Sudoku:
Bagging a Difficulty Metric
&
Building Up Puzzles

February 18, 2008

Abstract

Since its inception in 1979, Sudoku has experienced rapidly rising popularity and global interest. We present a difficulty rating metric and three puzzle generation algorithms for the popular Sudoku puzzle. Our metric focuses on the human difficulty of a puzzle, predicting the time an average Sudoku solver will require with $R^2 = 0.71$, rather than calculating an arbitrary computational metric. Furthermore, in predicting a continuous parameter, the metric is both extensible and versatile. It outperforms all other publicly available metrics we considered in predicting human difficulty of a large set of puzzles.

We also present 3 puzzle generation algorithms. The first, a library based algorithm, provides puzzles in O(1) time. The second uses Latin Squares to construct a valid solution grid, and then 'builds up' the puzzle leading to that solution from a blank grid. The third is a template-based generator that can be used to create puzzles with a desired initial configuration, mimicing popular human-constructed Sudoku puzzles. Each of these algorithms, particularly the first two, rapidly provides puzzles with a broad range of difficulties. Furthermore, each method is capable of generating a large number of new puzzles.

Finally, we propose a rapid method of transforming a single valid puzzle into many. The set of valid Sudoku puzzles is closed under several transformations, including row permutation within a band, for example. Using these transformations, we can convert a single puzzle into over 1 trillion, further expanding the efficacy of our generators.

3	4		6	7				
7		9		1				
1				4		3	7	2
2				8		1		
						6		
9	1		4	3		8		
8		5		6		4	1	9
6				5				
4				2				

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1 Introduction

Since its inception in 1979, Sudoku has experienced rapidly rising popularity and global interest. Sudoku puzzles are simple to understand, simple to try, though often not simple to solve.

1.1 History

Sudoku puzzles are related to number puzzles throughout history. The set of valid 9x9 Sudoku solutions are a subset of the 9x9 Latin Squares (invented in 1983 by Euler) and similar to the set of 9x9 Magic Squares, a puzzle invented prior to the 10th century AD.

The modern puzzle was first seen in 1979 in *Dell Magazines* called *Number Place*. Invented by the American architect Howard Garns, the puzzles soon became popular in Japan after being published by Nikoli, the first Japanese puzzle magazine [9].

Sudoku is short for "Su-ji wa dokushin ni kagiru" in Japanese, meaning "the numbers must be single."

1.2 Popularity

Sudoku has become a pop culture phenomenon dubbed the "fasting growing puzzle in the world" in 2005 by the world media [11]. Hundreds, if not thousands, of web sites exist to provide puzzle-addicts with their daily fix; nearly every modern newspaper includes puzzles on a daily or weekly basis.

As a result, the need for efficient and plentiful generation of puzzles has become a particularly profitable venture - CNN Money reports that one firm received "well over $1 million" in revenue in less than a year from a puzzle generating program! [8]

2 Definition of Sudoku

A traditional Sudoku puzzle (see Fig 1(a)) consists of a 9x9 grid of **cells** divided into 9 3x3 subsections called **blocks**.

A Sudoku **solution** (see Fig 1(b)) is such a grid with each cell containing a single number, meeting the follwoing conditions:

- Every cell contains a single number between 1 and 9
- Every row contains each of the numbers 1-9 exactly once
- Every column contains each of the numbers 1-9 exactly once
- Every box contains each of the numbers 1-9 exactly once

A Sudoku **puzzle** is a Sudoku grid with some of the numbers filled in, called **givens**. The givens in a **valid** Sudoku puzzle must satisfy the following conditions:

- The givens do not violate any of the above rules of Sudoku

- There must be a single Sudoku solution that contains the set of givens, i.e. the set of givens must lead to a unique solution.

3	4		6	7				
7		9		1				
1				4		3	7	2
2				8		1		
						6		
9	1		4	3		8		
8		5		6		4	1	9
6				5				
4				2				

(a) The Puzzle

3	4	2	6	7	5	9	8	1
7	8	9	3	1	2	5	6	4
1	5	6	8	4	9	3	7	2
2	6	4	5	8	7	1	9	3
5	3	8	2	9	1	6	4	7
9	1	7	4	3	6	8	2	5
8	2	5	7	6	3	4	1	9
6	7	1	9	5	4	2	3	8
4	9	3	1	2	8	7	5	6

(b) The Solution

Figure 1: Sudoku Puzzle and Solution

While variants abound (e.g. Killer-, Samurai-, and Hyper-Sudoku), for simplicity we consider only traditional 9x9 Sudoku puzzles.

