

# Rational Metareasoning in Problem-Solving Search

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February 12, 2014

# Rational Metareasoning in Problem-Solving Search

## Problem-Solving Search:

Search time depends dramatically on problem instance features other than problem size.

## (Limited) Rationality:

The agent acts to maximize its reward given limited resources.

## Metareasoning:

Reasoning about computations which help to choose the best action.

Rational Metareasoning

Rational Deployment of Heuristics in CSP

VOI-aware Monte Carlo Tree Search

Towards Rational Deployment of Multiple Heuristics in A\*

Insights into the Methodology

Summary and Future Work

# Outline

## Rational Metareasoning

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### Summary and Future Work

# Rational Metareasoning

- ▶ A problem-solving agent can perform *base-level* actions from a known set  $\{A_i\}$ .
- ▶ Before committing to an action, the agent may perform a sequence of *meta-level* deliberation actions from a set  $\{S_j\}$ .
- ▶ At any given time there is a base-level action  $A_\alpha$  that maximizes the agent's *expected utility*.

The **net VOI**  $V(S_j)$  of action  $S_j$  is the **intrinsic VOI**  $\Lambda_j$  less the cost of  $S_j$ :

$$V(S_j) = \Lambda(S_j) - C(S_j)$$

$$\Lambda(S_j) = \mathbb{E}(\mathbb{E}(U(A_\alpha^j)) - \mathbb{E}(U(A_\alpha)))$$

- ▶  $S_{j_{\max}}$  that maximizes the net VOI is performed:  
 $j_{\max} = \arg \max_j V(S_j)$ , if  $V(S_{j_{\max}}) > 0$ .
- ▶ Otherwise,  $A_\alpha$  is performed.

# Simplifying assumptions

- ▶ **Myopicity:**

- ▶ Meta-greedy: consider only the effect of single computational actions.
- ▶ Single-step: Assume all computations are complete, act as though a base-level action immediately follows the computation.

- ▶ **Subtree independence:** any computation updates the expected utility of a single action.

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# Constraint Satisfaction

- ▶ CSP backtracking search algorithms typically employ variable-ordering and value-ordering heuristics.
- ▶ Many value ordering heuristics are computationally heavy, e.g. heuristics *based on solution count estimates*.
- ▶ Principles of rational metareasoning can be applied to decide when to deploy the heuristics.



# Constraint Satisfaction

A constraint satisfaction problem (CSP) is defined by:

**variables**  $\mathcal{X} = \{X_1, X_2, \dots\}$ ,

**constraints**  $\mathcal{C} = \{C_1, C_2, \dots\}$ .

- ▶ Each *variable*  $X_i$  has a non-empty domain  $D_i$  of possible values.
- ▶ Each *constraint*  $C_i$  involves some subset of the variables—the *scope* of the constraint—and specifies the allowable combinations of values for that subset.
- ▶ An *assignment* that does not violate any constraints is called *consistent* (or solution).

# Value Ordering Model

Value ordering heuristics provide information about:

- ▶  $T_i$ —the expected time to find a solution containing an assignment  $X_k = y_{ki}$ ;
- ▶  $p_i$ —the probability that there is no solution consistent with  $X_k = y_{ki}$ .

The expected remaining search time in the subtree under  $X_k$  for ordering  $\omega$  is  $T^{s|\omega} = T_{\omega(1)} + \sum_{i=2}^{|D_k|} T_{\omega(i)} \prod_{j=1}^{i-1} p_{\omega(j)}$

- ▶ The current optimal base-level action is picking the  $\omega$  which optimizes  $T^{s|\omega}$ .  $T^{s|\omega}$  is minimal if the values are sorted by increasing order of  $\frac{T_i}{1-p_i}$ .
- ▶ The intrinsic VOI  $\Lambda_i$  of estimating  $T_i, p_i$  for the  $i$ th assignment is the expected decrease in the expected search time:  
$$\Lambda_i = \mathbb{E} [T^{s|\omega_-} - T^{s|\omega_{+i}}].$$

# Model Assumptions

1. Solutions are roughly evenly distributed in the search space, that is, the distribution of time to find a solution can be modeled by a Poisson process.
2. Finding all solutions for an assignment  $X_k = y_{ki}$  takes roughly the same time for all assignments to the variable  $X_k$ .
3. The expected time to find all solutions for an assignment divided by its solution count estimate is a reasonable estimate for the expected time to find a single solution.

