

Unravelling pre-eruptive P-T conditions by machine learning

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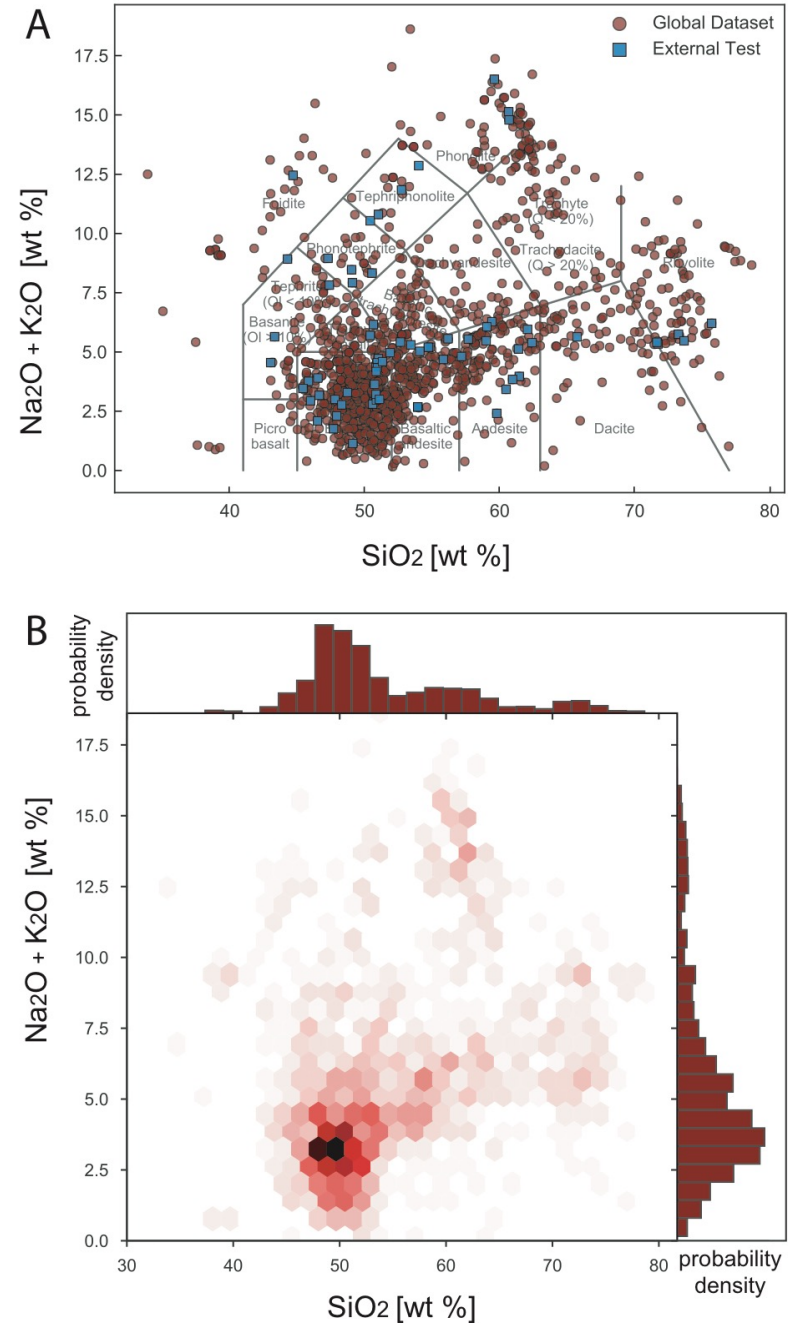
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We introduce a new approach, based on Machine Learning, to estimate the pre-eruptive temperatures and storage depths using clinopyroxene-melt pairs and clinopyroxene-only chemistry.

The method is calibrated for magmas of a wide compositional range, it complements existing models, and it can be applied independently of tectonic setting.