3 Prior Work

The combinatorics, algorithms, and solving techniques of Sudoku are well studied. In 2005, Felgenhauer and Jarvis showed that of the $\approx 5.25 * 10^{27}$ 9x9 Latin Squares, $\approx 6.671 * 10^{21}$ form valid Sudoku grids [3]. Royle hypothesizes the minimum number of clues required to produce a puzzle with unique solution is 17 [10]. Yato and Seta show that solving a Sudoku puzzle is NP-complete [12].

Solving techniques for humans and computers abound. Fowler details many logical strategies humans use to solve Sudoku puzzles, in 7 categories. We omit a lengthy discussion of these strategies. Suffice it to say that they range from the simple - examination of other elements in a given row/column - to the exotic - 'Swordfish', 'X-wing', and 'Forcing Chains' techniques [4]. Computational solving techniques range from brute force algorithms and recursive backtracking (a classic introductory computer science assignment), to stochastic methods, constraint solving algorithms, integer programming, genetic algorithms, and computer learning [1] [5] [6] [7].

Difficulty rating algorithms are widely acknowledged to be more effective at determining computational difficulty rather than apparent difficulty to a human solver. Metrics for determining human-difficulty tend to calculate a function of the techniques described by Fowler - more difficult puzzles will tend to require more difficult techniques more times. However, the choice of weights is often arbitrarily set by the programmer.

Publicly available generating algorithms vary in their approaches. The grand majority, however, use a randomized approach to generation. They repeatedly place a random number in a random position and then check the solvability of the puzzle until the puzzle has a unique solution.

According to Fowler, solving a Sudoku puzzle is easier than generating one, and generating a puzzle is easier than evaluating its difficulty [4]. This is confirmed by Sudoku aficionados' online forums.

4 Goals and Motivation

Goal - to provide a difficulty metric and puzzle generation algorithm that are **human-applicable** rather than arbitrary and esoteric.

4.1 Difficulty Metric

We seek to provide a difficultly metric that is:

- **accurate** - well-correlated to human difficulty data
- **versatile** - widely distributes Sudoku puzzles into difficulty levels
- **extensible** - the number and 'difficulty' of the levels can be changed. This can be achieved by making the metric **continuous** rather than discrete, and using **thresholding** to group into discrete levels

4.2 Puzzle Generation

We seek to provide a puzzle generation algorithm that is:

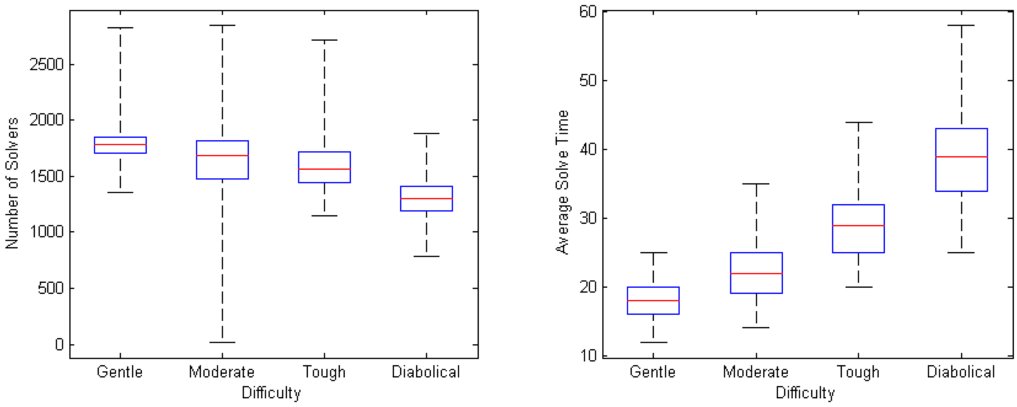
- **efficient** - provides puzzles quickly
- **customizable** - the user should be able to specify difficulty and receive a puzzle of that difficulty in response
- **versatile** - offers a range of difficulty levels
- **scalable** - can provide a few or many puzzles of a given difficulty

5 Data

Actual data derived from many individuals solving many puzzles is necessary to effectively evaluate the human-difficulty of a puzzle. Fortunately, the popularity of Sudoku puzzles makes this data easily available online.

The web site sudoku.org.uk records average solve time and the number of individuals to solve the Daily Sudoku puzzles, with puzzles rated for 4 difficulties.

First, we consider whether number of solvers or average solve time is a more effective measure of difficulty.



(a) Number of Solvers (b) Average Solve Time

Figure 2: Box plots of Distribution of Difficulty Measures for Puzzles of 4 Difficulties. Average Solve Time better differentiates between puzzle difficulties

As seen in Fig 2, the time taken to solve a puzzle better differentiates between puzzle difficulties. Time to solve also provides a more widely distributed 'true' difficulty.

Intuitively, solve time is a reasonable, accurate measure. Puzzle solvers often to consider a puzzle's difficulty to be the amount of time they spend working on it.

