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Inferring equations of state of the lower mantle minerals using Artificial Neural Networks (ANNs)

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Background

Motivation

Interpretation of information available from seismic images requires an understanding of the seismic properties of minerals at different pressure and temperature (P and T) environments. For example to interpret slow velocity structures like LLSVPs in terms of temperature and composition.

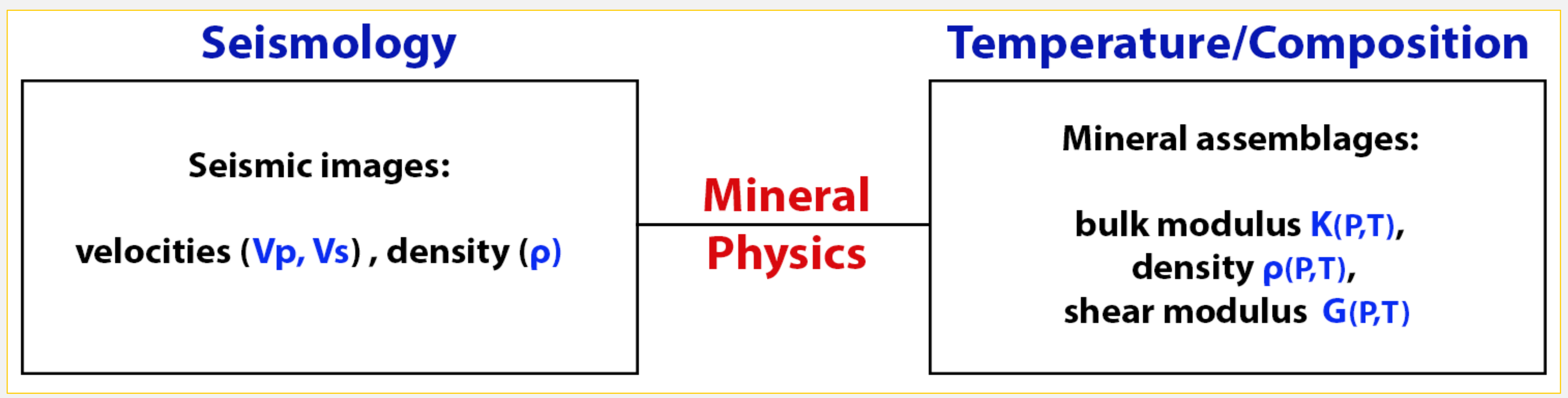

Figure 1: temperature & composition to seismic images.

$$V_p(P,T) = \sqrt{\frac{K(P,T)+4G(P,T)/3}{\rho(P,T)}}, \qquad V_s(P,T) = \sqrt{\frac{G(P,T)}{\rho(P,T)}}$$

Previous trends

1. Compress minerals either theoretically or experimentally to a very high P and T.
2. Fit the (experimental) data to some functions (mostly assuming the underlying physics is known, or sometimes ad-hoc).
3. Construct equations of state (EoS) based on data fitting.
4. Compute mineral properties (bulk modulus, density, thermal expansivity, etc.) based on those EoS at any pressure and temperature.

Problems

1. Pressure scale problem (i.e. no barometer to measure such high (lower mantle) pressures in high P and T experiments).
2. Different functions (EoS) can fit the experimental data equally well (i.e. no unified EoS), such that the derived elastic parameters are very different depending on the choice of EoS.
3. Uncertainties in temperature measurements, non-hydrostatic pressure, etc.

Artificial Neural Networks (ANNs)

Mixture Density Networks (MDNs)

1. An ANN can approximate any function at all [Nielsen, 2015].
2. Knowing the functional form beforehand (cf. data fitting) is not a prerequisite.
3. Standard ANNs combined with Gaussian Mixture Models (GMMs), then called MDNs [Bishop, 1994], can handle uncertainties.

