Ultra-fast interpretable machine-learning potentials

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I. PROPERTY DATA

TABLE I. *Derived properties.*

	Energy (meV/atom)	Forces (eV/Å)	Phonons (THz)	a_0 (Å)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)	E_{100} (eV)	E_{110} (eV)	E_{111} (eV)	E_V (eV)
DFT	**[225.4]**	**[1.496]**	**[2.254]**	**3.180**	**517.0**	**198.0**	**142.0**	**305.0**	**0.251**	**0.204**	**0.222**	**3.270**
UF_2	26.6	0.387	0.230	3.169	538.6	188.9	185.0	300.5	0.173	0.161	0.190	4.324
$UF_{2,3}$	5.1	0.152	0.263	3.176	558.4	231.4	158.7	333.7	0.240	0.203	0.223	3.283
LJ	110.0	1.400	3.914	3.105	506.2	600.9	599.4	566.7	0.345	0.325	0.348	4.334
Morse	40.0	0.480	1.139	3.230	135.8	126.3	126.1	129.1	0.171	0.170	0.174	2.894
EAM4	88.0	0.803	0.301	3.143	525.3	206.5	163.8	311.0	0.184	0.159	0.224	3.816
SNAP	14.2	0.189	0.270	3.166	653.8	335.4	124.2	433.4	0.227	0.196	0.261	2.048
qSNAP	9.9	0.167	0.256	3.176	497.0	179.2	101.9	281.1	0.249	0.202	0.245	2.574
GAP	6.2	0.169	0.291	3.178	596.4	253.7	142.0	363.5	0.268	0.216	0.177	3.342

II. MODEL PARAMETERS

TABLE II. *UF Potential hyperparameters selected in this work.*

	two-body						three-body					
	$r_{\mathrm{min},2}$ (Å)	$r_{\mathrm{cut},2}$ (Å)	knot spacing	basis functions	symmetry	λ_2	$r_{\mathrm{min},3}$ (Å)	$r_{\mathrm{cut},3}$ (Å)	knot spacing	basis functions	symmetry	λ_3
UF_2	1.5	5.5	linear	25	i-j = j-i	1E-08	-	-	-	-	-	-
$UF_{2,3}$	1.5	5.5	linear	25	i-j = j-i	1E-08	1.5	4.25	linear	915	i-j-k = i-k-j	1E-08

TABLE III. *SNAP/qSNAP hyperparameters selected in this work.*

	rcutfac (Å)	twojmax	rfac0	rmin0	quadraticflag	bzeroflag
SNAP	5.5	8	0.99363	0	0	0
qSNAP	5.5	6	0.99363	0	1	0

TABLE IV. *GAP hyperparameters selected in this work.*

	cutoff (Å)	l_max	n_max	atom_sigma	zeta	cutoff_transition_width	delta	f0	n_sparse	covariance_type	sparse_method
GAP	5.5	8	8	0.5	4	0.5	1	0	200	dot_product	cur_points

III. HYPERPARAMETER EXPLORATION IN UF POTENTIALS

TABLE V. *Basis functions and error vs. cutoff radius in $UF_{2,3}$ potential.*

r_{cut}	λ	RMSE_E (meV/atom)	RMSE_F (meV/Å)	$\|c \neq 0\|$	$\|c\|$	symmetry mask	cutoff mask
4.00	10^{-6}	7.380	0.205	924	2000	353	723
4.00	10^{-7}	7.311	0.203	924	2000	353	723
4.00	10^{-8}	7.309	0.203	924	2000	353	723
4.25	10^{-6}	6.335	0.179	915	2000	368	717
4.25	10^{-7}	6.344	0.176	915	2000	368	717
4.25*	10^{-8}*	6.340	0.176	915	2000	368	717
4.50	10^{-6}	42.973	1.553	905	2000	381	714
4.50	10^{-7}	6.116	0.171	905	2000	381	714
4.50	10^{-8}	6.115	0.171	905	2000	381	714
4.75	10^{-6}	5.731	0.168	903	2000	386	711
4.75	10^{-7}	5.576	0.163	903	2000	386	711
4.75	10^{-8}	5.575	0.163	903	2000	386	711
5.00	10^{-6}	5.326	0.159	899	2000	393	708
5.00	10^{-7}	5.190	0.156	899	2000	393	708
5.00	10^{-8}	5.189	0.156	899	2000	393	708
5.25	10^{-6}	35.824	1.414	889	2000	406	705
5.25	10^{-7}	5.208	0.154	889	2000	406	705
5.25	10^{-8}	5.210	0.154	889	2000	406	705
5.50	10^{-6}	32.388	1.310	888	2000	410	702
5.50	10^{-7}	5.106	0.152	888	2000	410	702
5.50	10^{-8}	5.107	0.152	888	2000	410	702

