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Bibliography

[1] Amira Abbas, David Sutter, Christa Zoufal, Aurélien Lucchi, Alessio Figalli, and Stefan Woerner. The power of quantum neural networks. *Nature Computational Science*, 1(6):403–409, 2021.

[2] Amir Adler, Mauricio Araya-Polo, and Tomaso Poggio. Deep learning for seismic inverse problems: Toward the acceleration of geophysical analysis workflows. *IEEE Signal Processing Magazine*, 38(2):89–119, 2021.

[3] D. Akhiyarov, A. Gherbi, B. Conche, and M. Araya-Polo. Fast machine learning-based oil slick detection on satellite imaging. *82nd EAGE Annual Conference & Exhibition*, 2021(1):1–5, 2021.

[4] V. Akshay, D. Rabinovich, E. Campos, and J. Biamonte. Parameter concentrations in quantum approximate optimization. *Phys. Rev. A*, 104:L010401, Jul 2021.

[5] Mahabubul Alam, Abdullah Ash-Saki, and Swaroop Ghosh. Analysis of Quantum Approximate Optimization Algorithm under Realistic Noise in Superconducting Qubits, 2019. arXiv:1907.09631.

[6] MD SAJID ANIS and et al. Qiskit: An open-source framework for quantum computing, 2021.

[7] Eric R Anschuetz and Bobak T Kiani. Beyond barren plateaus: Quantum variational algorithms are swamped with traps. *arXiv preprint arXiv:2205.05786*, 2022.

[8] Simon Apers and Ronald de Wolf. Quantum Speedup for Graph Sparsification, Cut Approximation and Laplacian Solving, 2019.

[9] Andrew Arrasmith, M. Cerezo, Piotr Czarnik, Lukasz Cincio, and Patrick J Coles. Effect of barren plateaus on gradient-free optimization. *Quantum*, 5:558, 2021.

[10] Andrew Arrasmith, Lukasz Cincio, Rolando D Somma, and Patrick J Coles. Operator sampling for shot-frugal optimization in variational algorithms. *arXiv preprint arXiv:2004.06252*, 2020.

[11] Frank Arute, Kunal Arya, Ryan Babbush, Dave Bacon, Joseph C. Bardin, Rami Barends, Rupak Biswas, Sergio Boixo, Fernando G. S. L. Brandao, David A. Buell, and et al. Quantum supremacy using a programmable superconducting processor. *Nature*, 574(7779):505–510, Oct 2019.

[12] Thomas Bäck. *Evolutionary algorithms in theory and practice - evolution strategies, evolutionary programming, genetic algorithms.* Oxford University Press, 1996.

[13] Lukas Balles, Javier Romero, and Philipp Hennig. Coupling Adaptive Batch Sizes with Learning Rates. In *Proceedings of the Thirty-Third Conference on Uncertainty in Artificial Intelligence (UAI)*, pages 410–419, 2017.

[14] Panagiotis Kl. Barkoutsos, Giacomo Nannicini, Anton Robert, Ivano Tavernelli, and Stefan Woerner. Improving Variational Quantum Optimization using CVaR, 2019. arXiv:1907.04769.

[15] J. E. Beasley. Or-library: Distributing test problems by electronic mail. *The Journal of the Operational Research Society*, 41(11):1069–1072, 1990.

[16] John Beasley. QUBO instances link - file bqpgka.txt. http://people.brunel.ac.uk/~mastjjb/jeb/orlib/bqpinfo.html.

[17] Kerstin Beer, Dmytro Bondarenko, Terry Farrelly, Tobias J. Osborne, Robert Salzmann, Daniel Scheiermann, and Ramona Wolf. Training deep quantum neural networks. *Nature Communications*, 11(1):808, 2020.

[18] Marcello Benedetti, Erika Lloyd, Stefan Sack, and Mattia Fiorentini. Parameterized quantum circuits as machine learning models. *Quantum Science and Technology*, 2019.

[19] Ville Bergholm, Josh A. Izaac, Maria Schuld, Christian Gogolin, and Nathan Killoran. Pennylane: Automatic differentiation of hybrid quantum-classical computations. *CoRR*, abs/1811.04968, 2018.

[20] Hans-Georg Beyer. *The theory of evolution strategies.* Natural computing series. Springer, 2001.

[21] Jacob Biamonte, Peter Wittek, Nicola Pancotti, Patrick Rebentrost, Nathan Wiebe, and Seth Lloyd. Quantum machine learning. *Nature*, 549(7671):195–202, 2017.

[22] Bernd Bischl, Giuseppe Casalicchio, Matthias Feurer, Pieter Gijsbers, Frank Hutter, Michel Lang, Rafael Gomes Mantovani, Jan N. van Rijn, and Joaquin Vanschoren. Openml benchmarking suites. In *Proceedings of the Neural Information Processing Systems Track on Datasets and Benchmarks*, 2021.

[23] Lennart Bittel and Martin Kliesch. Training variational quantum algorithms is np-hard. *Phys. Rev. Lett.*, 127:120502, Sep 2021.

[24] Xavier Bonet-Monroig, Hao Wang, Diederick Vermetten, Bruno Senjean, Charles Moussa, Thomas Bäck, Vedran Dunjko, and Thomas E. O'Brien. Performance comparison of optimization methods on variational quantum algorithms. *Phys. Rev. A*, 107:032407, Mar 2023.

[25] Michael Booth and Steven P. Reinhardt. Partitioning optimization problems for hybrid classical / quantum execution technical report, 2017.

[26] Fernando G. S. L. Brandão, Michael Broughton, Edward Farhi, Sam Gutmann, and Hartmut Neven. For Fixed Control Parameters the Quantum Approximate Optimization Algorithm's Objective Function Value Concentrates for Typical Instances, 2018. arXiv:1812.04170.

[27] Sergey Bravyi, David Gosset, and Robert König. Quantum advantage with shallow circuits. *Science*, 362(6412):308–311, 2018.

[28] Sergey Bravyi, Alexander Kliesch, Robert Koenig, and Eugene Tang. Obstacles to State Preparation and Variational Optimization from Symmetry Protection, 2019. arXiv:1910.08980.

