

# Errata

## Publication I

The early stopping and convergence criteria are described correctly in the Methods section (section 2.3), but there are unfortunate mistakes in the following two sentences in the Results section. A corrected version of Publication I is available as e-print arXiv:1703.10423.

Original sentence (rows 12–15 of section 3.1):

*The relaxation of the images on this rough estimate of the energy surface does not, however, bring the images too far from the initial placement because of the condition that images cannot be moved in a single iteration by more than a half of the initial distance between the images.*

Corrected sentence:

*[...] because of the condition that the relaxation phase is stopped early if the convergence measure, i.e., the mean of the magnitudes of the force components perpendicular to the path at the intermediate images, increases.*

Original sentence (rows 3–5 of the caption of figure 4):

*The convergence tolerance is  $0.001 \text{ eV}/\text{\AA}$  for the magnitude of the perpendicular component of the force on any one of the images.*

Corrected sentence:

*[...] for the mean of the magnitudes of the perpendicular force components at the intermediate images.*

## **Publications I and II**

The computational complexity of one inner iteration of the GP-NEB algorithm is claimed to be linear with respect to the number of degrees of freedom  $D$  (row 25 of section 2.3 in Publication I and the last three rows of section IV.A in Publication II). The computational cost of prediction of energy or any gradient component indeed scales linearly with respect to  $D$ , but since moving the images requires prediction of the whole gradient vector, the complexity of one inner iteration becomes quadratic with respect to  $D$ .