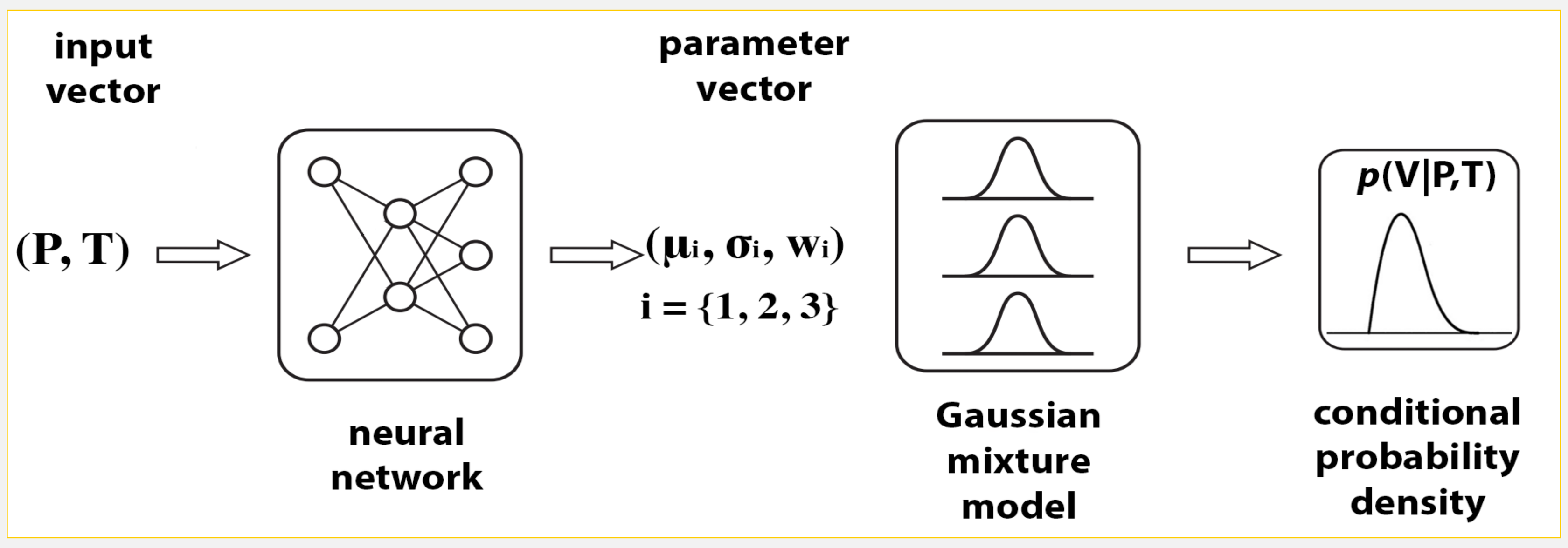

Figure 2: standard ANN combined with GMM [Bishop, 1994, modified] such that the network outputs have complete probabilistic description; μ, σ and w are mean, standard deviation and weight of each Gaussian kernels, respectively; P, T, V = pressure, temperature, volume.

$$p(V|P,T) = \sum_{i=1}^{m} w_i(P,T)\, \phi_i(V|P,T).$$

$$\phi_i(V|P,T) = \frac{1}{(2\pi)^{\frac{1}{2}}\sigma_i(P,T)} exp\left\{-\frac{\left|\left|V-\mu_i(P,T)\right|\right|^2}{2\sigma_i(P,T)^2}\right\}.$$

Procedure

1. Collect experimental Pressure-Temperature-Volume (P-T-V) data and uncertainties (1615 data for Periclase–MgO [Rijal et al., 2019]).
2. Construct a simple ANN with one hidden layer combined with GMM.
3. Use Gaussian noise to restrict overfitting.
4. Divide data into training and validation sets (validation set to restrict overfitting).
5. Standardize (mean=0, standard deviation=1) input data for better learning and optimization.
6. Train the network (using P, T as inputs and V as target).

Results (eg. MgO – Periclase)