[29] Sergey Bravyi, Alexander Kliesch, Robert Koenig, and Eugene Tang. Obstacles to state preparation and variational optimization from symmetry protection, 2019.

[30] Sergey Bravyi, Graeme Smith, and John A. Smolin. Trading classical and quantum computational resources. *Phys. Rev. X*, 6:021043, Jun 2016.

[31] Pavel Brazdil, Jan N. van Rijn, Carlos Soares, and Joaquin Vanschoren. *Metalearning: Applications to Automated Machine Learning and Data Mining*. Springer, 2nd edition, 2022.

[32] Leo Breiman. Random forests. *Mach. Learn.*, 45(1):5–32, October 2001.

[33] K. H. Brodersen, C. S. Ong, K. E. Stephan, and J. M. Buhmann. The balanced accuracy and its posterior distribution. In *2010 20th International Conference on Pattern Recognition*, pages 3121–3124, Aug 2010.

[34] Michael Broughton and et al. Tensorflow quantum: A software framework for quantum machine learning. *arXiv:2003.02989*, 2020.

[35] C. G. BROYDEN. The convergence of a class of double-rank minimization algorithms 1. general considerations. *IMA Journal of Applied Mathematics*, 6(1):76–90, 1970.

[36] Chris Cade, Lana Mineh, Ashley Montanaro, and Stasja Stanisic. Strategies for solving the fermi-hubbard model on near-term quantum computers. *Phys. Rev. B*, 102:235122, Dec 2020.

[37] Adam Callison and Nicholas Chancellor. Hybrid quantum-classical algorithms in the noisy intermediate-scale quantum era and beyond. *Phys. Rev. A*, 106:010101, Jul 2022.

[38] Matthias C. Caro, Elies Gil-Fuster, Johannes Jakob Meyer, Jens Eisert, and Ryan Sweke. Encoding-dependent generalization bounds for parametrized quantum circuits. *Quantum*, 5:582, 2021.

[39] Matthias C. Caro, Hsin-Yuan Huang, Nicholas Ezzell, Joe Gibbs, Andrew T. Sornborger, Lukasz Cincio, Patrick J. Coles, and Zoe Holmes. Out-of-distribution generalization for learning quantum dynamics. *arXiv preprint arXiv:2204.10268*, 2022.

[40] M. Cerezo, Andrew Arrasmith, Ryan Babbush, Simon C. Benjamin, Suguru Endo, Keisuke Fujii, Jarrod R. McClean, Kosuke Mitarai, Xiao Yuan, Lukasz Cincio, and Patrick J. Coles. Variational quantum algorithms. *Nature Reviews Physics*, 3(9):625–644, Sep 2021.

[41] M. Cerezo, Kunal Sharma, Andrew Arrasmith, and Patrick J Coles. Variational quantum state eigensolver. *npj Quantum Information*, 8(1):1–11, 2022.

[42] M. Cerezo, Akira Sone, Tyler Volkoff, Lukasz Cincio, and Patrick J Coles. Cost function dependent barren plateaus in shallow parametrized quantum circuits. *Nature Communications*, 12(1):1–12, 2021.

[43] Tianqi Chen and Carlos Guestrin. Xgboost: A scalable tree boosting system. *arXiv:1603.02754*, 2016.

[44] Cristina Cirstoiu, Zoe Holmes, Joseph Iosue, Lukasz Cincio, Patrick J. Coles, and Andrew Sornborger. Variational fast forwarding for quantum simulation beyond the coherence time. *npj Quantum Information*, 6(1):1–10, 2020.

[45] Iris Cong, Soonwon Choi, and Mikhail D Lukin. Quantum convolutional neural networks. *Nature Physics*, 15(12):1273–1278, 2019.

[46] Gavin E Crooks. Performance of the quantum approximate optimization algorithm on the maximum cut problem. *arXiv preprint arXiv:1811.08419*, 2018.

[47] Benjamin Doerr and Carola Doerr. Optimal static and self-adjusting parameter choices for the $(1+(\lambda, \lambda))$ genetic algorithm. *Algorithmica*, 80(5):1658–1709, 2018.

[48] Benjamin Doerr, Huu Phuoc Le, Régis Makhmara, and Ta Duy Nguyen. Fast genetic algorithms. In Peter A. N. Bosman, editor, *Proceedings of the Genetic and Evolutionary Computation Conference, GECCO 2017, Berlin, Germany, July 15-19, 2017*, pages 777–784. ACM, 2017.

[49] Carola Doerr, Hao Wang, Furong Ye, Sander van Rijn, and Thomas Bäck. Iohprofiler: A benchmarking and profiling tool for iterative optimization heuristics. *arXiv e-prints:1810.05281*, October 2018.

[50] Vedran Dunjko, Yimin Ge, and J. Ignacio Cirac. Computational speedups using small quantum devices. *Phys. Rev. Lett.*, 121:250501, Dec 2018.

[51] Iain Dunning, Swati Gupta, and John Silberholz. What Works Best When? A Systematic Evaluation of Heuristics for Max-cut and QUBO. *INFORMS Journal on Computing*, 30(3):608–624, 2018.

[52] Iain Dunning, Swati Gupta, and John Silberholz. What works best when? a systematic evaluation of heuristics for max-cut and qubo. *INFORMS J. on Computing*, 30(3):608–624, aug 2018.

[53] Katharina Eggensperger, Frank Hutter, Holger H. Hoos, and Kevin Leyton-Brown. Efficient benchmarking of hyperparameter optimizers via surrogates. In *Proceedings of the Twenty-Ninth AAAI Conference on Artificial Intelligence*, pages 1114–1120. AAAI Press, 2015.

[54] Gerald Kelechi Ekechukwu, Romain de Loubens, and Mauricio Araya-Polo. Long short-term memory-driven forecast of CO_2 injection in porous media. *Physics of Fluids*, 34(5):056606, May 2022.

[55] Suguru Endo, Zhenyu Cai, Simon C. Benjamin, and Xiao Yuan. Hybrid quantum-classical algorithms and quantum error mitigation. *Journal of the Physical Society of Japan*, 90(3):032001, 2021.

