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Machine Learning for Neuroscience

ML4NS

Summary and Overview

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From Day 1: What you are going to learn in this module

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- Primary machine learning topics and concepts
- Hands-on skills on how to:
  - Decide and choose suitable models
  - Design machine learning tasks/experiments
  - Choose and apply suitable metrics to evaluate the models
  - Identify and resolve common issues such as overfitting/underfitting

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From Day 1: By the end of this module

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- You should be able to:
  - Construct machine learning experiments
  - Create and run different probabilistic/statistical learning and deep learning models
  - Read and interpret existing work and assess their applicability/validity [to different use cases]
  - Be familiar with common concepts such as training/test, cross-validation, performance evaluation metrics
  - Learn common issues and pitfalls in developing ML models
  - Obtain practical experience in developing ML models and running (simple) experiments.

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Data and representations

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CCXVI divided by VI?

216/6?

ChatGPT
CCXVI divided by VI is equal to XXXIX, which is 39 in Roman numerals. Here's the breakdown:

CCXVI (216 in Roman numerals) divided by VI (6 in Roman numerals) equals XXXIX (39 in Roman numerals).

via: Goodfellow et al., Deep learning

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Categories of learning and intelligent systems

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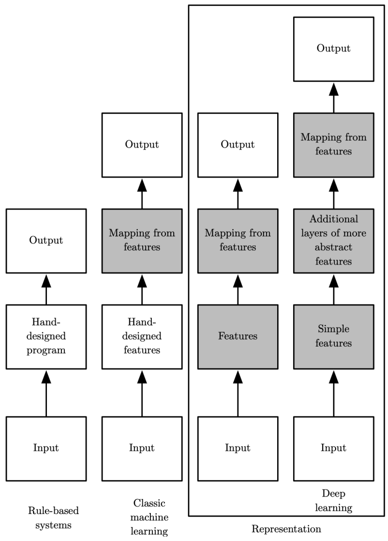

Source: Deep Learning, Ian Goodfellow et al, MIT press.

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Curse of dimensionality

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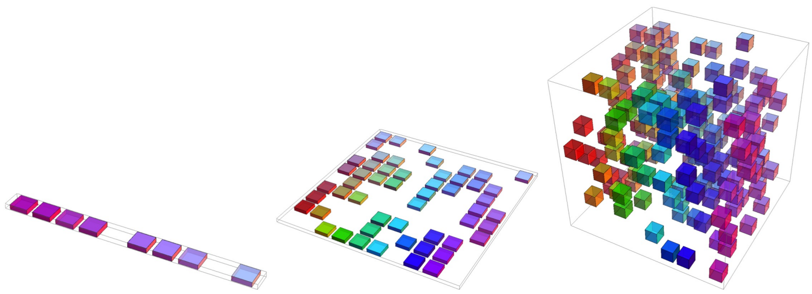

Overall, for d dimensions with v values we need $O(v^d)$ regions and examples

Source: Deep Learning, Ian Goodfellow et al, MIT press.

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Data/sample representation

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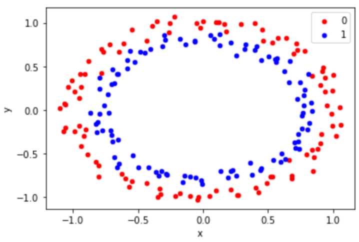

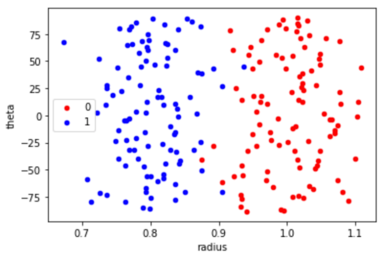

(x,y)

$$r=\sqrt{x^2+y^2}$$

$$\theta=\tan^{-1}\left(\frac{y}{x}\right).$$

<Code>

https://github.com/PBarnaghi/Basic-ML-Code/

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Manifold learning

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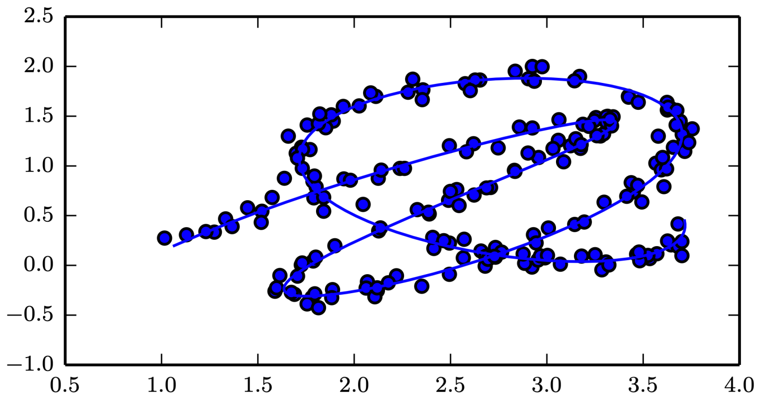

Source: Deep Learning, Ian Goodfellow et al, MIT press.

