Algorithms

Spectral graph analysis

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SAPIENZA
UNIVERSITÀ DI ROMA

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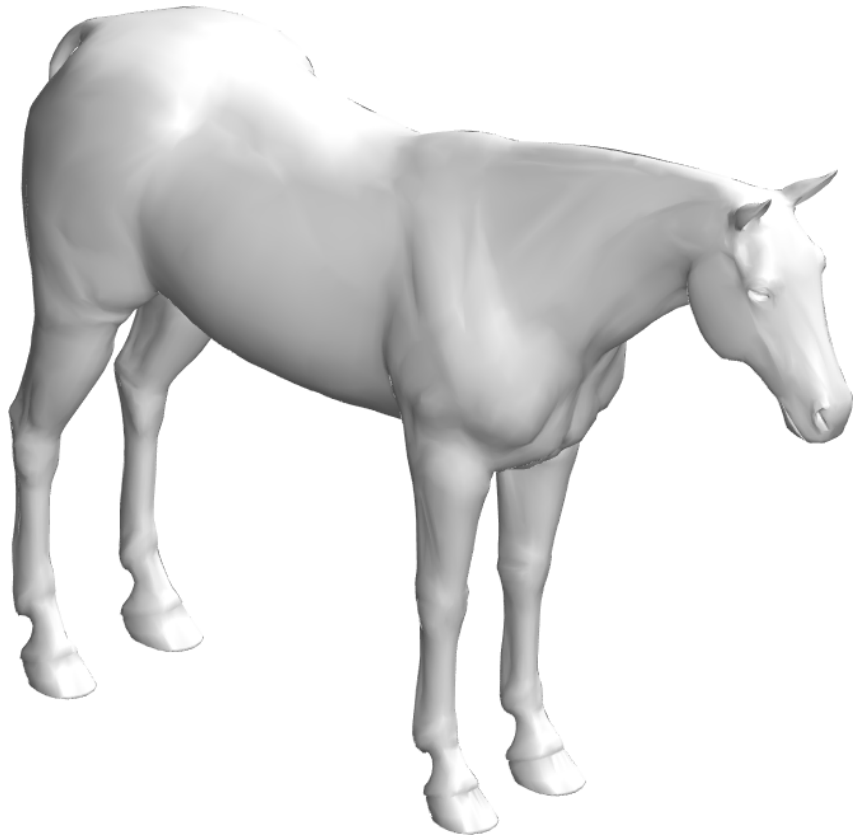
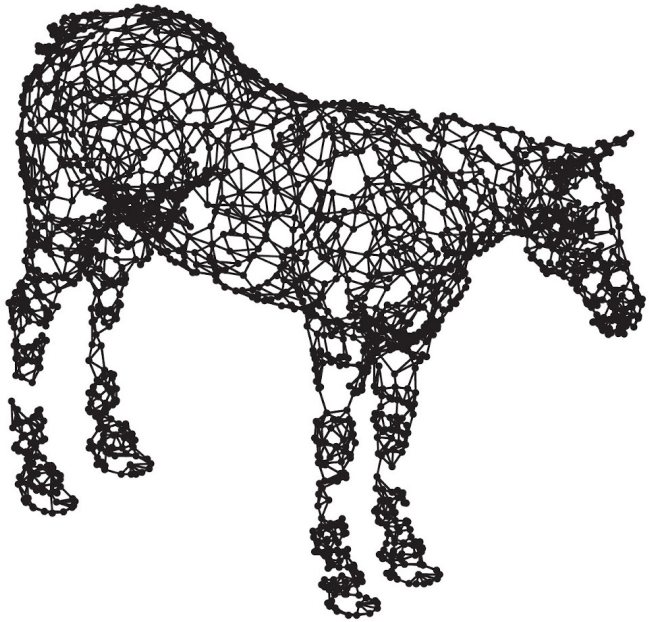
Discrete domains



smooth surface

(continuous domain with infinitely many points)

