

Stochastic Optimization

Marc Schoenauer



DataScience @ LHC Workshop 2015



Content

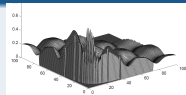
- 1 Setting the scene
- 2 Continuous Optimization
- 3 Discrete/Combinatorial Optimization
- 4 Non-Parametric Representations
- 5 Conclusion

- 1 Setting the scene
- 2 Continuous Optimization
- 3 Discrete/Combinatorial Optimization
- 4 Non-Parametric Representations
- 5 Conclusion

Stochastic Optimization

Hypotheses

- Search Space Ω with some topological structure
- Objective function \mathcal{F} assume some weak regularity



Hill-Climbing

- Randomly draw $x_0 \in \Omega$ and compute $\mathcal{F}(x_0)$ Initialisation
- Until(happy)
 - $y = \text{Best neighbor}(x_t)$ neighbor structure on Ω
 - Compute $\mathcal{F}(y)$
 - If $\mathcal{F}(y) \succ \mathcal{F}(x_t)$ then $x_{t+1} = y$ accept if improvement
else $x_{t+1} = x_t$

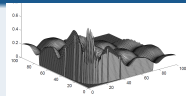
Comments

- Find *closest* local optimum defined by neighborhood structure
- Iterate from different x_0 's Until(very happy)

Stochastic Optimization

Hypotheses

- Search Space Ω with some topological structure
- Objective function \mathcal{F} assume some weak regularity



Stochastic (Local) Search

- Randomly draw $\mathbf{x}_0 \in \Omega$ and compute $\mathcal{F}(\mathbf{x}_0)$ Initialisation
- Until(happy)
 - $\mathbf{y} = \text{Random neighbor}(\mathbf{x}_t)$ neighbor structure on Ω
 - Compute $\mathcal{F}(\mathbf{y})$
 - If $\mathcal{F}(\mathbf{y}) \succ \mathcal{F}(\mathbf{x}_t)$ then $\mathbf{x}_{t+1} = \mathbf{y}$ accept if improvement
else $\mathbf{x}_{t+1} = \mathbf{x}_t$

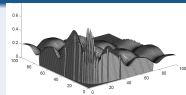
Comments

- Find one *close* local optimum defined by neighborhood structure
- Iterate, leaving current optimum Iterated Local Search

Stochastic Optimization

Hypotheses

- Search Space Ω with some topological structure
- Objective function \mathcal{F} assume some weak regularity



Stochastic (Local) Search – alternative viewpoint

- Randomly draw $\mathbf{x}_0 \in \Omega$ and compute $\mathcal{F}(\mathbf{x}_0)$ Initialisation
- Until(happy)
 - $\mathbf{y} = \text{Move}(\mathbf{x}_t)$ stochastic variation on Ω
 - Compute $\mathcal{F}(\mathbf{y})$
 - If $\mathcal{F}(\mathbf{y}) \succ \mathcal{F}(\mathbf{x}_t)$ then $\mathbf{x}_{t+1} = \mathbf{y}$ accept if improvement
else $\mathbf{x}_{t+1} = \mathbf{x}_t$

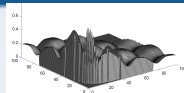
Comments

- Find one *close* local optimum defined by the Move operator
- Iterate, leaving current optimum Iterated Local Search

Stochastic Optimization

Hypotheses

- Search Space Ω with some topological structure
- Objective function \mathcal{F} assume some weak regularity



Stochastic Search

aka Metaheuristics

- Randomly draw $x_0 \in \Omega$ and compute $\mathcal{F}(x_0)$ Initialisation
- Until(happy)
 - $y = \text{Move}(x_t)$ stochastic variation on Ω
 - Compute $\mathcal{F}(y)$
 - $x_{t+1} = \text{Select}(x_t, y)$ stochastic selection, biased toward better points

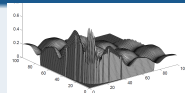
Comments

- Can escape local optima e.g., **Select** = Boltzman selection
- Iterate ?

Stochastic Optimization

Hypotheses

- Search Space Ω with some topological structure
- Objective function \mathcal{F} assume some weak regularity



Population-based Metaheuristics

- Randomly draw $\mathbf{x}_0^i \in \Omega$ and compute $\mathcal{F}(\mathbf{x}_0^i)$, $i = 1, \dots, \mu$ Initialisation
- Until(happy)
 - $\mathbf{y}^i = \text{Move}(\mathbf{x}_t^1, \dots, \mathbf{x}_t^\mu)$, $i = 1, \dots, \lambda$ stochastic variations on Ω
 - Compute $\mathcal{F}(\mathbf{y}^i)$, $i = 1, \dots, \lambda$
 - $(\mathbf{x}_{t+1}^1, \dots, \mathbf{x}_{t+1}^\mu) = \text{Select}(\mathbf{x}_t^1, \dots, \mathbf{x}_t^\mu, \mathbf{y}^1, \dots, \mathbf{y}^\lambda)$ $(\mu + \lambda)$ selection
= $\text{Select}(\mathbf{y}^1, \dots, \mathbf{y}^\lambda)$ (μ, λ) selection

Evolutionary Metaphor: 'natural' selection and 'blind' variations

- $\mathbf{y}^i = \text{Move}_m(\mathbf{x}_t^i)$ for some i : mutation
- $\mathbf{y}^i = \text{Move}_c(\mathbf{x}_t^i, \mathbf{x}_t^j)$ for some (i, j) : crossover

Metaheuristics: an Alternative Viewpoint

- Population and variation operators define a distribution on Ω
- \longrightarrow directly evolve a parameterized distribution $P(\theta)$