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Reference and sources

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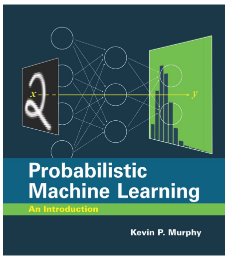
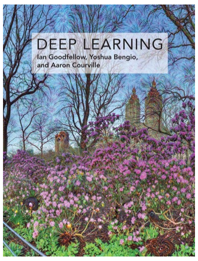
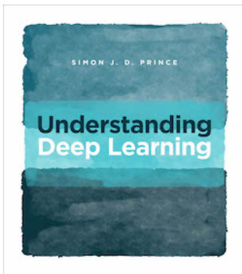


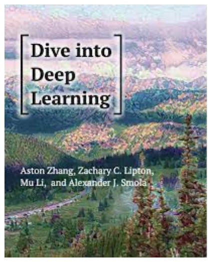
Probabilistic Machine Learning
Kevin P. Murphy, MIT Press



Deep Learning
Goodfellow et al., MIT Press



Understanding Deep Learning,
Simon J.D. Prince, MIT Press



Dive into Deep Learning
Aston Zhang et al.

Preprints:
Probabilistic Machine Learning: An Introduction, https://probml.github.io/pml-book/book1.html
Deep learning: https://www.deeplearningbook.org
Understanding Deep Learning, https://udlbook.github.io/udlbook/
Dive into deep learning, https://d2l.ai/index.html

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Linear models - training

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$$\alpha * Age + \beta * SleepQuality + \theta * CognitiveTestScore = Risk\_score$$

The question is how to learn the coefficients (weights in ML terms)?

Using training data.

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How to evaluate your LR model

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- Mean Absolute Error (MAE)
- Mean Squared Error (MSE)
- Root Mean Squared Error (RMSE)

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|\hat{y}_i - y_i|$$

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}$$

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Logistic regression

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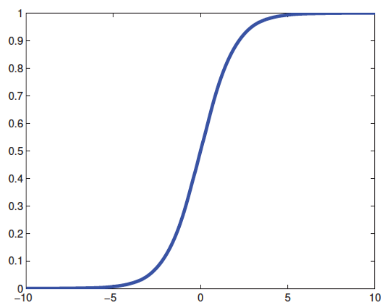
- The process of applying a linear combination of the inputs, as before, but then we pass this through a logistics function, is called logistic regression due to its similarity to linear regression (although it is a form of classification, not regression!).

$$\text{sigm}(\eta) \triangleq \frac{1}{1+\exp(-\eta)} = \frac{e^\eta}{e^\eta + 1}$$



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K-nearest neighbours - example

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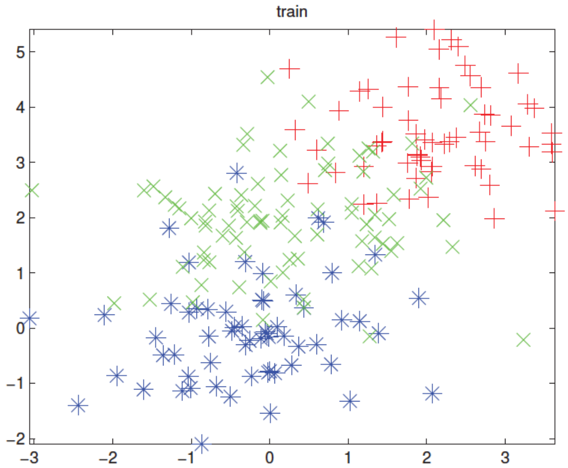

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Cross validation

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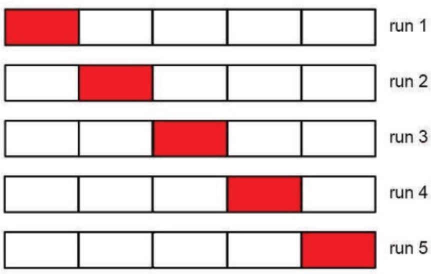
- The idea is simple: we split the training data into K folds; then, for each fold $k \in \{1, \ldots, K\}$, we train on all the folds but the k'th, and test on the k'th, in a round-robin fashion.



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Cross validation - in Scikit learn

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– https://scikit-learn.org/stable/modules/cross_validation.html#cross-validation

`sklearn.model_selection`: Model Selection

User guide: See the Cross-validation: evaluating estimator performance, Tuning the hyper-parameters of an estimator and Learning curve sections for further details.

