Landscape Net

An Application of the Landscape Theory in Machine Learning for Eigenvalue Counting

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Code available at
`https://github.com/nehcili/Wave-Localization`

Introduction

Experimental Setting

- $L^2(\mathbb{Z} \cap [1, 1000])$
- $-\Delta_{\mathbb{Z}} + V$ with periodic boundary conditions
- $V(x)$ are iid distributions for $x = 1, 2, 3, ..., 1000$
- $V(x) \geq 0$

Objective: approximate the eigenvalue counting

$$N_V(E) := \# \text{ of eigenvalues of } -\Delta_{\mathbb{Z}} + V \text{ less or equal to } E$$

Introduction

Method: We develop a neural net, the **Landscape Net**, to generalize landscape box counting.

Why?

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Why?

- David-Filoche-Mayboroda box counting $N^W(E)$

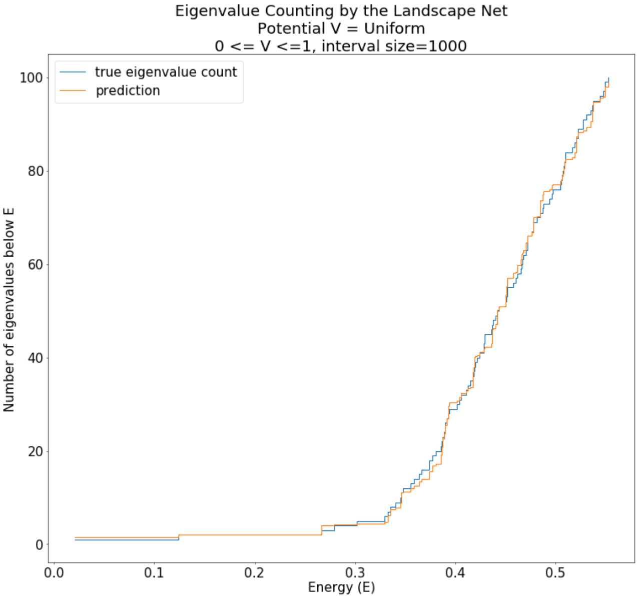
$$c_1 N^W(c_2 E) \leq N_V(E) \leq C_3 N^W(C_4 E)$$

  where $W = 1/u$ is the landscape potential.
  (Discrete case: Arnold-Filoche-Mayboroda-Wang-Zhang)
- More than just inequalities, box counting works well as a regression model with 2 parameters.

$$\text{predicted eigenvalue count} = c_1 N^W(c_2 E)$$

- Under fitting. It only has 2 parameters.

Results


Eigenvalue Counting by the Landscape Net
Potential V = Uniform
0 <= V <=1, interval size=1000
true eigenvalue count
prediction
Number of eigenvalues below E
Energy (E)
0
20
40
60
80
100
0.0
0.1
0.2
0.3
0.4
0.5

Results

- Testing on the bottom 10% of eigenvalues (100/1000 eigenvalues) from 30 samples,

$$\langle(\text{predicted } N_V(E) - \text{true } N_V(E))^2\rangle \approx 3$$

- Time complexity

Data generation*	Training*	Predicting one $N_V(E)$
0.0012s per eigenvalue	$\approx$ 1 hr	0.0025s

*Training data = bottom 10% of eigenvalues (100/1000 eigenvalues) from 300 samples.

Box counting as a neural net layer

Let us consider $E = 4$ and each box Q has length $= 2$ for illustration purpose.

$$\boxed{6}\boxed{5}\boxed{2}\boxed{1}\boxed{7}\boxed{3} \quad = \mathrm{W}$$

Box counting as a neural net layer

Let us consider $E = 4$ and each box Q has length $= 2$ for illustration purpose.

6	5	2	1	7	3	= W
-2	-1	2	3	-3	1	= E-W

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$$\boxed{-2}\boxed{-1}\boxed{2}\boxed{3}\boxed{-3}\boxed{1} \quad = \mathrm{E\text{-}W}$$

$$\boxed{-1} \quad = \sup(\mathrm{E\text{-}W}) \text{ on } Q\text{'s}$$

Box counting as a neural net layer

Let us consider $E = 4$ and each box Q has length $= 2$ for illustration purpose.

