CLEAN
Computational Laboratory for Energy And Nanoscience

Untangling nets - understanding deep learning and modern AI

I. Tamblyn

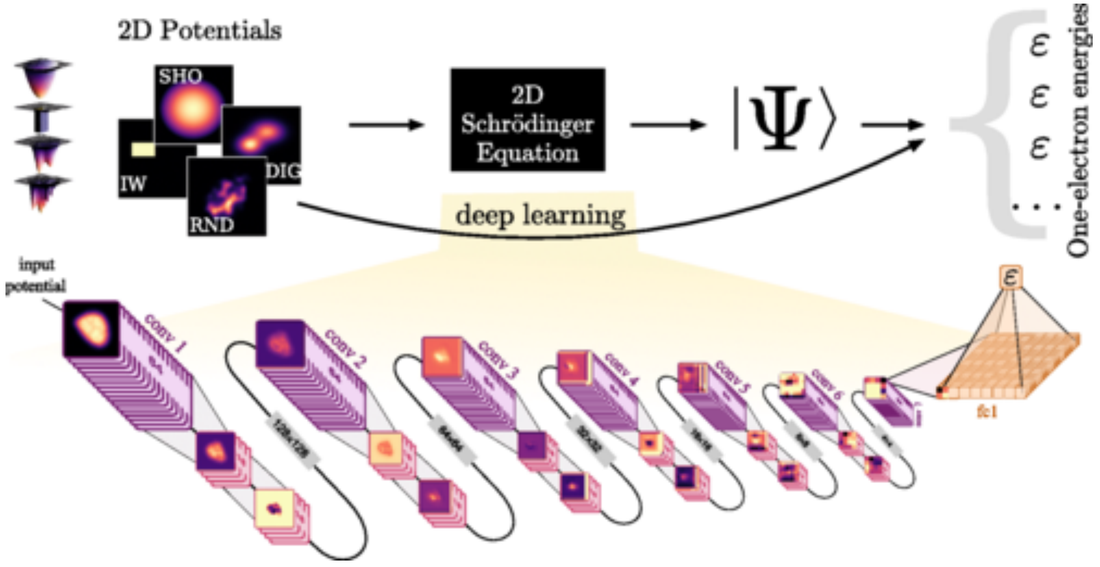
http://clean.energyscience.ca

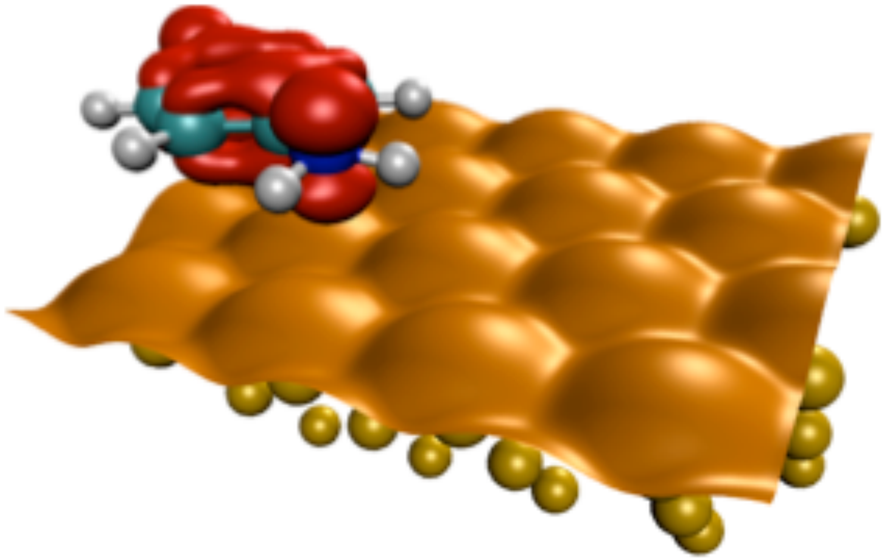
Deep learning and the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi$$

$$\hat{H} = -\frac{\hbar}{2m_e}\sum_i \nabla_i^2 + \sum_{i,I}\frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} - \frac{\hbar}{2}\sum_I \frac{\nabla_I^2}{M_I} + \frac{1}{2}\sum_{I\neq J}\frac{Z_I Z_J e^2}{|\mathbf{R}_I - \mathbf{R}_J|}$$

T_{elec} $V_{\text{e-i}}$ $V_{\text{e-e}}$ T_{ion} $V_{\text{i-i}}$





CT-64 TERMINAL SYSTEM

* 64 OR 32 CHARACTERS PER LINE
* UPPER AND lower case LETTERS
* FULL 8 BIT MEMORY
* 128 CHARACTER ASCII SET
* 110/220 Volt 50-60 Hz POWER SUPPLY
* SCROLLING OR PAGE MODE OPERATION
* CONTROL CHARACTER DECODING—32 COMBINATION
* PRINTS CONTROL CHARACTERS
* USABLE WITH ANY 8 BIT ASCII COMPUTER
* REVERSED BACKGROUND — HIGHLIGHTING

COMPLETE WITH — Chassis and cover, cursor control, 110-1200 Baud serial interface and keyboard. Optional monitor show in photo available.

Now you can buy it. The terminal that has all the features that people have been asking us to include. The CT-64 has all the functions that you could want in a terminal and they may be operated by either switches, or through a software program.

All cursor movements, home-up and erase, erase to end of line, erase to end of frame, read on, read off, cursor on, cursor off, screen reversal, scroll, no scroll, solid cursor, blinking cursor, page selection and a beeper to warn you of end of page; all are provided for your use in the CT-64.

You may also switch from upper case only teletype style operation to upper-lower case typewriter style operation. You can reverse the field on individual words to highlight them, or you can reverse the whole screen.

CT-64 is complete with keyboard, power supply serial interface and case. A matching 9 inch monitor with coordinated covers is also available to make a complete system.

CT-64 Terminal Kit	$325.00
MM-1 Monitor (assembled)	$175.00

SWTPC

219 W. Rhapsody

San Antonio, Texas 78216

Circle 29 on inquiry card.

You are right, it's just what I have been asking for.

☐ Enclose is $325.00 for the CT-64
☐ Send the MM-1 monitor too. ☐ Send Data
☐ or BAC _____ #_____
☐ or MC _____ Ex Date_____

NAME _____

ADDRESS _____

CITY _____ STATE _____ ZIP _____

Southwest Technical Products Corp.
219 W. Rhapsody, San Antonio, Texas 78216

READY for BUSINESS

We've got it all together—the cost effectiveness and reliability of our 6800 computer system with a high capacity 1.2 megabyte floppy disk system. . . PLUS—an outstanding new DOS and file management system.

1 MEGABYTE DISK SYSTEM

DMAF1 introduces a new level of capability to small computer systems. This disk system features two standard size floppy disk drives using the new double sided disk and two heads per drive. Usable storage space of over 600 kilobytes per drive, giving a total of over 1.0 megabyte of storage on line at all times. Ideal for small business applications, or for personal "super" systems.

DMA CONTROLLER

The controller occupies one main memory slot in an SS-50 bus and uses the Motorola MC-6844 DMA controller. The combination of a DMA type controller and double sided disks give the system speed of data transfer unobtainable with smaller drives.

OPERATING SYSTEM

To compliment this outstanding hardware we are supplying equally superior software. The disk operating system and file management system is called FLEX. It is one of the most flexible and complete DOS's available for small systems, but just as important; it is easy to use.

No one can match the variety of compatible peripherals offered by Southwest Technical Products for the SS-50 bus and the 6800 computer system. Now more than ever there is no reason to settle for less.

DMAF1 Disk System (assembled)	$2,095.00
DMAF1 Disk System (kit)	$2,000.00
68/2 Computer with 40K of memory (assembled)	$1,195.00

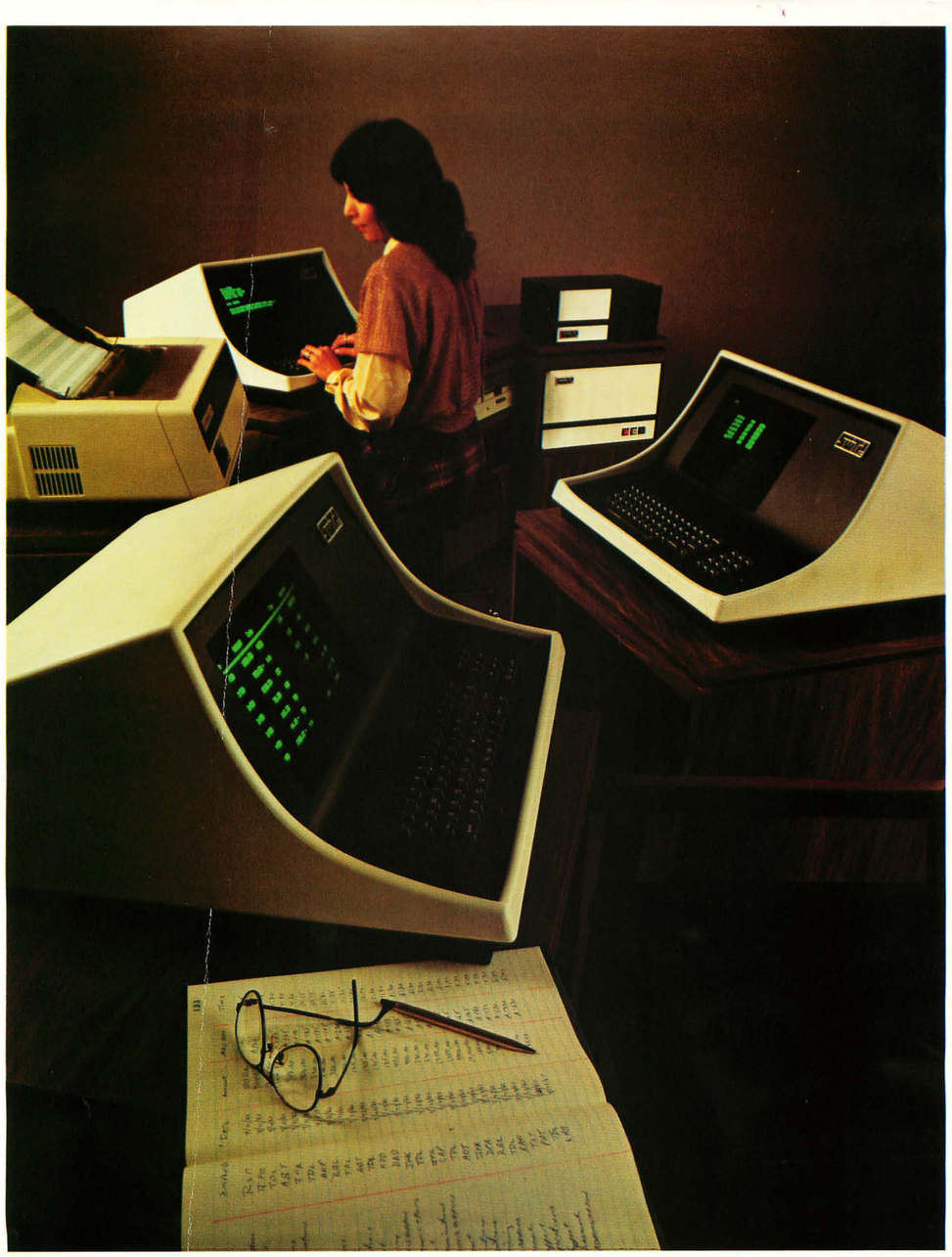
SYSTEMS - SOLUTIONS

If you have a problem that can be solved by a computer—we have a systems solution.

- Two central processors with maximum RAM capacities of 56K and 384 K bytes
- Three types of disk drives with capacities of 175K, 1.2M and 16M bytes
- Two dot matrix printers with 80 and 132 line capacity
- A Selectric typewriter interface and a daisy wheel printer

Match these to your exact need, add one or more of our intelligent terminals and put together a system from one source with guaranteed compatibility in both software and hardware.

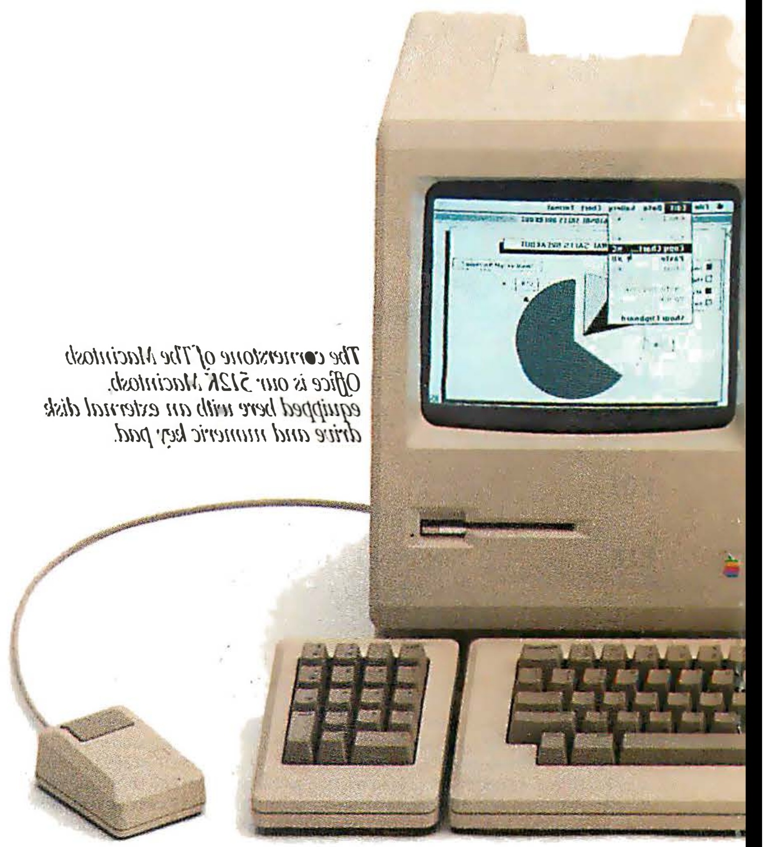
Southwest Technical Products systems give you unmatched power, speed and versatility. They are packaged in custom designed woodgrain finished cabinets. Factory service and support on the entire system and local service is available in many cities.



Macintosh Office.
add is people.

Macintosh XL, up to a full megabyte of RAM and a built-in 10 MB hard disk.

The AppleTalk Personal Network lets you connect up to 32 members of The Macintosh Office for an extremely low cost.



The cornerstone of The Macintosh Office is our 512K Macintosh, equipped here with an external disk drive and numeric key pad.

No, not computer systems people to help you design it. Or computer experts to show you how to use it.

But the kind of people who already make up most of your office.

Managers and professionals. People who spend most of their time selling products, services or, most importantly, ideas.

Because, unlike traditional office computer solutions, we didn't design The Macintosh™ Office around a mainframe. We designed it around an idea.

The idea that people, not mainframes, are the most important information centers in an office. And that most things in business are really accomplished by teams of 5 to 25 people who need to share information with each other. What we call the *workgroup.*

That's why we put Macintosh at the heart of The Macintosh Office. Its powerful, 32-bit technology reduces the time it takes to become productive with a computer from well over a work week, to just under a lunch hour.

For the first time, the people who could really use a computer — managers and professionals — had a computer they could really use. In their choice of sizes: Macintosh 128K, Macintosh 512K and Macintosh XL.

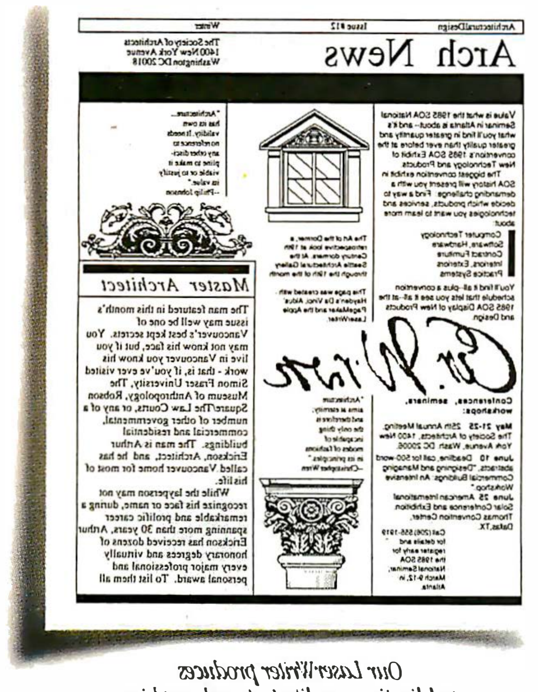
Then we designed a network solution for workgroups of 5 to 25. Instead of buildings of 500 to 2,500.

We call it the AppleTalk™ Personal Network. It's as easy to hook together as an extension cord. And almost as cheap. Less than $50* a desk, versus up to $1,200 for a typical network system.

Since the number one product of business is still paper, we found a way to make every sheet count. A breakthrough in printed communications called the LaserWriter printer. It produces publication-quality text and graphics. Making your presentations, reports and overheads more persuasive.

We've even found a way for The Macintosh Office to share offices with IBM.® An AppleTalk card that slips into an IBM PC, allowing it to trade information with Macintosh and access file servers.

Third party developers are also working on The Macintosh Office. Next month,



Our LaserWriter produces publication-quality text and graphics.

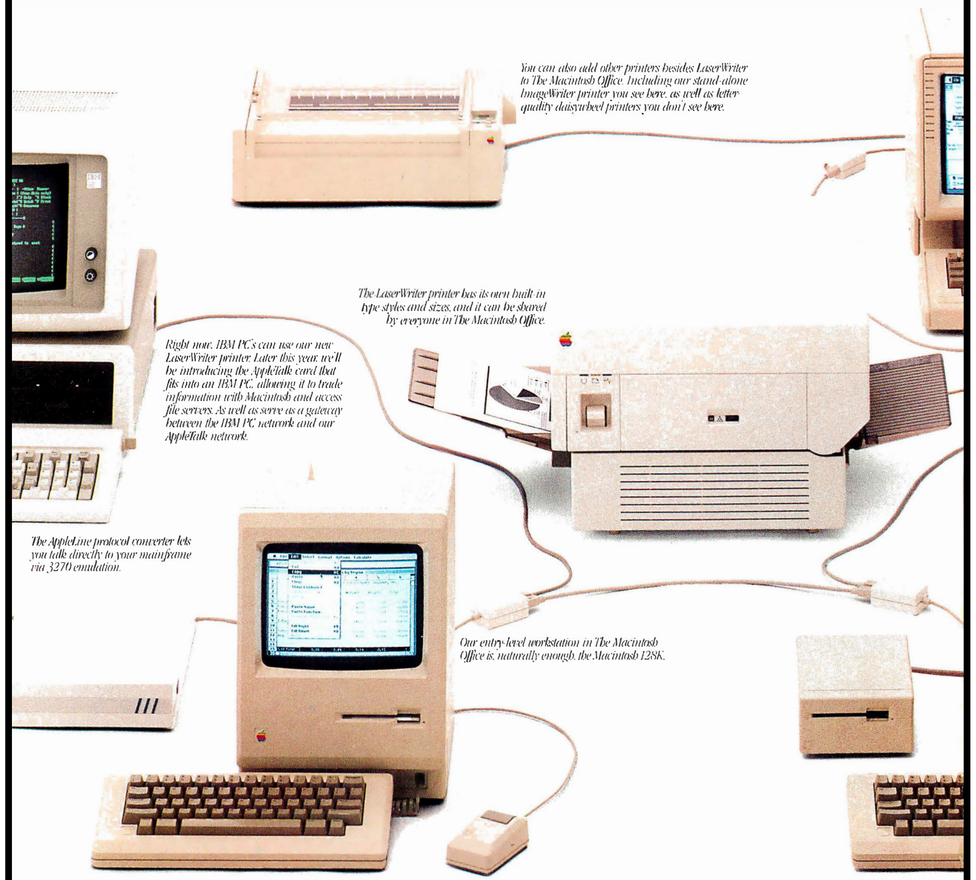
they'll be offering shared storage devices that let your workgroup share information. And they're writing a whole new generation of business software to go along with the 350 programs Macintosh already runs. Including Microsoft® Word, ThinkTank™ 512 and the new Jazz™ from Lotus.®

Now, there's only one more thing we'd like to add to this ad: call 800-446-3000.

We'll tell you how to get everything you need to turn your office into a Macintosh Office.

People not included.

Introducing The Macintosh Office. All you have to add is people.



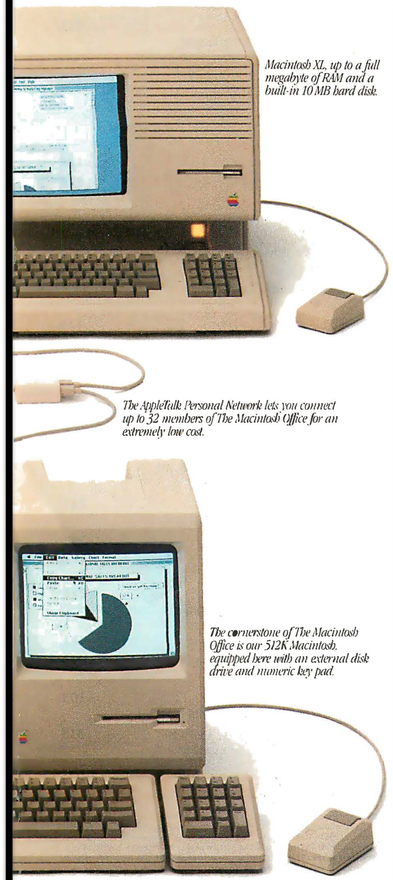
You can also add other printers besides LaserWriter to The Macintosh Office. Including our stand-alone ImageWriter printer you see here, as well as letter quality daisywheel printers you don't see here.