Distribution-based Metaheuristics

- Initialize distribution parameters θ_0
- Until(happy)
 - Sample distribution $P(\theta_t) \rightarrow y_1, \dots, y_\lambda \in \Omega$
 - Evaluate y_1, \dots, y_λ on \mathcal{F}
 - Update parameters $\theta_{t+1} \leftarrow F_\theta(\theta_t, y_1, \dots, y_\lambda, \mathcal{F}(y_1), \dots, \mathcal{F}(y_\lambda))$
includes selection

Covers

- Estimation of Distribution Algorithms
- Population-based Metaheuristics Evolutionary Algorithms
Particle Swarm Optimization, Differential Evolution, ...
- Deterministic algorithms

This is (mostly) Experimental Science

Theory

- lagging behind practice
- though rapidly catching up in recent years
- not discussed here

Results need to be experimentally validated

Experiments

Validation relies on

- | | |
|---|---------------|
| • grounded statistical validation | CPU costly |
| • informed (meta)parameter setting/tuning | CPU costly ++ |
| • reproducibility | Open Science |

From Solution Space to Search Space

Choices

- Objective function
- Search space representation
- and move operators / parameterized distribution

Approximation bias vs optimization error

This talk

- Non-convex, non-smooth objective parametric continuous optimization
→ Rank-based ML seeded identification of influencers
- Search spaces and crossover operators the TSP
- Non-parametric representations exploration vs optimization

- 1 Setting the scene
- 2 Continuous Optimization
 - The Evolution Strategy
 - The CMA-ES (Covariance Matrix Adaptation Evolution Strategy)
 - The Rank-based DataScience
- 3 Discrete/Combinatorial Optimization
- 4 Non-Parametric Representations
- 5 Conclusion

- 1 Setting the scene
- 2 Continuous Optimization
 - The Evolution Strategy
 - The CMA-ES (Covariance Matrix Adaptation Evolution Strategy)
 - The Rank-based DataScience
- 3 Discrete/Combinatorial Optimization
- 4 Non-Parametric Representations
- 5 Conclusion

Stochastic Optimization Templates

Population-based Metaheuristics

- Randomly draw $\mathbf{x}_0^i \in \Omega$ and compute $\mathcal{F}(\mathbf{x}_0^i)$, $i = 1, \dots, \mu$ Initialisation
- Until(happy)
 - $\mathbf{y}^i = \text{Move}(\mathbf{x}_t^1, \dots, \mathbf{x}_t^\mu)$, $i = 1, \dots, \lambda$ stochastic variations on Ω
 - Compute $\mathcal{F}(\mathbf{y}^i)$, $i = 1, \dots, \lambda$
 - $(\mathbf{x}_{t+1}^1, \dots, \mathbf{x}_{t+1}^\mu) = \text{Select}(\mathbf{x}_t^1, \dots, \mathbf{x}_t^\mu, \mathbf{y}^1, \dots, \mathbf{y}^\lambda)$ $(\mu + \lambda)$ selection
= $\text{Select}(\mathbf{y}^1, \dots, \mathbf{y}^\lambda)$ (μ, λ) selection

Distribution-based Metaheuristics

- Initialize distribution parameters θ_0
- Until(happy)
 - Sample distribution $P(\theta_t) \rightarrow \mathbf{y}_1, \dots, \mathbf{y}_\lambda \in \Omega$
 - Evaluate $\mathbf{y}_1, \dots, \mathbf{y}_\lambda$ on \mathcal{F}
 - Update parameters $\theta_{t+1} \leftarrow F_\theta(\theta_t, \mathbf{y}_1, \dots, \mathbf{y}_\lambda, \mathcal{F}(\mathbf{y}_1), \dots, \mathcal{F}(\mathbf{y}_\lambda))$

Distribution-based Metaheuristics

- Initialize distribution parameters θ_0
- Until(happy)
 - Sample distribution $P(\theta_t) \rightarrow \mathbf{y}_1, \dots, \mathbf{y}_\lambda \in \Omega$
 - Evaluate $\mathbf{y}_1, \dots, \mathbf{y}_\lambda$ on \mathcal{F}
 - Update parameters $\theta_{t+1} \leftarrow F_\theta(\theta_t, \mathbf{y}_1, \dots, \mathbf{y}_\lambda, \mathcal{F}(\mathbf{y}_1), \dots, \mathcal{F}(\mathbf{y}_\lambda))$

The (μ, λ) –Evolution Strategy

$$\Omega = \mathbb{R}^n$$

$P(\theta)$: normal distributions

Initialize distribution parameters $\mathbf{m}, \sigma, \mathbf{C}$, set population size $\lambda \in \mathbb{N}$

While not terminate

- 1 **Sample** distribution $\mathcal{N}(\mathbf{m}, \sigma^2 \mathbf{C}) \rightarrow \mathbf{y}_1, \dots, \mathbf{y}_\lambda \in \mathbb{R}^n$

$$\mathbf{y}_i \sim \mathbf{m} + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \quad \text{for } i = 1, \dots, \lambda$$

- 2 **Evaluate** $\mathbf{y}_1, \dots, \mathbf{y}_\lambda$ on \mathcal{F}

$$\text{Compute } \mathcal{F}(\mathbf{y}_1), \dots, \mathcal{F}(\mathbf{y}_\lambda)$$

- 3 **Select** μ best samples

$$\mathbf{y}_1, \dots, \mathbf{y}_\mu$$

- 4 **Update** distribution parameters

$$\mathbf{m}, \sigma, \mathbf{C} \leftarrow F(\mathbf{m}, \sigma, \mathbf{C}, \mathbf{y}_1, \dots, \mathbf{y}_\mu, \mathcal{F}(\mathbf{y}_1), \dots, \mathcal{F}(\mathbf{y}_\mu))$$

The (μ, λ) –Evolution Strategy (2)

