Transparency and reproducibility in artificial intelligence

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Benjamin Haibe-Kains[1,2,3,4,5]✉, George Alexandru Adam[3,5], Ahmed Hosny[6,7], Farnoosh Khodakarami[1,2], Massive Analysis Quality Control (MAQC) Society Board of Directors*, Levi Waldron[8], Bo Wang[2,3,5,9,10], Chris McIntosh[2,5,9], Anna Goldenberg[3,5,11,12], Anshul Kundaje[13,14], Casey S. Greene[15,16], Tamara Broderick[17], Michael M. Hoffman[1,2,3,5], Jeffrey T. Leek[18], Keegan Korthauer[19,20], Wolfgang Huber[21], Alvis Brazma[22], Joelle Pineau[23,24], Robert Tibshirani[25,26], Trevor Hastie[25,26], John P. A. Ioannidis[25,26,27,28,29], John Quackenbush[30,31,32] & Hugo J. W. L. Aerts[6,7,33,34]

ARISING FROM S. M. McKinney et al. *Nature* https://doi.org/10.1038/s41586-019-1799-6 (2020)

Breakthroughs in artificial intelligence (AI) hold enormous potential as it can automate complex tasks and go even beyond human performance. In their study, McKinney et al.[1] showed the high potential of AI for breast cancer screening. However, the lack of details of the methods and algorithm code undermines its scientific value. Here, we identify obstacles that hinder transparent and reproducible AI research as faced by McKinney et al.[1], and provide solutions to these obstacles with implications for the broader field.

The work by McKinney et al.[1] demonstrates the potential of AI in medical imaging, while highlighting the challenges of making such work reproducible. The authors assert that their system improves the speed and robustness of breast cancer screening, generalizes to populations beyond those used for training, and outperforms radiologists in specific settings. Upon successful prospective clinical validation and approval by regulatory bodies, this new system holds great potential for streamlining clinical workflows, reducing false positives, and improving patient outcomes. However, the absence of sufficiently documented methods and computer code underlying the study effectively undermines its scientific value. This shortcoming limits the evidence required for others to prospectively validate and clinically implement such technologies. By identifying obstacles hindering transparent and reproducible AI research as faced by McKinney et al.[1], we provide potential solutions with implications for the broader field.

Scientific progress depends on the ability of independent researchers to scrutinize the results of a research study, to reproduce the study's main results using its materials, and to build on them in future studies (https://www.nature.com/nature-research/editorial-policies/reporting-standards). Publication of insufficiently documented research does not meet the core requirements underlying scientific discovery[2,3]. Merely textual descriptions of deep-learning models can hide their high level of complexity. Nuances in the computer code may have marked effects on the training and evaluation of results[4], potentially leading to unintended consequences[5]. Therefore, transparency in the form of the actual computer code used to train a model and arrive at its final set of parameters is essential for research reproducibility. McKinney et al.[1] stated that the code used for training the models has "a large number of dependencies on internal tooling, infrastructure and hardware", and claimed that the release of the code was therefore not possible. Computational reproducibility is indispensable for high-quality AI applications[6,7]; more complex methods demand greater transparency[8]. In the absence of code, reproducibility falls back on replicating methods from textual description. Although, McKinney and colleagues[1] claim that all experiments and implementation details were described in sufficient detail in the supplementary methods section of their Article[1] to "support replication with non-proprietary libraries", key details about their analysis are lacking. Even with extensive description, reproducing complex computational pipelines based purely on text is a subjective and challenging task[9].

In addition to the reproducibility challenges inherent to purely textual descriptions of methods, the description by McKinney et al.[1] of the model development as well as data processing and training pipelines lacks crucial details. The definitions of several hyperparameters for the model's architecture (composed of three networks referred to as the breast, lesion and case models) are missing (Table 1). In their