Splitter Classes

`model_selection.GroupKFold`([n_splits])	K-fold iterator variant with non-overlapping groups.
`model_selection.GroupShuffleSplit`([...])	Shuffle-Group(s)-Out cross-validation iterator
`model_selection.KFold`([n_splits, shuffle, ...])	K-Folds cross-validator
`model_selection.LeaveOneGroupOut`()	Leave One Group Out cross-validator
`model_selection.LeavePGroupsOut`(n_groups)	Leave P Group(s) Out cross-validator
`model_selection.LeaveOneOut`()	Leave-One-Out cross-validator
`model_selection.LeavePOut`(p)	Leave-P-Out cross-validator
`model_selection.PredefinedSplit`(test_fold)	Predefined split cross-validator
`model_selection.RepeatedKFold`(*[, n_splits, ...])	Repeated K-Fold cross validator.
`model_selection.RepeatedStratifiedKFold`(*[, ...])	Repeated Stratified K-Fold cross validator.
`model_selection.ShuffleSplit`([n_splits, ...])	Random permutation cross-validator
`model_selection.StratifiedKFold`([n_splits, ...])	Stratified K-Folds cross-validator.
`model_selection.StratifiedShuffleSplit`([...])	Stratified ShuffleSplit cross-validator
`model_selection.StratifiedGroupKFold`([...])	Stratified K-Folds iterator variant with non-overlapping groups.
`model_selection.TimeSeriesSplit`([n_splits, ...])	Time Series cross-validator

Splitter Functions

`model_selection.check_cv`([cv, y, classifier])	Input checker utility for building a cross-validator.
`model_selection.train_test_split`(*arrays[, ...])	Split arrays or matrices into random train and test subsets.

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L1 Regularisation (Lasso)*

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– Lasso is an acronym for Least Absolute Shrinkage and Selection Operator.

– Lasso regression is a regression model that uses $\ell 1$ regularisation.

– In LASSO, we modify the optimisation function and add a coefficient, which is calculated based on the square of weights (parameters).

$$\sum_{i=1}^{n} (\hat{y}_i - y_i)^2 + \lambda \sum_{i=1}^{n} |\beta_i|$$

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L2 regularisation (Ridge)*

- Ridge regression sum of squared weight values as the penalty term in the optimisation function.

$$\sum_{i=1}^{n}(\hat{y}_i - y_i)^2 + \lambda \sum_{i=1}^{n} {\beta_i}^2$$

Lasso and Ridge

- The key difference between these two techniques is that lasso shrinks the less important feature's coefficient to zero, thus, removing some features altogether.
- In other words, $\ell 1$ regularisation works well for feature selection in case we have a huge number of features.

- Ridge reduces the complexity of the model by shrinking the coefficient (penalising higher weights).

Bayes Rule

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Likelihood

Prior

Posterior

$$p(A|B) = \frac{p(B|A).\,p(A)}{p(B)}$$

Marginalisation

Naïve Bayes

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- We call it Naïve because it assumes that all the features are independent. In practice, this is not always true – but this assumption allows us to apply the Bayesian theorem:

$$P(L \mid \text{features}) = \frac{P(\text{features} \mid L)P(L)}{P(\text{features})}$$

All in one place

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$$Precision = \frac{TP}{TP + FP}$$

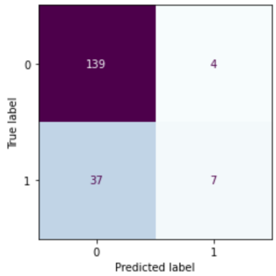
$$F_1 = 2 \times \frac{Precision \times Recall}{Precision\ + Recall}$$

$$Recall = \frac{TP}{TP + FN}$$

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

$$Sensetivity = \frac{TP}{TP + FN}$$

$$Specificity = \frac{TN}{TN + FP}$$



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Example – applying polynomial kernel

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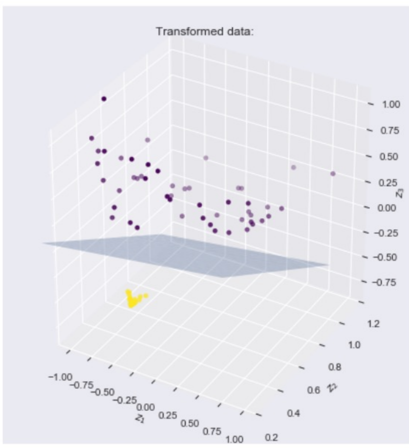

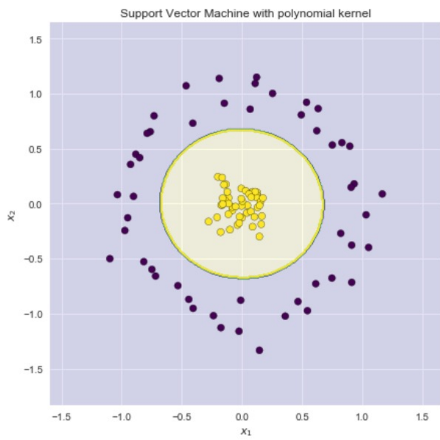

Source: https://xavierbourretsicotte.github.io/Kernel_feature_map.html

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A polynomial kernel

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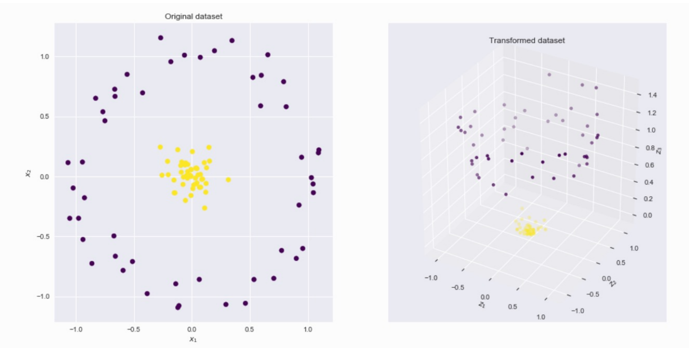
$$\phi(x_1, x_2) = (z_1, z_2, z_3) = (x_1, x_2, x_1^2 + x_2^2)$$

```
def feature_map_1(X):
    return np.asarray((X[:,0], X[:,1], X[:,0]**2 + X[:,1]**2)).T
```



