

Computational Intelligence

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- Design of Evolutionary Algorithms
 - Design Guidelines
 - Genotype-Phenotype Mapping
 - Maximum Entropy Distributions

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).

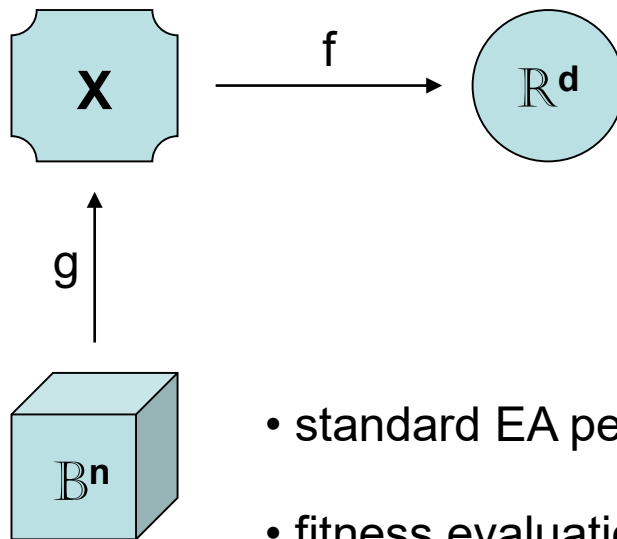
ad 1) different “schools“:

- (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 $f: X \rightarrow \mathbb{R}^d$

scenario: no standard algorithm for search space X available



- 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 $g: \mathbb{B}^n \rightarrow X$ is genotype-phenotype mapping
- selection operation independent from representation

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

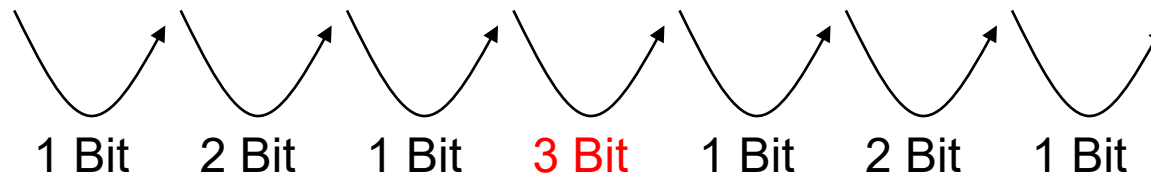
- Standard encoding for $b \in \mathbb{B}^n$

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

→ Problem: *hamming cliffs*

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

← genotype
← phenotype



↑
Hamming cliff

L = 0, R = 7
n = 3

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

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

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

$\oplus = \text{XOR}$

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: $000 \rightarrow 100 \Rightarrow \text{☹}$

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

- 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) $g: \mathbb{B}^n \rightarrow X$ can be computed efficiently (otherwise it is senseless)
- 2) $g: \mathbb{B}^n \rightarrow X$ is surjective (otherwise we might miss the optimal solution)
- 3) $g: \mathbb{B}^n \rightarrow X$ *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 .

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

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
 \Rightarrow 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 $x_1 < x_2 < \dots < x_n < \infty$

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

⇒ leads to nonlinear constrained optimization problem:

$$\begin{aligned} & - \sum_{k=1}^n p_k \log p_k \quad \rightarrow \max! \\ \text{s.t.} \quad & \sum_{k=1}^n p_k = 1 \end{aligned}$$

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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partial derivatives:

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

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

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

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



Knowledge available:

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

\Rightarrow leads to nonlinear constrained optimization problem:

$$\begin{aligned} & - \sum_{k=1}^n p_k \log p_k \quad \rightarrow \max! \\ \text{s.t.} \quad & \sum_{k=1}^n p_k = 1 \quad \text{and} \quad \sum_{k=1}^n k p_k = \nu \end{aligned}$$

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:

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

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

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

(continued on next slide)

