

## Corrections to proofs

- Line 67:  
 $f(x, \theta)$  should be  $f(\mathbf{x}, \theta)$
- Fig 1 caption should read:  
‘...design domain  $\chi$ ’ instead of ‘...design domain  $\mathbf{x}$ ’.
- In Equation 7,  $\log P(D_j|\theta_i^j, M_i)$  should read  $\log P(\mathcal{D}_j|\theta_i^j, M_i)$  as in Equation 5.
- on line 411, the sentence should read:  
where  $I_{\mathcal{H}}(\mathbf{y}|\mathbf{x}, \mathcal{D})$  denotes the hyper-volume improvement achieved by observing the outputs at  $\mathbf{x}$ , *E represents expectation*, and  $EI_{\mathcal{H}}(\mathbf{x}|\mathcal{D}, M_i)$  is the ordinary EHVI under model  $M_i$ .
- The sentence starting on line 416 should read:  
The optimal experiment to be performed next is  $\mathbf{x}^* = \underset{\mathbf{x} \in \mathcal{X}}{\operatorname{argmax}} EI_{\mathcal{H}}(\mathbf{x}|\mathcal{D})$ ,  
which is the one that maximizes the weighted average EHVI considering all the potential predictive models, *based on* the iteratively updated (posterior) model probabilities *given the observed data*.
- Line 436 should read:  
where  $I(y|\mathbf{x}, \mathcal{D})$  denotes the improvement achieved by observing the output of experiment  $\mathbf{x}$ , and  $EI(\mathbf{x}|\mathcal{D}, M_i)$  is the EI under model  $M_i$ .
- Caption for Figure 2 should read:  
Schematic of the proposed framework for an autonomous, efficient materials discovery system as a realization of Bayesian Optimization under Model Uncertainty (BOMU). Initial data and a set of candidate models are used to construct a stochastic representation of an experiment/simulation. Each model is evaluated in a Bayesian sense and its probability is determined. Using the model probabilities, an effective acquisition function is computed, which is then used to select the next point in the materials design space that needs to be queried. The process is continued iteratively until target is reached or budget is exhausted. *Adapted from the adaptive design strategy framework in [29].*