Artificial Immune Systems for Solving the Traveling Salesman Problem

A use of CLONALG in Pathfinding and Optimization

Bachelor Thesis

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Abstract

This thesis will examine the performance of artificial immune system algorithms, based on the clonal selection principle in solving traveling salesman problems. The CLONALG algorithm will be compared to a more conventional heuristic greedy algorithm. Furthermore variants with adaptive parameter control of the CLONALG will be compared to the original CLONALG. The results will show that the clonal algorithms can achieve better results under certain circumstances but are in their general form not as efficient as the heuristic algorithm. This thesis examines also if parameter control is beneficial in solving traveling salesman problems and shows that dynamic adaptation of certain parameters can enhance the performance of the algorithm.

Abbrevations

BIS Biological Immune System AIS Artificial Immune System

Ab Antibody Ag Antigen

TSP Traveling Salesman Problem

Keywords

Artificial Immune System Clonal Selection Algorithm Negative Selection Traveling Salesman Problem Bio-inspired approach AIS Machine learning

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Introduction

Textkörper mit Bild

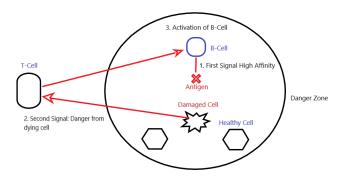


Figure 1.1: Danger Theory state of the art and stuff

Biological Immune System

A biological immune system (BIS) has many features that are useful in machine learning. It can be described with the following terms [?]:

- Distributed
- Parallel
- Multi-level
- Distinguishes between self and non-self
- Noise resistant
- Self-organized
- Associative memory

It is distributed because there is no need for a central control instance, the BIS acts where it need to and it does so immediately without supervising. It can operate on multiple parts of the body simultaneously thus it is parallel. The BIS works in different levels. At first there is the physical barrier, the skin and the body fluids. If this level fails the innate immune system responds, which is a pre-programmed immune reaction that can respond to known and non-changing threats. Finally, there is the adaptive immune system if all of the previous levels fail. This is the system most interesting for computational science, because of its ability to learn on its own. A very important ability of the BIS is the distinguishing between any self-element of the body and the non-self or potential threat. It is noise resistant because it can react to variations of known threats. The BIS does not need any supervising through the brain or any other central system to organize its work flow, therefore its self-organized. Finally, it has an associative memory which is used to react on similar and variant of threats already encountered. As mentioned above, the adaptive immune system is the most interesting part of the BIS for modelling an artificial immune system (AIS). The immune system uses many principles to be effective, in terms of computational science the principles of negative selection and clonal selection are specifically interesting.

2.1 Negative Selection

The adaptive immune system uses two kind of lymphocytes to counter a threat. The T-Lymphocyte and the B-Lymphocyte. Both have different roles but both lymphocytes must have the ability to distinguish between the self and the non-self-cells in the body. A fault in this system can not only lead to an infection, it could trigger an autoimmune reaction because a self-cell could be identified as a non-self threat. To avoid this the Lymphocytes are generated through the process of negative selection. While the B-Cells will be developed in the bone marrow and the T-Cells in the thymus the process is exactly the same. Both cell types are presented to a wide range of self-cells. If any of them react to such a self-cell, the Lymphocyte will be killed and another will be generated. This process is repeated till there are only B- and T-Cells which react to non-self cells [TAN16]. This process will be imitated in the AIS in generating detector sets.

After that the lymphocytes will be released into the tissue and the blood system. The B-cells are called antibodies (Ab) in this context, and any non-self cell is called an antigen (Ag). The B-cell has the ability to recognize and dock to a specific Ag. The ability to recognize an Ag is called affinity. If an Ab has a high affinity to an Ag it is especially good in recognizing and countering this Ag. Because the generation of Lymphocytes and therefore the affinity to different Ag's is random, additional measures are necessary to improve effectiveness.

2.2 Clonal Selection

If a B-Cell encounters an antibody it is able to proliferate (divide) into multiple terminal cells which are clones of the cell. The cell is not only cloned, the different clones will be mutated to improve the affinity to the antigen. The process of cloning and mutating will be repeated till a population and affinity threshold is reached which ensures the most efficient response to the Ag. Only the Ab's with the highest affinity score will be cloned and mutated. If the affinity is high enough, the B-Cell can proliferate into memory cells which will stay after the response and ensure that a secondary response to a similar Ag will be much faster than the initial one [DEC02]. This memory cells represent the associative memory of the adaptive immune system.

