THRML-Powered RBM Demonstration

A Thermodynamic Computing Inspired Probabilistic Model

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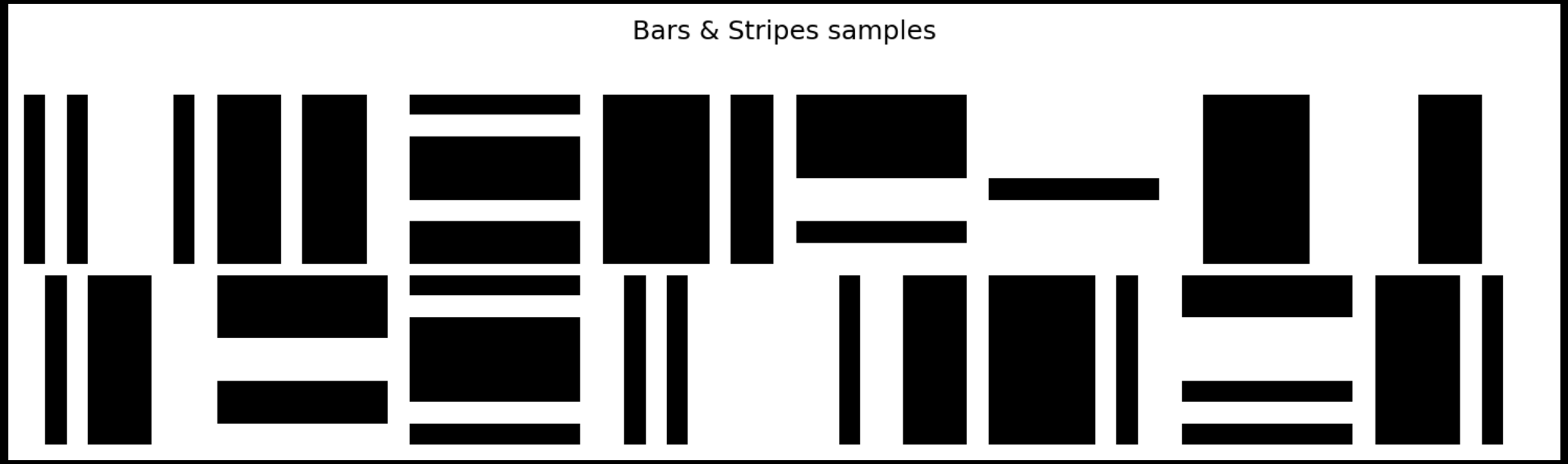
Overview

- Build a **Restricted Boltzmann Machine (RBM)** as an **Ising Energy-Based Model**
- Train it using **THRML's KL Gradient Estimator**
- Evaluate using:
  - 1-step **clamped reconstructions**
  - **THRML free-running sampling**
  - **Naive Python Gibbs sampling**
- Show how **THRML acts as a general Gibbs engine**
- Visualize learned filters and sampling results

Dataset: 8×8 Bars & Stripes

- Synthetic binary dataset used in EBM research
- Contains:
  - Horizontal bars
  - Vertical bars
  - Multiple bars per image
- Structured, multimodal, ideal for generative testing


Bars & Stripes samples

Training with THRML

THRML provides:

- **Block sampling** engine
- **KL divergence gradient estimator**
- **Factor graph representation**
- **Sampling schedules**
- Multi-chain sampling via `batch_shape`

We train RBM parameters:

- weights (W)
- visible biases (b_v), hidden biases (b_h)
- temperature parameter (\beta)

