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:

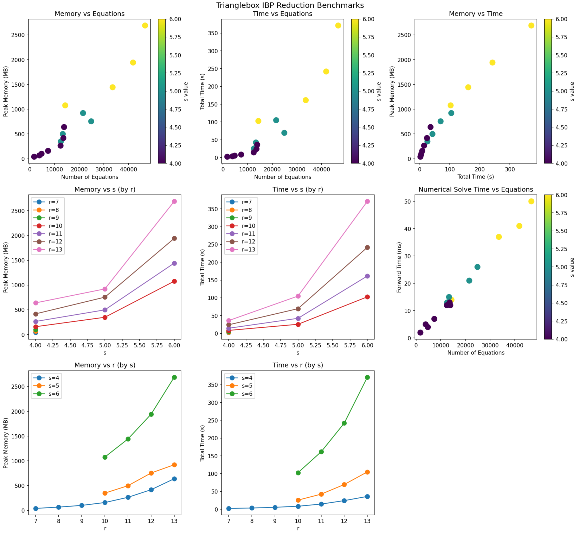

Figure 1: Kira Memory Scaling

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

Key Results

Triangle-Box Topology (arXiv:2502.05121)

Integral	Weight	Sequential	Parallel	Speedup	Maste
`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

```
┌───────────────────────────────────────────────────────┐
│                  Training Pipeline                   │
│                                                       │
│  ┌──────────────┐    ┌──────────────┐    ┌──────────────┐   │
│  │     Data     │ →  │    Model     │ →  │   Trained    │   │
│  │  Generation  │    │   Training   │    │  Checkpoint  │   │
│  └──────────────┘    └──────────────┘    └──────────────┘   │
└───────────────────────────────────────────────────────┘
                            ↓
┌───────────────────────────────────────────────────────┐
│                 Inference Pipeline                   │
│                                                       │
│  ┌──────────────┐    ┌──────────────┐    ┌──────────────┐   │
│  │   Starting   │ →  │     Beam     │ →  │    Master    │   │
│  │   Integral   │    │    Search    │    │  Integrals   │   │
│  └──────────────┘    └──────────────┘    └──────────────┘   │
│                          ↓                            │
│           ┌──────────────────────────┐                │
│           │  Condor Parallelization  │                │
│           │  (async + memoization)   │                │
```

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
                            │
          ┌─────────────────┴─────────────────┐
          │                                   │
          ▼                                   ▼
 ┌──────────────────┐               ┌──────────────────┐
 │ Expression Encoder │             │ Substitution Encoder│
 │ [CLS][TARGET][terms]            │ (full replacement) │
 │ 2-layer Transformer │            │ 2-layer Transformer │
 └────────┬─────────┘               └────────┬─────────┘
          │                                   │
          │        ┌────────────────┐         │
          │        │ Sector Encoder │         │
          │        └───────┬────────┘         │
          │                │                  │
          └────────────────┼──────────────────┘
                           │
                           ▼
```

Component Details

Component	Purpose	Architecture
Expression Encoder	Encode current expression + target	2-layer Transformer
Substitution Encoder	Encode reduction history	2-layer Transformer + attention pooling
Sector Encoder	Condition on target sector	Embedding + projection
Cross-Attention Scorer	Score actions by attending to expression	2-layer 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

```python
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 (~3-10x speedup)

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

P2: Batched Inference (~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 $\sim$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

```
┌────────────────────────────────────────────────────────────┐
│                      Main Controller                        │
│                                                            │
│  ┌─────────────┐  ┌─────────────┐  ┌─────────────┐         │
│  │ Work Queue  │  │    Cache    │  │  Straggler  │         │
│  │(non-masters)│  │(memoization)│  │  Detection  │         │
│  └─────────────┘  └─────────────┘  └─────────────┘         │
└────────────────────────────────────────────────────────────┘
                              │
               ┌──────────────┼──────────────┐
               ▼              ▼              ▼
          ┌──────────┐   ┌──────────┐   ┌──────────┐
          │Worker 1  │   │Worker 2  │   │Worker N  │
          │ (1 CPU)  │   │ (1 CPU)  │   │ (8 CPU)  │
          └──────────┘   └──────────┘   └──────────┘
               │              │              │
               └──────────────┼──────────────┘
                              ▼
```

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)	$\sim$20 hours
Time (parallel)	**115 minutes**
Speedup	$\sim$**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 $\sim$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_IBPreduction_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_IBPreduction_claude`
- arXiv: 2502.05121 (paper masters reference)