Lab Automation with Vision and AI: deep learning, object detection & classification

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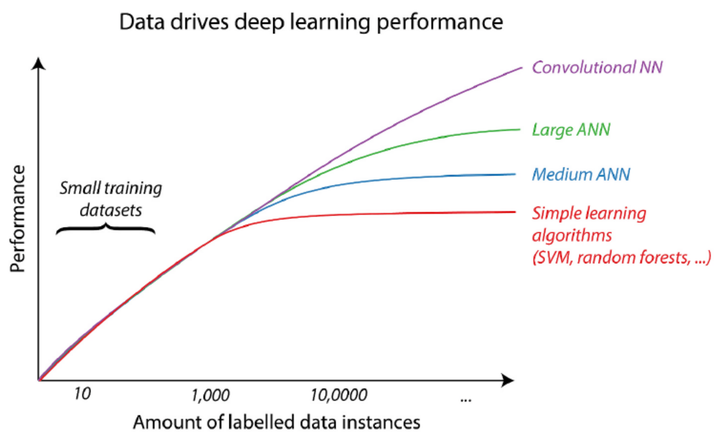
Introduction

Automation is the key to generating data for AI to learn from [1]. Automated experiments are faster, more accurate, consistent, self-documenting and reproducible. Automation augmented with AI can make intelligent decisions at many points in the research workflow, generating large training datasets for AI, thereby greatly increasing throughput of the design build test learn (DBTL) engineering cycle. High-throughput data generation and testing can facilitate drug discovery and, in the context of synthetic biology, optimize microbes and bioprocesses for the production of medicinal drugs. Consequently, as a proof of concept, I extended the Opentrons OT-2 liquid handling robot with low cost hardware components, the TensorFlow machine learning library, and the EfficientDet deep learning model [3] for object detection and classification of yeast colonies. My results show that very low cost intelligent automation can support high-throughput lab research.



① Performance of deep learning models continues to improve with more training data. Image [2]

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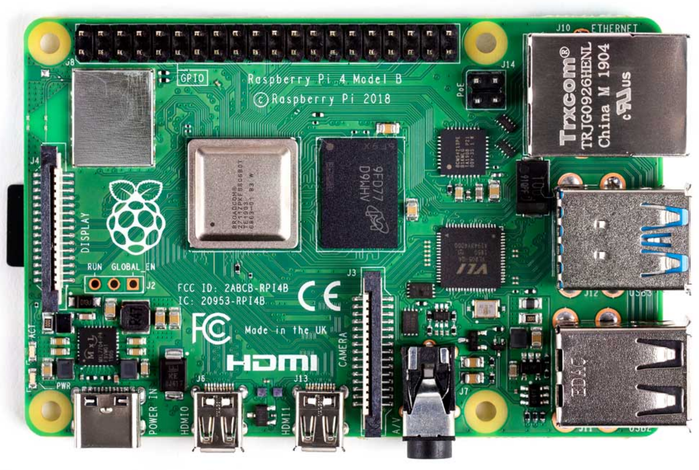
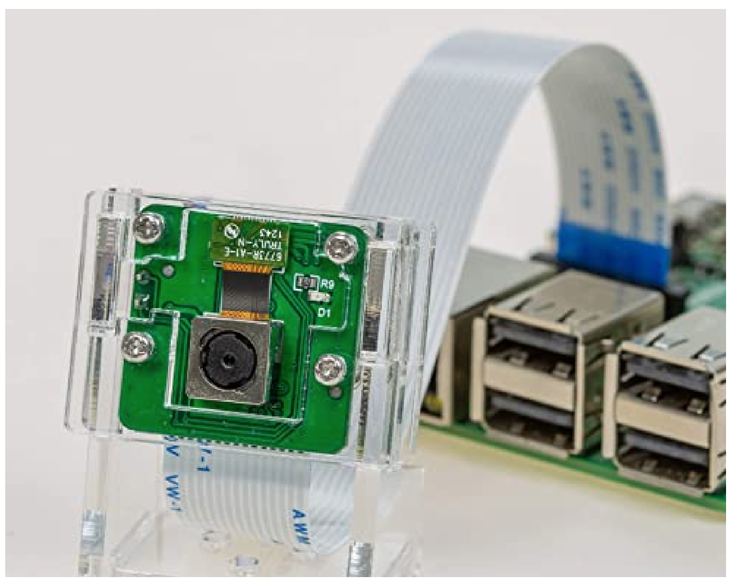
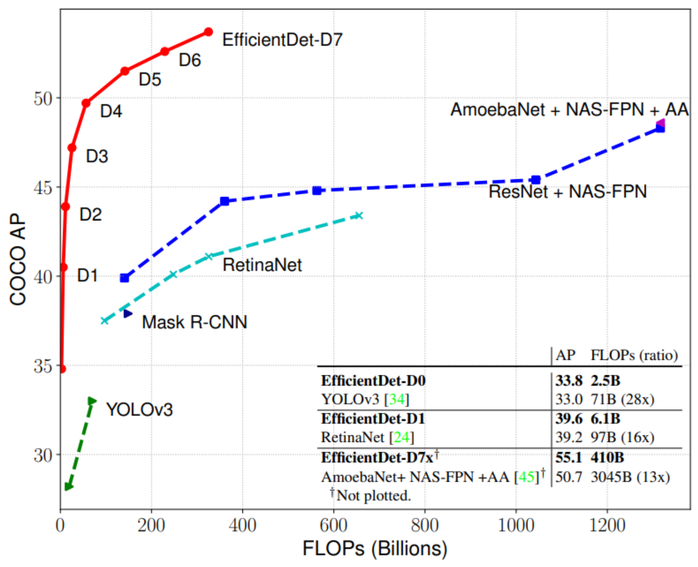
Materials and Methods



