

Computational Intelligence

Winter Term 2014/15

Prof. Dr. Günter Rudolph

Lehrstuhl für Algorithm Engineering (LS 11)

Fakultät für Informatik

TU Dortmund

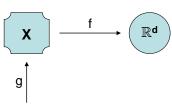
Design of Evolutionary Algorithms

Lecture 10

ad 1a) genotype-phenotype mapping

original problem $f: X \to \mathbb{R}^d$

scenario: no standard algorithm for search space X available





- \bullet standard EA performs variation on binary strings $b \in \mathbb{B}^n$
- fitness evaluation of individual b via (f ∘ g)(b) = f(g(b))
 where g: Bⁿ → X is genotype-phenotype mapping
- selection operation independent from representation

Design of Evolutionary Algorithms

Lecture 10

Three tasks:

- 1. Choice of an appropriate problem representation.
- 2. Choice / design of variation operators acting in problem representation.
- 3. Choice of strategy parameters (includes initialization).

ad 1) different "schools":

- (a) operate on binary representation and define genotype/phenotype mapping
 - + can use standard algorithm
 - mapping may induce unintentional bias in search
- (b) no doctrine: use "most natural" representation
 - must design variation operators for specific representation
 - + if design done properly then no bias in search



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Design of Evolutionary Algorithms

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Genotype-Phenotype-Mapping $\mathbb{B}^n \to [L, R] \subset \mathbb{R}$

 \bullet Standard encoding for $b \in \mathbb{B}^n$

$$x = L + \frac{R - L}{2^{n} - 1} \sum_{i=0}^{n-1} b_{n-i} 2^{i}$$

→ Problem: hamming cliffs

0							111			
	1	2	3	4	5	6	7			
1 Bit 2 Bit 1 Bit 3 Bit 1 Bit 2 Bit 1 Bit										

L = 0, R = 7n = 3

genotypephenotype

Hamming cliff

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Genotype-Phenotype-Mapping $\mathbb{B}^n \to [L, R] \subset \mathbb{R}$

• Gray encoding for $b \in \mathbb{B}^n$

Let $a \in \mathbb{B}^n$ standard encoded. Then $b_i = \left\{ \begin{array}{ll} a_i, & \text{if } i = 1 \\ a_{i\cdot 1} \oplus a_i, & \text{if } i > 1 \end{array} \right.$

000	001	011	010	110	111	101	100	← genotype
0	1	2	3	4	5	6	7	← phenotype

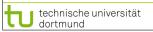
OK, no hamming cliffs any longer ...

 \Rightarrow small changes in phenotype "lead to" small changes in genotype

since we consider evolution in terms of Darwin (not Lamarck):

⇒ small changes in genotype lead to small changes in phenotype!

but: 1-Bit-change: $000 \rightarrow 100 \Rightarrow \odot$



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but: 1-Bit-cha

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Genotype-Phenotype-Mapping $\mathbb{B}^n \to \mathbb{P}^{log(n)}$

(example only)

 \bullet e.g. standard encoding for $b \in \mathbb{B}^n$

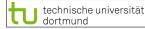
individual:

010	101	111	000	110	001	101	100	← genotype
0	1	2	3	4	5	6	7	← index

consider index and associated genotype entry as unit / record / struct; sort units with respect to genotype value, old indices yield permutation:

000	001	010	100	101	101	110	111	← genotype
3	5	0	7	1	6	4	2	← old index

= permutation



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ad 1a) genotype-phenotype mapping

typically required: strong causality

- → small changes in individual leads to small changes in fitness
- → small changes in genotype should lead to small changes in phenotype

but: how to find a genotype-phenotype mapping with that property?

necessary conditions:

- 1) g: $\mathbb{B}^n \to X$ can be computed efficiently (otherwise it is senseless)
- 2) g: $\mathbb{B}^n \to X$ is surjective (otherwise we might miss the optimal solution)
- 3) g: $\mathbb{B}^n \to X$ preserves closeness (otherwise strong causality endangered)

Let $d(\cdot, \cdot)$ be a metric on \mathbb{B}^n and $d_X(\cdot, \cdot)$ be a metric on X.

