Introduction to Metaheuristics
Estimation of Distribution

DrC. Alejandro Piad Morffis

Review: The metaheuristic framework

- given a black box function F
- define stop criteria
- while not stop do:
    - generate a new solution x_i (or many)
    - evaluate $y_i = F(x_i)$
    - update global best $y^* \leftarrow \min\{y^*, y_i\}$
    - learn something about F for next iteration (maybe)
- return global best y^*

Review: What can we learn…

- **… in local search?:**

Every metaheuristic learns some implicit **model** of the function to guide the search.

Can we make that model explicit?

Review: What can we learn...

- **... in local search?:**
  - Gradients

Every metaheuristic learns some implicit **model** of the function to guide the search.

Can we make that model explicit?

Review: What can we learn. . .

- **. . . in local search?:**
  - Gradients
  - Features of local optima

Every metaheuristic learns some implicit **model** of the function to guide the search.

Can we make that model explicit?

Review: What can we learn. . .

- **. . . in local search?:**
  - Gradients
  - Features of local optima
- **. . . in evolutionary search:?**

Every metaheuristic learns some implicit **model** of the function to guide the search.

Can we make that model explicit?

Review: What can we learn...

- **... in local search?:**
  - Gradients
  - Features of local optima
- **... in evolutionary search:?**
  - Components of good solutions

Every metaheuristic learns some implicit **model** of the function to guide the search.

Can we make that model explicit?

Review: What can we learn...

- **... in local search?:**
  - Gradients
  - Features of local optima
- **... in evolutionary search:?**
  - Components of good solutions
- **... in swarm optimization:?**

Every metaheuristic learns some implicit **model** of the function to guide the search.

Can we make that model explicit?

Review: What can we learn...

- **... in local search?:**
  - Gradients
  - Features of local optima
- **... in evolutionary search:?**
  - Components of good solutions
- **... in swarm optimization:?**
  - Features of the global landscape

Every metaheuristic learns some implicit **model** of the function to guide the search.

Can we make that model explicit?

Review: What can we learn...

- **... in local search?:**
  - Gradients
  - Features of local optima
- **... in evolutionary search:?**
  - Components of good solutions
- **... in swarm optimization:?**
  - Features of the global landscape
  - Features of local optima

Every metaheuristic learns some implicit **model** of the function to guide the search.

Can we make that model explicit?

Estimation of Distribution Algorithms

- given a black box function F
- **initialize** probabilistic model $\mathfrak{F}$
- define stop criteria
- while not stop do:
  - **sample** N new solutions $\{x_i\}$ from $\mathfrak{F}$
  - evaluate $\{y\}_i = \{F(x_i)\}$
  - update global best $y^* \leftarrow \min\{y^*, y_i ...\}$
  - **update** model $\mathfrak{F}$ for next iteration
- return global best y^*

Different EDAs differ in the selection of the model $\mathfrak{F}$

Types of models

What does the model estimates:

(The distribution of):

- the global optimum
- the local optima
- the best features
- fitness values
- ...

Types of models

What does the model estimates:

(The distribution of):

- the global optimum
- the local optima
- the best features
- fitness values
- ...

What assumptions the model encodes:

- Are components correlated?
- ...

PBIL: Genetic algorithms turn EDAs

Assuming the simplest possible model

PBIL: Genetic algorithms turn EDAs

Assuming the simplest possible model

- A fixed set of binary components i
- A binomial distribution for each component p_i
- Components are independent

PBIL: Genetic algorithms turn EDAs

Assuming the simplest possible model

- A fixed set of binary components i
- A binomial distribution for each component p_i
- Components are independent

Sample:

- For each component i, set $x_i = U(0,1) < p_i$

Update rule:

- For each component i:
  - compare solutions where $x_i = 0$ vs $x_i = 1$
  - if most solutions where $x_i = 0$ are better, decrease p_i
  - else, increase p_i

PBIL: Genetic algorithms turn EDAs

Some implementation details:

- Use a learning rate $r << 1$
- Adjust learning rate to balance exploration/exploitation

PBIL: Genetic algorithms turn EDAs

Some implementation details:

- Use a learning rate $r << 1$
- Adjust learning rate to balance exploration/exploitation

Extension to categorical distributions

- For each component i:
  - For each value b_{ij},
  - Compute all solutions where $x_i = b_{ij}$
  - Increase p_{ij} proportional to their fitness
- Renormalize probabilities

