Skoltech
Skolkovo Institute of Science and Technology

Thesis Changes Log

Name of Candidate: Evgenii Tsymbalov

PhD Program: Computational and Data Science and Engineering

Title of Thesis: Machine learning for elastic strain engineering

Supervisor: Associate Professor Alexander Shapeev

The thesis document includes the following changes in answer to the external review process.

I have corrected numerous typos and misprints as well as refined the bibliography list, as was pointed out by Jury members. Please find the changes log below:

Publications list:

- "Dropout Strikes Back: Improved Uncertainty Estimation via Diversity Sampled Implicit Ensembles": manuscript status changed from "Submitted to NeurIPS" to "In preparation";

Acknowledgements, page 9:

- "… Nadezhda Dontsu, Elena Ditte and many others …" → "… Nadezhda Dontsu, Elena Ditte, and many others …";
- "… for supporting me the in times of administrative troubles …" → "… for supporting me in times of administrative troubles …";
- "… for taking time to review my thesis and invaluable remarks and suggestions." → "… for taking the time to review my thesis and for invaluable remarks and suggestions."

Section 1.1
Page 10

- "For the last few decades, a microworld became a point of interest for the physicists." → "For the last few decades, a microworld became a point of interest for physicists.";

Section 1.2
Page 11

- "… one also need to work …" → "… one also needs to work …";

Section 1.3
Page 12

- "… findings in this area.This chapter …" → "…findings in this area. This chapter …";
- "… as the selected approaches to the training … " → "…as the selected approaches to the model training …";
- "… are provided in a Chapter 8." → "…are provided in Chapter 8.";

Section 2.2.1
Page 19

- Citation fixed: "(Perdew et al., 1996a)" → "(Perdew et al., 1996)";

Section 2.3.3
Page 27

- Citation fixed: “(Paszke et al., 2019b)” → “(Paszke et al., 2019)”;

Section 2.3.4
Page 28

- Citation fixed: “(Matthews et al., 2018a)” → “(Matthews et al., 2018)”;
- Citation fixed: “(Hafner et al., 2018b)” → “(Hafner et al., 2018)”;
- Citation fixed: “(Lee et al., 2017a)” → “(Lee et al., 2018)”;
- Citation fixed: “(Garnelo et al., 2018a)” → “(Garnelo et al., 2018)”;
- Citation fixed: “(Sun et al., 2018a)” → “(Sun et al., 2018)”;

Page 29

- Citations fixed: “Matthews et al. (2018b); Lee et al. (2017b)” → “Matthews et al. (2018); Lee et al. (2017)”;
- Citations fixed: “(Sun et al., 2018b; Garnelo et al., 2018b)” → “(Sun et al., 2018; Garnelo et al., 2018)”;
- “nad” → “and”;
- Citation fixed: “(Gal and Ghahramani, 2016a)” → “(Gal and Ghahramani, 2016)”;
- Citation fixed: “Gal (2016a)” → “Gal (2016)”;

Section 4.2.1
Page 45

- Citation fixed: “(Perdew et al., 1996b)” → “(Perdew et al., 1996)”;

Section 4.3.2
Page 51

- Citation fixed: “(Perdew et al., 1996b)” → “(Perdew et al., 1996)”;

Section 5.1
Page 57

- Citation fixed: “Paszke et al. (2019b)” → “Paszke et al. (2019)”;

Section 5.1.2
Page 61

- Citation fixed: “He et al. (2016a)” → “He et al. (2016)”;

Section 5.2.2
Page 66

- Citation fixed: “(Gal and Ghahramani, 2016b;” → “(Gal and Ghahramani, 2016;”;

Section 5.2.3
Page 73

- Citations fixed: “… in Matthews et al. (2018b) and Lee et al. (2017b), …” → “… in Matthews et al. (2018) and Lee et al. (2017), …”;

Section 5.2.5:
Page 76

- Subsubsections “Uncertainty estimation and diversification” and “Active learning” are now just a part of Section 5.2.5 (not indented as subsubsections);
- Classification metrics moved to the Appendix F devoted to image classification experiments;

Section 5.3.2
Page 82

- Citation fixed: “(Gal, 2016a)” → “(Gal, 2016)”;
- Citation fixed: “Hafner et al. (2018a)” → “Hafner et al. (2018)”;

Page 83

- Citation fixed: “(Gal, 2016b)” → “(Gal, 2016)”;

Section 5.4
Page 84
- Citation fixed: “(Gal, 2016a)” → “(Gal, 2016)”;

Section 6.4.1
Page 100
- Citation fixed: “Hafner et al. (2018a)” → “Hafner et al. (2018)”;

Section 8.1
Page 123
- “… an accuracy superior to the one of the specialized model …“ → “…an accuracy superior to one of the specialized model …“;

Page 124
- “… transitions induced by the strain, and used our model …” → “…transitions induced by the strain and used our model …”;

Section 8.2.2
Page 125
- “… yet the abilities for the thorough processing, cleaning, and selection are not.” → “… yet the abilities for processing, cleaning, and selection are not.”;

Page 126
- Citation fixed: “(Hafner et al., 2018b)” → “(Hafner et al., 2018)”;

Bibliography
General changes:
- Improved chemical formulae printing in articles’ titles.

