U.S. Department of Homeland Security
U.S. Citizenship and Immigration Services
2.27.2023

RE: Dr. Ryan-Rhys Griffiths

Dear Sir/Madam,

I am very happy to support Dr. Griffiths in his application as an outstanding research scholar. Dr. Griffith's principal area of research focus is Bayesian optimisation, a fast-growing subfield of machine learning. To this end, Dr. Griffiths has made many noteworthy contributions, advancing machine learning methodology as well as its applications to real-world problems. His work has received international recognition in both machine learning journals, conferences and workshops, as well as physics and chemistry journals, where in the latter case, he has applied Bayesian optimisation methodologies to tackle many novel problems.

I hold a titular professorship as a Chair in Statistical Data Science at the University of xxxxx I have held this position since 2018. In my position, I am currently supervising 5 Ph.D. students and 2 postdoctoral research associates. From 2015 to 2018, I worked mainly as a permanent senior researcher at xxxxx where I headed the Uncertainty Quantification and Optimal Design group. I defended my venia docendi (habilitation) in Statistics and Applied Probability before the Faculty of Science of the University of xxxxx in 2014 and my PhD in Applied Mathematics at the xxxxx in 2009. I am a longstanding member of the international machine learning community serving as Associate Editor of the Technometrics journal and the SIAM/ASA Journal on Uncertainty Quantification. I have also served as Meta-Reviewer and Area Chair for ICML and NeurIPS respectively, two of the three premier international machine learning conferences.

I first met Dr. Griffiths through an online encounter on the website ResearchGate where I received notification that we were both reading each other's research at the same time. At this point, I noticed that Dr. Griffiths was doing very interesting work in my own field of Gaussian processes and Bayesian optimisation. To provide an overview of the relevance of this line of research, Bayesian optimisation is a solution method for black-box optimisation

problems. Such problems are characterised chiefly by three properties: The absence of information about the underlying (black-box) function or its gradients, the expense of querying the function pointwise in terms of time or fiscal cost, and optionally, the presence of noise in the evaluations. Black-box optimisation problems are ubiquitous in industrial settings with some representative examples including machine learning hyperparameter tuning in the field of artificial intelligence, in geostatistics with the method known as Kriging, as well as in the field of computer experiments where the goal may be to optimise complex physics-based simulators. To solve black-box optimisation problems, Bayesian optimisation adopts a probabilistic surrogate model of the unknown black-box function, typically a Gaussian process. The surrogate model then trades off exploration and exploitation in the objective to suggest new locations at which to query the black-box leading to efficient and cost-effective optimisation. In my own work, I have contributed to the theory of Gaussian process regression and kernel methods, I have made significant methodological advances in parallelising Bayesian optimisation schemes via the Kriging-Believer algorithm, and I have successfully applied these methodologies across problems ranging from computer experiments to climate science and spatial statistics.

Following our initial online meeting in 2019, Dr. Griffiths has gone on to achieve notable international success in his research. In 2020, he jointly developed the heteroscedastic evolutionary Bayesian optimisation (HEBO) algorithm that won the 2020 NeurIPS Competition on Black-Box Optimisation. This was a major international competition sponsored by companies such as Meta and Twitter and received entries from many industrial research groups. The HEBO algorithm has subsequently been used to great effect in machine learning circles, the most recent of which I have seen included its use in the ATLAS experiments at the Large Hadron Collider at CERN. In his current role at Meta Research, Dr. Grffiths continues to push the state-of-the-art in Bayesian optimisation with his work on the Adaptive Experimentation team.

I will now discuss some of Dr. Griffiths's research contributions in technical detail. The aforementioned HEBO algorithm is the first Bayesian optimization algorithm to jointly consider heteroscedastic noise, non-stationarity of the underlying objective function, a multiobjective acquisition function optimization, and a scheme that is robust to model misspecification early in the Bayesian optimisation trace when there is little available data. The power of combining these modeling considerations was illustrated starkly in the results of the 2020 NeurIPS Black-Box Optimisation Competition, where HEBO outperformed incumbent state-of-the-art optimisers such as the TuRBO algorithm developed by Uber AI Labs. HEBO was subsequently published in the Journal of Artificial Intelligence Research, a leading international journal in the field of artifical intelligence and machine learning. A further key contribution of Dr. Griffiths's research has been the application of Gaussian process models to problems in molecular modeling. In 2022, Griffiths published a paper entitled, "Data-Driven Discovery of Molecular Photoswitches with Multioutput Gaussian Processes" in Chemical Science, a leading international chemistry journal. In this work, Dr. Griffiths leveraged multitask Gaussian process models to predict the properties of photoswitch molecules. To achieve this, Dr. Griffiths extended the Gaussian process framework to operate on molecular bit vector representations using the Tanimoto kernel. The novel machine learning methodology Dr. Griffiths developed outperformed a cohort of expert human chemists including PhD researchers and postdoctoral researchers. Furthermore, the methodology was put to practical effect in a laboratory screening when it was used to screen photoswitch candidates, resulting in the rapid discovery of a novel photoswitch molecule that may have taken years of human trial-and-error synthesis to identify. Such a method, possesses distinct advantages

as a method for accelerating the discovery of novel drug molecules and molecular materials in industry. Furthermore, the novel Gaussian process-Tanimoto kernel combination that Dr. Griffiths introduced subsequently formed the basis of the masters thesis of one of my students where we analysed the theoretical properties of the kernel and proposed a generalised extension.

Dr. Griffiths's innovations have significantly advanced the methodology of Bayesian optimization and Gaussian processes and have been deployed in applications ranging from the ATLAS experiment at CERN's Large Hadron Collider to drug discovery at AstraZeneca. To summarise my letter of support for Dr. Griffiths's consideration as an outstanding research scholar, I can strongly attest to Dr. Griffiths's outstanding research contributions to date in the field of machine learning and fully expect to see him achieve further global recognition for his efforts at Meta Research.

Sincerely,

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Professor, University of xxxxx
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