

Computational Intelligence

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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).

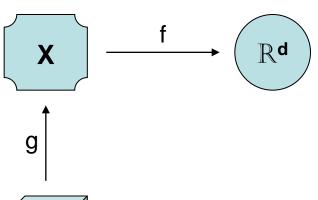
ad 1) different "schools":

- (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

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 $(f \circ g)(b) = f(g(b))$ where g: $\mathbb{B}^n \to X$ is genotype-phenotype mapping
- selection operation independent from representation

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

• 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*

000	001	010	011	100	101	110	111			
0	1	2 3		4	5	6	7			
1 B	Bit 2 E	Bit 1 E	3 l	Bit 1 ↑	Bit 2	Bit 1	Bit			
Hamming cliff										

depending de

L = 0, R = 7n = 3

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 $b_i = \left\{ \begin{array}{ll} a_i, & \text{if } i = 1 \\ a_{i-1} \oplus a_i, & \text{if } i > 1 \end{array} \right. \oplus = XOR$

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

OK, no hamming cliffs any longer ...

- ⇒ 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 → 100 ⇒ ☺

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

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.

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

Design of Evolutionary Algorithms

Lecture 07

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?

⇒ need design guidelines ...

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

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.

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

Formally:

Definition:

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*.

Knowledge available:

Discrete distribution with support $\{x_1, x_2, \dots x_n\}$ with $x_1 < x_2 < \dots x_n < \infty$ $p_k = P\{X = x_k\}$

⇒ leads to nonlinear constrained optimization problem:

$$-\sum_{k=1}^n p_k \, \log p_k \quad o ext{max!}$$
 s.t. $\sum_{k=1}^n p_k \, = \, 1$

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

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

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

partial derivatives:

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

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

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





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.
$$\sum_{k=1}^n p_k = 1 \qquad \text{and} \qquad \sum_{k=1}^n k \, p_k = \nu$$

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

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

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

partial derivatives:

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

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

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

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Excursion: Maximum Entropy Distributions

Lecture 07

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

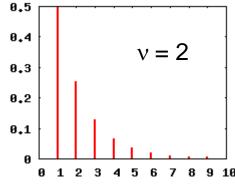
$$\Rightarrow$$
 discrete Boltzmann distribution $p_k = \frac{q^k}{\sum\limits_{i=1}^n q^i}$ $(q = e^b)$

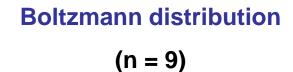
 \Rightarrow value of q depends on v via third condition: (\star)

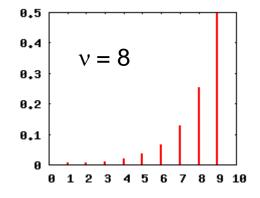
$$\sum_{k=1}^{n} k p_k = \frac{\sum_{k=1}^{n} k q^k}{\sum_{i=1}^{n} q^i} = \frac{1 - (n+1) q^n + n q^{n+1}}{(1-q)(1-q^n)} \stackrel{!}{=} \nu$$

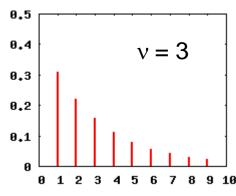
Excursion: Maximum Entropy Distributions

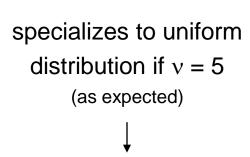
Lecture 07

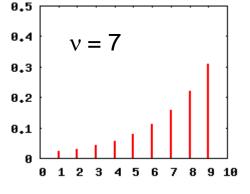


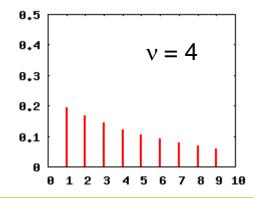


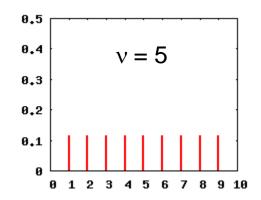


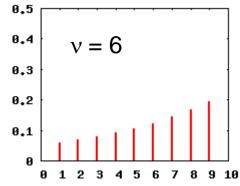












Knowledge available:

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

⇒ leads to nonlinear constrained optimization problem:

$$-\sum_{k=1}^n p_k \log p_k \longrightarrow \max!$$

s.t.
$$\sum_{k=1}^n p_k = 1 \quad \text{and} \quad \sum_{k=1}^n k \, p_k = \nu \quad \text{and} \quad \sum_{k=1}^n (k-\nu)^2 \, p_k = \eta^2$$

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_k

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

Linear constraints uniquely determine distribution:

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

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

III. $p_1 + 0 + p_3 = \eta^2$
 $p_1 = \frac{\eta^2}{2}$

III-I: $p_2 + 2p_3 = 1$ $p_3 = \frac{\eta^2}{2}$

III-II: $p_2 + 2p_3 = 1$ $p_3 = \frac{\eta^2}{2}$

$$\Rightarrow p = \left(\frac{\eta^2}{2}, 1 - \eta^2, \frac{\eta^2}{2}\right) \qquad \begin{array}{c} \eta^2 = \frac{1}{4} & \eta^2 = \frac{2}{3} & \eta^2 = \frac{4}{5} \\ \frac{0.5}{0.6} & \frac{0.5}{0.2} & \frac{0$$

Knowledge available:

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

⇒ leads to infinite-dimensional nonlinear constrained optimization problem:

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

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

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

Excursion: Maximum Entropy Distributions

Lecture 07

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

partial derivatives:

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

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

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

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Excursion: Maximum Entropy Distributions

Lecture 07

$$\Rightarrow e^{a-1} = \frac{1}{\sum_{k=0}^{\infty} (e^b)^k}$$

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

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

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

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

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

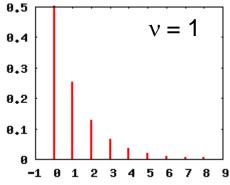
$$\sum_{k=0}^{\infty} k \, p_k \, = \, \frac{\sum_{k=0}^{\infty} k \, q^k}{\sum_{i=0}^{\infty} q^i} \, = \, \frac{q}{1-q} \, \stackrel{!}{=} \, \nu$$

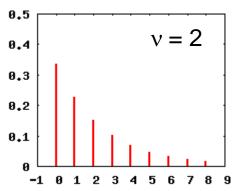
$$\Rightarrow q = \frac{\nu}{\nu + 1} = 1 - \frac{1}{\nu + 1}$$

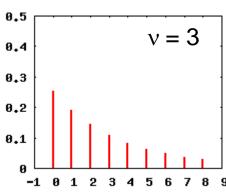
$$\Rightarrow p_k = \frac{1}{\nu+1} \left(1 - \frac{1}{\nu+1}\right)^k$$

Excursion: Maximum Entropy Distributions

Lecture 07



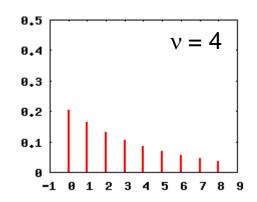


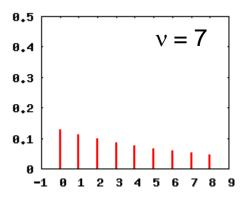


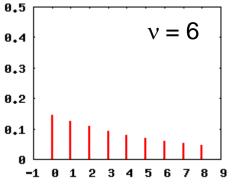
geometrical distribution

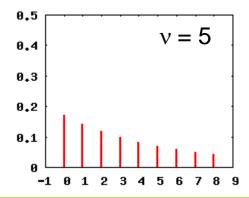
with E[x] =
$$v$$

$$p_k$$
 only shown for $k = 0, 1, ..., 8$









Overview:

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

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

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

support \mathbb{N} \Rightarrow not defined!