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

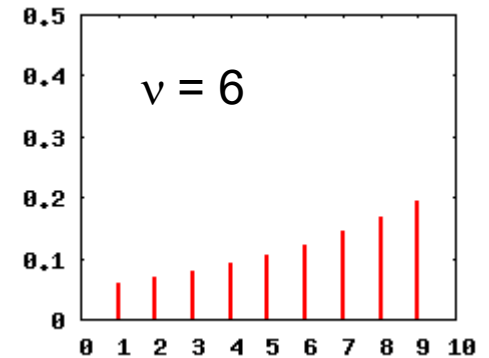
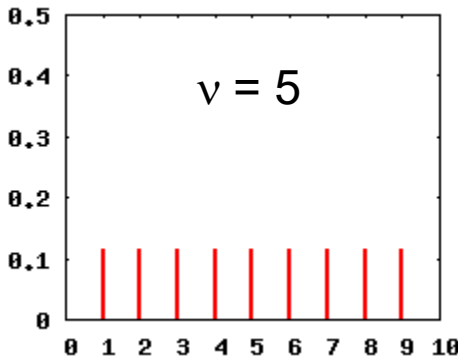
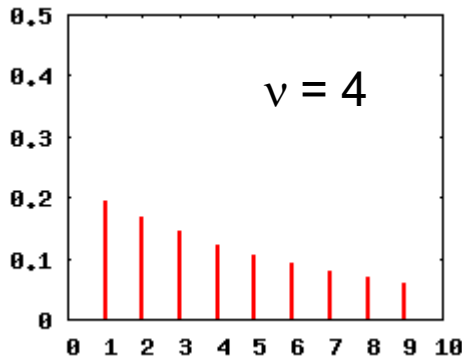
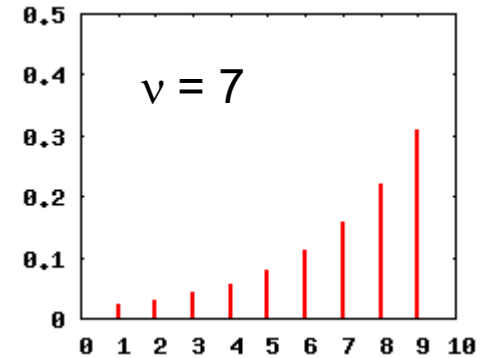
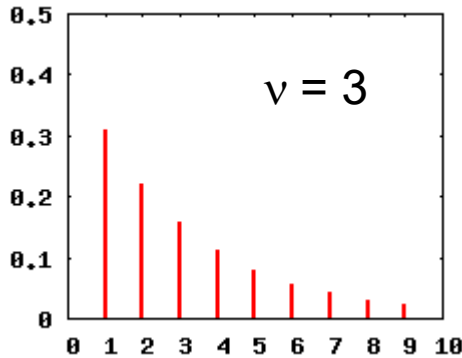
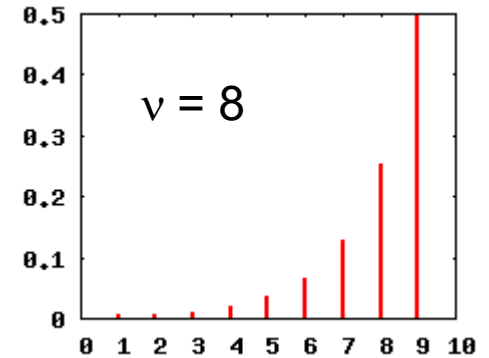
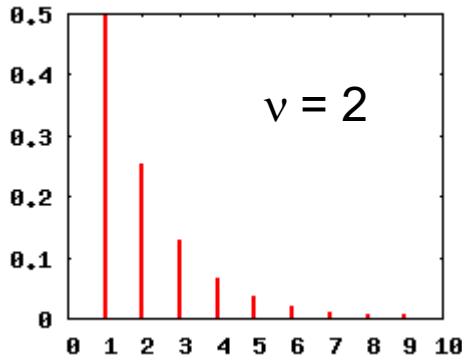
$$\Rightarrow \text{discrete Boltzmann distribution} \quad p_k = \frac{q^k}{\sum_{i=1}^n q^i} \quad (q = e^b)$$