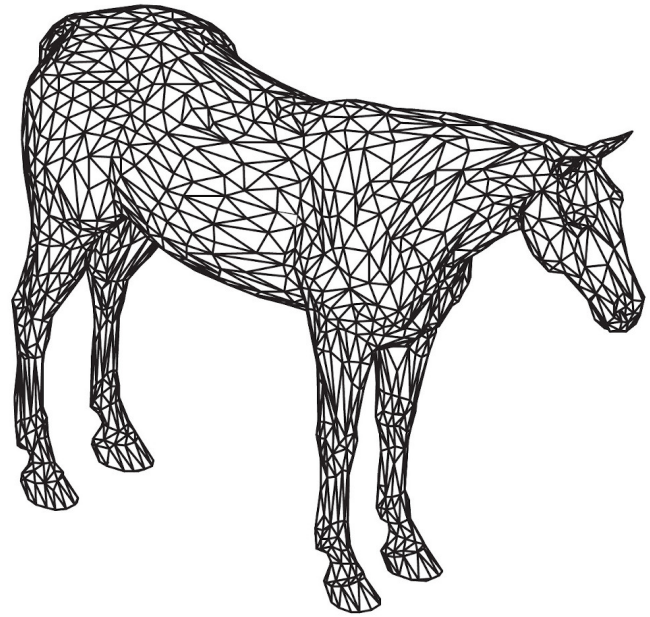
Discrete domains



Nearest neighbor graph

Vertices $\mathcal{V} = \{1, \ldots, n\}$

Edges $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$



Triangular mesh

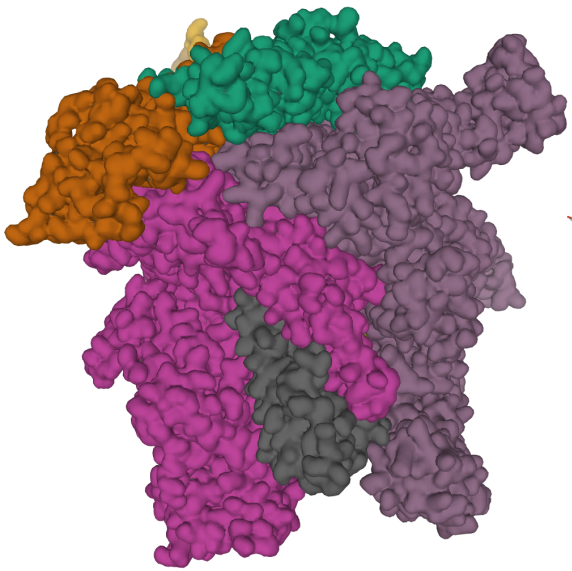
Vertices $\mathcal{V} = \{1, \ldots, n\}$

Edges $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$

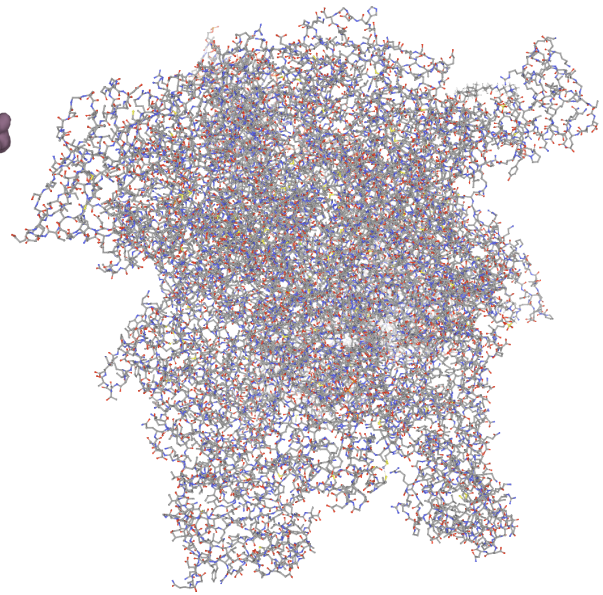
Faces $\mathcal{F} = \{(i, j, k) \in \mathcal{V} \times \mathcal{V} \times \mathcal{V} : (i, j), (j, k), (k, i) \in \mathcal{E}\}$

Discrete domains

Escherichia coli RNA polymerase
(`https://www.rcsb.org/3d-view/6WRD/1`)



coarse surface



atomic detail

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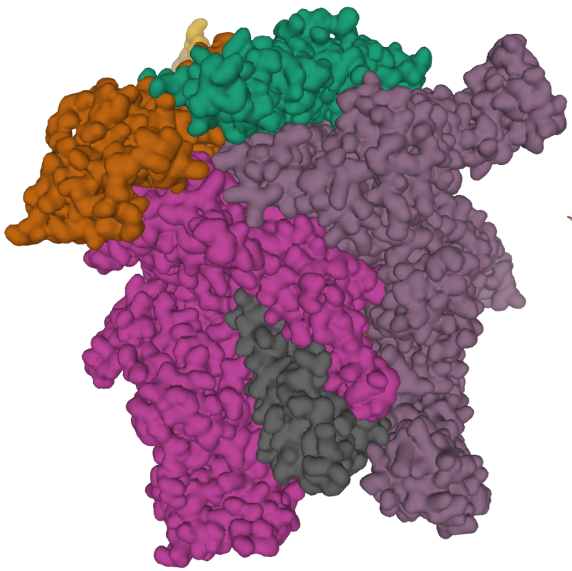

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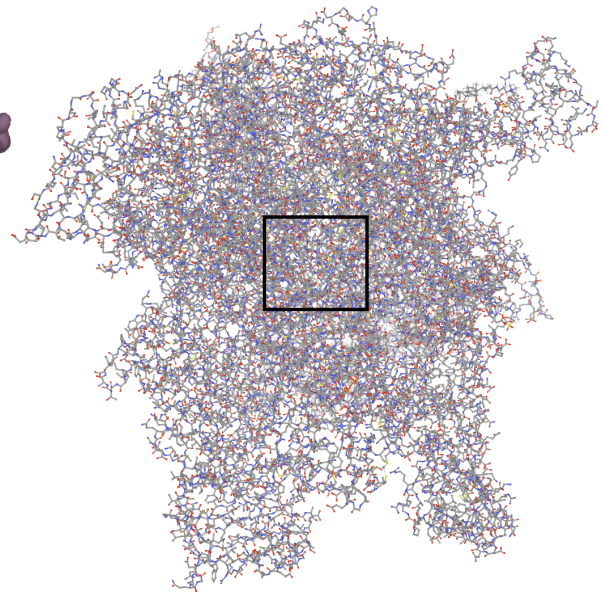