Gaussian Mutations

- **mean** vector $\mathbf{m} \in \mathbb{R}^n$ is the current solution
- the so-called **step-size** $\sigma \in \mathbb{R}_+$ controls the *step length*
- the **covariance matrix** $\mathbf{C} \in \mathbb{R}^{n \times n}$ determines the shape of the distribution ellipsoid

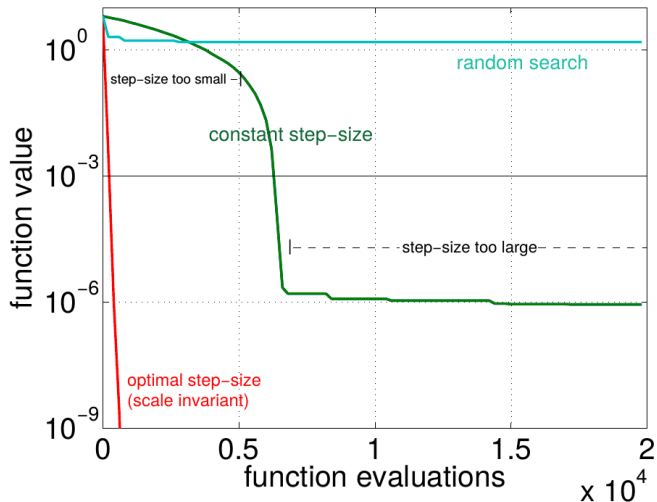
How to update \mathbf{m} , σ , and \mathbf{C} ?

- $$\mathbf{m} = \frac{1}{\mu} \sum_{i=1}^{i=\mu} x_{i:\lambda}$$

“Crossover” of best μ individuals

- Adaptive σ and \mathbf{C}

Need for adaptation

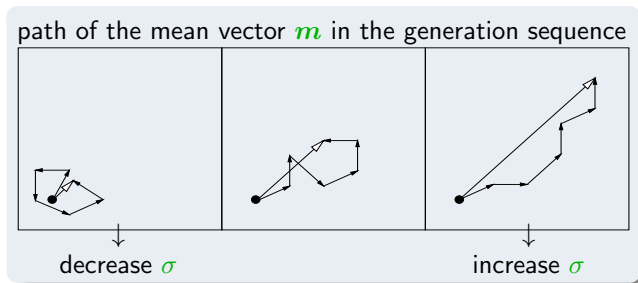


Sphere function $f(x) = \sum x_i^2, n = 10$

- 1 Setting the scene
- 2 Continuous Optimization
 - The Evolution Strategy
 - The CMA-ES (Covariance Matrix Adaptation Evolution Strategy)
 - The Rank-based DataScience
- 3 Discrete/Combinatorial Optimization
- 4 Non-Parametric Representations
- 5 Conclusion

Cumulative Step-Size Adaptation (CSA)

- Measure the length of the *evolution path*



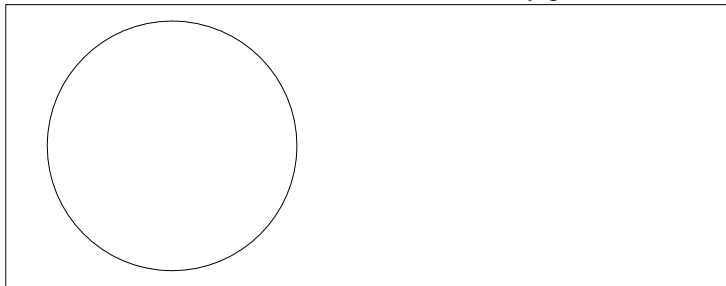
- Compare to random walk

without selection

Covariance Matrix Adaptation

Rank-One Update

$$\mathbf{m} \leftarrow \mathbf{m} + \sigma \mathbf{y}_w, \quad \mathbf{y}_w = \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda}, \quad \mathbf{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C})$$



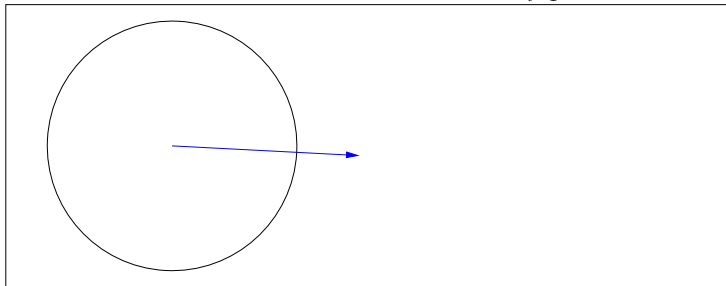
initial distribution, $\mathbf{C} = \mathbf{I}$

- new distribution: $\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \mathbf{y}_w \mathbf{y}_w^T$
- ruling principle: the adaptation increases the probability of successful steps, \mathbf{y}_w , to appear again

Covariance Matrix Adaptation

Rank-One Update

$$\mathbf{m} \leftarrow \mathbf{m} + \sigma \mathbf{y}_w, \quad \mathbf{y}_w = \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda}, \quad \mathbf{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C})$$



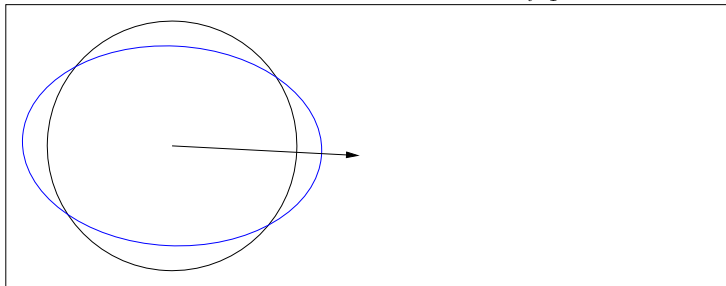
\mathbf{y}_w , movement of the population mean \mathbf{m} (disregarding σ)