The principles of negative selection and clonal selection are important concepts in designing an artificial immune system. The clonal selection aspect of the BIS is basically the learning system. The cloning process is a form of reinforcement learning and leads to a continues improvement [DEC02]. The mutation process itself is called affinity maturation. Random changes in the genes leads to changes in affinity in every single clone. The mutation process is inverse to the affinity level. Higher affinity level means lower mutation rate [DEC02]. Clonal selection is based on the basic evolutionary theory of Charles Darwin.

The three basic principles are [DEC02]:

- repertoire diversity (high population of Ab's)
- \bullet genetic variation (random changes to the population (blind variation))
- natural selection (high affinity Ab's will reproduce and maintained)

These are high level abstract concepts and are only used for a very brief overview of the immune system. The BIS is far more complex but the details are out of scope of this thesis.

Artificial Immune System

3.1 Basics of an AIS

A definition of an AIS is given by [TAN16]: "Articial Immune System (AIS) is a computational intelligence system inspired by the working mechanism and principles of the biological immune system" An AIS can be used in machine learning and is comparable to an artificial neural net in terms of different application fields. It shares some similarities with genetic algorithms due to the cloning and mutation process in clonal selection.

Generally speaking: a set of detectors (antibodies) react to a specific anomaly (antigen). This anomaly could be a malicious code, an IP address and port combination that is not allowed in the network or a pattern that has to be classified. What represents an antigen in the algorithm completely depends on the context and the use of the algorithm. An AIS can be used in an Intrusion Detection System [PAM17], learning and pattern recognition [DEC02], for recommender systems, data mining and clustering [BUR14] and optimization [NAN08].

The basic steps of an AIS can be summarized as [TAN16]:

- 1. Initialize/present antigen
- 2. Initialize antibody population
- 3. Calculate affinity for each antibody to the antigen
- 4. Check life cycle of each antibody and update it
- 5. If stopping condition met go to 6 else go to 3
- 6. Output antibody population

Step 2 and Step 4 are the steps where negative selection and clonal selection will be relevant in most forms of AIS algorithms.

At the time of writing there are mainly 5 concepts that are used in an AIS. The aforementioned negative selection, clonal selection and more recently the immune network theory, the danger theory and the dendritic cells theory.

3.2 Negative Selection in AIS

A typical AIS has a set of detectors which react to any non-self data of the system. The most common way to generate these detectors is to create them randomly and let them undergo a negative selection in which they are presented to self data sets. If one of the detectors recognizes a self data, therefore the affinity is high enough, it will be destroyed. In this case the AIS follows the process that is found in the BIS.

It is important to decide in which way affinity will be measured and which conditions will trigger an immune reaction. If the data that is used consists of numerical values, or is easily converted into a vector of those, the Euclidean distance [4] is commonly used as a mean to measure affinity [TAN16]: (Euclidean Distance Formula)

The Euclidean distance gives us the straight-line distance between two points in an Euclidean space. In the formula above xi and yi are values from two n-dimensional vector x and y.

Another possibility is the use of different variants of the Hammington distance [3]. The Hammington distance is the number of bits that must be changed in two bit strings of the same length to make both strings identical. A common variant of this is the use of the so called r-continues bits. In this case a detector recognizes an element if r continues bit are identical with the element.

Non-self element 0010110 Detector 0011101

In the example above the first 3 continues bit match in both strings. If the threshold of the detector is r = 3, it would react to this bit string if the number of continues bits is 3 or higher. In case of recommender systems another way to measure the affinity is to use the Pearson correlation [5]. But the Pearson correlation is not suited for optimization tasks or specifically the use in the travelling salesman problem.

3.3 Clonal Selection in an AIS

Negative Selection is good for generating a population of detectors. To mimic the learning abilities of the biological immune system, the clonal selection principle can be used. The CLONALG algorithm was proposed by [DEC02] in 2002 and is the foundation of many AIS algorithms that use the clonal selection principle. The CLONALG is also present in more recent variations of the AIS like in aiNet and in algorithms the utilize the immune network theory [CITACION NEEDED]. This thesis will focus on

the CLONALG algorithm and some of its variations, as these algorithms will be used to generate the data in Chapter 5.