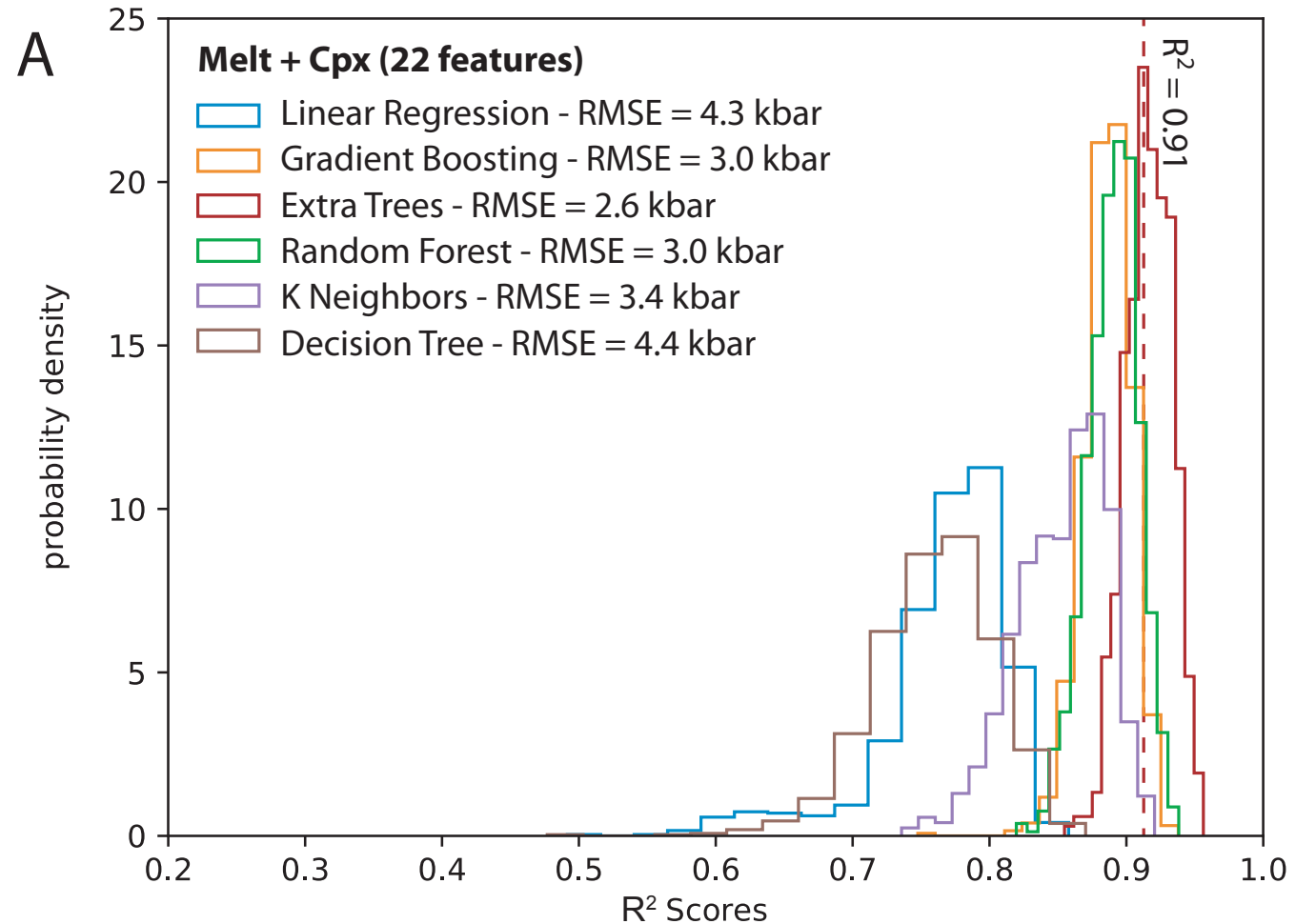
After the validation process, performances are assessed with test data never used during the training phase. We estimate the uncertainty using the Root Mean Square Error (RMSE) and the coefficient of determination (R^2).



