Landscape Theory for Tight-Binding Hamiltonians

Undergraduate Math/Stat Research Project Final Presentation

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Introduction

- Anderson localization is one of the central phenomena studied in modern mathematical physics, especially in dimensions 2 and 3. It originated with the Nobel-Prize winning discovery by P. W. Anderson.
- This project examines Landscape Theory. A new theory has unveiled a direct relationship between the random potential and the localized states.
- These physical ideas and applications can be expressed mathematically with fundamental precepts of linear algebra.

Schrödinger Matrix and its Eigenvalue Problem

- An example of 4×4 Schrödinger matrix:

$$H = \begin{pmatrix} v_1 & -1 & 0 & 0 \\ -1 & v_2 & -1 & 0 \\ 0 & -1 & v_3 & -1 \\ 0 & 0 & -1 & v_4 \end{pmatrix}, \quad v_1, v_2, v_3, v_4 \in \mathbb{R}.$$

- Eigenvalue problem of H, $H\vec{x} = \lambda\vec{x}, \lambda \in \mathbb{R}, \vec{x} \in \mathbb{R}^4$:

$$\begin{pmatrix} v_1 & -1 & 0 & 0 \\ -1 & v_2 & -1 & 0 \\ 0 & -1 & v_3 & -1 \\ 0 & 0 & -1 & v_4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \lambda \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}$$

Remark

The scalar λ such that $H\vec{x} = \lambda\vec{x}$ has a non-trivial solution $\vec{x} \in \mathbb{R}^4$ is called an eigenvalue of H, and the non-trivial solution $\vec{x}$ is called the associated eigenvector.

Landscape Theory for Schrödinger Matrices

- Landscape function, $\vec{u} \in \mathbb{R}^4$ satisfying:

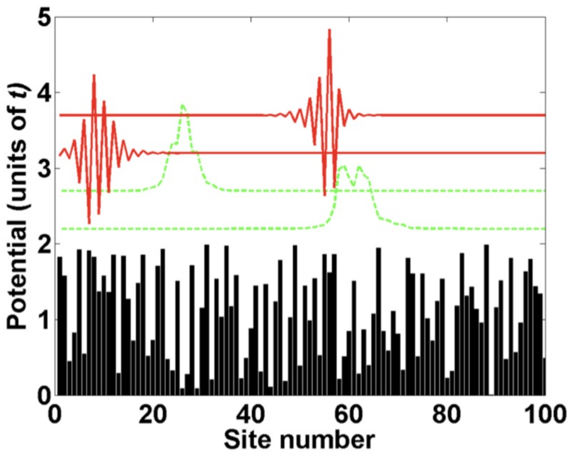
$$H\vec{u} = \begin{pmatrix} v_1 & -1 & 0 & 0 \\ -1 & v_2 & -1 & 0 \\ 0 & -1 & v_3 & -1 \\ 0 & 0 & -1 & v_4 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

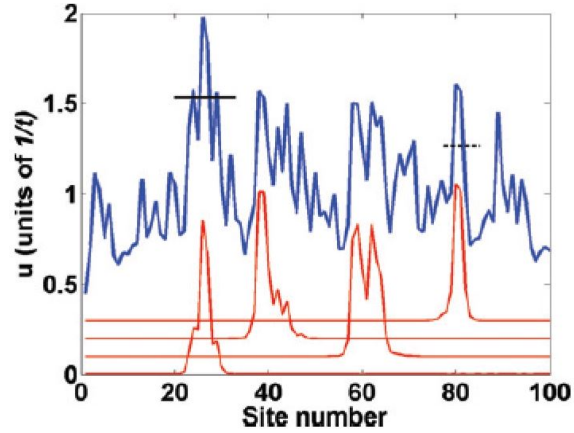
- Landscape theory (in $\mathbb{R}^4$): If $v_j \geq 2, j = 1, 2, 3, 4$, and $H\vec{x} = \lambda\vec{x}$, then we have

$$\frac{|x_j|}{\max\limits_{k=1,2,3,4} |x_k|} \leq \lambda u_j, \quad j = 1, 2, 3, 4.$$

- The theory holds true for general $n \times n$ Schrödinger matrices, and differential Schrödinger operators, proved by M. L. Lyra, S. Mayboroda and M. Filoche.
- The main goal of the project is to generalize the landscape theory to more complicated matrices.