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

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

Boltzmann distribution ($n = 9$)

specializes to uniform
distribution if $v = 5$
(as expected)



Knowledge available:

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

\Rightarrow leads to nonlinear constrained optimization problem:

$$\begin{aligned} & - \sum_{k=1}^n p_k \log p_k \quad \rightarrow \max! \\ \text{s.t.} \quad & \sum_{k=1}^n p_k = 1 \quad \text{and} \quad \sum_{k=1}^n k p_k = \nu \quad \text{and} \quad \sum_{k=1}^n (k - \nu)^2 p_k = \eta^2 \end{aligned}$$

solution: 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 $V[X] = \eta^2$

Linear constraints uniquely determine distribution:

$$\text{I. } p_1 + p_2 + p_3 = 1$$

$$\text{II. } p_1 + 2p_2 + 3p_3 = 2$$

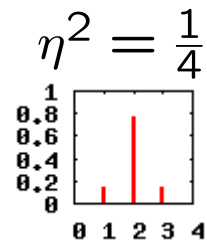
$$\text{III. } p_1 + 0 + p_3 = \eta^2$$

$$\text{II} - \text{I: } p_2 + 2p_3 = 1$$

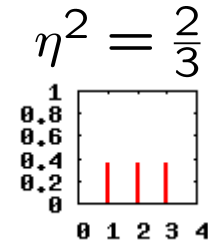
$$\text{I} - \text{III: } p_2 = 1 - \eta^2$$

$$\left. \begin{array}{l} p_1 = \frac{\eta^2}{2} \\ p_3 = \frac{\eta^2}{2} \end{array} \right\} \begin{array}{l} \uparrow \\ \text{insertion in III.} \end{array}$$

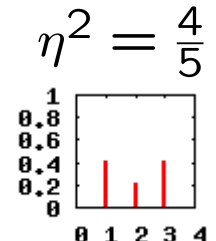
$$\Rightarrow p = \left(\frac{\eta^2}{2}, 1 - \eta^2, \frac{\eta^2}{2} \right)$$



unimodal



uniform



bimodal

Knowledge available:

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

\Rightarrow leads to infinite-dimensional nonlinear constrained optimization problem:

$$\begin{aligned} & - \sum_{k=0}^{\infty} p_k \log p_k \quad \rightarrow \max! \\ & \text{s.t.} \quad \sum_{k=0}^{\infty} p_k = 1 \quad \text{and} \quad \sum_{k=0}^{\infty} k p_k = \nu \end{aligned}$$

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:

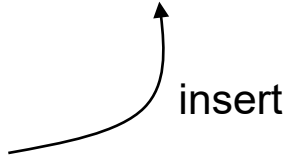
$$\frac{\partial L(p, a, b)}{\partial p_k} = -1 - \log p_k + a + b k \stackrel{!}{=} 0 \quad \Rightarrow \quad p_k = e^{a-1+bk}$$

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

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

(continued on next slide)

