A phase transition in the O'Doherty-Anstey model

Kris Innanen

ABSTRACT

In the O'Doherty-Anstey (OA) model, a stack of interfaces redistributes the amplitude of a transmitted wave pulse across a range of lags, and does so more and more widely as the reflectivities and number of interfaces grow. This is suggestive of a Maxwell-Boltzmann statistical model involving an ensemble of weighted raypaths, with a particular raypath and its weight playing the role of a system microstate, and lag playing the role of the energy. An artificial temperature, in the same units as the lag, is introduced, which measures in a bulk sense the reflection strengths and interface numbers in the stack. The partition function for such a model requires an estimate of the degeneracy of these states at each lag, which we argue is provided by one of the intermediate calculations in the OA model. Seeded by a real or simulated reflectivity series, a numerical estimate of the partition function allows the average lag to be calculated as a function of temperature. A critical transitional region dividing two distinct temperature regimes (one in which pulses are dominated by small lags and one in which pulses are dominated by lags of roughly the length of the input reflectivity) is observed.

INTRODUCTION

In the O'Doherty and Anstey (1971) model, a wave pulse transits a sequence of reflective interfaces, producing a direct arrival and a coda. As the number of interfaces and their reflection strengths change, the coda is re-distributed over lags l, which label discrete intervals of time (i.e., $\Delta\tau \times l$) after the arrival of the direct wave. In the calculation set out by the authors (OA), the reflectivity series is autocorrelated, and the positive lags of the result are auto-convolved and summed repeatedly, producing an estimate of the spectrum of the transmitted pulse. An intermediate result in this calculation is the set of contributions to the pulse at lag l from a generally very large number of raypaths, each being a contribution from a specific history of reflections and each with a weight determined by the reflectivity. In fact, at this stage in the OA calculation, the raypath (meaning a contributing reflection strength, at a particular lag, deriving from a certain zig-zag path through the medium) can be considered the logical unit of the model.

Two features of OA are striking: (1) that it favours small lags unless larger lags are enforced by the reflectivities and interface numbers, and (2) that as the geology changes to enforce larger lags, the number of possible raypaths contributing to any given lag grows rapidly. This is suggestive that a Maxwell-Boltzmann statistical model (e.g., Sears, 1959) may be appropriate to describe OA phenomena, with lag playing the role of energy, and a particular raypath and its weight playing the role of a system state.

Applying this model involves asking for the probability $P(l)$ of a particular raypath contributing at lag l. In a Maxwell-Boltzmann model, this $P(l)$ is determined to within a temperature T and a normalization factor, or partition function, Z. In this case, T is a parameter (with the same units as the lag) controlling the rate of increase in number of contributing raypaths as the lag increases. So, dialling it up or down simulates bulk changes in the reflection strengths and/or numbers of interfaces of the geology. Meanwhile, Z is a sum of P over all lags l, weighted by the degeneracy at each l, i.e., the number of distinct contributing raypaths. In statistical mechanical problems the partition function is generally difficult to determine or estimate. However, in OA, the lags are discrete and countable, and we assert that a quantity proportional to the degeneracy is actually determined during the OA calculation, seeded by a real or simulated reflectivity function.

With an estimate of Z in hand, the variability of the average lag $\langle l \rangle$ in the transmitted pulse as a function of lag-temperature T can be analyzed. A transition is predicted between states dominated by contributions at very small lag, and states dominated by lags at or near the length of the reflectivity series, as T increases past a critical point. This is a quasi-phase transition, as it is not discontinuous. Nevertheless it appears to mark a boundary between two clearly-defined regimes characteristic of the OA model and the gross features of an input reflectivity.