[56] Francesco A Evangelista, Garnet Kin-Lic Chan, and Gustavo E Scuseria. Exact parameterization of fermionic wave functions via unitary coupled cluster theory. *J. Chem. Phys.*, 151(24):244112, 2019.

[57] Edward Farhi, Jeffrey Goldstone, and Sam Gutmann. A quantum approximate optimization algorithm, 2014. arXiv:1411.4028.

[58] Edward Farhi and Aram W Harrow. Quantum supremacy through the quantum approximate optimization algorithm, 2016.

[59] Jan Faye. Copenhagen Interpretation of Quantum Mechanics. In Edward N. Zalta, editor, *The Stanford Encyclopedia of Philosophy*. Metaphysics Research Lab, Stanford University, Winter 2019 edition, 2019.

[60] Matthias Feurer, Katharina Eggensperger, Stefan Falkner, Marius Lindauer, and Frank Hutter. Auto-sklearn 2.0: Hands-free automl via meta-learning. *arXiv:2007.04074v2 [cs.LG]*, 2021.

[61] Alexey Galda, Xiaoyuan Liu, Danylo Lykov, Yuri Alexeev, and Ilya Safro. Transferability of optimal qaoa parameters between random graphs, 2021.

[62] Yimin Ge and Vedran Dunjko. A hybrid algorithm framework for small quantum computers with application to finding hamiltonian cycles. *Journal of Mathematical Physics*, 61(1):12201, Jan 2020.

[63] Joe Gibbs, Zoe Holmes, Matthias C. Caro, Nicholas Ezzell, Hsin-Yuan Huang, Lukasz Cincio, Andrew T. Sornborger, and Patrick J. Coles. Dynamical simulation via quantum machine learning with provable generalization. *arXiv preprint arXiv:2204.10269*, 2022.

[64] Fred Glover and Jin-Kao Hao. Efficient evaluations for solving large 0-1 unconstrained quadratic optimisation problems. *Int. J. Metaheuristics*, 1, 01 2010.

[65] Fred Glover, Gary Kochenberger, and Bahram Alidaee. Adaptive memory tabu search for binary quadratic programs. *Management Science*, 44:336–345, 03 1998.

[66] Fred W. Glover. *Tabu Search*, pages 1537–1544. Springer US, Boston, MA, 2013.

[67] Fred W. Glover, Zhipeng Lü, and Jin-Kao Hao. Diversification-driven tabu search for unconstrained binary quadratic problems. *4OR*, 8:239–253, 2010.

[68] Michel X. Goemans. Combining approximation algorithms for the prize-collecting tsp. *ArXiv*, abs/0910.0553, 2009.

[69] Michel X. Goemans and David P. Williamson. Improved Approximation Algorithms for Maximum Cut and Satisfiability Problems Using Semidefinite Programming. *J. ACM*, 42(6):1115–1145, November 1995.

[70] Max Hunter Gordon, M. Cerezo, Lukasz Cincio, and Patrick J. Coles. Covariance matrix preparation for quantum principal component analysis. *PRX Quantum*, 3:030334, Sep 2022.

[71] Gabriel Greene-Diniz, David Zsolt Manrique, Wassil Sennane, Yann Magnin, Elvira Shishenina, Philippe Cordier, Philip Llewellyn, Michal Krompiec, Marko J. Rančić, and David Muñoz Ramo. Modelling carbon capture on metal-organic frameworks with quantum computing, 2022.

[72] Andi Gu, Angus Lowe, Pavel A Dub, Patrick J. Coles, and Andrew Arrasmith. Adaptive shot allocation for fast convergence in variational quantum algorithms. *arXiv preprint arXiv:2108.10434*, 2021.

[73] G. G. Guerreschi and A. Y. Matsuura. QAOA for Max-cut requires hundreds of qubits for quantum speed-up. *Scientific Reports*, 9(1):6903, 2019.

[74] Gian Giacomo Guerreschi. Solving quadratic unconstrained binary optimization with divide-and-conquer and quantum algorithms, 2021.

[75] Nikolaus Hansen. Benchmarking a BI-Population CMA-ES on the BBOB-2009 Function Testbed. In *ACM-GECCO Genetic and Evolutionary Computation Conference*, Montreal, Canada, July 2009.

[76] Nikolaus Hansen, Youhei Akimoto, and Petr Baudis. CMA-ES/pycma on Github. Zenodo, DOI:10.5281/zenodo.2559634, February 2019.

[77] Nikolaus Hansen, Anne Auger, Raymond Ros, Steffen Finck, and Petr Posík. Comparing results of 31 algorithms from the black-box optimization benchmarking BBOB-2009. In Martin Pelikan and Jürgen Branke, editors, *Genetic and Evolutionary Computation Conference, GECCO 2010, Proceedings, Portland, Oregon, USA, July 7-11, 2010, Companion Material*, pages 1689–1696. ACM, 2010.

[78] Nikolaus Hansen and Andreas Ostermeier. Completely derandomized self-adaptation in evolution strategies. *Evol. Comput.*, 9(2):159–195, 2001.

