

# Visualizing Cauchy's Interlacing Property for Line Distance Matrices

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COV 2005, Koper

18.11.2005

Bioinformatics: study of DNA sequences

...ATGGTGC ACCTGAC TCCTGAG ...

...ATGGTGC TTACCTG ACAGACC ...

...GGTGCAC ATGACTT CTGAGCT ...

Comparison:

- finding optimal structural alignment is NP-hard
- similarities/differences
- relative positions (of A, C, G, T)

# Line distance matrices

Let  $\mathbf{t} = (t_1, t_2, \dots, t_n)$ ,  $t_1 < t_2 < \dots < t_n$ ,  $t_i \in \mathbb{R}$ , be a given vector.

A **line distance matrix**  $L \in \mathbb{R}^{n \times n}$  is defined as

$$(L)_{ij} = \begin{cases} t_i - t_j, & j \leq i, \\ t_j - t_i, & i < j. \end{cases}$$

$$L = \begin{pmatrix} 0 & t_2 - t_1 & t_3 - t_1 & t_4 - t_1 \\ t_2 - t_1 & 0 & t_3 - t_2 & t_4 - t_2 \\ t_3 - t_1 & t_3 - t_2 & 0 & t_4 - t_3 \\ t_4 - t_1 & t_4 - t_2 & t_4 - t_3 & 0 \end{pmatrix}$$

# Human $\beta$ -globin gene

The first exon of human  $\beta$ -globin gene:

ATGGTGCACCTGACTCCTGAG...

Positions of G in the sequence:

$$\mathbf{t} = (3, 4, 6, 12, 19, 21).$$

The corresponding line distance matrix:

$$L = \begin{pmatrix} 0 & 1 & 3 & 9 & 16 & 18 \\ 1 & 0 & 2 & 8 & 15 & 17 \\ 3 & 2 & 0 & 6 & 13 & 15 \\ 9 & 8 & 6 & 0 & 7 & 9 \\ 16 & 15 & 13 & 7 & 0 & 2 \\ 18 & 17 & 15 & 9 & 2 & 0 \end{pmatrix}.$$

# Properties of line distance matrices

- determined by its first row
- non-negative

$$L_{ij} > 0, \quad i \neq j$$

- symmetric
- real eigenvalues
- zeros on diagonal
- trace

$$\text{tr } L = \sum_{i=1}^n L_{ii} = 0$$

# Cauchy's interlacing theorem

## Theorem

Let  $A \in \mathbb{R}^{n \times n}$  be a **symmetric tridiagonal irreducible matrix**. Let  $A^{(1)}, A^{(2)}, \dots, A^{(n)}$  denote its principal (i.e., upper-left) square submatrices of dimension  $1, 2, \dots, n$ . Then the eigenvalues of  $A^{(k)}$  are **distinct**  $\lambda_k^{(k)} < \lambda_{k-1}^{(k)} < \dots < \lambda_1^{(k)}$  and they **strictly interlace**

$$\lambda_{j+1}^{(k+1)} < \lambda_j^{(k)} < \lambda_j^{(k+1)}$$

for  $k = 1, 2, \dots, n-1$  and  $j = 1, 2, \dots, k$ .

This is a basis for bisection algorithm for eigenvalue computation.

# The number of negative eigenvalues

## Theorem

For a **symmetric tridiagonal** matrix  $A \in \mathbb{R}^{n \times n}$  the number of negative eigenvalues is equal to the number of sign changes in the sequence

$$1, \det(A^{(1)}), \det(A^{(2)}), \dots, \det(A^{(n)}).$$

## Corollary

By shifting  $A$  by a multiple of the identity we can determine the number of eigenvalues in any interval  $[a, b)$ .

## Example

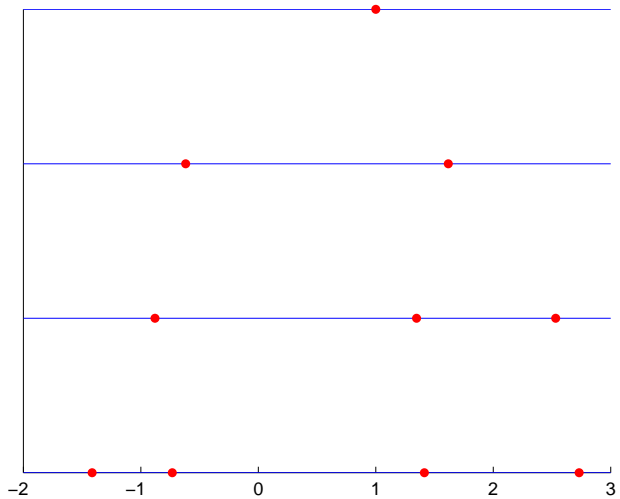
$$A = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 2 & 1 \\ 0 & 0 & 1 & -1 \end{pmatrix}$$

Then

$$\det A^{(1)} = 1, \det A^{(2)} = -1, \det A^{(3)} = -3, \det A^{(4)} = 4.$$

The matrix  $A$  has 2 negative eigenvalues.





# Cauchy's interlacing property

## Theorem

Let  $A \in \mathbb{R}^{n \times n}$  be a **symmetric matrix**. Let  $A^{(1)}, A^{(2)}, \dots, A^{(n)}$  denote its principal square submatrices of dimension  $1, 2, \dots, n$ . Then the eigenvalues of  $A^{(k+1)}$  and  $A^{(k)}$  **interlace**

$$\lambda_{j+1}^{(k+1)} \leq \lambda_j^{(k)} \leq \lambda_j^{(k+1)}$$

for  $k = 1, 2, \dots, n-1$  and  $j = 1, 2, \dots, k$ .