6 Our Difficulty Metric - Predicted Solve Time

We provide an predictor of Average Solve Time as a measure of difficulty, using a multiple regression model considering the number and type of solving logical strategies used to solve a puzzle. The program 'serate' (Sudoku Explainer) by Nicolas Juillerat is used to provide a list of strategies used.

6.1 Preliminary Model and Complexity

Our algorithm is as follows:

- Generation of the Model
  - Use 'serate' to generate a list of the usage of 31 logical strategies for each of 915 puzzles from sudoku.org.uk
  - Use linear multiple regression to calculate model coefficients
- Application of the Model on a Puzzle P
  - Use 'serate' to generate a list of the usage of 31 logical strategies required to solve P

– Apply the linear model to P

The algorithm is efficient in that it precomputes the 32 model coefficients. Calculation of the predictor given the strategies used is O(1). Computation of the metric is dominated by the determination of the logical strategies used to solve it, computed by 'serate'. Serate considers each possible logical strategy at each stage of solving the puzzle, hence is computationally intensive. On a modern computer, 15 puzzles are processed in 1 second.

6.2 Analysis via Bootstrapping

The model predicts solve time well when tested on the training data (see Fig 3, $R^2 = 0.711$).

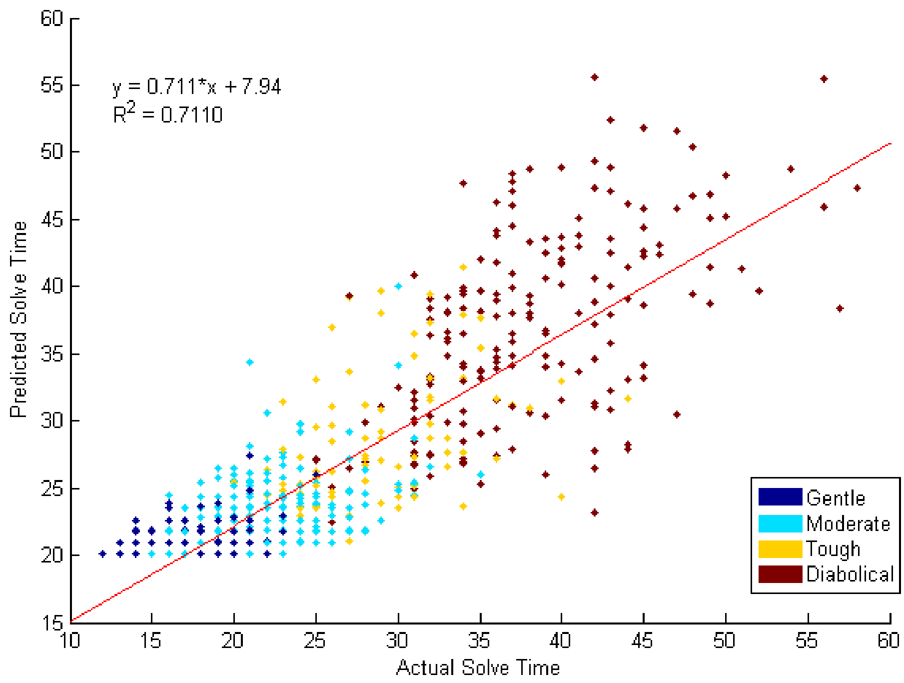


Figure 3: Relationship between Actual Solve Time and Predicted Solve Time, in minutes. Solve time is our difficulty metric

Bootstrapping is a technique in which a set of data is repeatedly divided into two groups - a training set and a test set. The training set is used to build a model, which is evaluated on the test set. By generating a distribution of performance, the technique provides a measure of the performance of a model on unseen data, that is, data not used to build the model.

Bootstrapping was used to evaluate the efficacy of the model in predicting the difficulty previously unseen data. The training set size was 604 samples, or 2/3 of the dataset.

Performance on the test set, as measured by the coefficient of determination R^2, can be seen in Fig 6.2. The mean R^2 is 0.6657, with a 95% confidence interval $CI = [0.6078, 0.7176]$, indicating a strong relationship between the predicted and actual solve time on the test set.