Our RBM/Ising energy function

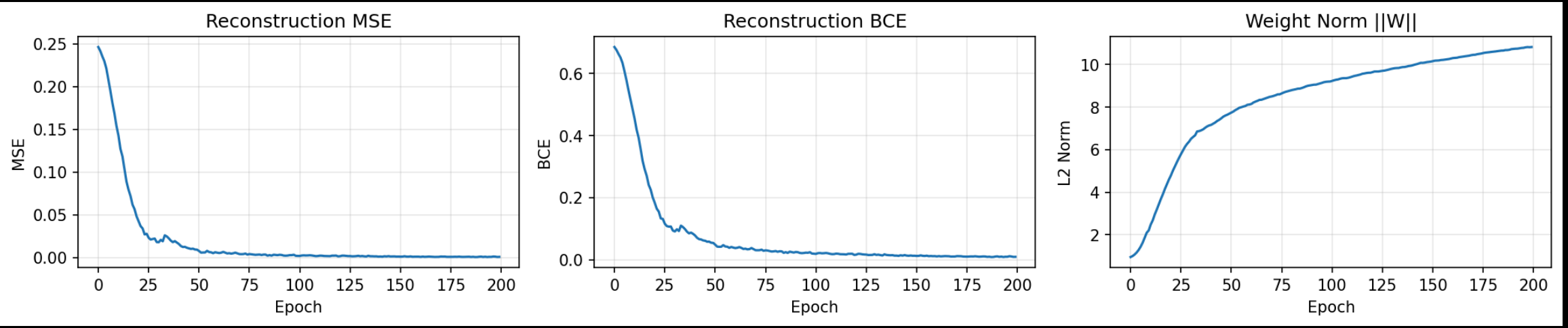
$$E(v,h) = -\beta \left[\sum_i b_i^{(v)} v_i + \sum_j b_j^{(h)} h_j + \sum_{i,j} W_{ij} v_i h_j \right]$$

directly taken from the Gibbs/Ising Hamiltonian, and each sum corresponds to a physical energy term

- 1st term, external field on visible spins
- 2nd term, external field on hidden spins
- Pairwise interaction energy