The LaserWriter printer has its own built in type styles and sizes, and it can be shared by everyone in The Macintosh Office.

Right now, IBM PC's can use our new LaserWriter printer. Later this year we'll be introducing the AppleTalk card that fits into an IBM PC, allowing it to trade information with Macintosh and access file servers. As well as serve as a gateway between the IBM PC network and our AppleTalk network.

The AppleLine protocol converter lets you talk directly to your mainframe via 3270 emulation.

Our entry-level workstation in The Macintosh Office is, naturally enough, the Macintosh 128K.



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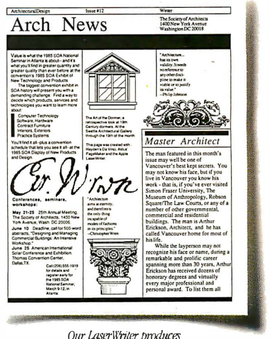

Arch News

Master Architect

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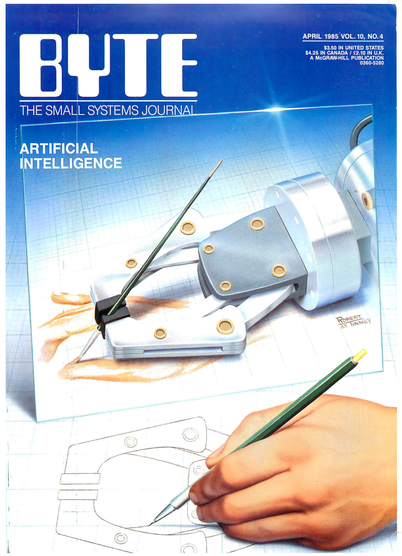
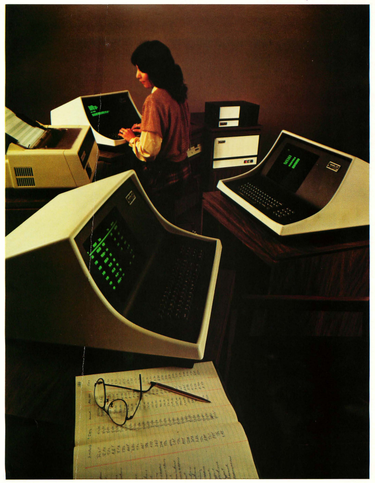
219 W. RHAPSODY
SAN ANTONIO, TEXAS 78216

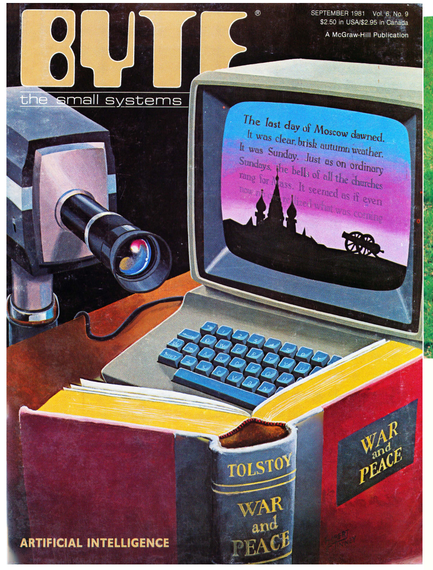
Circle 350 on inquiry card.





SWTPC
SOUTHWEST TECHNICAL PRODUCTS CORPORATION
219 W. RHAPSODY
SAN ANTONIO, TEXAS 78216 (512) 344-0241

Circle 334 on inquiry card.



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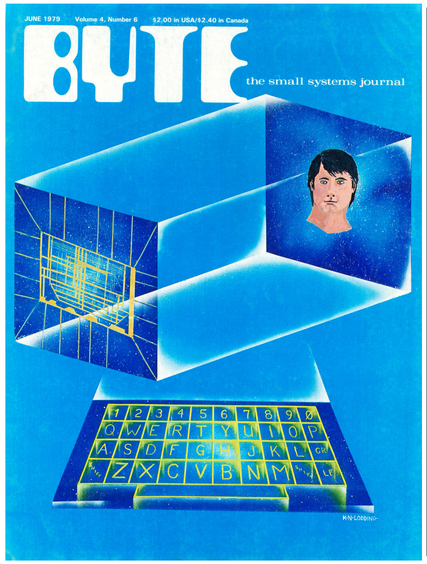
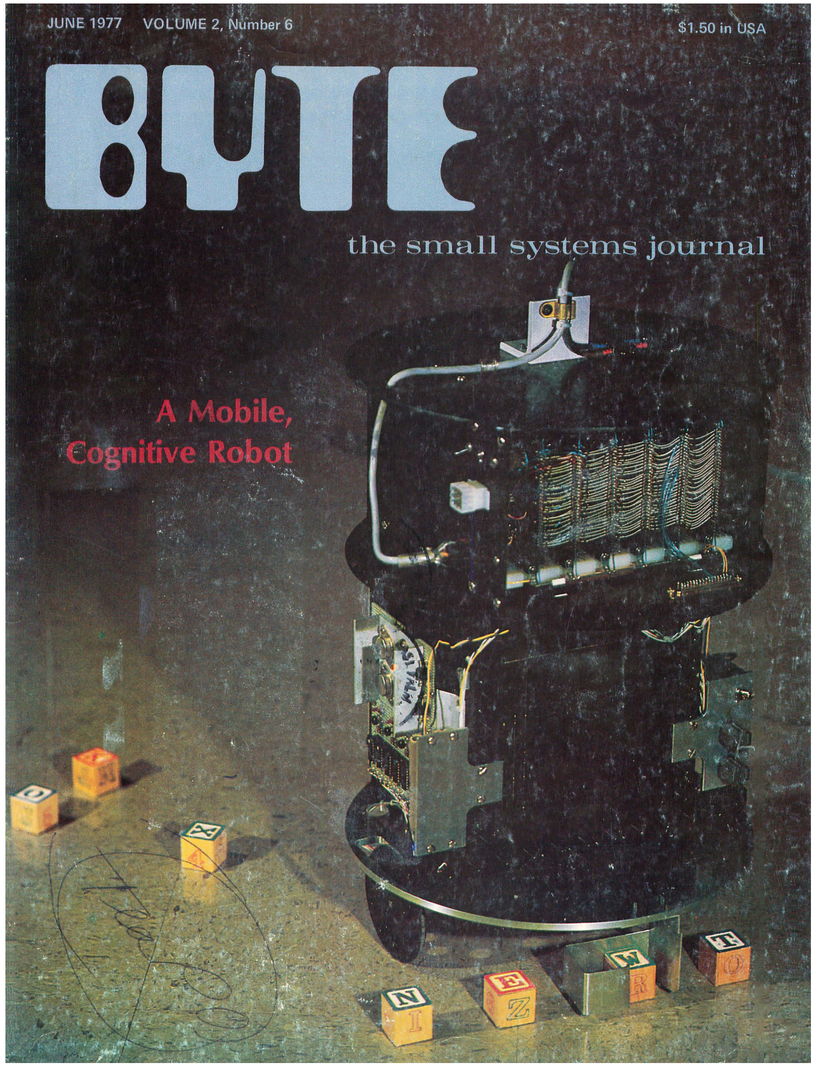
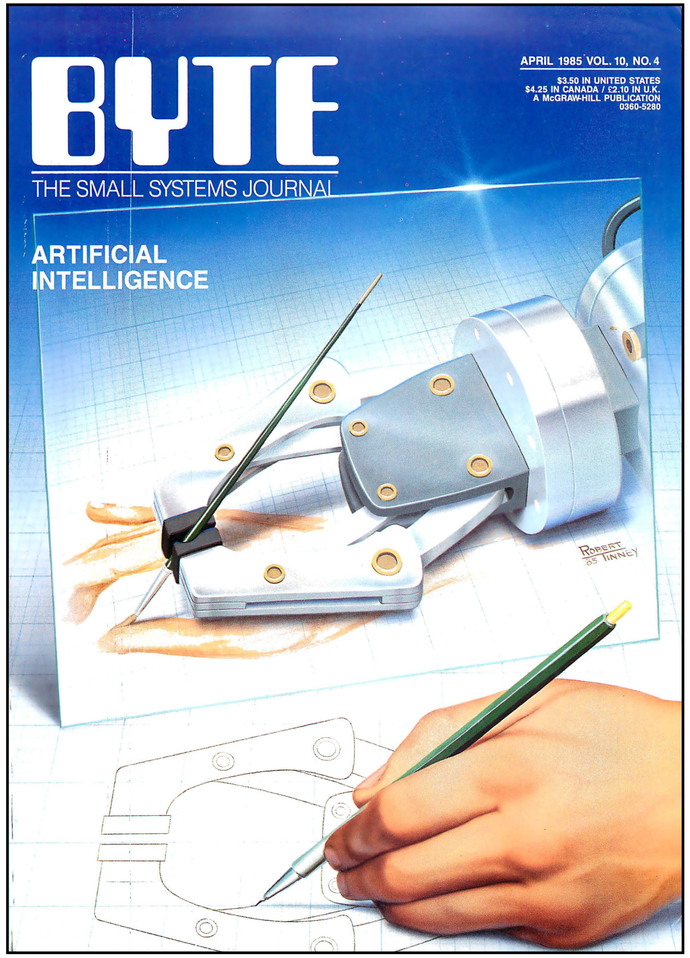




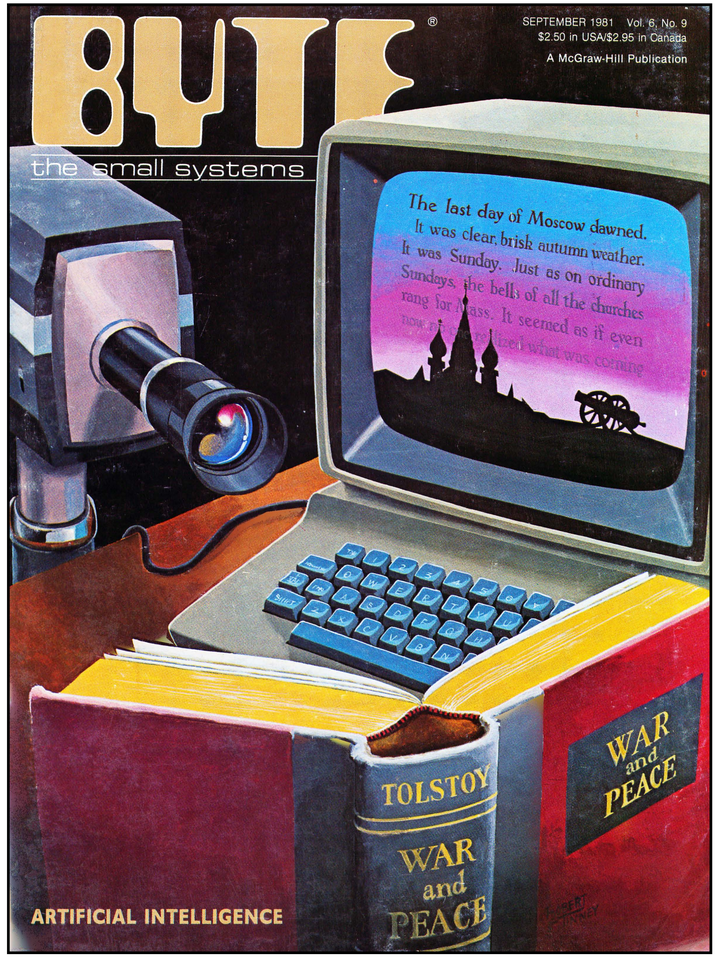
Cognitive Robot (1977)

Natural Language (1978)

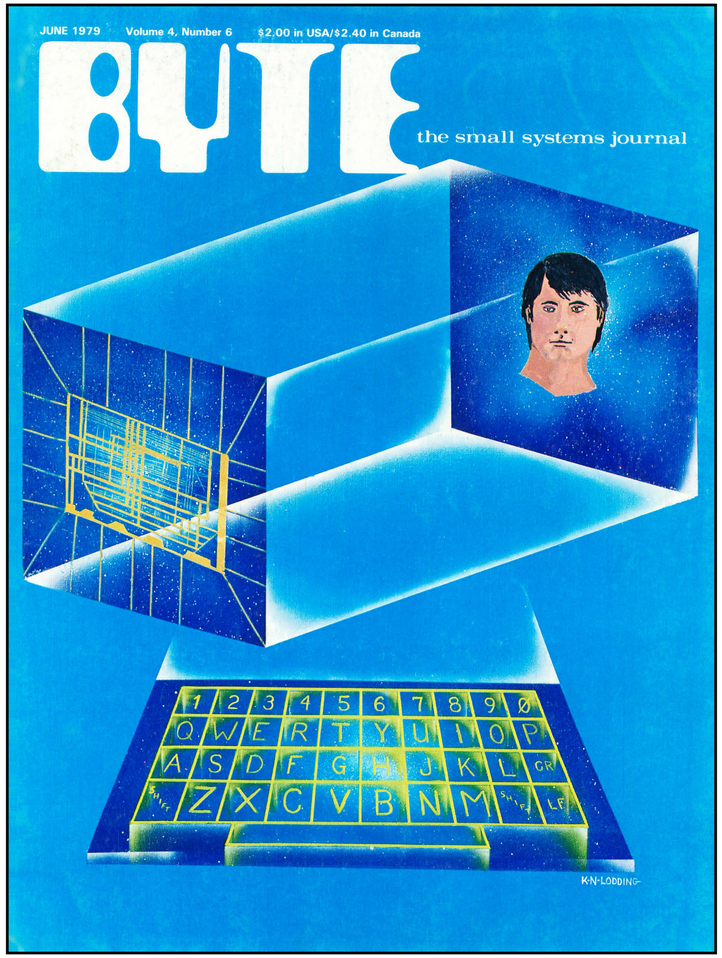
Artificial intelligence



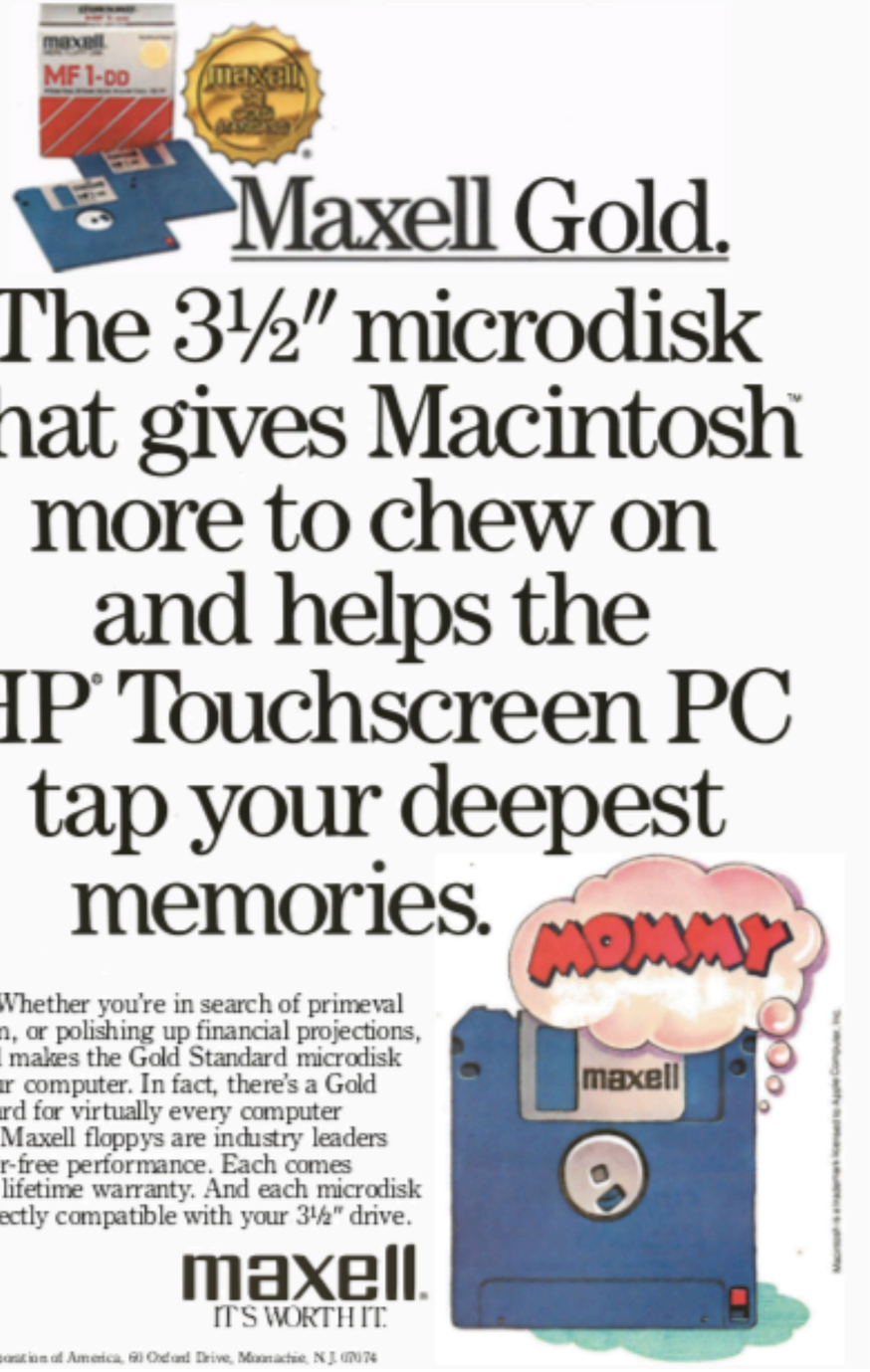
1979



1981



1985

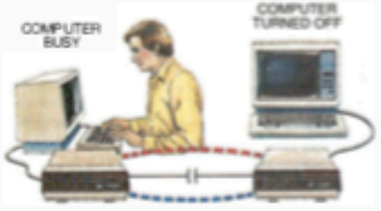


SR-12
640x400 non-interlaced resolution!

ProModem 1200... HOT-LINE

Our ProModem 1200 Makes Smart Modems Look Dumb

Send Or Receive 50 Pages Of Text Without Tying Up Your Computer



No wonder Smart Modems, Cats, and Maxwells cringe when compared to our $495 ProModem 1200, an expandable 1200/300 baud modem for use with all personal computers. It costs less, but is smarter than the rest.

And when you add our $99 Communications Buffer and Alphanumeric Display options, ProModem 1200 becomes a veritable genius!

Imagine, you unplug your computer, take it home for the weekend, and while you're gone, ProModem 1200 answers the phone, collects messages up to 50 pages long, sends out electronic mail, and displays all events with the exact time of each. Thanks to ProModem 1200, expensive, hard-to-use communications software isn't needed. The communications is in the modem, and electronic mail becomes a background function, where it belongs.

Simple To Install And Use

Our Communications Buffer is a 4 by 6 card that plugs into the ProModem 1200 motherboard. It comes with 2K of CMOS battery backed-up memory, expandable to 64K. Part of the memory is used as a dialing directory with the balance reserved for storage. For $99 more, a front panel Alphanumeric Display can be added to show time, date, and 24 status and help messages. These two powerful options can be included at time of purchase, or can be added later.

Hayes Compatible

ProModem 1200 is Hayes compatible but that's where the resemblance ends. Our standard $495 modem includes a real-time clock/calendar. Hayes charges hundreds more for a Smart Modem with a time-base. Nor do they have electronic mail capability at any price.

ProModem 1200 contains a battery backed-up real-time clock/calendar, a large dialing directory and can send or receive messages up to 50 pages long without tying up the computer.

Send for complete details and the name of the Prometheus dealer nearest you.

PHOTOGRAPHED BY PAUL AVIS. STYLED BY JANE SUTTON

BUILD THE HOME RUN CONTROL SYSTEM

PART 1: INTRODUCTION

BY STEVE CIARCIA

Energy management, convenience, and security in one package

Six years ago I presented an article on building a computer-controlled security system using an SDK-85 experimenters board. To this day, I still get letters asking for software and material sources. Since home/industrial energy and security management have been and still are a major interest (and little has been published since then), that article remains a popular reference for students and experimenters.

As I look back on it now, I realize that my first home-control computer was engineered properly but was about as user-friendly as ENIAC. It's time to re-address the subject, bring the design up to date, and make this home-control system a real friend.

I conceive of this project as a simple computer control system equally applicable in the home or factory. The choice of input sensors and output controls designates its primary application.

Whether for industrial or home use, control systems function similarly. Specific input data is analyzed and compared to a predetermined set of action parameters. If a favorable comparison exists, the designated task is performed. For example, if a light is to be turned on at 2:00 p.m., the control system sees a negative request-affirmation comparison until that time. At that instant, the output of the control system turns on the light and then continues with the next request. In a control system configured as an alarm, the inputs would be from contact closures, and the outputs would be to bells, automatic dialers, and other such items.

Whatever the application, control systems are designed to be either open loop or closed loop in function. An open-loop controller simply outputs its decision and forgets about it. Industrial control systems, on the other hand, require more assurance that the action has been performed. They close the loop by analyzing feedback signals from the operation being controlled. If

(continued)

Steve Ciarcia (pronounced "see-ARE-see-ah") is an electronics engineer and computer consultant with experience in process control, digital design, nuclear instrumentation, and product development. He is the author of several books about electronics. You can write to him at POB 582, Glastonbury, CT 06033.

