technische universität
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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 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

$\Rightarrow$ use maximum entropy distribution for sampling!

<u>properties:</u>

- distributes probability mass as uniform as possible

- additional knowledge can be included as constraints:
  $\rightarrow$ 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 { $x_1, x_2, \ldots x_n$ } with $x_1 < x_2 < \ldots x_n < \infty$

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

⇒ leads to nonlinear constrained optimization problem:

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

$$\text{s.t.} \quad \sum_{k=1}^{n} p_k = 1$$

<u>solution:</u> 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:

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

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

$$\Rightarrow \sum_{k=1}^{n} p_k = \sum_{k=1}^{n} e^{a-1} = n\, e^{a-1} \overset{!}{=} 1 \quad \Leftrightarrow \quad e^{a-1} = \frac{1}{n}$$

$$p_k = \frac{1}{n}$$

uniform distribution

■

Knowledge available:

Discrete distribution with support { 1, 2, …, n } with p_k = P { X = k } **and** E[X] = ν

$\Rightarrow$ leads to nonlinear constrained optimization problem:

$$-\sum_{k=1}^{n} p_k \log p_k \quad \rightarrow \text{max!}$$

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

<u>solution:</u> via Lagrange (find stationary point of Lagrangian function)

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

Excursion: Maximum Entropy Distributions

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

partial derivatives:

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

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

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

$$\Rightarrow \quad \sum_{k=1}^{n} p_k = e^{a-1} \sum_{k=1}^{n} (e^b)^k \stackrel{!}{=} 1$$

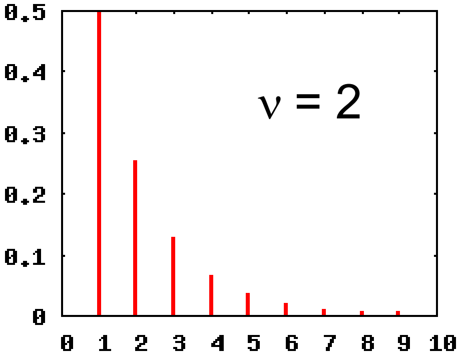
(continued on next slide)

$$\Rightarrow \quad e^{a-1} = \frac{1}{\sum\limits_{k=1}^{n} (e^b)^k} \qquad \Rightarrow \quad p_k = e^{a-1+b\,k} = \frac{(e^b)^k}{\sum\limits_{i=1}^{n} (e^b)^i}$$

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

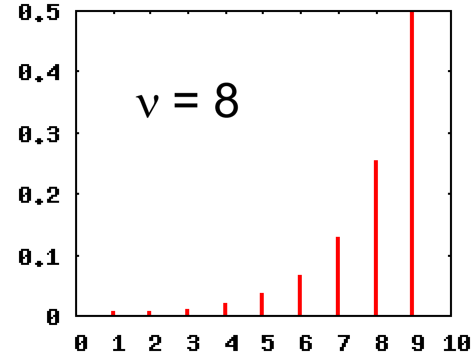
$\Rightarrow$ value of q depends on ν via third condition: (*)

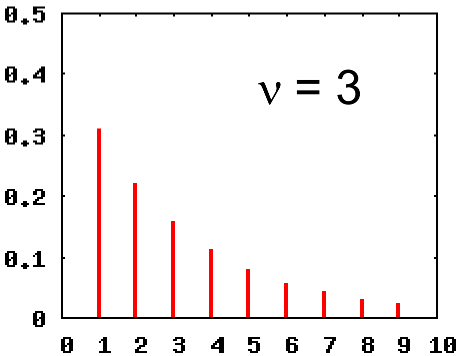
$$\sum_{k=1}^{n} k\, p_k = \frac{\sum\limits_{k=1}^{n} k\, q^k}{\sum\limits_{i=1}^{n} q^i} = \frac{1-(n+1)\, q^n + n\, q^{n+1}}{(1-q)\,(1-q^n)} \overset{!}{=} \nu$$



Boltzmann distribution

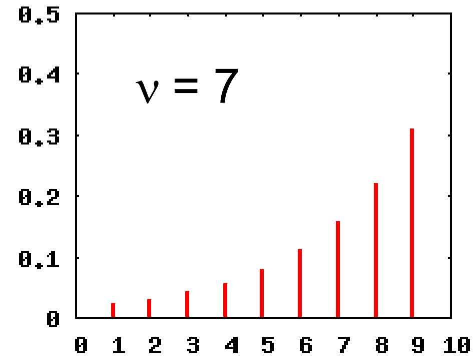
(n = 9)

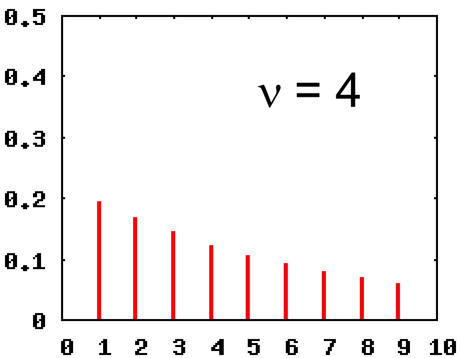


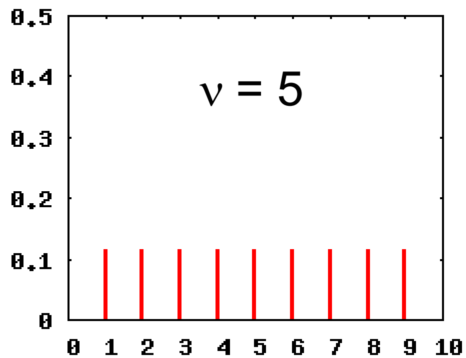


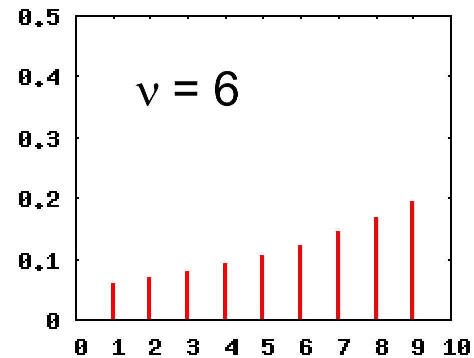
specializes to uniform distribution if ν = 5