[79] Matthew P. Harrigan, Kevin J. Sung, Matthew Neeley, Kevin J. Satzinger, Frank Arute, Kunal Arya, Juan Atalaya, Joseph C. Bardin, Rami Barends, Sergio Boixo, Michael Broughton, Bob B. Buckley, David A. Buell, Brian Burkett, Nicholas Bushnell, Yu Chen, Zijun Chen, Ben Chiaro, Roberto Collins, William Courtney, Sean Demura, Andrew Dunsworth, Daniel Eppens, Austin Fowler, Brooks Foxen, Craig Gidney, Marissa Giustina, Rob Graff, Steve Habegger, Alan Ho, Sabrina Hong, Trent Huang, L. B. Ioffe, Sergei V. Isakov, Evan Jeffrey, Zhang Jiang, Cody Jones, Dvir Kafri, Kostyantyn Kechedzhi, Julian Kelly, Seon Kim, Paul V. Klimov, Alexander N. Korotkov, Fedor Kostritsa, David Landhuis, Pavel Laptev, Mike Lindmark, Martin Leib, Orion Martin, John M. Martinis, Jarrod R. McClean, Matt McEwen, Anthony Megrant, Xiao Mi, Masoud Mohseni, Wojciech Mruczkiewicz, Josh Mutus, Ofer Naaman, Charles Neill, Florian Neukart, Murphy Yuezhen Niu, Thomas E. O'Brien, Bryan O'Gorman, Eric Ostby, Andre Petukhov, Harald Putterman, Chris Quintana, Pedram Roushan, Nicholas C. Rubin, Daniel Sank, Andrea Skolik, Vadim Smelyanskiy, Doug Strain, Michael Streif, Marco Szalay, Amit Vainsencher, Theodore White, Z. Jamie Yao, Ping Yeh, Adam Zalcman, Leo Zhou, Hartmut Neven, Dave Bacon, Erik Lucero, Edward Farhi, and Ryan Babbush. Quantum approximate optimization of non-planar graph problems on a planar superconducting processor. *Nature Physics*, 17(3):332–336, Mar 2021.

[80] Johan Håstad. Some Optimal Inapproximability Results. *J. ACM*, 48(4):798–859, July 2001.

[81] M. B. Hastings. Classical and Quantum Bounded Depth Approximation Algorithms, 2019. arXiv:1905.07047.

[82] Tobias Haug, Chris N. Self, and M. S. Kim. Large-scale quantum machine learning. *CoRR*, abs/2108.01039, 2021.

[83] Vojtěch Havlíček, Antonio D. Córcoles, Kristan Temme, Aram W. Harrow, Abhinav Kandala, Jerry M. Chow, and Jay M. Gambetta. Supervised learning with quantum-enhanced feature spaces. *Nature*, 567(7747):209–212, 2019.

[84] Dirk Heimann, Hans Hohenfeld, Felix Wiebe, and Frank Kirchner. Quantum deep reinforcement learning for robot navigation tasks. *CoRR*, abs/2202.12180, 2022.

[85] Hans Hinterberger. Exploratory data analysis. In *Encyclopedia of Database Systems*, pages 1080–1080. Springer US, Boston, MA, 2009.

[86] Wassily Hoeffding. A class of statistics with asymptotically normal distribution. *The Annals of Mathematical Statistics*, 19(3):293–325, 1948.

[87] Zoë Holmes, Andrew Arrasmith, Bin Yan, Patrick J. Coles, Andreas Albrecht, and Andrew T Sornborger. Barren plateaus preclude learning scramblers. *Physical Review Letters*, 126(19):190501, 2021.

[88] Zoë Holmes, Kunal Sharma, M. Cerezo, and Patrick J Coles. Connecting ansatz expressibility to gradient magnitudes and barren plateaus. *PRX Quantum*, 3:010313, Jan 2022.

[89] Holger H. Hoos, Frank Neumann, and Heike Trautmann. Automated Algorithm Selection and Configuration (Dagstuhl Seminar 16412). *Dagstuhl Reports*, 6(10):33–74, 2017.

[90] Hsin-Yuan Huang, Michael Broughton, Masoud Mohseni, Ryan Babbush, Sergio Boixo, Hartmut Neven, and Jarrod R McClean. Power of data in quantum machine learning. *Nature Communications*, 12(1):1–9, 2021.

[91] Hsin-Yuan Huang, Richard Kueng, and John Preskill. Predicting many properties of a quantum system from very few measurements. *Nature Physics*, 16(10):1050–1057, 2020.

[92] F. Hutter, Holger Hoos, and Kevin Leyton-Brown. An efficient approach for assessing hyperparameter importance. In *Proceedings of the 31th International Conference on Machine Learning, ICML 2014*, volume 32 of *JMLR Workshop and Conference Proceedings*, pages 1130–1144, 2014.

[93] Sofiène Jerbi, Lukas J. Fiderer, Hendrik Poulsen Nautrup, Jonas M. Kübler, Hans J. Briegel, and Vedran Dunjko. Quantum machine learning beyond kernel methods. *CoRR*, abs/2110.13162, 2021.

[94] Sofiène Jerbi, Casper Gyurik, Simon Marshall, Hans J. Briegel, and Vedran Dunjko. Parametrized quantum policies for reinforcement learning. In *Advances in Neural Information Processing Systems 34*, pages 28362–28375, 2021.

[95] Peter D Johnson, Jonathan Romero, Jonathan Olson, Yudong Cao, and Alán Aspuru-Guzik. Qvector: an algorithm for device-tailored quantum error correction. *arXiv preprint arXiv:1711.02249*, 2017.

[96] Abhinav Kandala, Antonio Mezzacapo, Kristan Temme, Maika Takita, Markus Brink, Jerry Chow, and Jay Gambetta. Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets. *Nature*, 549:242–246, 09 2017.

[97] Abhinav Kandala, Antonio Mezzacapo, Kristan Temme, Maika Takita, Markus Brink, Jerry M. Chow, and Jay M. Gambetta. Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets. *Nature*, 549(7671):242–246, 2017.

[98] Richard M. Karp. *Reducibility among Combinatorial Problems*, pages 85–103. Springer US, Boston, MA, 1972.

[99] Guolin Ke, Qi Meng, Thomas Finley, Taifeng Wang, Wei Chen, Weidong Ma, Qiwei Ye, and Tie-Yan Liu. Lightgbm: A highly efficient gradient boosting decision tree. *Advances in neural information processing systems*, 30:3146–3154, 2017.

[100] Sami Khairy, Ruslan Shaydulin, Lukasz Cincio, Yuri Alexeev, and Prasanna Balaprakash. Learning to optimize variational quantum circuits to solve combinatorial problems. *Proceedings of the AAAI Conference on Artificial Intelligence*, 34(03):2367–2375, April 2020.

[101] Subhash Khot. On the Power of Unique 2-prover 1-round Games. In *Proceedings of the Thiry-fourth Annual ACM Symposium on Theory of Computing*, STOC '02, pages 767–775, New York, NY, USA, 2002. ACM.