6	5	2	1	7	3	$=$ W
-2	-1	2	3	-3	1	$=$ E-W
		-1	3			$=$ sup(E-W) on Q's

Box counting as a neural net layer

Let us consider $E = 4$ and each box Q has length $= 2$ for illustration purpose.

$$\begin{array}{|c|c|c|c|c|c|}\hline 6 & 5 & 2 & 1 & 7 & 3 \\ \hline\end{array} = \text{W}$$

$$\begin{array}{|c|c|c|c|c|c|}\hline -2 & -1 & 2 & 3 & -3 & 1 \\ \hline\end{array} = \text{E-W}$$

$$\begin{array}{|c|c|c|}\hline -1 & 3 & 1 \\ \hline\end{array} = \text{sup(E-W) on } Q\text{'s}$$

Box counting as a neural net layer

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-1	3	1				$=$ sup(E-W) on Q's
0	1	1				$=$ apply Heaviside Θ

Box counting as a neural net layer

Let us consider $E = 4$ and each box Q has length $= 2$ for illustration purpose.

6	5	2	1	7	3	= W
-2	-1	2	3	-3	1	= E-W

-1	3	1	= sup(E-W) on Q's
0	1	1	= apply Heaviside Θ

2	= sum

Box counting as a neural net layer

Let us consider $E = 4$ and each box Q has length $= 2$ for illustration purpose.

	$\boxed{6\,|\,5\,|\,2\,|\,1\,|\,7\,|\,3}$		$=$ W
	$\boxed{-2\,|\,-1\,|\,2\,|\,3\,|\,-3\,|\,1}$		$=$ E-W
grader $sup_Q(E - W)$	$\boxed{-1\,|\,3\,|\,1}$		$=$ sup(E-W) on Q's
activation Θ	$\boxed{0\,|\,1\,|\,1}$		$=$ apply Heaviside Θ
(weighted) sum $w_Q = 1$	$\boxed{2}$		$=$ sum

Box counting as a neural net layer

Let us consider $E = 4$ and each box Q has length $= 2$ for illustration purpose.

	$\boxed{6}\boxed{5}\boxed{2}\boxed{1}\boxed{7}\boxed{3}$	= W
	$\boxed{-2}\boxed{-1}\boxed{2}\boxed{3}\boxed{-3}\boxed{1}$	= E-W
grader $f(W, E, Q)$	$\boxed{-1}\boxed{3}\boxed{1}$	= sup(E-W) on Q's
activation Θ, $\max(0, \cdot)$, etc.	$\boxed{0}\boxed{1}\boxed{1}$	= apply Heaviside Θ
weighted sum w_Q	$\boxed{2}$	= sum

Landscape net architecture

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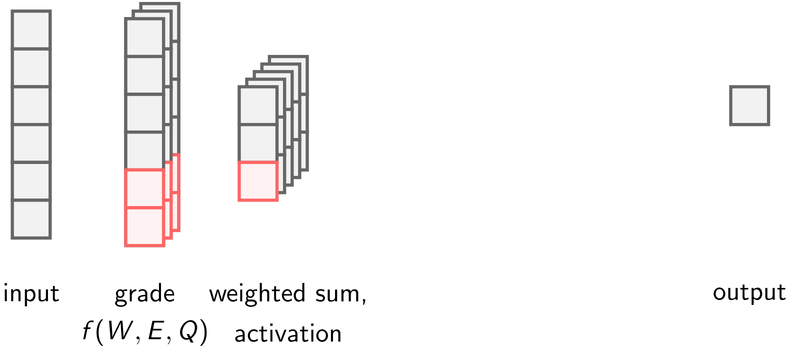
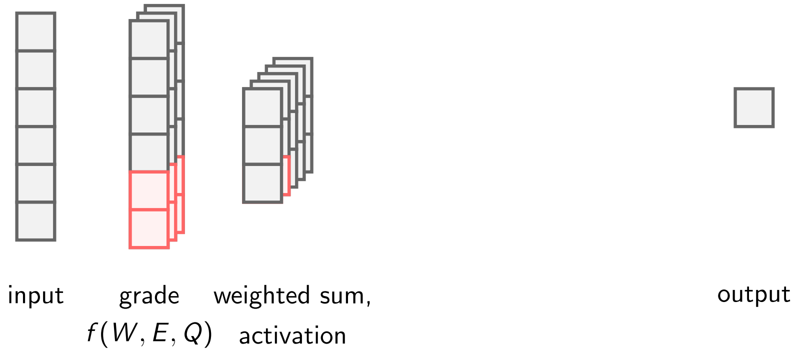
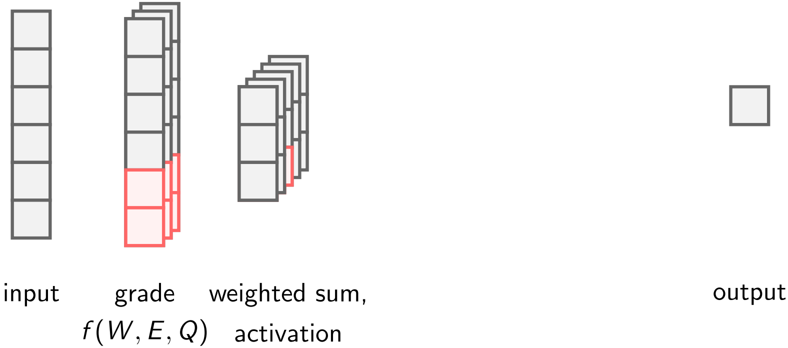


