

**Subject:** RE: Fitting Bayesian models to Wang & Engel  $f(x)$ s  
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**Date:** 11/5/18, 12:42 AM  
**To:** "e.wolkovich@ubc.ca" <e.wolkovich@ubc.ca>  
**CC:** Lizzie Wolkovich <wolkovich@fas.harvard.edu>

Dear Lizzie,

I am happy to hear from you.

I am just back from the east coast where my student Dan completed his qualifying exams (yay) and Cat is well. It was very nice to see them and see they are doing well. They will come to visit in December! Speaking of visits, you are most welcome to visit whenever. Next year would be great if you have time!

Thank you for your invitation. I do not know if I will be able to go next year to visit you. We are thinking to move for some months to New Zealand in 2020 and maybe next year it will be better if I do not travel too much. I will keep you in touch if I see I have the opportunity to come to Vancouver. However, you are always welcome in Avignon!

I also saw Nicole who is hoping to have a draft of her heat tolerance manuscript soon, we're planning to submit to Catalyst, a new journal Andy Walker suggested. If you know anything about it -- let me know.

Non, I do not know it. I just checked it and it is a Catalyst journal...? About chemical processes...? Is it not a little bit strange?

I have Bayesian modeler visiting Friday-Monday and I wanted to ask him to help me try to estimate  $T_{opt}$  and  $F_{star}$  values related to a Wang & Engel model in Stan. (basically just a fancy MCMC approach to search for best estimates of model parameters, I showed it to you briefly this summer)

I hope my answer does not arrive too late.

To do this I need to think \*a lot harder\* than I ever have about how these are estimated (e.g., in PMP). I have made up some fake data (attached) -- built off known values of all the parameters and the Wang & Engel functions -- which should help me test the model, but I am struggling to think through how to now ask Stan to fit the model (and test my test data!). Some questions if you have time (sorry for the short notice):

- In PMP do you fit/estimate  $T_{opt}$  and  $F^*$  at the same time? Or are they fit separately (and if so, how? Given that fitting  $T_{opt}$  seems to depend on knowing  $F^*$ )? I worry I am missing something fundamental ....

You have the choice to decide which parameters you want to fit. Usually they are fitted at the same time because if not, the value that you obtain for one (for example  $T_{opt}$ ) depend of the fixed values of the other. And maybe the fixed value that you have choosen is not the best. When you are fitting two parameters and typically one parameter of a function ( $T_{opt}$ ) and one parameter of a heat accumulation ( $F^*$ ) they are always correlated, but the database that you have, if it is quite enough large, it should look for the best combination of parameters.

- Do you have any code from PMP or such that may show how to do this? It would help me to have an example to work off.

PMP is using Metropolis algorithm and it is coded in Delphi. This is quite complicate to show you from the code (at least current version) because the code was developed in object language and they are many dependencies between classes.

If you don't have much time but can throw any references or files or such my way that would help too. No worries if you are too busy though!  
Like many things, I should have started on this sooner.

My hope is that I can work on getting some of the PMP models running in Stan, then we could see if it is a big improvement in fitting the models ....

I think it could be interesting to have a discussion about this topic by skype in order to be sure that we understand the same when we talk about fitting.

I can have some time this afternoon here (17 pm in France , 8 am in Vancouver). Let me know if it's useful for you.

All the best

Iñaki