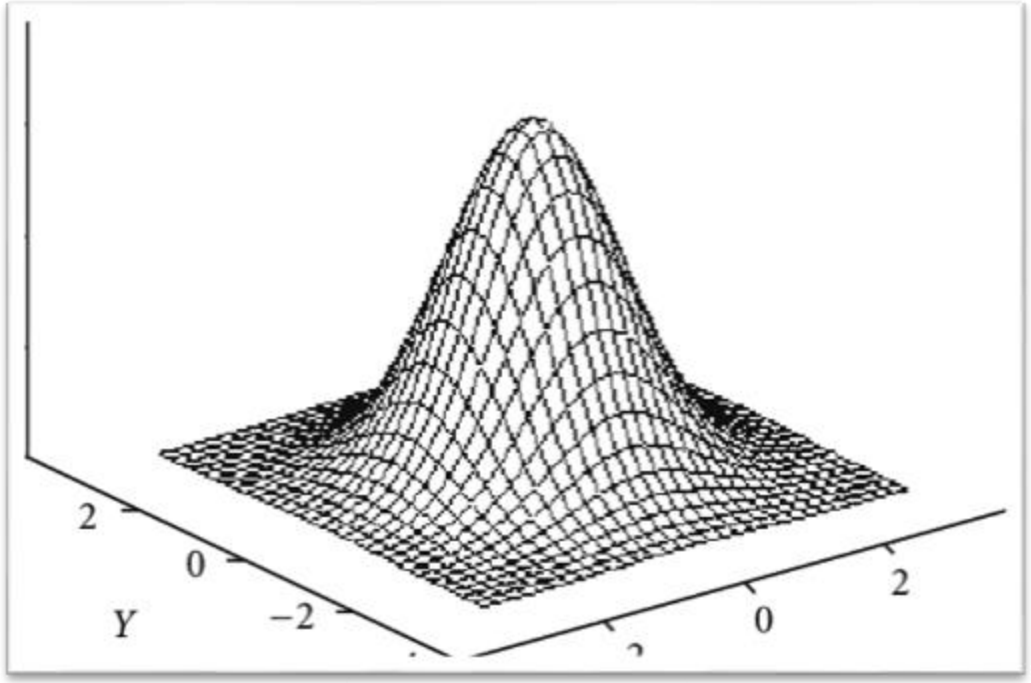
Mutations are Gaussian perturbations

Mutate each gene x by adding a number sampled from a Normal distribution N(0, σ^2)

$x' = x + N(0,\sigma^2) = x + \sigma\, N(0, 1)$

For genetic strings of length *n>1* (e.g. $\langle x_1, x_2 \rangle$), we sample the Normal distribution N(0, I), where I is the Identity Matrix



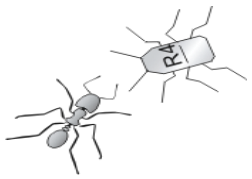


Standard deviation σ, *mutation step*, controls amount of change

ES (μ, λ) algorithm: Initialisation

1. Set up population size λ, number of parents μ, mutation step size $\boldsymbol{\sigma}$
2. Create real-valued vector **m** (also known as *population mean*)
3. Create population: generate λ offspring by adding mutations to **m**

$$\mathbf{x}_i = \mathbf{m} + \sigma\mathbf{N}_i(0, \mathbf{I}) \qquad \text{for } 0 < i \leq \lambda$$



ES (μ, λ) Algorithm: Selection and Reproduction

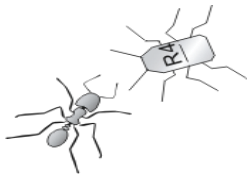
4. Evaluate λ individuals

5. Select μ parents with Truncated Rank Selection, e.g. top 25%

6. Update population mean vector **m** with *fitness-weighted* values of μ parents

   $\mathbf{m} = \sum_{i=1}^{\mu} \mathbf{w}_i \mathbf{x}_i$
   where $w_1 \geq w_2 \geq w_3 \geq w_\mu \geq 0$
   and $\sum_{i=1}^{\mu} \mathbf{w}_i = 1$

7. Go to step 3 ($\mathbf{x}_i = \mathbf{m} + \sigma \mathbf{N}_i(0, \mathbf{I})$ for $0 < i \leq \lambda$)



Co-evolution of mutation size

Mutation size σ can be added to genome of individuals and co-evolved $\langle x_1,\ldots,x_n, \sigma \rangle$

$\langle x, \sigma \rangle \rightarrow \langle x', \sigma' \rangle$

Mutation order is important…

1. $\sigma \rightarrow \sigma'$
2. $x \rightarrow x' = x + \sigma' N(0,1)$

…because quality of children $\langle x' ,\sigma' \rangle$ is evaluated twice

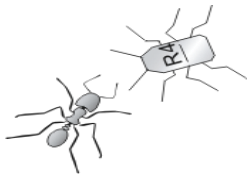
- Primary evaluation: x' is good if f(x') is good
- Secondary evaluation: σ' is good if the x' it created is good

(reversing mutation order this would not work)

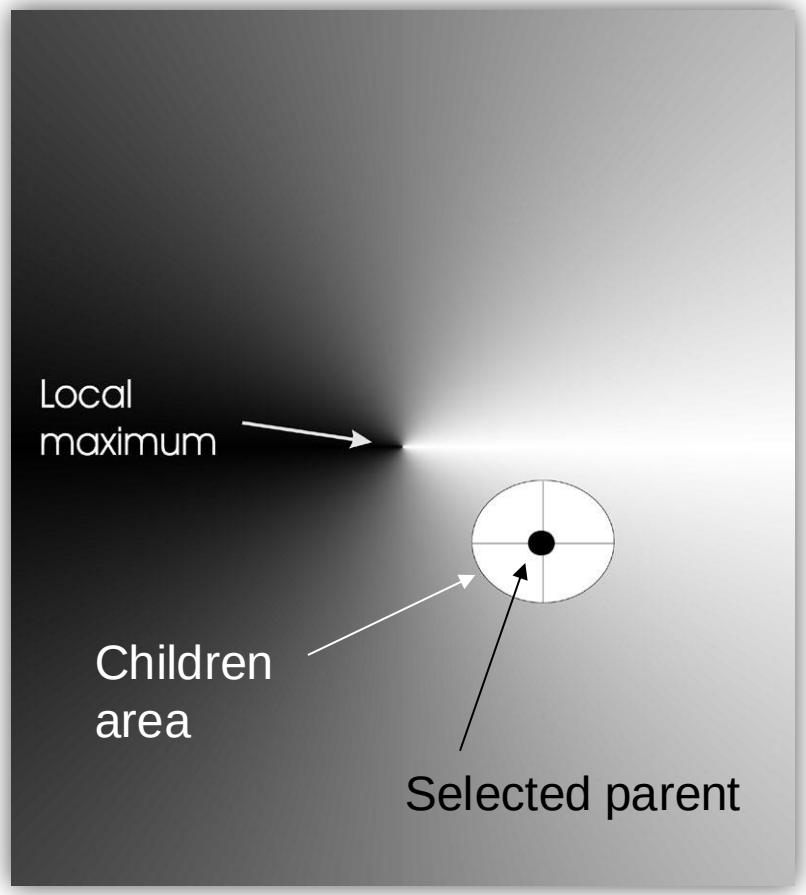
Mutations:

- $\sigma' = \sigma \bullet \exp(\tau N(0,1))$

  where $\tau \propto 1/ n^{½}$ where n = number of genes; boundary rule: if $\sigma' < \varepsilon_0 \Rightarrow \sigma' = \varepsilon_0$
- $x'_i = x_i + \sigma' N_i(0,1)$



One mutation step for all genes

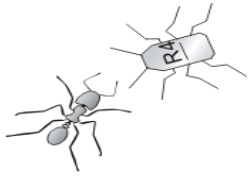


$\langle x_1, x_2, \sigma \rangle$

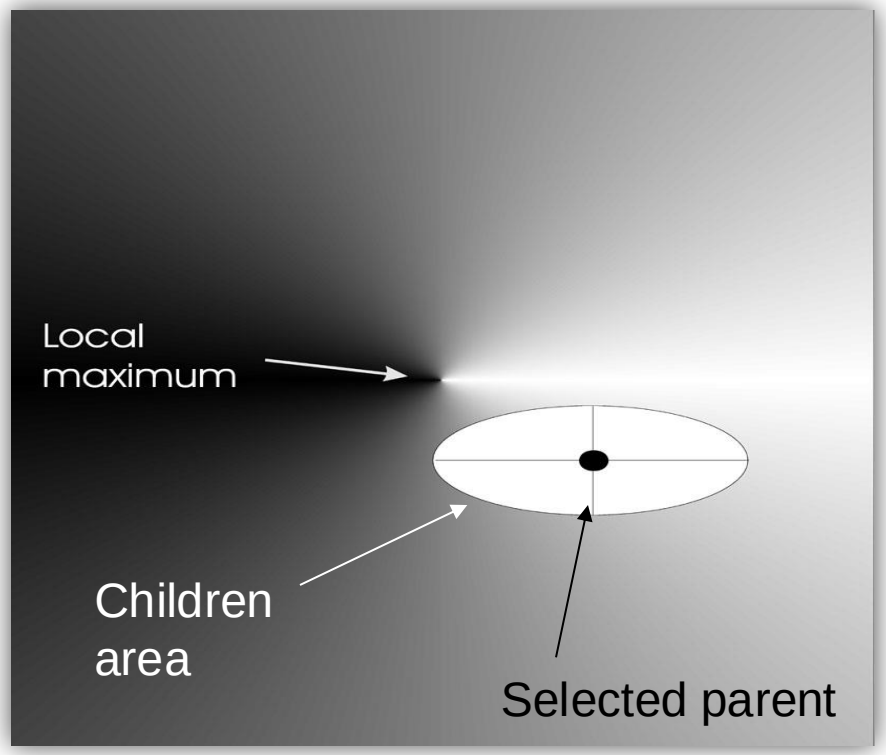
$\sigma' = \sigma \bullet \exp(\tau N(0,I))$
$x'_i = x_i + \sigma' N_i(0,I)$

where I is the Identity Matrix
where $\tau \propto 1/\sqrt{n}$
boundary rule $\sigma' < \varepsilon_0 \Rightarrow \sigma' = \varepsilon_0$

Adapted from: Eiben & Smith: http://www.evolutionarycomputation.org/slides/



Gene-wise, uncorrelated mutation steps



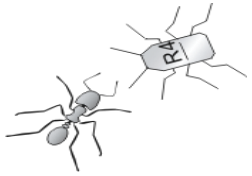
$\langle x_1, x_2, \sigma_1, \sigma_2 \rangle$

$\sigma'_i = \sigma_i \bullet \exp(\tau' N(0,1) + \tau N_i(0,1))$

$x'_i = x_i + \sigma'_i N_i(0,1)$

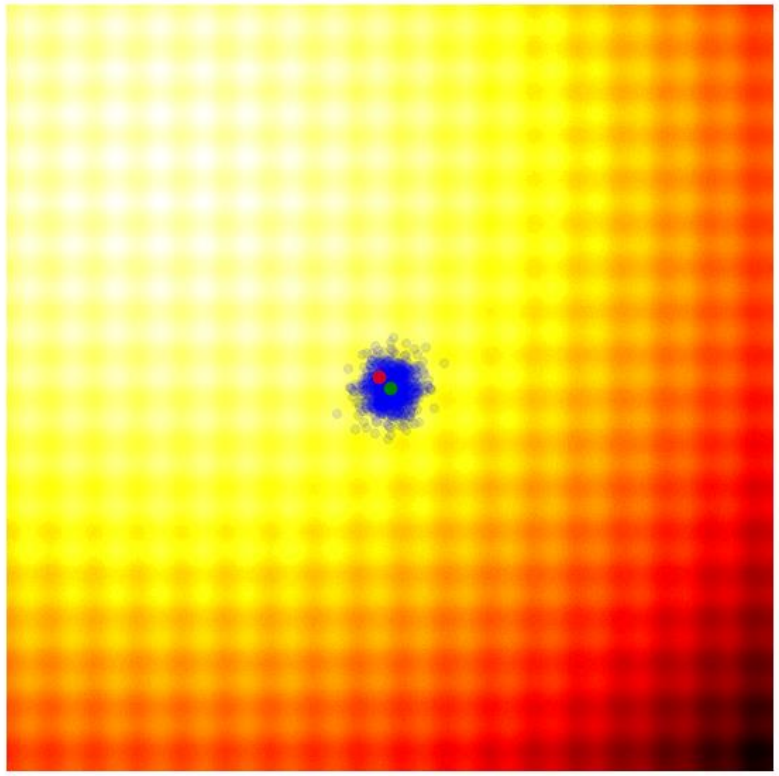
Two learning rate parameters:
τ' overall learning rate
τ gene-wise learning rate
$\tau' \propto 1/(2n)^{1/2}$ and $\tau \propto 1/(2n^{1/2})^{1/2}$
Boundary rule: $\sigma_i' < \varepsilon_0 \Rightarrow \sigma_i' = \varepsilon_0$