# Main Results

## Rational Value Ordering

The intrinsic VOI  $\Lambda_i$  of invoking the heuristic can be approximated as:

$$\Lambda_i \approx \mathbb{E} \left[ (T_1 - T_i) | D_k | \mid T_i < T_1 \right]$$

## VOI of Solution Count Estimates

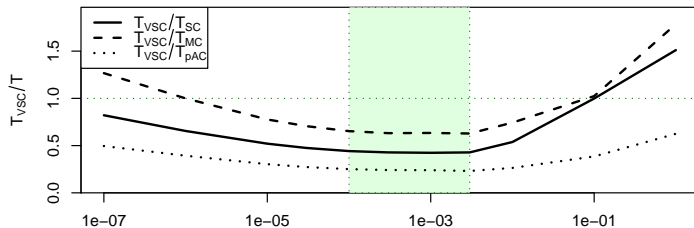
The net VOI  $V$  of estimating a solution count can be approximated as:

$$V \propto |D_k| e^{-v} \sum_{n=n_{\max}}^{\infty} \left( \frac{1}{n_{\max}} - \frac{1}{n} \right) \frac{v^n}{n!} - \gamma$$

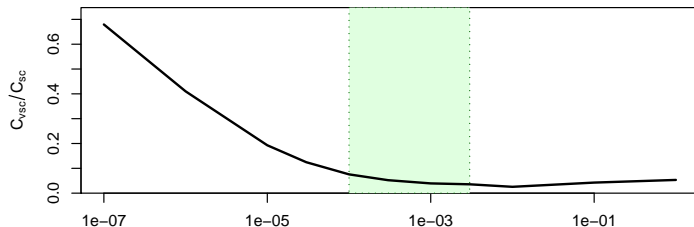
where the constant  $\gamma$  depends on the search algorithm and the heuristic, rather than on the CSP instance, and can be learned offline.

# Benchmarks

a. Search time

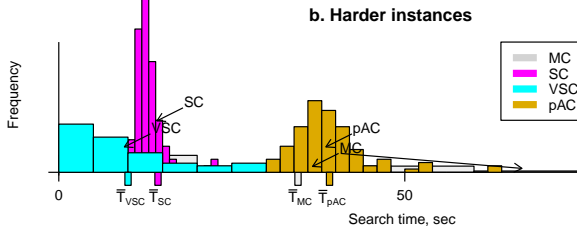
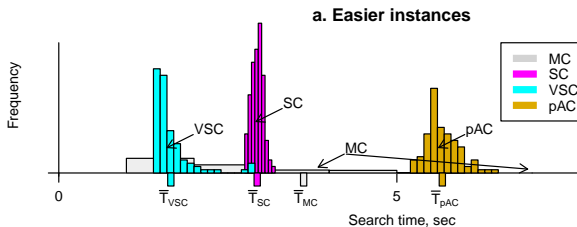


b. Solution count estimations



14 CSP Solver Competition 2005 Benchmarks  
solved for  $\gamma \in \{0, 10^{-7}, 10^{-6}, \dots, 1\}$

# Random Instances



100 Model RB Random Instances

# Generalized Sudoku

- ▶ Real-world problem instances often have much more structure than random instances generated according to Model RB.
- ▶ We repeated the experiments on randomly generated Generalized Sudoku instances— a highly structured domain.
- ▶ Relative performance on Generalized Sudoku was similar to Model RB.