3.3.1 CLONALG

The CLONALG algorithm mimics the clonal selection of the BIS on an abstract level. It will be applied mainly at step 4 in the basic AIS sequence in Chapter 3. The algorithm starts with generating a initial population C. It then calculates the affinity of the population to an antigen which is called the fitness. The n best antibodies of the population C will be chosen, determined by a fixed fitness value, and form the antibody set S. Every antibody in S will be cloned and represents our clone set P. Now the clone set will be mutated, every clone get randomly changed relatively to its affinity value. After the mutation the n best clones out of P are chosen. Then a new population will be generated and the process begins anew till a stopping condition is met.

A simple pseudocode can look like this, based on [RIFF09]:

Algorithm 1 Simple CLONALG pseudo code

Generate initial population C of A antibodies

Calculate Fitness(C)

while stopping condition not met do

S= Select the n best antibodies from C

P= Generate clones of the antibodies in S

Mutate(P)

C= Select the n best antibodies out of P

C = C + New population A-n

end

Usually the stopping condition is a given amount of evaluation where no increase in fitness is achieved or felt below a given threshold. The initial CLONALG algorithm as proposed by [DEC02] operates with static parameters and don't adjust anything besides the mutation. Different parameters are needed for different applications fields as was also stated in [DEC02]. This parameters must be changed beforehand and can't adapt dynamically during the runtime of the algorithm.

Although the algorithm is very simple and efficient in solving different tasks like multimodal problems or pattern recognition, drawbacks do exist [GARRET04]. Choosing how many member should be cloned is difficult. The lack of adaptive parameters can lead to inefficiency because of bad scalability and too many evaluations which could have been avoided [Garret04].

3.3.2 Adaptive CLONALG variants

To make the algorithm more efficient and adaptive, some variants where proposed. There are different parameter control strategies for the CLONALG algorithm. One of these variants is proposed by [RIFF09]. It is based on the idea of reinforcement learning. The antibody sets will be either rewarded for a high affinity or penalized for

a low one. This will be achieved through population control. The reward is the increase in antibody population for a given set and the penalty is the decrease in population [RIFF09]. The mutation factor is governed by the population size. This adaptive technique allows the algorithm to adjust the core parameters during runtime and makes it more efficient in problem solving and hardware usage as shown in [RIFF09]. Another method is proposed by [Garret04]. Some techniques from the evolutionary algorithms will be applied to the CLONALG in this approach. An algorithm based on this idea will be evaluated in chapter 5.

Traveling Salesman Problem

4.1 Background

One of the first publications of the traveling salesman problem was by the mathematician Karl Menger in the 1920's [Applegate 1991]. The problem itself was discussed earlier by Sir William Rowam Hamilton and Kirkman [Matai 2010]. It describes a graph with a certain amount of nodes with known distances between the nodes. The goal is to find a route where every node is visited exactly one time and the route ends at the node where it started. The route should be the shortest possible. ((example picture of an tsp))

The algorithmic complexity for a symmetric graph with n nodes is: $\frac{n(n-1)}{2}$ [Applegate 1991]. The graph is symmetric if the distance between two nodes n and m is the same as the distance between m and n. Asymetric traveling salesman problems also exist with a higher complexity of n(n-1)

The complexity of the problem is categorized as non-deterministic polynomial hard (NP-Hard). The runtime of an algorithm can scale exponentially with the number of nodes in the graph. No algorithm is able to solve the problem in polynomial time. Current algorithms work with heuristics to solve the TSP.

The TSP is common in many real world applications. Drilling of printed circuit boards, computer wiring, order picking in warehouses, vehicle routing and DNA sequencing are some fields where the TSP is present [Matai 2010].

4.2 Mathematical definition

The symmetric graph is defined as G = (V, E) where $V = \{1, ..., n\}$ are the vertex or the nodes and $E = \{(i, j) : i, j \in V, i < j\}$ are the edges or routes. Additionally there is an arc set $A = \{i, j) : i, j \in V, i\}$ which defines all routes in the graph, no route can be used twice. A cost matrix is defined on the edge or the arc set. Usually the cost matrix is calculated using the Euclidean distance. [Matai 2010].