- new distribution: $\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \mathbf{y}_w \mathbf{y}_w^T$
- ruling principle: the adaptation increases the probability of successful steps, \mathbf{y}_w , to appear again

Covariance Matrix Adaptation

Rank-One Update

$$\mathbf{m} \leftarrow \mathbf{m} + \sigma \mathbf{y}_w, \quad \mathbf{y}_w = \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda}, \quad \mathbf{y}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$$



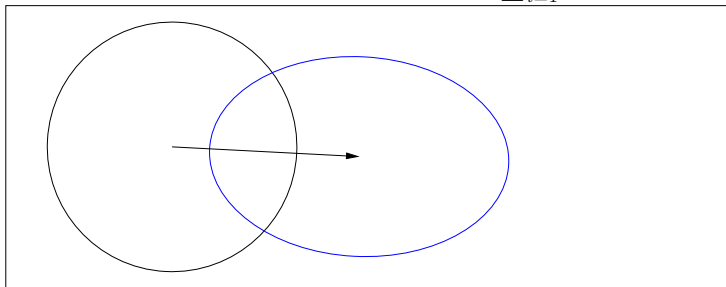
mixture of distribution \mathbf{C} and step \mathbf{y}_w , $\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \mathbf{y}_w \mathbf{y}_w^T$

- new distribution: $\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \mathbf{y}_w \mathbf{y}_w^T$
- ruling principle: the adaptation increases the probability of successful steps, \mathbf{y}_w , to appear again

Covariance Matrix Adaptation

Rank-One Update

$$\mathbf{m} \leftarrow \mathbf{m} + \sigma \mathbf{y}_w, \quad \mathbf{y}_w = \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda}, \quad \mathbf{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C})$$



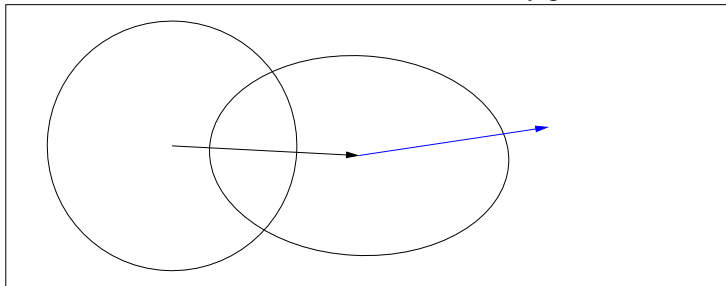
new distribution (disregarding σ)

- new distribution: $\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \mathbf{y}_w \mathbf{y}_w^T$
- ruling principle: the adaptation increases the probability of successful steps, \mathbf{y}_w , to appear again

Covariance Matrix Adaptation

Rank-One Update

$$\mathbf{m} \leftarrow \mathbf{m} + \sigma \mathbf{y}_w, \quad \mathbf{y}_w = \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda}, \quad \mathbf{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C})$$



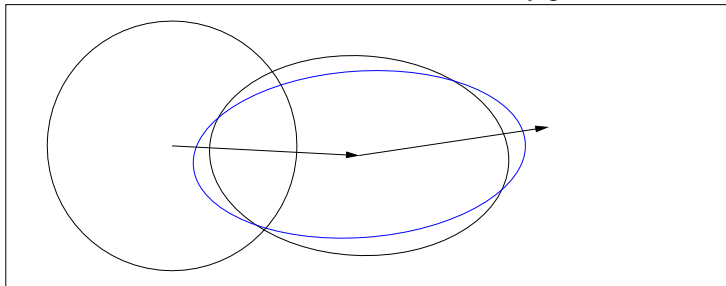
movement of the population mean \mathbf{m}

- new distribution: $\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \mathbf{y}_w \mathbf{y}_w^T$
- ruling principle: the adaptation increases the probability of successful steps, \mathbf{y}_w , to appear again

Covariance Matrix Adaptation

Rank-One Update

$$\mathbf{m} \leftarrow \mathbf{m} + \sigma \mathbf{y}_w, \quad \mathbf{y}_w = \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda}, \quad \mathbf{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C})$$



mixture of distribution \mathbf{C} and step \mathbf{y}_w ,

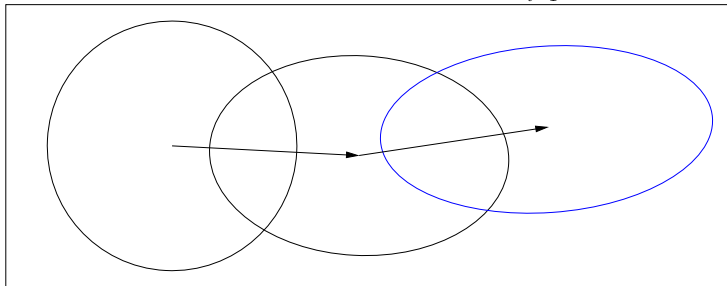
$$\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \mathbf{y}_w \mathbf{y}_w^T$$

- new distribution: $\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \mathbf{y}_w \mathbf{y}_w^T$
- ruling principle: the adaptation increases the probability of successful steps, \mathbf{y}_w , to appear again

Covariance Matrix Adaptation

Rank-One Update

$$\mathbf{m} \leftarrow \mathbf{m} + \sigma \mathbf{y}_w, \quad \mathbf{y}_w = \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda}, \quad \mathbf{y}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$$



- new distribution: $\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \mathbf{y}_w \mathbf{y}_w^T$
- ruling principle: the adaptation increases the probability of successful steps, \mathbf{y}_w , to appear again