[102] Subhash Khot, Guy Kindler, Elchanan Mossel, and Ryan O'Donnell. Optimal Inapproximability Results for MAX-CUT and Other 2-Variable CSPs? *SIAM J. Comput.*, 37(1):319–357, April 2007.

[103] Diederik P. Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *CoRR*, abs/1412.6980, 2015.

[104] Thomas N Kipf and Max Welling. Variational graph auto-encoders. *NIPS Workshop on Bayesian Deep Learning*, 2016.

[105] Gary Kochenberger, Jin-Kao Hao, Fred Glover, Mark Lewis, Zhipeng Lü, Haibo Wang, and Yang Wang. The unconstrained binary quadratic programming problem: a survey. *Journal of Combinatorial Optimization*, 28(1):58–81, Jul 2014.

[106] Gary A. Kochenberger and Fred Glover. *A Unified Framework for Modeling and Solving Combinatorial Optimization Problems: A Tutorial*, pages 101–124. Springer US, Boston, MA, 2006.

[107] Bálint Koczor and Simon C Benjamin. Quantum natural gradient generalised to non-unitary circuits. *arXiv preprint arXiv:1912.08660*, 2019.

[108] Lars Kotthoff. *Algorithm Selection for Combinatorial Search Problems: A Survey*, pages 149–190. Springer International Publishing, Cham, 2016.

[109] Jonas M Kübler, Andrew Arrasmith, Lukasz Cincio, and Patrick J Coles. An adaptive optimizer for measurement-frugal variational algorithms. *Quantum*, 4:263, 2020.

[110] Ryan LaRose, Arkin Tikku, Étude O'Neel-Judy, Lukasz Cincio, and Patrick J Coles. Variational quantum state diagonalization. *npj Quantum Information*, 5(1):1–10, 2019.

[111] Xinwei Lee, Yoshiyuki Saito, Dongsheng Cai, and Nobuyoshi Asai. Parameters fixing strategy for quantum approximate optimization algorithm. In *2021 IEEE International Conference on Quantum Computing and Engineering (QCE)*, pages 10–16, 2021.

[112] Per Kristian Lehre and Xin Yao. Crossover can be constructive when computing unique input–output sequences. *Soft Computing*, 15(9):1675–1687, 2011.

[113] Junde Li, Mahabubul Alam, and Swaroop Ghosh. Large-scale quantum approximate optimization via divide-and-conquer, 2021.

[114] Li Li, Minjie Fan, Marc Coram, Patrick Riley, and Stefan Leichenauer. Quantum Optimization with a Novel Gibbs Objective Function and Ansatz Architecture Search, 2019. arXiv:1909.07621.

[115] Qing-Song Li, Huan-Yu Liu, Qingchun Wang, Yu-Chun Wu, and Guo-Ping Guo. A unified framework of transformations based on the jordan–wigner transformation. *The Journal of Chemical Physics*, 157(13):134104, October 2022.

[116] Jin-Guo Liu and Lei Wang. Differentiable learning of quantum circuit born machines. *Physical Review A*, 98:062324, 2018.

[117] Yunchao Liu, Srinivasan Arunachalam, and Kristan Temme. A rigorous and robust quantum speed-up in supervised machine learning. *Nature Physics*, 17(9):1013–1017, 2021.

[118] S. Lloyd. Least squares quantization in pcm. *IEEE Transactions on Information Theory*, 28(2):129–137, 1982.

[119] Seth Lloyd, Masoud Mohseni, and Patrick Rebentrost. Quantum principal component analysis. *Nature Physics*, 10(9):631–633, September 2014. Number: 9 Publisher: Nature Publishing Group.

[120] Zhipeng Lü, Fred W. Glover, and Jin-Kao Hao. A hybrid metaheuristic approach to solving the ubqp problem. *Eur. J. Oper. Res.*, 207:1254–1262, 2010.

[121] Manuel López-Ibáñez, Jérémie Dubois-Lacoste, Leslie Pérez Cáceres, Mauro Birattari, and Thomas Stützle. The irace package: Iterated racing for automatic algorithm configuration. *Operations Research Perspectives*, 3:43–58, 2016.

[122] Carlos Ortiz Marrero, Mária Kieferová, and Nathan Wiebe. Entanglement-induced barren plateaus. *PRX Quantum*, 2(4):040316, 2021.

[123] Simon C. Marshall, Casper Gyurik, and Vedran Dunjko. High dimensional quantum machine learning with small quantum computers. *CoRR*, abs/2203.13739, 2022.

[124] Andreas Mayer and Svein Ove Aas. andim/noisyopt, May 2017.

[125] Jarrod R McClean, Sergio Boixo, Vadim N Smelyanskiy, Ryan Babbush, and Hartmut Neven. Barren plateaus in quantum neural network training landscapes. *Nature Communications*, 9(1):1–6, 2018.

[126] Jarrod R McClean, Nicholas C Rubin, Kevin J Sung, Ian D Kivlichan, Xavier Bonet-Monroig, Yudong Cao, Chengyu Dai, E Schuyler Fried, Craig Gidney, Brendan Gimby, Pranav Gokhale, Thomas Häner, Tarini Hardikar, Vojtěch Havlíček, Oscar Higgott, Cupjin Huang, Josh Izaac, Zhang Jiang, Xinle Liu, Sam McArdle, Matthew Neeley, Thomas O'Brien, Bryan O'Gorman, Isil Ozfidan, Maxwell D Radin, Jhonathan Romero, Nicolas P D Sawaya, Bruno Senjean, Kanav Setia, Sukin Sim, Damian S Steiger, Mark Steudtner, Qiming Sun, Wei Sun, Daochen Wang, Fang Zhang, and Ryan Babbush. Openfermion: the electronic structure package for quantum computers. *Quantum Sci. Technol.*, 2020.

[127] Matija Medvidovic and Giuseppe Carleo. Classical variational simulation of the quantum approximate optimization algorithm, 2020.

[128] Alexey A. Melnikov, Leonid Fedichkin, and Alexander Alodjants. Predicting quantum advantage by quantum walk with convolutional neural networks. *New Journal of Physics*, 21, 2019.