 $\forall x,\,y,\,z\in\mathbb{B}^n\colon d(x,\,y)\leq d(x,\,z)\ \Rightarrow d_X(g(x),\,g(y))\leq d_X(g(x),\,g(z))$

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ad 1b) use "most natural" representation

typically required: strong causality

- → small changes in individual leads to small changes in fitness
- → need variation operators that obey that requirement

but: how to find variation operators with that property?

 \Rightarrow need design guidelines ...

Lecture 10

ad 2) design guidelines for variation operators

a) reachability

every $x \in X$ should be reachable from arbitrary $x_0 \in X$ after finite number of repeated variations with positive probability bounded from 0

b) unbiasedness

unless having gathered knowledge about problem variation operator should not favor particular subsets of solutions ⇒ formally: maximum entropy principle

c) control

variation operator should have parameters affecting shape of distributions; known from theory: weaken variation strength when approaching optimum



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ad 2) design guidelines for variation operators in practice

binary search space $X = \mathbb{B}^n$

variation by k-point or uniform crossover and subsequent mutation

a) reachability:

regardless of the output of crossover we can move from $x\in\mathbb{B}^n$ to $y\in\mathbb{B}^n$ in 1 step with probability

$$p(x,y) = p_m^{H(x,y)} (1 - p_m)^{n - H(x,y)} > 0$$

where H(x,y) is Hamming distance between x and y.

Since min{ p(x,y): $x,y \in \mathbb{B}^n$ } = $\delta > 0$ we are done.



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b) unbiasedness

don't prefer any direction or subset of points without reason

⇒ use maximum entropy distribution for sampling!

properties:

- distributes probability mass as uniform as possible
- additional knowledge can be included as constraints:
- → under given constraints sample as uniform as possible

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Formally:

Definition:

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Let X be discrete random variable (r.v.) with $p_k = P\{X = x_k\}$ for some index set K. The quantity

$$H(X) = -\sum_{k \in K} p_k \log p_k$$

is called the **entropy of the distribution** of X. If X is a continuous r.v. with p.d.f. $f_X(\cdot)$ then the entropy is given by

$$H(X) = -\int_{-\infty}^{\infty} f_X(x) \log f_X(x) dx$$

The distribution of a random variable X for which H(X) is maximal is termed a **maximum entropy distribution**.

Lecture 10

Knowledge available:

Discrete distribution with support { $x_1,\,x_2,\,\ldots\,x_n$ } with $x_1 < x_2 < \ldots\,x_n < \infty$

$$p_k = \mathsf{P}\{X = x_k\}$$

⇒ leads to nonlinear constrained optimization problem:

$$-\sum_{k=1}^{n} p_k \log p_k \rightarrow \max!$$
s.t.
$$\sum_{k=1}^{n} p_k = 1$$

solution: via Lagrange (find stationary point of Lagrangian function)

$$L(p,a) = -\sum_{k=1}^{n} p_k \log p_k + a \left(\sum_{k=1}^{n} p_k - 1\right)$$



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Excursion: Maximum Entropy Distributions

Lecture 10

$$L(p, a) = -\sum_{k=1}^{n} p_k \log p_k + a \left(\sum_{k=1}^{n} p_k - 1\right)$$

partial derivatives:

$$\frac{\partial L(p,a)}{\partial p_k} = -1 - \log p_k + a \stackrel{!}{=} 0 \qquad \Rightarrow p_k \stackrel{!}{=} e^{a-1}$$

$$\frac{\partial L(p,a)}{\partial a} = \sum_{k=1}^n p_k - 1 \stackrel{!}{=} 0$$

$$\Rightarrow \sum_{k=1}^n p_k = \sum_{k=1}^n e^{a-1} = n e^{a-1} \stackrel{!}{=} 1 \quad \Leftrightarrow \quad e^{a-1} = \frac{1}{n}$$
uniform distribution