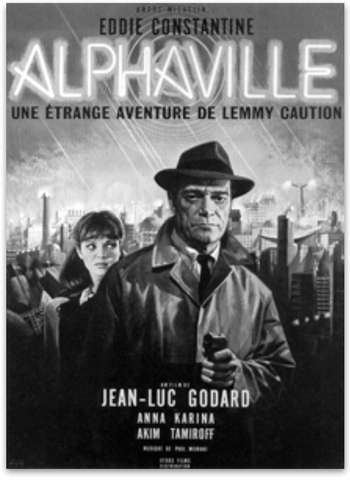
Artificial intelligence is not a new idea


METROPOLIS
EIN FILM VON FRITZ LANG
BRIGITTE HELM · GUSTAV FRÖHLICH
UFA FILM IM VERLEIM DER


DER HERR DER WELT
REGIE HARRY PIEL


THE SCIENCE-MONSTER WHO WOULD DESTROY THE WORLD!
M-G-M presents
The Invisible Boy
ROBBY THE ROBOT


FROM OUT OF SPACE.... A WARNING AND AN ULTIMATUM!
THE DAY THE EARTH STOOD STILL
FOR GENERAL EXHIBITION
MICHAEL RENNIE · PATRICIA NEAL · HUGH MARLOWE


EDDIE CONSTANTINE
ALPHAVILLE
UNE ÉTRANGE AVENTURE DE LEMMY CAUTION
JEAN-LUC GODARD
ANNA KARINA
AKIM TAMIROFF


An epic drama of adventure and exploration
2001: a space odyssey


SHALL WE PLAY A GAME

Nature 518, 529–533 (26 February 2015) doi:10.1038/nature14236

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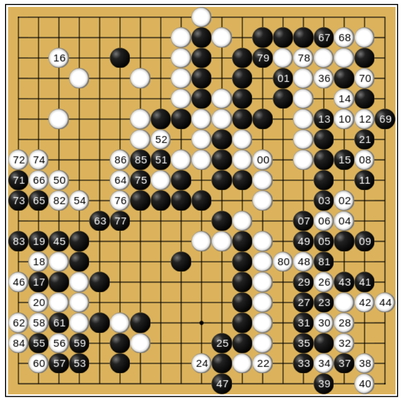
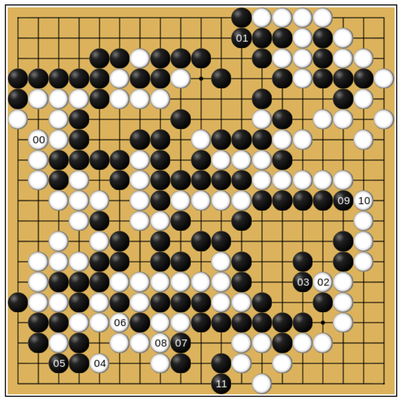
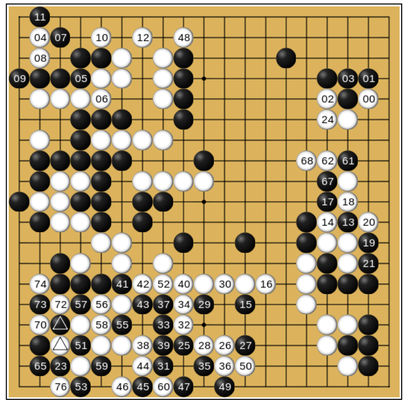
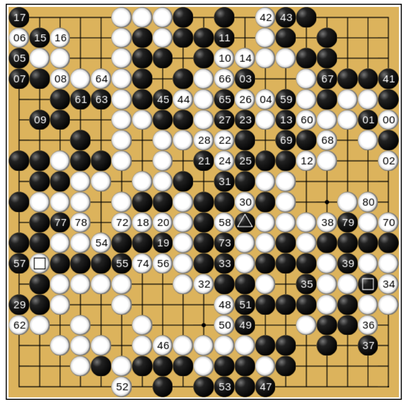
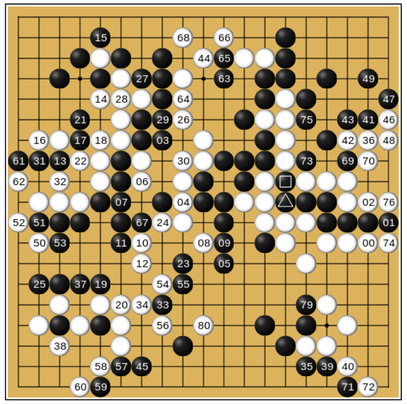




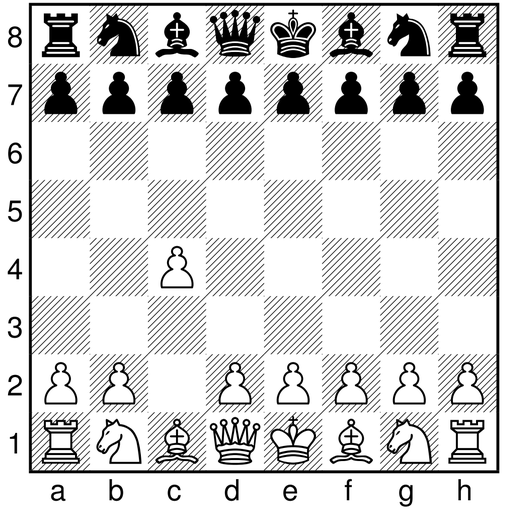




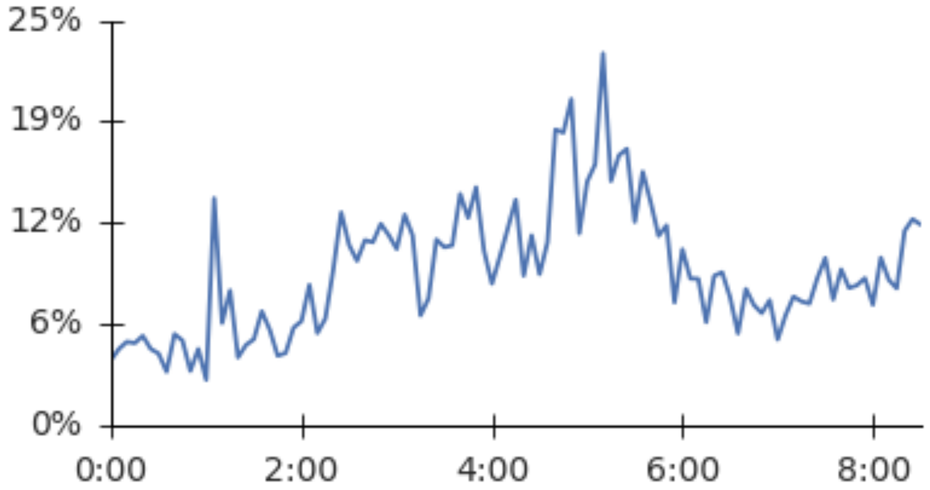
AlphaGo



A10: English Opening

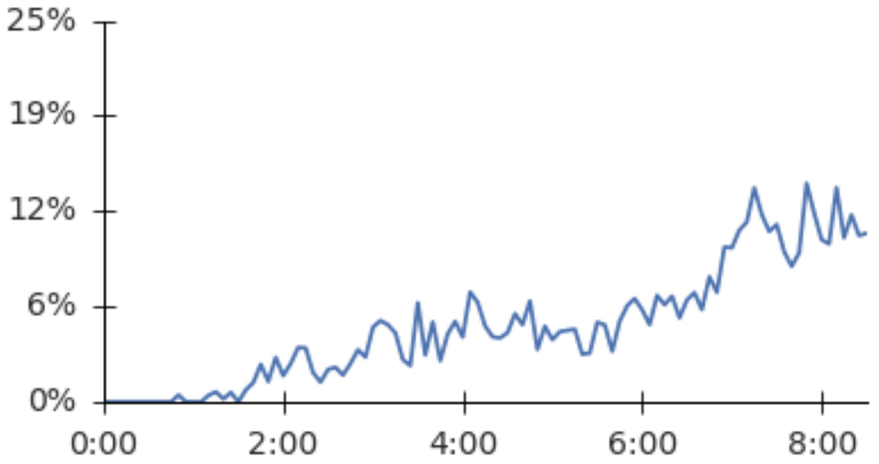


w 20/30/0, b 8/40/2

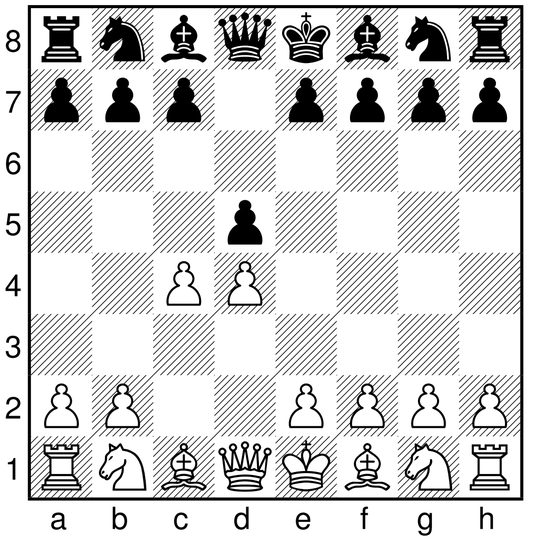


1...e5 g3 d5 cxd5 ♘f6 ♗g2 ♘xd5 ♘f3

D06: Queens Gambit



2...c6 ♘c3 ♘f6 ♘f3 a6 g3 c4 a4



w 16/34/0, b 1/47/2

arXiv:1712.01815v1 [cs.AI]

The Wolfram Language
Image Identification Project

#WolfAI

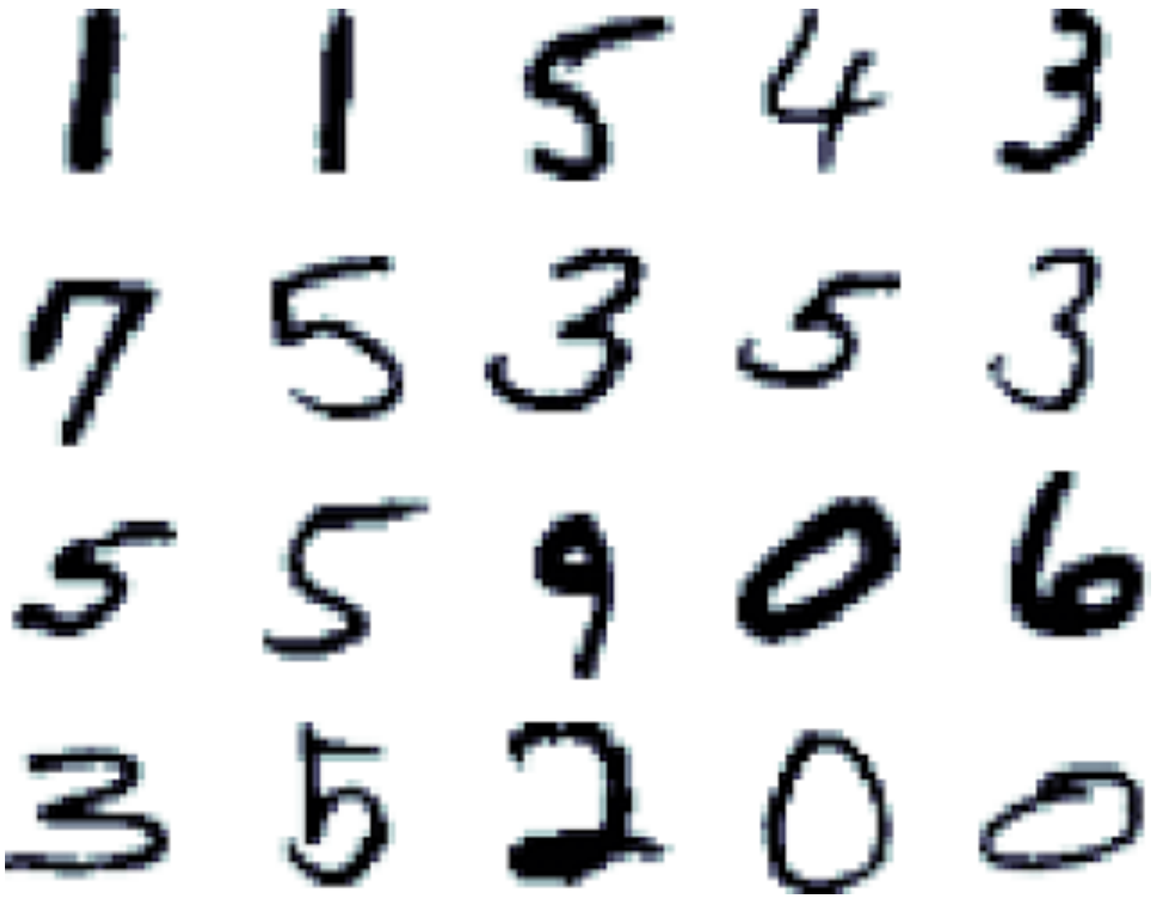
ImageIdentify[]

lightship

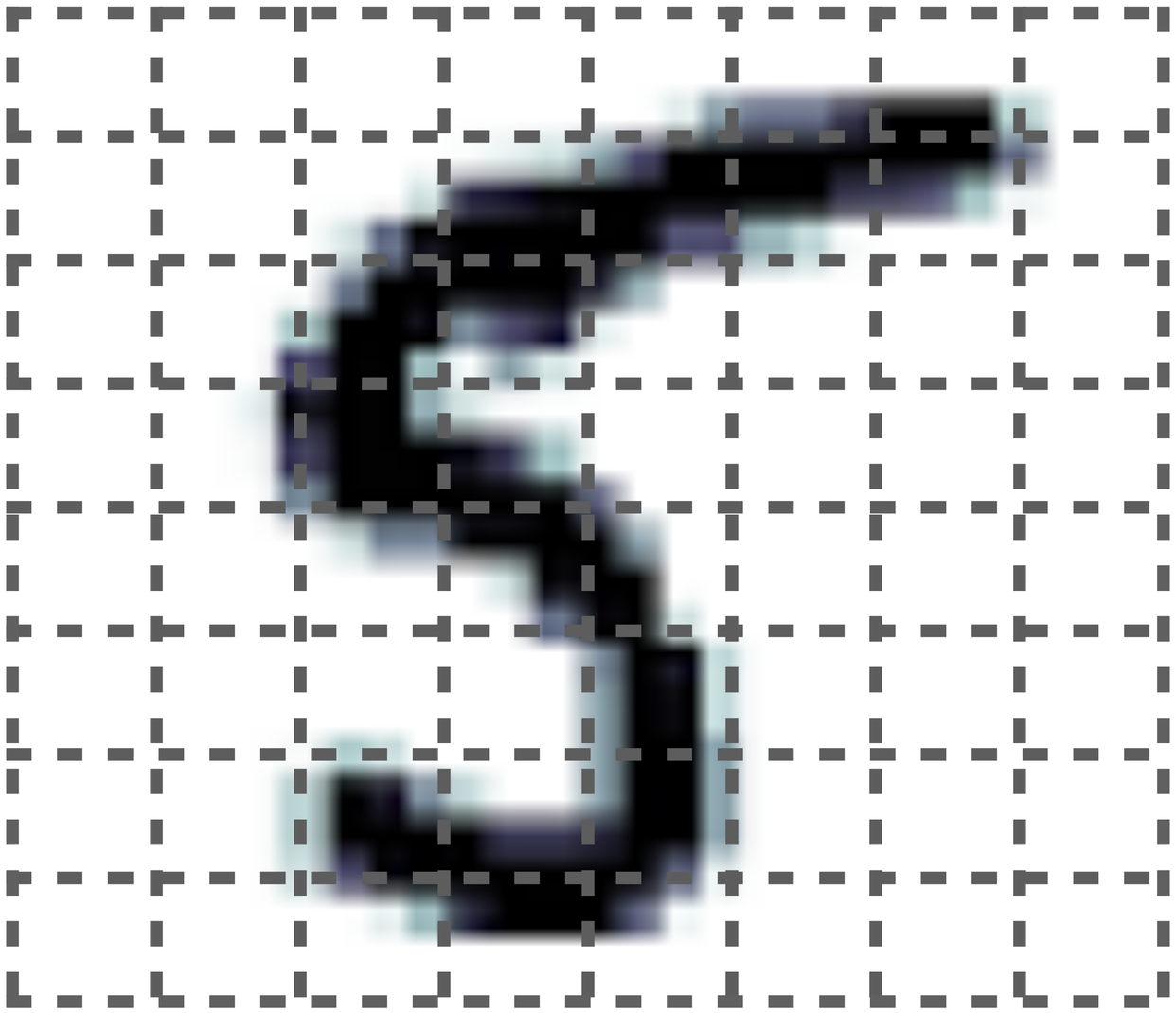
Lightship

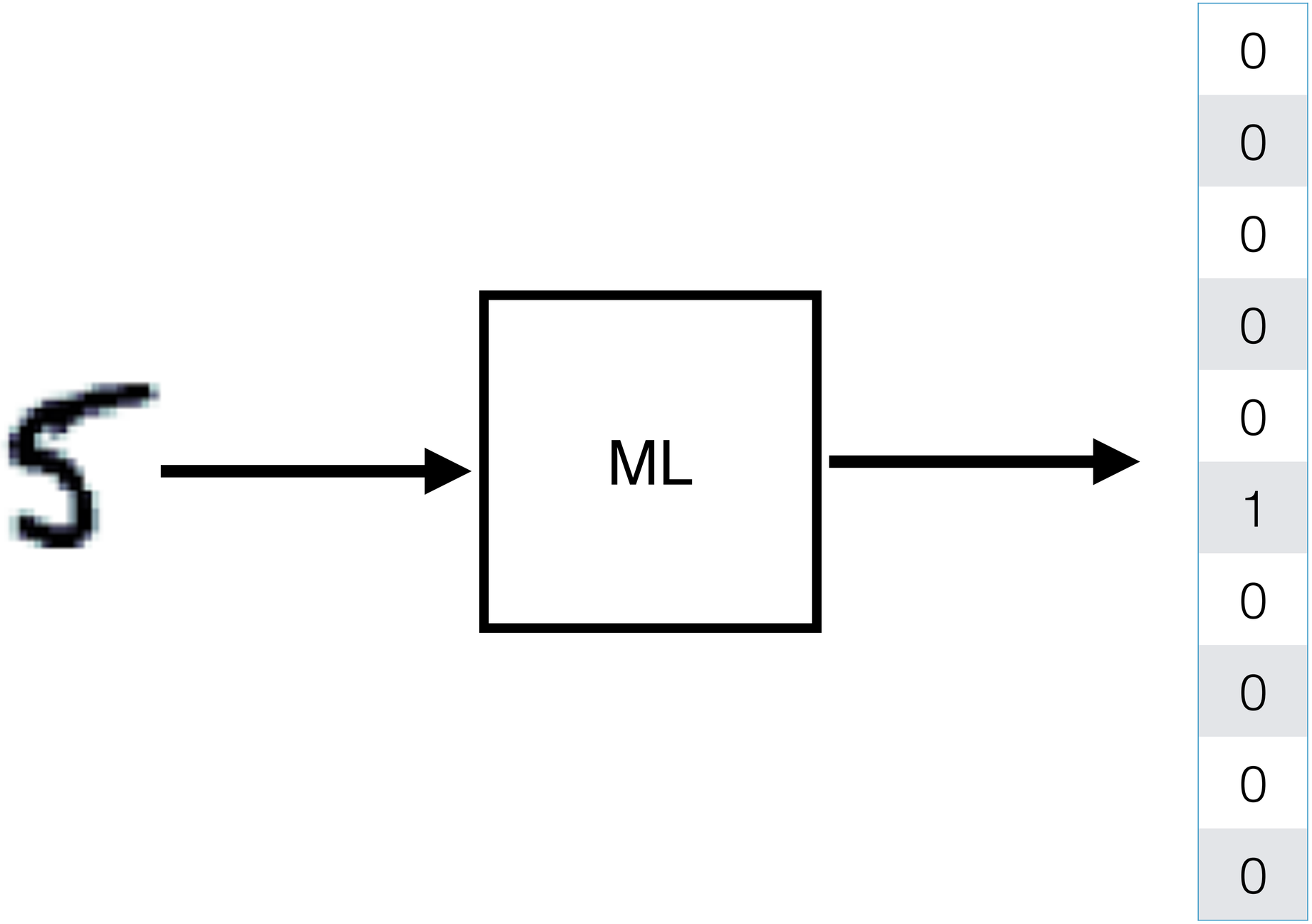
A lightvessel, or lightship, is a ship which acts as a lighthouse. They are used in waters that are too deep or otherwise unsuitable for lighthouse construction. Although there is some record of fire beacons placed on ships in Roman times, the first modern lightvessel was off the Nore sandbank at the mouth of the River Thames in England, placed there by its inventor Robert Hamblin in 1732.