Physical Applications



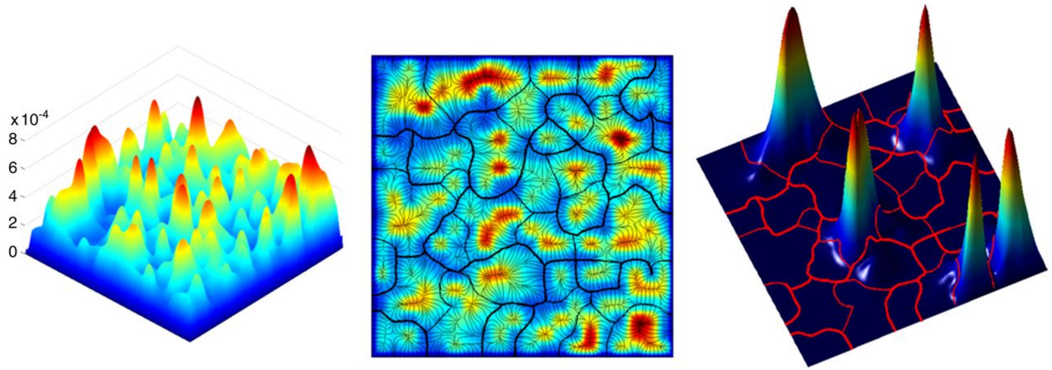


We consider a 100×100 Schrödinger matrix with the potential described by the black graph on the left.

Left figure, green: eigenvectors at small energies. Red: eigenvectors at large energies. Graphs have been shifted vertically.

Right figure, red: low energy eigenvectors. Blue: landscape function.

Physical Applications: More Complicated 2D Model



Left and middle figures: plot of the landscape function in a 2D continuous model.

Right figure: Red: contour plot of the “valleys” of the landscape function, together with five low energy eigenvectors.

In both cases, one can conjecture that peaks of landscape function correspond to localization centers of the eigenvectors.

Illustrations are taken from works of M. L. Lyra, S. Mayboroda and M. Filoche.

Our Model: a Long Range Schrödinger Matrix

In our expansion of landscape theory, we are interested in $n \times n$ matrices H of the form:

$$H = \begin{pmatrix} v_1 & -a_1 & -a_2 & \cdots & \cdots & -a_{n-2} & -a_{n-1} \\ -a_1 & v_2 & -a_1 & \cdots & \cdots & \cdots & -a_{n-2} \\ -a_2 & -a_1 & v_3 & \ddots & \ddots & \ddots & \vdots \\ \ddots & \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \cdots & \ddots & v_{n-2} & -a_1 & -a_2 \\ -a_{n-2} & \cdots & \cdots & \cdots & -a_1 & v_{n-1} & -a_1 \\ -a_{n-1} & -a_{n-2} & \cdots & \cdots & -a_2 & -a_1 & v_n \end{pmatrix}$$

where $a_i \geq 0,\ i = 1, \ldots, n-1$, and $v_j \in \mathbb{R}, j = 1, \ldots, n$.

Potential and Töplitz matrix

H is usually written as $H = V - H_0$, where (in the 6×6 case):

$$V = \begin{pmatrix} v_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & v_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & v_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & v_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & v_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & v_6 \end{pmatrix}, H_0 = \begin{pmatrix} 0 & a_1 & a_2 & a_3 & a_4 & a_5 \\ a_1 & 0 & a_1 & a_2 & a_3 & a_4 \\ a_2 & a_1 & 0 & a_1 & a_2 & a_3 \\ a_3 & a_2 & a_1 & 0 & a_1 & a_2 \\ a_4 & a_3 & a_2 & a_1 & 0 & a_1 \\ a_5 & a_4 & a_3 & a_2 & a_1 & 0 \end{pmatrix}$$

V is known as the potential, H_0 is known as a Töplitz matrix, and H is a natural generalization of the Schrödinger matrix.