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Excursion: Maximum Entropy Distributions

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Knowledge available:

Discrete distribution with support { 1, 2, ..., n } with $p_k = P \{ X = k \}$ and E[X] = v

⇒ leads to nonlinear constrained optimization problem:

$$-\sum_{k=1}^n p_k \log p_k \to \max!$$
 s.t.
$$\sum_{k=1}^n p_k = 1 \quad \text{and} \quad \sum_{k=1}^n k \, p_k = \nu$$

solution: via Lagrange (find stationary point of Lagrangian function)

$$L(p, a, b) = -\sum_{k=1}^{n} p_k \log p_k + a \left(\sum_{k=1}^{n} p_k - 1\right) + b \left(\sum_{k=1}^{n} k \cdot p_k - \nu\right)$$

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Excursion: Maximum Entropy Distributions

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$$L(p, a, b) = -\sum_{k=1}^{n} p_k \log p_k + a \left(\sum_{k=1}^{n} p_k - 1\right) + b \left(\sum_{k=1}^{n} k \cdot p_k - \nu\right)$$

partial derivatives:

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$$\frac{\partial L(p,a,b)}{\partial p_k} = -1 - \log p_k + a + b \cdot k \stackrel{!}{=} 0 \qquad \Rightarrow p_k = e^{a-1+b \cdot k}$$

$$\frac{\partial L(p,a,b)}{\partial a} = \sum_{k=1}^{n} p_k - 1 \stackrel{!}{=} 0$$

$$\frac{\partial L(p,a,b)}{\partial b} \stackrel{(*)}{=} \sum_{k=1}^{n} k \cdot p_k - \nu \stackrel{!}{=} 0 \qquad \sum_{k=1}^{n} p_k = e^{a-1} \sum_{k=1}^{n} (e^b)^k \stackrel{!}{=} 1$$

(continued on next slide)

Lecture 10

$$\Rightarrow e^{a-1} = \frac{1}{\sum_{k=1}^{n} (e^b)^k} \qquad \Rightarrow p_k = e^{a-1+bk} = \frac{(e^b)^k}{\sum_{i=1}^{n} (e^b)^i}$$

$$\Rightarrow$$
 discrete Boltzmann distribution $p_k = rac{q^k}{\sum\limits_{i=1}^n q^i}$ $(q=e^b)$

value of g depends on v via third condition: (*)

$$\sum_{k=1}^{n} k p_{k} = \frac{\sum_{k=1}^{n} k q^{k}}{\sum_{i=1}^{n} q^{i}} = \frac{1 - (n+1) q^{n} + n q^{n+1}}{(1-q) (1-q^{n})} \stackrel{!}{=} \nu$$

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Excursion: Maximum Entropy Distributions

Lecture 10

Knowledge available:

Discrete distribution with support $\{1, 2, ..., n\}$ with E[X] = v and $V[X] = n^2$

⇒ leads to nonlinear constrained optimization problem:

$$-\sum_{k=1}^n p_k \log p_k \to \max!$$
 s.t. $\sum_{k=1}^n p_k = 1$ and $\sum_{k=1}^n k \, p_k = \nu$ and $\sum_{k=1}^n (k-\nu)^2 \, p_k = \eta^2$

solution: in principle, via Lagrange (find stationary point of Lagrangian function)

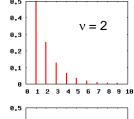
but very complicated analytically, if possible at all

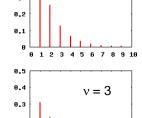
⇒ consider special cases only

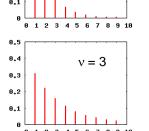
note: constraints are linear equations in p