CMA-ES in one slide

Input: $\mathbf{m} \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, λ

Initialize: $\mathbf{C} = \mathbf{I}$, and $\mathbf{p}_\mathbf{C} = \mathbf{0}$, $\mathbf{p}_\sigma = \mathbf{0}$,

Set: $c_\mathbf{C} \approx 4/n$, $c_\sigma \approx 4/n$, $c_1 \approx 2/n^2$, $c_\mu \approx \mu_w/n^2$, $c_1 + c_\mu \leq 1$,

$d_\sigma \approx 1 + \sqrt{\frac{\mu_w}{n}}$, and $w_{i=1 \dots \lambda}$ such that $\mu_w = \frac{1}{\sum_{i=1}^\mu w_i^2} \approx 0.3 \lambda$

While not terminate

$\mathbf{x}_i = \mathbf{m} + \sigma \mathbf{y}_i$, $\mathbf{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C})$, for $i = 1, \dots, \lambda$ sampling

$\mathbf{m} \leftarrow \sum_{i=1}^\mu w_i \mathbf{x}_{i:\lambda} = \mathbf{m} + \sigma \mathbf{y}_w$ where $\mathbf{y}_w = \sum_{i=1}^\mu w_i \mathbf{y}_{i:\lambda}$ update mean

$\mathbf{p}_\mathbf{C} \leftarrow (1 - c_\mathbf{C}) \mathbf{p}_\mathbf{C} + \mathbb{1}_{\{\|\mathbf{p}_\mathbf{C}\| < 1.5\sqrt{n}\}} \sqrt{1 - (1 - c_\mathbf{C})^2} \sqrt{\mu_w} \mathbf{y}_w$ cumulation for \mathbf{C}

$\mathbf{p}_\sigma \leftarrow (1 - c_\sigma) \mathbf{p}_\sigma + \sqrt{1 - (1 - c_\sigma)^2} \sqrt{\mu_w} \mathbf{C}^{-\frac{1}{2}} \mathbf{y}_w$ cumulation for σ

$\mathbf{C} \leftarrow (1 - c_1 - c_\mu) \mathbf{C} + c_1 \mathbf{p}_\mathbf{C} \mathbf{p}_\mathbf{C}^\mathbf{T} + c_\mu \sum_{i=1}^\mu w_i \mathbf{y}_{i:\lambda} \mathbf{y}_{i:\lambda}^\mathbf{T}$ update \mathbf{C}

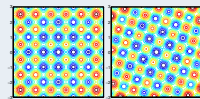
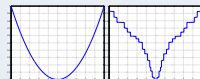
$\sigma \leftarrow \sigma \times \exp\left(\frac{c_\sigma}{d_\sigma} \left(\frac{\|\mathbf{p}_\sigma\|}{\mathbb{E}\|\mathcal{N}(\mathbf{0}, \mathbf{I})\|} - 1\right)\right)$ update of σ

Not covered on this slide: termination, restarts, active or mirrored sampling, outputs, and boundaries

Invariances: Guarantee for Generalization

Invariance properties of CMA-ES

- Invariance to **order preserving transformations** in function space
like all comparison-based algorithms
- Translation and **rotation invariance**
to *rigid transformations* of the search space



→ Natural Gradient in distribution space

NES, Schmidhuber et al., 08
IGO, Olliver et al., 11

CMA-ES is **almost parameterless**

- Tuning of a small set of functions
- Default values generalize to whole classes
- Exception: population size for multi-modal functions

Hansen & Ostermeier 2001

but see IPOP-CMA-ES Auger & Hansen, 05
and BIPOP-CMA-ES Hansen, 09

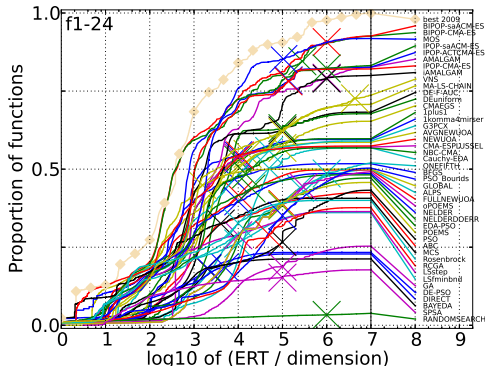
BBOB – Black-Box Optimization Benchmarking

- ACM-GECCO workshops, 2009-2015
- Set of 25 benchmark functions, dimensions 2 to 40
- With known difficulties (ill-conditioning, non-separability, ...)
- Noisy and non-noisy versions

<http://coco.gforge.inria.fr/>

Competitors include

- BFGS (Matlab version),
- Fletcher-Powell,
- DFO (Derivative-Free Optimization, [Powell 04](#))
- Differential Evolution
- Particle Swarm Optimization
- and many more



- 1 Setting the scene
- 2 Continuous Optimization
 - The Evolution Strategy
 - The CMA-ES (Covariance Matrix Adaptation Evolution Strategy)
 - The Rank-based DataScience
- 3 Discrete/Combinatorial Optimization
- 4 Non-Parametric Representations
- 5 Conclusion

Seeded Influencer Identification

Philippe Caillou & Michèle Sebag, coll SME Augure

Goal

- Find the **influencers** in a given social network
- from public data sources tweets, blogs, articles, ...
- Commercial goal: so as to bribe them :-)
- Scientific goal: with little user input

What is an Influencer?

No clear definition

- # followers?
- Highly retweeted? but # retweets disagrees with # followers
- Sources of information cascades?
- # invitations to join?
- Topic-specific PageRank?
- Presence on Wikipedia?