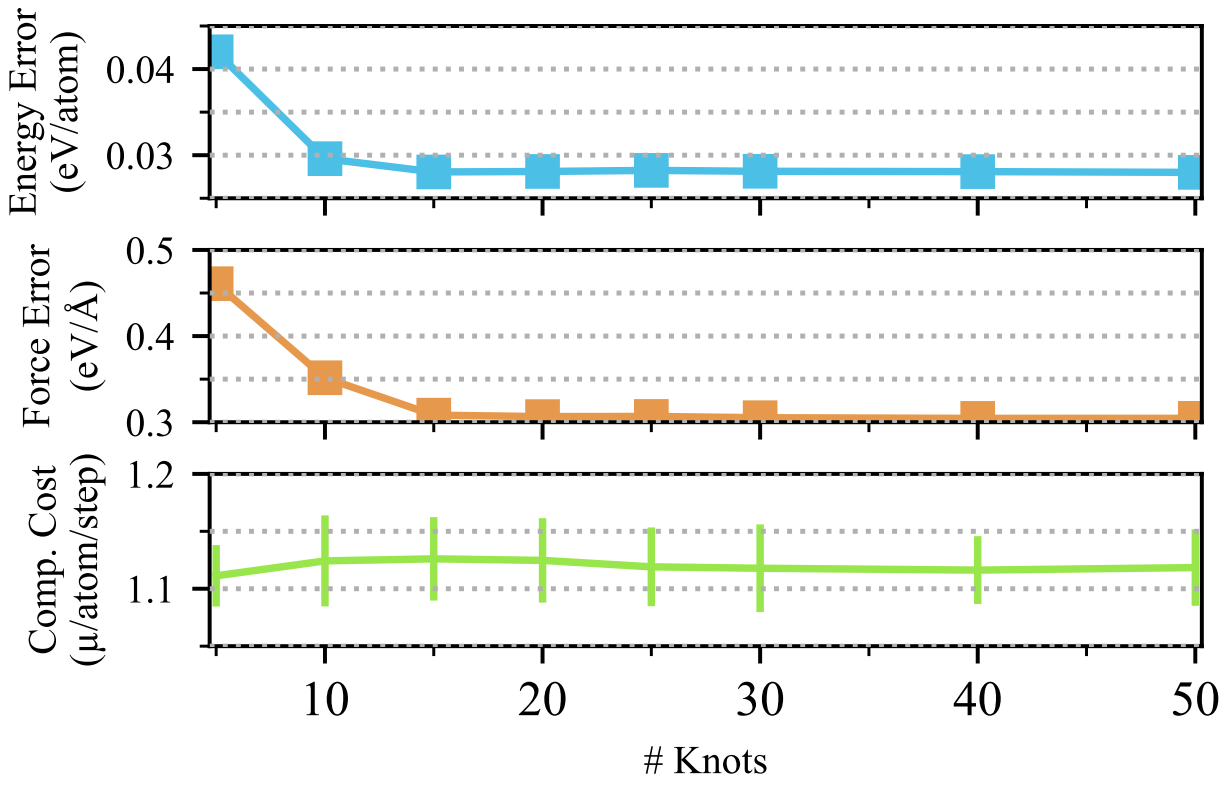

FIG. 1. *Convergence in two-body interaction properties with number of knots. Energy and force errors quickly converge with the number of knots, which, in turn, determine the number of basis functions. The computational cost of evaluation does not scale wtih the number of knots due to compact support.*