② Raspberry Pi 4 Model B: 1.5Hz Quad-core CPU, 8GB RAM. Runs the deep learning model that was trained on a PC. However, this could be replaced with a smaller device that just controls the camera and sends images to the laptop for analysis.



③ Raspberry Pi camera: Arducam Auto Focus Camera with Motorized Focus Lens, OV5647 5MP 1080P. A low resolution camera may be sufficient where images are reduced in size before being input to the object detection and classification model, i.e. 320x320, 384x384, 448x448, 512x512, or 640x640 pixels.



④ EfficientDet models provide a favorable accuracy versus computation trade-off and can be deployed onto small devices. Image [3]

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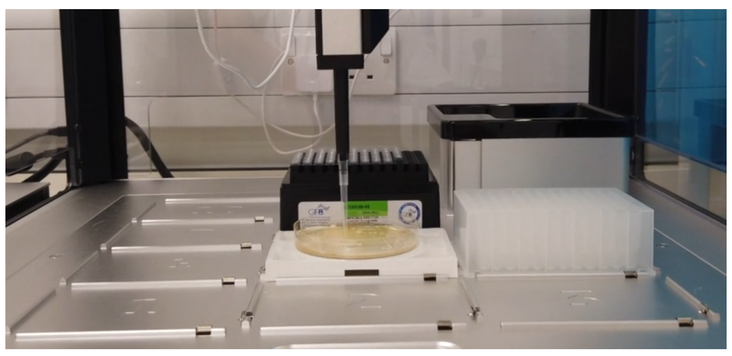
$$
\begin{aligned}
TPR &= tp/(tp+fn) \quad \text{sensitivity, hit rate} \\
FPR &= fp/(fp+tn) \\
Precision &= tp/(tp+fp) \\
Recall &= tp/(tp+fn) \\
Accuracy &= (tp+tn)/(tp+tn+fp+fn)
\end{aligned}
$$

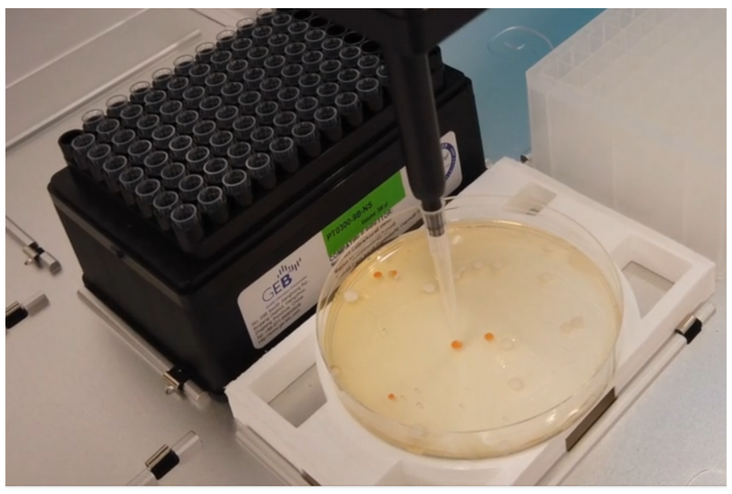
⑤ **Classification metrics**: True Positive Rate (TPR), False Positive Rate (FPR), true positives (tp), false positives (fp), true negatives (tn), false negatives (fn). Accuracy is a useful metric for applications where all classes are equally important.