Landscape net architecture



Landscape net architecture



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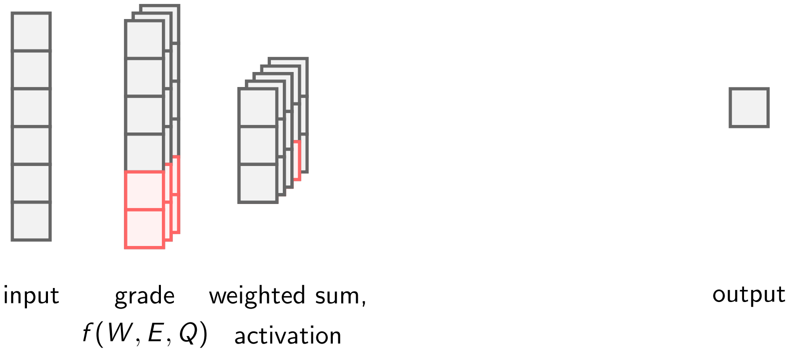

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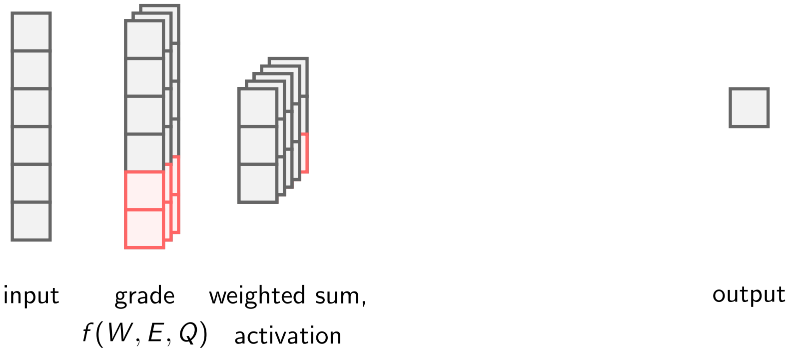

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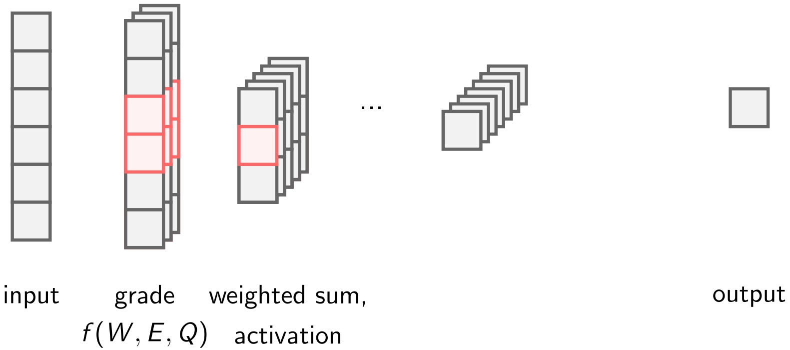

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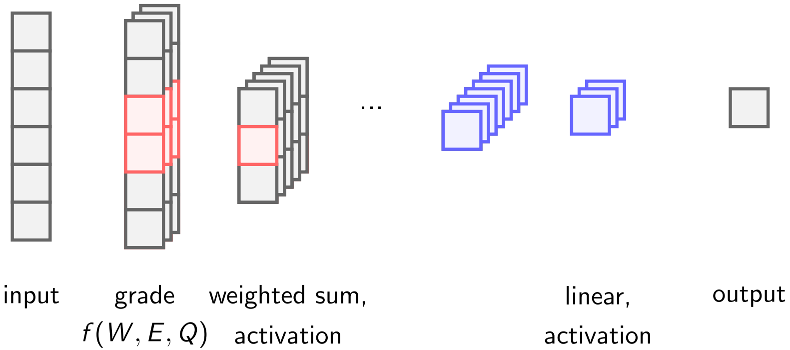