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# MCTS

**Monte Carlo Tree Search** helps in large search spaces. At each node:

- ▶ Repeats:
  1. **Selection:** select an action to explore.
  2. **Simulation:** simulates a rollout until a goal is reached.
  3. **Backpropagation:** updates the action value.
- ▶ Selects the best action.

**Adaptive** Generally, MCTS samples ‘good’ moves more frequently, but sometimes **explores** new directions.

# Multi-armed Bandit Problem and UCB

Multi-armed Bandit Problem:

- ▶ We are given a set of  $K$  arms.
- ▶ Each arm can be pulled multiple times.
- ▶ The reward is drawn from an **unknown** (but normally *stationary* and *bounded*) distribution.
- ▶ The **total reward** must be maximized.

**UCB** is near-optimal for MAB — solves *exploration/exploitation* tradeoff.

- ▶ pulls an arm that maximizes **Upper Confidence Bound**:

$$b_i = \bar{X}_i + \sqrt{\frac{c \log(n)}{n_i}}$$

- ▶ the cumulative regret is  $O(\log n)$ .

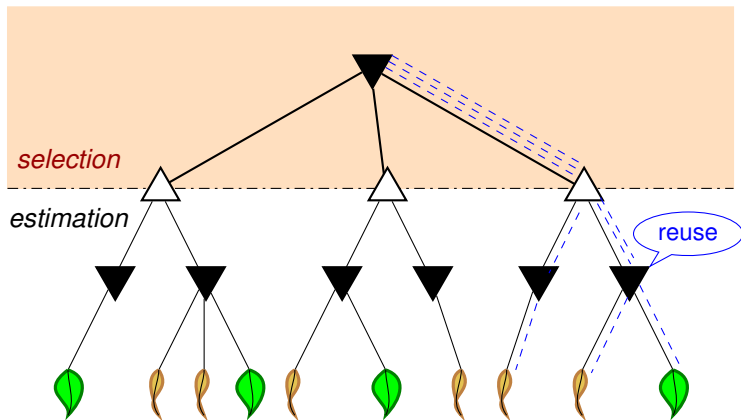
UCT (**U**pper **C**onfidence Bounds applied to **T**rees) is based on UCB.

- ▶ Adaptive MCTS.
- ▶ Applies the UCB selection scheme at each step of the rollout.
- ▶ Demonstrated good performance in Computer Go (MoGo, CrazyStone, Fuego, Pachi, ...) as well as in other domains.

However, the first step of a rollout is different:

- ▶ The purpose of MCTS is to choose an action with the greatest utility.
- ▶ Therefore, the **simple regret** must be minimized.

# MCTS Tree: Selection & Estimation



# Upper Bounds on Value of Information

Assuming that:

1. Samples are i.i.d. given the value of the arm.
2. The expectation of a selection in a belief state is equal to the sample mean.

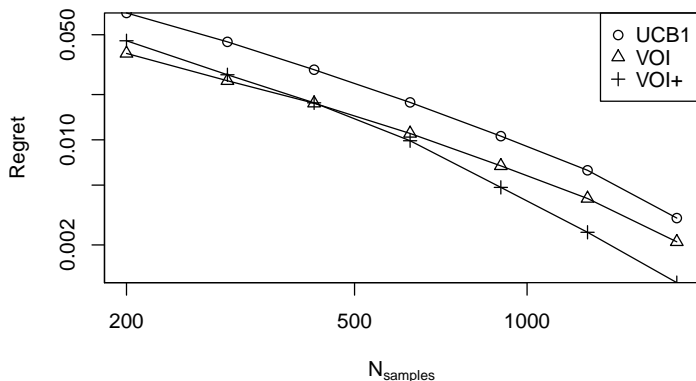
Upper bounds on intrinsic VOI  $\Lambda_i^b$  of testing the  $i$ th arm  $N$  times are (based on Hoeffding inequality):

