Rubik's Cube Solver: Integrating Classical Algorithms with Machine Learning Prediction

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1. Abstract & Objectives

The Rubik's Cube state space ($|G| \approx 4.3 \times 10^{19}$) presents a unique challenge for heuristic search. This project implements a comprehensive framework integrating **classical solvers** (Thistlethwaite and Kociemba) with an **AI-based predictive system**.

Key Objectives:

- Implementation of Thistlethwaite (Multi-phase) and Kociemba (Two-phase) algorithms.
- Creation of a reproducible benchmarking framework ($N = 5000$ dataset).
- Development of ML models to predict solver performance (runtime, moves, nodes) and enable **adaptive solver selection**.

2. Classical Algorithms: Theory

The solvers reduce the state space via group theory subgroups.

A. Thistlethwaite's Algorithm (Satisfaction) Decomposes the problem into 4 nested subgroups to limit search breadth:

$$G = G_0 \supset G_1 \supset G_2 \supset G_3 \supset \{e\}$$

- Uses 4 phases.
- Guarantee: Predictable, bounded runtime.
- Trade-off: Suboptimal solution lengths (30 moves).

B. Kociemba's Two-Phase Algorithm (Optimization) Optimizes the reduction into two stages using IDA* and Pattern Databases:

- Phase 1: Reach $G_1 = \langle U, D, R2, L2, F2, B2 \rangle$.
- Phase 2: Solve within G_1.
- Trade-off: Near-optimal solutions (19 moves) but heavy-tailed runtime distribution.

3. Classical Benchmark Results

We analyzed the trade-off between **Solution Quality** (Moves) and **Computational Cost** (Time/Nodes) on the midterm dataset ($N = 200$).

Table: Summary Statistics (Mean / Median)

Metric	Thistlethwaite	Kociemba
Runtime (s)	0.016 / 0.015	0.218 / 0.063
Solution Length	25.47 / 30.0	17.92 / 22.0
Nodes Expanded	142 / 149	4,150 / 1,486
Success Rate	100%	100%

Key Findings:

- **Kociemba** provides significantly shorter solutions ($\Delta \approx 7.5$ moves) but exhibits high variance (σ^2 is large).
- **Thistlethwaite** dominates in consistency and speed (Linear scaling).