A typical TSP consists of a set of cities (V), distances between the cities (E) and the cost measured in the euclidean distance between the cities (C). All TSP used in this thesis will follow this convention.

Evaluation

5.1 Setup

The CLONALG algorithm will be applied to a set of 17 different TSP problems from the TSP library TSPLIB95 [1]. The implementation follows the specification in [DEC02] and is provided by the OAT. The greedy search algorithm will be applied to the same set of problems. This algorithm is provided by the author of the OAT and uses a nearest neighbour technique with mutation and it is quite effective in solving the provided TSP.

The stopping criteria will be no improvement after a set amount of evaluations. No improvement means that the algorithm has not found a shorter route in it's actual iteration compared to the last one, this is often also called stagnation. The criteria for the results are:

- 1. Score
- 2. Time in ms
- 3. Evaluations
- 4. Percentage of optimal score

The score is measured as the summarized Euclidean distance of the presented best tour. The algorithm will be run multiple times on one TSP therefore the arithmetic mean of each criteria will be the end result. To compare the results the mean average error (MAE) of the average score will be used. The MAE is composed from the difference between the score of both algorithms divided through the score of the main compared algorithm, if we want to compare the performance of algorithm A1 to A2 the MAE is calculated as (A2 - A1)/A1. Positive MAE means better performance for A1. The CLONALG algorithm will be applied to the problem set multiple times with different parameters. The adaptive algorithms will be applied only once because of the dynamic parameters.

The parameters which will be altered are

- 1. Population size
- 2. Clone factor
- 3. Selection size
- 4. Random replacements

The first set of parameters will be the default parameters provided by the OAT as shown in table 5.1. The second one are the parameters that are proposed by DeCastro [DEC02] for solving TSP problems about the size of 30 nodes.

The adaptive variant of the CLONALG algorithm will use the default vaulues at the beginning and adjust the paramaters during runtime.

To measure the results, a modified version of the optimization algorithm toolkit (OAT) [2] will be used. The changes are a slightly different set of TSP Problems used in the domain and the addition of an adaptive CLONALG hybrid algorithm. The used TSP problems are listed in the appendix. The distances between the nodes in the TSP problem are measured as Euclidean distance. The implemented CLONALG algorithm is based on the specifications in [DEC02]. The adaptive variants expand the concept based on [RIFF09] and [GARRETT04]. Both algorithms will be applied 100 times on every single TSP problem.

The hardware is a i5-3320M dual core cpu with 2,60ghz each and 8gb of RAM, run on a Windows 10 operating system with only the minimal background tasks. All cpu and RAM usage shown in this thesis is after other processes are taken into account.

5.1.1 Evolution Strategy Parameter Control

The first CLONALG variation is based on [Garret04] and uses a idea from the evolution strategy[CITATION NEEDED]. The original managed to eliminate all parameters except population size from the CLONALG algorithm. This thesis uses a variant where the selection size n is eliminated. This is comparable to Variant C1-C4 from [Garret04. It uses a strategy parameter which will adjust the selection size. The strategy parameter itself will be adjusted by a evolution strategy constant of 1.3. This constant was empirically tested and proofed to be most effective [Garret04]. The adjustment is randomized, the strategy parameter will be either multiplied or divided by the constant based on a 50% chance. The strategy parameter itself will alter the selection size on each evaluation. The evolution strategy calls this evolution approximated by self evolution, however the difference to the original evolution strategy is, that we adjust a parameter indirectly through another parameter [Garret04]. Naturally the selection size still has to be initialized and can't be zero. [Garret04] proposed to start with a small number, the test runs in this thesis start with a selection size of 1. Another difference to the original CLONALG is the absence of random replacements. The population will only be altered by the clones and their mutations. The changes made to the original pseudo code in chapter 3 are shown in algorithm 2. This variant will be called CLONALG ESPC.

