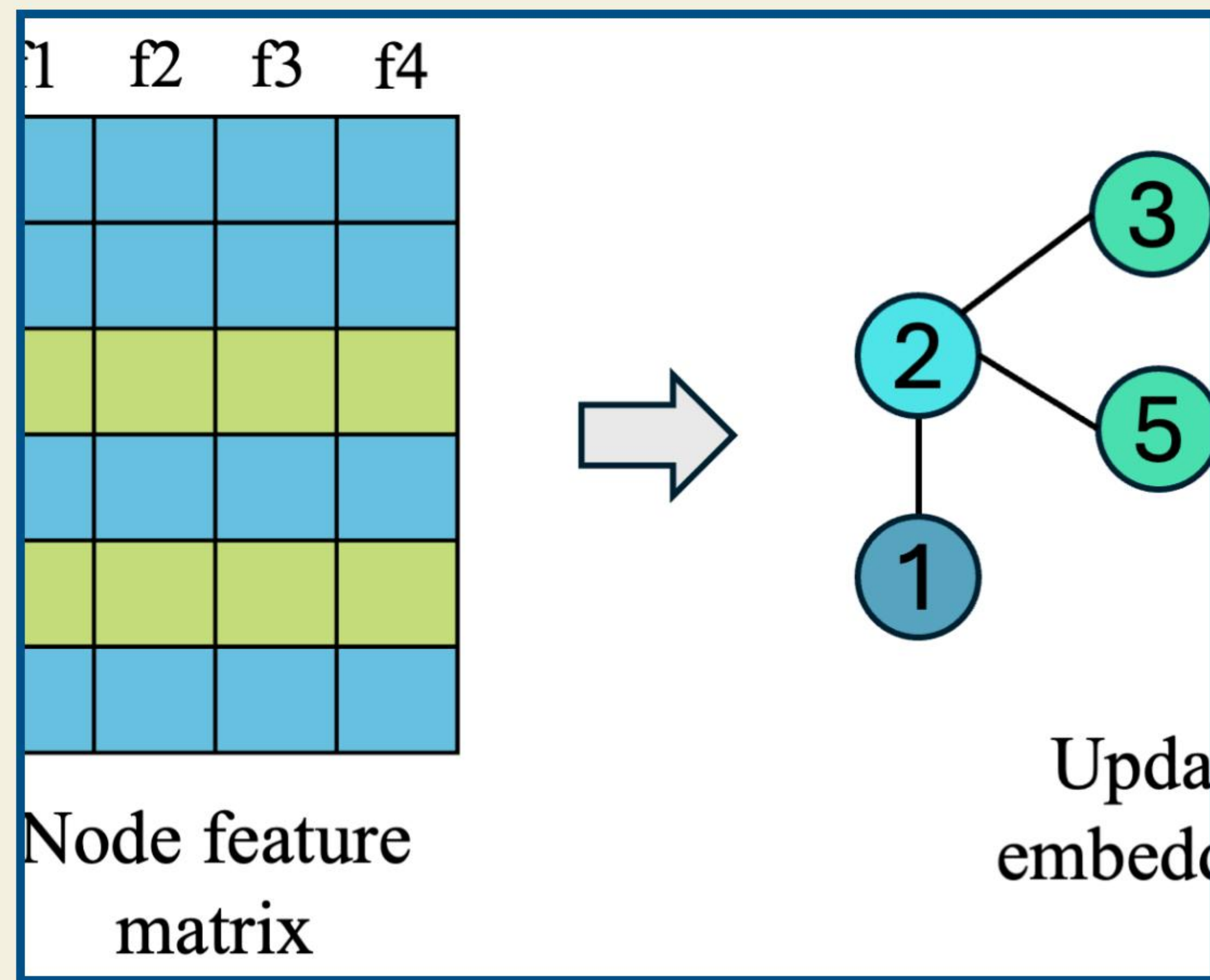


Topological Indices

An Explanation of the Wiener, Zagreb, & Randić Indices

What Are Topological Indices?