4. Analysis of Trade-offs

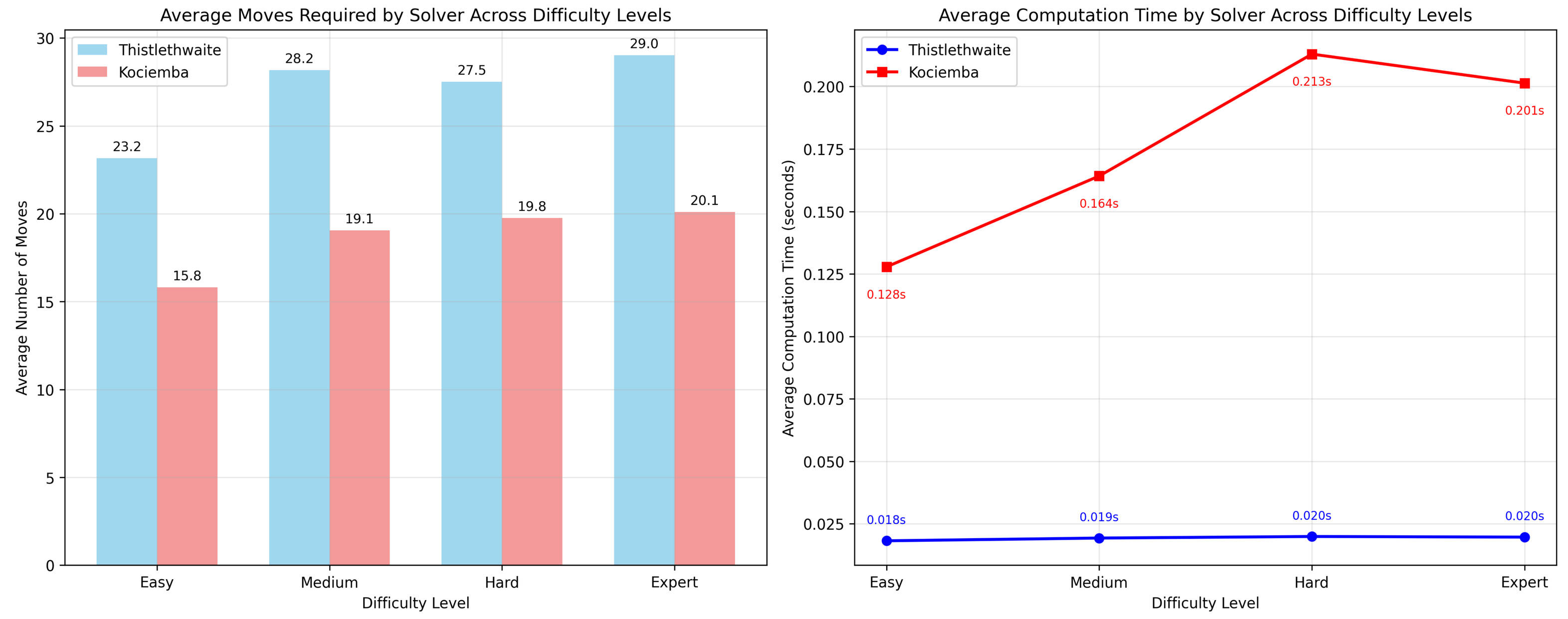


Figure: Mean Runtime and Move Count across difficulty levels. Note Kociemba's runtime spike in 'Expert' categories vs. Thistlethwaite's stability.

- **Kociemba:** produces substantially shorter solutions (18 moves mean / 22 median) but shows *high runtime variance* (median 0.063 s; mean inflated by outliers).
- **Thistlethwaite:** gives longer solutions (25–30 moves) with *predictable, low* runtimes (median 0.015–0.016 s) and tight variance.
- **Practical guideline:** use Thistlethwaite when consistent, real-time performance matters; use Kociemba when minimizing moves is the priority and occasional slow cases are acceptable.

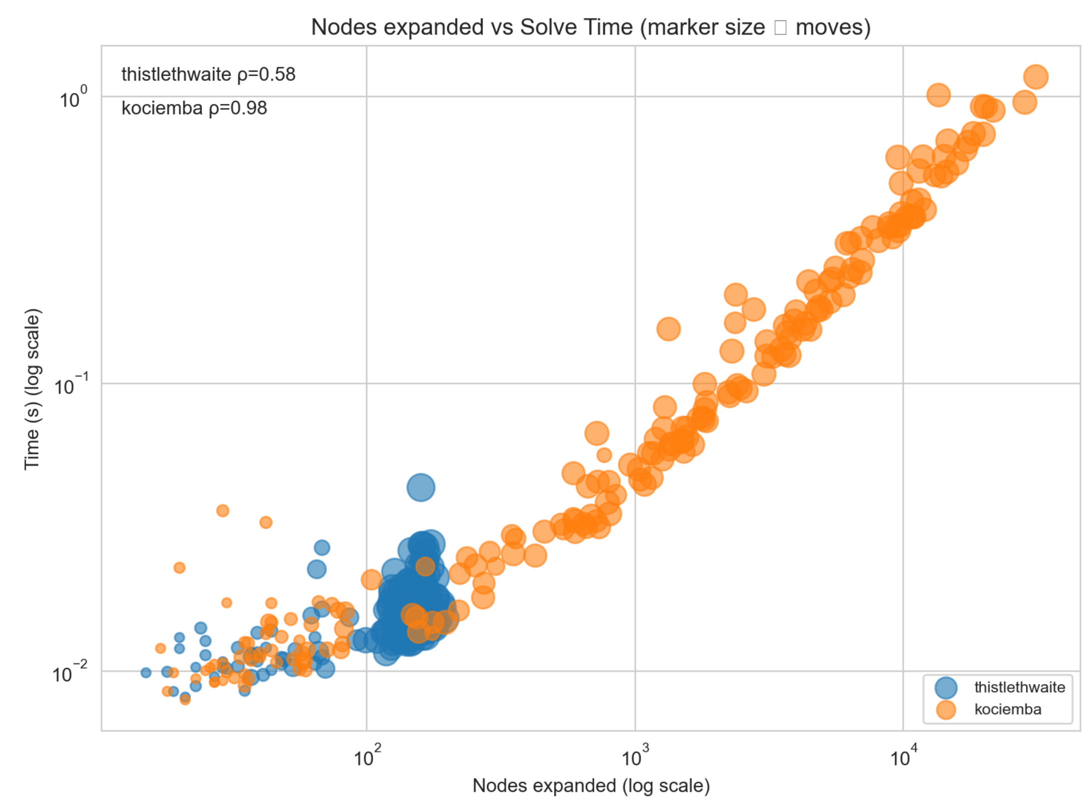


Figure: Nodes vs. Time (Log-Log). Thistlethwaite shows tight linear scaling; Kociemba shows heavy-tailed behavior due to heuristic sensitivity.

