# Modélisation en Géochimie

Questions for the part of C. Le Losq, 15 November 2021.

**Answers should be brief and to the point, no more than 4 sentences. Read the question several time prior to replying anything.**

## Context

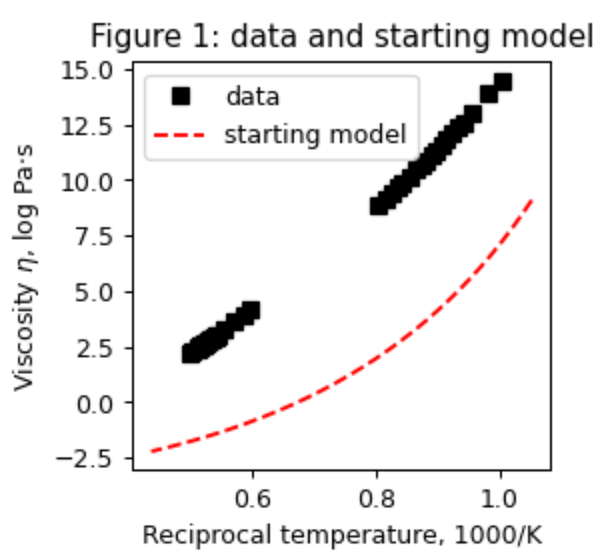
Melt configurational entropy $S^{conf}(T)$ (J mol$^{-1}$ K$^{-1}$) at temperature T (K) drives melt viscosity $\eta$ (Pa·s). It is equal to

$S^{conf}(T) = S^{conf}(T_g) + \int_{T_g}^{T} C_p^{conf}(T)/T dT$ , (eq. 1)

with $S^{conf}(T_g)$ the configurational entropy at the glass transition temperature $T_g$ , and $C_p^{conf}(T)$ (J K$^{-1}$) the melt configurational entropy at T. For silicate melts, $C_p^{conf}(T)$ can be calculated or measured. However, it is difficult to know $S^{conf}(T_g)$. Fortunately, $S^{conf}(T_g)$ can be calculated from viscosity measurements, solving an inverse problem. The direct mnodel is:

$\log \eta(T) = A_e + \frac{B_e}{TS^{conf}(T)}$ , (eq. 2)

with $A_e$ and $B_e$ adjustable parameters. $S^{conf}(T_g)$ is also considered as an adjustable parameter. For molten albite, a composition critical for granites, one can use published data and eq. 2, with starting values $A_e$ ~ -3.5, $B_e$ ~ 10 000 and $S^{conf}(T_g)$ = 9 +/- 2 J mol$^{-1}$ K$^{-1}$, to get the following figure.




Different methods allow adjusting $A_e$, $B_e$ and $S^{conf}(T_g)$, given a dataset composed of $i$ datapoints $\eta_i$.

#### Question 1

**Among the following propositions, which criterion could you use to adjust those parameters?**

*Choose the good answer. Several are possible.*

Answer A : $\min \sum_i (\eta_i - \eta_i^{\text{model}})^2$

Answer B : $\min \sum_i (\eta_i - \eta_i^{\text{model}})$

Answer C : $\min \sum_i \text{abs}(\eta_i - \eta_i^{\text{model}})$

*Note:* abs *corresponds to the notation for absolute value, and* min *for minimum.*

