

ML-Guided IBP Reduction

Neural Network Guided Integration-by-Parts Reduction of
Feynman Integrals

Two-Loop Triangle-Box Topology

The Problem

- ▶ **IBP reduction:** Express complex Feynman integrals as linear combinations of simpler “master” integrals
- ▶ **Challenge:** Exponential search space of IBP identities
- ▶ **Traditional approaches:** Laporta algorithm, Kira, FIRE

The Memory Wall

Traditional IBP codes hit **memory limits** as integrals grow more complex:

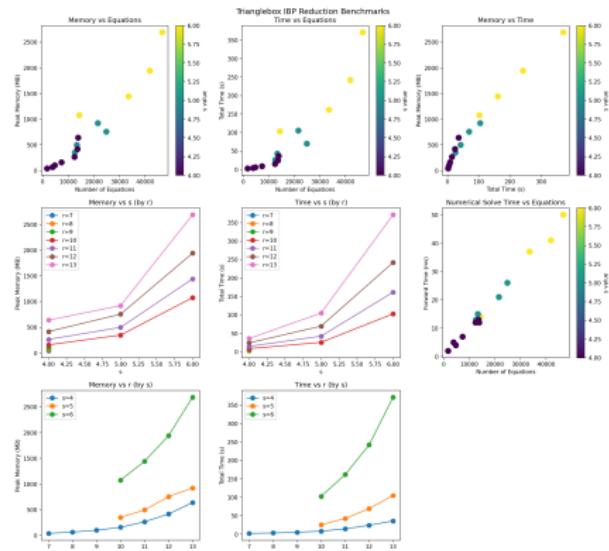


Figure 1: Kira Memory Scaling

Kira benchmarks: Memory grows exponentially with integral weight (r), reaching 2.5+ GB for $r=13$.

Our Solution

- ▶ **ML-guided beam search:** Train a neural network to score IBP actions
- ▶ **Hierarchical reduction:** Process sectors from highest to lowest
- ▶ **Parallel execution:** Distribute across Condor cluster for ~10x speedup
- ▶ **Constant memory:** Each one-step reduction is independent - no system accumulation

The Action Space: Key Innovation

Why Traditional IBP is Hard

- ▶ Infinite possible IBP identities (any seed, any operator)
- ▶ No clear way to choose which identity to apply
- ▶ Laporta: build giant linear system, solve globally

Our Approach: Finite Action Space

- ▶ Restrict to actions that **solve for a specific target integral**
- ▶ Each action = (IBP operator, seed shift)
- ▶ Enumerate only **valid actions** that eliminate the target
- ▶ Enables ML: classification over finite action set

Action Representation

Action = (ibp_op, delta)

- ▶ **ibp_op**: Which IBP/LI operator (0-15)
- ▶ **delta**: Shift from target to seed integral

Example

Target: $I[2,0,1,0,1,1,0]$, Action: (3, (-1,0,0,0,0,0,0))

IBP equation (op=3, seed=[1,0,1,0,1,1,0]):

$$c_1 \cdot I[2,0,1,0,1,1,0] + c_2 \cdot I[1,0,1,0,1,1,0] + c_3 \cdot I[1,0,2,0,1,1,0] + \dots$$

↑ target

Solve for target → express in terms of simpler integrals

Direct vs Indirect Actions

Direct Actions

- ▶ Target appears directly in the raw IBP equation
- ▶ Straightforward: apply IBP, solve for target

Indirect Actions (Key Innovation)

- ▶ Target does **not** appear in raw IBP equation
- ▶ But appears **after applying substitutions** from previous steps

Raw IBP: $c_1 \cdot I[A] + c_2 \cdot I[B] = 0$ (no target)

After subs: $c_1 \cdot I[A] + c_2 \cdot (\dots + c_3 \cdot I[\text{target}] + \dots) = 0$
↑ target appears!

