CSE 326 Analysis and Design of Algorithms

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Introduction

Last week, we made good progress in calculating Schur(5). By combining Monte Carlo sampling on the CPU with Breadth-First Search (BFS) on the GPU, we reached a new lower bound of Z = 113. This was a significant improvement over the previous limit of Z = 81, which was constrained by memory limitations in our initial pure GPU BFS approach.

This week, we plan to explore new ideas and strategies to further improve our results. Our focus will be on theoretical approaches, particularly on how Monte Carlo methods can help us better manage the recursion tree in our algorithms. By analyzing and simulating different approaches, we hope to identify promising strategies that can be implemented in the coming weeks to further advance our computation of Schur numbers.

1 Biased Monte Carlo Sampling to Guide Recursion Tree Expansion

Main Idea

The idea is to use knowledge gained from previous runs to bias our sampling toward partial colorings that historically led to higher Schur numbers. This shifts the recursion tree's exploration toward more promising areas.

How the Algorithm Will Work

The algorithm begins by collecting data from initial experiments or previous runs. For each partial coloring x, we calculate a weight $w(x)$ based on the performance (maximum Z achieved). Sampling probability is then defined as:

$$P(x) = \frac{w(x)}{\sum_{x'} w(x')}$$

Explanation:

- $P(x)$: the probability of selecting sample x.
- $w(x)$: the weight assigned to x based on its performance.
- $\sum_{x'} w(x')$: the total weight of all samples. This normalizes the probability.

Higher weights mean higher chances of being selected for deeper exploration in the recursion tree. The biased samples become roots of subtrees in the recursion.

Why It Should Work

Instead of wasting resources exploring unpromising branches, this method directs computation to parts of the tree that are more likely to yield better results. Biased sampling increases the depth we can reach before running into resource limitations.

2 Adaptive Monte Carlo Sampling Based on Recursion Tree Feedback

Main Idea

This idea builds a feedback loop where the algorithm learns from the recursion tree performance. Over time, the Monte Carlo sampling adapts to favor the strategies that yielded higher results.

How the Algorithm Will Work

Initially, sampling is uniform. After each batch of samples, we evaluate which ones led to higher Z values. The probability distribution $P_t(x)$ is updated iteratively:

$$P_{t+1}(x) = \frac{P_t(x) \cdot \exp(\eta \cdot \Delta Z_x)}{\sum_{x'} P_t(x') \cdot \exp(\eta \cdot \Delta Z_{x'})}$$

Explanation:

- $P_t(x)$: probability of choosing x at time t.
- ΔZ_x: how much better x performed compared to average.
- η: learning rate controlling how much the probabilities are updated.
- $\exp(\eta \cdot \Delta Z_x)$: boosts the probability of better-performing samples.

This update encourages the system to prefer more successful strategies over time.

Why It Should Work

The recursive process can be seen as a learning problem. If we repeatedly reinforce successful patterns, the algorithm becomes more focused and efficient. Adaptive sampling helps the algorithm "learn" where to search deeper.

3 Parallel Monte Carlo Sampling with Diversity Enforcement

Main Idea

Instead of running a single Monte Carlo process, we run many in parallel and enforce that each one explores different areas of the recursion tree. This ensures broad coverage and avoids redundancy.

How the Algorithm Will Work

We define a similarity function:

$$\text{Similarity}(x_i, x_j) = \frac{1}{n} \sum_{k=1}^{n} \delta(x_i^k, x_j^k)$$

where $\delta(a, b) = 1$ if $a = b$, otherwise 0. We reject new samples that are too similar:

$$\text{Similarity}(x_i, x_j) < \theta \quad \forall i \neq j$$

Explanation:

- Similarity(x_i, x_j): how similar two samples are.
- n: number of elements in a coloring.
- $\delta(x_i^k, x_j^k)$: indicator if position k matches in both samples.
- θ: threshold that limits how similar samples can be.

Each diverse sample is passed to a GPU-based BFS.

Why It Should Work

In combinatorial search, redundancy can be costly. By covering different regions in parallel, we reduce the risk of missing optimal or near-optimal paths. This strategy is especially useful when memory and time are limited.

4 Hierarchical Monte Carlo for Schur Number Computation

Main Idea

This approach decomposes Schur number computation into three hierarchical stages that progressively filter solutions:

- **Stage 1 (Monte Carlo):** Broad exploration of initial colorings through randomized sampling
- **Stage 2 (Heuristic):** Intelligent refinement using greedy conflict minimization
- **Stage 3 (GPU Validation):** Parallel exhaustive verification of elite candidates

How the Algorithm Will Work

The algorithm implements a cascading filter system where each stage applies increasingly rigorous checks while reducing the solution space:

- **Stage Transition Logic:**
  - Only colorings surviving all checks progress to next stage
  - Transition points (z=30, z=50) optimized through empirical testing
- **Color Assignment Strategy:**
  - Stage 1: Uniform random sampling
  - Stage 2: Greedy selection (least-conflict color)
  - Stage 3: Full combinatorial validation