$$\Lambda_{\alpha}^b < \frac{N\bar{X}_{\beta}^{n_{\beta}}}{n_{\alpha} + 1} \cdot 2 \exp \left( -1.37 (\bar{X}_{\alpha}^{n_{\alpha}} - \bar{X}_{\beta}^{n_{\beta}})^2 n_{\alpha} \right)$$
$$\Lambda_{i|i \neq \alpha}^b < \frac{N(1 - \bar{X}_{\alpha}^{n_{\alpha}})}{n_i + 1} \cdot 2 \exp \left( -1.37 (\bar{X}_{\alpha}^{n_{\alpha}} - \bar{X}_i^{n_i})^2 n_i \right)$$

Tighter bounds can be obtained (see the paper).

# VOI-based Sampling in Bernoulli Selection Problem

25 arms, 10000 trials:



UCB1 is always worse than VOI-aware policies (VOI, VOI+).

# Sampling in Trees

- ▶ Hybrid sampling scheme:
  1. At the *root node*: sample based on the VOI estimate.
  2. At *non-root nodes*: sample using UCT.
- ▶ Stopping criterion: Assuming sample cost  $c$  is known, stop sampling when intrinsic VOI is less than  $C = cN$ :

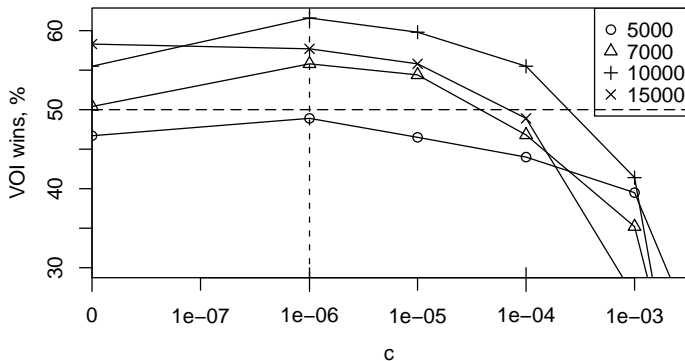
$$\frac{1}{N} \Lambda_{\alpha}^b \leq \frac{\bar{X}_{\beta}^{n_{\beta}}}{n_{\alpha} + 1} \Pr(\bar{X}_{\alpha}^{n_{\alpha} + N} \leq \bar{X}_{\beta}^{n_{\beta}}) \leq c$$
$$\frac{1}{N} \max_i \Lambda_i^b \leq \max_i \frac{(1 - \bar{X}_{\alpha}^{n_{\alpha}})}{n_i + 1} \Pr(\bar{X}_i^{n_i + N} \geq \bar{X}_{\alpha}^{n_{\alpha}}) \leq c$$
$$\forall i : i \neq \alpha$$

# Sample Redistribution

- ▶ The VOI estimate assumes that the information is **discarded** between states.
- ▶ MCTS **re-uses rollouts** generated at earlier search states.
- ▶ Either incorporate 'future' influence into the VOI estimate (*non-trivial!*).
- ▶ Or behave myopically w.r.t. search tree depth:
  1. Estimate VOI as though the information is discarded.
  2. Stop early if the VOI is below a certain threshold.
  3. Save the unused sample budget for search in future states.
- ▶ The cost  $c$  of a sample is  
the VOI of increasing a future budget by one sample.



# Playing Go Against UCT: Tuning the Sample Cost

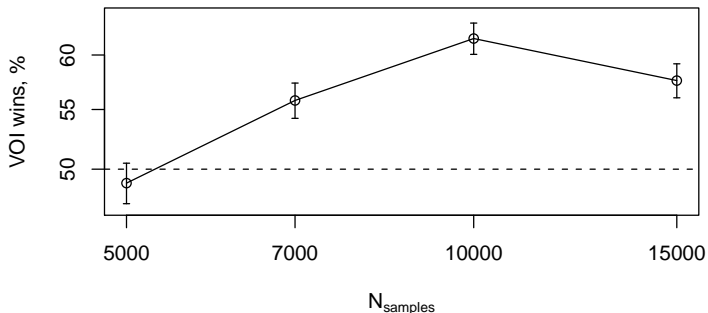


Best results for sample cost  $c \approx 10^{-6}$ :  
winning rate of **64%** for 10000 samples per ply.