Adapted from: Eiben & Smith: http://www.evolutionarycomputation.org/slides/

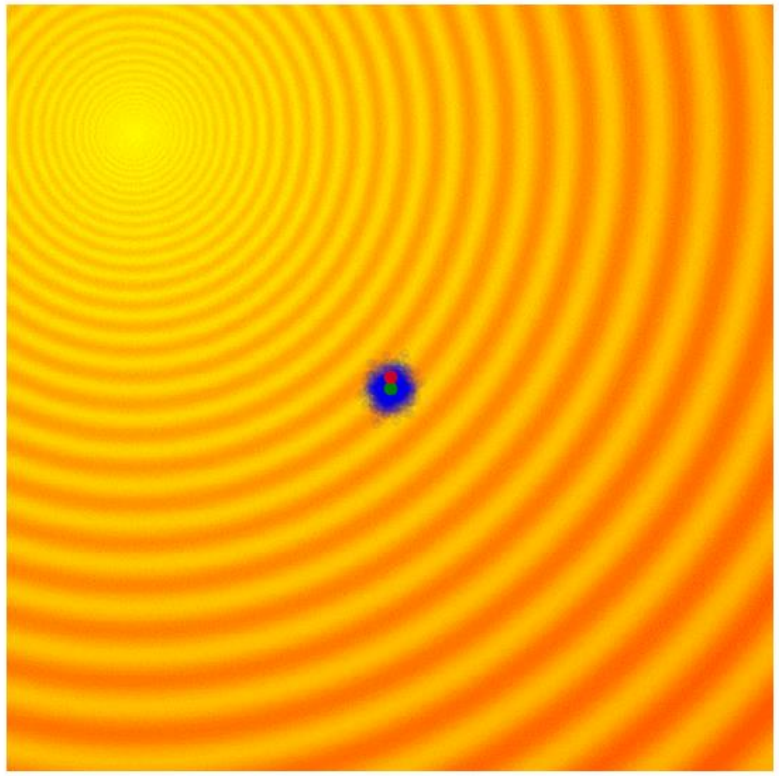


ES (μ, λ) algorithm with adaptive independent mutations

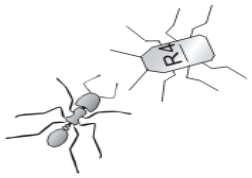
Shifted Schaffer-2D function



Shifted Rastrigin-2D function



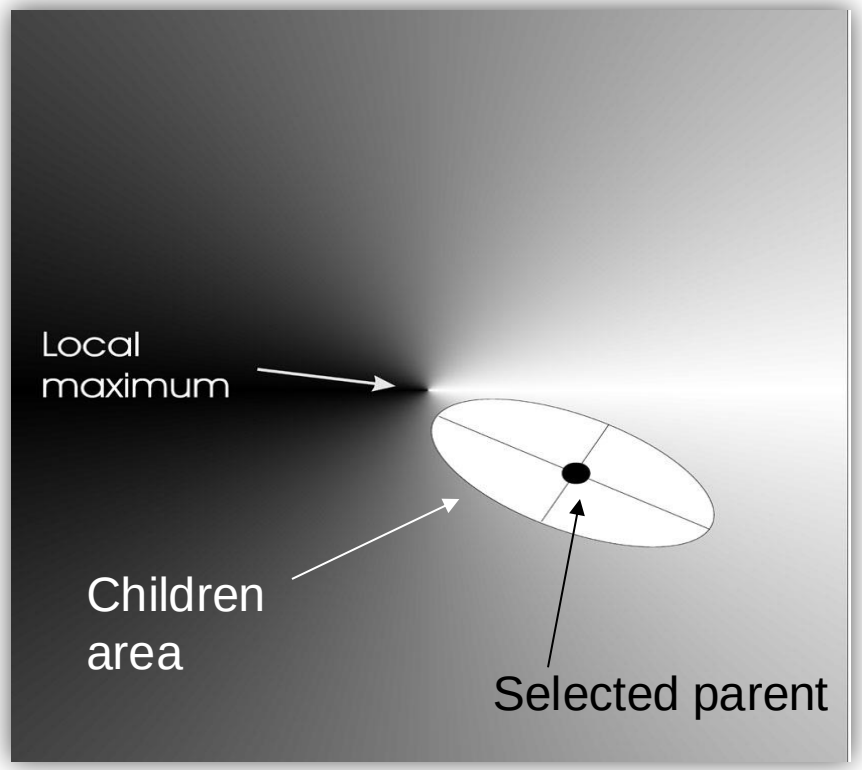
Green dot = mean solution
Blue dots = sampled solutions
Red dot = best solution



Source: http://blog.otoro.net/2017/10/29/visual-evolution-strategies/

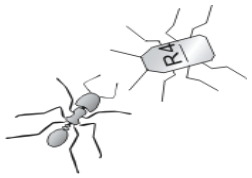
Correlated mutation steps

We want to tailor the size of each mutation in order to move each individual in the direction of the estimated gradient of the fitness distribution of the population



This can be done by using the Covariance matrix of the population instead of the Identity matrix to sample the mutation vector of each individual

Adapted from: Eiben & Smith: http://www.evolutionarycomputation.org/slides/

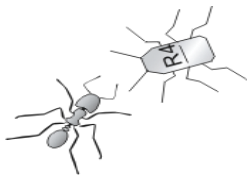


A reminder: Variance and Covariance

$$var(X) = \frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^2$$, $\bar{X}$ is the mean of the samples of X

$$covar(X,Y) = \frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})$$

$$covar(X,X) = var(X)$$

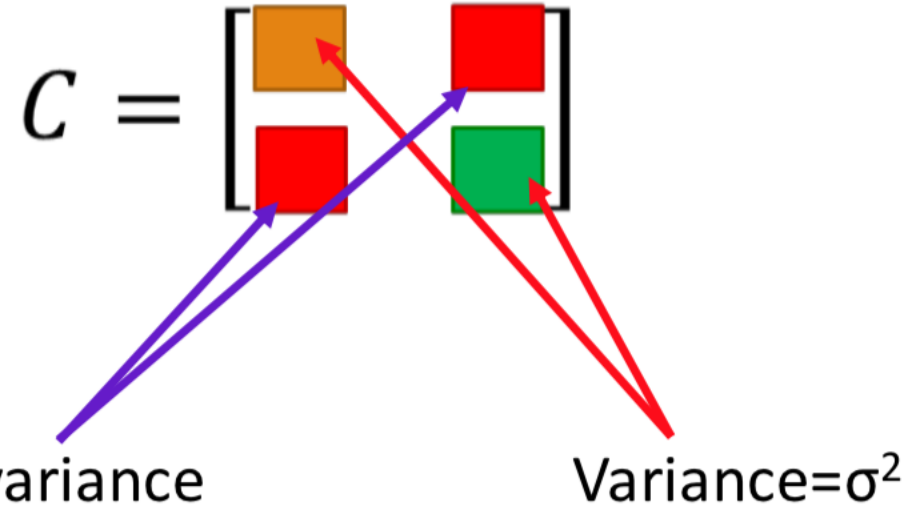


Covariance Matrix

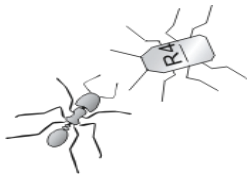
A Covariance Matrix is the matrix whose (ij) element is the covariance between the i and the j element of the data distribution.