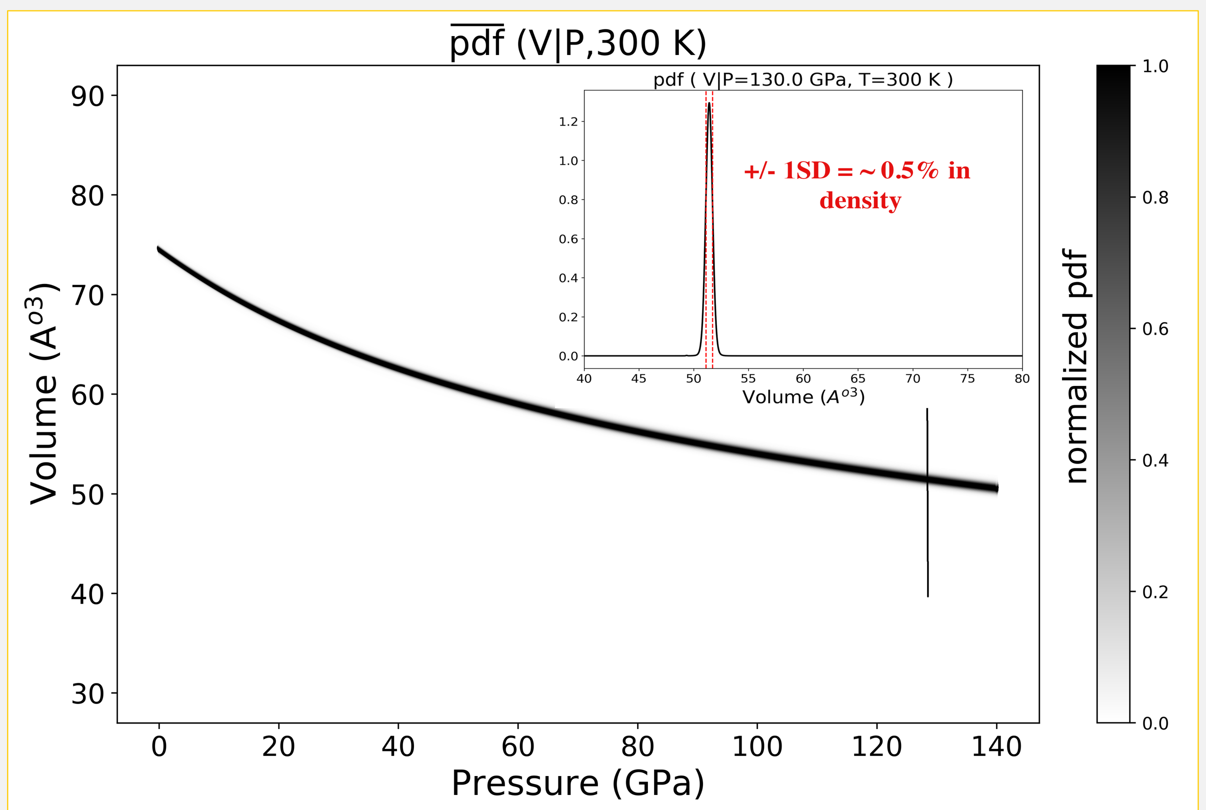

Figure 3: P-V EoS of MgO at 300K from ANNs with uncertainties; one standard deviation (SD) in density (/volume) is 0.5%.