Excursion: Maximum Entropy Distributions

Lecture 10

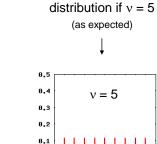






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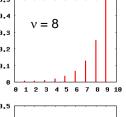


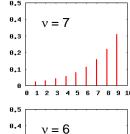
Boltzmann distribution

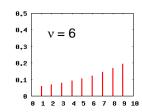
(n = 9)

specializes to uniform

v = 5







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Excursion: Maximum Entropy Distributions

Lecture 10

Special case: n = 3 and E[X] = 2 and $V[X] = n^2$

Linear constraints uniquely determine distribution:

i.
$$p_1 + p_2 + p_3 = 1$$

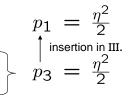
II.
$$p_1 + 2p_2 + 3p_3 = 2$$

I.
$$p_1 + p_2 + p_3 = 1$$

II. $p_1 + 2p_2 + 3p_3 = 2$
III. $p_1 + 0 + p_3 = \eta^2$

II.
$$p_1 + 2p_2 + 3p_3 = 2$$

III. $p_1 + 0 + p_3 = \eta^2$ $p_1 = \frac{\eta^2}{2}$
II. II. $p_2 + 2p_3 = 1$ $p_3 = \frac{\eta^2}{2}$ insertion in III. $p_3 = \frac{\eta^2}{2}$



$$\Rightarrow p = \left(\frac{\eta^2}{2}, 1 - \eta^2, \frac{\eta^2}{2}\right) \qquad \begin{array}{c} \eta^2 = \frac{1}{4} & \eta^2 = \frac{2}{3} & \eta^2 = \frac{1}{4} \\ \frac{1}{9 \cdot 1} & \frac{1$$









Lecture 10

Knowledge available:

Discrete distribution with unbounded support $\{0, 1, 2, ...\}$ and E[X] = v

⇒ leads to <u>infinite-dimensional</u> nonlinear constrained optimization problem:

$$-\sum_{k=0}^\infty p_k \log p_k \quad \to \max!$$
 s.t.
$$\sum_{k=0}^\infty p_k = 1 \quad \text{and} \quad \sum_{k=0}^\infty k \, p_k = \nu$$

solution: via Lagrange (find stationary point of Lagrangian function)

$$L(p,a,b) = -\sum_{k=0}^{\infty} p_k \log p_k + a \left(\sum_{k=0}^{\infty} p_k - 1\right) + b \left(\sum_{k=0}^{\infty} k \cdot p_k - \nu\right)$$



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Excursion: Maximum Entropy Distributions Lecture 10

$$\Rightarrow e^{a-1} = \frac{1}{\sum_{k=0}^{\infty} (e^b)^k} \qquad \Rightarrow p_k = e^{a-1+bk} = \frac{(e^b)^k}{\sum_{i=0}^{\infty} (e^b)^i}$$

set
$$q=e^b$$
 and insists that $q<1$ \Rightarrow $\sum_{k=0}^{\infty}q^k$ $=$ $\frac{1}{1-q}$ insert

$$p_k = (1-q)\,q^k$$
 for $k=0,1,2,\ldots$ geometrical distribution

it remains to specify q; to proceed recall that $\sum_{k=0}^{\infty} k \, q^k \, = \, \frac{q}{(1-q)^2}$

Excursion: Maximum Entropy Distributions

Lecture 10

$$L(p, a, b) = -\sum_{k=0}^{\infty} p_k \log p_k + a \left(\sum_{k=0}^{\infty} p_k - 1\right) + b \left(\sum_{k=0}^{\infty} k \cdot p_k - \nu\right)$$

partial derivatives:

$$\frac{\partial L(p,a,b)}{\partial p_k} = -1 - \log p_k + a + b \cdot k \stackrel{!}{=} 0 \qquad \Rightarrow p_k = e^{a-1+b \cdot k}$$

$$\frac{\partial L(p,a,b)}{\partial a} = \sum_{k=0}^{\infty} p_k - 1 \stackrel{!}{=} 0$$

$$\frac{\partial L(p,a,b)}{\partial b} \stackrel{(\clubsuit)}{=} \sum_{k=0}^{\infty} k \cdot p_k - \nu \stackrel{!}{=} 0 \qquad \sum_{k=0}^{\infty} p_k = e^{a-1} \sum_{k=0}^{\infty} (e^b)^k \stackrel{!}{=} 1$$

