Oleksandr Voroshylov (6590822) 7.05.2014

Übung zur Vorlesung Struktur und Simulation.

Aufgabe 1

Gegeben $S=-k\sum p_i \log(p_i)$. Fuer $p_i=\frac{1}{N}$ zeigen dass $S=k\log(N)$

Loesung: $S=-k\sum_{i=0}^{N}\frac{1}{N}\log(\frac{1}{N})$ => $S=k\sum_{i=0}^{N}\frac{1}{N}\log(N)$ => $S=\frac{k}{N}\log(N)\sum_{i=0}^{N}1$ =>

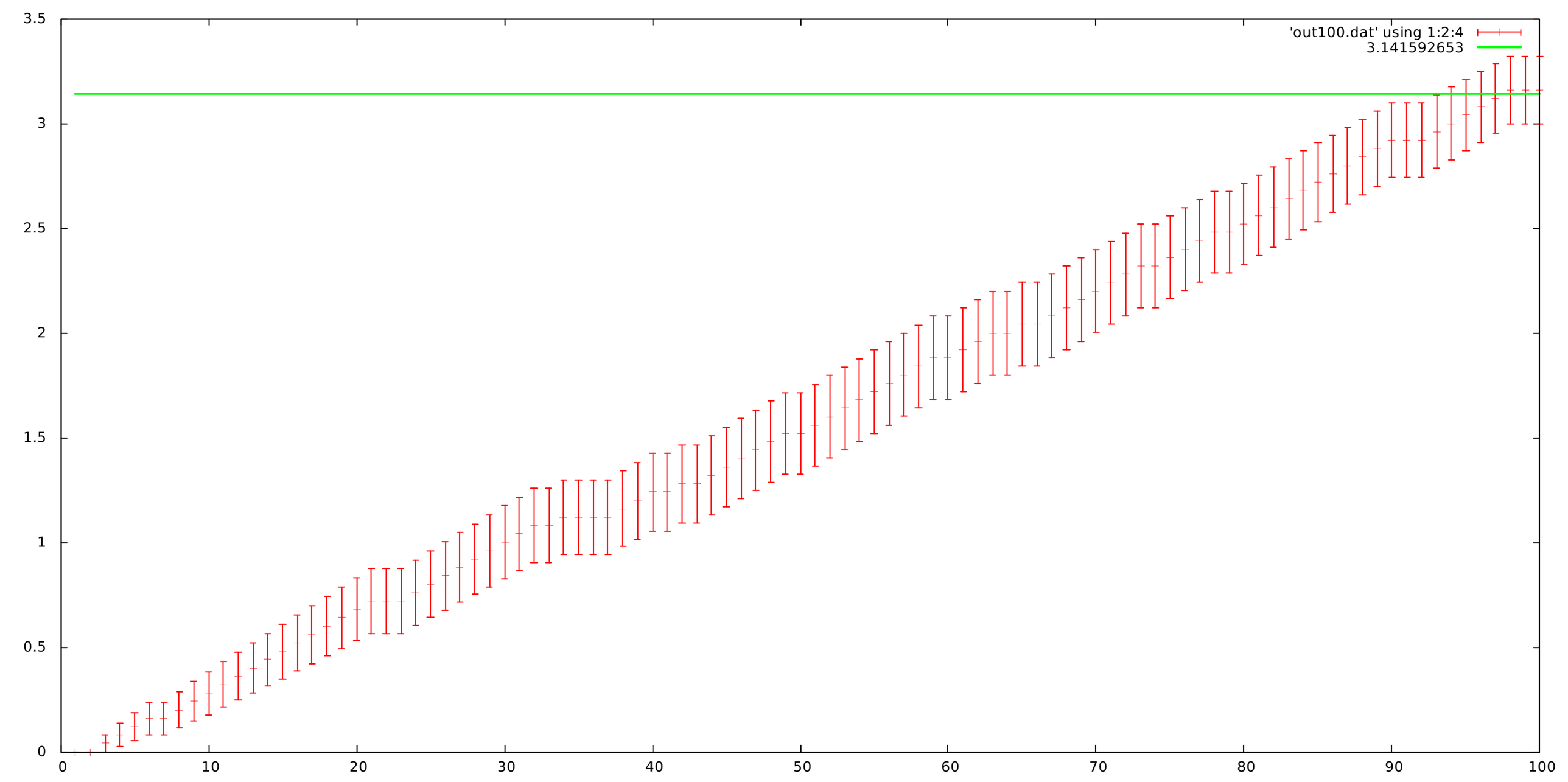
$S=\frac{Nk}{N}\log(N)$ => $S=k\log(N)$

Aufgabe 2

aufgabe2.py

State	E	e^(-E/RT)	p	p*Log(p)
T= 3K				
	1	0 1.0	1.5051660576620003e-35	-1.2068658517805181e-33
	2	-1 2.577554114851961e+17	3.879646965462193e-18	-1.5553810211655957e-16
	3	-2 6.643785214990277e+34	1.0	0.0
		Z: 6.643785214990277e+34		S: 1.5553810211655957e-16
T= 300K				
	1	0 1.0	0.21174035343869668	-0.32870456071133425
	2	-1 1.4931797031726477	0.31616639809726466	-0.3640613795467765
	3	-2 2.229585625966756	0.47209324846403866	-0.35434316154485274
		Z: 4.722765329139404		S: 1.0471091018029635
T= 300000K				
	1	0 1.0	0.33319970630782186	-0.3661908921680369
	2	-1 1.0004009882494296	0.3333333154747647	-0.3662040944616284
	3	-2 1.0008021372904352	0.3334669782174134	-0.3662172484627384
		Z: 3.001203125539865		S: 1.0986122350924037

