Identifying Ideal Stratigraphic Cycles Using a Quantitative Optimization Method

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Abstract

The ideal cycle concept is poorly defined yet implicit and potentially useful in many stratigraphic analyses. A new method provides a quantitative definition of ideal cycles, and a simple, robust method to analyse stratal order and quantify stratigraphic interpretations. The method calculates transition probability (TP) matrices from a vertical succession of strata for all possible permutations of facies class row numbering in the matrices. The ordering of facies classes that gives highest transition probabilities along a diagonal of the TP matrix can be taken as a quantitative definition an ideal cycle for the strata being analysed. Application to a synthetic example shows how an ideal cycle can be identified, even in noisy strata, without any assumptions about or knowledge of cyclicity. Application of the method to two outcrop examples shows how it can be useful to define the most optimal cycle and determine how much evidence is present for ordered and cyclical strata.

Introduction

In stratigraphic analysis there is a long history of attempts to identify cyclical strata based on bed-by-bed analysis of facies successions (Miall, 2010), but so long as methods are qualitative and poorly defined, progress in understanding facies cyclicity will be limited. Understanding what order and cyclicity are present in strata is fundamentally important because strata record the history of Earth surface processes, including long term climate change. Identification of order and cyclicity can help resolve patterns of Earth surface processes. Understanding order and cyclicity is also important for predictive models of stratal heterogeneity, useful for example in evaluation of subsurface water and hydrocarbon resources.

In the context of a succession of sedimentary facies, a cycle is a series of connected events, for example depositional facies, which return to a particular starting point (Schwarzacher, 1975; Goldhammer, 2003;). Parasequences and high-frequency sequences are examples of cycles, often defined on the basis of facies, indicating depositional environment linked to changes in external forcing factors such as relative sea-level or climate change (e.g. Catnuneanu, 2006). This approach is a continuation of much older ideas of an ideal cycle (Duff and Walton, 1962; Duff et al. 1967). Identifying characteristic or idealised cycles has often been based on an optimistic assumption that underlying order is present, even if partly or mostly obscured by noise (Pearn, 1964; Schwarzacher, 1975; Burgess, 2006), with a few notable more quantitative exceptions (e.g. Powers and Easterling, 1982; Xu and Maccarthy, 1998, and see techniques described in Sadler, 2004). This paper introduces a method to quantitatively define ideal cycles as the arrangement of facies classes in a vertical succession that best represents any ordered cyclical repetition of facies present. This optimised most cyclic arrangement of facies classes can be used to determine the degree of evidence present for order in the strata.

Identifying order using transition probability matrices

Burgess (2016) presented a method to calculate the degree or order present in a vertical succession of strata by constructing a facies transition probability (TP) matrix T (Fig 1) and calculating a value *m* that summarises the matrix structure.

$$m = argmax_{j=1..F-1}\left\{\frac{\sum diag(T_j) + \sum diag(T_{-(F-j)})}{F}\right\} - argmin_{j=1..F-1}\left\{\frac{\sum diag(T_j) + \sum diag(T_{-(F-j)})}{F}\right\}$$

where *F* is the number of facies classes, in this case 5, *j* is the offset value from the main matrix diagonal, *diag* is a function to find all elements in a diagonal of *T* with offset *j*, and *argmin* and *argmax* are mathematical functions to find the minimum and maximum values in a series composed ofall cells in the *j*th offset diagonal (Burgess, 2016). The value *m* ranges from 0 (perfectly disordered) to 1 (perfectly asymmetrically cyclical) and usefully summarizes the degree of order present in a TP matrices constructed from a facies succession. Comparison between *m* from the observed strata and *m* calculated for TP matrices from many shuffled realizations of the same strata indicates how ordered or otherwise the strata are.

Very importantly, the *m* value calculated for a TP matrix depends on how facies classes are numbered and therefore how they are arranged in the matrix rows and columns. This dependence can be used in an optimization process to show what arrangement of facies classes best represents any cyclicity present in the strata.

Identifying an Ideal Cyclothem: A Synthetic Example

Matlab code to perform the analysis described below and worked examples are available from the GSA data repository entry number ###.