Note:

- non-strict interlacing

# Eigenvalues of line distance matrices

## Theorem

Let  $L \in \mathbb{R}^{n \times n}$  be a **line distance matrix**, defined by a vector  $\mathbf{t}$  and let  $L^{(i)} := L(1 : i, 1 : i)$ ,  $i = 1, 2, \dots, n$  be its principal submatrices. Let

$$\lambda_i(L^{(i)}) \leq \lambda_{i-1}(L^{(i)}) \leq \dots \leq \lambda_2(L^{(i)}) \leq \lambda_1(L^{(i)})$$

be the eigenvalues of the matrix  $L^{(i)}$ . Then  $\lambda_1(L^{(i)}) > 0$ ,  $\lambda_2(L^{(i)}) < 0$  for  $i > 1$  and  $\lambda_1(L^{(1)}) = 0$ .

## Corollary

A line distance matrix has exactly one positive eigenvalue.

## Corollary

$\lambda_2(L^{(i)}) = 0$ ,  $i > 1$  iff  $t_j = t_{j+1}$  for some  $j < i$ .

# Key observations

Let  $\lambda_j^{(i)} := \lambda_j(L^{(i)})$  and let  $p_i(x) := \det(L^{(i)} - xI)$  denote the characteristic polynomial of the matrix  $L^{(i)}$ . Then

$$\det L^{(i)} = -2^{i-2}(t_1 - t_i) \prod_{j=1}^{i-1} (t_j - t_{j+1}).$$

Since  $\text{trace } L^{(i)} = \sum_{j=1}^i \lambda_j^{(i)} = 0$ ,  $\det L^{(i)} = \prod_{j=1}^i \lambda_j^{(i)} \neq 0$  and  $L_{jk} > 0$  for  $j \neq k$ ,

$$\lambda_1^{(i)} > 0, \quad \lambda_i^{(i)} < 0, \quad i > 1,$$

and

$$\lambda_1^{(1)} = 0.$$

Cauchy's interlacing theorem implies

$$\lambda_2^{(2)} \leq \lambda_1^{(1)} \leq \lambda_1^{(2)}.$$

Therefore

$$\lambda_2^{(2)} < 0.$$

Similarly,

$$\lambda_3^{(3)} \leq \lambda_2^{(2)} \leq \lambda_2^{(3)} \leq \lambda_1^{(2)} \leq \lambda_1^{(3)}.$$

Since  $p_3(0) > 0$ ,  $\lambda_2^{(2)} < 0$ ,  $\lambda_1^{(2)} > 0$  and  $p_3(x) = -x^3 + \dots$ ,

$$\lambda_2^{(3)} < 0.$$

Inductive supposition:  $\lambda_2^{(i-1)} < 0$ .

Cauchy's interlacing theorem implies

$$\lambda_3^{(i-1)} \leq \lambda_3^{(i)} \leq \lambda_2^{(i-1)} \leq \lambda_2^{(i)} \leq \lambda_1^{(i-1)} \leq \lambda_1^{(i)}.$$

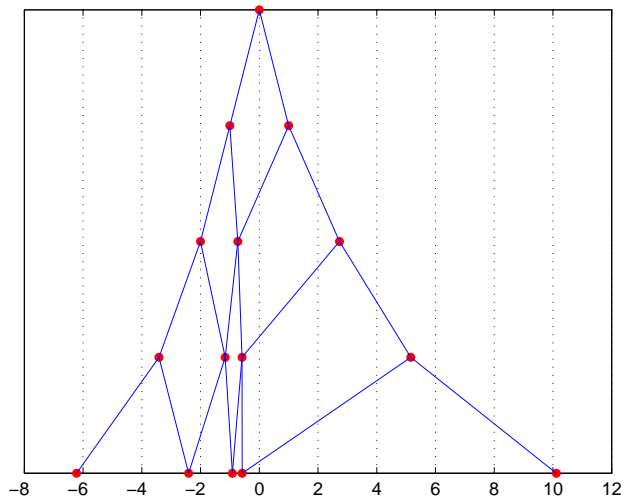
Recall  $\lambda_1^{(i)} > 0$  and  $\lambda_j^{(i)} < 0$ ,  $j \geq 3$ .

Since  $p_i(x) = (-1)^i x^i + \dots$  and  $\text{sign}(p_i(0)) = (-1)^{i+1}$ ,

$$\lambda_2^{(i)} < 0.$$

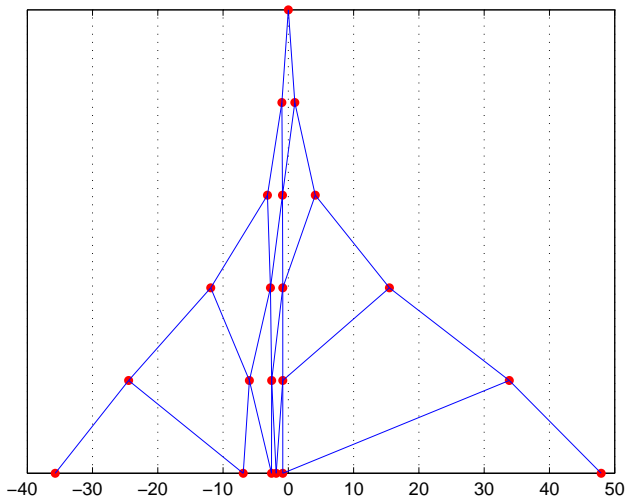


# Visualization





# Visualization: $\beta$ -globin



- eigenvalue positions

$$|\lambda| \leq \sum_{j=2}^n t_j - (n-1)t_1$$

- study of partial sums  $\left(\sum_{i=1}^j \lambda_i^{(k)}\right)_j$
- generalization to proteins
- comparison of methods on real life data