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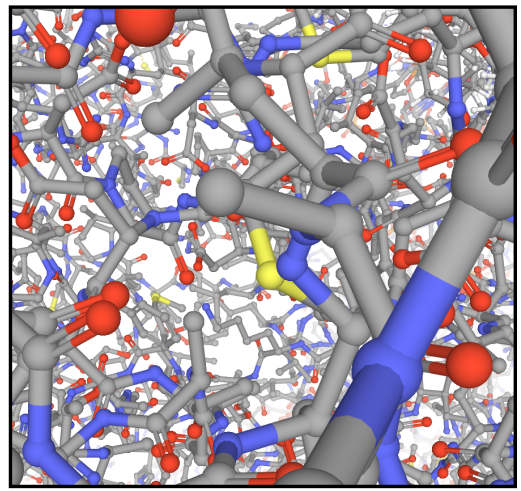
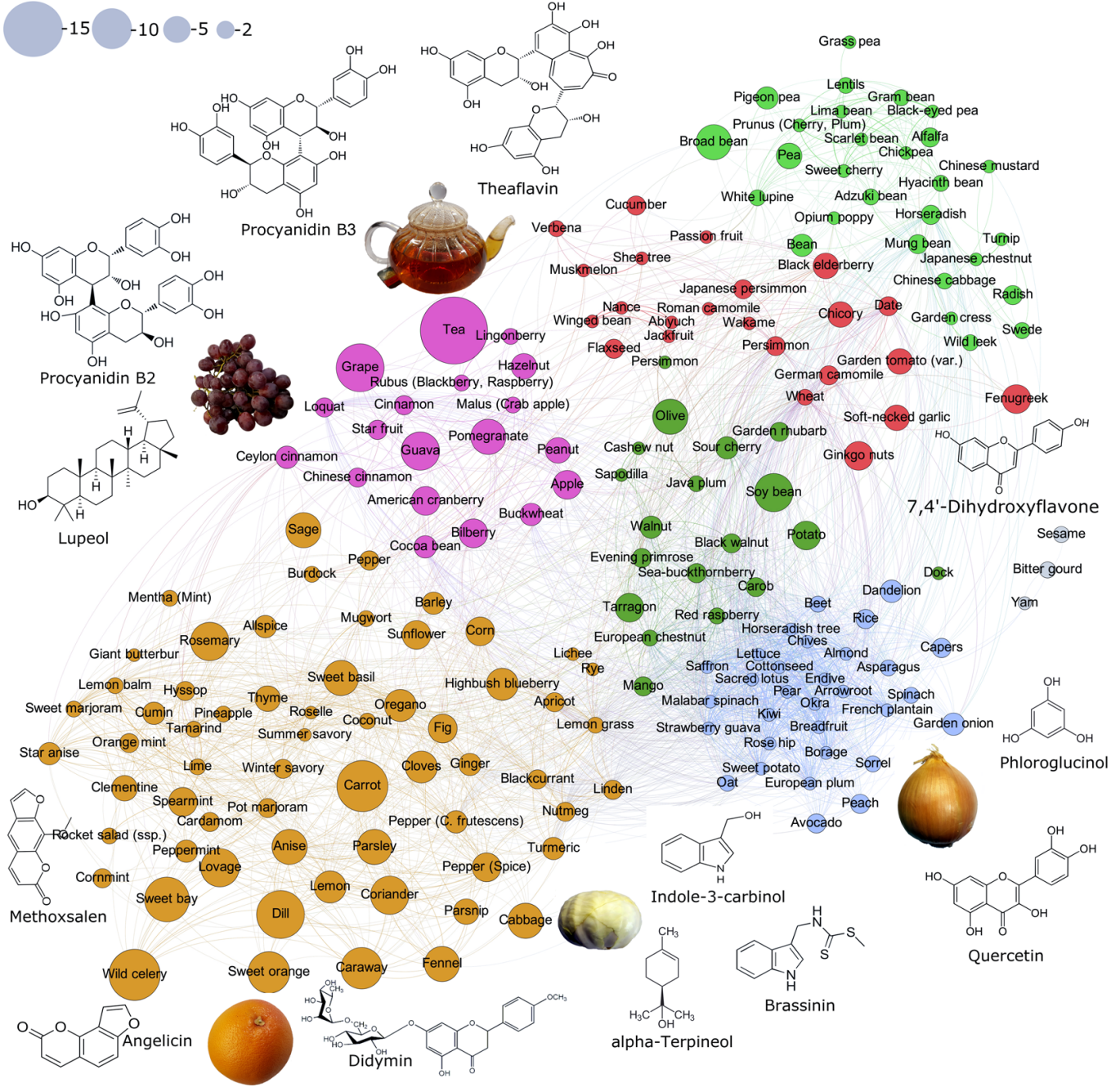
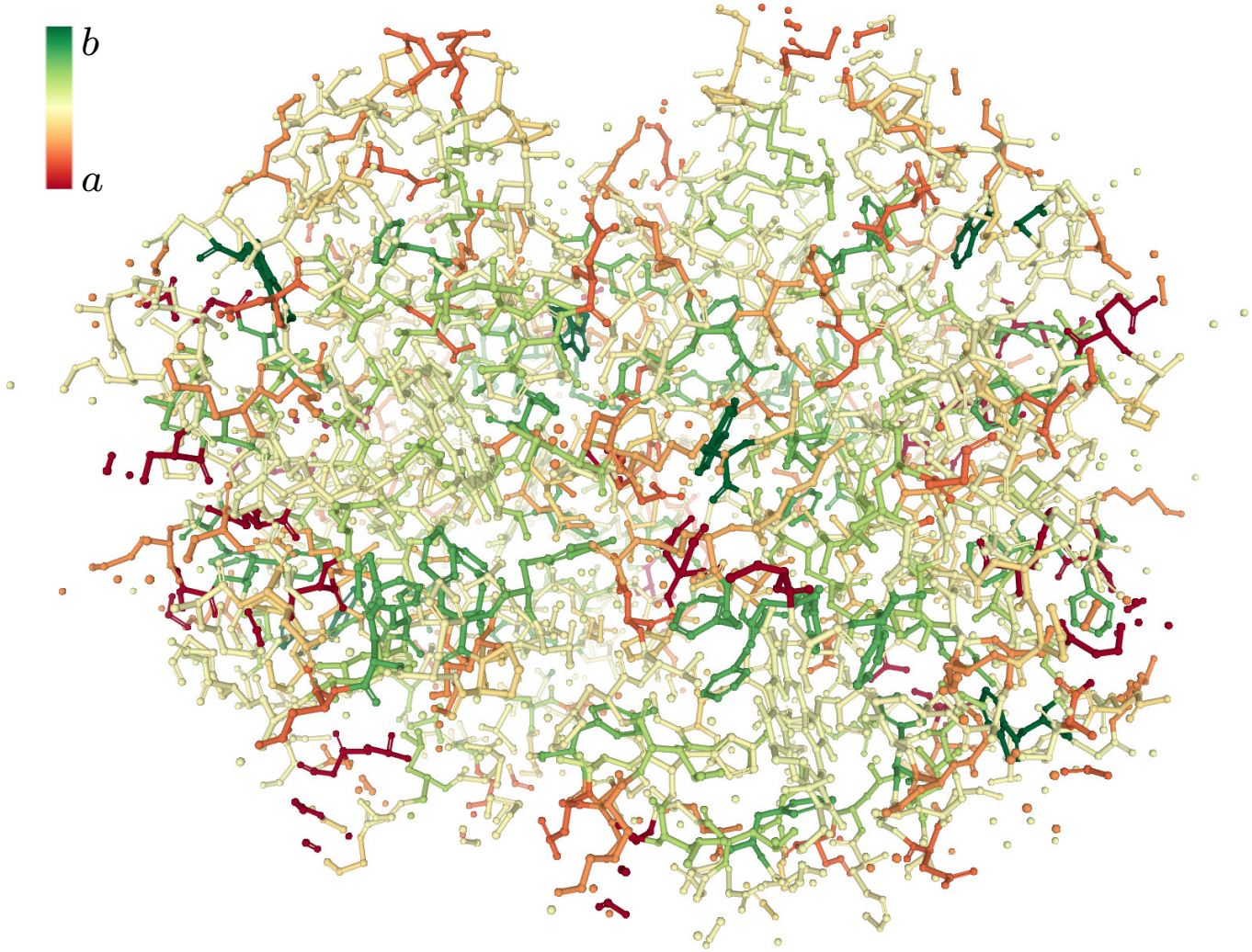