- They are numerical values (descriptors) derived from the graph structure of a molecule.
- In this graph:
 - **Atoms** = Vertices (Nodes)
 - **Bonds** = Edges (Links)
- They are a core part of **Cheminformatics**.
- Used to predict a molecule's chemical and physical properties without experimentation.
- This is known as **QSAR/QSPR** (Quantitative Structure-Activity/Property Relationship).



The Wiener Index (W)

The Pioneer of Distance-Based Indices

Wiener Index: The Concept

- ✓ **Core Idea:** Measures the overall "compactness" or "extension" of a molecule.
- ✓ **Type:** A **distance-based** index, introduced by Harry Wiener in 1947.
- ✓ **How it Works:** It is the sum of the shortest distances (number of bonds) between **all unique pairs** of atoms in the molecule.
- ✓ **Result:**
 - ✓ A compact, highly-branched molecule has a **low** W .
 - ✓ A long, linear molecule has a **high** W .

Wiener Index: The Formula

$$W(G) = \frac{1}{2} \sum_u \sum_v d(u, v)$$

$W(G)$ is the Wiener Index of the graph G .

Σ (Sigma) means "the sum of".

u and v are two different vertices (atoms).

$d(u,v)$ is the distance (shortest path) between u and v .

$1/2$ is used to avoid double-counting (since $d(u,v)$ is the same as $d(v,u)$).

The Zagreb Indices (M_1 & M_2)

The Classic Degree-Based Indices

Zagreb Indices: The Concept

- ✓ **Core Idea:** Measure molecular branching and complexity.
- ✓ **Type: Degree-based** indices, focusing on the **degree** of each atom (d_v).
- ✓ **Degree (d_v):** The number of bonds a specific atom has.
- ✓ **M_1 (First Zagreb Index):** Sum of the **squares of the degrees** of all atoms. It's a measure of atom "busyness".
- ✓ **M_2 (Second Zagreb Index):** Sum of the **products of degrees** for all **bonds** (adjacent atoms).

Zagreb Indices: The Formulas

First Zagreb Index (M_1)

$$M_1 (G) = \sum_{v \in V} (d_v)^2$$

Sum (Σ) over all **vertices** v .

d_v is the degree of vertex v .

Second Zagreb Index (M_2)

$$M_2 (G) = \sum_{uv \in E} (d_u \cdot d_v)$$

Sum (Σ) over all **edges** E .

d_u and d_v are the degrees of the two atoms u and v connected by that edge.

The Randić Index (R)

The Connectivity & Branching Index

Randić Index: Concept & Formula

The Concept

- Also known as the **Connectivity Index**.
- It is one of the most successful and widely used indices for measuring molecular branching.
- Also **degree-based**, calculated by summing values for each bond.
- A **lower** Randić Index (R) indicates **more** branching.