A synthetic example of a plausible perfectly cyclical facies succession (Fig. 1B) starts with medium sandstone, passes upwards into fine sandstone siltstone, limestone and mudstone, then repeats. If row numbering in a TP matrix constructed from these strata reflects this cyclicity, such that the row order for the facies classes in the TP matrix is the same as the order of the facies classes in the cycles, then the transition probabilities in the j=1 j=-4 TP matrix diagonal would be 1, and the m value for the matrix would be 1 (Fig. 1A) (Burgess, 2016). However, different row orders for the facies classes may lead to lower values of m. Note that the stratal succession does not change with different row orders, only the facies numbering and therefore which row in the TP matrix each facies class occupies.

Knowing the nature of the cyclicity *a priori* would allow facies coding and therefore row order for the TP matrix to be selected to best represent the cyclicity, to generate a TP matrix with the highest probabilities aligned along the j=1 j=-4 matrix diagonal, and a m value as close as obtainable to one. However, to avoid *a priori* assumptions about the cyclicity thought to be present, all possible facies class codings can be explored to determine which produces the TP matrix or matrices with the greatest number of the highest transition probabilities aligned along the j=1 j=-4 offset diagonal. For n facies classes there are factorial n (n!) possible arrangements of the facies classes on the TP matrix rows and columns, so for $n \leq 10$ it is computationally inexpensive (i.e. minutes) to calculate all of the TP matrices to find those with the highest m values. Note that for n>10 a refined algorithm or a powerful computer will be required.

To demonstrate how this method works a synthetic 15m thick succession of strata composed of fifty lithological units classified as five distinct facies (Fig. 1B) has been analysed. The succession was generated initially with a perfectly cyclical arrangement of facies, as described above, but then random variation was introduced by changing the lithology of ten units distributed approximately evenly through the succession. The result is a succession of synthetic strata containing five lithofacies that are variable in terms of their up-section transitions, but which nevertheless appears to show some evidence for cyclicity. For example, at 7m and 10m in the vertical succession, there are clear fining-upward arrangements of facies from medium sandstone to mudstone, and at 13m there is also a clear coarsening-upward arrangement of facies (Fig. 1B). If observed in nature caution would be necessary because such apparent order can arise by chance, requiring careful comparison with random models (Burgess, 2016). Here however we know the origin of the strata, so it is possible to assess how remnant cyclicity present in the synthetic strata can be extracted despite being obscured by imposed noise.

Calculating a TP matrix for the strata based on a facies coding and row ordering that does not reflect the cyclicity present in the strata (Fig. 1D) generates a m statistic of 0.199. This low m value occurs because there is little concentration of highest probabilities on the offset-one diagonal of the matrix (Fig. 1C). Calculating TP matrices for all 5! 120 row ordering permutations of the TP matrix shows that 5 of 120 permutations have the highest m values of 0.679 arising from high transition probability values concentrated along the j=1 j=-4 offset diagonal (Fig. 1E). These 5 permutations all have an arrangement of facies classes (Fig. 1F) that is the same as the order in the fining-upward cycle originally defined in these synthetic strata before the random noise was added.

This example demonstrates how this method can extract the most cyclical arrangement of facies classes from synthetic strata, even when the strata include a substantial random component. The arrangement of facies classes extracted in this way can be considered an optimised, or ideal cycle. The next section shows how the method can be applied for the same purpose to outcropping vertical successions, or to vertical succession from boreholes.

Identifying an Ideal Cycle: Outcrop Examples

Pennsylvanian siliciclastic strata, Illinois – order revealed

Pennsylvanian (Upper Carboniferous) strata around the world have been repeatedly interpreted as cyclical and forced by glacioeustasy, and were one of the original sources of the concept of an ideal cycle (Duff and Walton, 1962; Duff et al. 1967; Olszewski and Patzkowsky, 2003). Pennsylvanian strata in the continental USA include classic sections in Illinois studied by Weller (1930) and interpreted as cyclical. Wanless (1957) logged ~70 m of strata composed of 48 lithofacies units and ten distinct lithofacies classes, (Fig. 2A). Lithofacies analysis defined an ideal cycle with an overall fining-upward pattern, passing from terrestrial to marine deposition (Fig. 2B). More recently Wilkinson et al. (2003) and Burgess (2016) suggested via two independent quantitative analyses of the observed facies succession that there is not strong evidence to support this interpretation; an *m* value of 0.187 fell within the range generated from the randomly shuffled strata giving a probability (*p)* value of 0.6, providing no evidence for order in the strata.