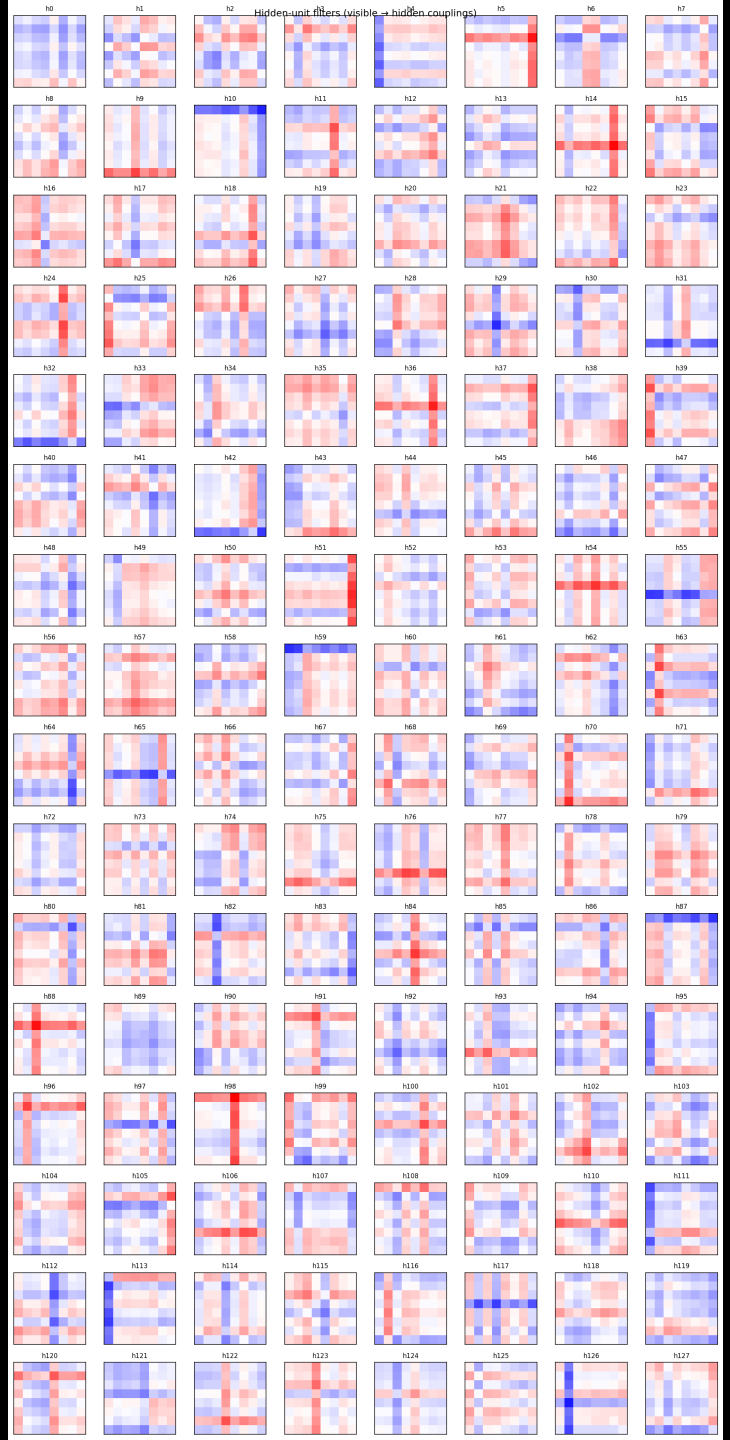
Training Curves

- **MSE** drops sharply → good reconstructions
- **BCE** approaches ~0 → near-perfect predictions
- Weight norm increases steadily → filters specialize


Reconstruction MSE
MSE
0.25
0.20
0.15
0.10
0.05
0.00
0
25
50
75
100
125
150
175
200
Epoch
Reconstruction BCE
BCE
0.6
0.4
0.2
0.0
0
25
50
75
100
125
150
175
200
Epoch
Weight Norm ||W||
L2 Norm
10
8
6
4
2
0
25
50
75
100
125
150
175
200
Epoch

Learned Hidden Unit Filters

- Each hidden unit learns a **feature detector**
- Filters resemble:
  - Vertical bars
  - Horizontal bars
  - Crossings
  - Composite stripe patterns
- RBM learns a **distributed encoding** of the dataset


Hidden-unit filters (visible → hidden couplings)
h0 h1 h2 h3 h4 h5 h6 h7
h8 h9 h10 h11 h12 h13 h14 h15
h16 h17 h18 h19 h20 h21 h22 h23
h24 h25 h26 h27 h28 h29 h30 h31
h32 h33 h34 h35 h36 h37 h38 h39
h40 h41 h42 h43 h44 h45 h46 h47
h48 h49 h50 h51 h52 h53 h54 h55
h56 h57 h58 h59 h60 h61 h62 h63
h64 h65 h66 h67 h68 h69 h70 h71
h72 h73 h74 h75 h76 h77 h78 h79
h80 h81 h82 h83 h84 h85 h86 h87
h88 h89 h90 h91 h92 h93 h94 h95
h96 h97 h98 h99 h100 h101 h102 h103
h104 h105 h106 h107 h108 h109 h110 h111
h112 h113 h114 h115 h116 h117 h118 h119
h120 h121 h122 h123 h124 h125 h126 h127