[1]Princess Margaret Cancer Centre, University Health Network, Toronto, Ontario, Canada. [2]Department of Medical Biophysics, University of Toronto, Toronto, Ontario, Canada. [3]Department of Computer Science, University of Toronto, Toronto, Ontario, Canada. [4]Ontario Institute for Cancer Research, Toronto, Ontario, Canada. [5]Vector Institute for Artificial Intelligence, Toronto, Ontario, Canada. [6]Artificial Intelligence in Medicine (AIM) Program, Brigham and Women's Hospital, Harvard Medical School, Boston, MA, USA. [7]Radiation Oncology and Radiology, Dana-Farber Cancer Institute, Brigham and Women's Hospital, Harvard Medical School, Boston, MA, USA. [8]Department of Epidemiology and Biostatistics and Institute for Implementation Science in Population Health, CUNY Graduate School of Public Health and Health Policy, New York, NY, USA. [9]Peter Munk Cardiac Centre, University Health Network, Toronto, Ontario, Canada. [10]Department of Laboratory Medicine and Pathobiology, University of Toronto, Ontario, Canada. [11]SickKids Research Institute, Toronto, Ontario, Canada. [12]Child and Brain Development Program, CIFAR, Toronto, Ontario, Canada. [13]Department of Genetics, Stanford University School of Medicine, Stanford, CA, USA. [14]Department of Computer Science, Stanford University, Stanford, CA, USA. [15]Dept. of Systems Pharmacology and Translational Therapeutics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA, USA. [16]Childhood Cancer Data Lab, Alex's Lemonade Stand Foundation, Philadelphia, PA, USA. [17]Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, MA, USA. [18]Department of Biostatistics, Johns Hopkins Bloomberg School of Public Health, Baltimore, MD, USA. [19]Department of Statistics, University of British Columbia, Vancouver, British Columbia, Canada. [20]BC Children's Hospital Research Institute, Vancouver, British Columbia, Canada. [21]European Molecular Biology Laboratory, Genome Biology Unit, Heidelberg, Germany. [22]European Molecular Biology Laboratory, European Bioinformatics Institute, EMBL-EBI, Hinxton, UK. [23]McGill University, Montreal, Quebec, Canada. [24]Montreal Institute for Learning Algorithms, Quebec, Canada. [25]Department of Statistics, Stanford University School of Humanities and Sciences, Stanford, CA, USA. [26]Department of Biomedical Data Science, Stanford University School of Medicine, Stanford, CA, USA. [27]Department of Medicine, Stanford University School of Medicine, Stanford, CA, USA. [28]Meta-Research Innovation Center at Stanford (METRICS), Stanford, CA, USA. [29]Department of Epidemiology and Population Health, Stanford University School of Medicine, Stanford, CA, USA. [30]Department of Biostatistics, Harvard T.H Chan School of Public Health, Boston, MA, USA. [31]Channing Division of Network Medicine, Brigham and Women's Hospital, Boston, MA, USA. [32]Department of Data Science, Dana-Farber Cancer Institute, Boston, MA, USA. [33]Radiology and Nuclear Medicine, Maastricht University, Maastricht, The Netherlands. [34]Cardiovascular Imaging Research Center, Massachusetts General Hospital, Harvard Medical School, Boston, MA, USA. *A list of authors and their affiliations appears at the end of the paper. ✉e-mail: bhaibeka@uhnresearch.ca

Table 1 | Essential hyperparameters for reproducing the study for each of the three models

	Lesion	Breast	Case
Learning rate	Missing	0.0001	Missing
Learning rate schedule	Missing	Stated	Missing
Optimizer	Stochastic gradient descent with momentum	Adam	Missing
Momentum	Missing	Not applicable	Not applicable
Batch size	4	Unclear	2
Epochs	Missing	120,000	Missing

Table 2 | Frameworks to share code, software dependencies and deep-learning models

Resource	URL
Code	
BitBucket	https://bitbucket.org
GitHub	https://github.com
GitLab	https://about.gitlab.com
Software dependencies	
Conda	https://conda.io
Code Ocean	https://codeocean.com
Gigantum	https://gigantum.com
Colaboratory	https://colab.research.google.com
Deep-learning models	
TensorFlow Hub	https://www.tensorflow.org/hub
ModelHub	http://modelhub.ai
ModelDepot	https://modeldepot.io
Model Zoo	https://modelzoo.co
Deep-learning frameworks	
TensorFlow	https://www.tensorflow.org/
Caffe	https://caffe.berkeleyvision.org/
PyTorch	https://pytorch.org/

publication, McKinney et al.[1] did not disclose the settings for the augmentation pipeline; the transformations used are stochastic and can considerably affect model performance[10]. Details of the training pipeline were also missing. Without this key information, independent reproduction of the training pipeline is not possible.

Numerous frameworks and platforms exist to make artificial intelligence research more transparent and reproducible (Table 2). For the sharing of code, these include Bitbucket, GitHub and GitLab, among others. The many software dependencies of large-scale machine learning applications require appropriate control of the software environment, which can be achieved through package managers including Conda, as well as container and virtualization systems, including Code Ocean, Gigantum, Colaboratory and Docker. If virtualization of the McKinney et al.[1] internal tooling proved to be difficult, they could have released the computer code and documentation. The authors could have also created small artificial examples or used small public datasets[11] to show how new data must be processed to train the model and generate predictions. Sharing the fitted model (architecture along with learned parameters) should be simple aside from privacy concerns that the model may reveal sensitive information about the set of patients used to train it. Nevertheless, techniques for achieving differential privacy exist to alleviate such concerns. Many platforms allow sharing of deep learning models, including TensorFlow Hub, ModelHub.ai, ModelDepot and Model Zoo with support for several frameworks such as PyTorch and Caffe, as well as the TensorFlow library used by the authors. In addition to improving accessibility and transparency, such resources can considerably accelerate model development, validation and transition into production and clinical implementation.