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Excursion: Maximum Entropy Distributions

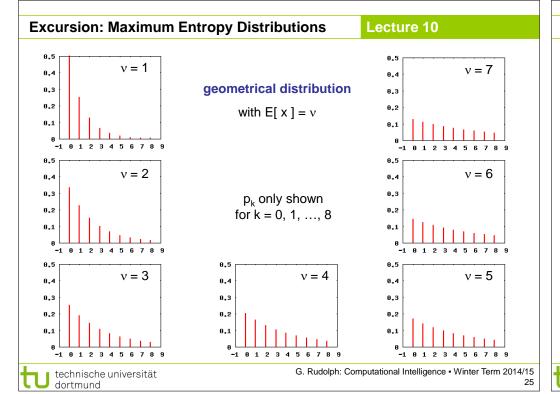
Lecture 10

 \Rightarrow value of q depends on v via third condition: (*)

$$\sum_{k=0}^{\infty} k p_k = \frac{\sum_{k=0}^{\infty} k q^k}{\sum_{i=0}^{\infty} q^i} = \frac{q}{1-q} \stackrel{!}{=} \nu$$

$$\Rightarrow q = \frac{\nu}{\nu + 1} = 1 - \frac{1}{\nu + 1}$$

$$\Rightarrow p_k = \frac{1}{\nu+1} \left(1 - \frac{1}{\nu+1} \right)^k$$



Lecture 10

Overview:

support { 1, 2, ..., n } ⇒ discrete uniform distribution

and require $E[X] = \theta$ ⇒ Boltzmann distribution

and require $V[X] = \eta^2$ ⇒ N.N. (**not** Binomial distribution)

support N ⇒ not defined!

and require $E[X] = \theta$ ⇒ *geometrical* distribution

and require $V[X] = \eta^2$ \Rightarrow ?

support \mathbb{Z} ⇒ not defined!

and require $E[|X|] = \theta$ ⇒ bi-geometrical distribution (discrete Laplace distr.)

and require $E[|X|^2] = \eta^2$ ⇒ N.N. (discrete Gaussian distr.)



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Excursion: Maximum Entropy Distributions

Lecture 10

support [a,b] $\subset \mathbb{R}$ ⇒ uniform distribution

support \mathbb{R}^+ with $\mathsf{E}[\mathsf{X}] = \theta$ ⇒ Exponential distribution

support $\mathbb R$

with $E[X] = \theta$, $V[X] = \eta^2$ \Rightarrow normal / Gaussian distribution N(θ , η^2)

support \mathbb{R}^n

with $E[X] = \theta$

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and Cov[X] = C \Rightarrow multinormal distribution N(θ , C)

> expectation vector $\in \mathbb{R}^n$ covariance matrix $\in \mathbb{R}^{n,n}$

positive definite: $\forall x \neq 0 : x'Cx > 0$

Excursion: Maximum Entropy Distributions

Lecture 10

for permutation distributions?

→ uniform distribution on all possible permutations

```
set v[j] = j for j = 1, 2, ..., n
for i = n to 1 step -1
  draw k uniformly at random from { 1, 2, ..., i }
  swap v[i] and v[k]
endfor
```

generates permutation uniformly at random in Θ(n) time

Guideline:

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Only if you know something about the problem a priori or

if you have learnt something about the problem during the search

⇒ include that knowledge in search / mutation distribution (via constraints!)