Strata from Wanless (1957) are reanalysed here to calculate optimized transition probability matrix permutations. Initial lithofacies coding and hence initial matrix row positions are as defined by the ideal cycle of Wanless (1957) shown in Wilkinson et al. (2003) (Fig. 2B) except that three intervals of no exposure have been assumed to be a continuation of the fine-grained lithology either above or below. Analysis of the vertical succession as logged gives a *m* value of 0.206 (Fig 2C&D), slightly higher than the value of 0.187 given in Burgess (2016) which did not re-code the intervals of no exposure. Since there are 10 lithofacies there are 3628800 facies arrangement permutations. For each permutation a TP matrix and associated *m* value was calculated. Of the 3628800 permutations tested, ten showed maximum *m* values of 0.489 arising from high probabilities concentrated along the j=1 j=-4 offset diagonal (Fig. 2E). Although each of these ten permutations has a different row numbering for the facies classes, the order of facies classes is the same (Fig. 2F). These permutations could represent a quantitatively derived definition of the ideal cycle for these strata.

The Wanless (1957) ideal cycle (Fig 2B) and this optimized version have similarities; the first five facies in both cycles are identical, with the same transitions through sandstone to coal in each case. Differences arise in the limestones and shales where optimization has identified the highest transition probabilities. Carrying out the same analysis previously performed in Burgess (2016) but using the optimised facies ordering gives a *m* value of 0.489. This lies well outside the range of *m* values generated from randomly shuffled otherwise equivalent successions (Fig. 2G), leading to a *p* value of 0.0 which indicates that the observed arrangement of strata is unlikely to occur by chance so can be considered to contain significant order. This demonstrates how application of this new method, in combination with the comparison against randomly shuffled successions (Burgess, 2016), can work well to identify ordered strata.

Santonian carbonate strata, northern Spain – disorder prevails

Carbonate strata in the Rio Carreu river gorge on the flanks of the San Corneli anticline in the Spanish Pyrenees have been previously interpreted by Pomar et al. (2005) as “simple sequences and parasequences according to internal lithofacies arrangement and inferred sea-level cyclicity”. Pomar et al. (2005) defined these stratal units on the basis of “persistent occurrence of lithofacies grouped into two facies assemblages” defining rudist buildups that form parasequences and sequences (Figure 5 in Pomar et al., 2005). Subsequent analysis Burgess (2016) showed no evidence of preferred transitions between facies, suggesting no preferred arrangement of lithofacies and hence raising doubts about identification of sequences and parasequences on that basis.

The Rio Carreu vertical succession is 163m thick, with 61 stacked facies units composed of 6 distinct lithofacies classes (Pomar et al., 2005; Burgess, 2016) (Fig. 3A). The top 80m of the succession is composed of alternations of just two facies representing more distal strata, so this analysis is limited to the lower 80m that represent platform margin strata interpreted as cyclical by Pomar et al. (2005). Construction of a TP matrix for these strata following the facies coding from Burgess (2016) gives a m value of 0.242 which is well within the range of what is likely to occur by chance (Fig 3F). Since there are six distinct lithofacies there are 6! or 720 possible permutations for TP matrix row numbering. Calculating these 720 TP matrices shows that the highest m value of 0.291 occurs in 48 permutations, of which 18 have a highest sum concentration of probabilities along the j=1 j=-4 offset diagonal.

A key difference with the previous Pennsylvanian cyclothem example is that in this case the *m* values are lower because transition probabilities in the optimised matrices are lower. Certain transitions occur more frequently than others in these 18 optimised arrangements, for example sheetstone to benthic-foraminifer-rich grainstones, and rudist grainstone to pillarstone. However, overall each of the 18 optimal facies arrangements are different, so it is not possible to identify any single ideal cycle (Fig 3C, D and E). Analysing the Rio Carreu strata encoded with one of the optimized facies codings (Fig. 3C) gives an *m* value that falls within the range of *m* values generated by randomly shuffled but otherwise equivalent strata (Fig. 3F), giving a *p* value of 0.201 and providing no evidence for order in the strata. In this case the optimization process supports the original analysis in Burgess (2016) that cast substantial doubt on the interpretations of ordered vertical successions of strata presented by Pomar et al. (2005).