For a distribution with two dimensions A (gene x) and B (gene y):

$$\begin{pmatrix} cov(A,A) & cov(A,B) \\ cov(B,A) & cov(B,B) \end{pmatrix} = \begin{pmatrix} var(A) & cov(A,B) \\ cov(B,A) & var(B) \end{pmatrix}$$

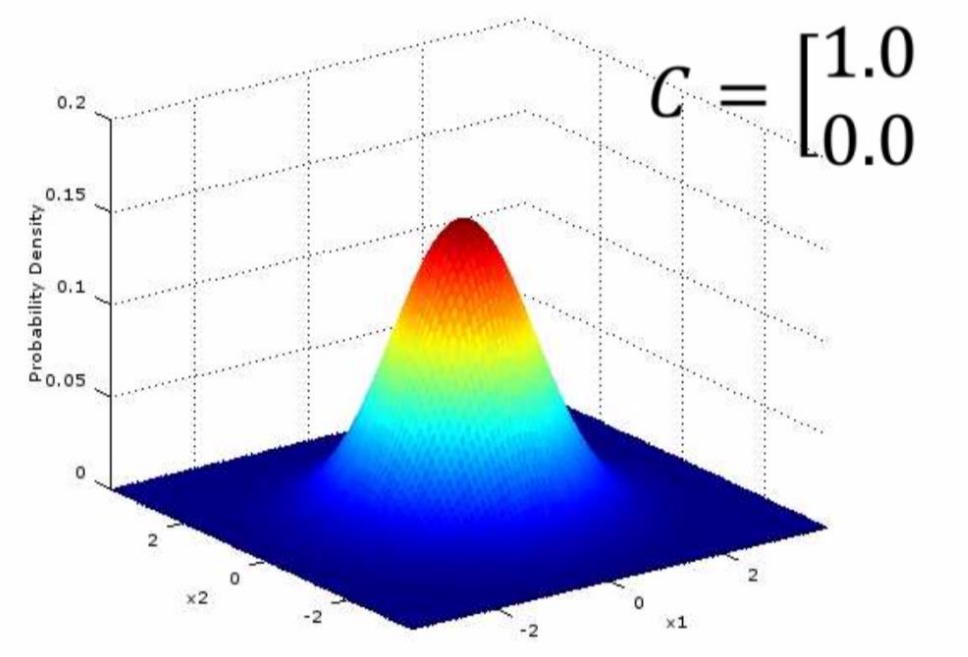


Adapted from: https://www.slideshare.net/OsamaSalaheldin2/cmaes-presentation

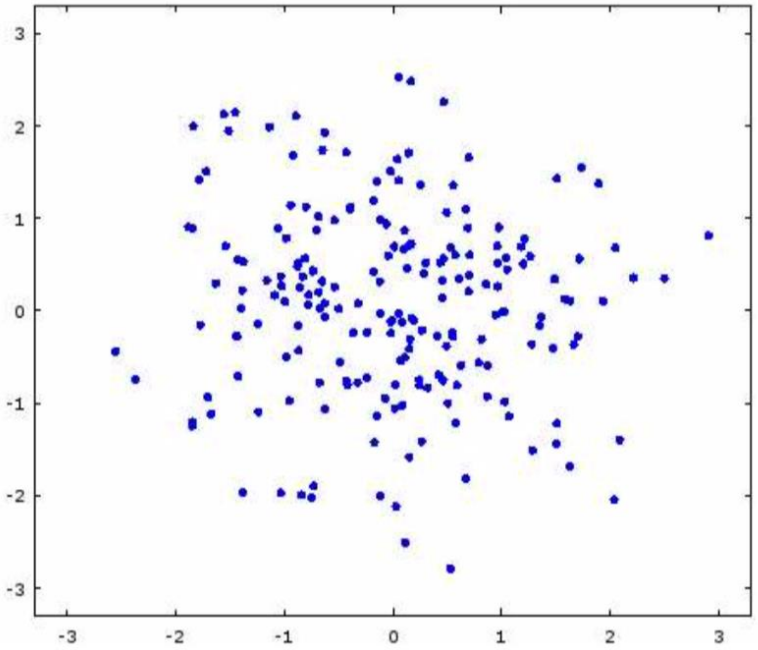


Covariance Matrix of variables that don't covary with equal variance

If two elements x, y do not covary and normally distributed, the covariance matrix is equivalent to σ N(0, I)



$$C = \begin{bmatrix} 1.0 & 0.0 \\ 0.0 & 1.0 \end{bmatrix}$$



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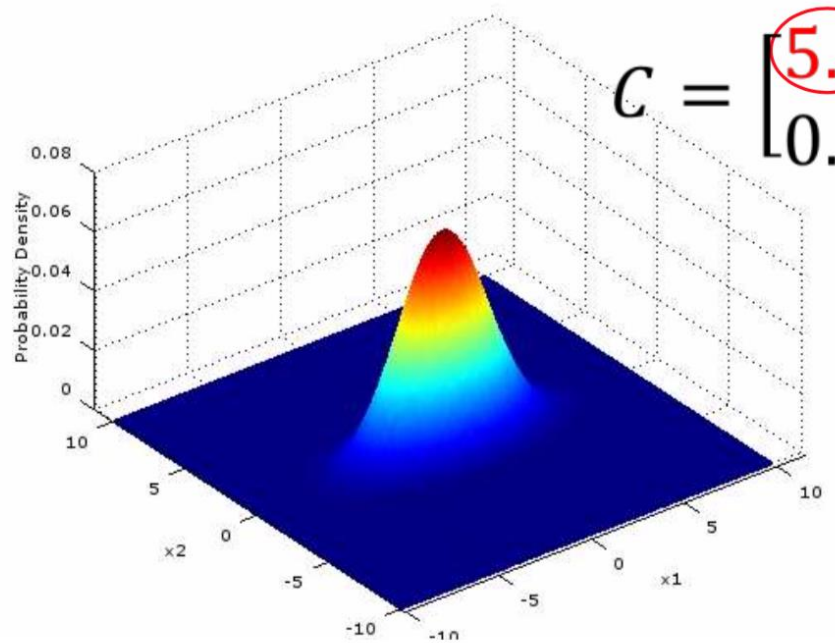
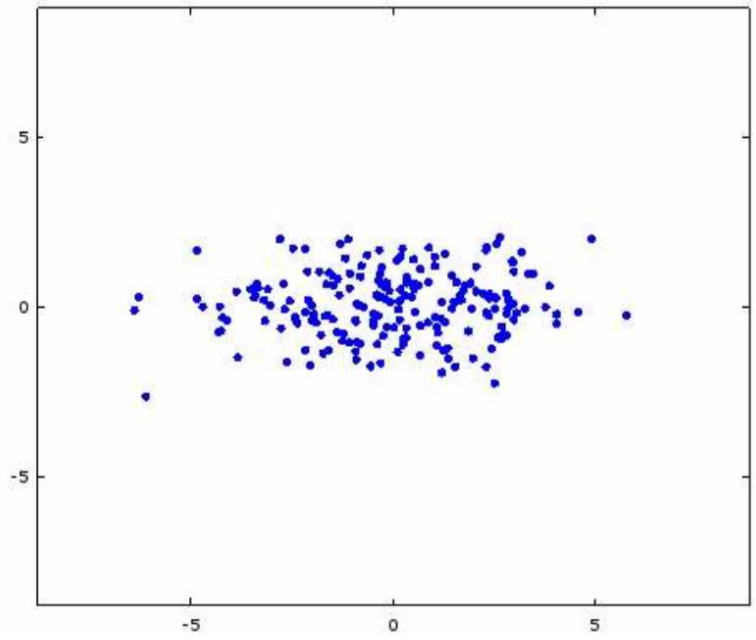
Covariance Matrix of variables that don't covary with different variance