THE O'DOHERTY-ANSTEY (OA) MODEL

The OA model begins with a reflectivity series which in the z-transform domain is

$$R(z) = r(0) + r(1)z + ... + r(N)z^N. \tag{1}$$

The first order of multiples is approximated as

$$M(z) = -R(z)R({}^1\!/\!_z)\big|_{\text{lags}>0}, \tag{2}$$

and the remaining orders are included through autoconvolution to produce an estimate of the transmitted pulse:

$$F(z) = M(z) + \frac{1}{2!}M^2(z) + ... + \frac{1}{n!}M^n(z) + ... = \exp M(z). \tag{3}$$

After this, the OA model is refined to estimate the reflection response of the layers. Here we will instead continue to analyze the transmitted pulse and its coda. Collecting terms of common lag in F we have

$$F(z) \approx f(0) + f(1)z + f(2)z^2 + ... + f(L)z^L, \tag{4}$$

where the zero-lag term $f(0)$ is zero by (2). At non-zero lags the amplitude $f(l)$ at lag l is the sum total of all weighted raypath contributions with the correct delay. These contributions are in general positive or negative, and they interfere to determine $f(l)$, which is also consequently either positive or negative. However, once computed, its sign will no longer be relevant for our purposes (our interest being in the strength of a contribution, whether positive or negative), and so we consider instead the envelope of $f(l)$:

$$\text{oa}(l) = \sqrt{f(l)^2 + f^*(l)^2}, \tag{5}$$

where f^* is the quadrature counterpart of f (e.g., Taner et al., 1979). The calculations in the next section will make use of this intermediate quantity $\text{oa}(l)$, the envelope of the transmitted OA pulse.

MAXWELL-BOLTZMANN STATISTICS OF THE OA MODEL

Let $P(l)$ represent the probability that the reflectivity will produce a raypath contributing at lag l. This is analogous in standard statistical mechanics to setting up the probability that a system will be in a state with the lth allowable energy E_l. Consequently, a Boltzmann distribution is induced of the form

$$P(l) = \frac{1}{Z(\beta)} e^{-\beta l}, \tag{6}$$

where $\beta = 1/T$ is the inverse temperature, and the temperature is a parameter in units of lag. The partition function is

$$Z(\beta) = c' \sum_{l=1}^{\infty} g(l) e^{-\beta l}, \tag{7}$$

where c' is a scale factor and $g(l)$ is the degeneracy, or multiplicity function (Kittel, 1969), which in this case is the number of distinct raypaths which contribute at lag l. The upper limit reflects the fact that in principle infinite lags are permitted; these very large lags are negligible contributors to Z, and in practice an upper limit L can be selected.

The autoconvolutions within equation (3) can be interpreted as an accounting of all raypaths (including their relative weights) contributing to a given lag. Therefore we assert that oa(l) is proportional to the $g(l)$ in (7). This produces a computable form for the partition function:

$$Z(\beta) = c \sum_{l=1}^{L} \text{oa}(l) e^{-\beta l}, \tag{8}$$

with the new constant c absorbing the proportionality. From this ensemble averages are obtainable, for instance the average lag and its fluctuation are

$$\langle l \rangle = -\frac{\partial}{\partial \beta} \left(\log \sum_{l=1}^{L} \text{oa}(l) e^{-\beta l} \right), \tag{9}$$

and

$$\Delta l^2 = \frac{\partial^2}{\partial \beta^2} \log \left(\sum_{l=1}^{L} \text{oa}(l) e^{-\beta l} \right), \tag{10}$$

respectively. The oa(l) will normally be available as numerical quantities, and only in special instances might they be available as analytical functions of β. Hence the derivatives in (9)-(10) will normally be estimated through differencing.

PHASE TRANSITION

Phase transitions in simple 1D models are typified by (1) availability of forbidden infinite energy (here lag) states, and (2) a greater degeneracy at higher states than at the lowest state.

Because both of these conditions are in place within the OA model as set out above, the presence of a transition is therefore plausible. We seek that transition in the variation of the average lag of a pulse $\langle l \rangle$ as a function of the logarithm of the lag temperature, i.e., $\log T$. The details of the reflectivity series used to seed the estimate of the degeneracy function are presumed to have a strong influence on these variations. We therefore consider both a random reflectivity drawn from a normal distribution with various standard deviations, and by raising these reflectivity values by a small integer power.