Indirect actions leverage reduction history for deeper reductions

Subsector Filtering

The Problem

Arbitrary IBP actions can introduce integrals in **higher sectors** → explosion

Solution: Subsector Constraint

Only allow actions where all resulting integrals are in **subsectors** of target

Sector Hierarchy

Sector 63 [1,1,1,1,1,1] (6 propagators)

↓ subsectors

Sector 62 [0,1,1,1,1,1] (5 propagators)

Sector 61 [1,0,1,1,1,1] (5 propagators)

↓

...lower sectors...

Result: Reductions flow downward through sector hierarchy

Why This Works

Finite + Learnable

- ▶ Typically 10-100 valid actions per state
- ▶ Model learns which actions lead to successful reductions

Hierarchical Structure

- ▶ Subsector filtering ensures monotonic progress
- ▶ Never introduces integrals harder than current target

Substitution Chains

- ▶ Indirect actions enable multi-step reasoning
- ▶ Model implicitly learns useful substitution patterns

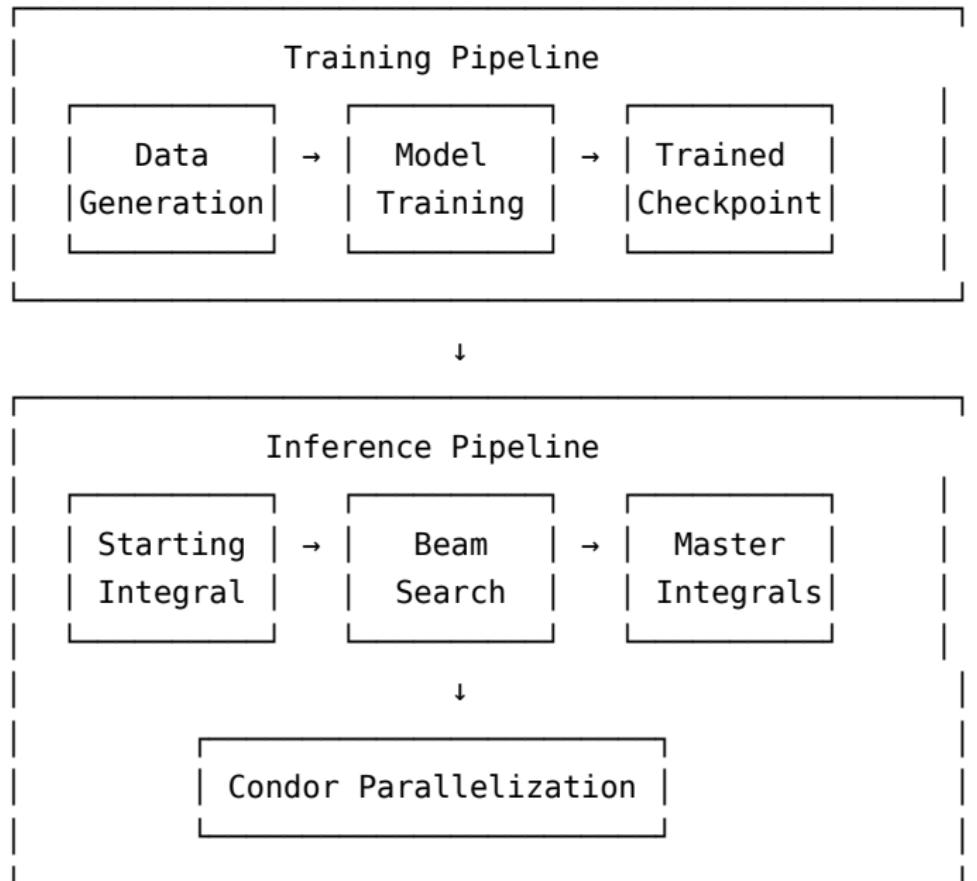
Key Results

Triangle-Box Topology (arXiv:2502.05121)

| Integral | Weight | Seq. | Par. | Speedup | Masters |
|-------------------|--------|---------------|----------------|-------------|---------|
| I[2,0,2,0,1,1,0] | (6,0) | 5 min | - | - | 4 |
| I[1,1,1,1,1,1,-3] | (6,3) | 73 min | 12 min | 6x | 16 |
| I[3,2,1,3,2,2,-6] | (13,6) | ~20 hr | 115 min | ~10x | 16 |