Veselkov et al, "HyperFoods: Machine intelligent mapping of cancer-beating molecules in foods", Nature 2019

Attributed graphs

Often we have additional attributes on top of the graph structure.



amino acid hydrophobicity

Attributed graphs

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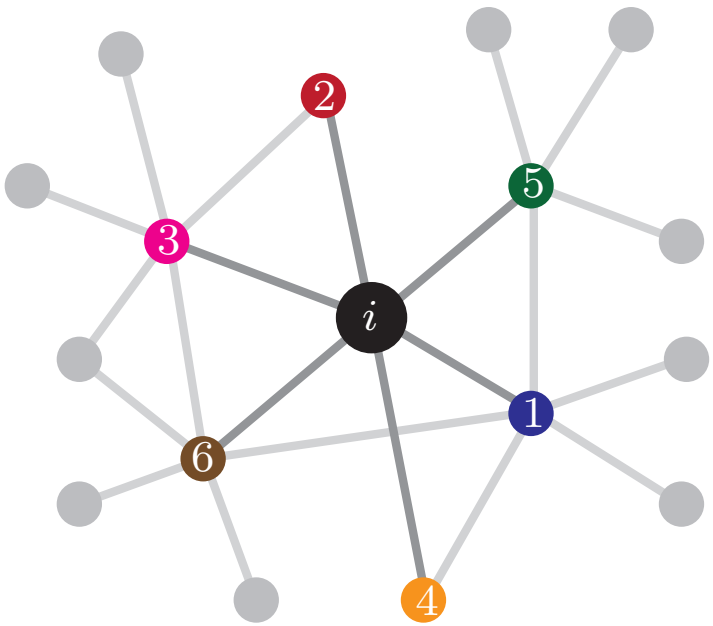
Per-node attributes can be encoded as vectors.



n nodes

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ \\ \\ \vdots \end{bmatrix}$$

$\mathbf{x} \in \mathbb{R}^n$

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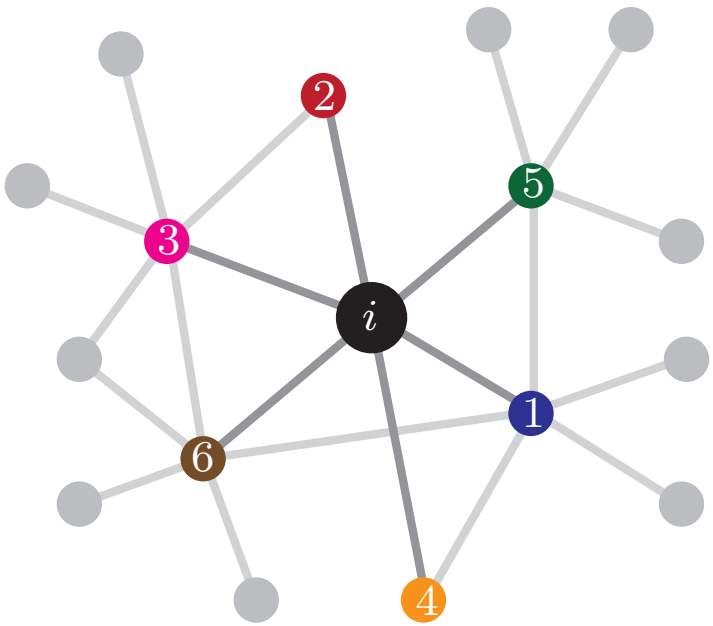

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The vertex ordering is arbitrary and can be permuted.