# Playing Go Against UCT:

## Winning Rate vs. Number of Samples per Ply

Sample cost  $c$  fixed at  $10^{-6}$ :



Best results for *intermediate*  $N_{\text{samples}}$ :

- ▶ When  $N_{\text{samples}}$  is too low, poor moves are selected.
- ▶ When  $N_{\text{samples}}$  is too high, the VOI of further sampling is low.

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$A^*$

Apply all heuristics to initial state  $s_0$

Insert  $s_0$  into OPEN

**while** OPEN *not empty* **do**

$n \leftarrow$  best node from OPEN

**if** Goal( $n$ ) **then**

        └ **return** trace( $n$ )

**foreach** child  $c$  of  $n$  **do**

        └ Apply  $h_1$  to  $c$

        └ insert  $c$  into OPEN

    └ Insert  $n$  into CLOSED

**return** FAILURE

# Lazy A\*

Apply all heuristics to initial state  $s_0$

Insert  $s_0$  into OPEN

**while** OPEN *not empty* **do**

$n \leftarrow$  best node from OPEN

**if** Goal( $n$ ) **then**

        └ **return** trace( $n$ )

**if**  $h_2$  was not applied to  $n$

**then**

        └ Apply  $h_2$  to  $n$

        └ re-insert  $n$  into OPEN

        └ **continue**      //next node in OPEN

**foreach** child  $c$  of  $n$  **do**

        └ Apply  $h_1$  to  $c$

        └ insert  $c$  into OPEN

└ Insert  $n$  into CLOSED

**return** FAILURE

# Rational Lazy $A^*$

Apply all heuristics to initial state  $s_0$

Insert  $s_0$  into OPEN

**while** OPEN *not empty* **do**

$n \leftarrow$  best node from OPEN

**if**  $Goal(n)$  **then**

        └ **return** trace( $n$ )

**if**  $h_2$  was not applied to  $n$  and  $h_2$  is likely to pay off **then**

        └ Apply  $h_2$  to  $n$

        └ re-insert  $n$  into OPEN

        └ **continue**      //next node in OPEN

**foreach** child  $c$  of  $n$  **do**

        └ Apply  $h_1$  to  $c$

        └ insert  $c$  into OPEN

└ Insert  $n$  into CLOSED

**return** FAILURE

# Rational Decision

- ▶ When does computing  $h_2$  pay off?
- ▶ Suppose  $h_2$  was computed for state  $s$ . Then either:
  1.  $s$  will be expanded later on anyway
  2. an optimal goal is found before  $s$  is expanded
- ▶ Computing  $h_2$  pays off only in outcome 2 — call this “ $h_2$  is helpful”

*“It is difficult to make predictions, especially about the future”*

— Yogi Berra / Neils Bohr

# Towards a Rational Decision

- ▶ Myopic assumption: this is the *last* meta-level decision to be made, and henceforth the algorithm will act like lazy  $A^*$ .
- ▶ When a node re-emerges from the open list, compare the regret of computing  $h_2$  as in lazy  $A^*$ , vs. just expanding the node.
- ▶ Note: if rational lazy  $A^*$  is indeed better than lazy  $A^*$ , the myopic assumption results in an upper bound on the regret.