Conclusions

1. This new method defines optimised or ideal cycles using quantitative analyses of a vertical facies succession to identify the most ordered cyclical repetition of facies present in strata.
2. The analysis is an optimization method calculating all possible permutations of TP matrices, given different facies codings and hence facies class row ordering in the matrices. Permutations with the highest *m* values arising from concentrations of high transition probabilities along the j=1 j=-4 offset diagonal of the TP matrix indicate facies codings representing the most ordered arrangement of facies classes in the TP matrix, and may define an ideal cycle.

3. Application to two outcrop examples shows how the method can be useful either to reveal order that was previously not apparent, or to demonstrate a lack of evidence for order.
4. Since robust identification of order in strata provides key evidence to underpin interpretations of controls on strata, for example climatic or relative sea-level variations, this new method should be a useful quantitative addition to sequence stratigraphic analysis.

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Figure Captions

Figure 1. **A.** A TP matrix for perfectly ordered cyclical strata. Transition probabilities are shown in each cell; the top left cell shows the probability of a transition from mudstone (mst) to medium sandstone (msst). The *j* values indicate the offset of matrix diagonals from the main matrix diagonal. Cells on the main diagonal do not contain probability values because no transitions are allowed between the same facies in this method. Note the offset-one diagonal cells (j=1) contain probability values of 1 because this is a TP matrix for perfectly cyclical strata. **B.** The15m thick synthetic succession composed of 50 lithofacies units classified into five facies classes was generated as perfectly cyclical repetitions of the five classes, but random variation was added, with on-average 1-2 out of order facies units occurring in each cycle. An arbitrary start point defines cycles as medium sandstone (msst), fine sandstone (fsst) siltstone (slt), limestone (lst), mudstone (mst), and repeat. Resulting strata are variable in terms of up-section transitions, but still show some evidence for cyclicity. **C.** A TP matrix calculated for the succession with facies ordering shown in **D.** The matrix has a low *m* value of 0.199 because high transition probability cells are not aligned along a *j*=1 *j*=-4 diagonal. **E.** In contrast, one of the five permutations of the facies coding that aligns high transition probabilities along the j=1 j=-4 diagonal leading to a higher *m* value of 0.679. The facies class arrangement (**F**) represents the most cyclical order present in the strata, successfully revealed by the optimization method.

Figure 2. **A.** Pennsylvanian strata from section number 5, Sangamon River in Illinois, from Wanless (1957). Eleven distinct lithofacies are recognized in the strata, including clean sandstones, sandy shales, shale, coal, and both freshwater and marine limestones. These

facies classes can be arranged in an ideal cycle (**B**) according to Wanless (1957). Using this ordering (**D**) generates a transition probability matrix (**C**) with little concentration of high probabilities on any diagonal and consequently *m*=0.206. (**E**) is the TP matrix from one of 10 permutation generated by the optimization process with an *m* value of 0.489 due to a concentration of high transition probabilities along the offset-one diagonal. **G.** When tested against randomly shuffled versions of the same strata this facies coding (vertical red line) reveals good evidence for order in the strata, suggesting the facies class order shown in **F** can be considered optimum for this succession.

Figure 3. **A.** A vertical section from Santonian carbonate strata in the Rio Carreu river gorge, northern Spain, showing six facies classes described in Pomar et al. (2005). Wpst is wackestone-packstone, bfgst is benthic foram grainstone, shst is coral-sponge-rudist sheetstone, mxst is coral-rudist mixstone, pillst is dense hippuritid pillarstone, and rgst is rudist bearing grainstone. **B.** TP matrix calculated using the facies class order indicated by Pomar et al. (2005) has a low *m* value of 0.242 and highest probability values are not clustered on the j=1 j=-4 offset diagonal. In this case, a random selection of the 18 TP matrices showing the highest *m* values with the most j=1 j=-4 offset diagonal clustering from the 720 possible row ordering permutations (**C**, **D**, and **E**) have *m* values of only 0.291, show little clustering on the j=1 j=-4 offset diagonal, and all show different vertical arrangements of the facies. **F**. Comparing one of the highest scoring facies class orders (vertical red line) with randomly shuffled versions of the strata coded in the same way indicates that the strata fall within the range of successions that could occur by chance, confirming that there is no evidence from this analysis for order in these strata.