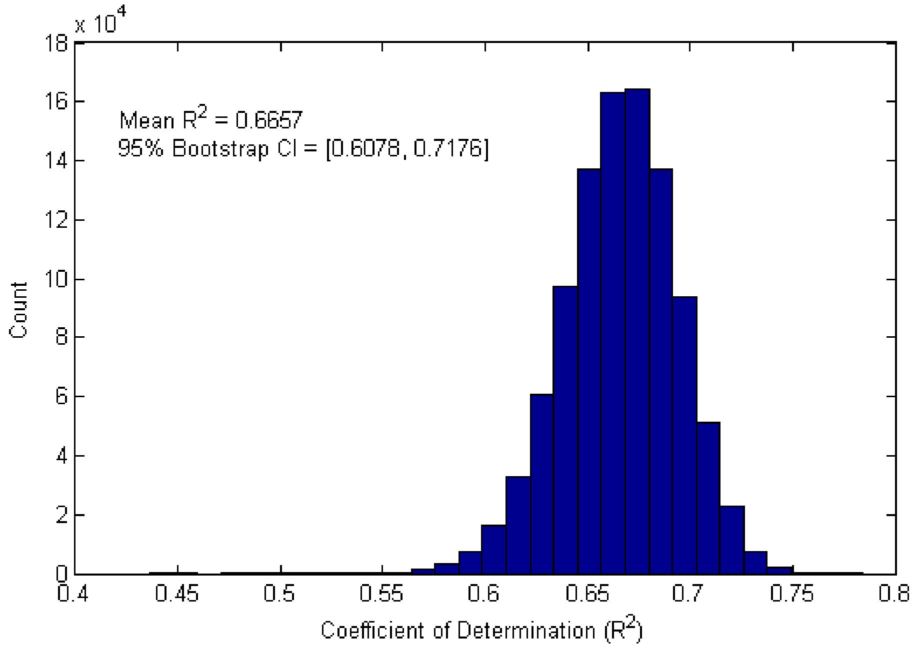


Figure 4: Bootstrapping Results: Performance of Model on Test Set

6.3 Meta-Model via Pseudo-Bagging

Bagging, or bootstrap aggregating, can be used to improve the stability and accuracy of regression models, reducing variance and helping to avoid overfitting [2].

We use a slight modification to the traditional bagging procedure here - instead of having each bootstrap model contribute equally to the final predictor, we weight the contributions by the R^2 of that model, so better models contribute more.

Because our model is linear, this does NOT increase the complexity of the meta-model. The coefficient of a predictor x_i in the meta-model is the weighted sum of the coefficients in each model. The final meta-model is only a list of 32 coefficients.

The meta-model was generated from the 1 million bootstrap iterations described in the previous section.

6.4 Analysis of Meta-Model

Further bootstrapping was used to evaluate the efficacy of the meta-model. Due to computational limits, we could not iterate over 1-million-iteration meta-models. Rather, to estimate the effectiveness of this technique in general, 100 bootstrap iterations were conducted, generating a 10,000-iteration meta-model each time. In each outer iteration, 311 random samples were reserved for testing and 604 samples were passed to the meta-model generator. The generator used 398 of those samples for training and the remaining 206 samples for test, to determine the model weights.

Each meta-model was then evaluated on the 311 test samples. The distribution of performance on the test set can be seen in Fig 6.4

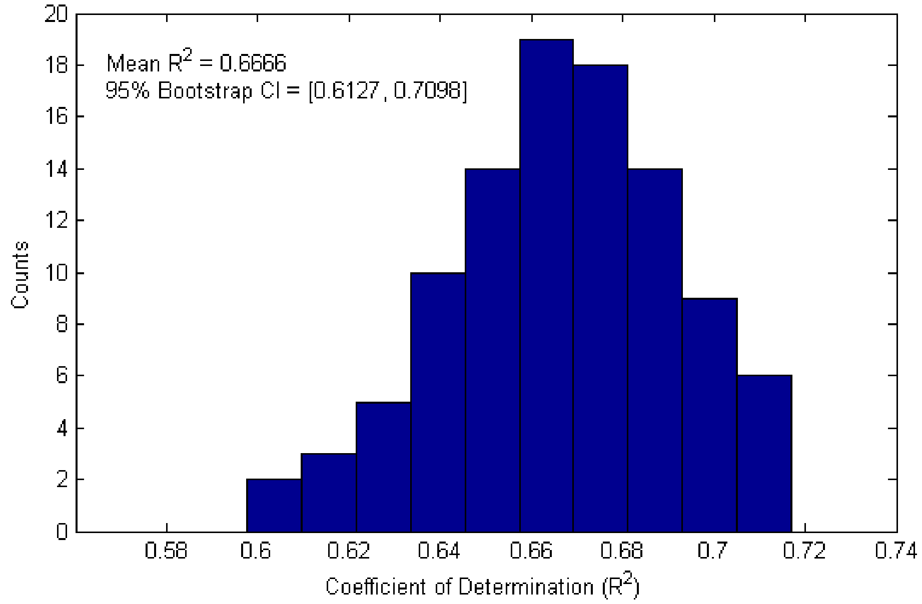


Figure 5: Bootstrapping Results: Performance of Meta-Model on Test Set

7 Practical Analysis of our metric

7.1 Applicability

Our metric is

- **accurate - well-correlated** to human solve times, with $R^2 = 0.71$
- **versatile - widely distributes Sudoku puzzles** into difficulty, as solve times are well distributed

- **extensible** - by computing a **continuous** parameter, allowing specification of difficult bounds

7.2 Comparison to Other Difficulty Metrics

We consider the correlation between the difficulty rating and actual average solve time for four publicly available metrics and four naive metrics we designed in Table 1. Table 2 describes the function of these metrics. Our metric focuses on human difficulty rather than arbitrary computational metrics, so out performs the other metrics we consider in predicting difficult for a human solver.