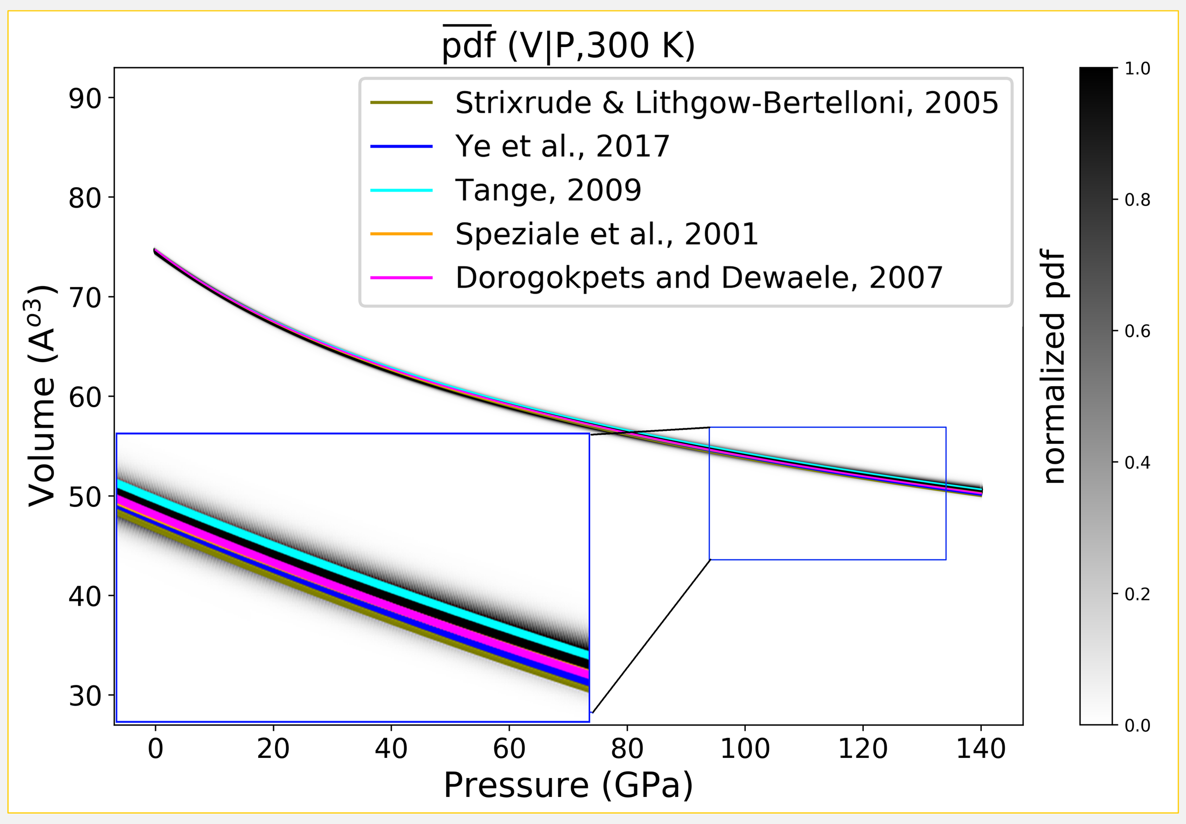

Figure 4: P-V EoS of MgO at 300K from ANNs with uncertainties; zoomed around 120 GPa to compare with previous studies [Rijal et al., 2019].

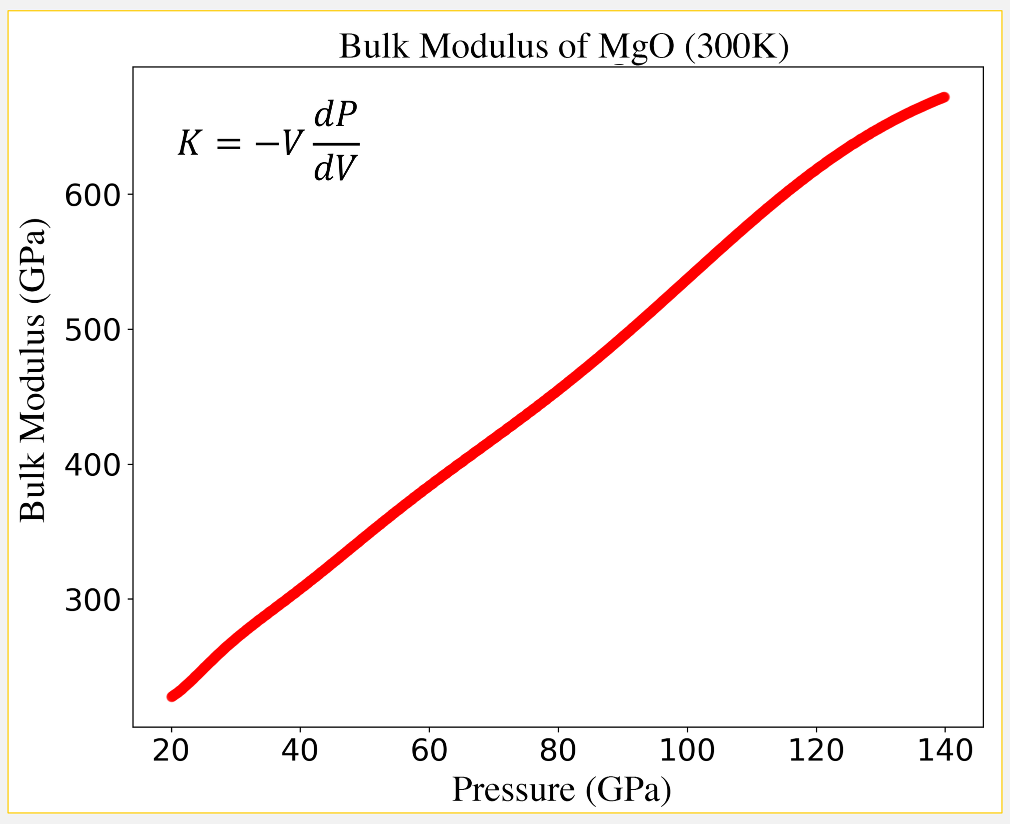

Figure 5: bulk modulus of MgO at 300K from ANNs without uncertainties (MDN to be implemented).

Findings

1. ANN outputs show uncertainty in density (/volume) at the base of lower mantle (~135GPa, but at 300K) is approx. +/-0.5% (+/-1SD).
2. Previously published EoS show as much as 1.5% density difference among them, and thus derived elastic parameters can be very different (depending on the functional form of the EoS used).
3. (Most) previously published EoS fall within +/- 2SD of our ANNs derived EoS.

Ongoing/Future work

1. Implement MDNs to approximate derivatives (i.e. bulk modulus and thermal expansivity) of an unknown mapping and quantify uncertainties.
2. Compute uncertainties in shear modulus.
3. Compute uncertainties in primary and shear wave velocities.
4. Apply the same procedures to other lower mantle minerals.
5. Interpret seismic images in terms of temperature and composition.

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