Lecture 10

every recombination results

- mutation of z may then lead

to any $z^* \in \mathbb{Z}^n$ with positive

probability in one step

in some $z \in \mathbb{Z}^n$

ad 2) design guidelines for variation operators in practice

integer search space $X = \mathbb{Z}^n$

- a) reachability
- b) unbiasedness
- c) control
- ad a) support of mutation should be \mathbb{Z}^n
- ad b) need maximum entropy distribution over support \mathbb{Z}^n
- ad c) control variability by parameter
 - → formulate as constraint of maximum entropy distribution



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Design of Evolutionary Algorithms

Lecture 10

ad 2) design guidelines for variation operators in practice

 $X = \mathbb{Z}^n$

task: find (symmetric) maximum entropy distribution over \mathbb{Z} with $E[|Z|] = \theta > 0$

⇒ need analytic solution of a ∞-dimensional, nonlinear optimization problem with constraints!

$$H(p) = -\sum_{k=-\infty}^{\infty} p_k \log p_k \quad \longrightarrow \quad \max!$$

 $p_k = p_{-k} \quad \forall k \in \mathbb{Z}$, (symmetry w.r.t. 0) s.t.

$$\sum_{k=-\infty}^{\infty} p_k = 1 , \qquad \text{(normalization)}$$

$$p_k = p_{-k} \quad \forall k \in \mathbb{Z} \,,$$
 (symmetry w.r.t. 0
$$\sum_{k=-\infty}^{\infty} p_k = 1 \,,$$
 (normalization)
$$\sum_{k=-\infty}^{\infty} |k| \, p_k = \theta \qquad \qquad \text{(control "spread")}$$
 $p_k \geq 0 \quad \forall k \in \mathbb{Z} \,.$ (nonnegativity)

$$p_k \geq 0 \quad \forall k \in \mathbb{Z} \ .$$
 (nonnegativity)

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Design of Evolutionary Algorithms

Lecture 10

result:

a random variable Z with support \mathbb{Z} and probability distribution

$$p_k := P\{Z = k\} = \frac{q}{2-q} (1-q)^{|k|}, k \in \mathbb{Z}, q \in (0,1)$$

symmetric w.r.t. 0, unimodal, spread manageable by *q* and has max. entropy

generation of pseudo random numbers:

 $Z = G_1 - G_2$

where

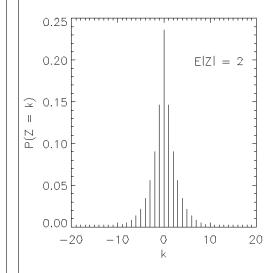
$$U_i \sim U(0,1) \ \Rightarrow \ G_i = \left| \frac{\log(1 - U_i)}{\log(1 - q)} \right| \ , \ i = 1, 2.$$

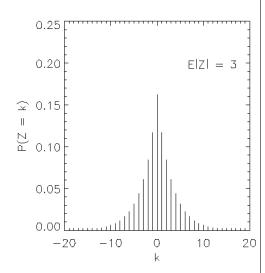
stochastic independent!

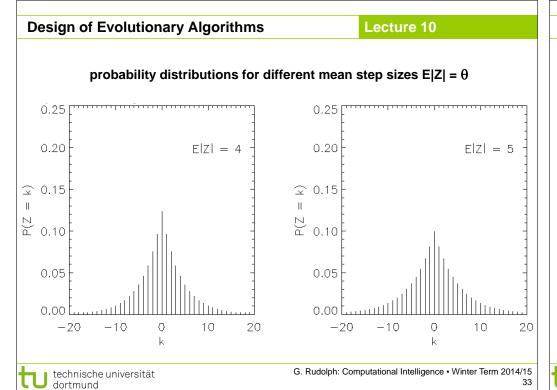
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Lecture 10

probability distributions for different mean step sizes $E|Z| = \theta$







Lecture 10

How to control the spread?