Source: https://xavierbourretsicotte.github.io/Kernel_feature_map.html

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Example: SVM for a linearly separable set of 2d-points

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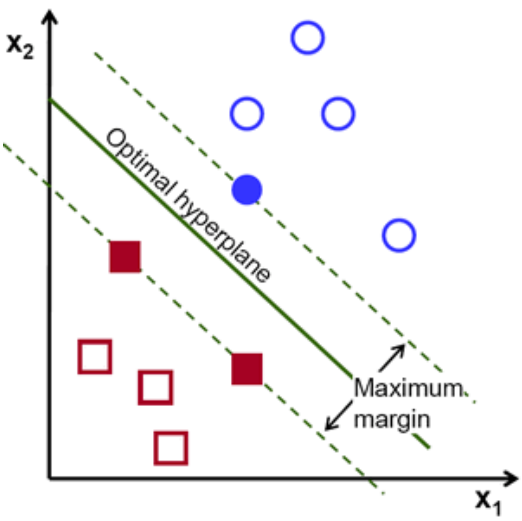

Source: https://vovkos.github.io/doxyrest-showcase/opencv/sphinx_rtd_theme/page_tutorial_introduction_to_svm.html

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Decision Making Using DTs

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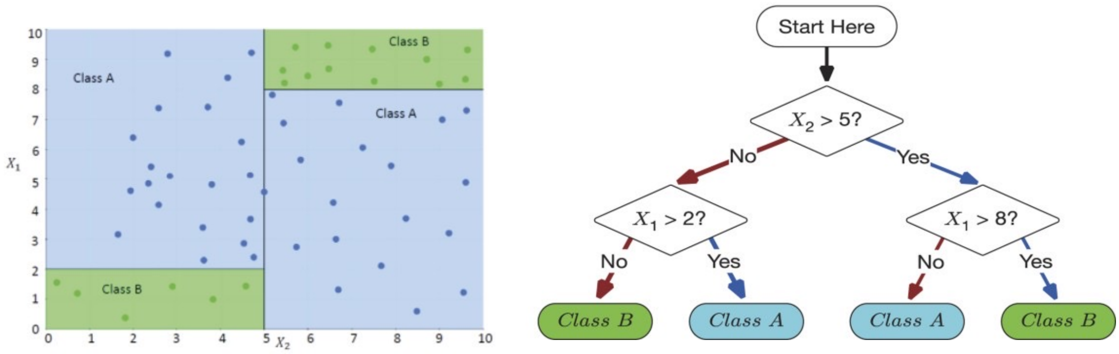

Source: Valdes, G., Luna, J., Eaton, E. *et al.* MediBoost: a Patient Stratification Tool for Interpretable Decision Making in the Era of Precision Medicine. *Sci Rep* 6, 37854 (2016). https://doi.org/10.1038/srep37854

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Structure of Random Forests

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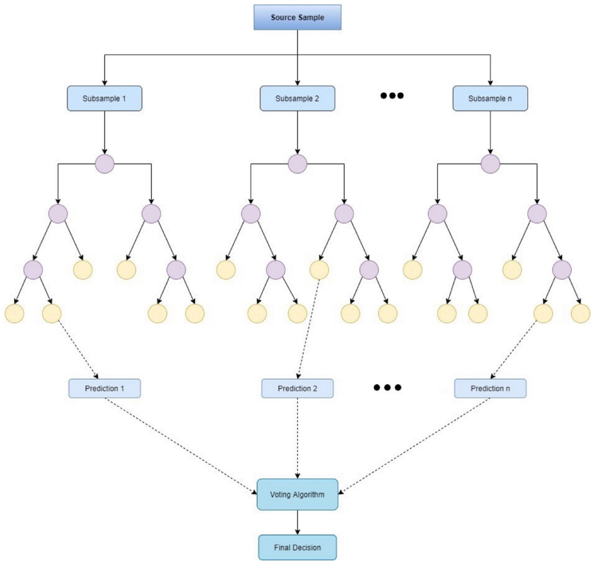

Source: Malebary, S.J., Khan, Y.D. Evaluating machine learning methodologies for identification of cancer driver genes. *Sci Rep* **11**, 12281 (2021). https://doi.org/10.1038/s41598-021-91656-8

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NN with an activation function