- ▶ Results match Kira exactly
- ▶ Reduces to exact 16 paper masters from arXiv:2502.05121

System Architecture



Part 1: Data Generation

Data Generation: Scrambling Approach

Key Insight

Instead of collecting reduction trajectories (expensive), **reverse the process**: 1. Start from master integrals 2. Apply random IBP identities to increase complexity 3. Record each step - becomes training data when reversed

Constraints During Scrambling

- ▶ Only apply IBPs that don't introduce higher-sector integrals
- ▶ Stay within target sector and subsectors
- ▶ Ensures training data reflects valid reduction paths

Data Generation: Coverage

Sector Coverage

- ▶ All 63 non-trivial sectors covered
- ▶ Uses 16 paper masters for their respective sectors
- ▶ Uses corner integrals for remaining sectors

Dataset Statistics

| Split | Samples | Size |
|------------|----------|--------|
| Train | 946,168 | 3.8 GB |
| Validation | 118,271 | 480 MB |
| Test | ~118,000 | 480 MB |

Data Format

Each training sample contains:

```
{  
    'sector_mask': [1,0,1,0,1,1],  # 6-bit sector encoding  
    'expr': [                      # Current expression  
        ([1,0,2,0,1,1,0], 107),     # (integral, coefficient)  
        ([1,0,1,0,1,1,0], 303),  
        ...  
    ],  
    'subs': [                      # Substitution history  
        (key_integral, [(repl_int1, coeff1), ...]),  
        ...  
    ],  
    'target_integral': [1,0,2,0,1,1,0], # Integral to eliminate  
    'valid_actions': [(ibp_op, delta), ...],  
    'label': 3  # Index of correct action  
}
```

Part 2: Model Architecture

Model: IBPActionClassifierV5

Overview

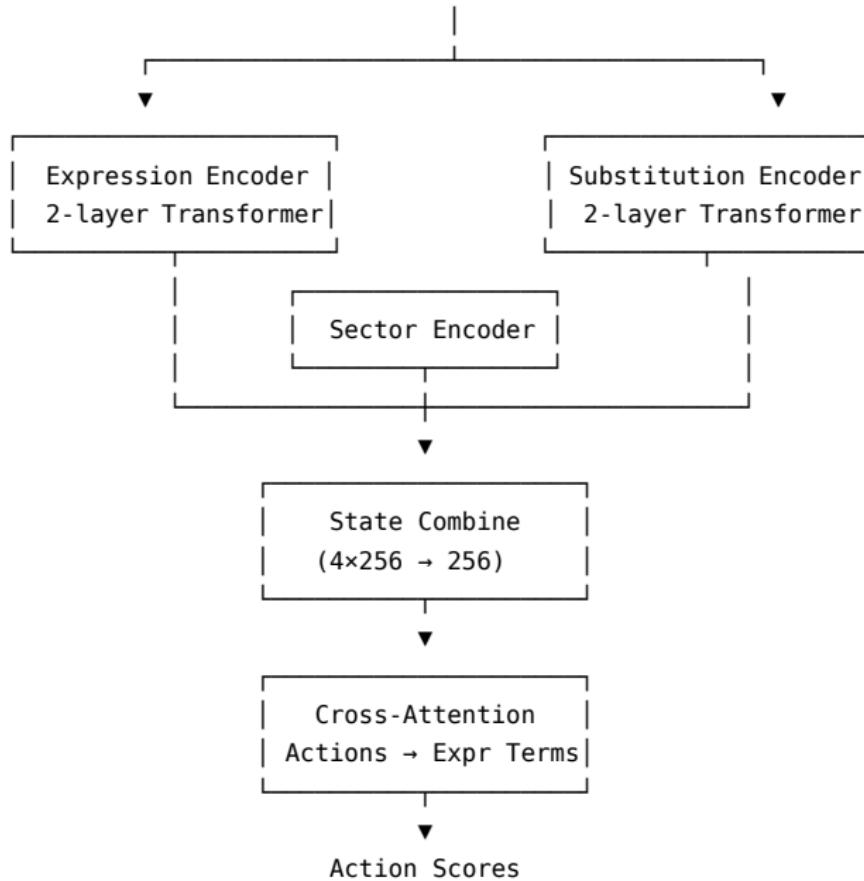
- ▶ **Task:** Score candidate IBP actions given current reduction state
- ▶ **Architecture:** Transformer-based with specialized encoders
- ▶ **Parameters:** 7.7M
- ▶ **Best validation accuracy:** 90.77%

