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Author Correction: Optimization of Molecules via Deep Reinforcement Learning

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This Article contains errors.

Penalized logP is reported in this Article for our methods in a non-normalised form. Previous research (which we compared to in the original Tables 1 and 2), starting with JT-VAE¹ normalized the logP to be zero mean and unit standard deviation based on the training set. To correctly compare with previous research, our penalized logP was recalculated into a normalised form. This resulted in changes of numerical values for Penalized logP in Table 1, and numerical values for MolDQN-naïve and MolDQN-bootstrap Improvement in Table 2. The corrected versions of these tables are included below as Tables 1 and 2.

	Penalized logP				QED			
	1st	2nd	3rd	Validity	1st	2nd	3rd	Validity
random walk ^a	−0.65	−1.72	−1.88	100%	0.64	0.56	0.56	100%
greedy ^b	9.05	—	—	100%	0.39	—	—	100%
ϵ -greedy, $\epsilon = 0.1$ ^b	9.10	9.05	9.05	100%	0.914	0.910	0.906	100%
JT-VAE ^c	5.30	4.93	4.49	100%	0.925	0.911	0.910	100%
ORGAN ^c	3.63	3.49	3.44	0.4%	0.896	0.824	0.820	2.2%
GCPN ^c	7.98	7.85	7.80	100%	0.948	0.947	0.946	100%
MolDQN-naïve	8.69	8.68	8.67	100%	0.934	0.931	0.930	100%
MolDQN-bootstrap	9.01	9.01	8.99	100%	0.948	0.944	0.943	100%
MolDQN-bootstrap	—	—	—	—	0.948	0.948	0.948	100%

Table 1. Top three unique molecule property scores found by each method. ^a“random walk” is a baseline that chooses a random action for each step. ^b“greedy” is a baseline that chooses the action that leads to the molecule with the highest reward for each step. ^c“ ϵ -greedy” follows the “random” policy with probability ϵ , and “greedy” policy with probability $1-\epsilon$. In contrast, the ϵ -greedy MolDQN models choose actions based on predicted Q-values rather than rewards. ^cvalues are reported in You *et al.*².

δ	JT-VAE ^a		GCPN ^a		MolDQN-naïve		MolDQN-bootstrap	
	Improvement	Success	Improvement	Success	Improvement	Success	Improvement	Success
0.0	1.91 ± 2.04	97.5%	4.20 ± 1.28	100%	4.83 ± 1.30	100%	4.88 ± 1.30	100%
0.2	1.68 ± 1.85	97.1%	4.12 ± 1.19	100%	3.79 ± 1.32	100%	3.80 ± 1.30	100%
0.4	0.84 ± 1.45	83.6%	2.49 ± 1.30	100%	2.34 ± 1.18	100%	2.44 ± 1.25	100%
0.6	0.21 ± 0.71	46.4%	0.79 ± 0.63	100%	1.40 ± 0.92	100%	1.30 ± 0.98	100%

Table 2. Mean and standard deviation of penalized logP improvement in constrained optimization tasks. δ is the threshold of the similarity constraint $\text{SIM}(\mathbf{m}, \mathbf{m}_0) \geq \delta$. The success rate is the percentage of molecules satisfying the similarity constraint. ^avalues are reported in You *et al.*².

Additionally, in the Discussion, subsection “Constrained optimization”:

“Using Welch’s t -test³⁰ for $N = 800$ molecules, we found that both variants of MolDQN gives a highly statistically significant improvement over GCPN for all values of δ with $t < -8$. The bootstrap variant also significantly outperforms the naive model (except for $\delta = 0.2$) with $t < -3$.”

should read:

“Using Welch’s t -test³⁰, we found that on $\delta = 0.2$, both variants of MolDQN gives a statistically significant lower improvement comparing to GCPN with $P < 1e-7$; on $\delta = 0.4$, the differences are insignificant at a 1% level with $P = 0.016$ for MolDQN naive and $P = 0.43$ for MolDQN bootstrap; on $\delta = 0.0$ and 0.6 , both variants of MolDQN gives a statistically significant higher improvement comparing to GCPN with $P < 1e-22$. The differences between two variants of MolDQN are statistically insignificant at a 1% level with $P > 0.036$.”

Furthermore, Figure S7 was updated. The corrected version is shown below as Figure 1.

Figure 1.

Lastly, References 13 and 18 were incorrectly given as:

13. Jin, W., Barzilay, R. & Jaakkola, T. Junction tree variational autoencoder for molecular graph generation. arXiv preprint arXiv:1802.04364 (2018).

18. You, J., Liu, B., Ying, Z., Pande, V. & Leskovec, J. Graph convolutional policy network for goal-directed molecular graph generation. arXiv preprint arXiv:1806.02473 (2018).

The correct references are listed below as references 1 and 2.

These changes do not affect the conclusions of the Article.

References

1. Jin, W., Barzilay, R. & Jaakkola, T. Junction Tree Variational Autoencoder for Molecular Graph Generation. In *Proceedings of the 35th International Conference on Machine Learning* (eds. Dy, J. & Krause, A.) vol. **80**, 2323–2332 (PMLR, 2018).
2. You, J., Liu, B., Ying, Z., Pande, V. & Leskovec, J. Graph Convolutional Policy Network for Goal-Directed Molecular Graph Generation. In *Advances in Neural Information Processing Systems 31* (eds. Bengio, S. et al.) 6410–6421 (Curran Associates, Inc., 2018).

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