⑥ The colony picker configuration: The laptop communicates directly with the R Pi and the robot, and relays new colony coordinates from the R Pi to the robot. Image: Opentrons.com

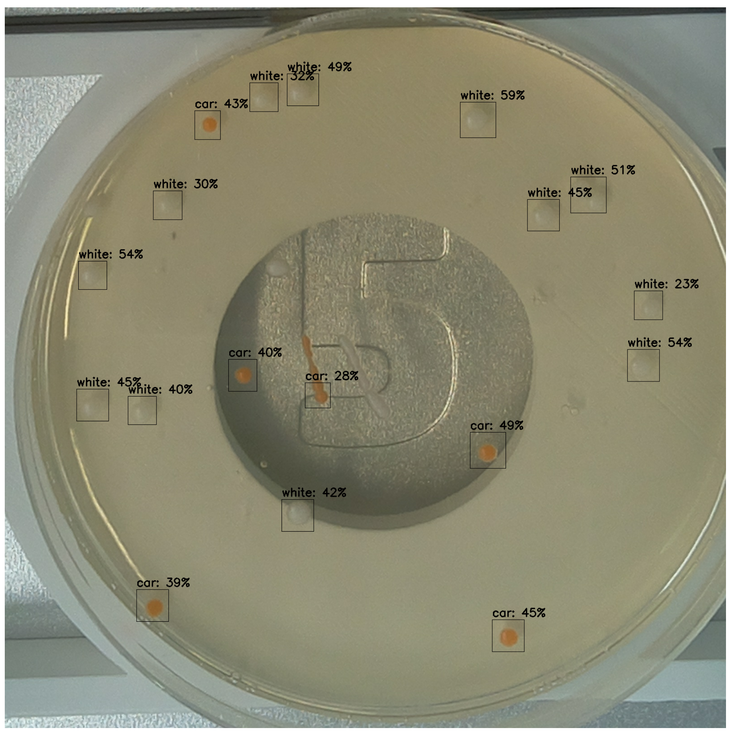
Results



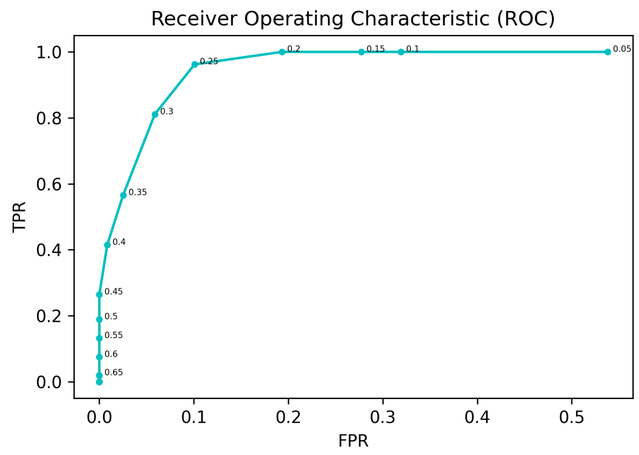
⑦ Opentrons robot with colony picker extension. The robot has just received a list of colony coordinates and is picking a colony.



⑧ Opentrons pipette picking a detected carotene yeast colony.



⑨ Bounding boxes are drawn around detected yeast colonies and classified as carotene (orange) or white. The deep learning model was trained on 50 original plus 150 augmented images for 50 epochs; these colonies were detected with ≥ 20% confidence. Post process filtering: where predicted bounding boxes overlapped, only the prediction with the highest confidence was used. Precision is more important than recall where false positives are associated with a relatively high cost.



⑩ The ROC curve shows the true positive rate versus false positive rate trade-off. This trade-off depends heavily on labeling accuracy and the complexity of the images and their classes. Precision will be a better metric for some applications.

Conclusions

Low cost open source lab automation + AI can support the design build test learn (DBTL) engineering cycle used in synthetic biology to optimize drug production, and in many other labs where high-throughput data generation and testing plays an important role such as drug discovery. Post process filtering can be optimized to reduce required training time, increase precision, and reduce false positive costs. Although more training data tends to improve prediction accuracy, 50 original images may be sufficient for some applications. For more challenging applications, automation + AI can generate more training data during each DBTL cycle and, as a result, make better predictions over time.

References

[1] Pablo Carbonell, Tijana Radivojevic, and Héctor García Martín. Opportunities at the Intersection of Synthetic Biology, Machine Learning, and Automation. *ACS Synthetic Biology*, 8(7):1474–1477, 2019.

[2] Christopher E. Lawson, Jose Manuel Martí, Tijana Radivojevic, Sai Vamshi R. Jonnalagadda, Reinhard Gentz, Nathan J. Hillson, Sean Peisert, Joonhoon Kim, Blake A. Simmons, Christopher J. Petzold, Steven W. Singer, Aindrila Mukhopadhyay, Deepti Tanjore, Joshua G. Dunn, and Hector Garcia Martin. Machine learning for metabolic engineering: A review. *Metabolic Engineering*, 63(October 2020):34–60, 2021.

[3] Mingxing Tan, Ruoming Pang, and Quoc V Le. EfficientDet: Scalable and Efficient Object Detection, 2020.

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