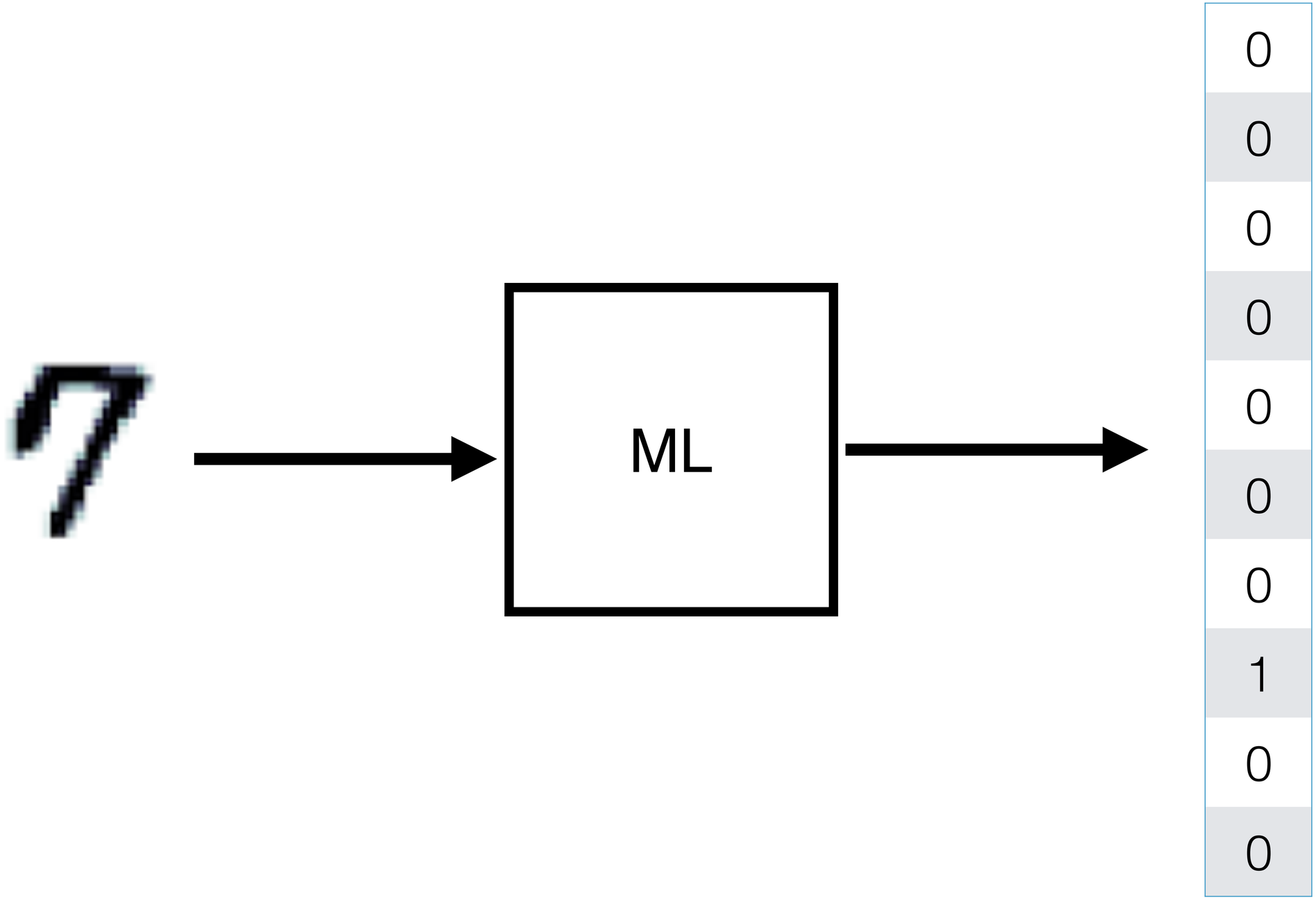
Google images

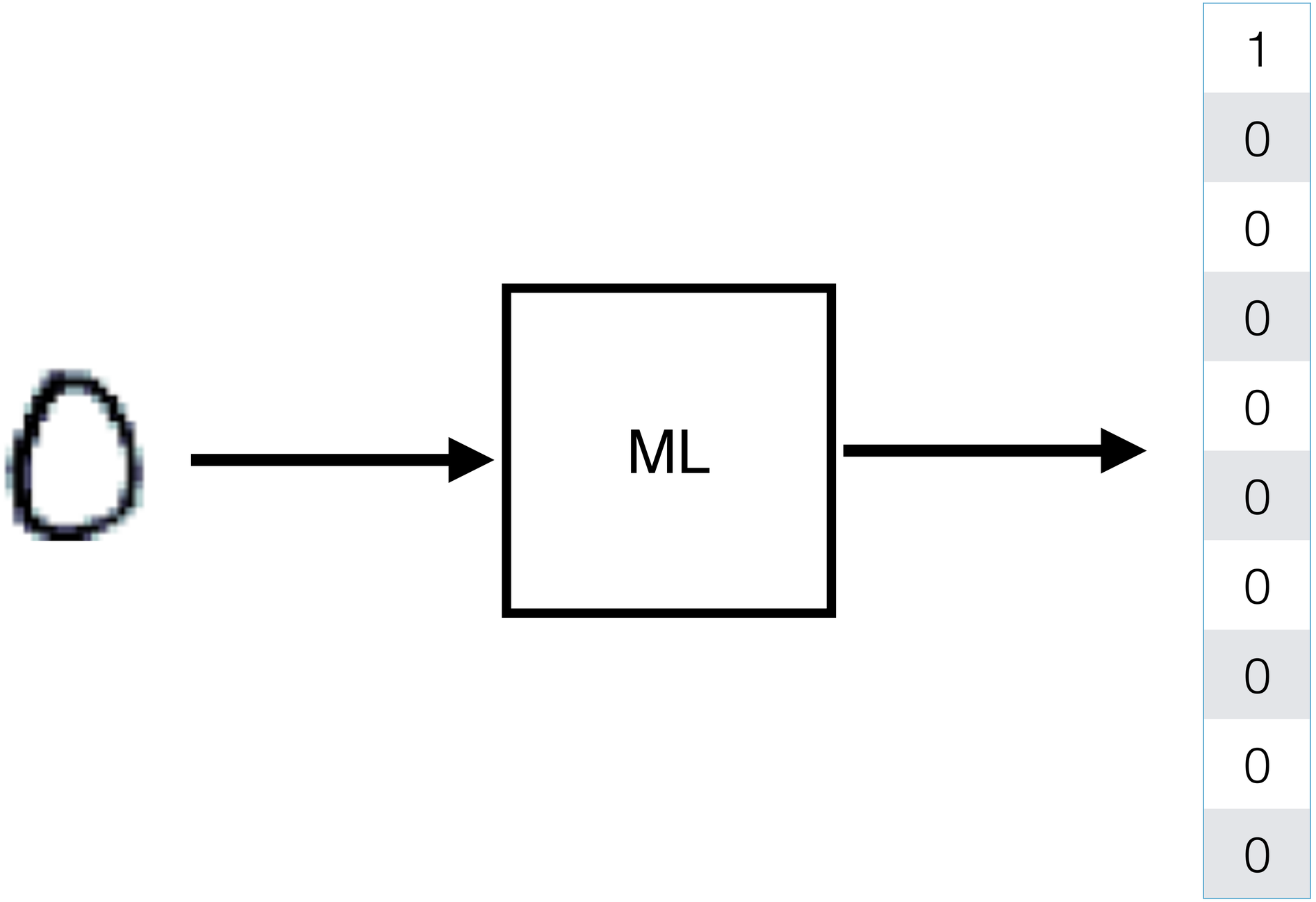


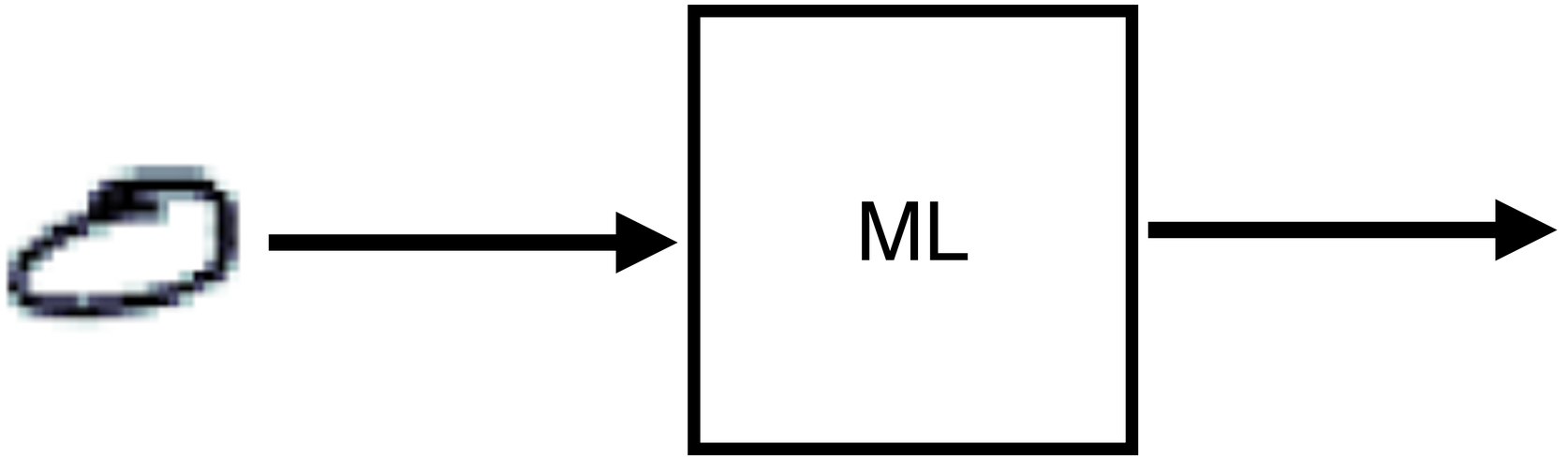
MNIST Training set




ML
0
0
0
0
0
1
0
0
0
0


ML
0
0
0
0
0
0
0
0
1
0
0


ML
1
0
0
0
0
0
0
0
0
0

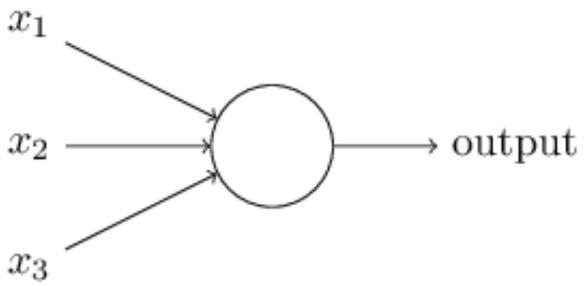


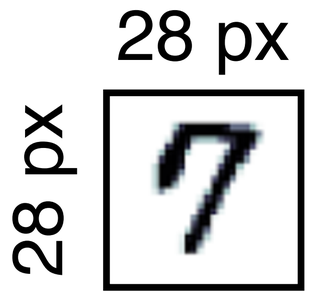
1
0
0
0
0
0
0
0
0
0

ML

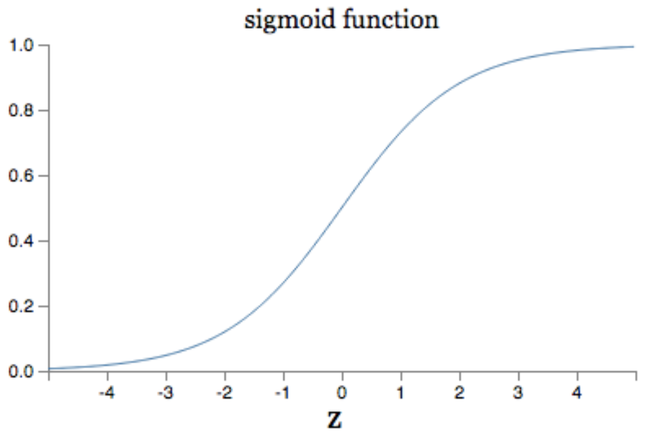
1
0
0
0
0
0
0
0
0
0

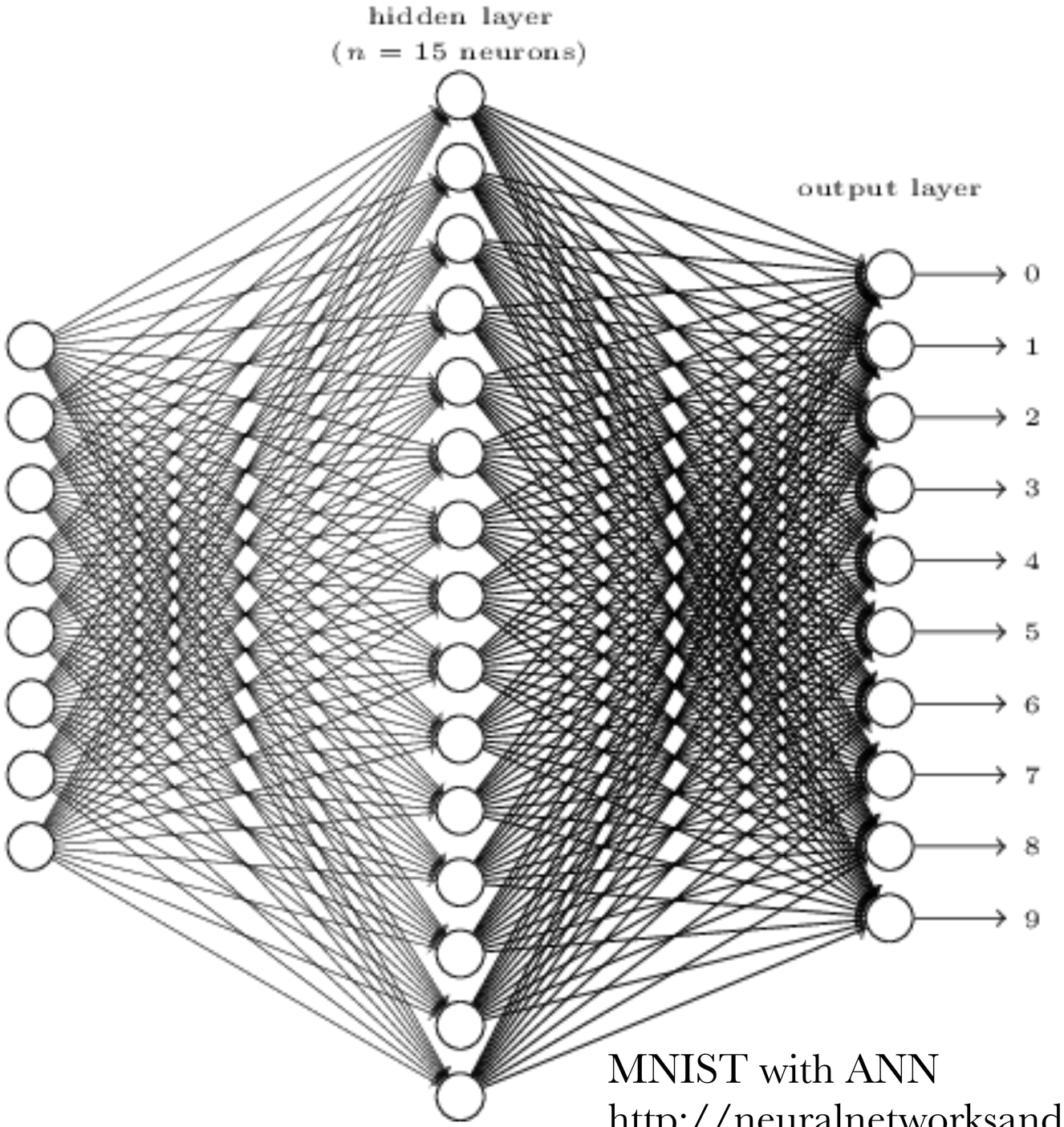
After lots of training, the ML algorithm can accurately classify new data



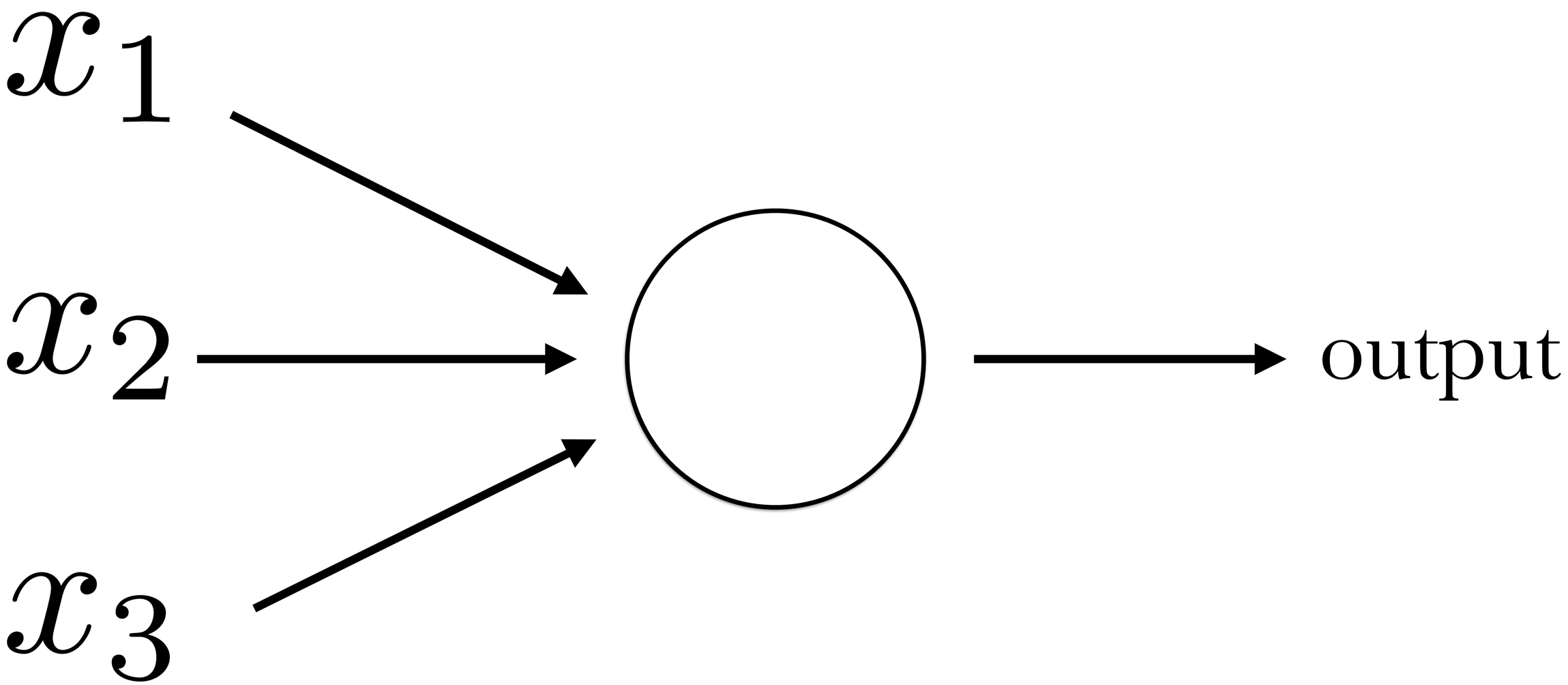


input layer
(784 neurons)