Another crucial aspect of ensuring reproducibility lies in access to the data the models were derived from. In their study, McKinney et al.[1] used two large datasets under license, properly disclosing this limitation in their publication. The sharing of patient health information is highly regulated owing to privacy concerns. Despite these challenges, the sharing of raw data has become more common in biomedical literature, increasing from under 1% in the early 2000s to 20% today[12]. However, if the data cannot be shared, the model predictions and data labels themselves should be released, allowing further statistical analyses. Above all, concerns about data privacy should not be used as a way to distract from the requirement to release code.

Although sharing of code and data are widely seen as a crucial part of scientific research, the adoption varies across fields. In fields such as genomics, complex computational pipelines and sensitive datasets have been shared for decades[13]. Guidelines related to genomic data are clear, detailed and, most importantly, enforced. It is generally accepted that all code and data are released alongside a publication. In other fields of medicine and science as a whole, this is much less common, and data and code are rarely made available. For scientific efforts in which a clinical application is envisioned and human lives would be at stake, we argue that the bar of transparency should be set even higher. If a dataset cannot be shared with the entire scientific community, because of licensing or other insurmountable issues, at a minimum a mechanism should be set so that some highly-trained, independent investigators can access the data and verify the analyses.

The lack of access to code and data in prominent scientific publications may lead to unwarranted and even potentially harmful clinical trials[14]. These unfortunate lessons have not been lost on journal editors and their readers. Journals have an obligation to hold authors to the standards of reproducibility that benefit not only other researchers, but also the authors themselves. Making one's methods reproducible may surface biases or shortcomings to authors before publication[5]. Preventing external validation of a model will likely reduce its impact, as it also prevents other researchers from using and building upon it in future studies. The failure of McKinney et al. to share key materials and information transforms their work from a scientific publication open to verification and adoption by the scientific community into a promotion of a closed technology.

We have high hopes for the utility of AI methods in medicine. Ensuring that these methods meet their potential, however, requires that these studies be scientifically reproducible. The recent advances in computational virtualization and AI frameworks are greatly facilitating the implementations of complex deep neural networks in a more structured, transparent, and reproducible way. Adoption of these technologies will increase the impact of published deep-learning algorithms and accelerate the translation of these methods into clinical settings.

Reporting summary

Further information on research design is available in the Nature Research Reporting Summary linked to this paper.

Data availability

No data have been generated as part of this manuscript.

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Author contributions B.H.-K. and G.A.A. wrote the first draft of the manuscript. B.H.-K. and H.J.W.L.A. designed and supervised the study. A.H., F.K., T.S., R.K., S.-A.S., W.T., R.D.W., C.E.M., W.J., J.D., C.F., L.W., B.W., C. McIntosh, A.G., A.K., C.S.G., T.B., M.M.H., J.T.L., K.K., W.H., A.B., J.P., R.T., T.H., J.P.A.I. and J.Q. contributed to the writing of the manuscript.

Competing interests A.H. is a shareholder of and receives consulting fees from Altis Labs. M.M.H. received a GPU Grant from Nvidia. H.J.W.L.A. is a shareholder of and receives consulting fees from Onc.AI. B.H.K. is a scientific advisor for Altis Labs. C.M. holds an equity position in Bridge7Oncology and receives royalties from RaySearch Laboratories. A.K. is on the SAB of ImmuneAI Inc, a consultant for Biogen Inc., a scientific co-founder of RavelBio Inc. and a shareholder of Freenome Inc. G.A.A., F.K., L.W., B.W., C.S.G., J.T.L., W.H., A.B., J.P., R.T., T.H., J.P.A.I. and J.Q. declare no other competing interests related to the manuscript.

Additional information
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[35]National Center for Toxicological Research, US Food and Drug Administration, Jefferson, AR, USA. [36]Immuneering Corporation, Cambridge, MA, USA. [37]Engineering Science Department, Oxford e-Research Centre, University of Oxford, Oxford, UK. [38]SAS Institute Inc, Cary, NC, USA. [39]Weill Cornell Medicine, New York, NY, USA. [40]Q2 Solutions, Morrisville, NC, USA. [41]Hospital Virgen del Rocio, Sevilla, Spain. [42]Fondazione Bruno Kessler, Trento, Italy.