Key Innovation (V5)

Full substitution encoding - encode not just the key integral but the complete replacement expression

Model Architecture Diagram

Inputs: Expression, Target, Substitutions, Sector, Actions



Component Details

| Component | Purpose |
|-------------------------------|-----------------------------|
| Expression Encoder | Encode expression + target |
| Substitution Encoder | Encode reduction history |
| Sector Encoder | Condition on sector |
| Cross-Attention Scorer | Score actions vs expression |

All use 2-layer architectures (Transformer or cross-attention)

Model Hyperparameters

- ▶ Embedding dimension: 256, Attention heads: 4
- ▶ Total parameters: 7,696,709

Part 3: Training

Training Configuration

```
epochs = 30
batch_size = 256
learning_rate = 0.0004
weight_decay = 1e-5
optimizer = AdamW
```

Training Results

- ▶ **Best checkpoint:** Epoch 22
- ▶ **Validation accuracy:** 90.77% (top-1)
- ▶ **Top-5 accuracy:** ~98%
- ▶ **Training time:** ~800s per epoch on GPU

Training Curves

Key Observations

- ▶ Model converges by epoch 20-25
- ▶ Validation accuracy plateaus at ~91%
- ▶ No significant overfitting observed
- ▶ Top-5 accuracy very high (~98%) - beam search can recover from top-1 mistakes

Part 4: Beam Search Inference

Beam Search Algorithm

```
def beam_search(start_integral, beam_width=20):
    beam = [start_state]

    while not all_masters(beam[0]):
        candidates = []
        for state in beam:
            for action in get_valid_actions(state):
                score = model.score(state, action)
                new_state = apply_action(state, action)
                candidates.append((new_state, score))

        # Keep top-k by score
        beam = sorted(candidates, key=score)[:beam_width]

    return beam[0]
```

Beam Search Optimizations

P1: Equation Caching ($\sim 3\text{-}10x$ speedup)

- ▶ IBP equation generation is expensive (sympy operations)
- ▶ Cache `get_raw_equation` results
- ▶ Reuse across beam states with shared history

P2: Batched Inference ($\sim 50x$ speedup)

- ▶ Prepare all action candidates as numpy arrays
- ▶ Single batched forward pass through model
- ▶ Eliminates per-action inference overhead

Combined Effect

- ▶ Per-step time: 10-90s \rightarrow 0.1-5s
- ▶ Makes deep reductions feasible

Hierarchical Reduction Strategy

Algorithm

1. Find highest-level sector with non-master integrals
2. Run beam search to eliminate all non-masters in that sector
3. Move to next highest sector
4. Repeat until only masters remain

Example: I[2,0,2,0,1,1,0]

| Sector | Level | Steps |
|--------------|-------|------------|
| 53 | 4 | 53 |
| 52 | 3 | 17 |
| 49 | 3 | 4 |
| 37 | 3 | 42 |
| 21 | 3 | 46 |
| ... | ... | ... |
| Total | - | 176 |