Validation process on Pressure estimations

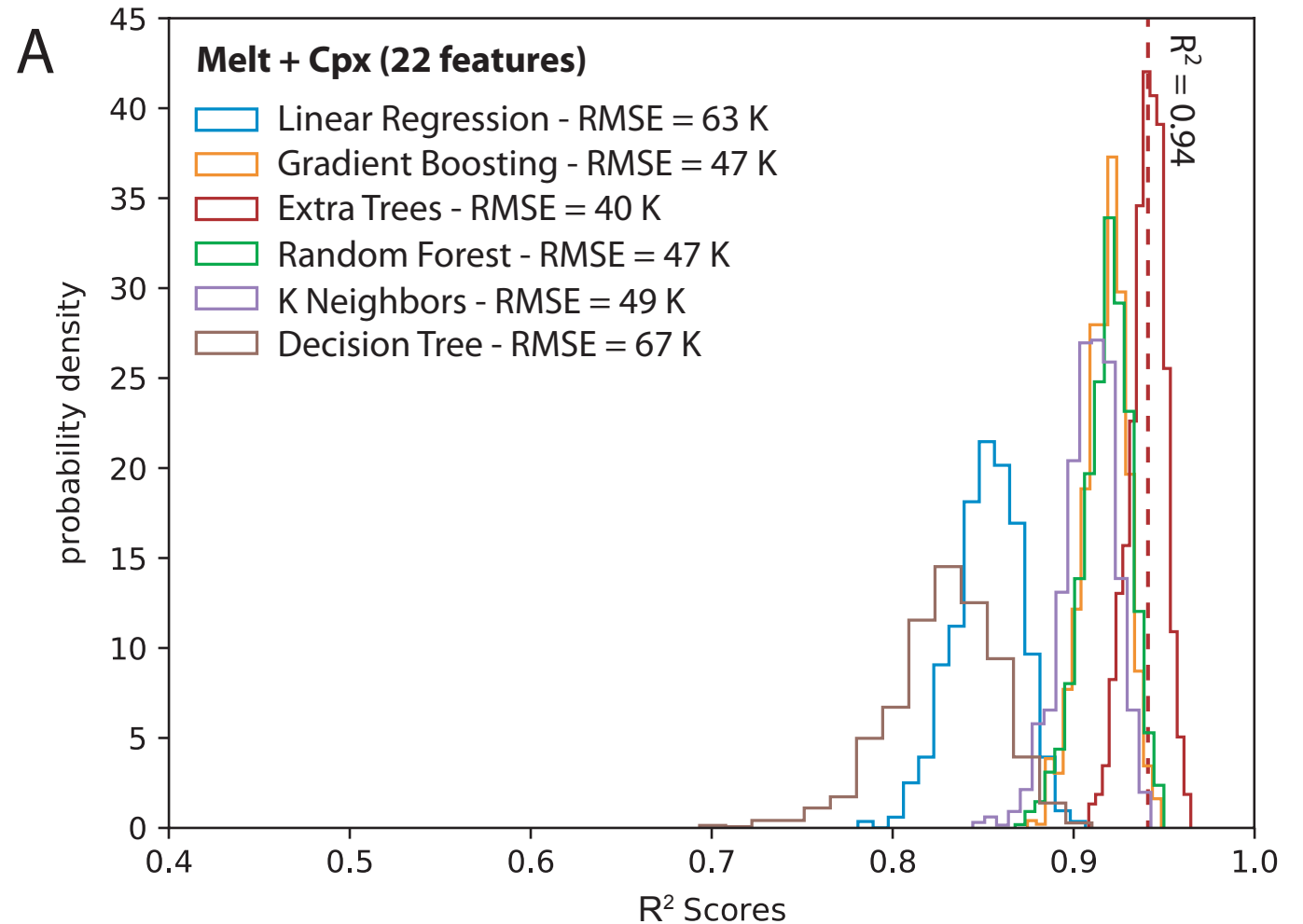
The Extra Tree Regression technique (ETR; Geurts et al., 2006) is the best performing ML algorithm, with a R^2 probability density distribution characterized by a modal value equal to 0.91 and a RMSE value of 2.6 kbar.