MNIST with ANN
http://neuralnetworksanddeeplearning.com


x_1
x_2
x_3
output

$$x_1 \times w_1 =$$

$$x_2 \times w_2 =$$

$$x_3 \times w_3 =$$

1 x w_1 =

128 x w_2 =

200 x w_3 =

1 X 0.8743234 =

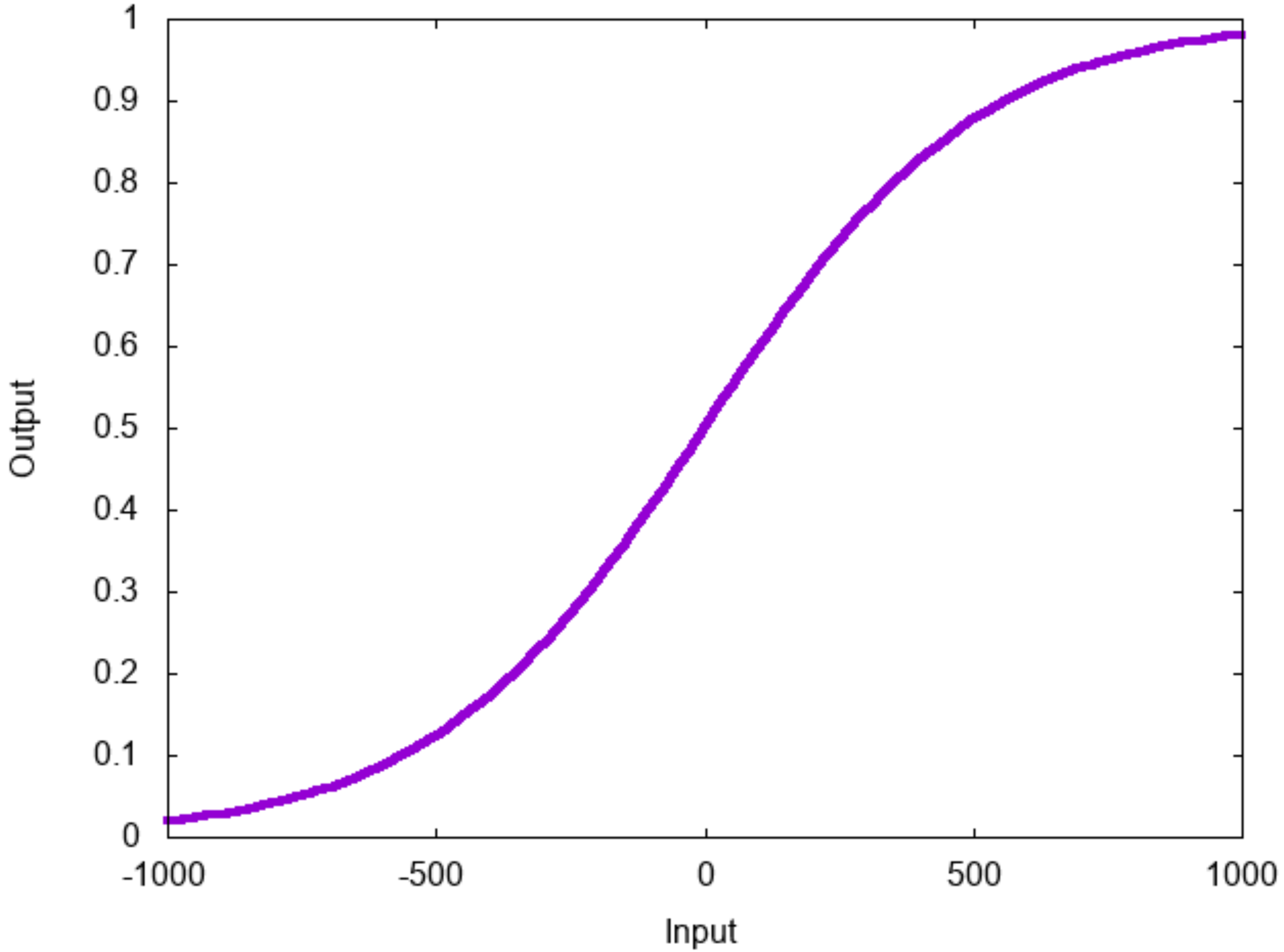
128 X 0.3765123 =

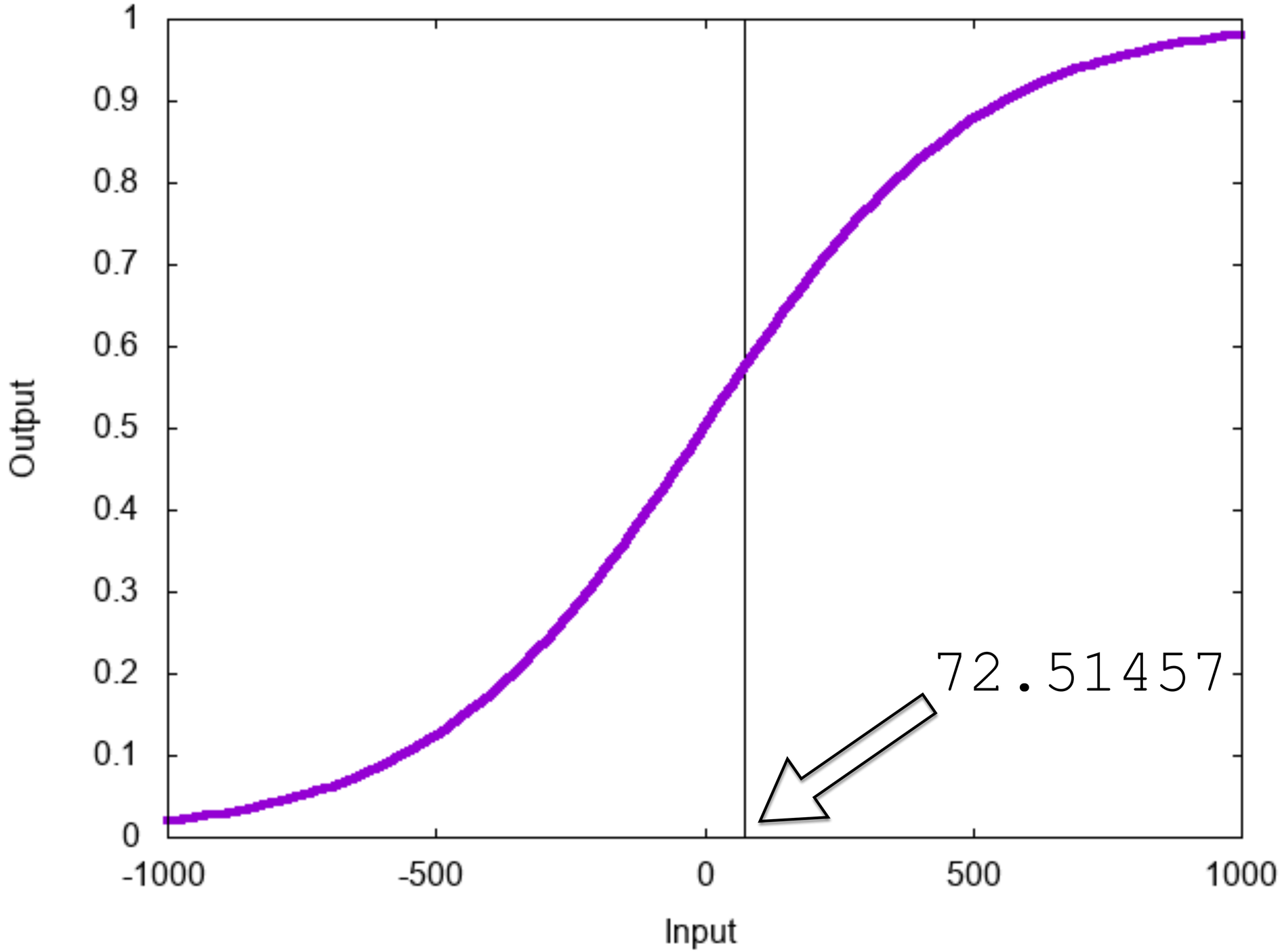
200 X 0.1172334 =

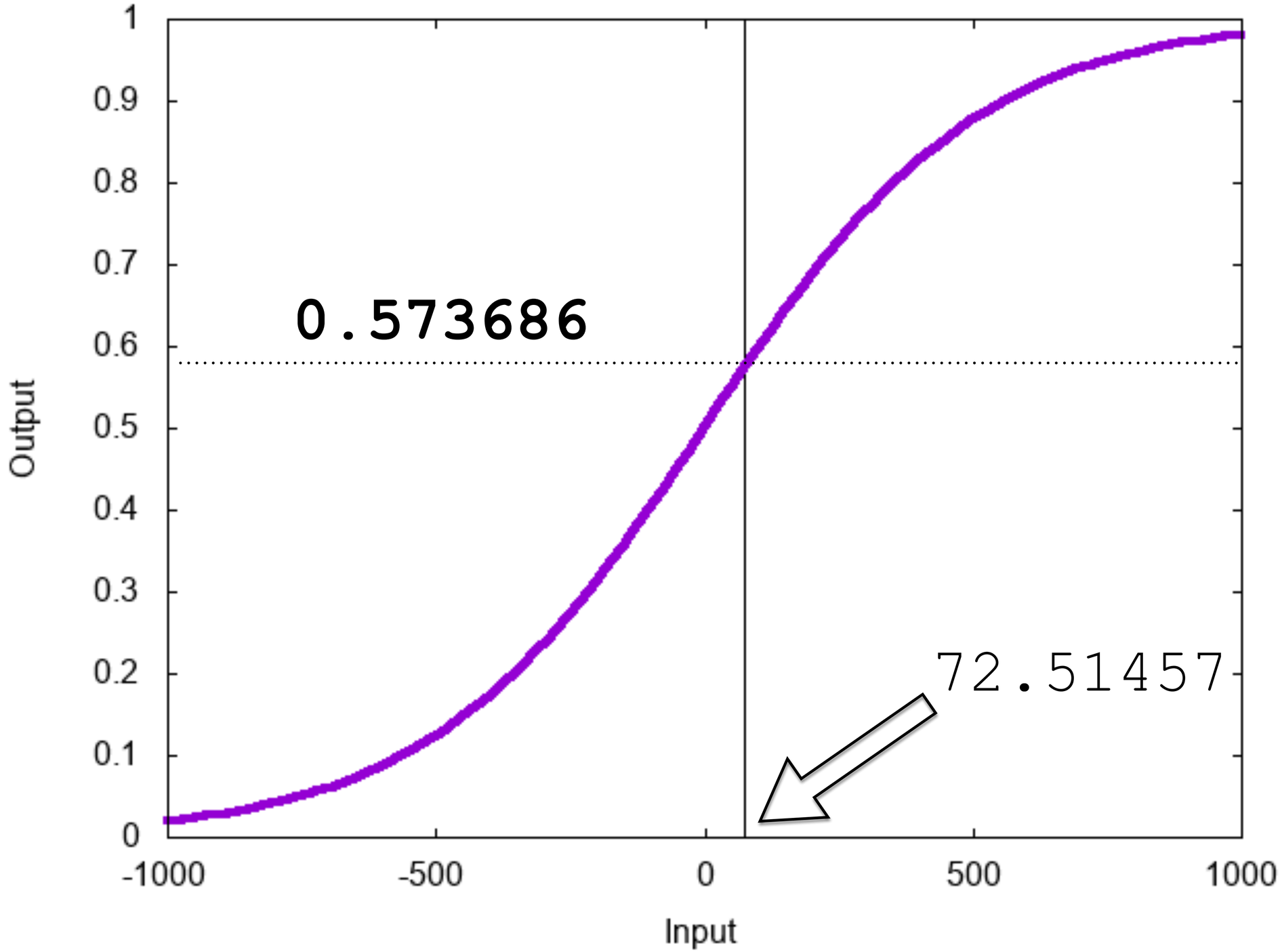
1	X	0.8743234	=	0.8743234
128	X	0.3765123	=	48.1935744
200	X	0.1172334	=	23.44668

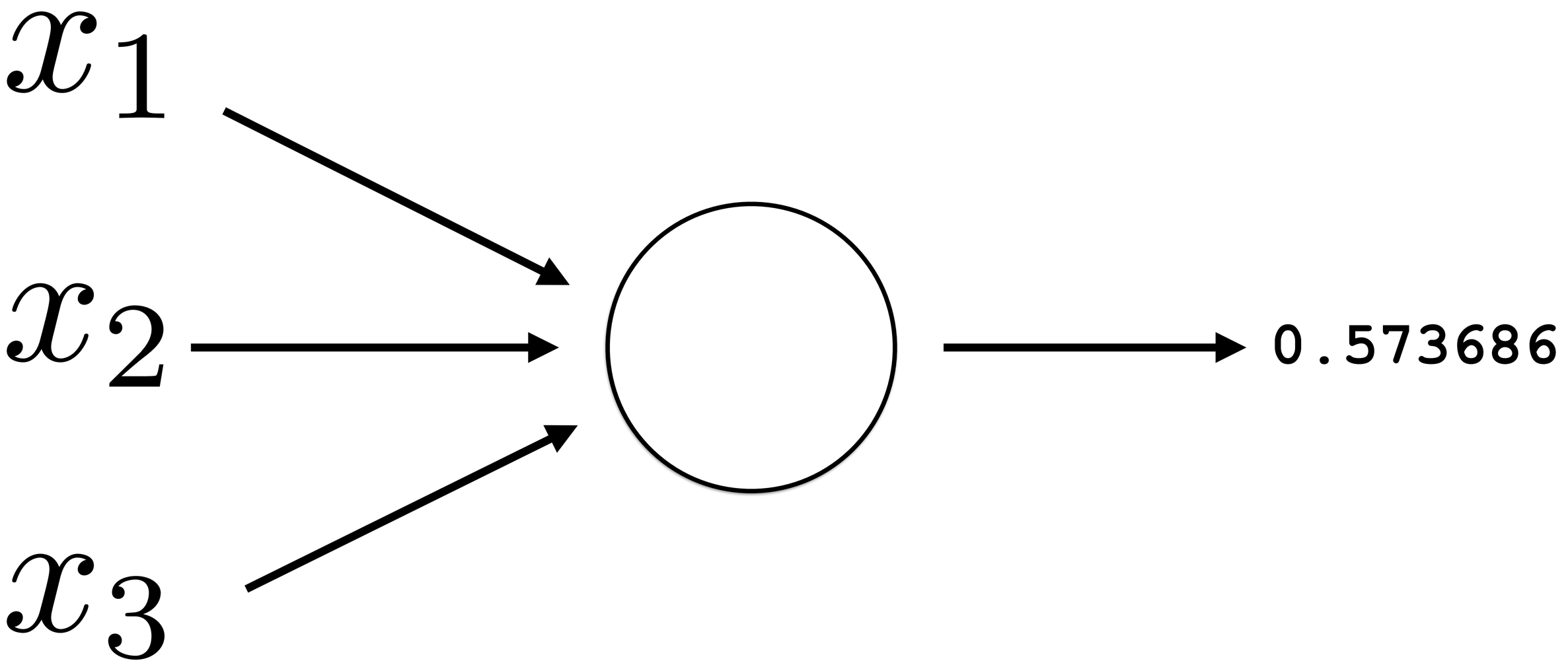
1	X	0.8743234	=	0.8743234
128	X	0.3765123	=	48.1935744
200	X	0.1172334	=	23.44668

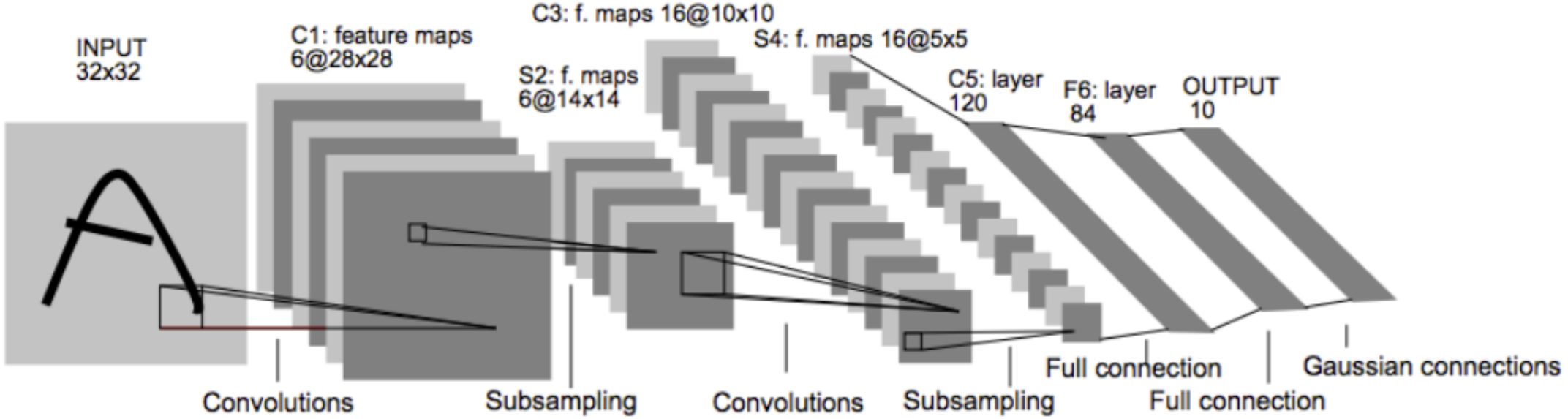
sum is 72.51457 [store a *few* decimals]

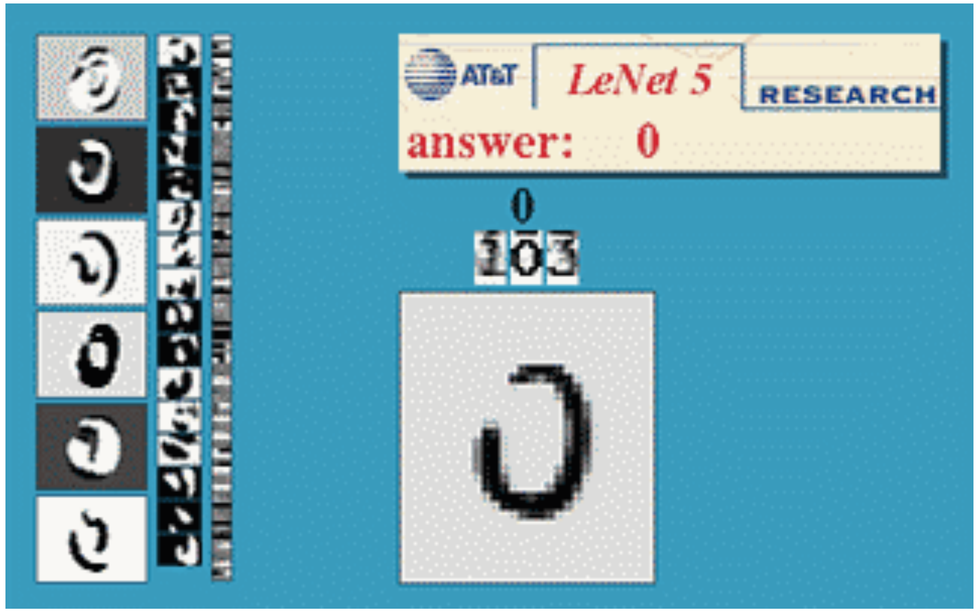

1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Output
-1000
-500
0
500
1000
Input

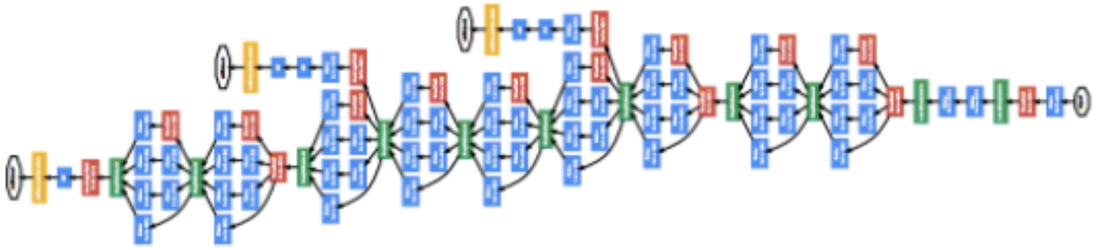

1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Output
-1000
-500
0
500
1000
Input
72.51457


1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Output
0.573686
72.51457
-1000
-500
0
500
1000
Input


x_1
x_2
x_3
0.573686

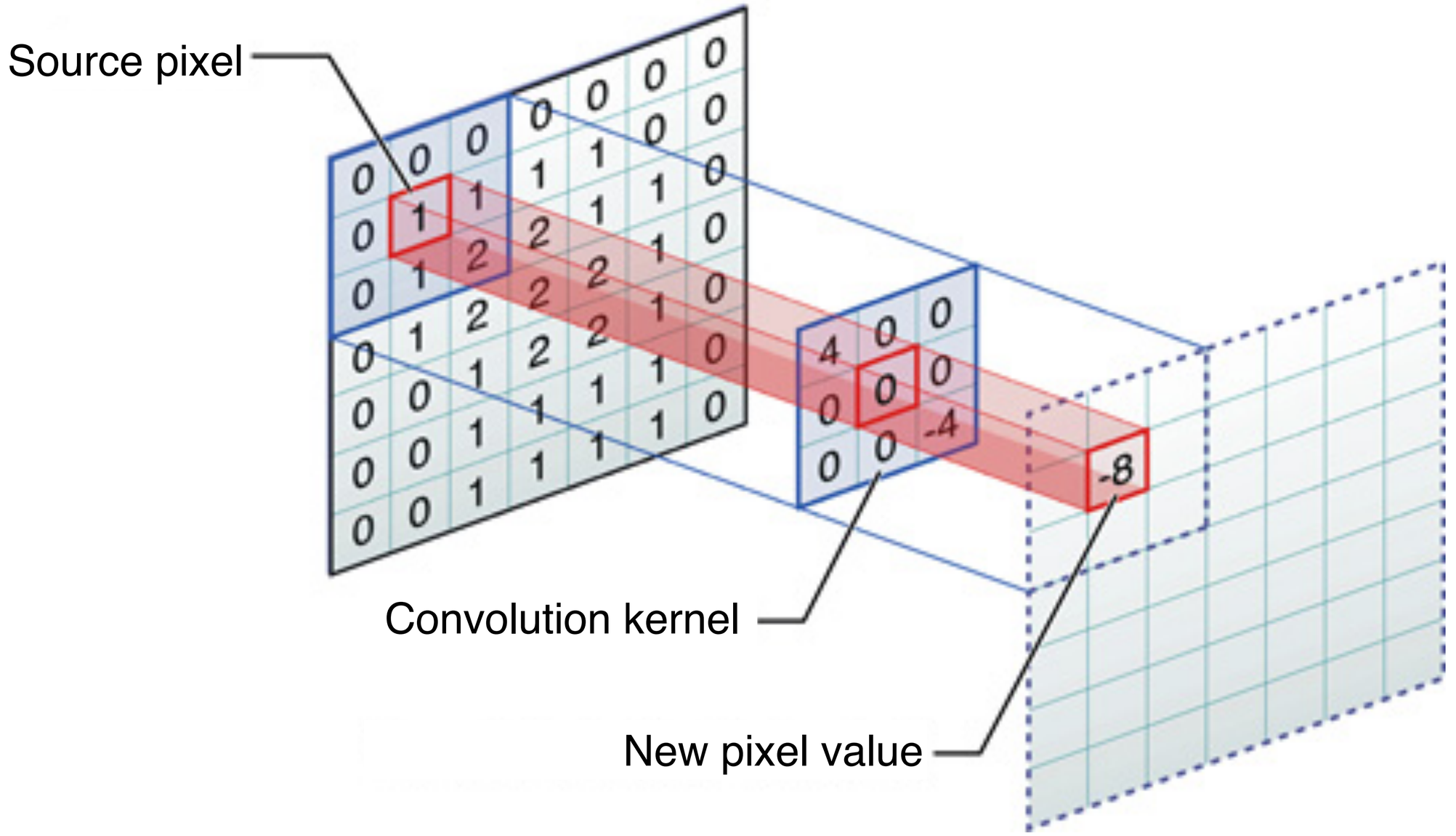






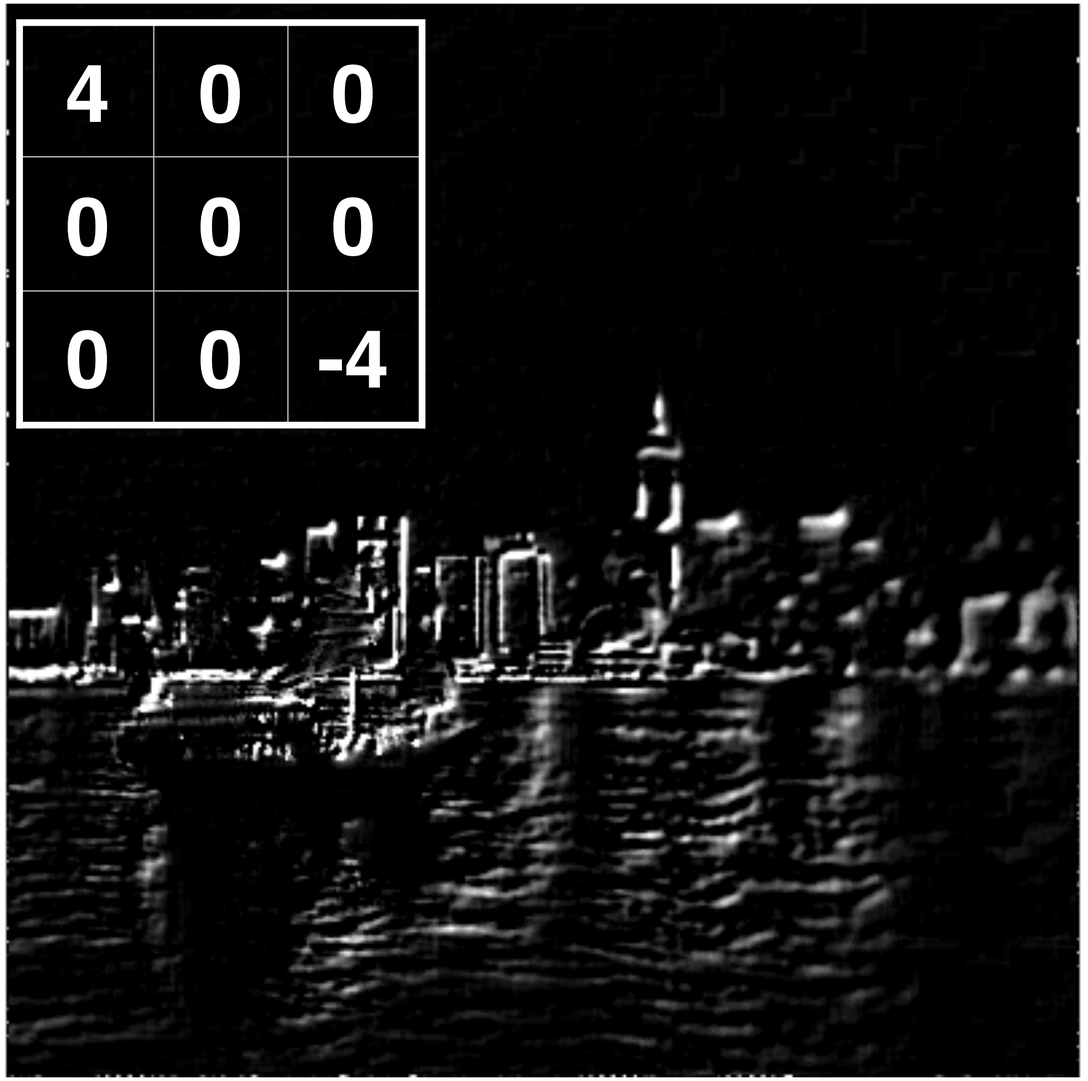
(GoogleNet, 22 layers!)

Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner, Proceedings of the IEEE, November 1998




```
(4 x 0)
(0 x 0)
(0 x 0)
(0 x 0)
(0 x 1)
(0 x 1)
(0 x 0)
(0 x 1)
+ (-4 x 2)
-8
```

https://developer.apple.com


4 0 0
0 0 0
0 0 -4

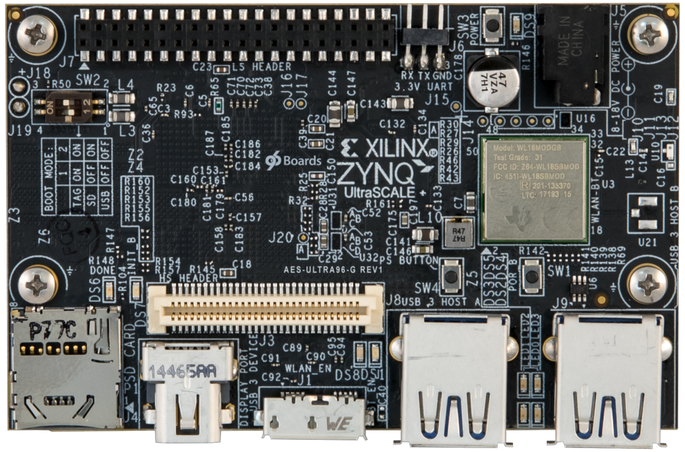

-1 -1 -1
-1 8 -1
-1 -1 -1

Nvidia

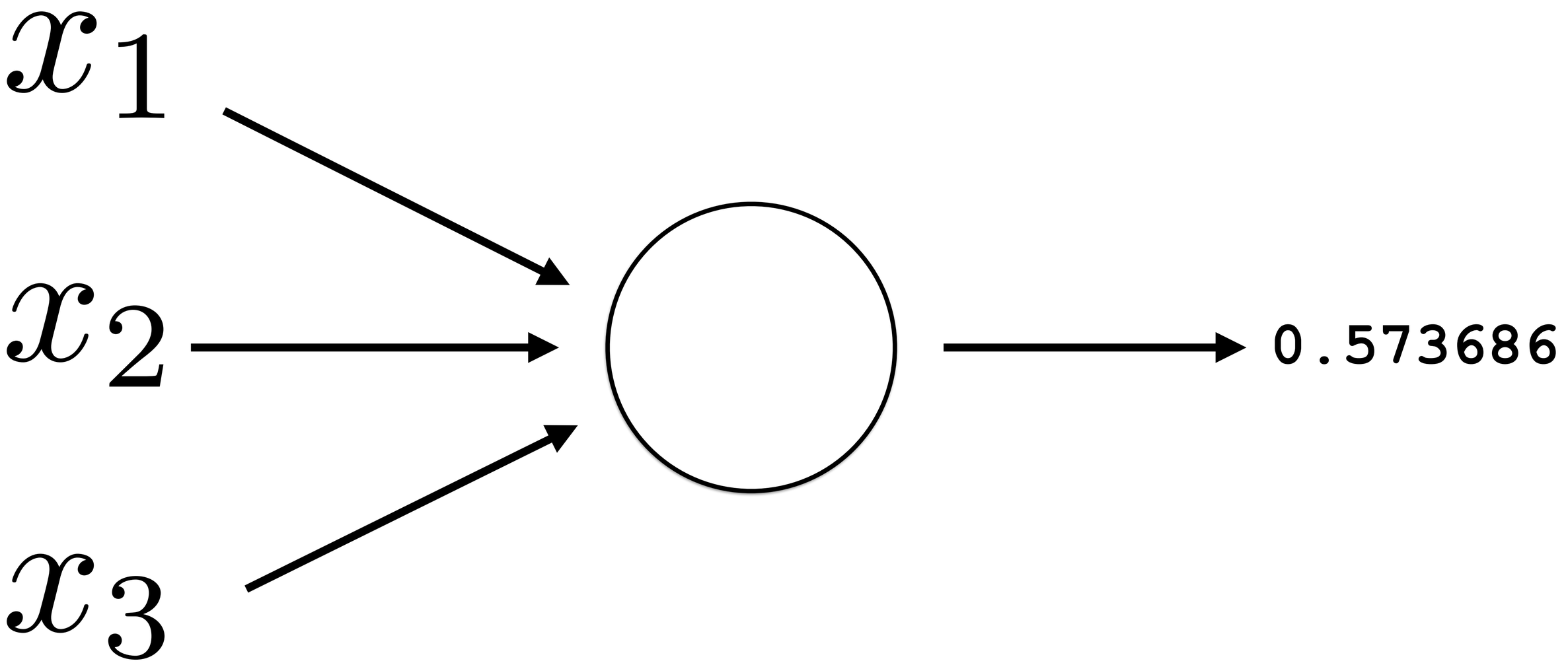
Apple

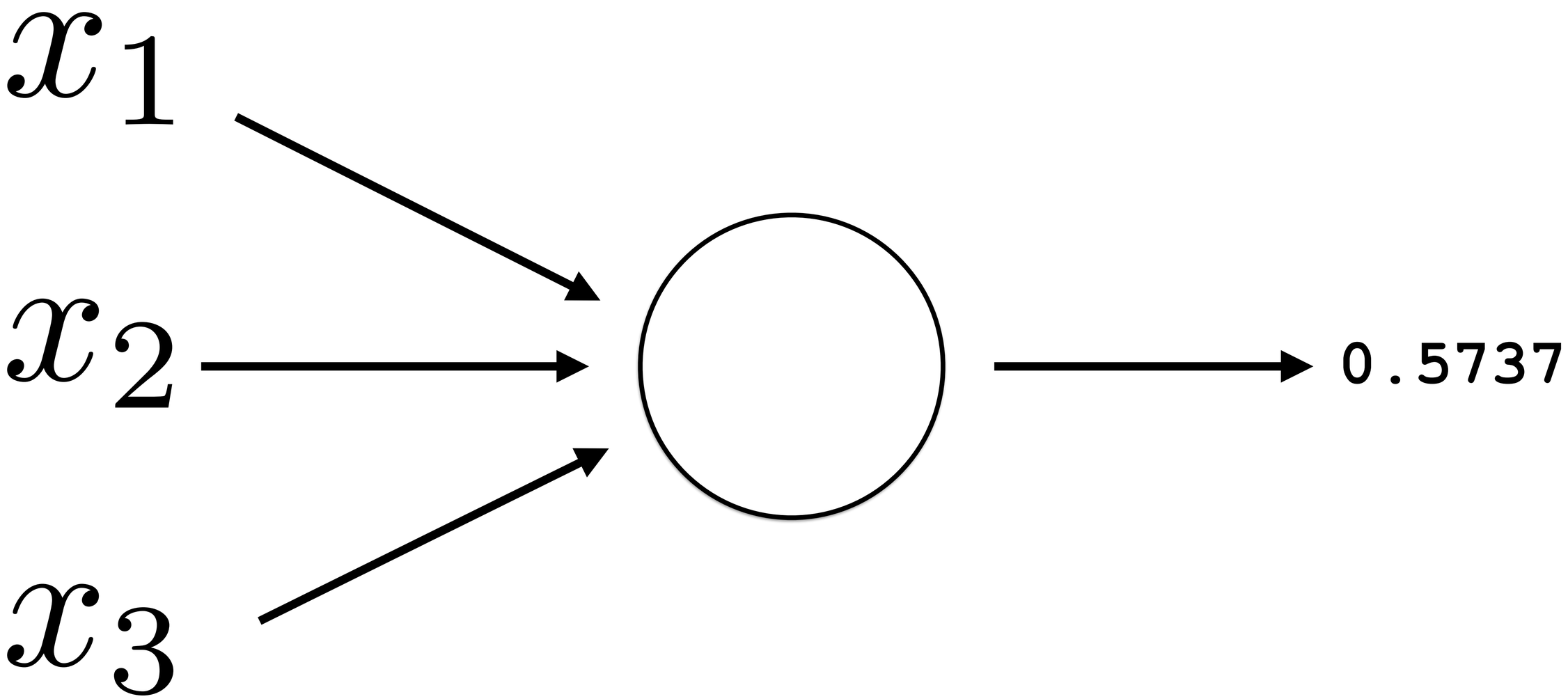
Intel Movidius and AVX-512

96boards.ai



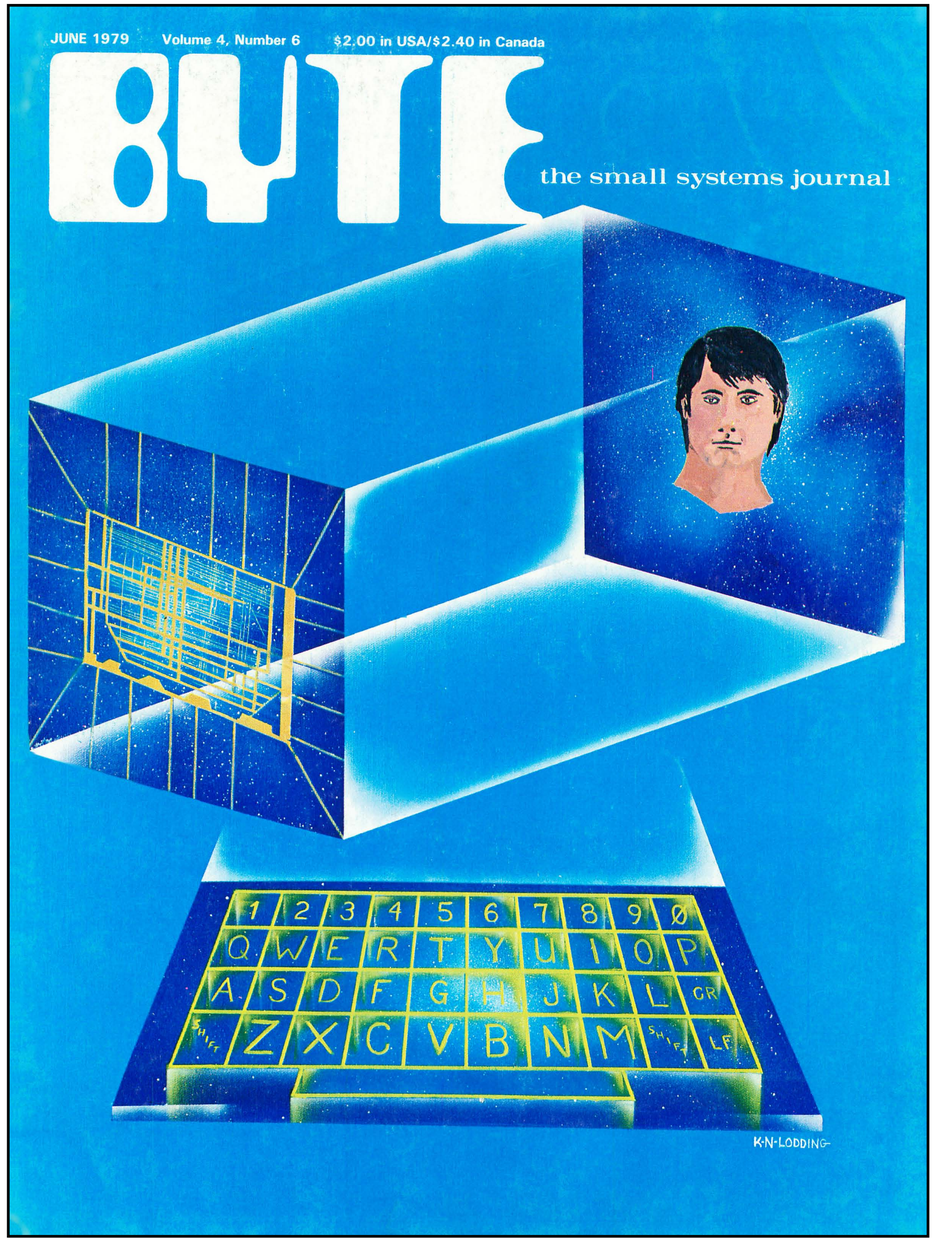
Google TPUv3


x_1
x_2
x_3
0.573686

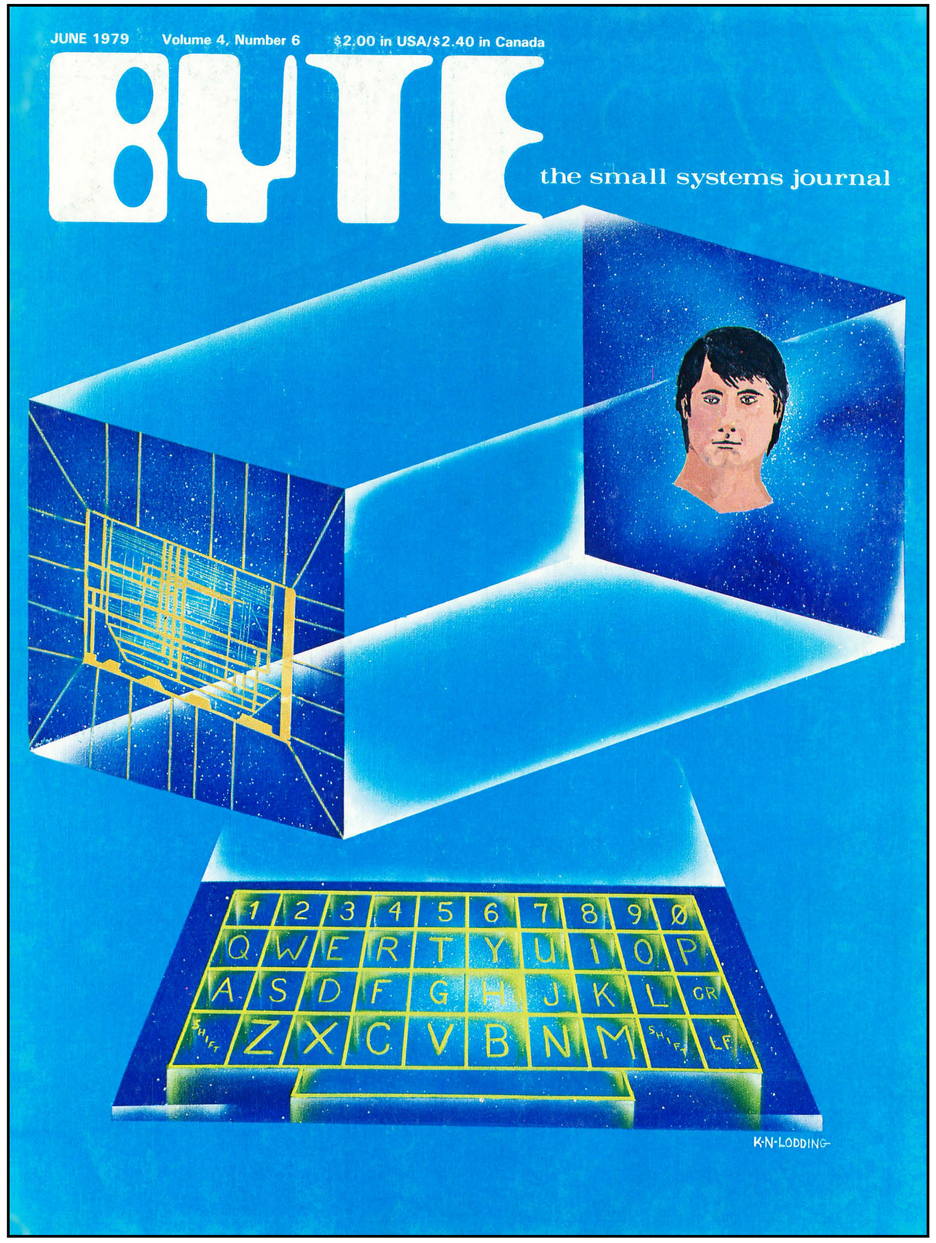


Half-precision math = tensor cores

Where do I get the weights???


JUNE 1979 Volume 4, Number 6 $2.00 in USA/$2.40 in Canada
BYTE
the small systems journal
1 2 3 4 5 6 7 8 9 Ø
Q W E R T Y U I O P
A S D F G H J K L GR
SHIFT Z X C V B N M SHIFT LF
K·N·LODDING

1985



1985

Arco, Exxon, Phillips Petroleum, Texaco Inc., The Upjohn Co. We also acknowledge the donors of the Petroleum Research Fund, administered by the American Chemical Society (grant 16144-AC2 to M.H.E., grant 14805-AC2 to S.A.M.) for support. S.A.M. acknowledges NSERC (grant A2644) for partial support.

Received 19 May; accepted 15 July 1986.

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3. Boulton, G. S. *et al. Nature* **298**, 437–441 (1982).
4. Wehmiller, J. F. in *Quaternary Dating Methods* (ed. Mahaney, W. C.) 171–193 (Elsevier, Amsterdam, 1984).
5. Engel, M. H., Zumberge, J. E. & Nagy, B. *Analyt. Biochem.* **82**, 415–422 (1977).
6. Bada, J. L. A. *Rev. Earth planet. Sci.* **13**, 241–268 (1985).