Beam Restart Strategy (V11+)

Problem

After weight improvement, beam often contains suboptimal states that will never succeed

Solution: Beam Restart

1. Run beam search until weight improves
2. **Stop and restart** with only the best state
3. Prunes dead ends, enables deeper exploration

Impact

- ▶ Essential for high-weight integrals
- ▶ $I[1,1,1,1,1,1,-3]$: 1,416 steps across 45 sectors
- ▶ $I[3,2,1,3,2,2,-6]$: 46,345 steps across 62 sectors

Part 5: Parallelization

Parallelization Motivation

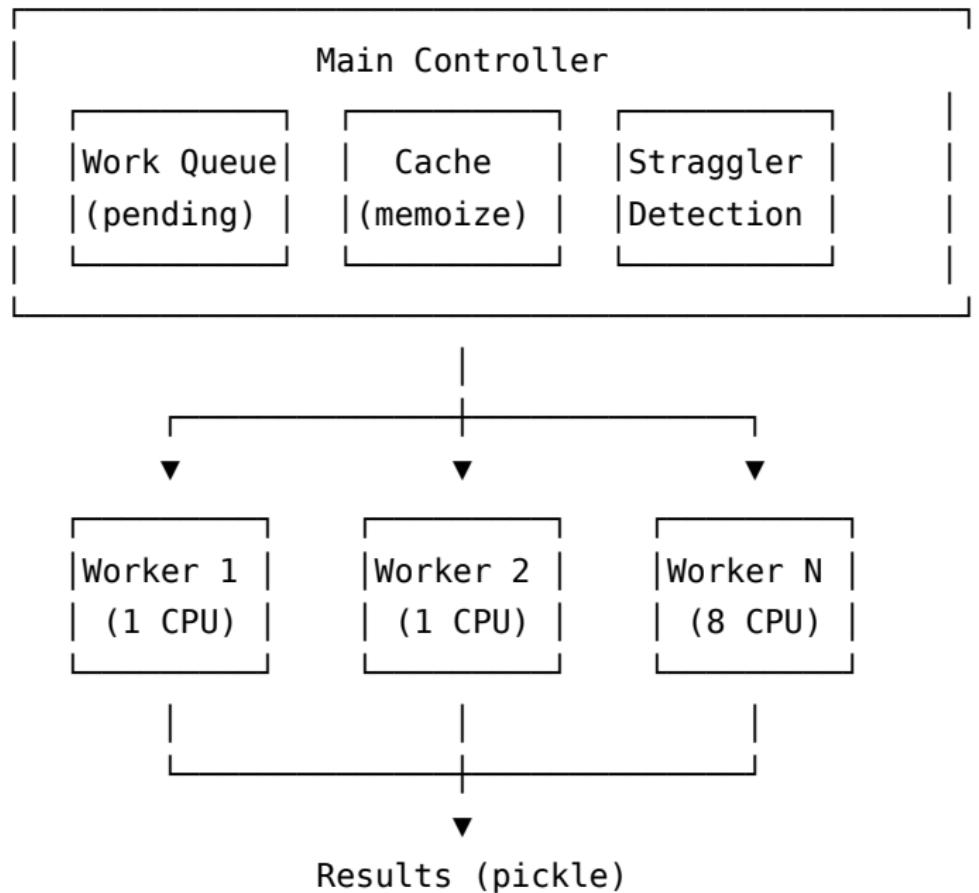
The Bottleneck

- ▶ Sequential reduction of $I[3,2,1,3,2,2, -6]$ takes ~20 hours
- ▶ Single-threaded beam search on CPU
- ▶ Many independent integrals could be processed in parallel

Key Insight

Each one-step reduction is independent - distribute across workers!