PBIL: Genetic algorithms turn EDAs

Some implementation details:

- Use a learning rate $r << 1$
- Adjust learning rate to balance exploration/exploitation

Extension to categorical distributions

- For each component i:
  - For each value b_{ij},
  - Compute all solutions where $x_i = b_{ij}$
  - Increase p_{ij} proportional to their fitness
- Renormalize probabilities

Alternative formulation:

- Compute marginal distribution from K best solutions
- Interpolate model using learning rate

UMDA: Moving to continuous spaces

Model:

- Each component is a normal distribution $N(\mu_i, \sigma_i)$
- Start with large σ values

Update rule:

- Computer marginal distribution of best solutions
- Compute μ_b, σ_b
- Interpolate

Removing the independence constraint

Instead of N independent Gaussian univariate distributions, use a multivariate distribution

- A vector $\vee$ of μ_i means
- A matrix Σ of σ_{ij} covariance pairs

Update rule:

- Keep the best $M < N$ solutions
- Update mean
- Update covariance matrix on solution pairs

Better idea: **CMA-ES**

CMA-ES

Updating the covariance matrix w.r.t. solutions naively is suboptimal. (Why?)

CMA-ES

Updating the covariance matrix w.r.t. solutions naively is suboptimal. (Why?)

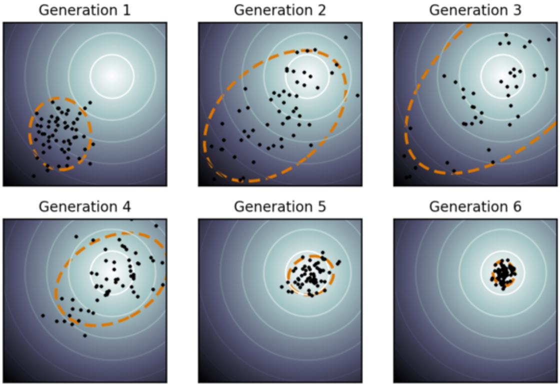
CMA-ES updates the covariance matrix such that it produces new solutions in the **direction of the best search steps** seen so far.

Details are involved:

- Compute incremental evolution path: *If the mean moves in a similar direction, the path length increases.*
- Update step-size σ in a similar way.
- Compute covariance matrix.

CMA-ES

Adapts much quicker to the function landscape.



State-of-the-art in continuous optimization.

Towards general-purpose domains

What happens when the domain is too complex?:

- Continuous and discrete parameters
- Conditional parameters (hierarchical)

Example: Optimizing in the space of computer programs.

- Analytic regression
- Compiler optimization
- AutoML

Towards general-purpose domains

What happens when the domain is too complex?:

- Continuous and discrete parameters
- Conditional parameters (hierarchical)

Example: Optimizing in the space of computer programs.

- Analytic regression
- Compiler optimization
- AutoML

Define the search space with a probabilistic grammar

Probabilistic Grammatical Evolution

Model:

- Associate probabilities to grammar productions
- Sample in DFS order

Update rule:

- Select $K < N$ best solutions
- Compute marginal probability of used productions
- Update model by interpolation

What is the fundamental problem with PGE?

You have to evaluate many solutions for a single model update. For e.g., AutoML, this can be prohitive.

Bayesian Optimization

Can we estimate with a single solution?

Bayesian Optimization

Can we estimate with a single solution?

- Assume F can be approximated by, e.g., a mixture of Gaussians
- Bake uncertainty into the sampling process

Bayesian Optimization

Can we estimate with a single solution?

- Assume F can be approximated by, e.g., a mixture of Gaussians
- Bake uncertainty into the sampling process

Update rule:

- Build $\mathfrak{F}$ from previous evaluations
- Construct **acquisition function** G
- Find global optimum in G

Examples of acquisition functions:

- Probability of improvement
- Expected improvement
- Confidence bounds
- ...

Some conclusions

Why estimation of distribution works:

- EDAs are some of the most robust optimization strategies
- Easy to incorporate domain knowledge (e.g., what general shape you expect the function to have)
- Some empirical and formal convergence guarantees

Other considerations:

- PBIL / UMDA are simple and good enough for most cases.
- Bayesian Optimization is the fastest when F is very costly.
- **Do not** reimplement CMA-ES! Use a library instead.
- PGE is Turing-complete :)

Time to practice!