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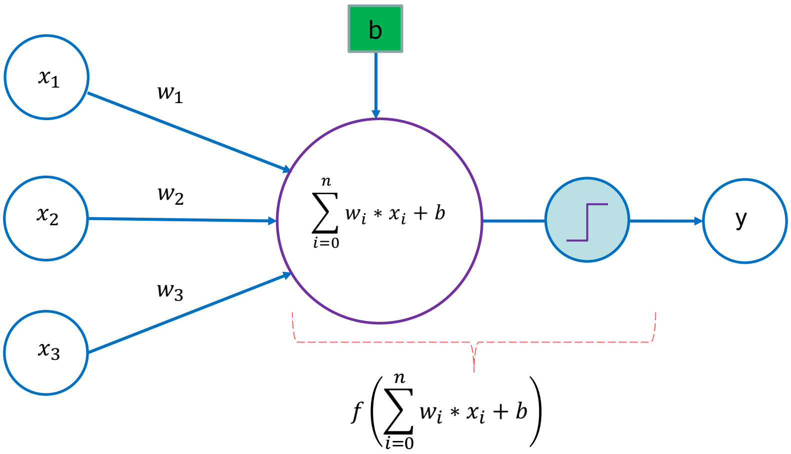

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Rectified Linear Units (ReLU)

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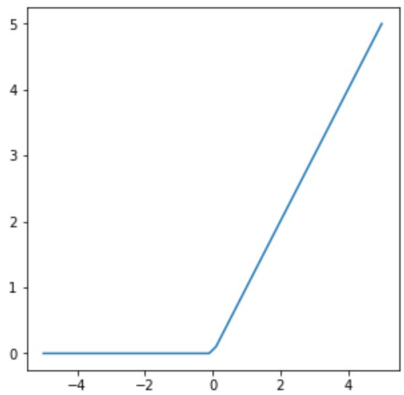
```
def relu(z):
    return np.maximum(0,z)
```



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Images a vectors

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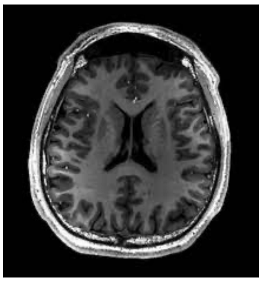
- Using images by *flattening* the images means overlooking the spatial relation between pixels.
- This deeply unsatisfying approach could be a very simple solution in order to feed the resulting one-dimensional vectors through a fully connected MLP or other probabilistic models.



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Example – edge detection: kernel

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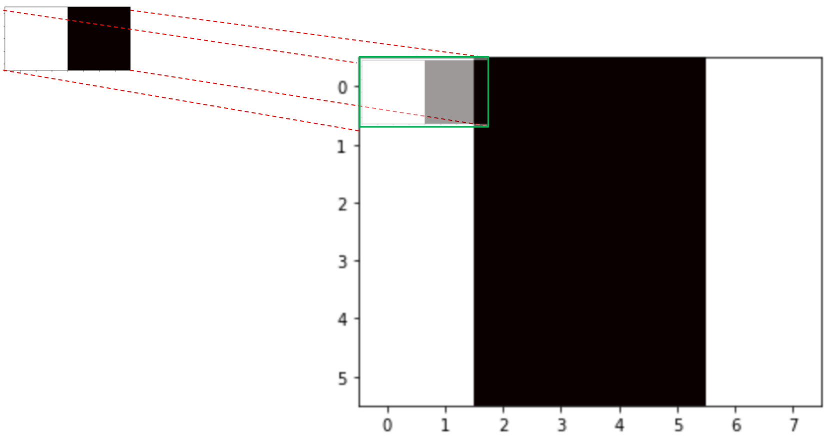
```
K = torch.tensor([[1.0, -1.0]])
```



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CNN kernels

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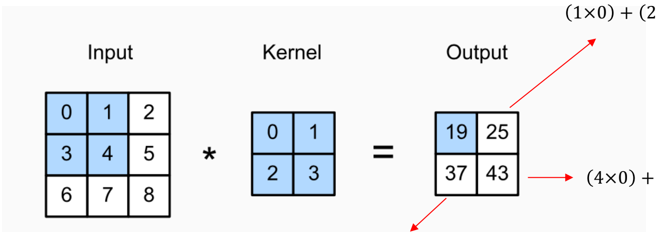
$(1\times0) + (2\times1) + (4\times2) + (5\times3) = 25$



$(4\times0) + (5\times1) + (7\times2) + (8\times3) = 43$

$(3\times0) + (4\times1) + (6\times2) + (7\times3) = 37$

Two-dimensional cross-correlation operation. The shaded portions are the first output element as well as the input and kernel tensor elements used for the output computation:

$(0\times0) + (1\times1) + (3\times2) + (4\times3) = 19.$

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Padding: example

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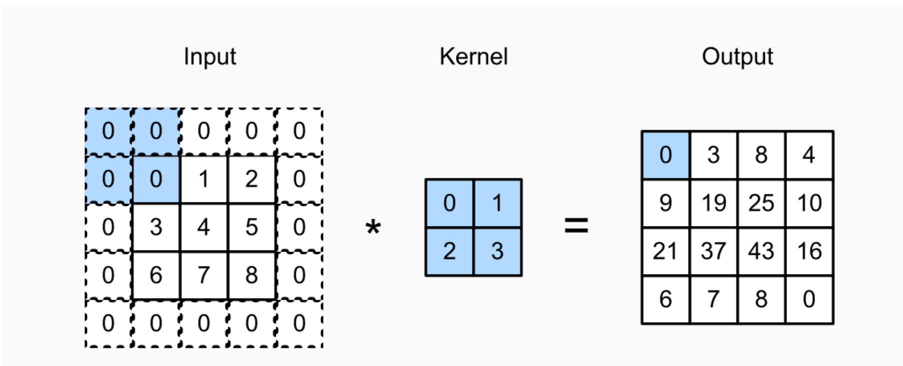

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Pooling

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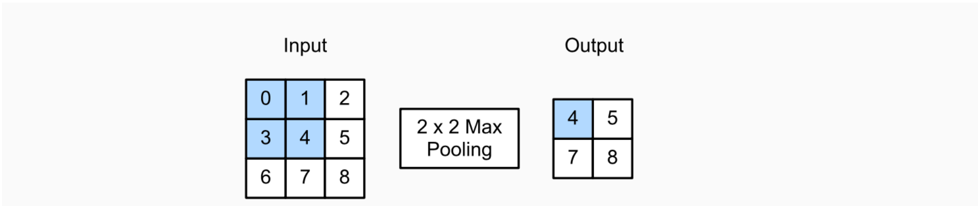
- Like convolutional layers, *pooling* operators consist of a fixed-shape window that is slid over all regions in the input according to its stride, computing a single output for each location traversed by the fixed-shape window (sometimes known as the *pooling window*).



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Compressed notion for LeNet-5

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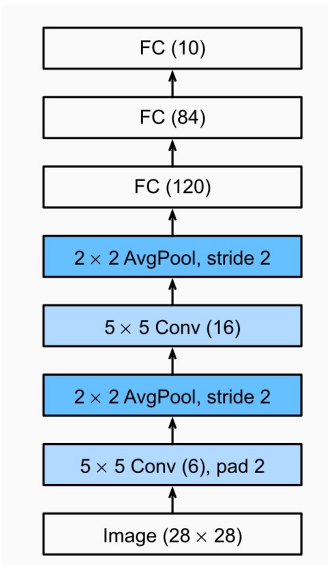

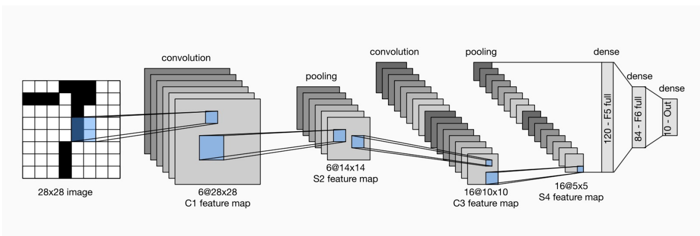

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Autoencoder

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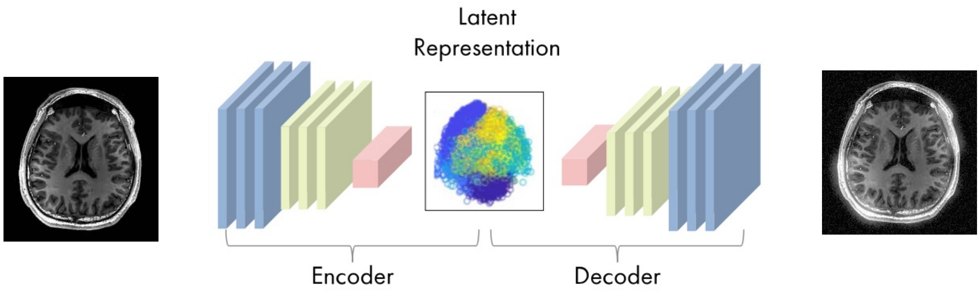

Source for the middle image: https://uk.mathworks.com/discovery/autoencoder.html

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ML deployments in real-world settings

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- The systems are often used for decision support and have humans in the loop.
- However, the trustworthiness, reliability and robustness of the systems/models must be considered and investigated prior to the deployments.
- The users' perceptions of the system and appropriate training should be also considered.

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Responsible and ethical machine learning

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- Anticipate risks and potential issues
- Actively engage and think of solutions
- Work with domain experts and learn about the context and conditions of data collection, and the use of system/model.
- Create feedback loops (before and after deployment)
- Plan for update and maintenance

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Hidden technical debt in real-world ML systems

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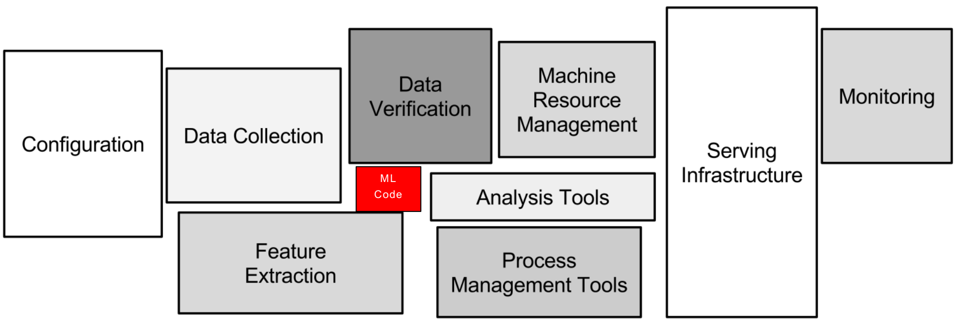
- It is important to note that in several applications, only a small fraction of real-world ML systems comprise the ML code.