	Metric	R^2
Our Final Metric	mcm2280	0.7103
Others' Metrics	serate	0.5610
	suexrat9	0.5324
	suexrate	0.4848
	Fowler #r	0.4275
Our Naive Metrics	Singles Cell#	0.1052
	Singles SumPoss	0.0488
	Intelligent BruteForce	0.0460
	Seed Count	0.0419

Table 1: Performance of Various Metrics

Metric	Description
mcm2280	Uses a linear meta-model considering the number and type of strategy necessary to solve a puzzle
serate	Uses the number and type of strategy necessary to solve a puzzle, with weights set by the programmer
suexrat9	Improved version of suexrate, but faster and less canonical
suexrate	Conducts a depth-first search with minimal logic and takes the number of nodes in the search tree
Fowler #r	Uses the number and type of strategy necessary to solve a puzzle, grouping some strategies together, with the weights set by the programmer
Singles Cell#	Counts the number of cells solvable by the simplest techniques
Singles SumPoss	Evaluates the number of possibilities remaining for each cell using the simplest techniques and takes the sum over all cells
Intelligent BruteForce	Considers the number of recursive calls when solving a puzzle using recursive backtracking
Seed Count	Counts the number of givens in the puzzle

Table 2: Description of Metrics

8 Our Puzzle Generation Algorithms

An effective way to generate many puzzles is to transform an existing one. We first discuss the valid transformations on a Sudoku puzzle and then provide 3 algorithms to generate puzzles of desired difficulties.

8.1 Puzzle Transformation

Much as a Latin Square can be permuted to form a new Latin Square, so can a completed Sudoku be permuted to form a new Sudoku. However, care must be taken to ensure that the permutations do not place more than one of a given number into a block. We restrict permuting rows or columns to permutations within a **band** or **stack** to prevent this from occurring. A band is a set of three blocks that are horizontally contiguous, and a stack is the vertical equivalent.

This results in the following valid permutations: (see Fig 6)

1. Row permutation within a band
2. Column permutation within a stack
3. Symbol permutation: exchanging all instances of a given number with another, for instance replacing all 1's with 4's and all 4's with 1's

4. Transposition

In addition, we allow the following two permutations:

5. Band Permutation: Swapping two of the bands
6. Stack Permutation: Swapping two of the stacks

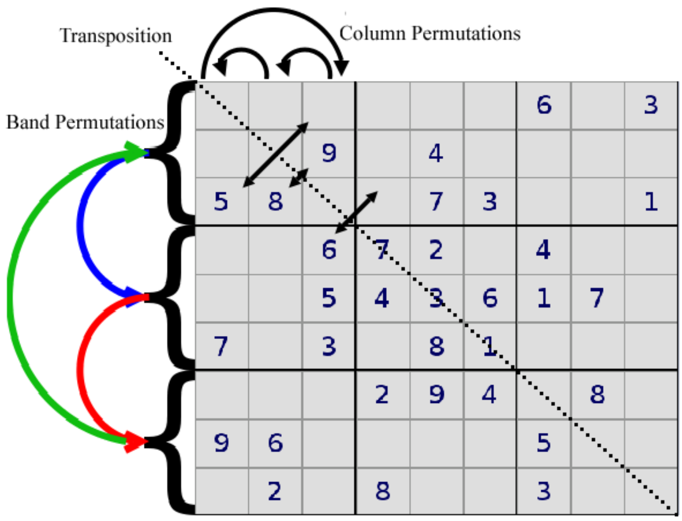


Figure 6: Valid 9x9 Sudoku Permutations

Transforming a puzzle, while maintaining its difficulty and other properties, dramatically alters its appearance and creates a new puzzle, different from the original. The magnitude of change can be seen in Fig 7, a puzzle we generate using the Build Up Generator B, before and after transformation.

8.2 Generator A: Library-based Generator

A library based puzzle generator is extremely efficient and generates a large spread of puzzle difficulties.

8.2.1 Algorithm

Preprocessing
Large sets of valid Sudoku puzzles are available. We produce a library from 100,000 puzzles available online by preprocessing the difficulty of each puzzle.
Generation
Using a Hash Table, a puzzle of requested difficulty can be retrieved and transformed nearly instantaneously.