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#### Question 2

**Give the name(s) of the criterion(s) you selected.**

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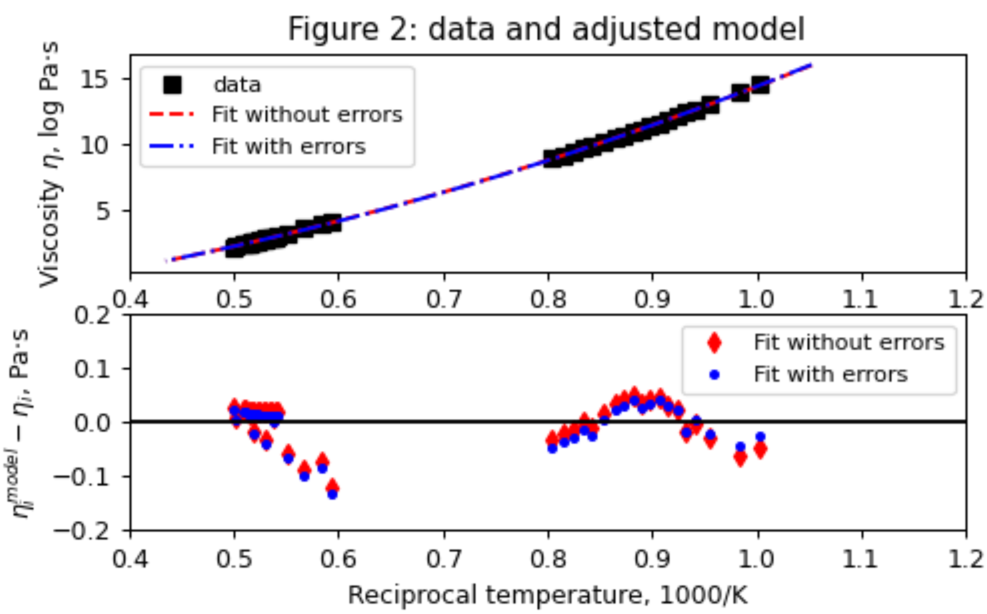
After fighting with the documentation of `scipy`, one founds that he can use the function `curve_fit` to adjust model parameters. One finds out that data errors $\sigma_i$ can be provided to `curve_fit`. Using errors or not result in slightly different results, as visible in figure 2.

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#### Question 3

There is no real significant visible difference between the two results. The user may actually think that the fit without data errors is better. **Is that a good thinking? Justify your answer. How data errors are taken into account by a criterion like least squares? (tip: write the equation)**

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#### Question 4

Looking online, one finds that errors affecting model parameter can be better explored (sometimes) with Markov-Chain Monte Carlo (MCMC) methods. However, those methods involve changing the paradigm regarding how one considers adjusting model variables.

**What MCMC methods actually do? Why they can provide better estimations of errors on model parameters, particularly in the case of strongly non-linear problems involving many parameters?**

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### Question 5

**For each affirmation, indicate if it is True or False. If you think precisions are necessary, add a one sentence comment.**

a) The log posterior probability of the model is the sum of the model log likelihood and the model log prior probability.

b) The model prior probability is always a multidimentional Gaussian distribution.

c) Covariance of model parameters is critical for calculating uncertainties on model predictions.

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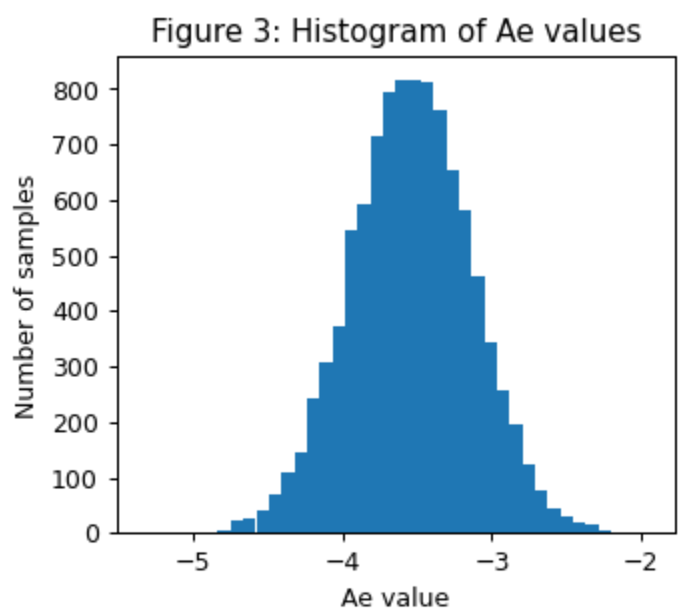
### Question 6

For the $A_e$ parameter, one finds a value of -3.56 log Pa·s with `curve_fit` , which could be considered as the "best" value. With MCMC methods, one finds 10000 possible values forming the histogram visible in figure 3. **What is this histogram representing?**

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### Question 7

Our user thinks that, given this histrogram, a model with Ae = -3.0 is worse than one with a value of -3.5. **Is this reasonning valid ? Justify your answer.**

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**Question 8**

**What other method can allow us to get an estimation of the above histogram? Add a brief description of what this method does.**

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**Question 9**

One knows that the Hamiltonian Monte Carlo method may be quite good at exploring the model space, but have no idea about how to implement them. **What should the user do?**

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**Question 10**

A user wrote a Metropolis Hasting MCMC algorithm to fit the above data. However, the algorithm is behaving weirdly, it is not converging toward the answer at all, as shown in the figure below. The acceptance rates are very low, well below 10%.

**What hyperparameters should be tuned to improve convergence ? What typical values of the acceptance rates the user should aim at?**