We must be able to adapt $q \in (0,1)$ for generating Z with variable $E|Z| = \theta$! self-adaptation of q in open interval (0,1)?

 \longrightarrow make mean step size E[|Z|] adjustable!

$$E[|Z|] = \sum_{k=-\infty}^{\infty} |k| p_k = \theta = \frac{2(1-q)}{q(2-q)} \Leftrightarrow q = 1 - \frac{\theta}{(1+\theta^2)^{1/2}+1}$$

$$\in \mathbb{R}_+ \qquad \qquad \in (0,1)$$

$$\to \theta \text{ adjustable by mutative self adaptation} \qquad \to \text{get q from } \theta$$

like mutative step size size control of σ in EA with search space \mathbb{R}^n !

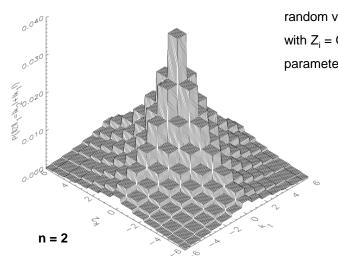
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Lecture 10

n - dimensional generalization



random vector $Z = (Z_1, Z_2, ..., Z_n)$ with $Z_i = G_{1,i} - G_{2,i}$ (stoch. indep.); parameter q for all $G_{1,i}$, $G_{2,i}$ equal

Design of Evolutionary Algorithms

Lecture 10

n - dimensional generalization

$$P{Z_i = k} = \frac{q}{2-q} (1-q)^{|k|}$$

$$P\{Z_1 = k_1, Z_2 = k_2, \dots, Z_n = k_n\} = \prod_{i=1}^n P\{Z_i = k_i\} = \prod_{i=1}^n P\{Z_i = k_i\} = \prod_{i=1}^n P\{Z_i = k_i\}$$

$$\left(\frac{q}{2-q}\right)^n \prod_{i=1}^n (1-q)^{|k_i|} = \left(\frac{q}{2-q}\right)^n (1-q)^{\sum_{i=1}^n |k_i|}$$

$$= \left(\frac{q}{2-q}\right)^n (1-q)^{\|k\|_1}.$$

- \Rightarrow n-dimensional distribution is symmetric w.r.t. ℓ_i norm!
- ⇒ all random vectors with same step length have same probability!

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How to control $E[|| Z ||_1]$?

$$E[\|Z\|_1] = E\left[\sum_{i=1}^n |Z_i|\right] = \sum_{i=1}^n E[|Z_i|] = n \cdot E[|Z_1|]$$
by def. | linearity of E[·] | identical distributions for Z_i

$$n \cdot E[|Z_1|] = n \cdot \frac{2(1-q)}{q(2-q)} \Leftrightarrow q = 1 - \frac{\theta/n}{(1+(\theta/n)^2)^{1/2}+1}$$

$$= \theta \qquad \text{self-adaptation} \qquad \text{calculate from } \theta$$



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Excursion: Maximum Entropy Distributions

Lecture 10

ad 2) design guidelines for variation operators in practice

continuous search space $X = \mathbb{R}^n$

- a) reachability
- b) unbiasedness
- c) control

leads to CMA-ES

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Design of Evolutionary Algorithms

Lecture 10

Algorithm:

individual : $(x,\theta) \in \mathbb{Z}^n \times \mathbb{R}_+$

mutation : $\theta^{(t+1)} = \theta^{(t)} \cdot \exp(N)$, $N \sim N(0, 1/n)$.

if $heta^{(t+1)} < 1$ then $heta_{t+1} = 1$

calculate new q for G_i from θ_{t+1}

 $\forall j = 1, \dots, n : X_j^{(t+1)} = X_j^{(t)} + (G_{1,j} - G_{2,j})$

recombination: discrete (uniform crossover)

selection : (μ, λ) -selection

(Rudolph, PPSN 1994)

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