Algorithm 2 CLONALG variant with dynamic selection size

```
Set strategy paramater Sp

Generate initial population C of A antibodies

Oc=Calculate Fitness(C)

while stopping condition not met do

S= Select the n best antibodies from C

P= Generate clones of the antibodies in S

Mutate(P)

C= Select the n best antibodies out of P

C= C + New population A-n

If C has better fitness than Oc then

n=Sp * 1.3 OR n= Sp/1.3

else

n=n

end if
```

5.2 Results

5.2.1 CLONALG un-tuned

The algorithms are run 100 times on every TSP. The stopping criteria are no improvements after 10000 iterations of the algorithm. This number is chosen to give the algorithm enough time without restricting it to a specific amount of seconds. The cpu usage spiked around 58% and was average around 30% for all algorithms. This is because the more costly operations like sorting, selection, cloning and mutation will be done in exactly the same way in all algorithms.

The parameters for the original CLONALG are shown in Table 5.1.

The parameter C is the initial population, n is the selection size for cloning, B is the cloning factor (how many clones of the chosen n will be done) and d are the random replacements to keep the new population partially randomized. [DEC02] proposed some tuning to the default parameters for more efficiency in solving TSP. The replacement value d should always be between 5-20% of the population. Higher ratios tend to randomize too much while lower ratios can still produce good results but less reliable and efficient.

	С	n	В	d
Default	50	50	0.1	5
Tuned	300	150	2.0	60

Table 5.1: Tuning parameters

When comparing the results it is clearly seen that the CLONALG algorithm is worse on average than the greedy search algorithm as shown in table 5.2. However the CLONALG was able to find the best solution to ulysses22 with a MAE of 0.117 while the greedy search algorithm could not. The overall time for solving all problems was also shorter for the CLONALG. The number of evaluations is mostly smaller for the CLONALG which shows that stagnation started earlier in this algorithm. The average MAE compared to the greedy algorithm is -0.524. The average MAE calculated on the best score is in the same range with -0.546. The mean average error of -0.009 is small for berlin52 which highlights that CLONALG performs equal or better on small TSP under 50 nodes but is less efficient at more difficult TSP than the greedy algorithm.

TSP	Avgerage Score	Best Score	Best Per-	MAE com-	Average
			centage	pared to	Evalua-
				Greedy	tions
a280	26483.99	25581	891.8960838	-0.885322038	38462.71
berlin52	11077.22	9369	24.22434368	-0.009083507	132557.69
lin105	69431.08	62981	338.0068155	-0.666910122	59348.99
pcb442	649513.41	631174	1143.006814	-0.795694149	38322.66
pr2392	14231642.92	14122859	3635.889819	-0.971810641	32506.49
pr76	299815.73	267781	147.5808763	-0.486638576	73496.26
st70	1765.09	1510	123.7037037	-0.382569727	82887.36
tsp225	31309.96	29905	663.6618999	-0.822318521	41252.29
ulysses22	7273.04	6901	0	0.117078966	27588.51
ch130	31453	29391	381.0310966	-0.630750644	46159.77
ch150	37883.24	36015	451.7003676	-0.660824945	47285.45
eil101	2126.54	1954	210.6518283	-0.525482709	56058.04
eil51	654.65	552	29.57746479	-0.103093256	115597.85
eil76	1377.39	1194	121.9330855	-0.407509856	67914.53
kroA100	96214.68	86675	307.2690537	-0.572862998	60339.55
kroC100	94471.33	85368	311.4318762	-0.550283351	60015.33
kroD100	93282	84305	295.9096459	-0.557829485	57958.20

Table 5.2: CLONALG untuned performance

5.2.2 CLONALG tuned

Comparing the tuned algorithm to the original one shows, that the tuned parameter are not suited for this TSP setup. The tuned CLONALG has a worse average score in solving all 17 TSP compared to the untuned CLONALG. The unexpected outcome is, that the tuned algorithm performs better if the TSP is larger. The MAE on pr2392, which is the largest TSP in the setup, is only -0.014 but the MAE of ulysses22, the smallest TSP, is -0.305. The algorithm could not find the best solution for ulysses22. The average MAE was -0.253 compared to the untuned algorithm. This is especially unexpected because the parameters where tuned by [DEC02] for a 30 node TSP. In their tests, the tuned algorithm behaved better on this specific TSP than the un-tuned one. This shows that the chosen parameters do not work well when the stopping criteria