(as expected)









Knowledge available:

Discrete distribution with support { 1, 2, …, n } with E[X] = ν **and** V[X] = η^2

$\Rightarrow$ leads to nonlinear constrained optimization problem:

$$-\sum_{k=1}^{n} p_k \log p_k \quad \rightarrow \text{max!}$$

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

<u>solution:</u> in principle, via Lagrange (find stationary point of Lagrangian function)

but very complicated analytically, if possible at all

$\Rightarrow$ consider special cases only

note: constraints are linear equations in p_k

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

Linear constraints uniquely determine distribution:

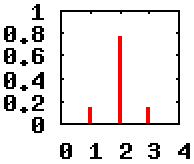
$$
\begin{array}{llcl}
\text{I.} & p_1 + p_2 + p_3 & = & 1 \\
\text{II.} & p_1 + 2\,p_2 + 3\,p_3 & = & 2 \\
\text{III.} & p_1 + 0 + p_3 & = & \eta^2
\end{array}
$$

$$
\begin{array}{llcl}
\text{II – I:} & p_2 + 2\,p_3 & = & 1 \\
\text{I – III:} & p_2 & = & 1 - \eta^2
\end{array}
\Bigg\} \quad p_3 = \frac{\eta^2}{2}
$$

insertion in III. $\Rightarrow \quad p_1 = \frac{\eta^2}{2}$

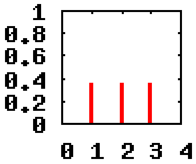
$$\Rightarrow \quad p = \left(\frac{\eta^2}{2}, 1 - \eta^2, \frac{\eta^2}{2} \right)$$

$\eta^2 = \frac{1}{4}$



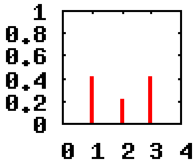
unimodal

$\eta^2 = \frac{2}{3}$



uniform

$\eta^2 = \frac{4}{5}$



bimodal

Knowledge available:

Discrete distribution with unbounded support { 0, 1, 2, … } and E[X] = ν

⇒ leads to infinite-dimensional nonlinear constrained optimization problem:

$$-\sum_{k=0}^{\infty} p_k \log p_k \quad \rightarrow \text{max!}$$

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

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

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

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

partial derivatives:

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

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

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

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

(continued on next slide)

$$\Rightarrow \quad e^{a-1} = \frac{1}{\sum\limits_{k=0}^{\infty} (e^b)^k} \qquad \Rightarrow \quad p_k = e^{a-1+b\,k} = \frac{(e^b)^k}{\sum\limits_{i=0}^{\infty} (e^b)^i}$$

insert

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

$$\Rightarrow \quad p_k = (1-q)\, q^k \quad \text{for} \quad k = 0, 1, 2, \ldots$$

geometrical distribution

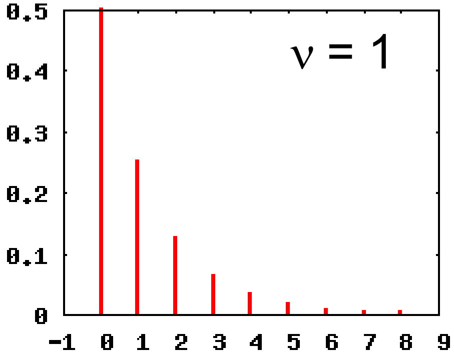
it remains to specify q; to proceed recall that $\sum\limits_{k=0}^{\infty} k\, q^k = \frac{q}{(1-q)^2}$

⇒ value of q depends on ν via third condition: (*)

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

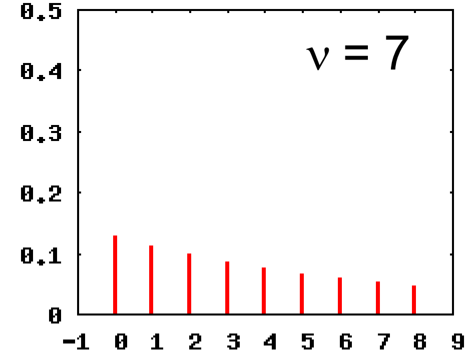
⇒ $$q = \frac{\nu}{\nu+1} = 1 - \frac{1}{\nu+1}$$

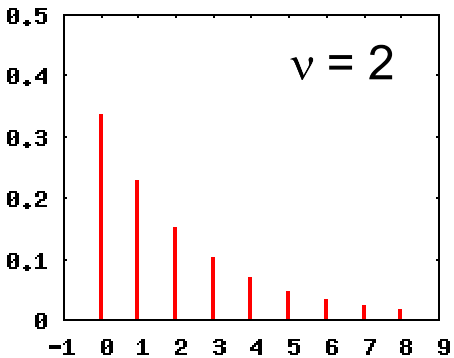
⇒ $$p_k = \frac{1}{\nu+1}\left(1 - \frac{1}{\nu+1}\right)^k$$



geometrical distribution

with E[x] = ν





p_k only shown
for k = 0, 1, …, 8