Random reflectivity case

In Figure 1 an example reflectivity drawn from a normal distribution with standard deviation of 0.05 is illustrated.

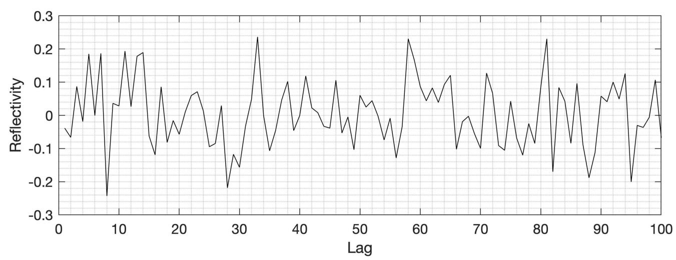

FIG. 1. 100-point random reflectivity with coefficients drawn from a zero-mean normal distribution with standard deviation of 0.05.

Reflectivities of this type, but with varying standard deviation and varying maximum number of samples, are used to seed Boltzmann distributions, and the partition function and average $\langle l \rangle$ are computed, the latter with (9). This are plotted against the logarithm of the lag-temperature T, which is a parameter in (**??**), in Figures 2a-b. Clear transition regions are visible in a sigmoid-shaped responses, with the high temperature maximum being the most sensitive feature of the curves. No discontinuity or precise critical temperature is produced, but all curves to have a unique point of maximum slope, which is identified with dashed lines on the plots.

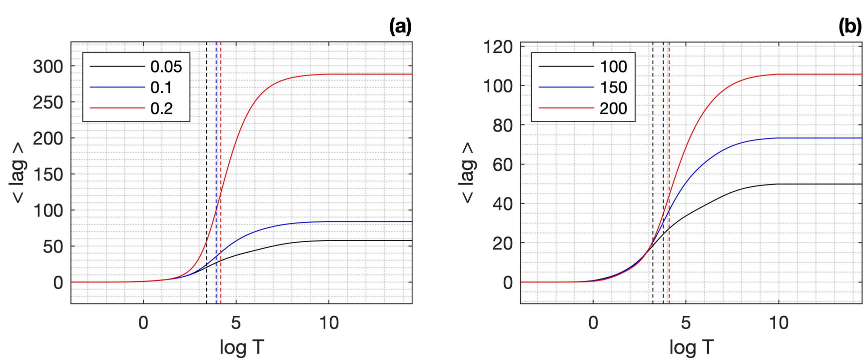

FIG. 2. Plots of $\langle l \rangle$ versus the logarithm of the lag-temperature T (solid), with points of maximum change identified as transition points (dashed). (a) Three curves corresponding to increasing reflectivity values, with standard deviations of 0.05 (black), 0.1 (blue), and 0.2 (red). (b) Three curves corresponding to increasing reflectivity series length, with 100 points (black), 150 points (blue), and 200 points (red).

Spiky reflectivity case

Reflectivities can be more realistically simulated by drawing values from a normal distribution and raising the values to a small integer power (Margrave and Lamoureux, 2019). Two examples are illustrated in Figure 3a-b, with the same reflectivity raised to the 3rd and 5th power.

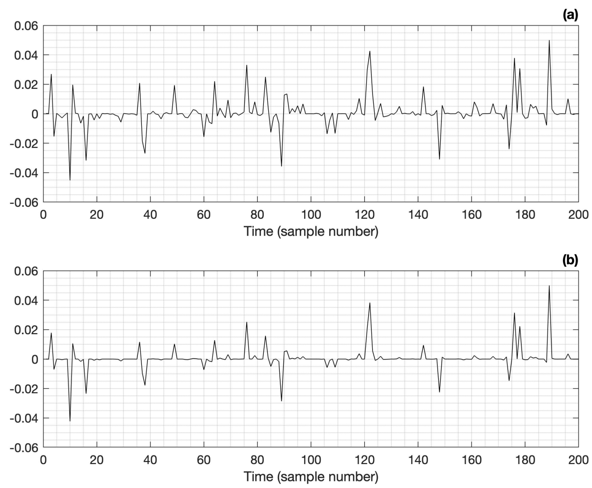

FIG. 3. Random (Gaussian) reflectivities raised to the (a) 3rd and (b) 5th power.