Adjacency matrices

Graph connectivity can be encoded in adjacency matrices

Let $|V| = n$, $|E| = e$, $|F| = m$ for a mesh $M = (V, E, F)$

Adjacency matrices: Vertex-to-vertex

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Let $|V| = n$, $|E| = e$, $|F| = m$ for a mesh $M = (V, E, F)$

The vertex-to-vertex adjacency is defined as the $n \times n$ binary matrix:

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & \cdots & 1 \\ \vdots & \cdots & \cdots & \cdots & \vdots \\ \vdots & \cdots & \cdots & \cdots & \vdots \\ 1 & 0 & 1 & \cdots & 0 \end{pmatrix}$$

where $a_{ij} = 1$ if vertex v_i is connected to v_j (that is, $e_{ij} \in E$)

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- The diagonal is always 0
- $\mathbf{A}$ is symmetric (assuming undirected graphs)
- Each row and column has at least one 1 (that is, $\sum_{ij} a_{ij} = 2e$)

Adjacency matrices as operators

From a linear algebra perspective:

- Per-node attributes are functions $f : V \to \mathbb{R}^k$.
- Adjacency matrices as operators that can be applied to functions.

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$$\begin{pmatrix} g_1 \\ g_2 \\ \vdots \\ g_n \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & \cdots & 1 \\ \vdots & \cdots & \cdots & \cdots & \vdots \\ \vdots & \cdots & \cdots & \cdots & \vdots \\ 1 & 0 & 1 & \cdots & 0 \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{pmatrix}$$

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One can construct new operators such as $\mathbf{I} - \mathbf{A}$:

$$g(v_i) = f(v_i) - \sum_{e_{ij} \in E} f(v_j)$$

And similarly for more complex (but still linear) operations.

Graph Laplacian

Given an attributed graph $G = (V, E)$, consider this condition on node v_i:

$$f(v_i) - \frac{1}{d_i} \sum_{j:(i,j)\in E} f(v_j) = 0$$

where d_i is the degree of v_i.

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In matrix notation, we define the $n \times n$ symmetric matrix $\mathbf{L}$ as:

$$L_{ij} = \begin{cases} 1 & \text{if } i = j \\ -\frac{1}{d_i} & \text{if } e_{ij} \in E \\ 0 & \text{otherwise} \end{cases}$$

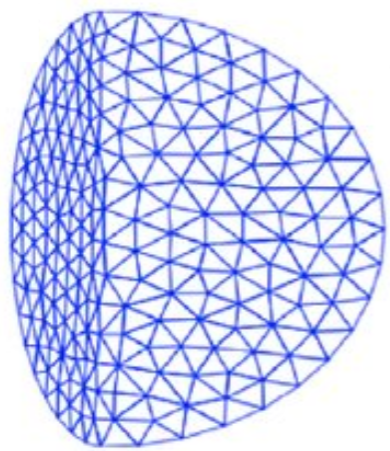
called the graph Laplacian of G.

Example

Consider the planar graph $G = (V, E)$ with per-node attributes:

$$f(v_i) = \{x_i, y_i\},$$

which are 2D coordinates for all the nodes.



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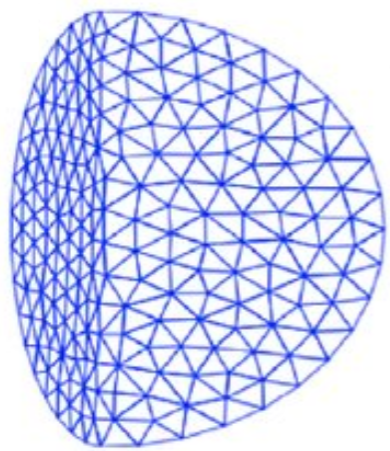

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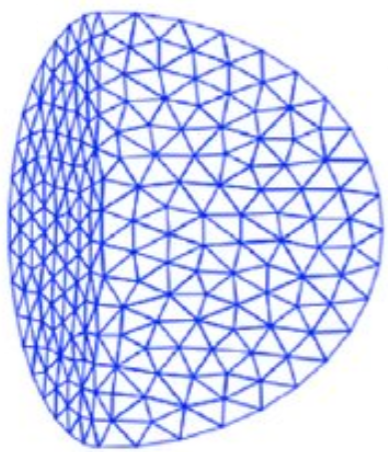
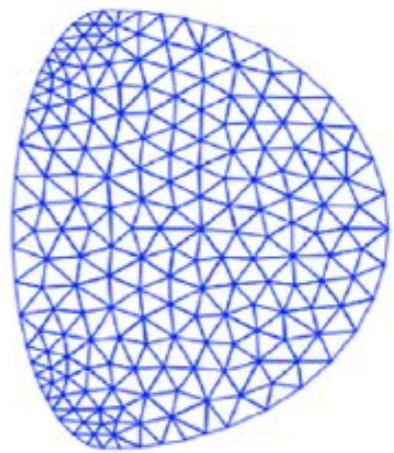
The equation $\mathbf{LF} = \mathbf{0}$ is satisfied if all the v_i are in the barycenter of their immediate neighbors (except for the boundary vertices).