Async Parallel Architecture



Key Parallelization Features

1. Async Work Distribution

- ▶ Submit all pending non-masters immediately
- ▶ Don't wait for level synchronization
- ▶ Process results as they arrive

2. Memoization Cache

- ▶ Store: integral → reduced expression
- ▶ Avoid redundant work (~55,000 cache hits!)
- ▶ Critical when stragglers produce already-cached results

3. Straggler Detection

- ▶ Jobs >30 min are killed and resubmitted
- ▶ Resubmit with 8 CPUs (parallel beam search)
- ▶ Prevents slow integrals from blocking progress

Parallel Performance

I[3,2,1,3,2,2,-6] Results

| Metric | Value |
|------------------------|--------------------|
| Time (sequential) | ~20 hours |
| Time (parallel) | 115 minutes |
| Speedup | ~10x |
| Jobs submitted | 21,096 |
| Stragglers resubmitted | 24 |
| Cache hits | 55,075 |
| Final masters | 16 |

Part 6: Results

Validation Against Kira

I[2,0,2,0,1,1,0] (Sector 53)

| Method | Masters | Result |
|---------------|---------|-----------------|
| Kira | 4 | Reference |
| Our V5 | 4 | Matches exactly |

Our reduction produces the **exact same master basis** as professional IBP software.

Scaling Results

| Integral | Weight | Time | Steps | Masters |
|-------------------|--------|-----------------|---------|---------|
| I[2,0,2,0,1,1,0] | (6,0) | 5 min | 176 | 4 |
| I[1,1,1,1,1,1,-3] | (6,3) | 12 min* | 1,416 | 16 |
| I[3,2,1,3,2,2,-6] | (13,6) | 115 min* | 131,769 | 16 |

*With parallel execution

Final Reduction Example

$I[3,2,1,3,2,2,-6] \rightarrow 16$ Paper Masters

Final expression (mod 1009):

171 * $I[1,0,1,1,1,1,0]$

854 * $I[1,1,0,1,1,1,0]$

377 * $I[1,1,1,1,1,0,0]$

160 * $I[-1,1,1,1,1,0,0]$

100 * $I[0,1,1,1,1,0,0]$

647 * $I[1,-1,1,0,1,1,0]$

9 * $I[1,-1,1,1,1,0,0]$

... (16 masters total)

Matches arXiv:2502.05121 basis exactly!

Part 7: Conclusions

Key Contributions

1. **ML-guided IBP reduction** that matches professional software (Kira)
2. **Constant memory usage** - avoids the memory wall of traditional approaches
3. **Hierarchical beam search** with restart strategy for deep reductions
4. **Async parallel execution** with ~10x speedup
5. **Straggler handling** for robust distributed computing
6. **Paper-masters-only mode** for clean minimal basis

Technical Innovations

Model

- ▶ Full substitution encoding (V5)
- ▶ Cross-attention action scoring
- ▶ Target-aware expression encoding

Inference

- ▶ Equation caching (3-10x speedup)
- ▶ Batched model inference (50x speedup)
- ▶ Beam restart strategy

Parallelization

- ▶ Async one-step distribution
- ▶ Memoization cache ($\sim 55k$ hits)
- ▶ Automatic straggler resubmission

Future Work

1. **GPU workers** for faster beam search
2. **Adaptive timeouts** based on sector statistics
3. **More integrals** - test on other two-loop families
4. **Training on successful paths** - use reduction results to improve model
5. **Path optimization** - shorten saved reduction paths

Code Availability

Repository: github.com/davidshih17/RL_IBPrediction_claude

Key Files

- ▶ `models/classifier_v5.py` - Model architecture
- ▶ `scripts/eval/hierarchical_reduction_async.py` - Parallel reduction
- ▶ `scripts/eval/reduce_integral_onestep_worker.py` - Condor worker
- ▶ `docs/parallelization.md` - Detailed documentation

Thank You

Questions?

Contact

- ▶ Repository:
github.com/davidshih17/RL_IBPrediction_claude
- ▶ arXiv: 2502.05121 (paper masters reference)