Need for

- Topic-specific features
- **and** graph features
- **and** user input no generic ground truth

Seeded Influencer Ranking

Input

- A social network
- (Big) Data of user interactions Tweets, blogs, messages, ...
- Some identified influencers

The global picture

- Derive features representing the users using content and traces
- Optimize scoring function giving highest scores to known influencers
- return best-k scoring users the most (known + new) influencers

Search Space and Learning Criterion

The scoring function

- Each individual is described by d features
- Non-linear score h defined by pair (v, a) in $\mathbb{R}^d \times \mathbb{R}^d$

$$x_i \in \mathbb{R}^d$$

$$h_{v,a}(x) = \sum_{i=1}^d v_i |x_i - a_i|$$

A rank-based criterion

- Each score $h_{v,a}$ induces a ranking $R_{v,a}$ on the dataset
- Goal: Known influencers (KIs) ranked highest

Best has rank n

Non-convex optimization

$$\text{ArgMax}_{(v,a)} \left\{ \sum_{x_i \in \text{KI}} R_{v,a}(x_i) \right\}$$

→ Stochastic Optimizer

e.g., sep-CMA-ES

Domains

- **Fashion:** 18/23 influencers with twitter account
- **SmartPhones:** 69/206 influencers with twitter account
- **Social Influence:** 39/39 influencers with twitter account
- **Wine:** 28/235 influencers with twitter account, coming from public sources (e.g., *Time Magazine*)
- **Human Resources:** 99 influencers from the *100 most influential people in HR and recruiting on twitter*

Sources

- random 10% of all retweets of November 2014
- 100M tweets, 45M unique tweets,
- with origin-destination pairs → 43M nodes graph
- only words in at least 0.001% and at most 10% tweets considered → 10.5M candidates

Features

100 Content-based Features

foreach medium eventually

- Foreach user x , identify $\mathcal{W}(x)$, the N words with max tf-idf
term frequency - inverse document frequency
- 50 words that appear most often in all $\mathcal{W}(\text{influencer})$
- 50 words with max sum of tf-idf over $\bigcup \mathcal{W}(\text{influencer})$
- each selected word is a feature for x : 0 if not present in $\mathcal{W}(x)$, ti-idf otherwise
Many are null for most candidates

6 Network Features

- from the weighted graph of retweets
centrality, PageRank, ...

5 Social Features

- from tweeter user profiles
tweets, # followers, ...

Seeded Influencer Identification: Discussion

Results

- Better than using only social features
- Found unexpected influencers
- Confirmed by experts

Forthcoming application

- Unveil some influential xxx-sceptics Global warming, genocides, ...

- 1 Setting the scene
- 2 Continuous Optimization
- 3 Discrete/Combinatorial Optimization
 - The Crossover Controversy
 - The TSP Illustration
- 4 Non-Parametric Representations
- 5 Conclusion

- 1 Setting the scene
- 2 Continuous Optimization
- 3 Discrete/Combinatorial Optimization
 - The Crossover Controversy
 - The TSP Illustration
- 4 Non-Parametric Representations
- 5 Conclusion

Stochastic Optimization Templates (reminder)

Population-based Metaheuristics

- Randomly draw $\mathbf{x}_0^i \in \Omega$ and compute $\mathcal{F}(\mathbf{x}_0^i)$, $i = 1, \dots, \mu$ Initialisation
- Until(happy)
 - $\mathbf{y}^i = \text{Move}(\mathbf{x}_t^1, \dots, \mathbf{x}_t^\mu)$, $i = 1, \dots, \lambda$ stochastic variations on Ω
 - Compute $\mathcal{F}(\mathbf{y}^i)$, $i = 1, \dots, \lambda$
 - $(\mathbf{x}_{t+1}^1, \dots, \mathbf{x}_{t+1}^\mu) = \text{Select}(\mathbf{x}_t^1, \dots, \mathbf{x}_t^\mu, \mathbf{y}^1, \dots, \mathbf{y}^\lambda)$ $(\mu + \lambda)$ selection
= $\text{Select}(\mathbf{y}^1, \dots, \mathbf{y}^\lambda)$ (μ, λ) selection

Distribution-based Metaheuristics

- Initialize distribution parameters θ_0
- Until(happy)
 - Sample distribution $P(\theta_t) \rightarrow \mathbf{y}_1, \dots, \mathbf{y}_\lambda \in \Omega$
 - Evaluate $\mathbf{y}_1, \dots, \mathbf{y}_\lambda$ on \mathcal{F}
 - Update parameters $\theta_{t+1} \leftarrow F_\theta(\theta_t, \mathbf{y}_1, \dots, \mathbf{y}_\lambda, \mathcal{F}(\mathbf{y}_1), \dots, \mathcal{F}(\mathbf{y}_\lambda))$

Stochastic Optimization Templates (reminder)

Population-based Metaheuristics

- Randomly draw $\mathbf{x}_0^i \in \Omega$ and compute $\mathcal{F}(\mathbf{x}_0^i)$, $i = 1, \dots, \mu$ Initialisation
- Until(happy)
 - $\mathbf{y}^i = \text{Move}(\mathbf{x}_t^1, \dots, \mathbf{x}_t^\mu)$, $i = 1, \dots, \lambda$ stochastic variations on Ω
 - Compute $\mathcal{F}(\mathbf{y}^i)$, $i = 1, \dots, \lambda$
 - $(\mathbf{x}_{t+1}^1, \dots, \mathbf{x}_{t+1}^\mu) = \text{Select}(\mathbf{x}_t^1, \dots, \mathbf{x}_t^\mu, \mathbf{y}^1, \dots, \mathbf{y}^\lambda)$ $(\mu + \lambda)$ selection
= $\text{Select}(\mathbf{y}^1, \dots, \mathbf{y}^\lambda)$ (μ, λ) selection

Crossover or not Crossover

Issues with crossover

- Crossover ubiquitous in nature
though not in all bacteria
- Showed to mainly work on dynamical problems
Compared to ILS, SA, Ch. Papadimitriou et al., 15