If the two elements x, y do not covary, but x has larger variance

$$C = \begin{bmatrix} 5.0 & 0.0 \\ 0.0 & 1.0 \end{bmatrix}$$





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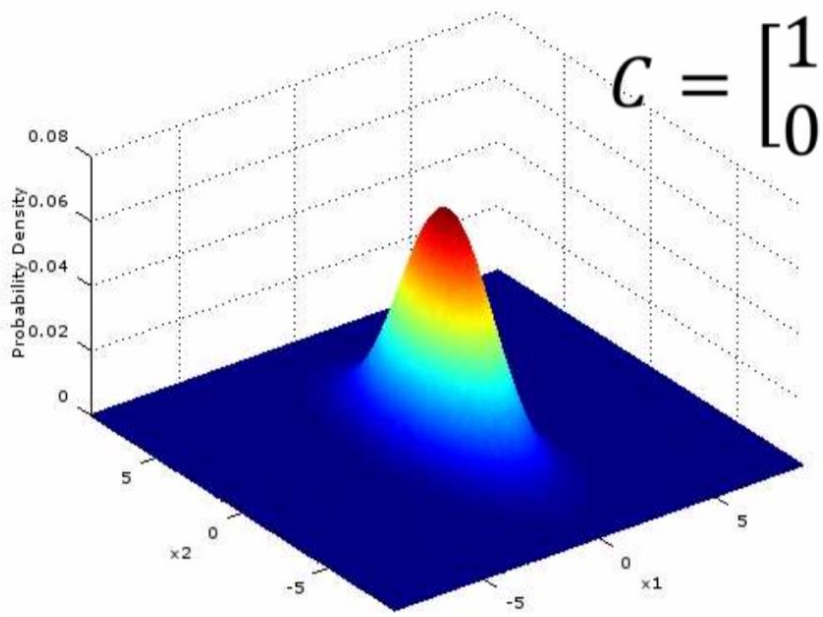
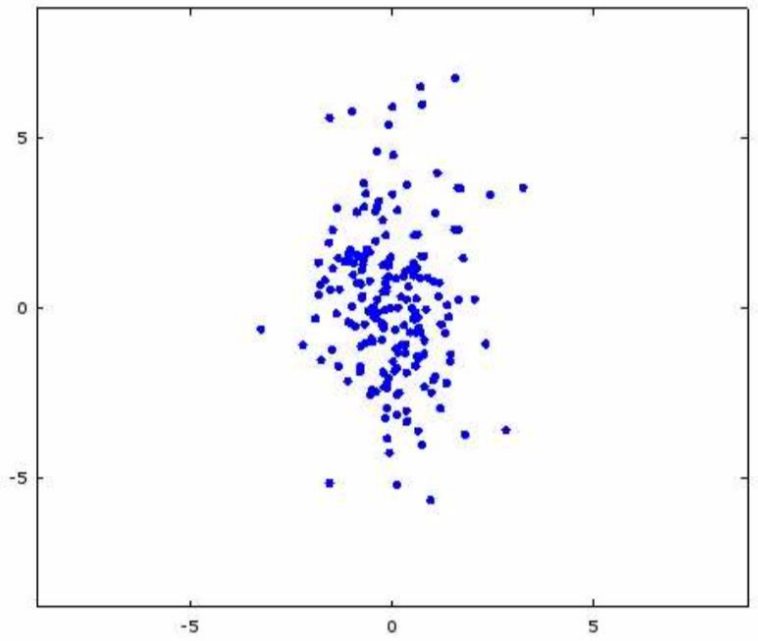
Covariance Matrix of variables that don't covary with different variance

If the two elements x, y do not covary, but y has larger variance

$$C = \begin{bmatrix} 1.0 & 0.0 \\ 0.0 & 5.0 \end{bmatrix}$$





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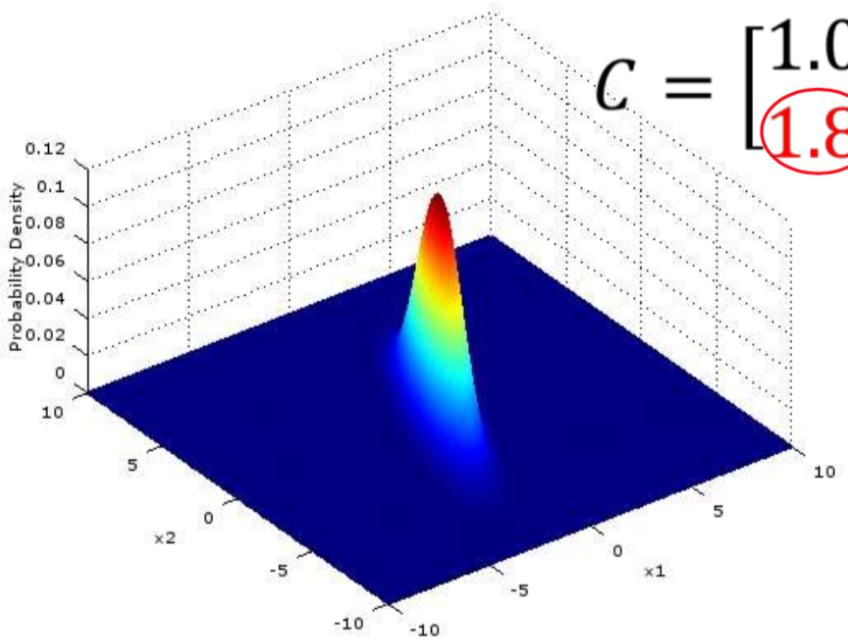
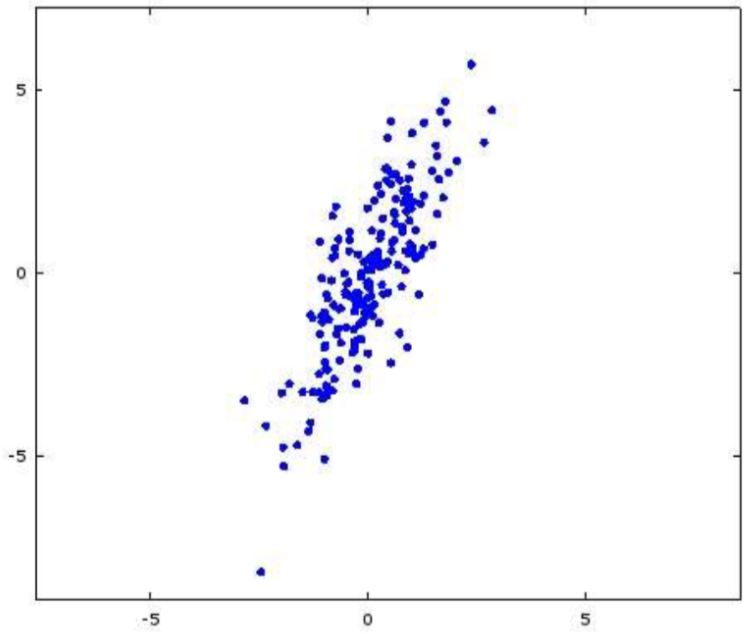
Covariance Matrix of variables that covary with different variance

