

Problem to be solved: predicting magnetism (ferromagnetic, antiferromagnetic, or nonmagnetic) from structural and chemical descriptors.

Typical Approach: neutron scattering experiments (time and resources expensive), and only ~1600 materials have such experimental data.

Data set: Materials from the “Materials Project” database (~ tens of thousands of materials).

Descriptors:

- Elements in the compound.
- Oxidation state of each element. (implicitly encoding the SOC)
- Number of ions in the compound.
- Space group.
- Volume of unit cell.
- Density.

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