The Formula

$$R(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_u \cdot d_v}}$$

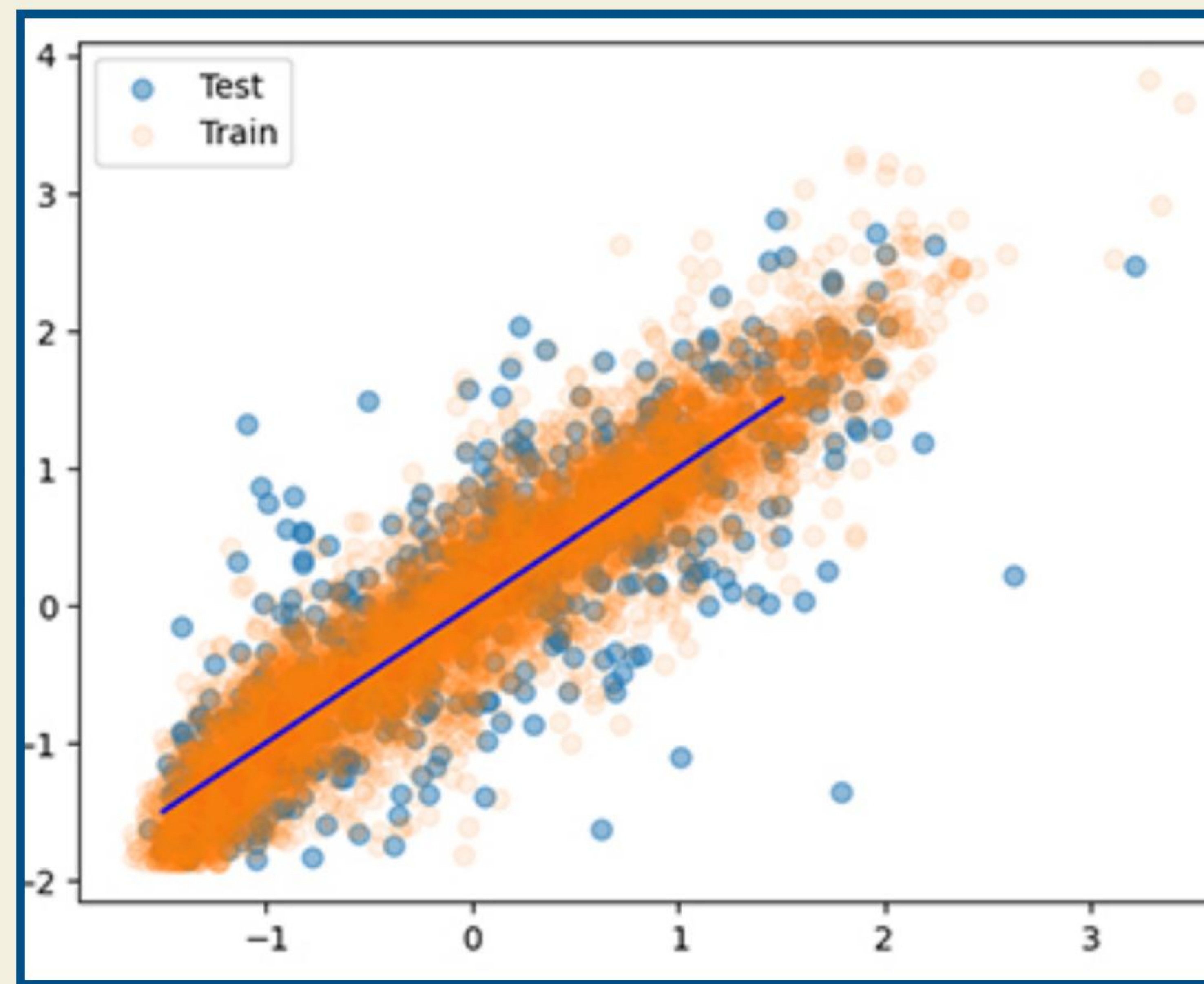
Sum (Σ) over all **edges** E (bonds).

d_u and d_v are the degrees of the two atoms connected by the bond.

Summary & Applications

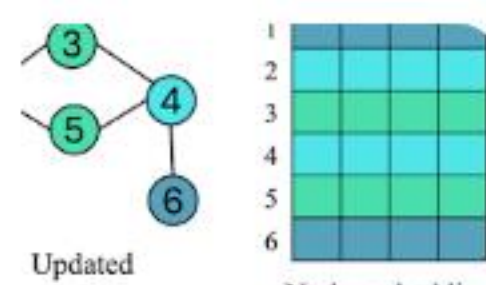
Why Use These Indices?

- **Wiener (W):** Predicts properties related to molecular volume and compactness (e.g., boiling point, density).
- **Zagreb (M_1, M_2):** Correlate with the total π -electron energy and measure branching.
- **Randić (R):** Highly successful at predicting properties like boiling points, surface area, and toxicity.
- All are vital for **QSAR/QSPR**, allowing scientists to predict a molecule's properties and activity **before** it is synthesized.



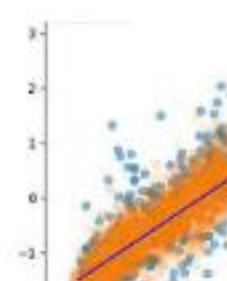
Questions?

Image Sources



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