Learning representations by back-propagating errors

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* Institute for Cognitive Science, C-015, University of California, San Diego, La Jolla, California 92093, USA
† Department of Computer Science, Carnegie-Mellon University, Pittsburgh, Philadelphia 15213, USA

There have been many attempts to design self-organizing neural networks. The aim is to find a powerful synaptic modification rule that will allow an arbitrarily connected neural network to develop an internal structure that is appropriate for a particular task domain. The task is specified by giving the desired state vector of the output units for each state vector of the input units. If the input units are directly connected to the output units it is relatively easy to find learning rules that iteratively adjust the relative strengths of the connections so as to progressively reduce the difference between the actual and desired output vectors[2]. Learning becomes more interesting but

† To whom correspondence should be addressed.

y_i, of the units that are connected to j and of the weights, w_{ji}, on these connections

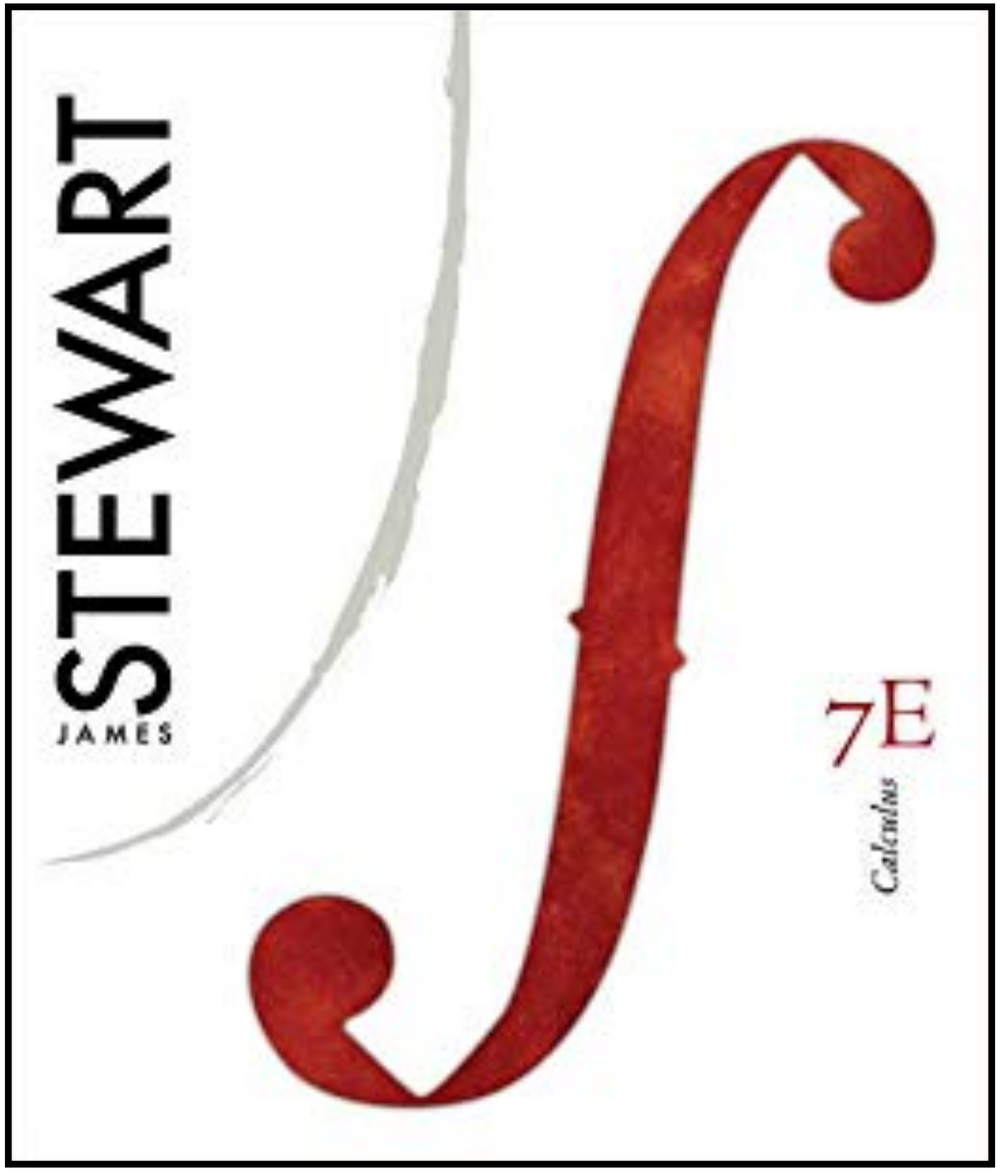
$$x_j = \sum_i y_i w_{ji} \quad (1)$$

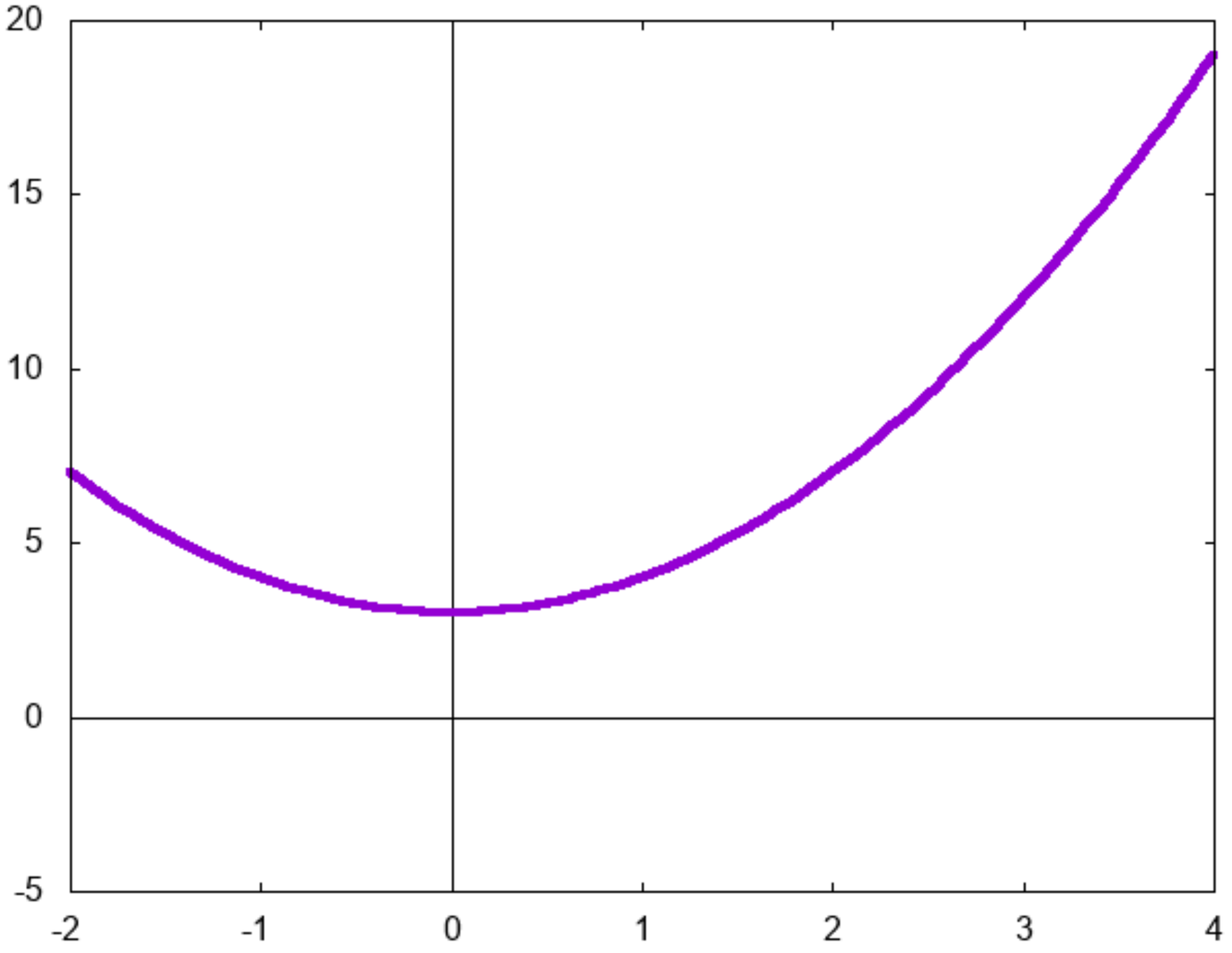
Units can be given biases by introducing an extra input to each unit which always has a value of 1. The weight on this extra input is called the bias and is equivalent to a threshold of the opposite sign. It can be treated just like the other weights.

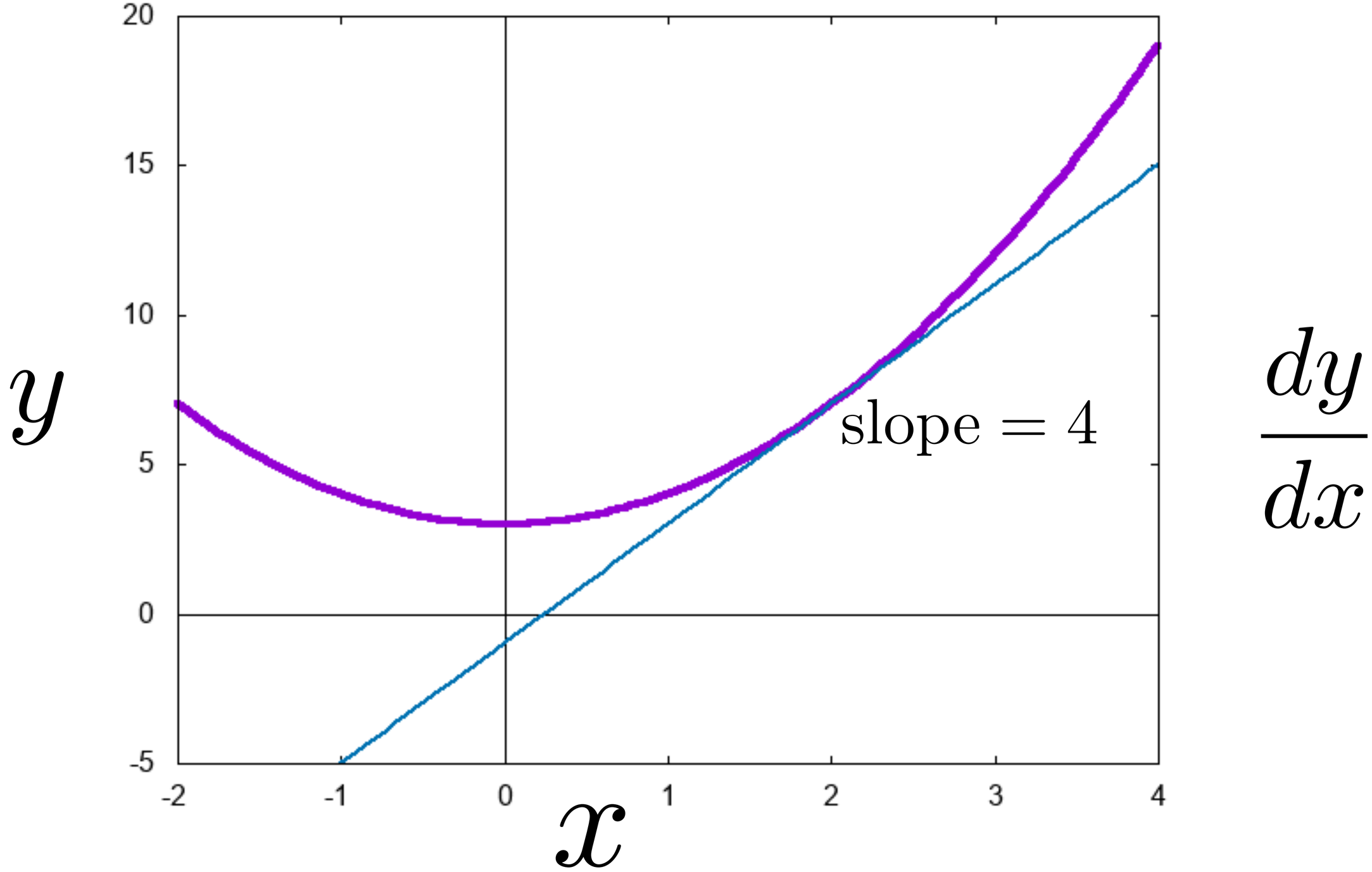
A unit has a real-valued output, y_j, which is a non-linear function of its total input

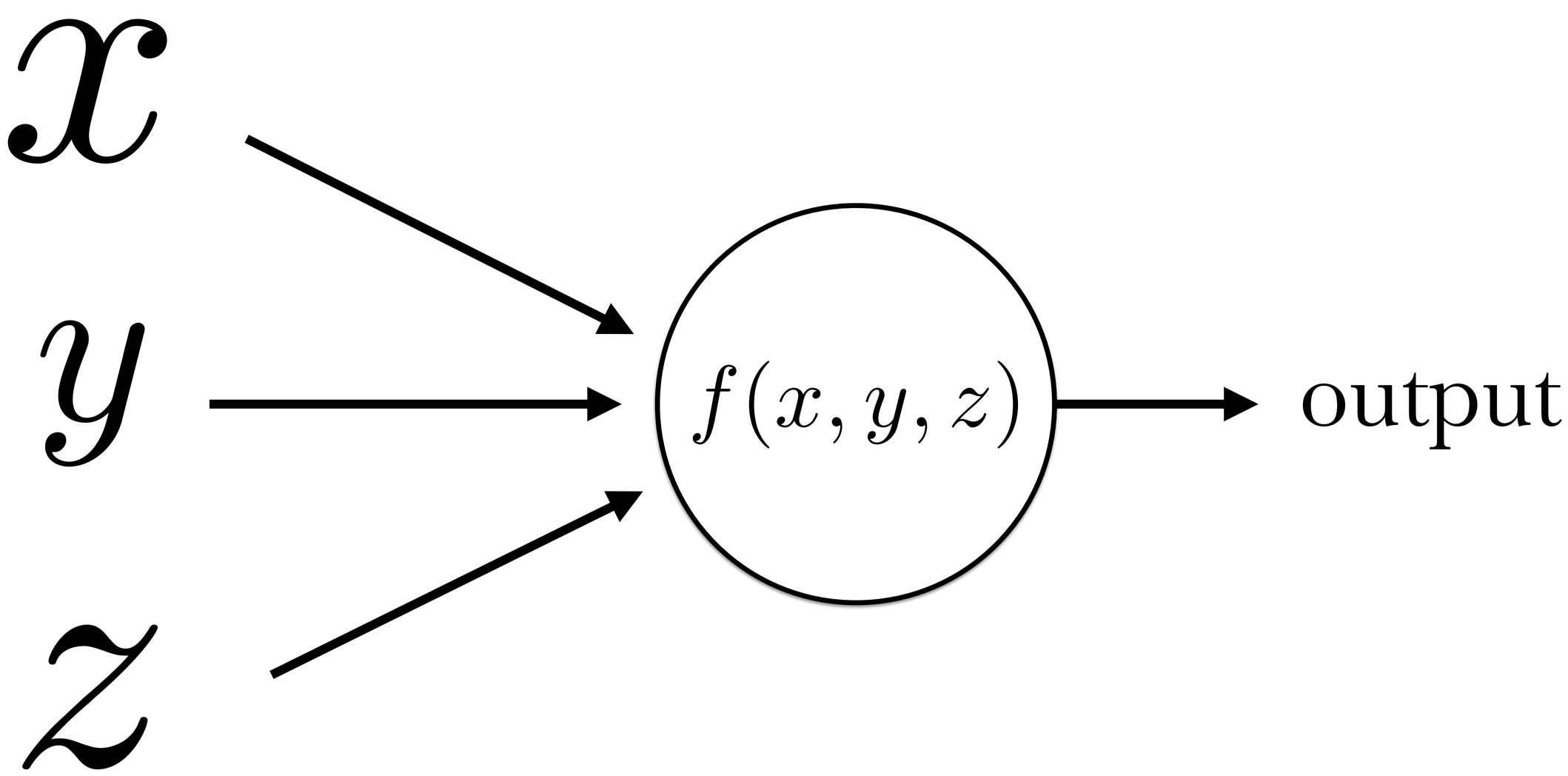
$$y_j = \frac{1}{1+e^{-x_j}} \quad (2)$$

1986


STEWART
JAMES
7E
Calculus


20
15
10
5
0
-5
-2
-1
0
1
2
3
4


20
15
10
5
0
-5
-2
-1
0
1
2
3
4
y
x
slope $= 4$
$\frac{dy}{dx}$


x
y
z
$f(x, y, z)$
output

$$f(x, y, z)$$

$$df = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy + \frac{\partial f}{\partial z}dz$$ partial derivatives!

if x, y, z depend on t

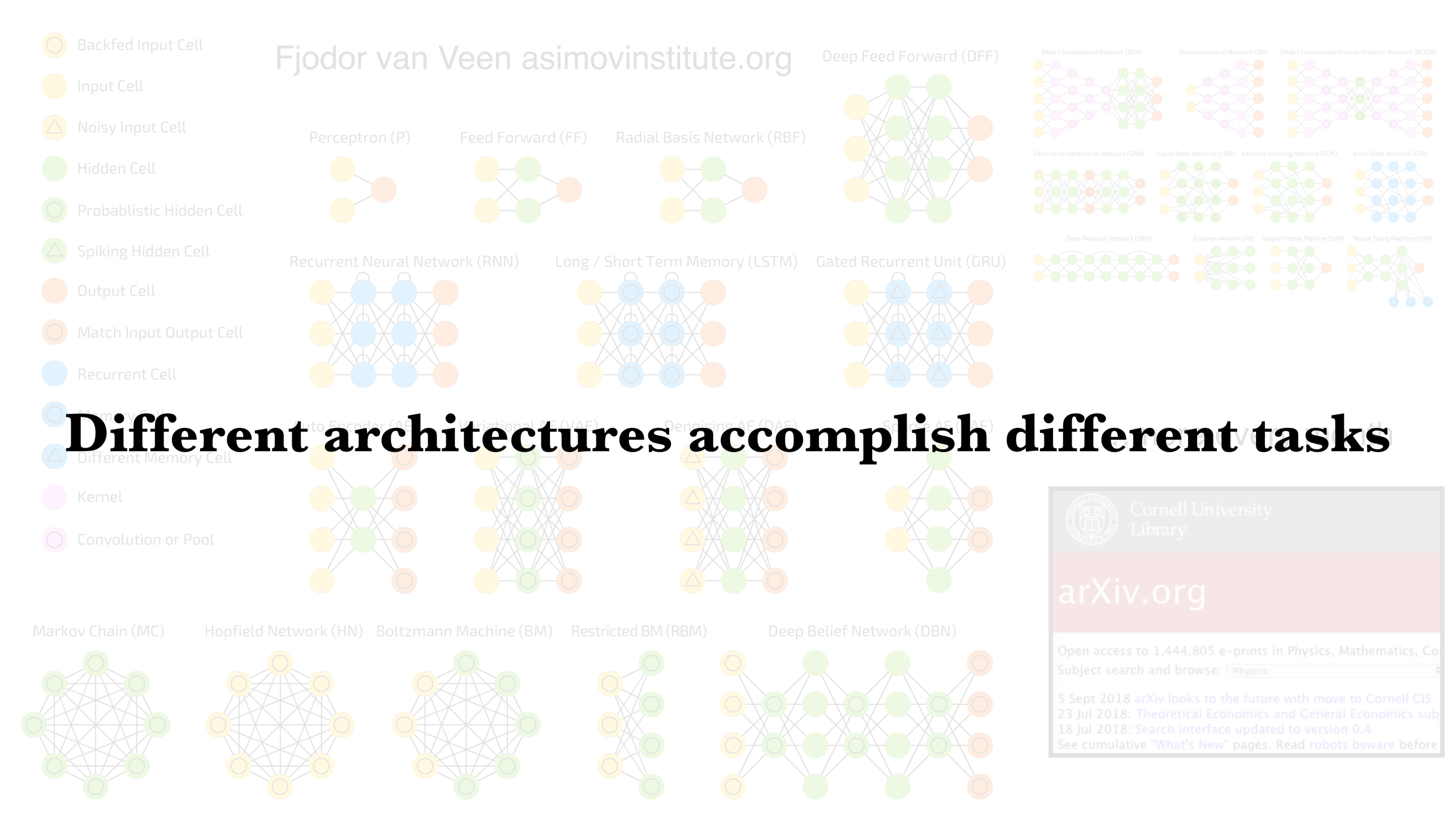
$$\frac{df}{dt} = \frac{\partial f}{\partial x} \cdot \frac{dx}{dt} + \frac{\partial f}{\partial y} \cdot \frac{dy}{dt} + \frac{\partial f}{\partial z} \cdot \frac{dz}{dt} + \frac{\partial f}{\partial t}$$ chain rule!