Crossover or not Crossover

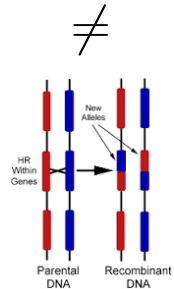
Issues with crossover

- Crossover ubiquitous in nature
though not in all bacteria
- Showed to mainly work on dynamical problems
Compared to ILS, SA, Ch. Papadimitriou et al., 15



Yes, but

- Most artificial crossover operators exchange chunks of solutions
- Nature does not exchange “organs”
- but chunks of programs that builds the solution



Crossover or not Crossover

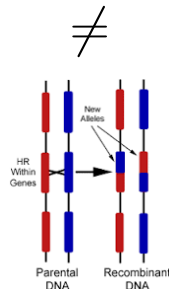
Issues with crossover

- Crossover ubiquitous in nature
though not in all bacteria
- Showed to mainly work on dynamical problems
Compared to ILS, SA, Ch. Papadimitriou et al., 15



Yes, but

- Most artificial crossover operators exchange chunks of solutions
- Nature does not exchange “organs”
- but chunks of programs that builds the solution

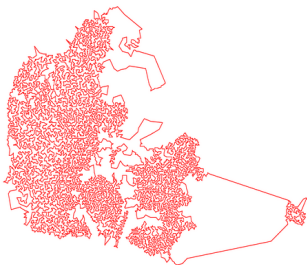


Better no crossover than a poor crossover

- 1 Setting the scene
- 2 Continuous Optimization
- 3 Discrete/Combinatorial Optimization
 - The Crossover Controversy
 - The TSP Illustration
- 4 Non-Parametric Representations
- 5 Conclusion

The Traveling Salesman Problem

Find shortest Hamiltonian circuit on n cities



dk11455.tsp

Permutation Representation

- Ordered list of cities:
no semantic link with the objective
- Blind exchange of chunks meaningless,
and leads to unfeasible circuits

Edge Representation

- List of all edges of the tour: **unordered**
clearly related to objective
- but blind exchange of edges doesn't
work either

Challenge or opportunity?

- A strong exact solver
- A very strong heuristic solver

Concorde

LKH-2

LKH-2

- Local Search
- Deep k-opt moves
- Many ad hoc heuristics

efficient implementation

Multi-trial LKH-2

- Iterated Local Search
- Using ... a crossover operator between best-so-far and new local optima
- Iterative Partial Transcription,
a particular case of GPX

Mobius et al., 99-08

next slide

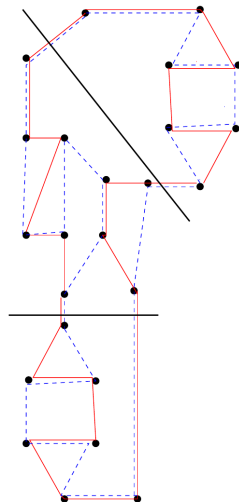
Most best known results on non-exactly solved instances, up to 10M cities

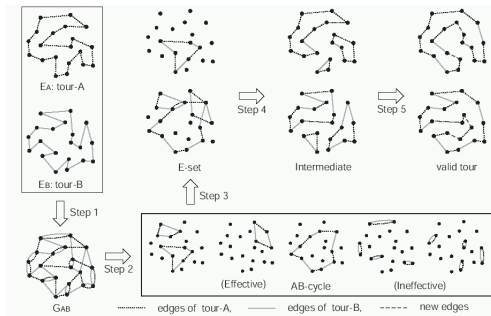
Respectful and Transmitting crossover

- Find k -partitions of cost 2 if exist $O(n)$
- Chooses best of $2^k - 2$ solutions $O(k)$
 - All common edges are kept
 - No new edge is created

Two possible hybridizations

- Evolutionary Algorithm using GPX and iterated 2-opt as mutation operator
Some best results on small instance $< 10k$ cities
- Replacing IPT in LKH-2 heuristic
Improved some state-of-the-art results





The EAX crossover

- 1 Merge A and B
- 2 Alternate A/B edges
- 3 Local, then global choice strategy
- 4 Use sub-tours to remove parent edges
- 5 Local search for minimal new edges

The EAX algorithm

- Foreach randomly chosen parent pair typically 300 iterations
- apply EAX N times typically 30
- keep best of parents + N offspring diversity-preserving selection

Best known results on several instances $\dots \leq 200k$ cities

Meta or not Meta?

- GPX can be applied to other graph problems
- EAX is definitely a specialized TSP operator

Take Home Message

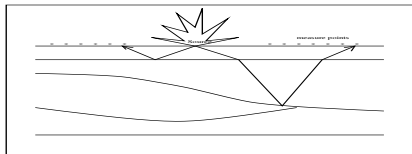
- Efficient crossovers might exist
- for semantically relevant representations
- but require domain knowledge . . . and fine-tuning

- 1 Setting the scene
- 2 Continuous Optimization
- 3 Discrete/Combinatorial Optimization
- 4 Non-Parametric Representations
 - The Velocity Identification
 - The Planning Decomposition
- 5 Conclusion

- 1 Setting the scene
- 2 Continuous Optimization
- 3 Discrete/Combinatorial Optimization
- 4 **Non-Parametric Representations**
 - The Velocity Identification
 - The Planning Decomposition
- 5 Conclusion

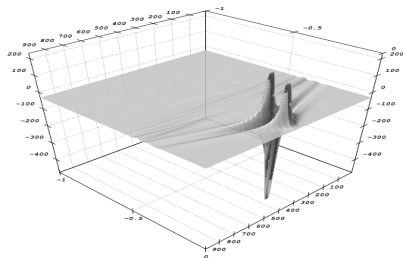
Identification of Spatial Geological Models