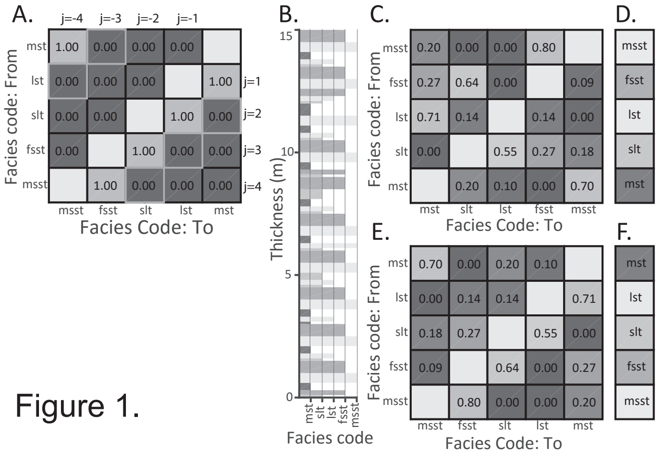
A.
j=-4
j=-3
j=-2
j=-1
j=1
j=2
j=3
j=4
Facies code: From
Facies Code: To
B.
Thickness (m)
Facies code
C.
Facies code: From
Facies Code: To
D.
E.
Facies code: From
Facies Code: To
F.

Figure 1.

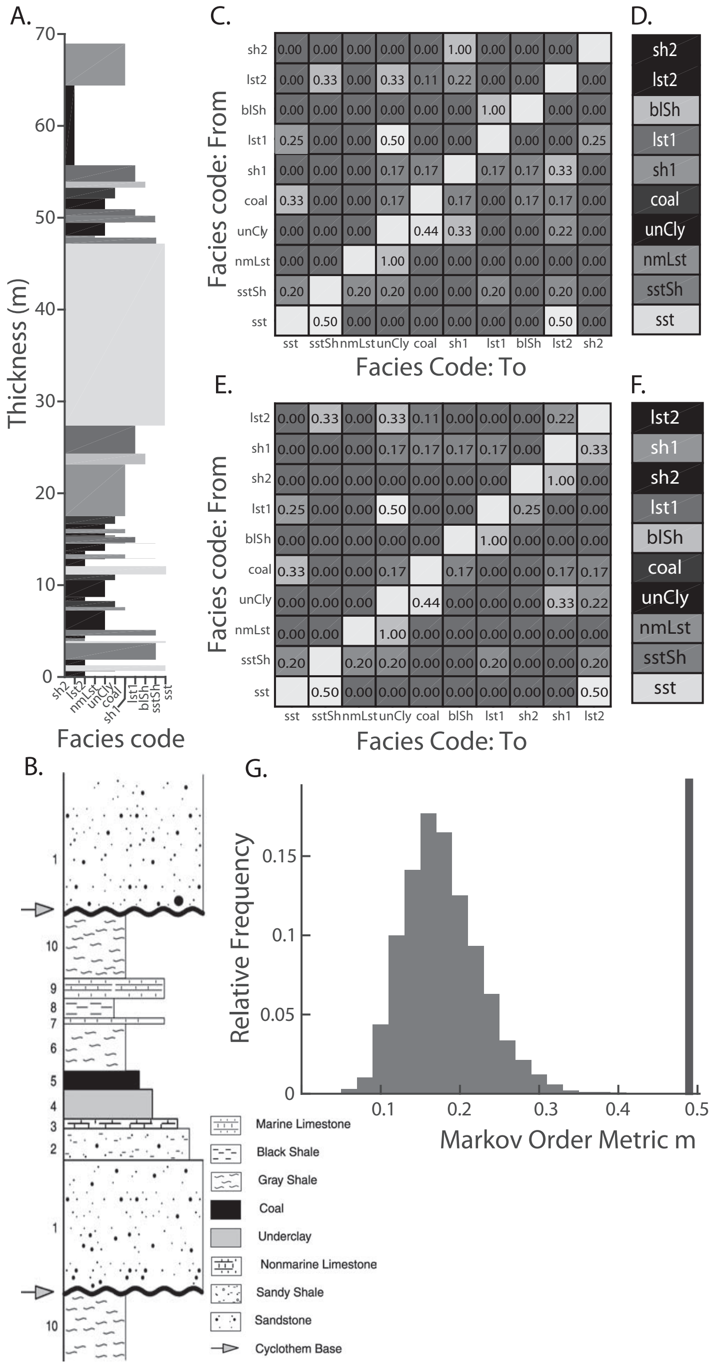
A.
Thickness (m)
Facies code
sh2 lst2 nmLst unCly coal sh1 lst1 blSh sstSh sst
C.
Facies code: From
Facies Code: To
sh2 lst2 blSh lst1 sh1 coal unCly nmLst sstSh sst
D.
E.
F.
lst2 sh1 sh2 lst1 blSh coal unCly nmLst sstSh sst
B.
Marine Limestone
Black Shale
Gray Shale
Coal
Underclay
Nonmarine Limestone
Sandy Shale
Sandstone
Cyclothem Base
G.
Relative Frequency
Markov Order Metric m