$\mathbf{LF} \neq \mathbf{0}$



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Laplacian eigen-decomposition

Consider the spectral decomposition of the Laplacian:

$$\mathbf{L}\mathbf{u} = \lambda\mathbf{u}$$

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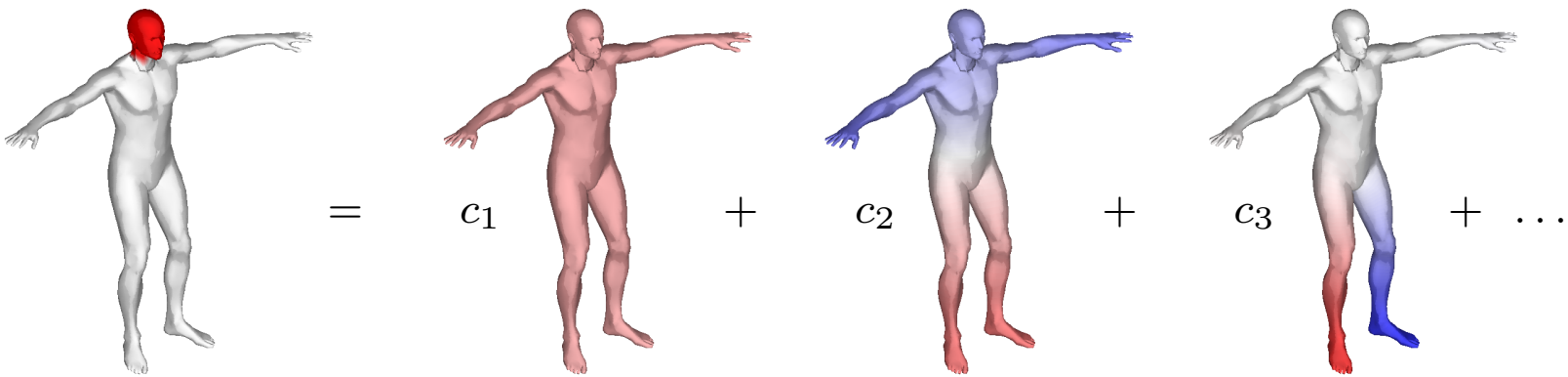
Any given function $f : V \to \mathbb{R}$ can be written as a unique linear combination of the Laplacian eigenvectors $\{\mathbf{u}_i\}$:



$\mathbf{f}$ $\mathbf{u}_1$ $\mathbf{u}_2$ $\mathbf{u}_3$

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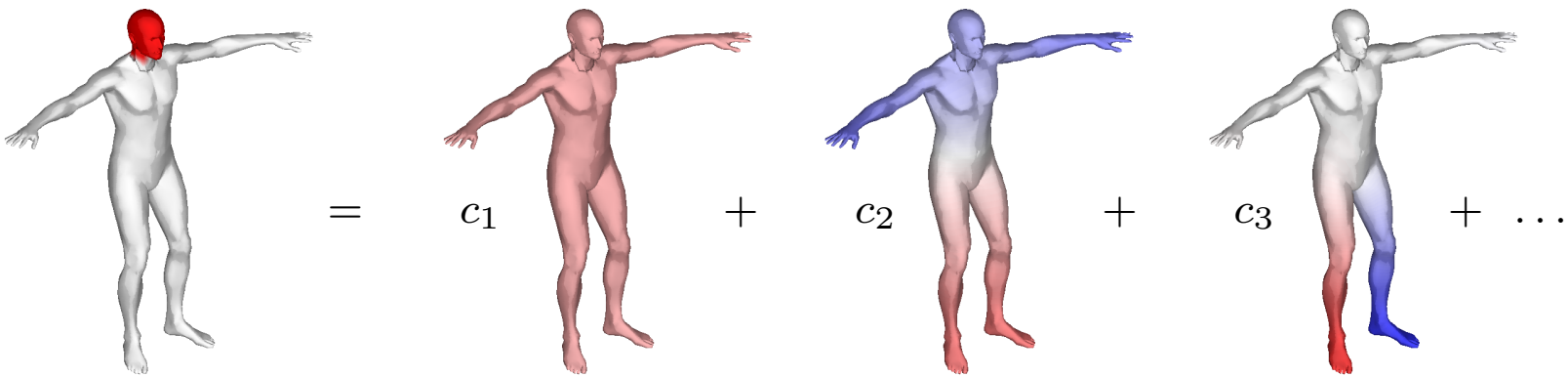

Since each eigenvector $\mathbf{u}_i$ can be interpreted as a function $u_i : V \to \mathbb{R}$, they are also called eigenfunctions.

Spectrum

The spectrum is the set of Laplacian eigenvalues.

It has a canonical ordering, and the first eigenvalue is always $= 0$:

$$0 = \lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots \to 2$$

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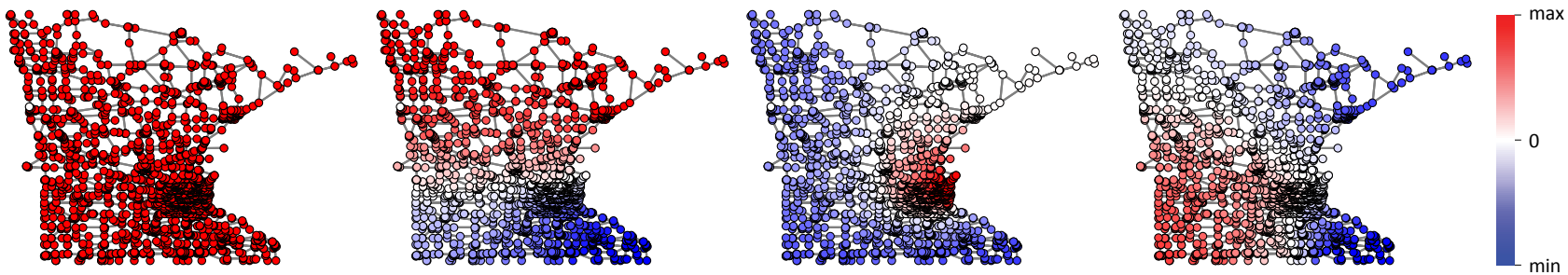
The eigenfunctions follow the ordering of the eigenvalues.