MS, Ehinger, Braunschweig, 98



The direct problem

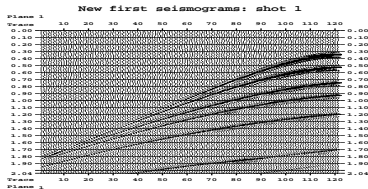
- Function ϕ
- applied to model \mathcal{M}
- Find result $\mathcal{R} = \phi(\mathcal{M})$
→ numerical simulation



(simulated) 3D seismogram

The inverse problem

- Given experimental results \mathcal{R}^*
- find model \mathcal{M}^*
- such that $\phi(\mathcal{M}^*) = \mathcal{R}^*$
→ $\text{Arg Min}_{\mathcal{M}} \{ \|\phi(\mathcal{M}) - \mathcal{R}^*\|^2 \}$



120 × 2D seismogram

Voronoi Representation

The solution space

- Velocities in some 3D domain
- Blocky model *piecewise constant*

Values on a grid/mesh

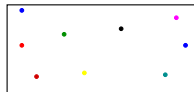
- Thousands of variables
- Uncorrelated

Voronoi representation

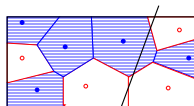
- List of labelled Voronoi sites
- Velocity = site label inside each cell

Variation Operators

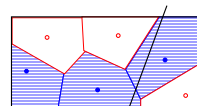
- Geometric exchange *crossover*
- Add, remove, move sites *mutations*



Variable unordered list of Voronoi sites, and corresponding 'colored' Voronoi diagram



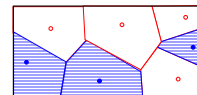
Parent 1



Parent 2



Offspring 1



Offspring 2

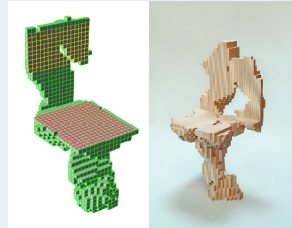
The crossover operator

Other Voronoi successes

Evolutionary chairs

- Minimize weight
- Constraint on stiffness

Permanent collection of
Beaubourg Modern Art Museum



The Seroussi architectural competition

- A building for private exhibitions
- Optimize natural lightning of paintings *all year round*
- Room seeds for adaptive room desing

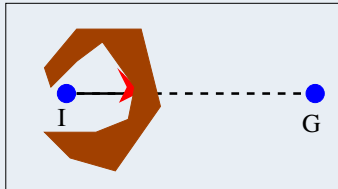


1st price (out of 8 submissions)

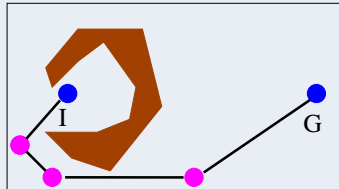
- 1 Setting the scene
- 2 Continuous Optimization
- 3 Discrete/Combinatorial Optimization
- 4 **Non-Parametric Representations**
 - The Velocity Identification
 - The Planning Decomposition
- 5 Conclusion

The TGV paradigm

Improve a dummy algorithm



Cannot directly go from I to G



Can go sequentially from I to the intermediate stations, and to G

→ evolve the sequence of intermediate 'stations'

Representation

- Variable-length ordered lists of (●₁, ●₂, ●₃)

Variation operators

- Chromosome-like swap
- Move, add or remove intermediate stations

variable-length crossover

mutations

AI Planning problem $(\mathcal{S}, \mathcal{A}, I, G)$

- Given a state space \mathcal{S} and a set of actions \mathcal{A} conditions, effects
- An initial state I and a goal state G possibly partially defined
- Find optimal sequence of actions from I to G .

Many complete / satisficing planners

biennial IPC since 1998

Evolving intermediate states

- Search space: Variable-length ordered lists of states (S_1, \dots, S_l)
- Solve $(\mathcal{S}, \mathcal{A}, S_i, S_{i+1})$ using a given planner “dummy”
- All sub-problems solved \rightarrow solution of initial problem

Highlights

J. Bibaï et al., 09-11

- Solves instances where ‘dummy’ planner fails
- Silver Medal, Humies Awards, GECCO 2010
- Winner, satisficing track, IPC 2011
- First multi-objective planner, IJCAI 2013

M. Khouadjia et al.

Non-Parametric Representations: Discussion

Further examples

- Spatial geological models: horizontal layers + geological parameters
patented
- Neural Networks HyerNeat, Stanley 07; Compressed NNs, Schmidhuber 10

Non-parametric representations

- Explore larger search spaces, but with some constraints
→ explore a sub-variety of the whole space
- Modifies both the approximation bias
how far from the true optimum is the best solution under the streetlight?
- and the optimization error our algorithm is not perfect

Optimization as an exploratory tool

- 1 Setting the scene
- 2 Continuous Optimization
- 3 Discrete/Combinatorial Optimization
- 4 Non-Parametric Representations
- 5 Conclusion

The Black-Box Hypothesis

Meta or not Meta?

- A continuum of embedded classes of problems
Where does Black Box start? e.g., GPX and EAX
- Continuous optimization: at least the dimension is known
- The more information the better e.g. multimodality for restarts
- Learn about \mathcal{F} during the search
→ online tuning beyond distribution parameters

Not Covered Today

General

- Statistical tests Tutorials available
- From parameter setting to hyper-heuristics Programming by Optimization, Hoos, 2014
Burke et al., 08-15
- Multi-objective Full track with own conferences

Continuous

- Surrogates ML helping Optimization
- Constraints from Lagrangian to specific approaches
- Noise handling e.g., using Höfdding or Bernstein inequalities

Other Representations/Paradigms

- Genetic Programming Search a space of programs
- Generative Developmental Systemsthat build the solution

Flexibility