Spherical Harmonics, CG Coefficients, and CGCNN

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Overview

- Spherical Harmonics $\rightarrow$ Just 2-parameter functions!

- Clebsch-Gordon Coefficients $\rightarrow$ Just look them up in a table!

- An example of a Crystal Graph Convolutional Neural Network (CGCNN)

Spherical Harmonics

JUST A NICE SET OF TWO-PARAMETER FUNCTIONS!

Origin: Spherical Laplacian

If you haven't seen differential equations before, don't worry! I just want you to see this in case it comes up again.

Apply Laplace's equation to an arbitrary function in spherical coordinates:

$$\nabla^2 f(\phi, \theta, r) = 0$$

$$\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial^2\phi}\right] f = 0$$

Origin: Spherical Laplacian cont.

Now, we make the assumption (which works for Laplace's equation) that the solution is separable such that it is a product of simpler functions: $f(\theta, \phi, r) = \Theta(\theta)\Phi(\phi)R(r)$.

Then we may isolate the angular dependence into a function $Y_\ell^m(\theta, \phi)$, which satisfies:

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial^2\phi}\right]Y_\ell^m = 0$$

These functions, termed the spherical harmonics, take the form:

$$Y_\ell^m(\theta, \phi) = C_{m\ell}P_\ell^m(\cos\theta)e^{-im\phi}$$

where $P_\ell^m(x)$ are the associated Legendre polynomials, and $C_{m\ell}$ is just some constant/normalization coefficient.

Note that their value is in general a complex number. Also note that $Y_\ell^m = 0$ for $m > \ell$ and $m < \ell$, where m and ℓ must be integers.

Origin: Irreducible Representation of SO(3)

Spherical Harmonics also may be taken as the basis set for irreducible representations of the group of rotations in 3-space ($SO(3)$).

We can always decompose functions defined on a surface of a sphere as a linear combination of these spherical harmonics as below:

$$f(\theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{m=\ell} c_{\ell,m} Y_\ell^m(\theta, \phi)$$

Spherical Harmonics Practically

Spherical harmonics are just two-dimensional functions!!!

They have some nice properties that make them indispensable for dealing with functions on the surface of spheres (they form an orthonormal basis).

A nice way to visualize them is to plot their magnitude as the radius in three dimensional space (where the input is the pair of angles θ, ϕ). See this ipython notebook to play with them: `https://alexheilman.com/products/ipy/spherical_harm_vis.ipy`

Tensor Products of SO(3)

Say we want to describe the product of two spherical harmonics in terms of a third (equivalent to the product) spherical harmonic expansion.

$$Y_{\ell_1}^{m_1}(\Omega)Y_{\ell_2}^{m_2}(\Omega) = \sum_{\ell_3,m_3}\sqrt{\frac{(2\ell_1+1)(2\ell_2+1)}{4\pi(2\ell_3+1)}}C_{\ell_1 m_1 \ell_2 m_2}^{\ell_3 m_3}C_{\ell_1 0 \ell_2 0}^{\ell_3 0}Y_{\ell_3 m_3}(\Omega)$$

where $C_{\ell_1 m_1 \ell_2 m_2}^{LM}$ are Clebsch-Gordon coefficients.

In physics, they're most often used for addition of angular momenta. In fact, this is the most common application of them. Hence, sometimes CG coefficients are often given the alternative notation:

$$C_{\ell_1 m_1 \ell_2 m_2}^{LM} = \langle j_1 m_1 j_2 m_2 | LM \rangle$$

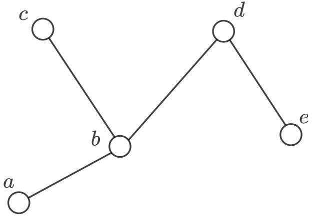
CG Practically

They're just numbers.

LOOK THEM UP IN A TABLE!

Graphs (Not Plots of Functions)

Graphs are mathematical objects. They're just sets of nodes and edges that connect two nodes.



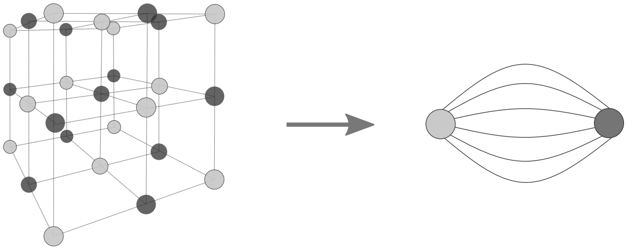
$$\mathcal{V} : \{a, b, c, d, e\}$$

$$\mathcal{E} : \{(a, b), (b, c), (b, d), (d, e)\}$$

Undirected Graph

Crystal Graphs

Now, we'd like to encode crystalline structures as graphs and associate physical information with the graph elements:



For an overview of the usual techniques, see `https://alexheilman.com/halfbaked/crystalgraphs`

Graph Convolutional Neural Networks

Graph neural networks act on and update the node features based upon the connectivity of the graph, while preserving the underlying graph structure.

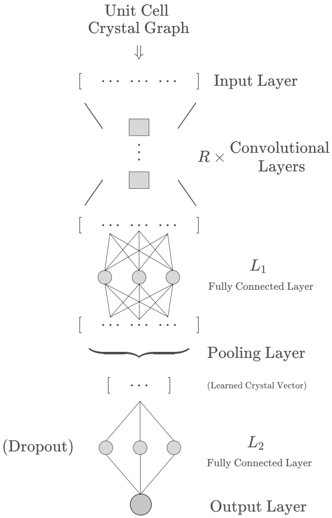
For a nice overview of basic graph networks and convolution see:
`https://distill.pub/2021/gnn-intro/`
`https://distill.pub/2021/understanding-gnns/`

Machine Learning & Materials Science

Most state-of-the-art machine learning models applied to materials science utilize graph networks.

One of the original models is Tian Xie and Jeffrey Grossman's Crystal Graph Convolutional Neural Network (CGCNN).

CGCNN Architecture



A schematic of the basic CGCNN architecture is presented aside.

Note that both edge and node features are generally used, but node features are the only ones updated.

For the corresponding paper, see `https://link.aps.org/doi/10.1103/PhysRevLett.120.145301`.