Thus we can talk of the "first" k eigenfunctions:



First 4 eigenfunctions of a graph Laplacian

Band-limited approximation

Each eigenvalue quantifies the oscillations of its associated eigenfunction.

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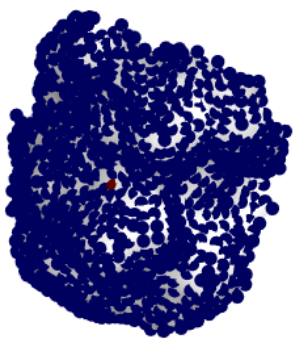
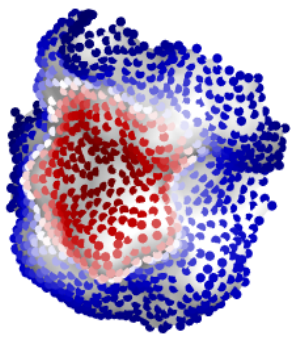
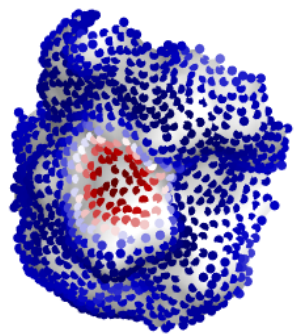
Using the first k eigenfunctions to approximate a given function:



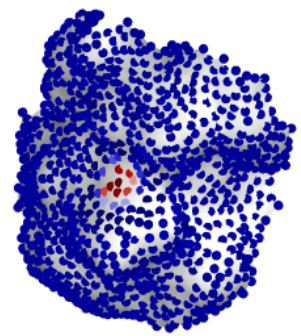
$k = n$



$k = 10$



$k = 30$



$k = 100$

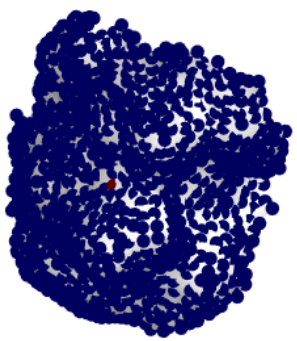
Band-limited approximation

Each eigenvalue quantifies the oscillations of its associated eigenfunction.

Small eigenvalues are associated to smooth eigenfunctions.

Using the first k eigenfunctions to approximate a given function:

- Reduces high-frequency noise.



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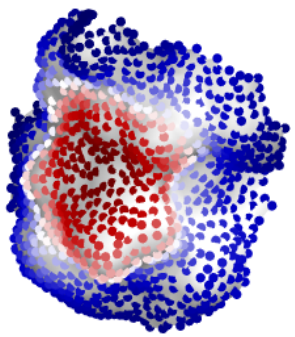

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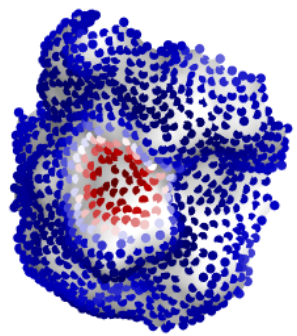

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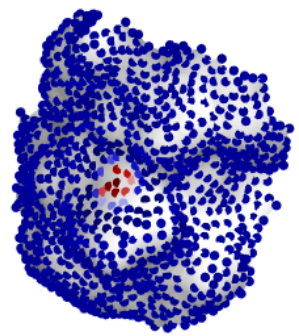

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Band-limited approximation

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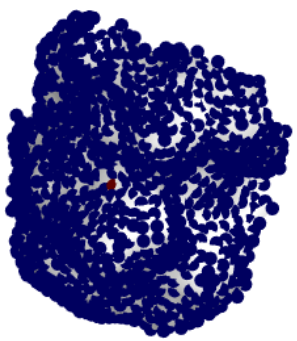
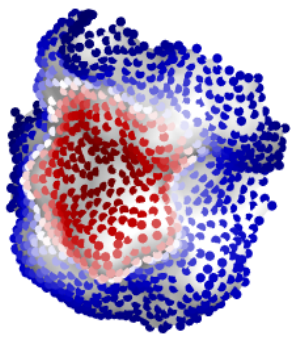
Small eigenvalues are associated to smooth eigenfunctions.

Using the first k eigenfunctions to approximate a given function:

- Reduces high-frequency noise.
- Enables efficient algorithms.
  Manipulate and store $k \ll n$ coefficients instead of n function values.



$k = n$



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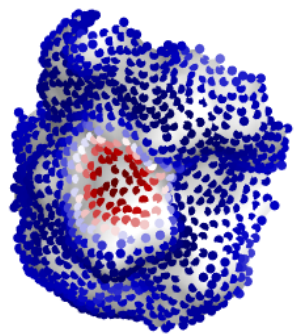
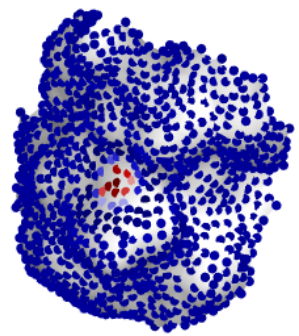


$k = 30$



$k = 100$

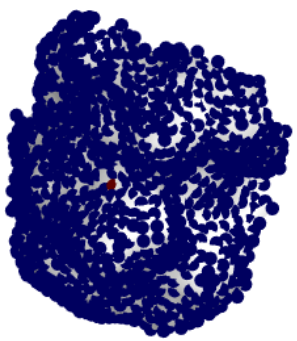
Band-limited approximation

Each eigenvalue quantifies the oscillations of its associated eigenfunction.