Differences in the $\langle l \rangle$ versus $\log T$ curves (Figure 3) for different degrees of sparseness in the above sense appear minimal.

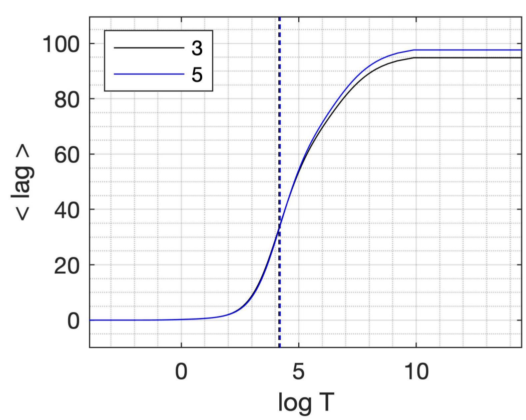

FIG. 4. $\langle l \rangle$ versus $\log T$ for reflectivity series generated from Gaussian processes raised to integer powers of 3 and 5.

DISCUSSION AND CONCLUSIONS

A Maxwell-Boltzmann statistical model of the probable average lags, normalized by a process of enumeration defined by the OA model, evidently predicts a transition between two different regimes of average lag. The low T regime is associated with simpler raypath geometries (i.e., more simple geological media with fewer interfaces), which favour smaller lags, as well as lower reflection coefficients, and the high T regime correspondingly with the larger number of raypath geometries capable of producing larger lags, and higher reflection coefficients, which keep the contributions from more complex raypaths contributing non-negligibly.

A particular raypath with its characteristic zig-zag shape is the template for a state in this statistical model. As is common with 1D statistical-mechanical models that produce phase transitions, there is a rapid growth the the number of available states (raypaths) as the energy (lag) grows. This is the mathematical explanation for the transition as it appears in Figures (2) and (4). This growth in number of accessible states is the same phenomenon O'Doherty and Anstey invoke to argue that in a periodic medium multiple reflections in the coda eventually outweigh the direct pulse, described in a different language. It adds to that phenomenon however the idea of two regimes – one dominated by the direct wave and one by the coda – and a transition from one to the other akin to a liquid changing state as the geological model is varied smoothly.

(1) The use of Maxwell-Boltzmann statistics, (2) the use of the OA model (which produces only an approximation of the transmitted pulse), and (3) the identification of the OA model as providing an estimate of the degeneracy, are the three main assumptions in this calculation. They are each justifiable in their own way, but each are ultimately assertions, and each could be replaced with something else and produce a different result. Any set of assumptions which, as the lag grows, allows a rapidly increasing number of raypaths to contribute, should be expected to produce something at least qualitatively similar.

ACKNOWLEDGEMENTS

The sponsors of CREWES are gratefully thanked for continued support. This work was funded by CREWES industrial sponsors, NSERC (Natural Science and Engineering Research Council of Canada) through the grant CRDPJ 543578-19, and in part by an NSERC-DG.

REFERENCES

Kittel, C., 1969, Phase transition of a molecular zipper: American Journal of Physics, **37**, 917.

Margrave, G. F., and Lamoureux, M. P., 2019, Numerical methods of exploration seismology with algorithms in MATLAB: Cambridge University Press, 1st edn.

O'Doherty, R. F., and Anstey, N. A., 1971, Reflections on amplitudes: Geophysical Prospecting, **19**, 430–458.

Sears, F. W., 1959, An introduction to thermodynamics, the kinetic theory of gases, and statistical mechanics: Addison-Wesley Publishing, 4th edn.

Taner, M. T., Koehler, F., and Sheriff, R. E., 1979, Complex seismic trace analysis: Geophysics, **44**, No. 6, 1041–1063.