[129] Stefano Mensa, Emre Sahin, Francesco Tacchino, Panagiotis Kl. Barkoutsos, and Ivano Tavernelli. Quantum machine learning framework for virtual screening in drug discovery: a prospective quantum advantage. *CoRR*, abs/2204.04017, 2022.

[130] K. Mitarai, M. Negoro, M. Kitagawa, and K. Fujii. Quantum circuit learning. *Physical Review A*, 98:032309, 2018.

[131] Kosuke Mitarai, Makoto Negoro, Masahiro Kitagawa, and Keisuke Fujii. Quantum circuit learning. *Physical Review A*, 98(3):032309, 2018.

[132] Tom M. Mitchell. *Machine learning, International Edition*. McGraw-Hill Series in Computer Science. McGraw-Hill, 1997.

[133] Felix Mohr and Jan N. van Rijn. Learning curves for decision making in supervised machine learning - A survey. *CoRR*, abs/2201.12150, 2022.

[134] Nikolaj Moll, Panagiotis Barkoutsos, Lev S. Bishop, Jerry M. Chow, Andrew Cross, Daniel J. Egger, Stefan Filipp, Andreas Fuhrer, Jay M. Gambetta, Marc Ganzhorn, Abhinav Kandala, Antonio Mezzacapo, Peter Müller, Walter Riess, Gian Salis, John Smolin, Ivano Tavernelli, and Kristan Temme. Quantum optimization using variational algorithms on near-term quantum devices. *Quantum Science and Technology*, 2017. arXiv:1710.01022.

[135] Charles Moussa, Henri Calandra, and Vedran Dunjko. To quantum or not to quantum: towards algorithm selection in near-term quantum optimization. *Quantum Science and Technology*, 5(4):044009, 2020.

[136] Charles Moussa, Max Hunter Gordon, Michal Baczyk, M. Cerezo, Lukasz Cincio, and Patrick J. Coles. Resource frugal optimizer for quantum machine learning. *arXiv:2211.04965*, 2022.

[137] Charles Moussa, Jan N. van Rijn, Thomas Bäck, and Vedran Dunjko. Hyperparameter importance of quantum neural networks across small datasets. In Poncelet Pascal and Dino Ienco, editors, *Discovery Science*, pages 32–46, Cham, 2022. Springer Nature Switzerland.

[138] Charles Moussa, Hao Wang, Thomas Bäck, and Vedran Dunjko. Unsupervised strategies for identifying optimal parameters in quantum approximate optimization algorithm. *EPJ Quantum Technology*, 9(1), 2022.

[139] Charles Moussa, Hao Wang, Henri Calandra, Thomas Bäck, and Vedran Dunjko. Tabu-driven quantum neighborhood samplers. In Christine Zarges and Sébastien Verel, editors, *Evolutionary Computation in Combinatorial Optimization*, pages 100–119, Cham, 2021. Springer International Publishing.

[140] Ken M Nakanishi, Keisuke Fujii, and Synge Todo. Sequential minimal optimization for quantum-classical hybrid algorithms. *Physical Review Research*, 2(4):043158, 2020.

[141] Quynh T. Nguyen, Louis Schatzki, Paolo Braccia, Michael Ragone, Martin Larocca, Frederic Sauvage, Patrick J. Coles, and M. Cerezo. A theory for equivariant quantum neural networks. *arXiv preprint arXiv:2210.08566*, 2022.

[142] Michael A. Nielsen and Isaac L. Chuang. *Quantum Computation and Quantum Information*. Cambridge University Press, Cambridge, 2000.

[143] Michael A. Nielsen and Isaac L. Chuang. *Quantum Computation and Quantum Information: 10th Anniversary Edition*. Cambridge University Press, 2011.

[144] Michael A Nielsen et al. The fermionic canonical commutation relations and the jordan-wigner transform. *School of Physical Sciences The University of Queensland*, 59, 2005.

[145] niko, Youhei Akimoto, yoshihikoueno, Dimo Brockhoff, Matthew Chan, and ARF1. Cma-es/pycma: r3.0.3, April 2020.

[146] Randal S. Olson, Nathan Bartley, Ryan J. Urbanowicz, and Jason H. Moore. Evaluation of a Tree-based Pipeline Optimization Tool for Automating Data Science. In *Proceedings of the Genetic and Evolutionary Computation Conference 2016*, GECCO '16, pages 485–492, New York, NY, USA, 2016. ACM.

[147] Gintaras Palubeckis. Multistart tabu search strategies for the unconstrained binary quadratic optimization problem. *Annals of Operations Research*, 131:259–282, 10 2004.

[148] Gintaras Palubeckis. Iterated tabu search for the unconstrained binary quadratic optimization problem. *Informatica (Vilnius)*, 2, 01 2006.

[149] Christos H. Papadimitriou and Mihalis Yannakakis. Optimization, approximation, and complexity classes. *Journal of Computer and System Sciences*, 43(3):425 – 440, 1991.

[150] Tianyi Peng, Aram W. Harrow, Maris Ozols, and Xiaodi Wu. Simulating large quantum circuits on a small quantum computer. *Phys. Rev. Lett.*, 125:150504, Oct 2020.

[151] Adrián Pérez-Salinas, Alba Cervera-Lierta, Elies Gil-Fuster, and José I. Latorre. Data re-uploading for a universal quantum classifier. *Quantum*, 4:226, 2020.

[152] Alberto Peruzzo, Jarrod McClean, Peter Shadbolt, Man-Hong Yung, Xiao-Qi Zhou, Peter J Love, Alán Aspuru-Guzik, and Jeremy L O'brien. A variational eigenvalue solver on a photonic quantum processor. *Nature Communications*, 5(1):1–7, 2014.

[153] Arthur Pesah, M. Cerezo, Samson Wang, Tyler Volkoff, Andrew T Sornborger, and Patrick J Coles. Absence of barren plateaus in quantum convolutional neural networks. *Physical Review X*, 11(4):041011, 2021.