Source: Sculley et al., Hidden Technical Debt in Machine Learning Systems, NeurIPS, 2015.

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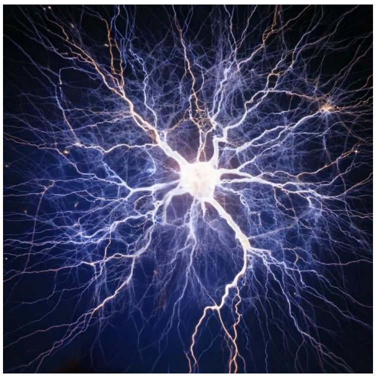
Applications



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Neuroscience inspired machine learning

nature communications

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Article | Open access | Published: 22 January 2025

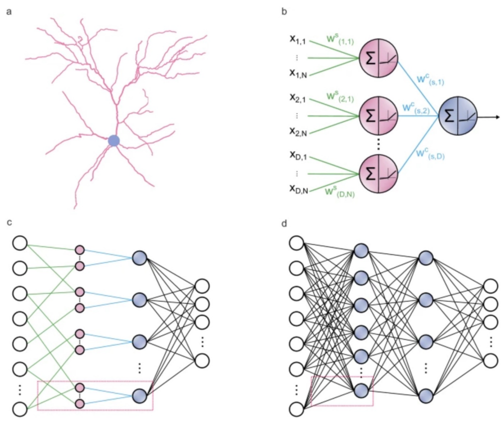
Dendrites endow artificial neural networks with accurate, robust and parameter-efficient learning

Spyridon Chavlis & Panayiota Poirazi

Nature Communications **16**, Article number: 943 (2025) | Cite this article

13 Altmetric | Metrics

Fig. 1: Schematic representation of the dendritic ANN (dANN) compared to a classical vanilla ANN (vANN).



Chavlis, S., Poirazi, P. Dendrites endow artificial neural networks with accurate, robust and parameter-efficient learning. *Nat Commun* **16**, 943 (2025). https://doi.org/10.1038/s41467-025-56297-9

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Neuroscience inspired machine learning

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"…build a Hodgkin–Huxley (HH) network with rich internal complexity, where each neuron is an HH model, and prove that the dynamical properties and performance of the HH network can be equivalent to a bigger leaky integrate-and-fire (LIF) network, where each neuron is a LIF neuron with simple internal complexity."


nature computational science

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Article | Published: 16 August 2024

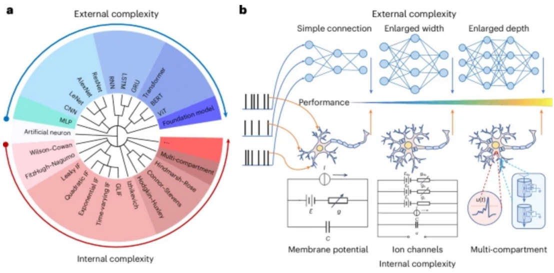
Network model with internal complexity bridges artificial intelligence and neuroscience

Linxuan He, Yunhui Xu, Weihua He, Yihan Lin, Yang Tian, Yujie Wu, Wenhui Wang, Ziyang Zhang, Junwei Han, Yonghong Tian, Bo Xu & Guoqi Li

Nature Computational Science 4, 584–599 (2024) | Cite this article

4907 Accesses | 2 Citations | 147 Altmetric | Metrics

Fig. 1: The internal and external complexity of neurons and networks.



He, L., Xu, Y., He, W. *et al.* Network model with internal complexity bridges artificial intelligence and neuroscience. *Nat Comput Sci* **4**, 584–599 (2024). https://doi.org/10.1038/s43588-024-00674-9

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Machine learning for neurodegenerative conditions

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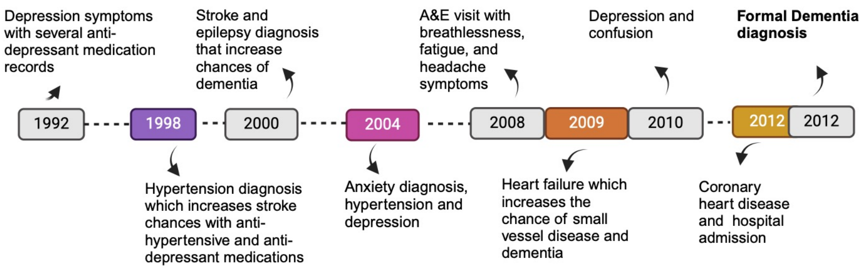