- **Thistlethwaite scaling:** points cluster tightly along an almost-linear trend (near $T \propto N_e$); mean/median nodes are low (143 / 150) and runtime variance is small.
- **Kociemba scaling:** shows a heavy-tailed scatter — median cases are moderate but *rare* instances trigger massive node expansion (mean nodes median), driven by IDA*/heuristic sensitivity.
- **Constant-factor trade-off:** Thistlethwaite has slightly higher per-node overhead (table lookups / subgroup checks) but avoids worst-case blowups; Kociemba often has cheaper per-node work yet can require far more nodes on hard instances.

5. ML Prediction Performance

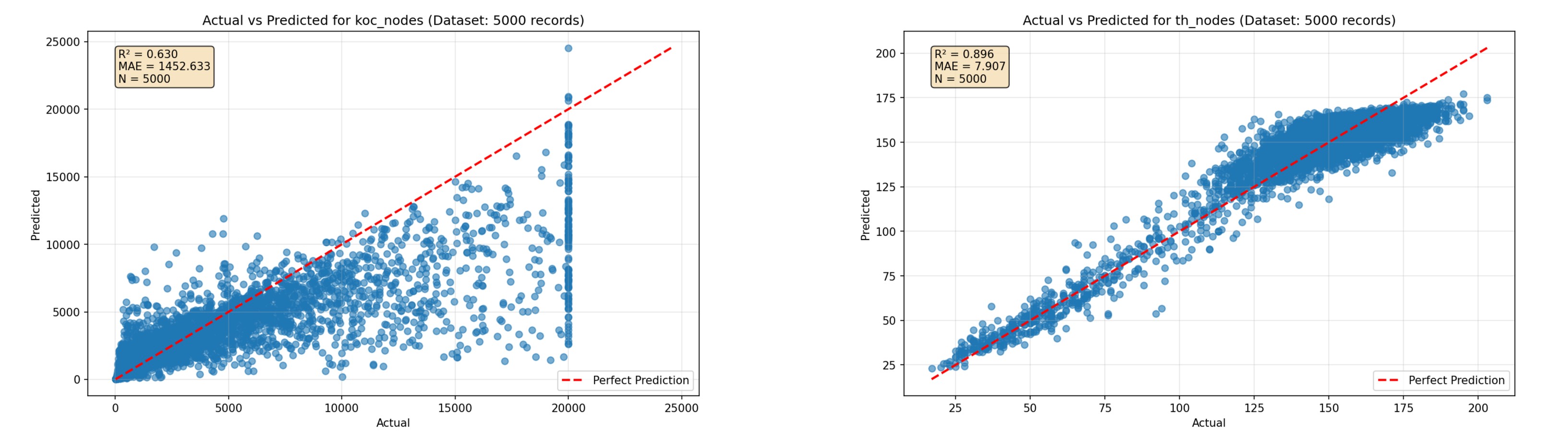
We trained Random Forest models on 25 static cube features (e.g., `solution_score`, `orientation_entropy`) to predict solver behavior ($N = 5000$).

Target	R^2 (Held-out)	CV R^2	Insight
Thistlethwaite Moves	0.998	0.997	Highly Deterministic
Kociemba Moves	0.998	0.997	Heuristics align with reality
Kociemba Nodes	0.630	0.661	Hard to predict (IDA*)
Kociemba Time	0.240	0.266	Implementation overhead

Adaptive Classification (Solver Selection): The system decides: *"Should we use Thistlethwaite to avoid Kociemba's worst-case?"*

- **Accuracy:** 94.2% (Held-out test split).
- **Feature Importance:** `solution_score` and `solution_variance` are the dominant predictors.

6. Prediction Accuracy Analysis Across Metrics



(a) Confusion matrix (raw counts) for 'avoid$_k$ociemba'.

(b) Confusion matrix (normalized by true class) for 'avoid$_k$ociemba'.

Figure: Actual vs. Predicted analysis for node expansion. The model for `Thistlethwaite` (right) shows high linearity due to deterministic phases, while `Kociemba` (left) shows higher variance ($R^2 = 0.630$) due to IDA* heuristic sensitivity.

7. Conclusion & Future Work

Conclusion:

- Established a clear dichotomy: Thistlethwaite for **predictability**, Kociemba for **optimality**.
- Demonstrated that ML can accurately predict solution length ($R^2 \approx 0.99$) but resource usage is inherently chaotic for IDA*.
- The hybrid system effectively selects the optimal solver based on constraints.

Future Work:

- Deep Learning (GNNs) to capture spatial dependencies better than static features.
- Online learning to adapt solver selection during deployment.

References

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4. F. Agostinelli et al. Solving the Rubik's Cube with Deep Reinforcement Learning. Nature MI, 2019.