Nonlinear and dynamical models for temperature reconstructions from multi proxy data in bivalve shells

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The fact that bivalve shells that are sampled from the same environment show almost the same chemical signature, suggests that such shells properly record their environment and thus offer potential to reconstruct the paleo-environment. Many efforts have been made to understand the link between the chemical signatures of the shells and their environment. Although we now have some insights in these processes, accurate temperature reconstructions are still not possible. The main problem is the fact that the incorporation of different proxies is influenced by a set of different environmental parameters for a given point in time.
In this work several approaches have been proposed to improve the temperature reconstructions. In a first instance we hoped that the combination of several proxies in a multi-proxy model would help to resolve the influences of the different environmental parameters. Even though the first results based on linear multiple regression were promising, clear nonlinear proxy environmental relationships observed in some datasets encouraged us to explore the potential of nonlinear multi-proxy models and dynamical models. At first the introduction of nonlinear models seemed to have improved the reconstructions significantly. However, this appeared to be an artifact, due to the fact that the nonlinear models used normalized data. It turned out that a similar improvement could be achieved by normalizing the data before doing a linear multiple regression analysis. The introduction of dynamical models appeared to improve model performance even more than the use of multi-proxy models.
The main achievements in this work are summarized in Fig. 1 where the model performances of the most important model types are given in root mean squared errors (RMSEs). Fig. 1 shows how the linear static models based on raw data that are generally used in sclerochronology can be improved by introducing: multi proxy models as done in Chapter 1, nonlinear models as done in Chapter 2, and dynamical models as done in Chapter 4. On the other hand the figure shows that the optimization of the proxy combination introduced in Chapter 3 and used in Chapter 5, may result in worse reconstructions.
Fig. 1 clearly quantifies the improvements achieved by the different steps made in this work and makes clear that the **best reconstructions are obtained by linear dynamical models that use Mg-information**. In the following sections every important step in this work is disused individually.

		Static		Dynamic	
		Raw data	Norm. data	Raw data	Norm. data
Mg	Linear	4.12 Lit	2.43	5.44	1.34 Ch4
	Nonlinear	3.35	2.67	4.88	1.35
MgSrBaPb	Linear	Ch1 2.45	2.21	3.96	1.37
	Nonlinear	2.87	Ch2 2.19	14.79	3.34
Best comb	Linear	MgSrBaPb: 2.45	MgSrPb: 1.96	MgSr: 5.67	Ch5 MgPb: 1.42
	Nonlinear	MgSrBa: 3.05	MgBaPb: Ch3 2.34	Pb: 2.66	MgPb: 1.07

Fig. 1. In order to show how much the temperature reconstructions could be improved in this work, the model performances in RMSE (in ˚C) are given for different model types. The static linear Mg model obtained on raw (not-normalized data) is considered as the best reconstruction before this work. The arrow 'Ch1' represents the introduction of multi-proxy models in Chapter 1. The arrow 'Ch2' represents the introduction of nonlinear models in Chapter 2. The arrows 'Ch3' and 'Ch5' represent the proxy optimization process described in Chapter 3 and 5. The arrow 'Ch4' represents the introduction of dynamical models in Chapter 4.

1. The use of multi-proxy models
Two reasons are presented to promote the use of multi-proxy models. (1) The first one was algebraic and indicated that when the incorporation of a proxy is influenced by several environmental forcers, the environmental parameters themselves can only be described by a combination of proxies. (2) The second reason was statistical and stated that the uncertainty on a measurement is lower when more measurements are combined.
Along this work it became clear that the second reason is of higher importance. Since the improvement on the temperature reconstruction was higher by multiplying the data of one proxy than by measuring additional proxies, we have to conclude that the best improvements on temperature reconstructions are not obtained by combining proxies into a multi-proxy model.

2. The use of dynamical models
The introduction of dynamical models appeared to be much more powerful than expected (up to 2 °C in RMSE sense). Three reasons can be put forward to explain these improvements: (1) more data can be used for a reconstruction, resulting in a lower uncertainty, (2) future and past proxy data coupled to one temperature measurement during the training of the model could have reduced errors made for the unknown shell growth, and (3) the more flexible time basis can pull initially more complex proxy environmental relationships towards a linear model. The latter fact can explain why the reconstructions obtained by linear dynamical models are satisfying, even though the relationship between the proxies and their environment is clearly nonlinear.

3. The use of nonlinear models
The observation that several proxy-environmental relationships showed substantial nonlinearities encouraged the use of nonlinear models for temperature reconstruction. However, we observed that linear models performed equally if not better than nonlinear models provided both models are based on normalized data. The failure of the nonlinear models is caused by extrapolation errors: when proxy signatures of the validation data are (slightly) different from the training data, the reconstructions often show very large errors (RMSEs up to 700 °C). For more robust nonlinear models a larger training dataset should be used, solving these extrapolation problems: the more information is given in the training set, the more information is incorporated in the model and the fewer the number of extrapolations that have to be carried out during the reconstructions.

4. The use of normalized data
An important observation is the fact that the use of normalized data has a major positive impact on the reconstruction performance of all models. The overall pattern of a proxy signal appeared to be more informative than elemental concentrations or ratios. Non-normalized elemental ratios often show site specific concentration shifts or amplitude differences, which are incorrectly interpreted as temperature differences. As a result, models based on non-normalized elemental ratios are site specific and cannot be used for wider environments, which is not the case for models based on normalized data that appeared to be very generic.

5. About the proxies
A large part of the work presented in this thesis is based on the combination of two datasets that are originally published by Vander Putten *et al.* (2000) and Gillikin *et al.* (2006a). In the studied datasets four proxies were available: Mg/Ca, Sr/Ca, Ba/Ca and Pb/Ca ratios. The Mg/Ca-ratios appeared to be the most powerful temperature proxy, which confirms conclusions in the current sclerochronology literature. However, tests using the models on other species showed that models based on calcite Mg/Ca-data cannot be extrapolated to on aragonitic shells. On the other hand, we did observe that Ba/Ca ratios carry a lot of temperature information, but because the Ba/Ca ratios show to be much more site specific, the proxy cannot be extrapolated to a wide variety of environments. Pb/Ca and Sr/Ca do not carry a lot of temperature information, but combining them with Mg/Ca-ratios appears to be successful in some cases. The combination of Mg/Ca ratios with the other elemental rations can help to explain the variation in the proxy-signals. It is likely that the Sr/Ca ratios and Ba/Ca ratios explain the variations in Mg/Ca ratios that are coupled to shell growth, or to salinity variations. On the other hand Pb/Ca ratios may explain some metabolic or ontogenetic variations.