[154] Evan Peters, João Caldeira, Alan Ho, Stefan Leichenauer, Masoud Mohseni, Hartmut Neven, Panagiotis Spentzouris, Doug Strain, and Gabriel N. Perdue. Machine learning of high dimensional data on a noisy quantum processor. *npj Quantum Information*, 7(1):161, 2021.

[155] Svatopluk Poljak and Zsolt Tuza. Maximum cuts and large bipartite subgraphs. *Combinatorial optimization.(DIMACS series in discrete mathematics and theoretical computer science 20.)*, pages 181–244, 1995.

[156] John Preskill. Quantum Computing in the NISQ era and beyond. *Quantum*, 2:79, August 2018.

[157] Michael Ragone, Quynh T. Nguyen, Louis Schatzki, Paolo Braccia, Martin Larocca, Frederic Sauvage, Patrick J. Coles, and M. Cerezo. Representation theory for geometric quantum machine learning. *arXiv preprint arXiv:2210.07980*, 2022.

[158] H. Razip and M. N. Zakaria. Combining approximation algorithm with genetic algorithm at the initial population for np-complete problem. In *2017 IEEE 15th Student Conference on Research and Development (SCOReD)*, pages 98–103, 2017.

[159] Mathys Rennela, Sebastiaan Brand, Alfons Laarman, and Vedran Dunjko. Hybrid divide-and-conquer approach for tree search algorithms, 2020.

[160] Jonathan Romero, Ryan Babbush, Jarrod R McClean, Cornelius Hempel, Peter J Love, and Alán Aspuru-Guzik. Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz. *Quantum Science and Technology*, 4(1):014008, 2018.

[161] Jonathan Romero, Jonathan P Olson, and Alan Aspuru-Guzik. Quantum autoencoders for efficient compression of quantum data. *Quantum Science and Technology*, 2(4):045001, 2017.

[162] Gili Rosenberg, Mohammad Vazifeh, Brad Woods, and Eldad Haber. Building an iterative heuristic solver for a quantum annealer. *Computational Optimization and Applications*, 65:845–869, 2016.

[163] Manas Sajjan, Junxu Li, Raja Selvarajan, Shree Hari Sureshbabu, Sumit Suresh Kale, Rishabh Gupta, and Sabre Kais. Quantum computing enhanced machine learning for physico-chemical applications. *CoRR*, arXiv:2111.00851, 2021.

[164] Andrea Saltelli and I.M. Sobol. Sensitivity analysis for nonlinear mathematical models: Numerical experience. *Matematicheskoe Modelirovanie*, 7, 1995.

[165] A. L. Samuel. Some studies in machine learning using the game of checkers. *IBM Journal of Research and Development*, 3(3):210–229, 1959.

[166] Raffaele Santagati, Alan Aspuru-Guzik, Ryan Babbush, Matthias Degroote, Leticia Gonzalez, Elica Kyoseva, Nikolaj Moll, Markus Oppel, Robert M. Parrish, Nicholas C. Rubin, Michael Streif, Christofer S. Tautermann, Horst Weiss, Nathan Wiebe, and Clemens Utschig-Utschig. Drug design on quantum computers, 2023.

[167] Frederic Sauvage, Sukin Sim, Alexander A. Kunitsa, William A. Simon, Marta Mauri, and Alejandro Perdomo-Ortiz. Flip: A flexible initializer for arbitrarily-sized parametrized quantum circuits, 2021.

[168] N. Schetakis, D. Aghamalyan, M. Boguslavsky, and P. Griffin. Binary classifiers for noisy datasets: a comparative study of existing quantum machine learning frameworks and some new approaches. *CoRR*, abs/2111.03372, 2021.

[169] Maria Schuld, Ville Bergholm, Christian Gogolin, Josh Izaac, and Nathan Killoran. Evaluating analytic gradients on quantum hardware. *Physical Review A*, 99(3):032331, 2019.

[170] Maria Schuld, Alex Bocharov, Krysta M Svore, and Nathan Wiebe. Circuit-centric quantum classifiers. *Physical Review A*, 101(3):032308, 2020.

[171] Maria Schuld and Nathan Killoran. Is quantum advantage the right goal for quantum machine learning? *Corr*, abs/2203.01340, 2022.

[172] Maria Schuld, Ilya Sinayskiy, and Francesco Petruccione. The quest for a quantum neural network. *Quantum Information Processing*, 13(11):2567–2586, 2014.

[173] Maria Schuld, Ilya Sinayskiy, and Francesco Petruccione. An introduction to quantum machine learning. *Contemporary Physics*, 56(2):172–185, 2015.

[174] Maria Schuld, Ryan Sweke, and Johannes Jakob Meyer. Effect of data encoding on the expressive power of variational quantum-machine-learning models. *Physical Review A*, 103:032430, 2021.

[175] Abhinav Sharma, Jan N. van Rijn, Frank Hutter, and Andreas Müller. Hyperparameter importance for image classification by residual neural networks. In *Discovery Science - 22nd International Conference*, volume 11828 of *Lecture Notes in Computer Science*, pages 112–126. Springer, 2019.

[176] Kunal Sharma, M. Cerezo, Lukasz Cincio, and Patrick J Coles. Trainability of dissipative perceptron-based quantum neural networks. *Physical Review Letters*, 128(18):180505, 2022.

[177] Ruslan Shaydulin, Ilya Safro, and Jeffrey Larson. Multistart Methods for Quantum Approximate Optimization, 2019. arXiv:1905.08768.

[178] Ruslan Shaydulin, Hayato Ushijima-Mwesigwa, Ilya Safro, Susan Mniszewski, and Yuri Alexeev. Quantum Local Search for Graph Community Detection. In *APS March Meeting Abstracts*, volume 2019 of *APS Meeting Abstracts*, page C42.009, January 2019.

[179] Sukin Sim, Peter D. Johnson, and Alán Aspuru-Guzik. Expressibility and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms. *Advanced Quantum Technologies*, 2(12):1900070, 2019.

[180] Andrea Skolik, Sofiene Jerbi, and Vedran Dunjko. Quantum agents in the gym: a variational quantum algorithm for deep q-learning. *CoRR*, abs/2103.15084, 2021.