Landscape Theory for the Generalized Model

Theorem (B–C–G–L–L–L, 19)

Let H be defined as in the previous slide. If

$$v_j > 2\sum_{i=1}^{n-1} a_i, \; j = 1, \ldots, n$$

and $H\vec{x} = \lambda\vec{x}$, *then* $\forall j = 1, \cdots, n$

$$\frac{|x_j|}{\max\limits_{1\le k\le n} |x_k|} \le \lambda u_j, \qquad \textit{where} \quad H\vec{u} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}.$$

Outline of the Proof

The proof of the initial landscape theorem is built off three points:

- That the Schrödinger matrix, H, is invertible
  - This is ensured by the structure of H.
- That there exists a landscape function $\vec{u}$
  - This follows from the invertibility of H.
- The positivity of H^{-1} and $\vec{u}$
  - The positivity of H^{-1} ensures positivity of landscape function.

The process is the same for our expanded model.

Power Series Expansion Proof

We developed a new method of proving both the initial landscape theory and our generalized model. One key ingredient is the following power series expansion formula for any square matrices A, B: If A is invertible and $\|A^{-1}B\| < 1$, then

$$(A - B)^{-1} = \sum_{k=0}^{\infty} \left(A^{-1}B\right)^k A^{-1}. \tag{1}$$

We are applying the above formula to $A = V$ and $B = H_0$, where $H = V - H_0$ is our original matrix and we decompose H into the diagonal part V and the off diagonal part H_0.

Power Series Expansion Proof (Continued)

We will provide a 3×3 example of this theory:

$$H = \begin{pmatrix} v_1 & -a_1 & -a_2 \\ -a_1 & v_2 & -a_1 \\ -a_2 & -a_1 & v_3 \end{pmatrix} = \begin{pmatrix} v_1 & 0 & 0 \\ 0 & v_2 & 0 \\ 0 & 0 & v_3 \end{pmatrix} - \begin{pmatrix} 0 & a_1 & a_2 \\ a_1 & 0 & a_1 \\ a_2 & a_1 & 0 \end{pmatrix} = V - H_0$$

In order to satisfy the criterion $\|V^{-1}H_0\| < 1$, we employ the following conditions:

$$\|V^{-1}\| \leq \max_{1 \leq j \leq n} v_j^{-1} \tag{2}$$

$$\|H_0\| \leq 2 \sum_{i=1}^{n-1} a_i \tag{3}$$

Stronger Result (Work in Progress)

Conjecture

Let H be defined as it has been previously. If

$$v_j \geq 2\sum_{i=1}^{n-1} a_i \;\; > 0 \; j = 1, \ldots, n \; and \; H\vec{x} = \lambda\vec{x}, \; then \; \forall j = 1, \cdots, n$$

$$\frac{|x_j|}{\max\limits_{1 \leq k \leq n} |x_k|} \leq \lambda u_j, \qquad where \quad H\vec{u} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}.$$

Remark

A special case of this conjecture occurs when only $a_1 \neq 0$*, and that is the original landscape theory.*

Further General Applications

- Overall, we generalize the matrices

$$H = \begin{pmatrix} v_1 & -1 & 0 \\ -1 & v_2 & -1 \\ 0 & -1 & v_3 \end{pmatrix} \longrightarrow H = \begin{pmatrix} v_1 & -a_1 & -a_2 \\ -a_1 & v_2 & -a_1 \\ -a_2 & -a_1 & v_3 \end{pmatrix}$$

- Extended matrix has further off diagonal entries
- These represent interactions which are further than nearest-neighbor.
- Gives a more complicated model, but describes more realistic physical systems.
- The power series method can be easily extended to higher dimensional lattices.

Thank You!