					2	6	7	
	7	1			5			3
2								
						8		2
		3						4
	8		3		4		9	
				9		3	6	
	6		1			4		
1				5				

(a) Before Transformation

8		1						
			9			6		1
	7		3					
3	9			2		4		
4			8			5		
				6	9			3
		7					6	
	4		2					5
					3			7

(b) After Transformation

Figure 7: Transformation of a Generated Puzzle

8.2.2 Applicability

Our library consists of 100,000 puzzles with a range of difficulties (Fig 8).

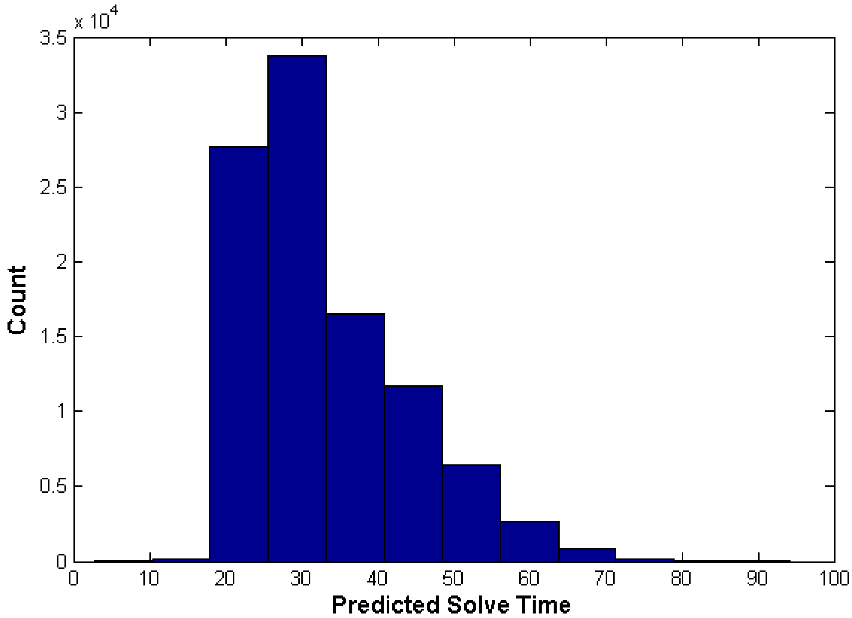


Figure 8: Library Generator - Difficulty Distribution

Furthermore, each puzzle can be transformed to generate $2{*}9!{*}6^8 = 1,218,998,108,160$ other puzzles. At a rate of one puzzle per second, it would take a solver 38 millenia to complete these puzzles. Note that our library consists of 100,000 puzzles before transformation.

8.2.3 Complexity

By creating a library of puzzles with their difficulties, we avoid having to compute difficulty and checking validity, both time-consuming operations, on fly. If the puzzles are stored in a Hash Table indexed by their difficulty, retrieving a puzzle of desired difficulty is O(1). Transforming the puzzle also takes O(1) time.

8.2.4 Sample Puzzles

	7	9	8			3		
5					9			
	1					2		
			9				2	8
8			2		7			
	6							
	5		6	8			4	
				1			9	3
	2	4						1

(a) Predicted Difficulty: 2.81 minutes

				8	1			
1	3		4				9	
6	9			2				
			8			5		
		8		6		3		
		3	6					5
	4	9					6	
2	8			4				7

(b) Predicted Difficulty: 27.39 minutes

9			8			1		
		4		3				
				5			2	7
2		5						9
	6			8	5		4	
		3					6	
			1			3		
5				4				2
					3		8	4

(c) Predicted Difficulty: 52.40 minutes

							2	7
				6	4	3		5
9					1			
		2				7	5	
		4						8
6				9	5			
		9	5	8				2
	1		3					
	8				6			

(d) Predicted Difficulty: 71.68 minutes

Figure 9: Library Generator - Sample Puzzles of 4 Different Difficulties

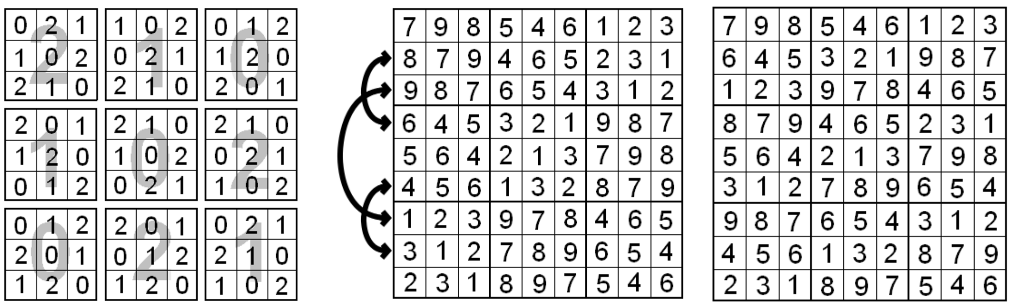
8.3 Generator B: Build-up from Solution

Instead of picking random numbers to seed a blank puzzle, we start with a valid solution and generate a puzzle leading to that solution.