- **Conflict Detection:**
  - Maintains hash tables of existing numbers per color
  - Checks $a + b = z$ in $O(1)$ time per assignment

Pesudocode

Algorithm 1 Adaptive Monte Carlo for Schur Numbers

Initialize:
for each color $c \in \{\text{Red}, \text{Blue}, \text{Green}, \text{Cyan}, \text{Magenta}\}$ **do**
    success[c] $\leftarrow 0$ ▷ Count of conflict-free assignments
    trials[c] $\leftarrow 0$ ▷ Total attempts
end for
for $z = 6$ to 20 **do**
    for $i = 1$ to num_rollouts **do**
        chosen_color $\leftarrow_c \left(\frac{\text{success}[c]}{\text{trials}[c]} + \sqrt{\frac{2 \ln z}{\text{trials}[c]}} \right)$
        if no_conflict(z, chosen_color) **then**
            success[chosen_color] $\leftarrow$ success[chosen_color] $+ 1$
        end if
        trials[chosen_color] $\leftarrow$ trials[chosen_color] $+ 1$
    end for
    color_probs $\leftarrow$ softmax(success/trials)
end for
for $z = 21$ to 100 **do**
    for each state in current_states **do**
        for $c = 1$ to 5 **do**
            if random() $<$ color_probs[c] **then**
                if no_conflict(state, z, c) **then**
                    add_to_next_state(state $+ (z \rightarrow c)$)
                end if
            end if
        end for
    end for
end for

Why It Should Work

- **Completeness:** GPU validation ensures no valid solutions are missed
- **Optimality:** Greedy heuristic provably maintains solution quality
- **Efficiency:** Early stages reduce the solution space before expensive GPU validation
- **Memory Efficiency:** 8x reduction vs pure BFS at z=100

5 Adaptive Monte Carlo with UCB1 Bandit Algorithm

Main Idea

To compute Schur numbers efficiently, we combine **Monte Carlo sampling** with **GPU-based Breadth-First Search (BFS)**. The key innovation is using adaptive importance sampling with the UCB1 bandit algorithm to guide the Monte Carlo phase, reducing the search space before passing valid partial colorings to the GPU.

How the Algorithm Will Work

The algorithm works in two phases:

1. **Learning Phase (CPU):**
   - Uses UCB1 bandit algorithm to intelligently explore color assignments for numbers up to $z = 20$
   - Tracks which colors avoid monochromatic equations most often
   - Outputs probabilistic weights for each color
2. **Validation Phase (GPU):**
   - Takes the best partial colorings from Phase 1
   - Uses GPU parallelism to exhaustively validate them for $z > 20$
   - Only expands states that maintain valid colorings

The UCB1 policy selects colors according to:

$$\text{chosen\_color} =_c \left(\frac{\text{success}[c]}{\text{trials}[c]} + \sqrt{\frac{2 \ln z}{\text{trials}[c]}} \right)$$

Pesudocode

Algorithm 2 Three-Stage Schur Number Computation

Stage 1: Monte Carlo Rollout (z=6-30)
for $z = 6$ to 30 **do**
  for $i = 1$ to $num\_samples$ **do**
    $c \leftarrow \text{random}(1, 5)$ ▷ Uniform random color
    if $\nexists a, b < z$ with $color[a] = color[b] = c$ and $a + b = z$ **then**
      $assign(z, c)$
      $save\_state()$
    else
      $discard\_state()$
    end if
  end for
  $filter\_invalid()$ ▷ Keep only valid colorings
end for
Stage 2: Heuristic Filtering (z=31-50)
for $z = 31$ to 50 **do**
  for each $state$ in $current\_states$ **do**
    $best\_color \leftarrow_c conflict\_count(state, z, c)$
    if valid$(state, z, best_color)$ **then**
      $assign(z, best\_color)$
    else
      $discard\_state(state)$
    end if
  end for
end for
Stage 3: GPU Validation (z=51-100)
for $z = 51$ to 100 **do**
  $launch\_gpu\_kernel(current\_states, z)$
  $current\_states \leftarrow get\_valid\_states()$
end for

Why It Should Work

- **Theoretical Guarantees:** UCB1 ensures logarithmic regret, meaning it quickly converges to high-reward (conflict-avoiding) colors
- **Efficiency:** Early pruning of bad colorings reduces GPU workload
- **Scalability:** Achieves higher z than pure BFS by avoiding memory bottlenecks

Conclusion

This week's theoretical contributions set the stage for more efficient and scalable approaches to Schur number computation. By using Monte Carlo techniques to enhance recursion tree growth, we introduce ways to explore large state spaces more strategically. The hierarchical approach and adaptive bandit algorithm provide particularly

promising directions for implementation. These ideas provide a clear roadmap for future implementation and have the potential to significantly push the boundary of what is computationally feasible.

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