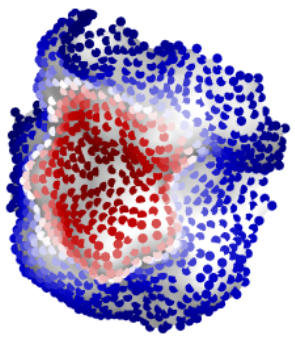
Small eigenvalues are associated to smooth eigenfunctions.

Using the first k eigenfunctions to approximate a given function:

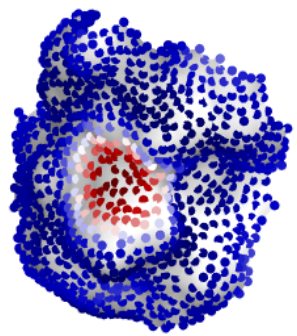
- Reduces high-frequency noise.
- Enables efficient algorithms.
  Manipulate and store $k \ll n$ coefficients instead of n function values.
- Guarantees invariance to deformations.



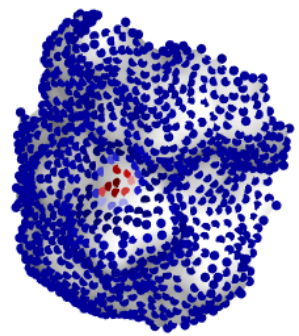
$k = n$



$k = 10$



$k = 30$



$k = 100$

Multiplicity

For a given graph G, an eigenvalue might appear multiple times, e.g.:

$$\lambda_{16} = \lambda_{17} = 1.1451$$

In this example, we say that eigenvalue 1.1451 has multiplicity 2.

Multiplicity is known to be related to symmetries in the graph.

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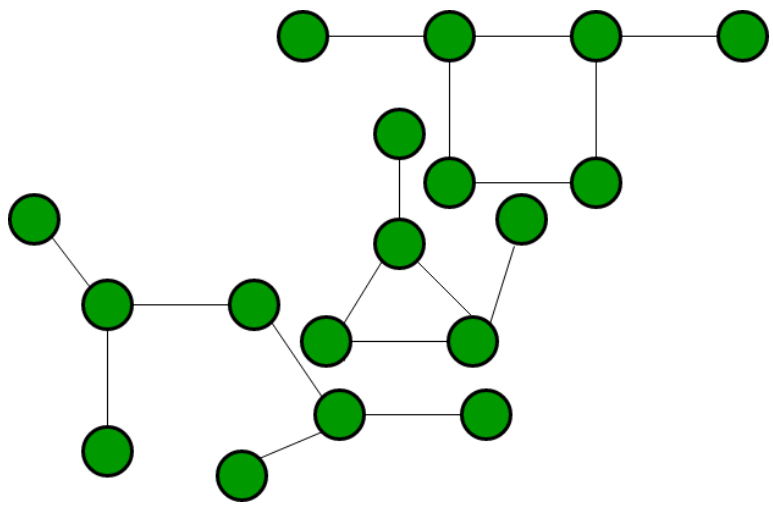
The multiplicity of $\lambda_1 = 0$ counts the connected components in G:



$$\lambda_1 = \lambda_2 = \lambda_3 = 0$$

Informativity

Spectral quantities encode a whole lot of information about the underlying structure (a surface or a graph).

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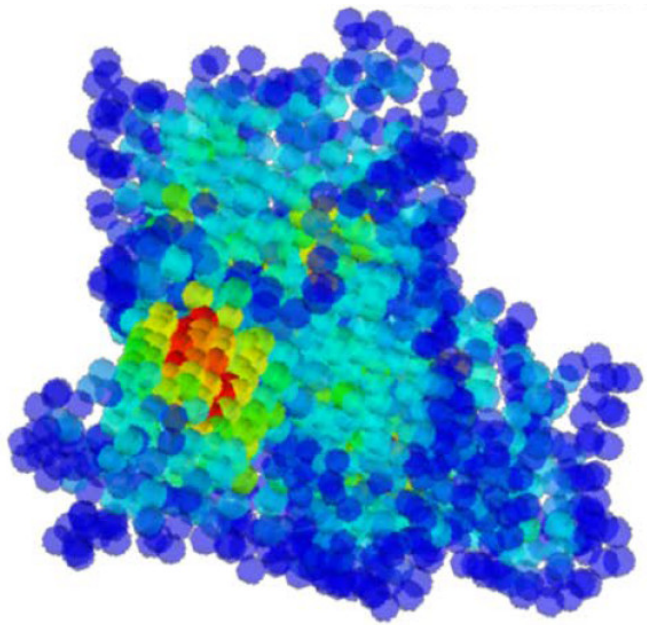
For example, eigenfunctions localize around hot spots of vibrational energy (active sites in the case of enzymes).



glutamate synthase

Chalopin et al, "Universality of fold-encoded localized vibrations in enzymes", Nature 2019

Exercise

- Implement an algorithm to compute the graph Laplacian.
- Compute it for the Minnesota road map graph (see webpage).
- Compute its eigenvectors and eigenvalues using NumPy (you can use this function)
- Plot and send me an image with the first 20 eigenvectors (visualized by coloring the graph nodes), and a bar plot of the first 50 eigenvalues.