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

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

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

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

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

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

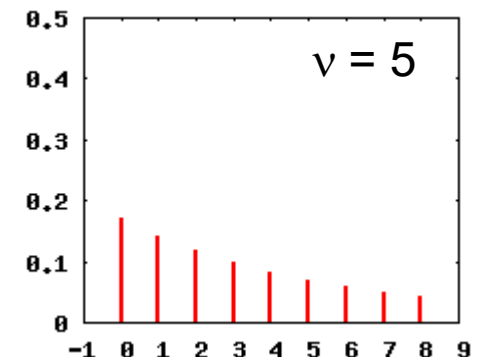
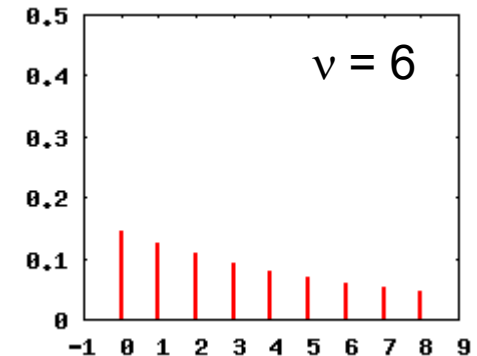
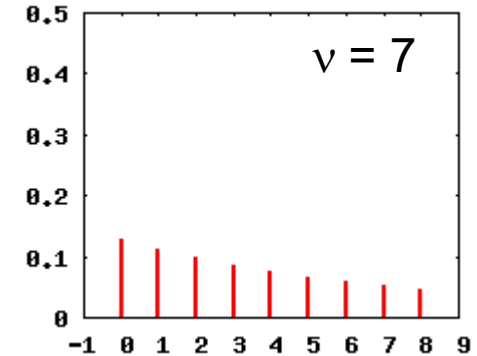
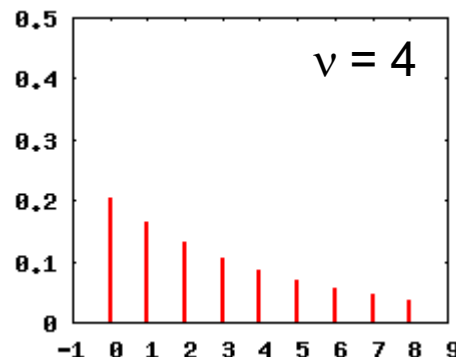
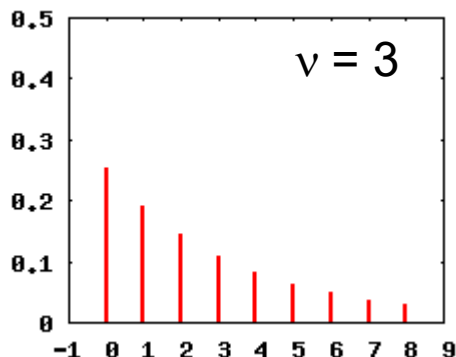
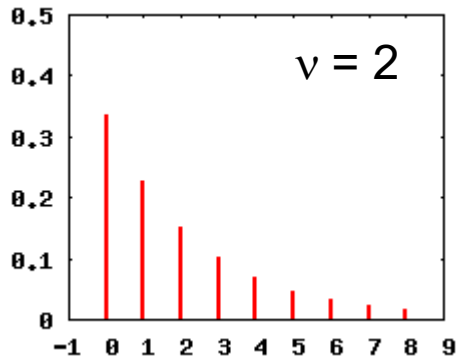
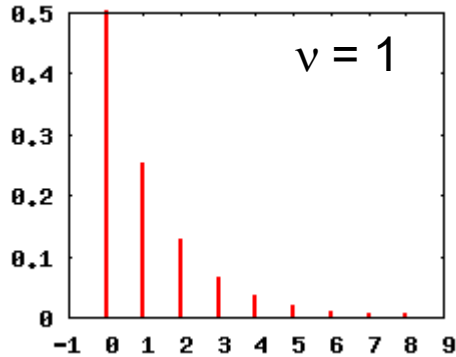
$$\Rightarrow q = \frac{\nu}{\nu + 1} = 1 - \frac{1}{\nu + 1}$$

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

geometrical distribution

with $E[x] = \nu$

p_k only shown
for $k = 0, 1, \dots, 8$



Overview:

support $\{ 1, 2, \dots, n \}$ \Rightarrow *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.)

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

support \mathbb{R}^+ with $E[X] = \theta$ \Rightarrow 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 $\text{Cov}[X] = C$ \Rightarrow multinormal distribution $N(\theta, C)$

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

```
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
 $\Theta(n)$ time

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!)