[181] I. M. Sobol. Sensitivity estimates for nonlinear mathematical models. *Mathematical Modelling and Computational Experiments*, 1(4):407–414, 1993.

[182] J. C. Spall. Multivariate stochastic approximation using a simultaneous perturbation gradient approximation. *IEEE Transactions on Automatic Control*, 37(3):332–341, 1992.

[183] James C Spall. An overview of the simultaneous perturbation method for efficient optimization. *Johns Hopkins apl technical digest*, 19(4):482–492, 1998.

[184] Daniel Stilck França and Raul Garcia-Patron. Limitations of optimization algorithms on noisy quantum devices. *Nature Physics*, 17(11):1221–1227, 2021.

[185] James Stokes, Josh Izaac, Nathan Killoran, and Giuseppe Carleo. Quantum natural gradient. *Quantum*, 4:269, 2020.

[186] Michael Streif and Martin Leib. Comparison of QAOA with Quantum and Simulated Annealing, 2019. arXiv:1901.01903.

[187] Michael Streif and Martin Leib. Training the quantum approximate optimization algorithm without access to a quantum processing unit, 2019.

[188] Ryan Sweke, Jean-Pierre Seifert, Dominik Hangleiter, and Jens Eisert. On the quantum versus classical learnability of discrete distributions. *Quantum*, 5:417, 2021.

[189] Ryan Sweke, Frederik Wilde, Johannes Jakob Meyer, Maria Schuld, Paul K Fährmann, Barthélémy Meynard-Piganeau, and Jens Eisert. Stochastic gradient descent for hybrid quantum-classical optimization. *Quantum*, 4:314, 2020.

[190] AV Uvarov and Jacob D Biamonte. On barren plateaus and cost function locality in variational quantum algorithms. *Journal of Physics A: Mathematical and Theoretical*, 54(24):245301, 2021.

[191] Laurens van der Maaten and Geoffrey Hinton. Visualizing data using t-sne. *Journal of Machine Learning Research*, 9(86):2579–2605, 2008.

[192] Jan N. van Rijn and Frank Hutter. Hyperparameter importance across datasets. In *Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, KDD 2018*, pages 2367–2376. ACM, 2018.

[193] Guillaume Verdon, Michael Broughton, Jarrod R. McClean, Kevin J. Sung, Ryan Babbush, Zhang Jiang, Hartmut Neven, and Masoud Mohseni. Learning to learn with quantum neural networks via classical neural networks, 2019. arXiv: 1907.05415.

[194] Hanrui Wang, Jiaqi Gu, Yongshan Ding, Zirui Li, Frederic T. Chong, David Z. Pan, and Song Han. Quantumnat: Quantum noise-aware training with noise injection, quantization and normalization. *CoRR*, abs/2110.11331, 2021.

[195] Hanrui Wang, Zirui Li, Jiaqi Gu, Yongshan Ding, David Z. Pan, and Song Han. Qoc: Quantum on-chip training with parameter shift and gradient pruning. *CoRR*, abs/2202.13239, 2022.

[196] Minjie Wang, Da Zheng, Zihao Ye, Quan Gan, Mufei Li, Xiang Song, Jinjing Zhou, Chao Ma, Lingfan Yu, Yu Gai, Tianjun Xiao, Tong He, George Karypis, Jinyang Li, and Zheng Zhang. Deep graph library: A graph-centric, highly-performant package for graph neural networks. *arXiv preprint arXiv:1909.01315*, 2019.

[197] Samson Wang, Enrico Fontana, M. Cerezo, Kunal Sharma, Akira Sone, Lukasz Cincio, and Patrick J Coles. Noise-induced barren plateaus in variational quantum algorithms. *Nature Communications*, 12(1):1–11, 2021.

[198] Yang Wang, Zhipeng Lü, Fred W. Glover, and Jin-Kao Hao. Path relinking for unconstrained binary quadratic programming. *Eur. J. Oper. Res.*, 223:595–604, 2012.

[199] Richard A. Watson and Thomas Jansen. A building-block royal road where crossover is provably essential. In *Proc. of Genetic and Evolutionary Computation Conference (GECCO'07)*, pages 1452–1459. ACM, 2007.

[200] Dave Wecker, Matthew B. Hastings, and Matthias Troyer. Progress towards practical quantum variational algorithms. *Physical Review A*, 92:042303, Oct 2015.

[201] Madita Willsch, Dennis Willsch, Fengping Jin, Hans De Raedt, and Kristel Michielsen. Benchmarking the quantum approximate optimization algorithm. *Quantum Information Processing*, 19(7):197, Jun 2020.

[202] Leonard Wossnig. Quantum machine learning for classical data. *CoRR*, abs/2105.03684, 2021.

[203] Cheng Xue, Zhao-Yun Chen, Yu-Chun Wu, and Guo-Ping Guo. Effects of Quantum Noise on Quantum Approximate Optimization Algorithm, 2019. arXiv:1909.02196.

[204] Sheir Yarkoni, Elena Raponi, Thomas Bäck, and Sebastian Schmitt. Quantum annealing for industry applications: introduction and review. *Reports on Progress in Physics*, 85(10):104001, sep 2022.

[205] Jie Zhou, Ganqu Cui, Shengding Hu, Zhengyan Zhang, Cheng Yang, Zhiyuan Liu, Lifeng Wang, Changcheng Li, and Maosong Sun. Graph neural networks: A review of methods and applications, 2018.

[206] Leo Zhou, Sheng-Tao Wang, Soonwon Choi, Hannes Pichler, and Mikhail D. Lukin. Quantum Approximate Optimization Algorithm: Performance, Mechanism, and Implementation on Near-Term Devices, 2018. arXiv:1812.01041.

[207] Leo Zhou, Sheng-Tao Wang, Soonwon Choi, Hannes Pichler, and Mikhail D. Lukin. Quantum approximate optimization algorithm: Performance, mechanism, and implementation on near-term devices, 2018. arXiv:1812.01041.

[208] Christa Zoufal, Aurélien Lucchi, and Stefan Woerner. Quantum generative adversarial networks for learning and loading random distributions. *npj Quantum Information*, 5(1):103, 2019.