State	E	e^(-E/RT)	p	p*Log(p)
T=300K				
(1, 1)		-5 7.422674044658944	0.09900260169200192	-0.22895432249481829
(1, 2)		-1 1.4931797031726477	0.019915824744339252	-0.07799516244171611
(1, 3)		-2 2.229585625966756	0.02973790528019095	-0.10453863308702062
(2, 1)		-1 1.4931797031726477	0.019915824744339252	-0.07799516244171611
(2, 2)		-7 16.549487356208104	0.22073477766579955	-0.3334846450762381
(2, 3)		-3 3.3291720031790426	0.044404036579251835	-0.1382930371709111
(3, 1)		-2 2.229585625966756	0.02973790528019095	-0.10453863308702062
(3, 2)		-3 3.3291720031790426	0.044404036579251835	-0.1382930371709111
(3, 3)		-9 36.898499126520164	0.4921470874346344	-0.34892128499607766
		Z: 74.9745351920241		S: 1.5530139179664297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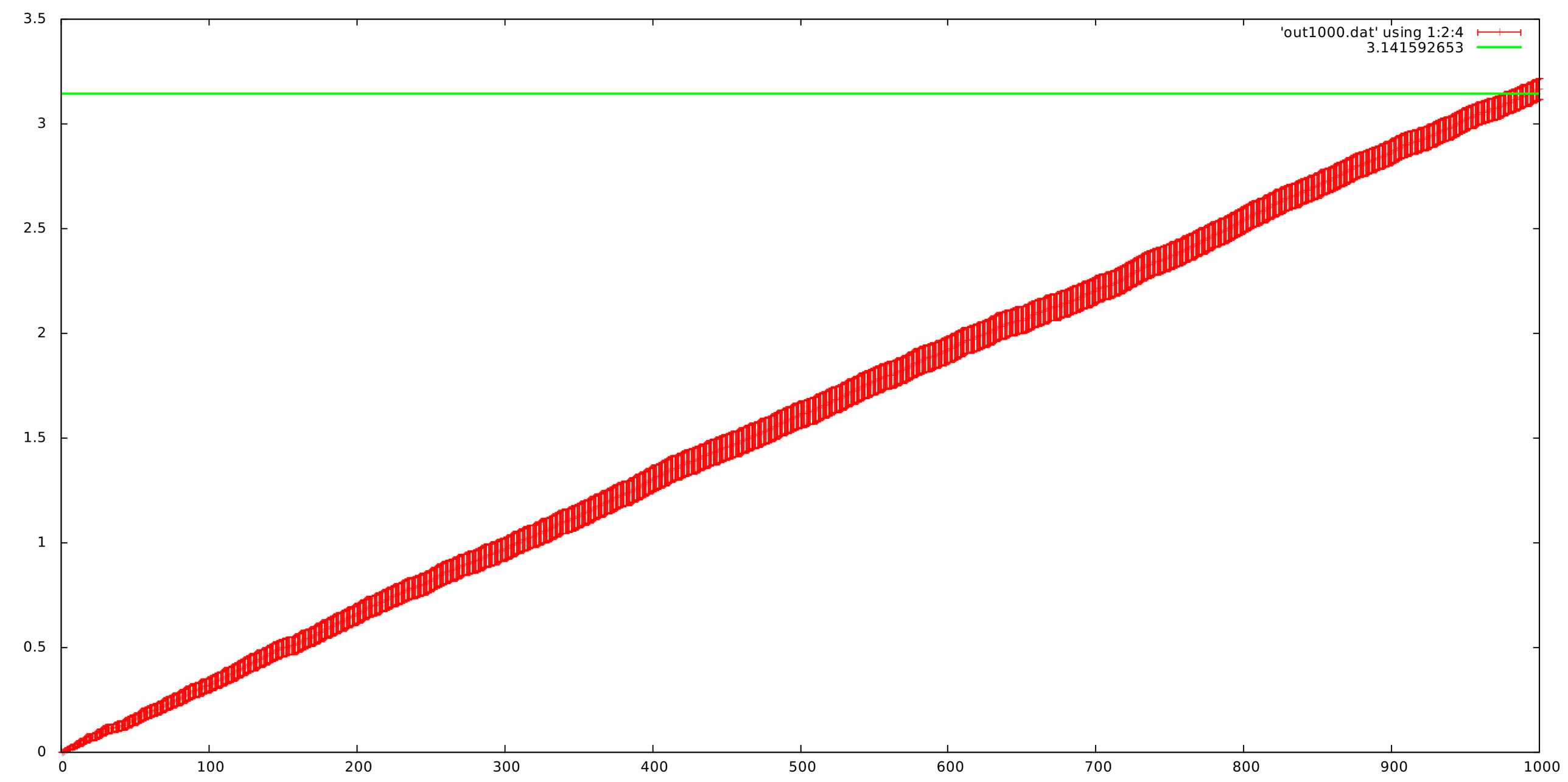
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