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ML in Parkinson's Disease

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nature medicine

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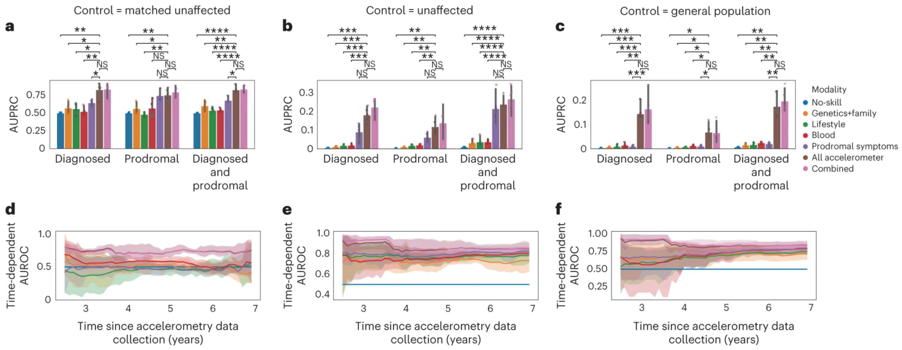
Article | Published: 03 July 2023

Wearable movement-tracking data identify Parkinson's disease years before clinical diagnosis

Ann-Kathrin Schalkamp, Kathryn J. Peall, Neil A. Harrison & Cynthia Sandor



chalkamp, AK., Peall, K.J., Harrison, N.A. *et al.* Wearable movement-tracking data identify Parkinson's disease years before clinical diagnosis. *Nat Med* **29**, 2048–2056 (2023). https://doi.org/10.1038/s41591-023-02440-2

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ML in Dementia Care

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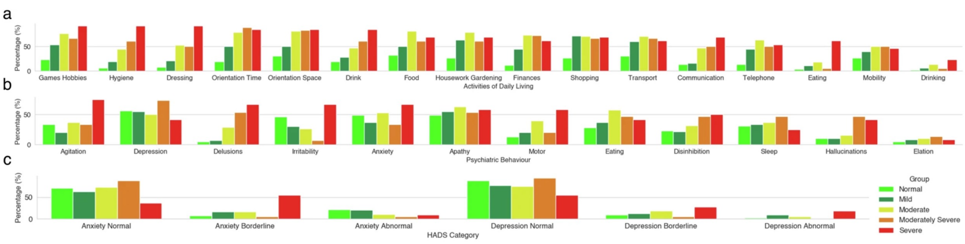
nature > communications medicine > articles > article

Article | Open access | Published: 10 January 2025

Longitudinal study of care needs and behavioural changes in people living with dementia using in-home assessment data

Chloe Walsh, Alexander Capstick, Nan Fletcher-Lloyd, Jessica True, CR&T Group, Ramin Nilforooshan & Payam Barnaghi

Communications Medicine **5**, Article number: 14 (2025) | Cite this article



Walsh, C., Capstick, A., Fletcher-Lloyd, N. *et al.* Longitudinal study of care needs and behavioural changes in people living with dementia using in-home assessment data. *Commun Med* **5**, 14 (2025). https://doi.org/10.1038/s43856-024-00724-3

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ML in comorbidities associated with neurodegenerative conditions

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An interpretable machine learning tool for in-home monitoring of agitation episodes in people living with dementia: a proof-of-concept study

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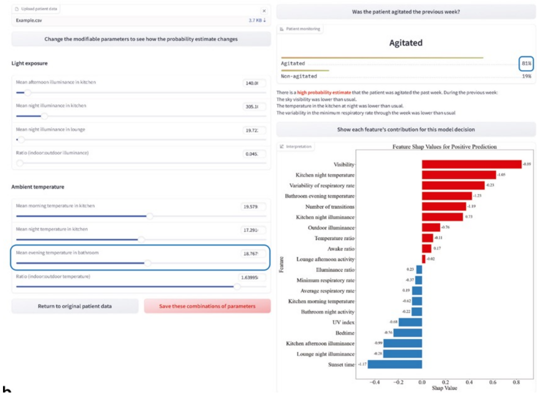

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Review Questions

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Q1

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- What machine learning libraries you have worked with before?

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Q2

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- What is the difference between L1 and L2 norms for regularisation and when you use them.

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Q3

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- If you have a dataset with an imbalanced number of samples, how do you deal with this problem?

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Q4

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- If we give you a set of data (imagine imaging data or electronic healthcare records) and ask you to design a machine learning model. Where and how would you start designing your model?

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Q5

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- If you are given a dataset, how do you decide which model would be the most efficient model to solve your problem?

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Q6

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- Suppose you are given a dataset to cluster. How do you decide what number of clusters would be the most suitable for the dataset?

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Q7

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- How would you ensure the model you designed is not overfitted?

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If you have any questions

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- Please feel free to arrange a meeting or email (p.barnaghi@imperial.ac.uk).
- My office: 928, Sir Michael Uren Research Hub, White City Campus.

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