8.3.1 Latin Squares for Solution Generation

To quickly and effectively generate a solution, we use the 12 unique 3x3 Latin Squares.

- Select nine 3x3 Latin Squares, with replacement.
- Place each of these squares into one of the blocks in a blank grid.
- Select another 3x3 Latin Square and match each cell with the corresponding *block* in the Sudoku grid. (Fig 10(a)).
- Each cell now has a pair of numbers. Treat these pairs as base 3 numbers, and convert to base 10, adding 1 (Fig 10(b)).
- Each cell now has the numbers 1-9. However blocks contain duplicates.
- Swap the 2nd & 4th rows, 3rd & 7th rows, and 6th & 8th rows preserving the row and column properties, and adding the desired property for blocks.
- This produces a valid Sudoku solution (Fig 10(c)).



(a) Selection of Latin Squares (b) Conversion to Base 10 (c) Sudoku Solution

Figure 10: Producing a Sudoku Solution from Latin Squares

8.3.2 Intelligent Brute Force Solver

We use a created an 'intelligent' recursive-backtracking brute-force sudoku solver to determine the number of solutions for a set of givens to ensure uniqueness.

Instead of recursing on the next cell sequentially, it calculates the number of possible values in all cells via the simplest logic techniques, and *recurses on the most constrained cell.*

In practice, this 'Intelligent Brute Force' algorithm performs on average ≈ 300 times fewer recursive calls than a conventional recursive-backtracking brute-force algorithm.

8.3.3 Algorithm

This generator

- Uses latin squares to generate a valid Sudoku solution
- Places 40 values from that solution on a blank board
- Iteratively removes values, checking that the puzzle is still valid, until the appropriate difficulty is generated.
- Transforms the generated puzzle

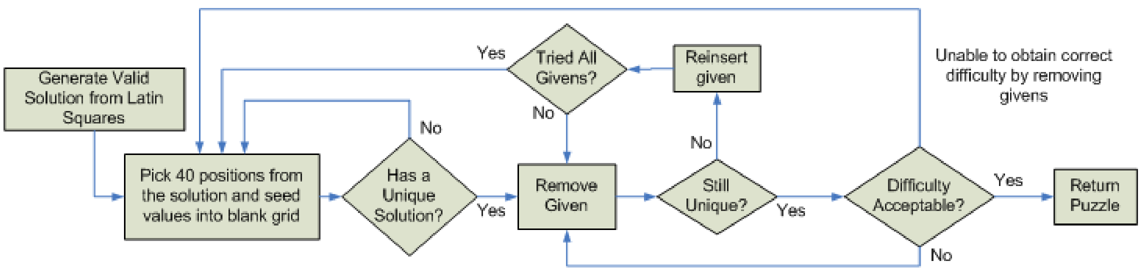


Figure 11: Flow Chart of Bottom Up Generator

8.3.4 Complexity

The complexity of this algorithm is defined by the number of calls to the Intelligent Brute Forcer to check solution uniqueness. We have calculated amortized statistics for the generation of a puzzle:

- 3 puzzles generated per second, before transformation
- More than 1.2 trillion puzzles can be produced from each nearly instantaneously
- 103 calls to the Intelligent Brute Forcer per generated puzzle
- 2.3 failed placements of the initial 40 values, per puzzle generated

8.3.5 Sample Puzzles

		4	1					
9					5	3		
	3				6			5
		8		9		4		
		5	3			6		
	2					8		
	5			6		1		
7					2		4	9
								2

(a) Predicted Difficulty: 8.23 minutes

				5		3		
		8	7					
	1		3					
					8			
		4		2	1		8	
		9						7
5				3				9
		6		8		7		4
			4		5	2		

(b) Predicted Difficulty: 28.78 minutes

			3					
	7	2			6			9
6								
	9		5				1	8
		1			8	4	6	
				1	3			
				9	1			5
	5	4						
			8		4			6

(c) Predicted Difficulty: 45.84 minutes

1			8		9		7	6
						8		
6	4				5			9
				4		9		
		9			7			
	5				8		1	
			3	1				
2		4						
				9			8	

(d) Predicted Difficulty: 82.74 minutes

Figure 12: Build up Generator - Sample Puzzles of 4 Different Difficulties

This algorithm generates puzzles with a range of difficulties (Fig 13).