The modal R^2 of other ML algorithms presented here ranges between 0.7 and 0.9, with the RMSE of 3-4.4 kbar.



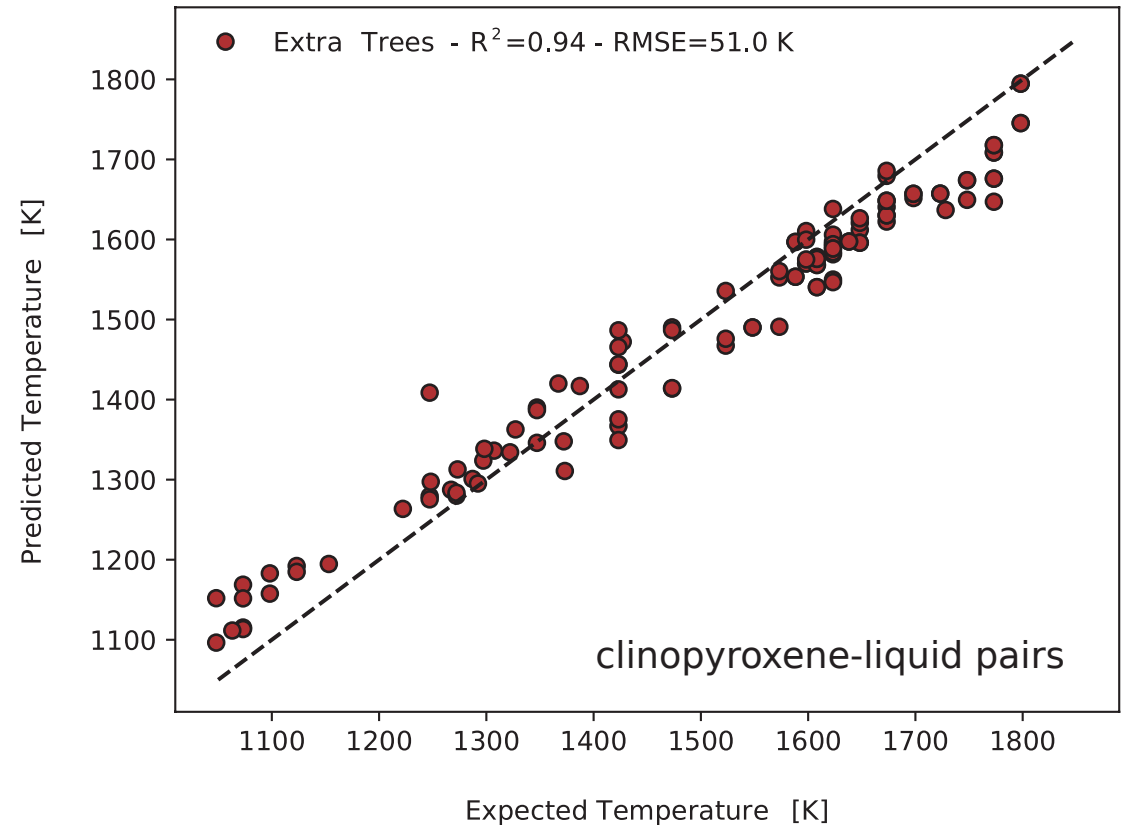
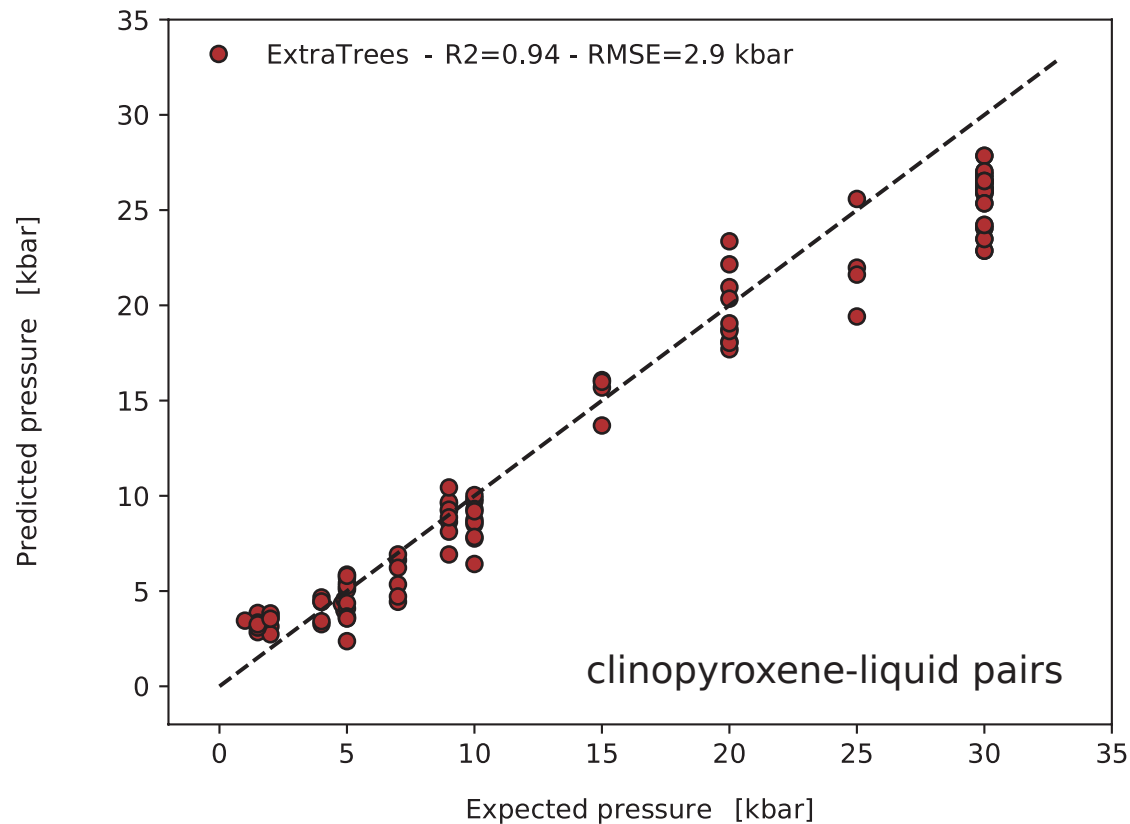
Validation process on Temperature estimations

As for the pressure estimates, the Extra Tree Regression technique shows the best distribution of R^2 , with a modal value of 0.94 and a RMSE equal to 40 K (Fig. 3A)



Independent test on Pressure and Temperature estimations

The good pressure and temperature predictive performances of the ETR is confirmed by its application to the test dataset, which was never used during the training and validation phase. Figures below highlight R^2 scores for the ETR algorithm of 0.94 for both pressure and temperature estimates with RMSEs of 2.9 kbar and 51, respectively.



Conclusions

We reported a new approach based on Machine-Learning to estimate pre-eruptive temperatures and pressures. The approach does not assume any *a-priori* knowledge of chemical exchange between the crystal and the carrier melt.

Our results highlight that this approach can be applied on a wide compositional range.

It complements existing models and can be used as an independent check to validate the results obtained by current calibrations based on the thermodynamic of the system.