If the two elements x, y covary, and y has larger variance

$$C = \begin{bmatrix} 1.0 & 1.8 \\ 1.8 & 5.0 \end{bmatrix}$$





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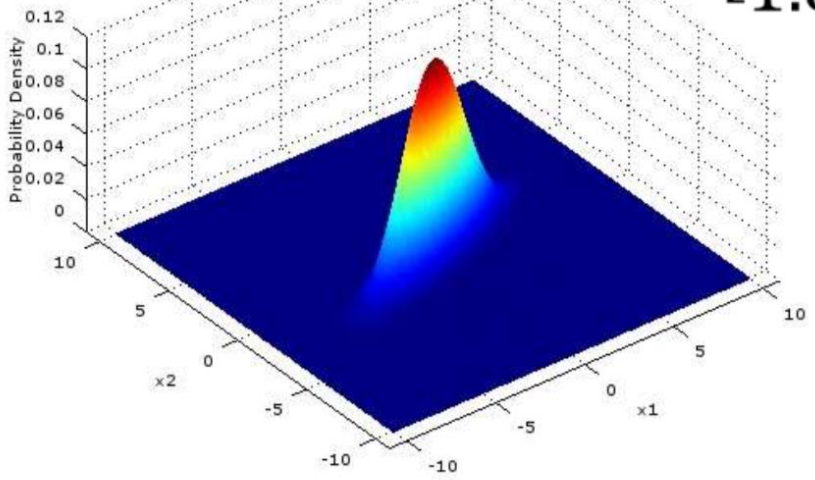
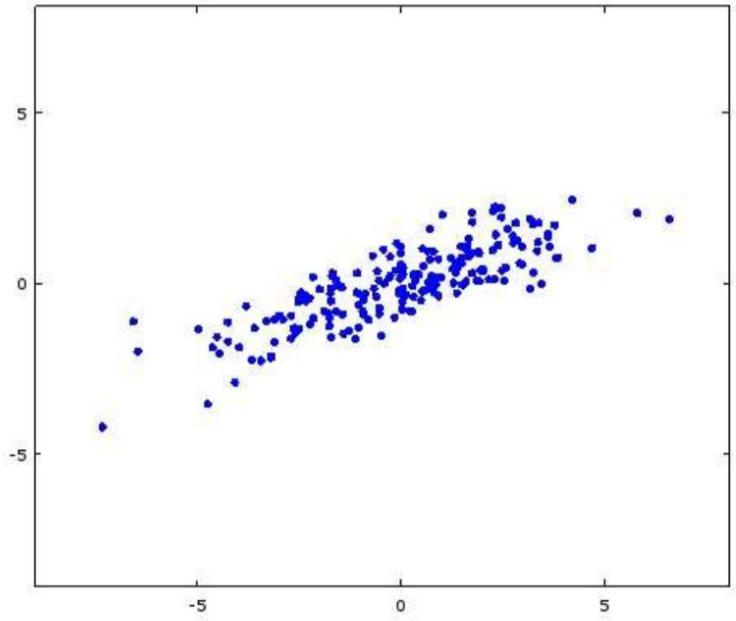
Covariance Matrix of variables that covary with different variance

If the two elements x, y covary, and x has larger variance

$$C = \begin{bmatrix} 5.0 & 1.8 \\ 1.8 & 1.0 \end{bmatrix}$$





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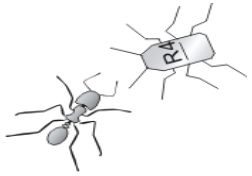
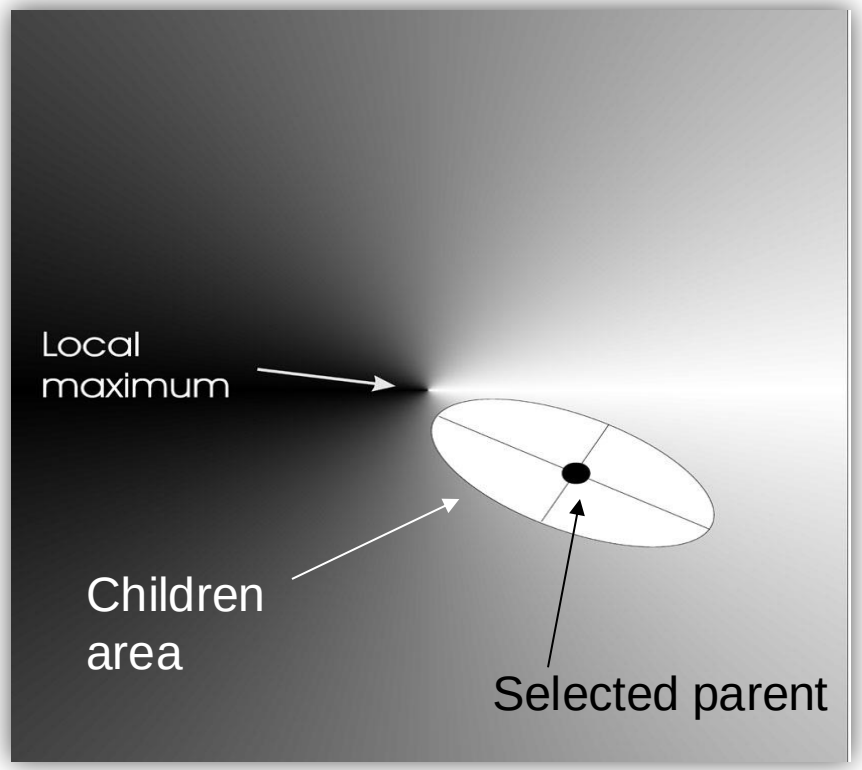
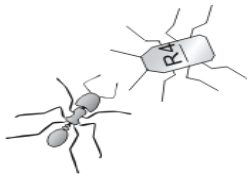


Covariance Matrix Adaptation ES (CMA-ES)

Take larger steps in the direction of highest variance, i.e. the population should move faster in the direction of the eigenvalue corresponding to the largest eigenvector of the covariance matrix of the fitness distribution of the current population



Hansen N, Ostermeier A (2001). *Evolutionary Computation*, **9**(2), 159–195.

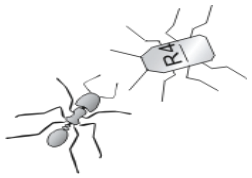


CMA-ES Algorithm: Initialise population

1. Initialise Covariance Matrix **C** as n x n Identity Matrix
2. Set up individual **m** (e.g., solution guess or at the distribution center)
3. Set up initial mutation step size vector σ
4. Generate λ offspring from **m**

$$\mathbf{x}_i = \mathbf{m} + \mathbf{N}_i(\sigma^2, \mathbf{C}) \qquad \text{for } 0< i \leq \lambda$$

notice that **m** represents an estimate of the population mean



CMA-ES Algorithm: Selection and Reproduction

5. Evaluate λ individuals of the population

6. Identify μ parents with Truncated Rank Selection, e.g. top 25%

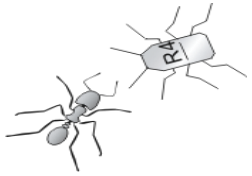
7. Update population mean using weighted values of μ parents

   $\mathbf{m} = \sum_{i=1}^{\mu} \mathbf{w}_i \mathbf{x}_i$
   where $w_1 \geq w_2 \geq w_3 \geq w_\mu \geq 0$
   and $\sum_{i=1}^{\mu} \mathbf{w}_i = 1$

