Rational Metareasoning in Problem-Solving Search

July 30, 2013

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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

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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_{α} that maximizes the agent's *expected utility*.

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

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

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

- ▶ $S_{j_{\text{max}}}$ that maximizes the net VOI is performed: $j_{\text{max}} = \arg \max_{j} V(S_{j})$, if $V(S_{j_{\text{max}}}) > 0$.
- Otherwise, A_{α} 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
$$\mathscr{X} = \{X_1, X_2, ...\}$$
, constraints $\mathscr{C} = \{C_1, C_2, ...\}$.

- 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 ω 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 ω which optimizes $T^{s|\omega}$. $T^{s|\omega}$ is minimal if the values are sorted by increasing order of $\frac{T_i}{1-D_i}$.
- ► The intrinsic VOI Λ_i of estimating T_i, p_i for the *i*th assignment is the expected decrease in the expected search time: $\Lambda_i = \mathbb{E} \left[T^{s|\omega_-} T^{s|\omega_{+i}} \right]$.

Model Assumptions

- 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 Λ_i of invoking the heuristic can be approximated as:

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

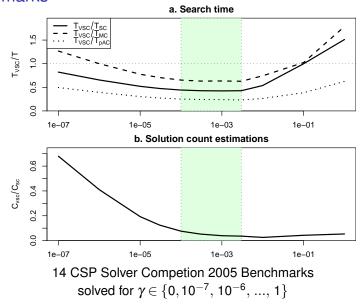
VOI of Solution Count Estimates

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

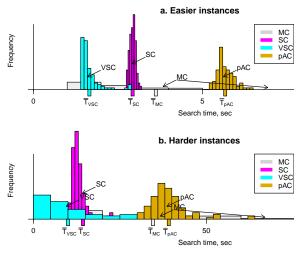
$$V \propto |D_k|e^{-\nu}\sum_{n=n_{\text{max}}}^{\infty} \left(\frac{1}{n_{\text{max}}} - \frac{1}{n}\right) \frac{v^n}{n!} - \gamma$$

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

Benchmarks



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 **C**arlo **T**ree **S**earch 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:

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

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

UCT

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.

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.

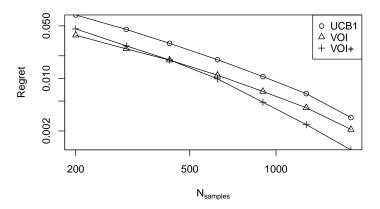
Upper bounds on intrinsic VOI Λ_i^b of testing the *i*th arm N times are (based on Hoeffding inequality):

$$\begin{split} & \Lambda_{\alpha}^{b} < \frac{N \overline{X}_{\beta}^{n_{\beta}}}{n_{\alpha} + 1} \cdot 2 \exp\left(-1.37 (\overline{X}_{\alpha}^{n_{\alpha}} - \overline{X}_{\beta}^{n_{\beta}})^{2} n_{\alpha}\right) \\ & \Lambda_{i|i \neq \alpha}^{b} < \frac{N (1 - \overline{X}_{\alpha}^{n_{\alpha}})}{n_{i} + 1} \cdot 2 \exp\left(-1.37 (\overline{X}_{\alpha}^{n_{\alpha}} - \overline{X}_{i}^{n_{i}})^{2} n_{i}\right) \end{split}$$

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:

$$\frac{1}{N} \Lambda_{\alpha}^{b} \leq \frac{\overline{X}_{\beta}^{n_{\beta}}}{n_{\alpha} + 1} \Pr(\overline{X}_{\alpha}^{n_{\alpha} + N} \leq \overline{X}_{\beta}^{n_{\alpha}}) \leq c$$

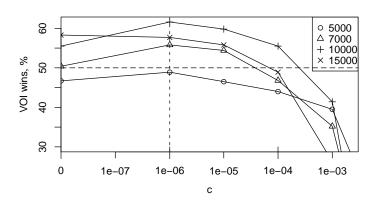
$$\frac{1}{N} \max_{i} \Lambda_{i}^{b} \leq \max_{i} \frac{(1 - \overline{X}_{\alpha}^{n_{\alpha}})}{n_{i} + 1} \Pr(\overline{X}_{i}^{n_{i} + N} \geq \overline{X}_{\alpha}^{n_{\alpha}}) \leq c$$

$$\forall i : i \neq \alpha$$

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

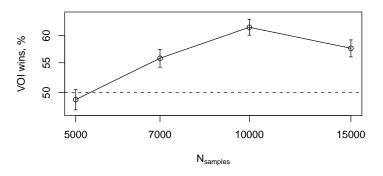


Best results for sample cost $c \approx 10^{-6}$: winning rate of **64%** for 10000 samples per ply.



Playing Go Against UCT: Winning Rate vs. Number of Samples per Ply

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



Best results for *intermediate N_{samples}*:

- ▶ When N_{samples} is too low, poor moves are selected.
- ▶ When *N_{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 so into Open
while OPEN not empty do
    n \leftarrow \text{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 so into Open
while OPEN not empty do
    n \leftarrow \text{best node from OPEN}
   if Goal(n) then
       return trace(n)
   if h2 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 so into Open
while OPEN not empty do
    n \leftarrow \text{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 h₂ pays off only in outcome 2 call this "h₂ 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 h₂ 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 h₂ 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

- ▶ h₁ weighted manhattan distance
- ▶ h₂ lookahead to depth I with h₁

	Generated			Time		
1	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	0.588	0.533	0.464
8	740,464	740,464	793,126	0.648	0.527	0.377
10	611,975	611,975	889,220	0.843	0.671	0.371
12	454,130	454,130	807,846	0.927	0.769	0.429

Empirical Evaluation: Planning Domains

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

		623 Commonly Solved			
Alg	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	22,774,804	108,132,460	
selmax	747	0.89	54,557,689	193,980,693	
LA*	747	0.79	22,790,804	108,201,244	
RLA*	750	0.77	25,742,262	110,935,698	

RLA* solves the most problems, and is fastest on average



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- Rational metareasoning works best when:
 - Ubiquitous heuristic evaluation of the search space decreases the total search time.
 - The heuristic computation time constitutes a significant part of the total search time.
- lt 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