	Compute $h_2$	Bypass $h_2$
$h_2$ helpful	0	$\sim b(s)t_1 + (b(s) - 1)t_2$
$h_2$ not helpful	$\sim t_2$	0

$b(s)$  denotes the number of successors of  $s$

*Disclaimer: for the exact analysis, see the paper*



# From Regret to Rational Decision

	Compute $h_2$	Bypass $h_2$
$h_2$ helpful	0	$\sim b(s)t_1 + (b(s) - 1)t_2$
$h_2$ not helpful	$\sim t_2$	0

- ▶ Suppose that the probability of  $h_2$  being helpful is  $p_h$
- ▶ Then the rational decision is to compute  $h_2$  iff:

$$\frac{t_2}{t_1} < \frac{p_h b(s)}{1 - p_h b(s)}$$

## Approximating $p_h$

$$\frac{t_2}{t_1} < \frac{p_h b(s)}{1 - p_h b(s)}$$

- ▶ We can directly measure  $t_1$ ,  $t_2$  and  $b(s)$ , but need to approximate  $p_h$
- ▶ If  $s$  is a state at which  $h_2$  was helpful, then we computed  $h_2$  for  $s$ , but did not expand  $s$ . Denote the number of such states by  $B$ .
- ▶ Denote by  $A$  the number of states for which we computed  $h_2$ .
- ▶ We can use  $\frac{A}{B}$  as an estimate for  $p_h$
- ▶ To get an estimate which is more stable, we use a weighted average with  $k$  fictitious examples giving an estimate of  $p_{init}$ :

$$\frac{(A + p_{init} \cdot k)}{B + k}$$

- ▶ We use  $p_{init} = 0.5$  and  $k = 1000$

# Empirical Evaluation: Weighted 15 Puzzle

- ▶  $h_1$  — weighted manhattan distance
- ▶  $h_2$  — lookahead to depth  $l$  with  $h_1$

$l$	Generated			Time		
	$A^*$	$LA^*$	$RLA^*$	$A^*$	$LA^*$	$RLA^*$
2	1,206,535	1,206,535	1,309,574	0.707	0.820	0.842
4	1,066,851	1,066,851	1,169,020	0.634	0.667	0.650
6	889,847	889,847	944,750	<b>0.588</b>	0.533	0.464
8	740,464	740,464	793,126	0.648	<b>0.527</b>	0.377
10	611,975	611,975	889,220	0.843	0.671	<b>0.371</b>
12	<b>454,130</b>	<b>454,130</b>	807,846	0.927	0.769	0.429

# Empirical Evaluation: Planning Domains

- ▶  $h_{LA}$  — admissible landmarks
- ▶  $h_{LM-CUT}$  — landmark cut

Alg	Solved	623 Commonly Solved		
		Time (GM)	Expanded	Generated
$h_{LA}$	698	1.18	183,320,267	1,184,443,684
$h_{LM-CUT}$	697	0.98	23,797,219	114,315,382
max	722	0.98	<b>22,774,804</b>	<b>108,132,460</b>
selmax	747	0.89	54,557,689	193,980,693
$LA^*$	747	0.79	<b>22,790,804</b>	<b>108,201,244</b>
$RLA^*$	<b>750</b>	<b>0.77</b>	25,742,262	110,935,698

- ▶  $RLA^*$  solves the most problems, and is fastest on average

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# Insights into the Methodology

- ▶ Rational metareasoning works best when:
  1. Ubiquitous heuristic evaluation of the search space *decreases* the total search time.
  2. The heuristic computation time constitutes *a significant part* of the total search time.
- ▶ It is important to identify the right metareasoning decision.
- ▶ Simple utility and information model serve well.
- ▶ Tunable parameters should reflect algorithm implementation rather than problem set.

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## Novel techniques:

- ▶ “Rational Deployment of heuristics in CSP” demonstrated derivation of the belief model from the algorithm rather than problem set.
- ▶ “VOI-aware Monte-Carlo tree search” provided distribution-independent upper bounds for semi-myopic VOI estimates in Monte-Carlo sampling.
- ▶ “Towards rational deployment of Multiple Heuristics in A\*”, introduced a novel area of application of rational metareasoning—optimal search in optimization problems.

## Future research:

- ▶ Whether a dramatic breakthrough in performance is possible.
- ▶ Rational metareasoning when action costs and state utilities are not commensurable.



Thank You