5. Update **C** covariance matrix with new **C** computed for **m** distribution

6. Adapt mutation step size vector $\boldsymbol{\sigma}$

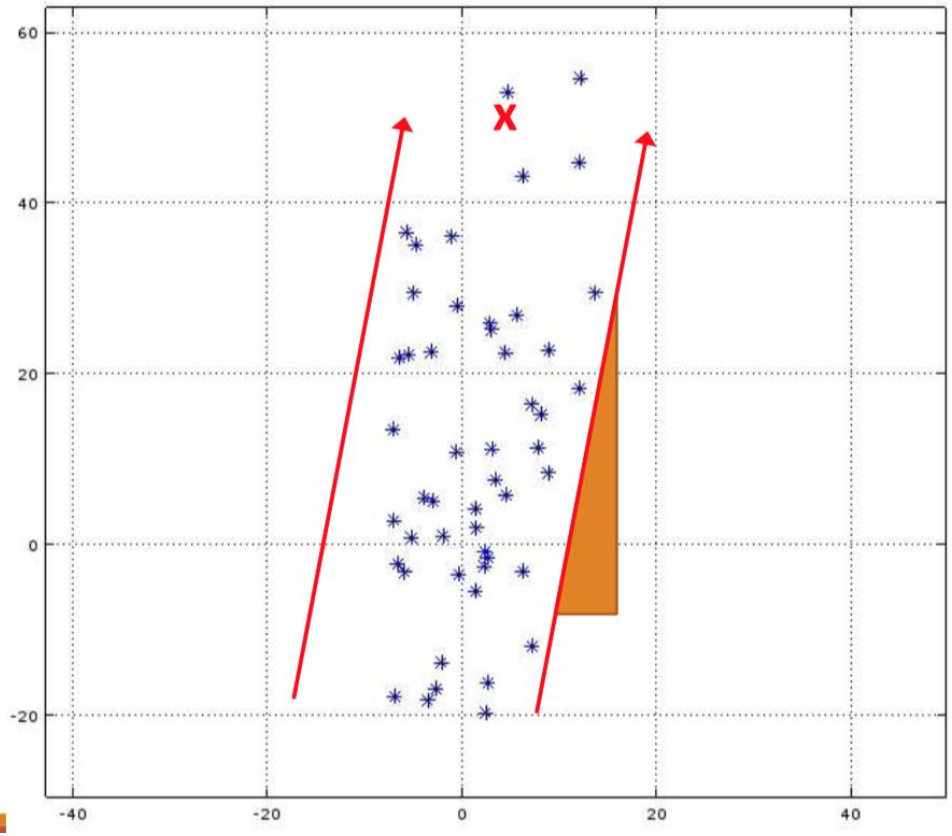
7. Go to step 4 ($\mathbf{x}_i = \mathbf{m} + \mathbf{N}_i(\sigma^2, \mathbf{C})$ for $0< i \leq \lambda$)



An example of CMA-ES at work

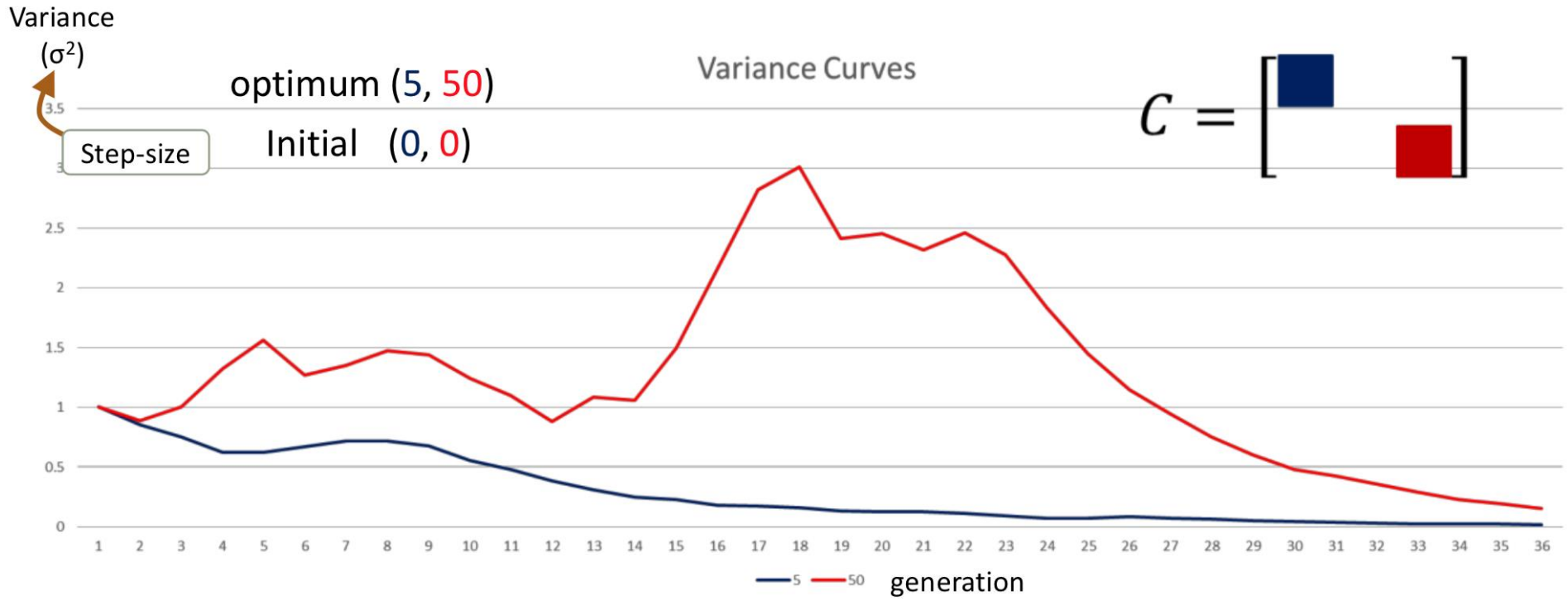
- A practical run of CMA-ES
  - The optimum solution is (5, 50)
  - The initial guess is (0, 0)
  - The population moves faster towards the direction of the second component (50)