IV. REPRODUCTION OF PAIR AND TWO-AND-THREE-BODY POTENTIALS WITH UF POTENTIALS

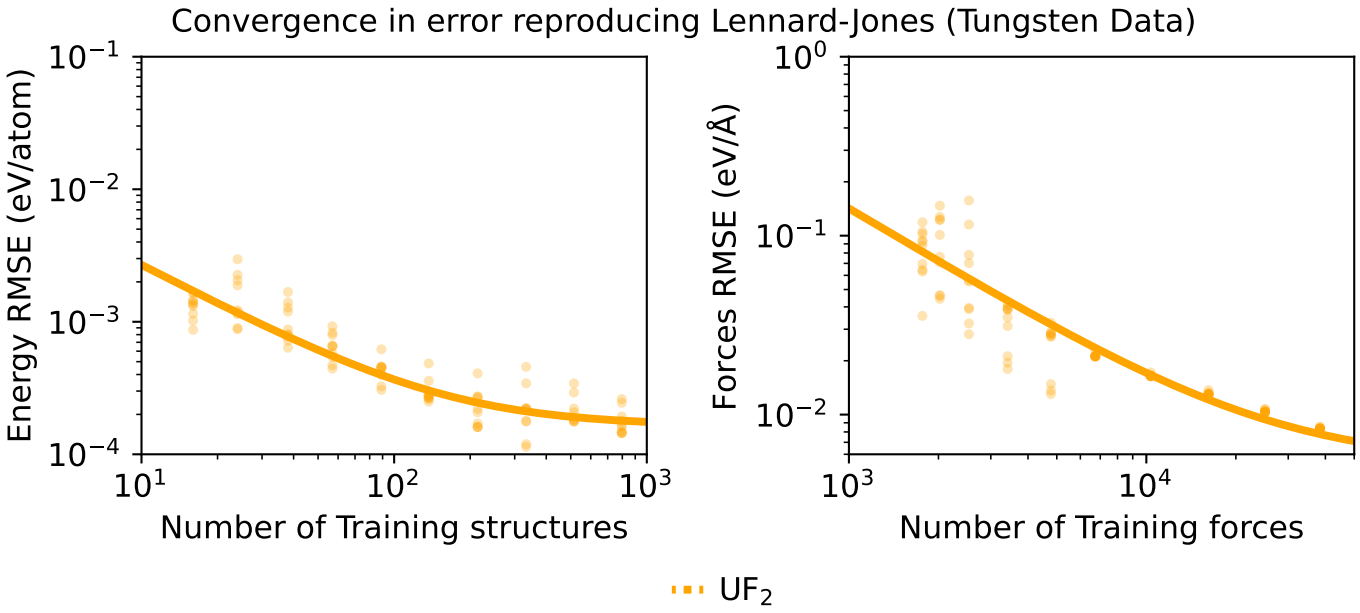

FIG. 2. *Convergence in errors in reproducing the Lennard-Jones potential with the two-body UF potential. The dataset used to construct these learning curves contain various elemental tungsten configurations (e.g. bcc, vacancy, gamma surfaces) and was previously constructed by Szlachta et al. to fit GAP potentials [1].*

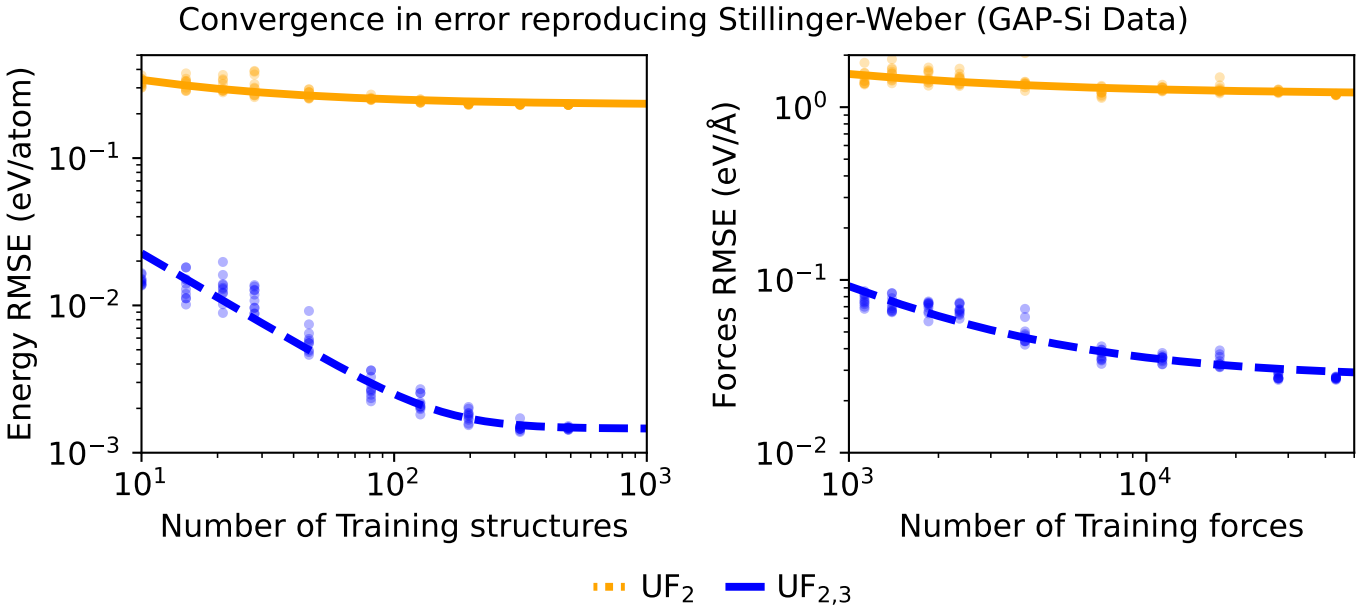

FIG. 3. *Convergence in errors in reproducing the Stillinger-Weber potential with the UF_2 and $UF_{2,3}$ potentials. The dataset used to construct these learning curves contain various elemental silicon configurations (e.g. diamond, hexagonal, β-Sn, amorphous) and was previously constructed by Bartók et al. to fit GAP potentials [2].*

[1] Szlachta, W. J., Bartók, A. P. & Csányi, G. Accuracy and transferability of Gaussian approximation potential models for tungsten. *Phys. Rev. B* **90**, 104108 (2014).
[2] Bartók, A. P., Kermode, J., Bernstein, N. & Csányi, G. Machine learning a general-purpose interatomic potential for silicon. *Physical Review X* **8** (2018).