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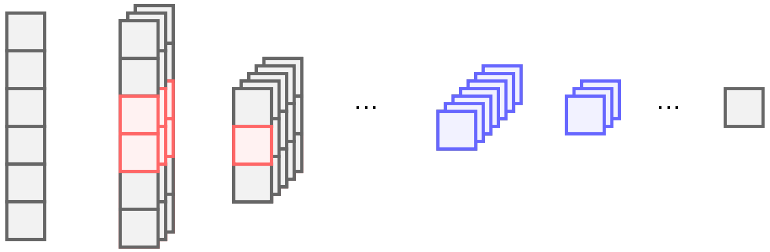


	input	grade	weighted sum,		linear,	output
		$f(W,E,Q)$	activation		activation	
parameters:		10k	60k		3k	

Ansatz for f

- Let ρ be the true density, we would like to have

$$f(W, E, Q) = \int_Q dx\, \rho(x).$$

- In dimension d, the semi-classical expansion ($-\hbar^2\Delta + V$ and $\hbar \to 0$) of ρ is

$$\begin{aligned}\rho(x) =& \hbar^{-d} \int_{\mathbb{R}^d} dp\, 1_{\{p^2 + W(x) - E < 0\}} \text{ (Weyl term)} \\ & + \hbar^{-d+2} \sum_i A_i(V(x), W(x), \nabla W(x)) B_i(E - W(x)) \\ & + O(\hbar^{-d+4}),\end{aligned}$$

for some local functions A_i and B_i.

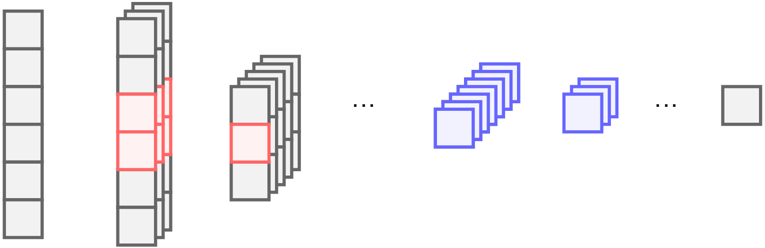
Ansatz for f

- We choose f to have the same form as the first 2 lowest order terms

$$f(W, E, Q) = \sum_{x \in Q} w_x A(V(x), W(x), W'(x)) B(E - W(x))$$

where each A and B are constructed from layers of neural nets and w_x are weights.

Thank you!



input

grade $f(W, E, Q)$

weighted sum, activation

linear, activation

output

parameters: 10k 60k 3k

Semi-classical expansions

For any meromorphic function f which is analytic on a tabular neighborhood of the real line, if $\rho(x) = f(-\hbar^2\Delta + V)(x,x)$ and W is the associated landscape potential, then as $\hbar \to 0$,

$$
\begin{aligned}
\rho = \hbar^{-d} \int_{\mathbb{R}^d} dp\, f(p^2 + W) \\
+\hbar^{-d+2} \Bigg(-\frac{1}{2}\Delta W \int_{\mathbb{R}^d} dp\, f''(p^2 + W) \\
+ 2W^{-1}\Delta W \int_{\mathbb{R}^d} dp\, p^2 f''(p^2 + W) \\
- \frac{1}{3}|\nabla W|^2 \int_{\mathbb{R}^d} dp\, f'''(p^2 + W) \\
+ (2W^{-1}|\nabla W|^2 + \frac{2}{3}\Delta W) \int_{\mathbb{R}^d} dp\, p^2 f'''(p^2 + W) \\
+ \frac{1}{2}|\nabla W|^2 \int_{\mathbb{R}^d} dp\, p^2 f''''(p^2 + W) \Bigg) + O(\hbar^{-d+4})
\end{aligned}
$$

Types of potentials considered

1. constant 1
2. uniform
3. standard exponential
4. poisson
5. power
6. bernoulli
7. chisquare
8. rayleigh
9. laplace
10. normal
11. logistic

Future direction

- Optimization: reduction of parameters, hyperparameter tuning, scalability, training on additional classes of potentials
- Larger domain/higher dimension
- Obtaining eigenvalue counting by using signatures of $H - E$ instead of explicity eigenvalue computation
- Approximating the density ρ itself