$$C = \begin{bmatrix} 1.4011 & 2.0368 \\ 2.0368 & 11.8843 \end{bmatrix}$$



Source: https://www.slideshare.net/OsamaSalaheldin2/cmaes-presentation

An example of CMA-ES at work



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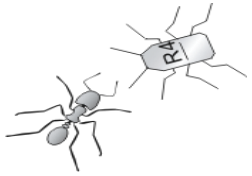
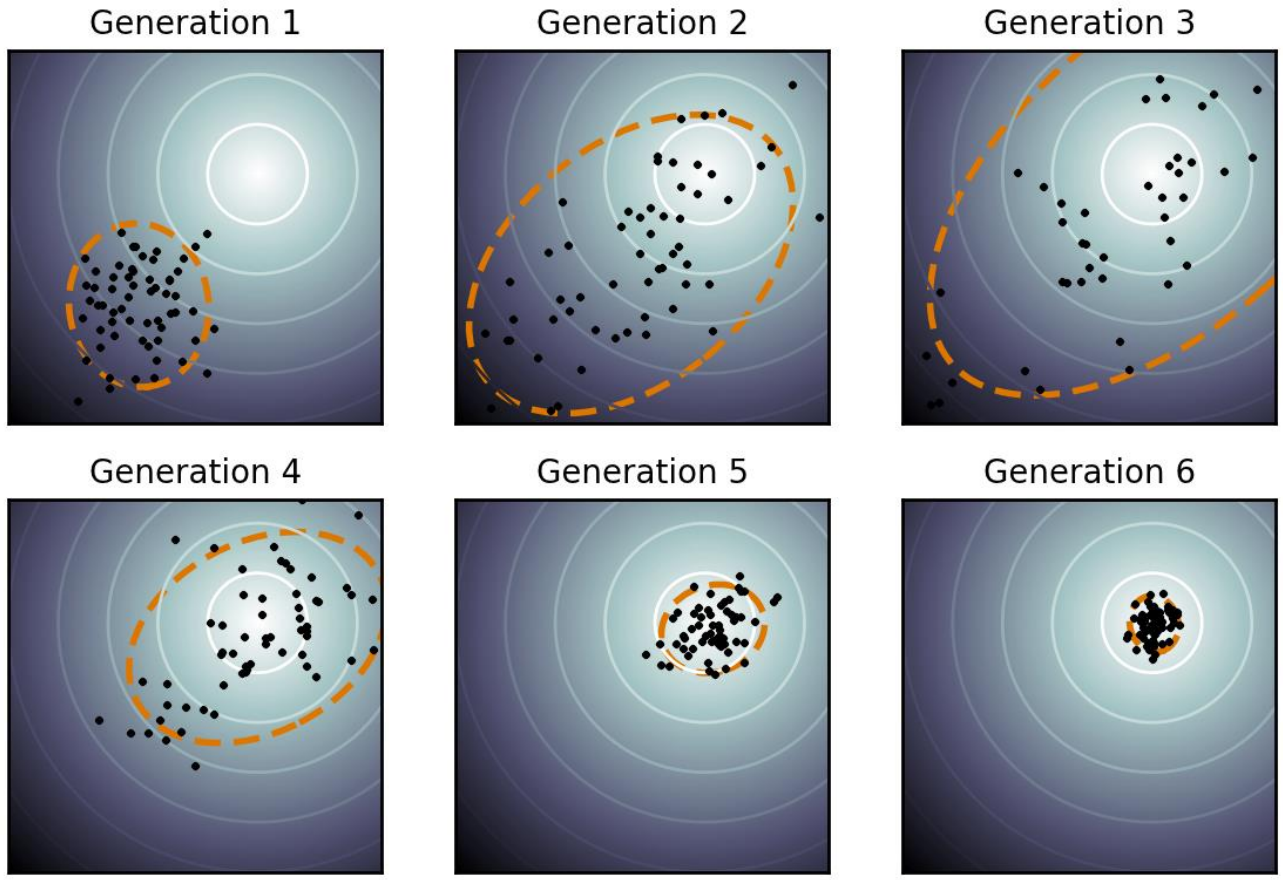
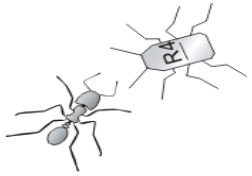


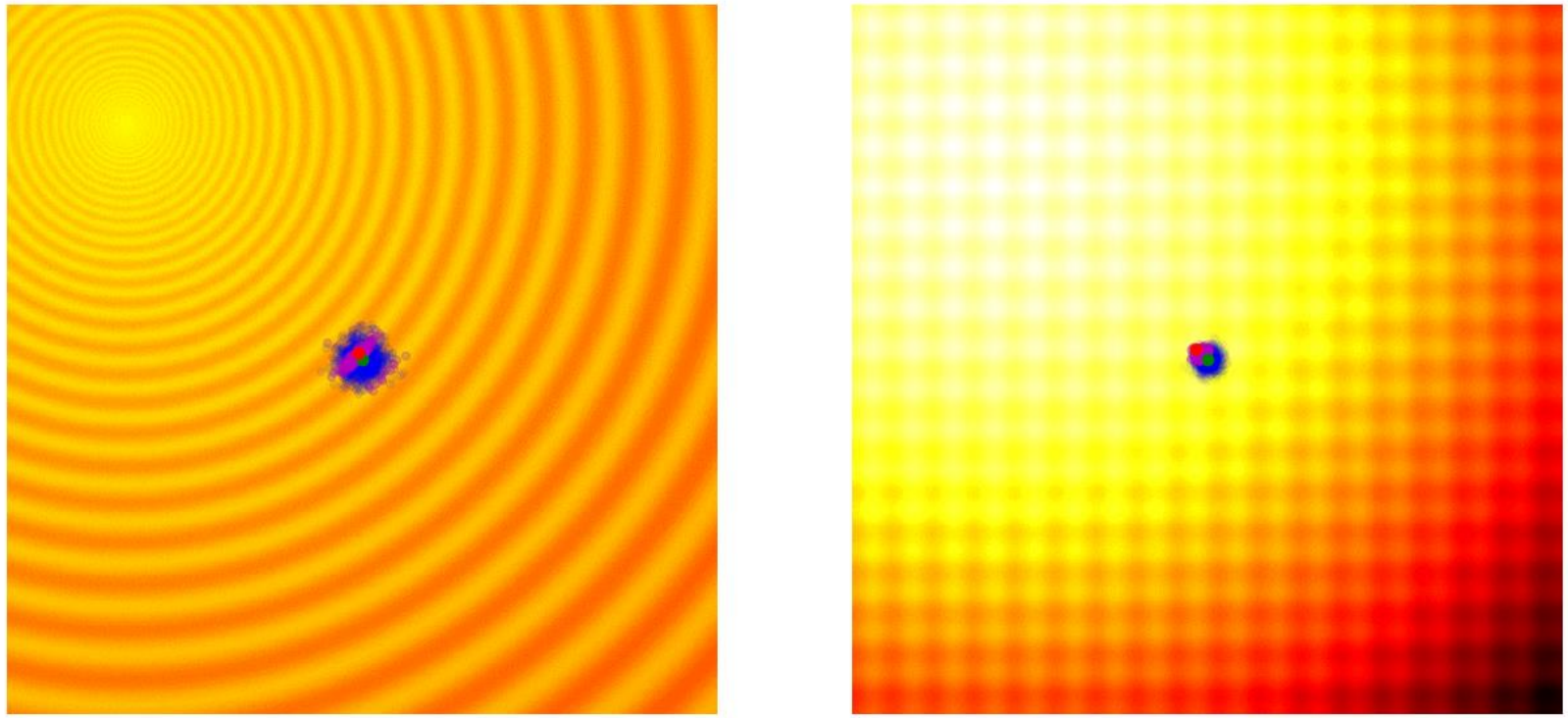
CMA-ES at work



- Full details of **C** and σ updates: https://arxiv.org/abs/1604.00772
- Computer code: https://github.com/CMA-ES



CMA-ES adapts direction and spread



CMA-ES is currently the most powerful evolutionary algorithm for real-value optimization, but for >10K variables it becomes computationally very expensive

Source: http://blog.otoro.net/2017/10/29/visual-evolution-strategies/