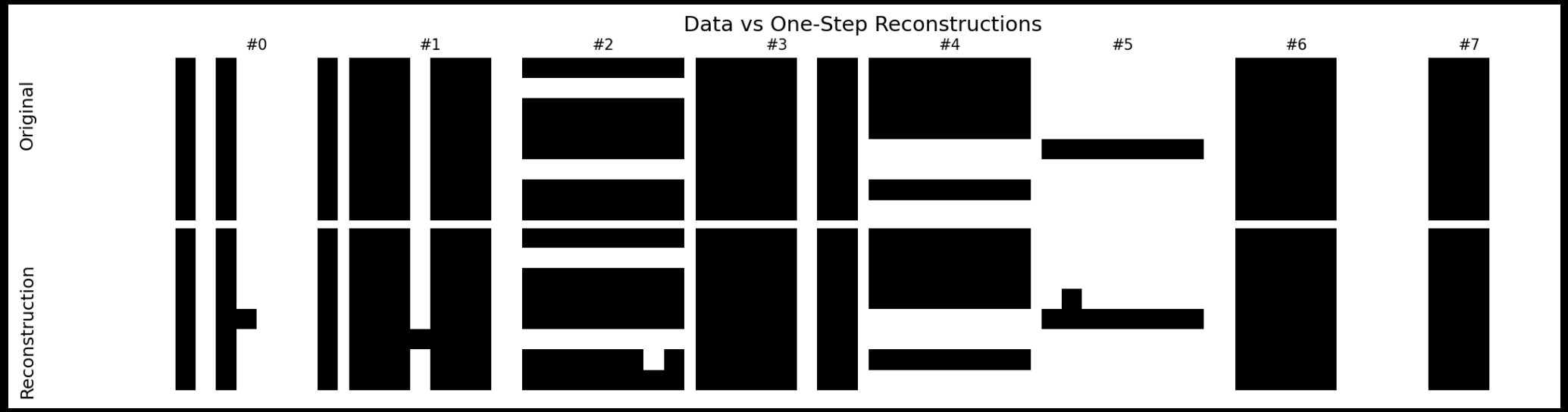
Clamped 1-Step Reconstructions

Process:

1. Clamp visibles to data
2. Sample (h \sim p(h|v))
3. Sample (v' \sim p(v|h))

Purpose:

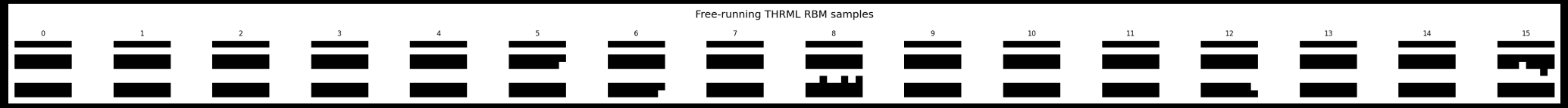
- Validate training
- Check encoder–decoder consistency
- Ensure stable attractor basins


Data vs One-Step Reconstructions
#0
#1
#2
#3
#4
#5
#6
#7
Original
Reconstruction

THRML Free-Running Sampling

- Start from random spins
- Run full Gibbs chain (no clamping)
- THRML explores the learned energy landscape
- Produces pure model samples

Shows true generative behavior of the RBM.


Free-running THRML RBM samples
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15

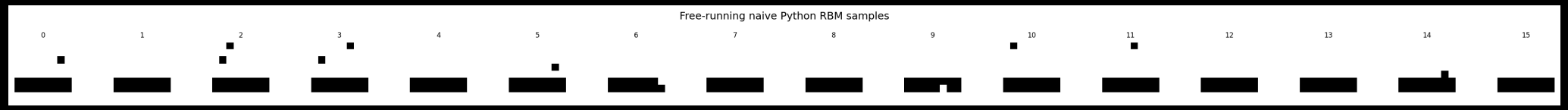
Naive Python Gibbs Sampling (Baseline)

Why?

- Validate correctness of THRML sampler
- Check if a hand-written sampler produces similar samples

Results:

- Python sampler produces Bars & Stripes
- Confirms correctness of learned energy landscape
- THRML behaves consistently with standard RBM sampling


Free-running naive Python RBM samples
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15

Why Three Sampling Modes?

1. Clamped Reconstructions

- ✓ Measure training quality
- ✓ Checks encoder/decoder mapping
- ✓ Local consistency

2. THRML Free-Running Sampling

- ✓ Explore full Boltzmann distribution
- ✓ Checks generative behavior
- ✓ Shows learned modes

3. Naive Gibbs Sampling

- ✓ Baseline sanity check
- ✓ Confirms THRML correctness
- ✓ Ensures consistent energy landscape

What We Learned

RBM Learning

- RBM trained via THRML achieves extremely low recon error
- Filters reflect dataset structure

Energy Landscape

- THRML free-running samples match Bars & Stripes
- Energy minima match dataset modes

Sampler Validation

- Python Gibbs sampler matches THRML outputs
- Confirms correctness of THRML's block sampler

THRML as a Gibbs Engine

Benefits

- Eliminates hand-written Gibbs loops
- Works for **arbitrary** factor graphs
- Supports multi-chain sampling
- Hardware-friendly (GPU/TPU acceleration)
- Clean integration with EBMs

Takeaway

THRML can serve as a **general-purpose thermodynamic sampling engine** for probabilistic models.

Conclusion

We successfully:

- Built a THRML-powered RBM
- Learned structured representations
- Generated high-quality samples
- Validated sampler correctness
- Demonstrated the feasibility of using THRML as a Gibbs engine

A strong foundation for larger EBMs and future thermodynamic computing systems.

Thank You

Questions?

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