Page 128
- “… with the atlas detector at the lhc.” → “with the ATLAS detector at the LHC.”;
- “… properties of 2d materials …” → “… properties of 2D materials …”;
- “… A python framework …” → “… A Python framework …”;

Page 129
- “Rademacher and gaussian complexities …” → “Rademacher and Gaussian complexities …”;
- “… network is np-complete.” → “… network is NP-complete.”;

Page 130
- “Bypassing the kohn-sham equations …” → “Bypassing the Kohn-Sham equations …”;
- “… based on Gaussian processes” → “… based on Gaussian processes”;
- “Jumping nlp curves: …” → “Jumpling NLP curves: …”;

Page 131
- “Xgboost: …” → “XGBoost: …”;
- “Mxnet: …” → “MXNet: …”;

Page 132
- “… for improving condition?based maintenance …” → “… for improving condition-based maintenance …”;
- “Aflowlib.org: …” → “AFLOWLIB.ORG: …”;
- “Maximum likelihood from incomplete data via the em algorithm.” → “Maximum likelihood from incomplete data via the EM algorithm.”;

Page 133
- “Uci machine learning repository” → “UCI machine learning repository”;
- Citations merged: Gal, Y. (2016a), Gal, Y. (2016b);
- “Dropout as a bayesian approximation …” → “Dropout as a Bayesian approximation …”;
- “Deep bayesian active learning …” → “Deep Bayesian active learning …”;
- “Implementing the nelder-mead simplex algorithm with adaptive parameters.” → “Implementing the Nelder-Mead simplex algorithm with adaptive parameters.”;

Page 134

- "Dppy: Dpp sampling with python." → "DPPy: DPP sampling with Python.";

Page 135

- "Energy gaps and a zero-field quantum hall effect in graphene by strain engineering." → "Energy gaps and a zero-field quantum Hall effect in graphene by strain engineering.";
- "Elastic properties of van der waals epitaxy grown bismuth telluride 2d nanosheets." → "Elastic properties of van der Waals epitaxy grown bismuth telluride 2D nanosheets.";
- Citations merged: Hafner et al. (2018a), Hafner et al. (2018b);
- Citations merged: He et al. (2016a), He et al. (2016b);

Page 136

- "Why relu networks …" → "Why ReLU networks …";
- "scalable learning of bayesian neural networks." → "scalable learning of Bayesian neural networks.";
- "Assessment of the heyd–scuseria–ernzerhof screened coulomb hybrid functional." → "Assessment of the Heyd–Scuseria–Ernzerhof screened Coulomb hybrid functional.";

Page 137

- "Lightgbm: …" → "LightGBM: …";

Page 138

- "The mnist database of handwritten digits." → "The MNIST database of handwritten digits.";

Page 139

- "… using the gw-approximation." → "… using the GW-approximation.";
- "A bayesian encourages dropout." → "A Bayesian encourages dropout.";
- Citations merged: Matthews et al. (2018a), Matthews et al. (2018b);
- "Prediction of dispersion relation and pbgs in 2-d pcs by using artificial neural networks." → "Prediction of dispersion relation and PBGs in 2D PCs by using artificial neural networks.";
- "Mdl-based decision tree pruning." → "MDL-based decision tree pruning.";

Page 140

- "Multiscale computational understanding and growth of 2d materials: a review." → "Multiscale computational understanding and growth of 2D materials: a review.";
- "Structured bayesian pruning via log-normal multiplicative noise" → "Structured Bayesian pruning via log-normal multiplicative noise";

Page 141

- Citations merged: Paszke et al. (2019a), Paszke et al. (2019b);
- "Pytorch: An imperative style, high-performance deep learning library." → "PyTorch: An imperative style, high-performance deep learning library.";

Page 142

- Citations merged: Perdew, J.P., Burke, K., and Ernzerhof, M. (1996a), (1996b);
- "Catboost: unbiased boosting with categorical features." → "CatBoost: unbiased boosting with categorical features.";

Page 143

- "gdb-17" → "GDB-17";

Page 144

- "Implementation and performance of the frequency-dependent gw method within the paw framework." → "Implementation and performance of the frequency-dependent GW method within the PAW framework.";
- "Ani-1: an extensible neural network potential with dft accuracy at force field computational cost." → "ANI-1: an extensible neural network potential with DFT accuracy at force field computational cost.";

Page 145

- Citations merged: Sun et al. (2018a), Sun et al. (2018b);

Page 146

- "Scipy 1.0: fundamental algorithms for scientific computing in python." → "SciPy 1.0: fundamental algorithms for scientific computing in Python.";

Page 147

- "Fashion-mnist" → "Fashion-MNIST";
- "A new hybrid exchange–correlation functional using the coulomb-attenuating method (cam-b3lyp)" → "A new hybrid exchange–correlation functional using the Coulomb-attenuating method (CAM-B3LYP)";

- “Model gw band structure of inas and gaas …” → “Model GW band structure of InAs and GaAs …”;

Appendix F
Page 158

- Classification metrics description is added.