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

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

support \mathbb{Z} \Rightarrow not defined!

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

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

Excursion: Maximum Entropy Distributions

Lecture 07

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

⇒ uniform distribution

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

support \mathbb{R}

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

support \mathbb{R}^n

with $E[X] = \theta$

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:

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

for permutation distributions?

→ uniform distribution on all possible permutations

```
 \begin{array}{l} \text{set } v[j] = j \text{ for } j = 1, \ 2, \ \dots, \ n \\ \\ \text{for } i = n \text{ to } 1 \text{ step } -1 \\ \\ \text{draw } k \text{ uniformly at random from } \{\ 1, \ 2, \ \dots, \ i\ \} \\ \\ \text{swap } v[i] \text{ and } v[k] \\ \\ \text{endfor} \\ \end{array} \right) \begin{array}{l} \text{generates permutation uniformly at random in } \\ \\ \Theta(n) \text{ time} \\ \end{array}
```

Guideline:

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!)

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

- every recombination results in some $z \in \mathbb{Z}^n$
- mutation of z may then lead to any $z^* \in \mathbb{Z}^n$ with positive probability in one step
- ad b) need maximum entropy distribution over support \mathbb{Z}^n
- ad c) control variability by parameter
 - → formulate as constraint of maximum entropy distribution

ad 2) design guidelines for variation operators in practice

 $X = \mathbb{Z}^n$

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

 \Rightarrow need <u>analytic</u> solution of a ∞ -dimensional, nonlinear optimization problem with constraints!

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

s.t.

$$p_k = p_{-k} \quad \forall k \in \mathbb{Z}$$
 ,

(symmetry w.r.t. 0)

$$\sum_{k=0}^{\infty} p_k = 1,$$

(normalization)

$$\sum_{k=-\infty}^{\infty} p_k = \sum_{k=-\infty}^{\infty} |k| p_k = \theta$$

(control "spread")

$$k = -\infty$$
 $p_k \geq 0 \quad \forall k \in \mathbb{Z}$.

(nonnegativity)

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:

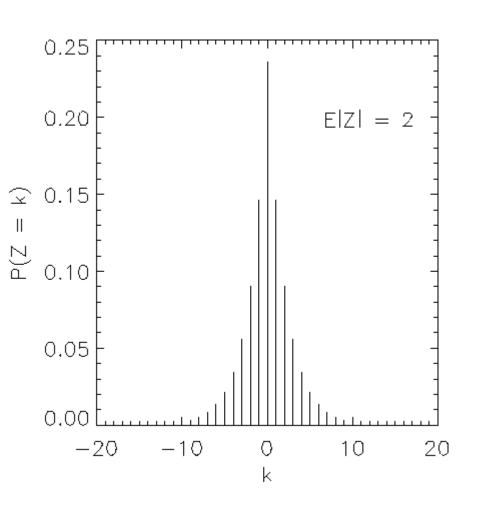
$$Z = G_1 - G_2$$

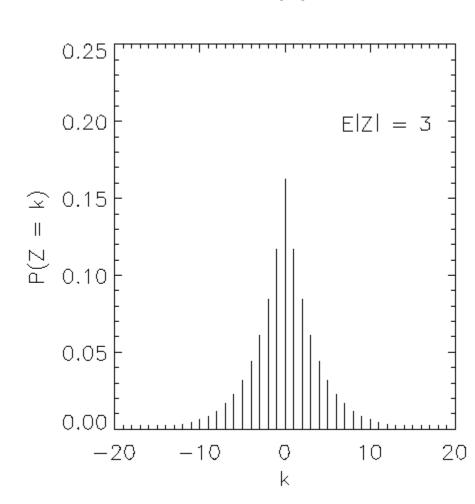
where

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

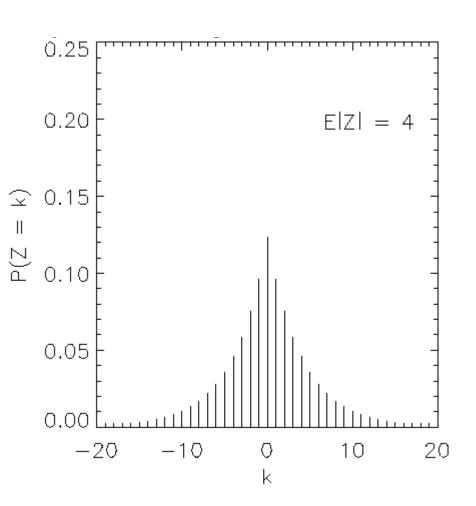
stochastic independent!

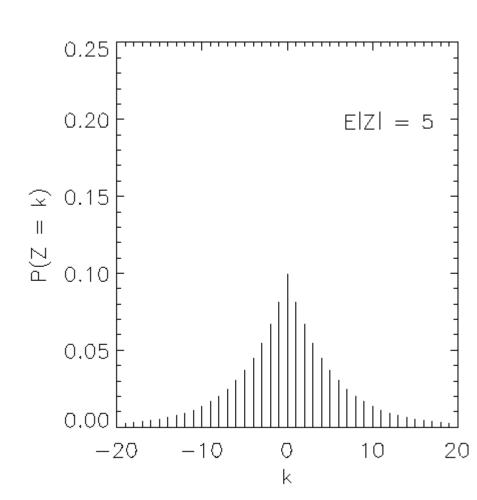
probability distributions for different mean step sizes $E|Z| = \theta$





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





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!

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

$$\in \mathbb{R}_+$$

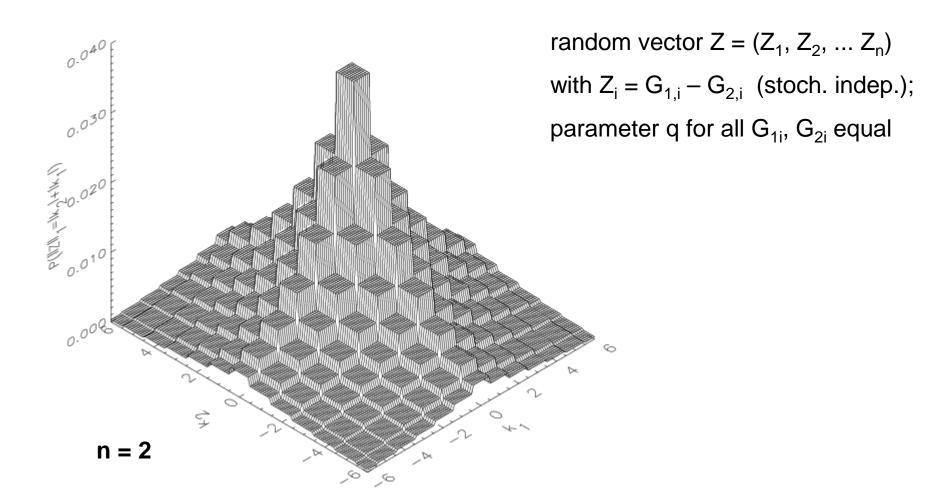
$$\in (0,1)$$

 $\rightarrow \theta$ adjustable by mutative self adaptation

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

 \rightarrow get q from θ

n - dimensional generalization



n - dimensional generalization

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

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

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

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

- \Rightarrow n-dimensional distribution is symmetric w.r.t. ℓ_1 norm!
- ⇒ all random vectors with same step length have same probability!

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

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

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

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
$$\theta^{(t+1)} < 1$$
 then $\theta_{t+1} = 1$

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 :
$$(\mu, \lambda)$$
-selection

(Rudolph, PPSN 1994)

ad 2) design guidelines for variation operators in practice

<u>continuous search space</u> $X = \mathbb{R}^n$

- a) reachability
- b) unbiasedness
- c) control
- ⇒ leads to CMA-ES!