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Reporting Summary

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Our web collection on statistics for biologists contains articles on many of the points above.

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Data collection	No data have been generated as part of this manuscript.
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n/a	Involved in the study
☒	☐ ChIP-seq
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Reply to: Transparency and reproducibility in artificial intelligence

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Check for updates

Scott Mayer McKinney[1]✉, Alan Karthikesalingam[2], Daniel Tse[1], Christopher J. Kelly[2], Yun Liu[1], Greg S. Corrado[1] & Shravya Shetty[1]✉

REPLYING TO B. Haibe-Kains et al. *Nature* https://doi.org/10.1038/s41586-020-2766-y (2020)

We thank the authors of the accompanying Comment[1] for their interest in our work[2] and their thoughtful contribution. We agree that transparency and reproducibility are paramount for scientific progress. In keeping with this principle, the largest data source used in our publication is available to the academic community. Any researcher can apply for access to the OPTIMAM database (https://medphys.royalsurrey.nhs.uk/omidb/getting-access), which our institution helped fund. The broad accessibility of the database was part of the reason we pursued this collaboration. In fact, since our article came out, another group has already published results on this very dataset[3].

The other dataset, from the United States, was shared with our research team after approval from the hospital system's Institutional Review Board (IRB). The IRB judged that the potential benefits of the research outweighed the minimal privacy risks associated with sharing de-identified data with a trusted party capable of and committed to safeguarding these data. As the authors understand, we are not at liberty to share data that we do not own. More generally, widely releasing data considerably alters the risk–benefit calculus for patients, so institutions must be thoughtful about how and when they do this. Because of these considerations, large medical image datasets with associated breast cancer outcomes are rarely made openly available[3–5]. However, as our support for the OPTIMAM database demonstrates, we endorse such efforts where practical. Although there are some small, publicly available mammography datasets[6], restricting published research to such datasets would provide an extremely limited picture of an algorithm's clinical applicability.

The commenters[1] asked for more information concerning the training of our deep learning models. We strove to document all relevant machine learning methods while keeping the paper accessible to a clinical and general scientific audience. We thank the authors for highlighting the omission of some hyperparameters. We have supplied the requested methodological details and further elaborated on our data augmentation strategies in an Addendum[7] to our original Article[2].

The authors of the Comment[1] suggest open-sourcing all the code associated with this project. Most of our work builds on open-source implementations, such as ResNet (https://github.com/tensorflow/models/blob/master/research/slim/nets/resnet_v1.py), MobileNet (https://github.com/tensorflow/models/blob/master/research/slim/nets/mobilenet/mobilenet_v2.py), multidimensional image augmentation (https://github.com/deepmind/multidim-image-augmentation), and the Tensorflow Object Detection API (https://github.com/tensorflow/models/tree/master/research/object_detection), all of which were released by our institution. Much of the remaining code concerns data input–output and the orchestration of the training process across internal compute clusters, both of which are of scant scientific value and limited utility to researchers outside our organization. Given the extensive textual description in the supplementary information of our Article[2], we believe that investigators proficient in deep learning should be able to learn from and expand upon our approach.

The authors[1] further suggest releasing a containerized version of our model for others to apply to new images. It is important to note that regulators commonly classify technologies such as the one proposed here as 'medical device software' or 'software as a medical device'. Unfortunately, the release of any medical device without appropriate regulatory oversight could lead to its misuse. As such, doing so would overlook material ethical concerns. Because liability issues surrounding artificial intelligence in healthcare remain unresolved[8], providing unrestricted access to such technologies may place patients, providers, and developers at risk. In addition, the development of impactful medical technologies must remain a sustainable venture to promote a vibrant ecosystem that supports future innovation. Parallels to hardware medical devices and pharmaceuticals may be useful to consider in this regard. Finally, increasing evidence suggests that a model's learned parameters may inadvertently expose properties of its training set to attack; how to safeguard potentially susceptible models is the subject of active research[9]. As our training data are private or under restricted access, sharing the model openly seems premature and may introduce risks that are not well characterized. On the basis of these concerns, we deliberately approach sharing artefacts derived from patient data (even if de-identified) with an abundance of caution.

No doubt the commenters[1] are motivated by protecting future patients as much as scientific principle. We share that sentiment. This work serves as an initial proof of concept, and is by no means the end of the story. We intend to subject our software to extensive testing before its use in a clinical environment, working alongside patients, providers and regulators to ensure efficacy and safety.

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[1]Google Health, Palo Alto, CA, USA. [2]Google Health, London, UK. ✉e-mail: scottmayer@google.com; sshetty@google.com

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