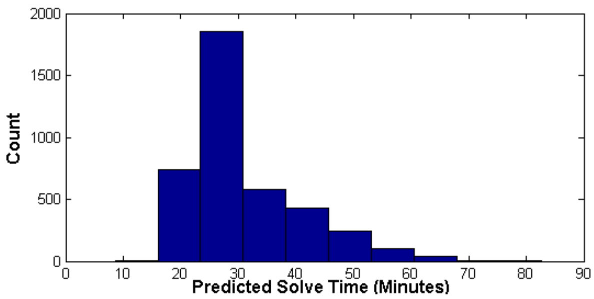


Figure 13: Build Up Generator - Difficulty Distribution

8.4 Generator C: Template Generation

Puzzles provided by the puzzle magazine *Nikoli* are prefered by some Sudoku enthusiasts because they are all human-generated. This is often reflected in their symmetry or their conformation to a specific pattern of locations of givens.

We provide an algorithm with this functionality.

8.4.1 Algorithm

- Read a template from the user
- Iterate:
  - Generate a valid solution using Latin Squares
  - Place the appropriate values in the template locations
  - Return if the puzzle has a unique solution
- Tranform the puzzle ONLY with symbol permutation

8.4.2 Complexity

The performance of this algorithm varies substantially with the template provided. In the worst case, if there are no valid puzzles with that pattern, it will run in $O(9^n)$ time, where n is the number of locations in the template.

If sufficiently many cells are given in the template, however, it is efficient. The 'MCM' puzzle on the first page and those below were generated via this algorithm. It produced approximately 1 puzzle per minute, before transformation. Each puzzle could be symbol permuted to $9! = 362,880$ other valid puzzles.

We note that we generate puzzles from one class of solution grids, namely those generated by Latin Squares. It is possible that there exists a valid puzzle of another class that our algorithm will not find.

8.4.3 Sample Puzzles

Because these puzzles are more constrained, this algorithm generates puzzles with a smaller range of difficulties.

1	2		5	6				
8		4		7				
5				8		6	4	1
6				3		2		
						9		
2	3		7	9		1		
4		1		5		7	6	2
3				2				
9				1				

(a) Predicted Difficulty: 18.43 minutes

8	9		5	7				
5		4		2				
2				4		8	6	5
6				9		1		
						5		
1	2		4	5		7		
3		8		1		4	5	7
4				8				
7				6				

(b) Predicted Difficulty: 21.36 minutes

1	9		2	5				
7		3		4				
2				3		1	9	5
9				8		7		
						6		
5	8		4	9		2		
4		5		6		3	2	7
8				1				
6				7				

(c) Predicted Difficulty: 25.94 minutes

3	8		7	4				
1		2		5				
4				1		7	9	8
7				9		8		
						5		
9	4		1	3		6		
8		4		7		9	5	1
6				8				
5				2				

(d) Predicted Difficulty: 28.99 minutes

Figure 14: Template Generator - Sample 'MCM' Puzzles of 4 Different Difficulties

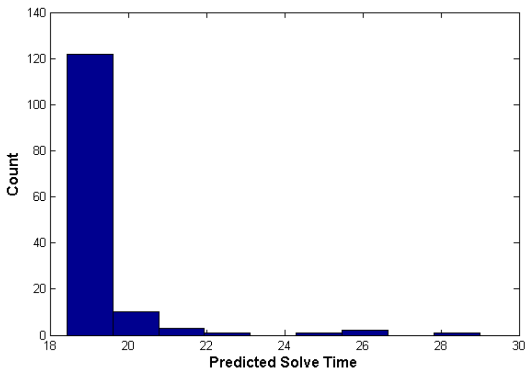


Figure 15: Template Generator - Difficulty Distribution for 'MCM' puzzles

9 Conclusion

Sudoku puzzle rating and generation algorithms abound. Our model differs in that we focus on the human-applicability of our rating and generation algorithms. Rather than defining parameters used to rate difficulty by hand, we use multiple regression and bootstrap aggregation to better model the predicted time an average solver will require to complete a puzzle.

We present difficulty rating metric that outperforms all other metrics we consider in predicting the average solve time for a set of 915 puzzles. Furthermore, we demonstrate that this metric is extensible and versatile. We also provide a suite of puzzle generation algorithms. We provide a library based algorithm that provides many puzzles in O(1) time; a generator that uses a solution to 'build up' a puzzle; and a template-based generator that can be used to mimic popular human-constructed Sudoku puzzles. Each of these algorithms, particularly the first two, rapidly provide puzzles with a broad range of difficulties. Furthermore, each method is capable of generating a large number of new puzzles.

Further work could explore a more direct puzzle generation algorithm that makes use of the unique nature of our difficulty metric. By applying the logical strategies we consider in reverse to selectively remove givens from a completed grid, a puzzle that requires certain strategies to solve could be constructed, effectively tailoring the puzzle to conform to a desired difficulty. This could potentially generate puzzles of a desired difficulty more efficiently.

References

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