Figure 2.

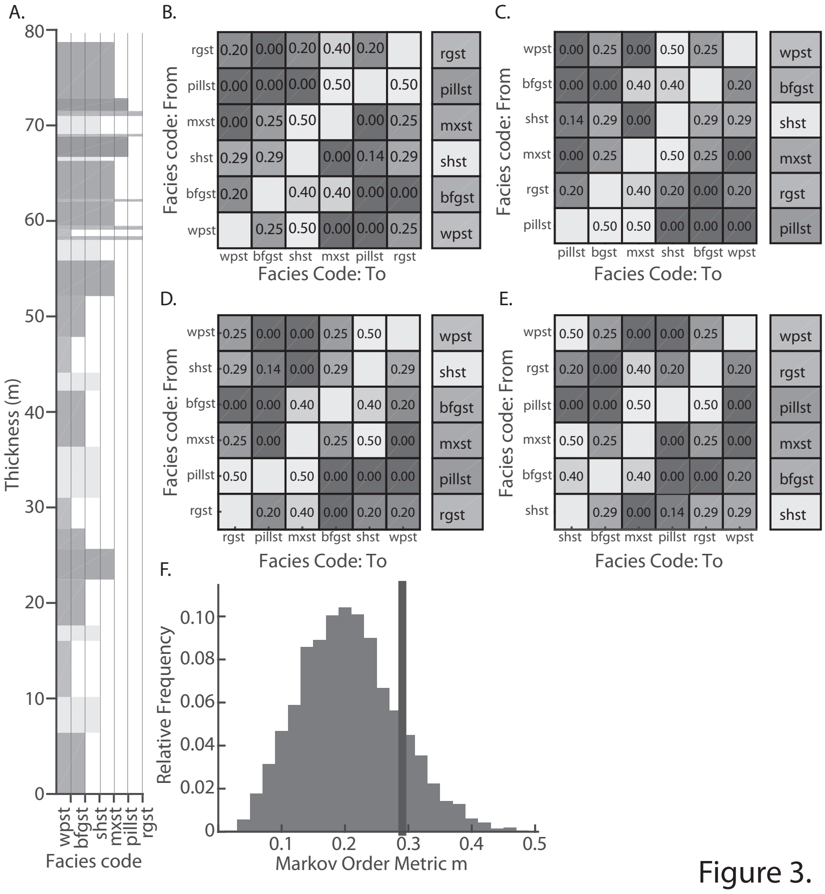
A.
B.
C.
D.
E.
F.
Thickness (m)
Facies code
Facies code: From
Facies Code: To
Relative Frequency
Markov Order Metric m

Figure 3.