-0.472116051

-0.308886101

-0.282774782

-0.288957516

-0.277346275

13879.30

13296.35

13492.89

13778.59

14173.76

TSP	Avgerage Score	Best Score	Best Percentage	MAE com-	Average
				pared to	Evalua-
				CLONALG	tions
a280	29313.63	27910	982.202404	-0.09652984	12173.27
berlin52	22284.75	20861	176.5977194	-0.502923748	13140.05
lin105	95696.8	89181	520.2169831	-0.274468112	12437.46
pcb442	695194.14	680524	1240.194572	-0.065709314	12179.71
pr2392	14434730.31	14288477	3679.700396	-0.014069358	11541.92
pr76	445633.5	418899	287.2992539	-0.327214561	12718.28
st70	2826.17	2672	295.8518519	-0.375448045	12650.36
tsp225	35353.65	32603	732.5587334	-0.114378289	12485.88
ulysses22	10459.55	9389	36.05274598	-0.304650774	13776.71
ch130	38766.46	36521	497.7250409	-0.188654316	13543.46
ch150	45610.23	43708	569.5465686	-0.169413529	12907.27
eil101	2773.71	2685	326.8680445	-0.233322878	13245.55

174.6478873

235.6877323

489.5169627

510.5884621

485.1930121

are 10000 evaluations without improvement.

Table 5.3: CLONALG tuned performance

1170

1806

125461

126691

124611

5.2.3 CLONALG ESPC

1240.14

134148.49

132863.13

129082.57

1993

eil51

eil76

kroA100

kroC100

kroD100

The variant with an adaptive selection size shows only a insignificant worse performance with an average MAE of -0.009. The interesting behaviour is seen in the average MAE calculated on the best score with 0.039. This value shows that the adaptive CLONALG is better in finding the shorter route but will also produce some worse ones in the long run. The MAE on the best score was better for all TSP except pcb442, pr76, st70 and eli76. This results highlight that a adaptive selection size altered with the evolution strategy and combined with no random replacements can be beneficial for finding the shorter route. On average the CLONALG ESPC needed less evaluations to terminate, the stagnation started earlier in this variant. The overall runtime was nearly identical for the original CLONALG and the ESPC with close to 19 minutes for the complete run.

TSP	Average	Best	Best	Per-	MAE	com-	MAE on Best	Average			
	Score	Score	centage		pared	to	Score	Evalu-			
					CLONA	ALG		tions			
a280	26559.75	24949	867.3904	1614	-0.0028	52436	0.025331677	34025.59			
berlin52	11120.65	9241	22.52718	3112	-0.0039	05347	0.013851315	173022.70			
lin105	74683.73	60638	321.7122	2192	-0.0703	31918	0.038639137	48963.38			
pcb442	652981.26	637838	1156.130	0608	-0.0053	10796	-0.010447794	35590.02			
pr2392	14259316.88	14060841	3619.484	1329	-0.0019	40763	0.004410689	31152.73			
pr76	316531.58	278997	157.9507	7947	-0.0528	09423	-0.040201149	64605.41			
st70	1912.1	1511	123.8518	3519	-0.0768	84054	-0.000661813	68687.03			
tsp225	31963.99	29509	653.5495	5403	-0.0204	61463	0.013419635	36970.86			
ulysses22	7499.74	6901	0		-0.0302	27715	0	27280.05			
ch130	30748.35	27332	347.3322	2422	0.02291	6677	0.075332943	45024.26			
ch150	38069.35	34981	435.8609	9069	-0.0048	8871	0.029558903	40273.29			
eil101	2111.16	1622	157.8696	5343	0.00728	35094	0.204685573	53395.42			
eil51	650.27	536	25.82159	9624	0.00673	35664	0.029850746	118097.23			
eil76	1405.74	1221	126.9516	5729	-0.0201	67314	-0.022113022	62993.43			
kroA100	91818.4	75100	252.8803	3684	0.04788	80163	0.15412783	62252.60			
kroC100	94006.78	82471	297.4697	7576	0.00494	1665	0.035127499	57812.68			
kroD100	88897.32	75500	254.5599	9699	0.04932	22972	0.116622517	58883.91			

Table 5.4: ESPC performance

Related work

Conclusio

Appendix A

Appendix

List of TSP problems taken from TSPLIB95 library:

a280

berlin52

ch130

ch150

eil101

eil51

eil76

kroA100

kroC100

kroD100

lin 105

pcb442

pr2392

pr76

st70

tsp225

ulysses22

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1.1	Danger Theory																	

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