LOTS of online resources

http://cs231n.stanford.edu/slides/2016/winter1516_lecture4.pdf

Weights are learned by *training* on DATA

Follow the *slopes* to minimize the error
(just like a curve fit in **Excel**)

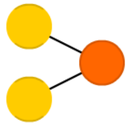


Different architectures accomplish different tasks

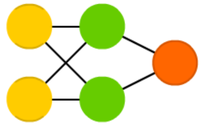
Fjodor van Veen asimovinstitute.org

- Backfed Input Cell
- Input Cell
- Noisy Input Cell
- Hidden Cell
- Probablistic Hidden Cell
- Spiking Hidden Cell
- Output Cell
- Match Input Output Cell
- Recurrent Cell
- Memory Cell
- Different Memory Cell
- Kernel
- Convolution or Pool

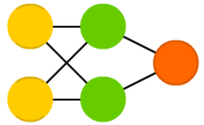
Perceptron (P)



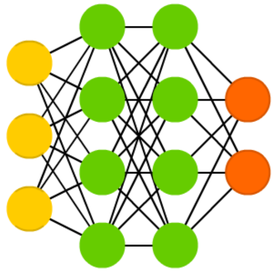
Feed Forward (FF)



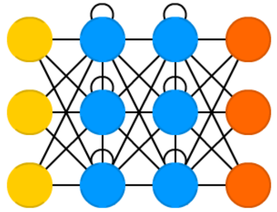
Radial Basis Network (RBF)



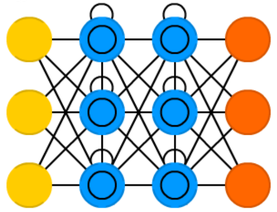
Deep Feed Forward (DFF)



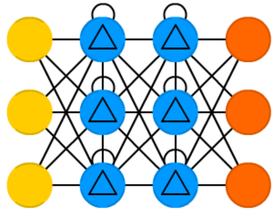
Recurrent Neural Network (RNN)



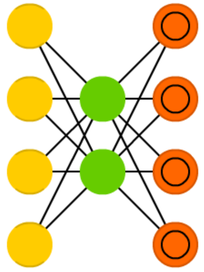
Long / Short Term Memory (LSTM)



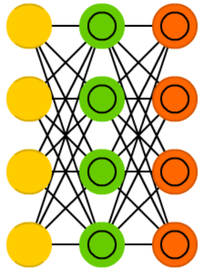
Gated Recurrent Unit (GRU)



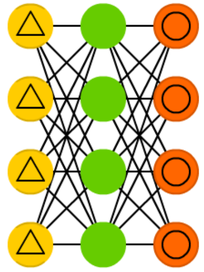
Auto Encoder (AE)



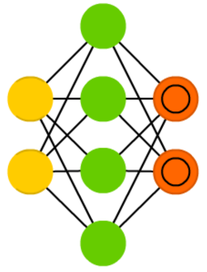
Variational AE (VAE)



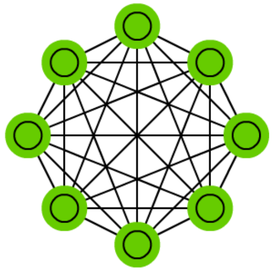
Denoising AE (DAE)



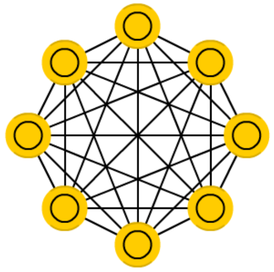
Sparse AE (SAE)



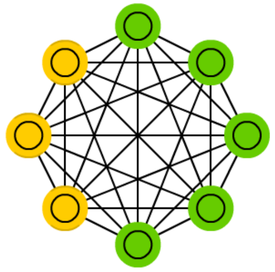
Markov Chain (MC)



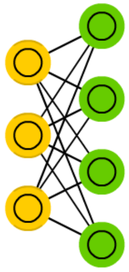
Hopfield Network (HN)



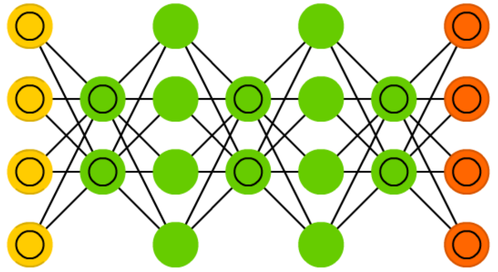
Boltzmann Machine (BM)

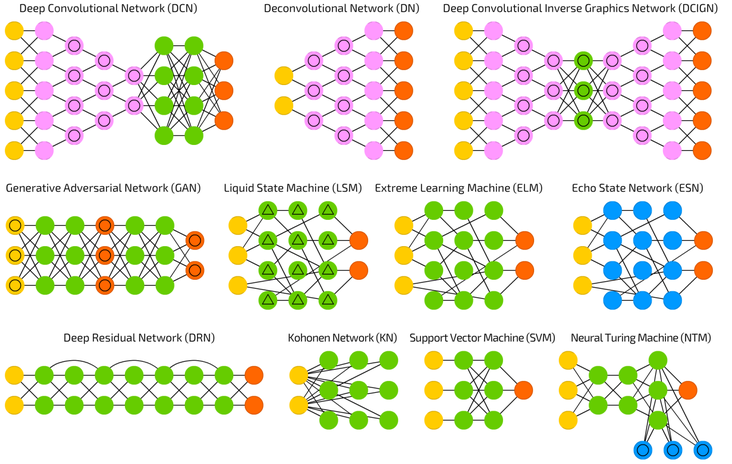


Restricted BM (RBM)

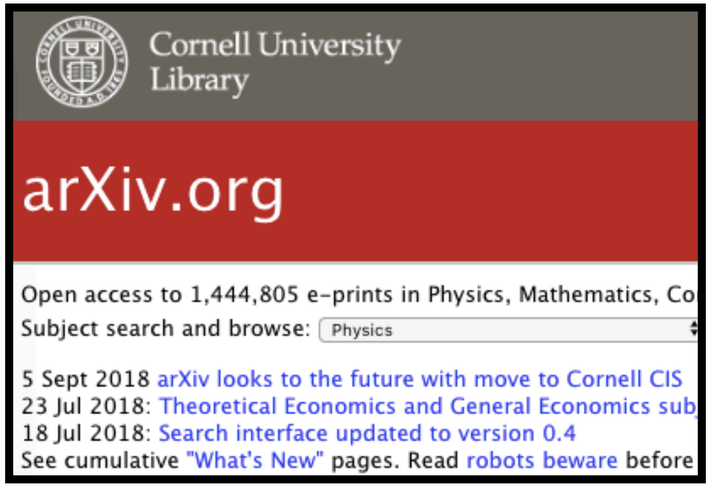


Deep Belief Network (DBN)

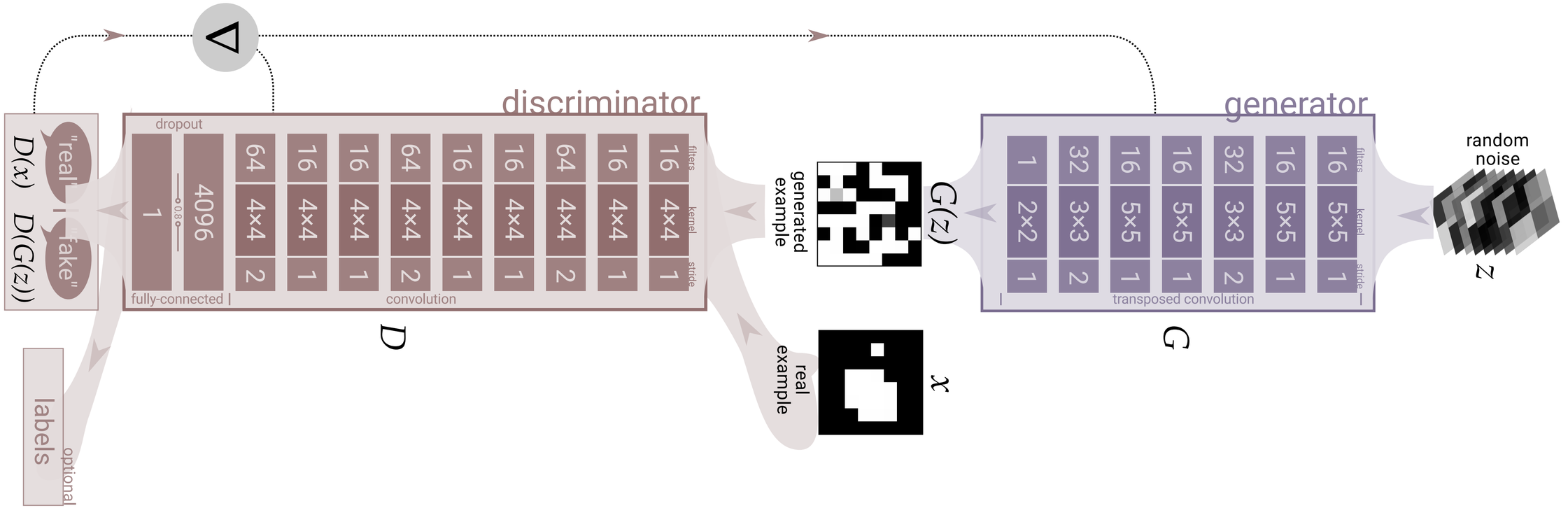




…more every month



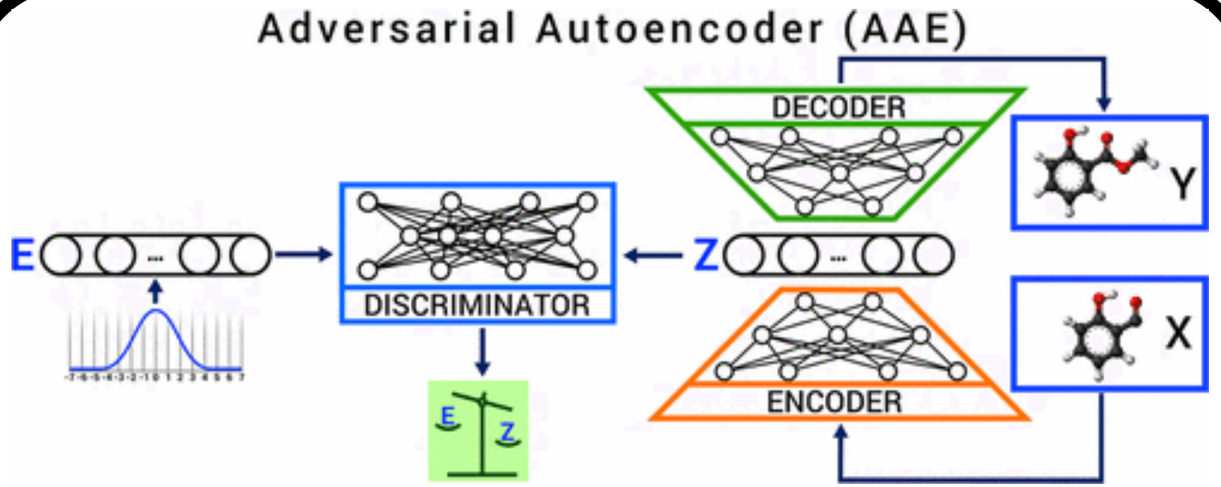
Generative adversarial networks[1]



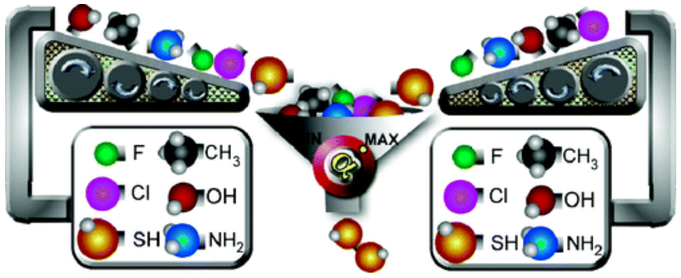
[1] Goodfellow, et al, 5423, NIPS 2014

Radford et al., ICRL 2016

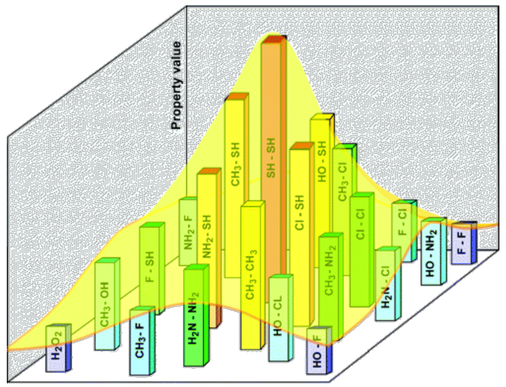
Given some observations…

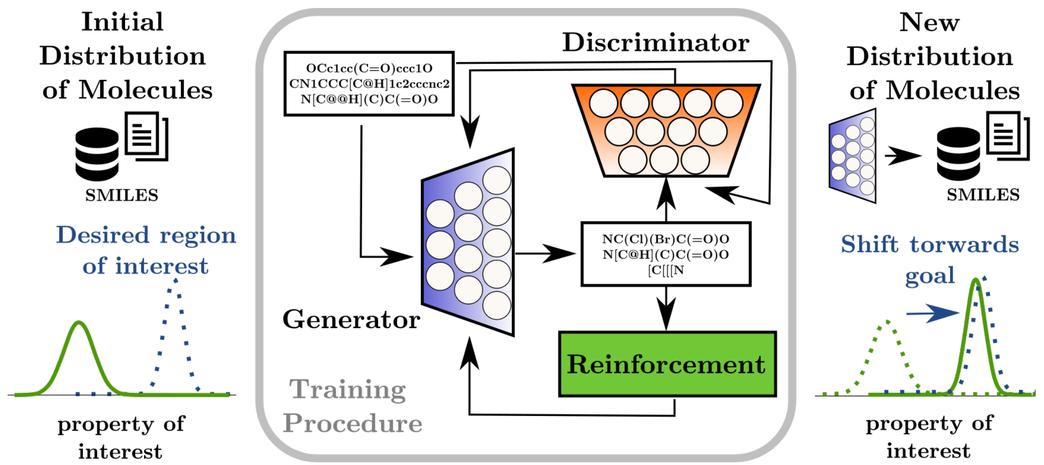


10.1021/acs.molpharmaceut.7b00346



Wang, JACS, 128, 3228, (2006)





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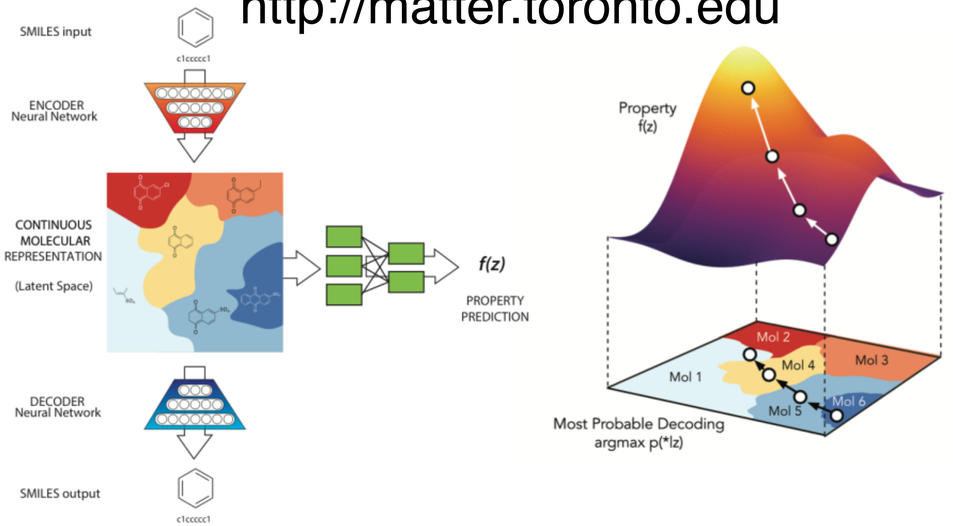
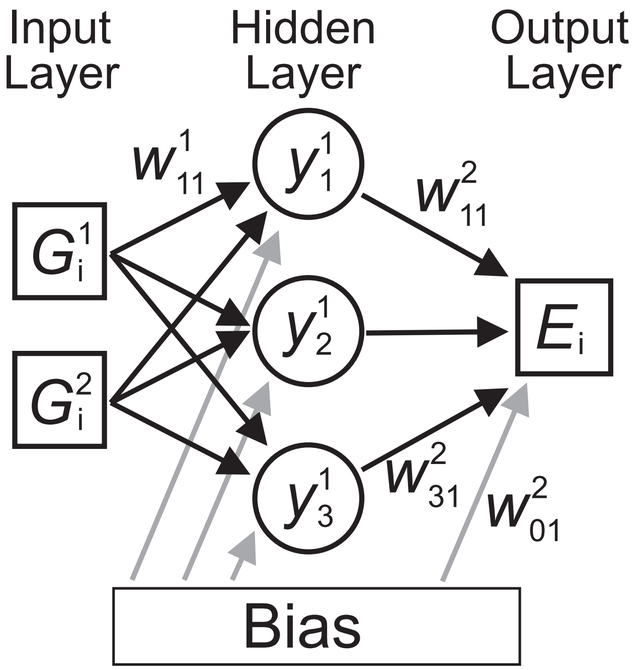
http://matter.toronto.edu



Given a structure…

symmetry basis functions



what are its “properties”?

Beeler & Parrinello, PRL 98, 146401 (2007)

How shall I describe it?

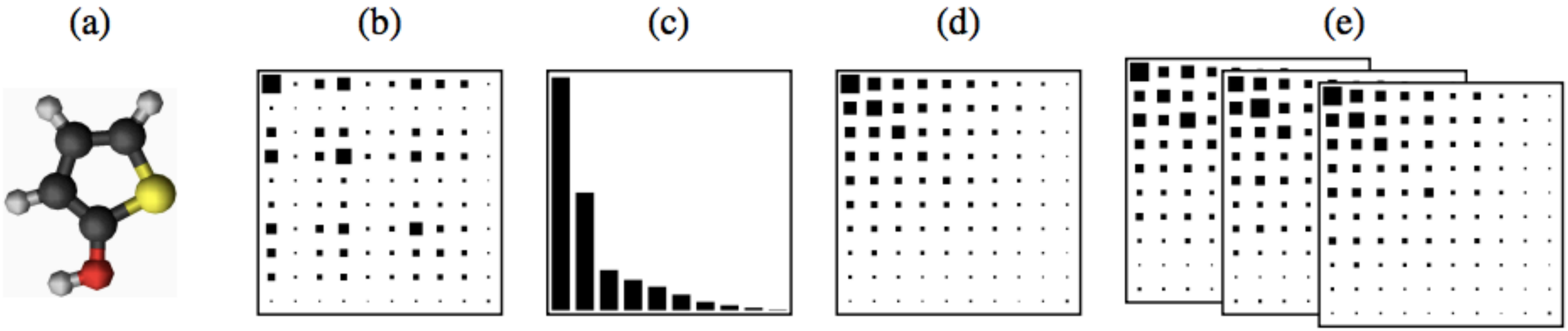
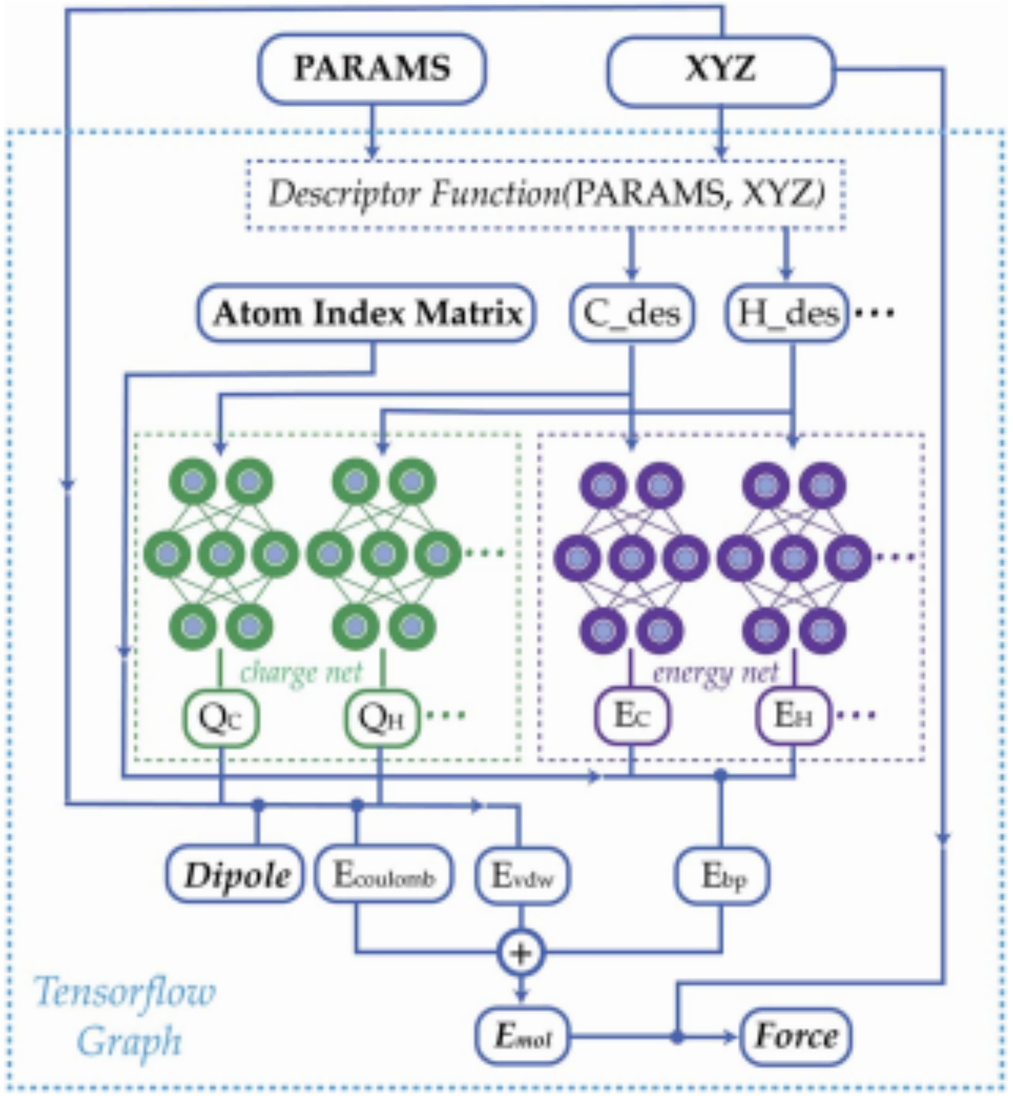


Figure 1: Different representations of the same molecule: (a) raw molecule with Cartesian coordinates and associated charges, (b) original (non-sorted) Coulomb matrix as computed by Equation 1, (c) eigenspectrum of the Coulomb matrix, (d) sorted Coulomb matrix, (e) set of randomly sorted Coulomb matrices.

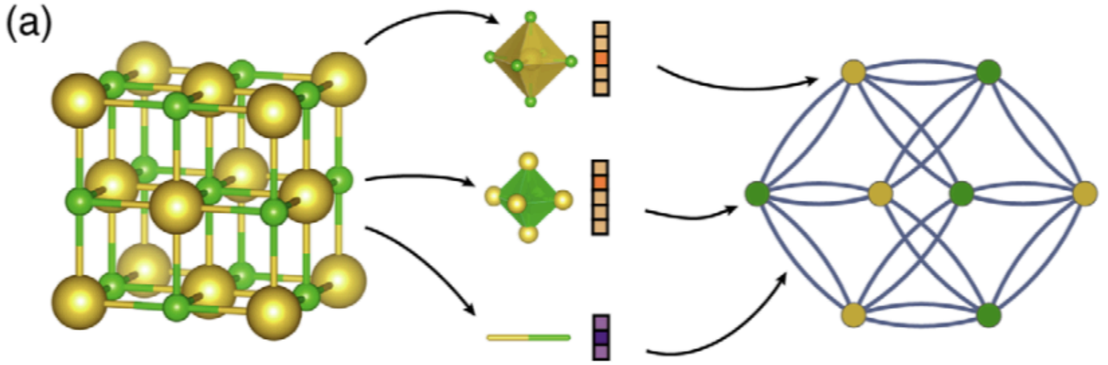
Learning Invariant Representations of Molecules for Atomization Energy Prediction, NIPS, 2012

Convolutional graph

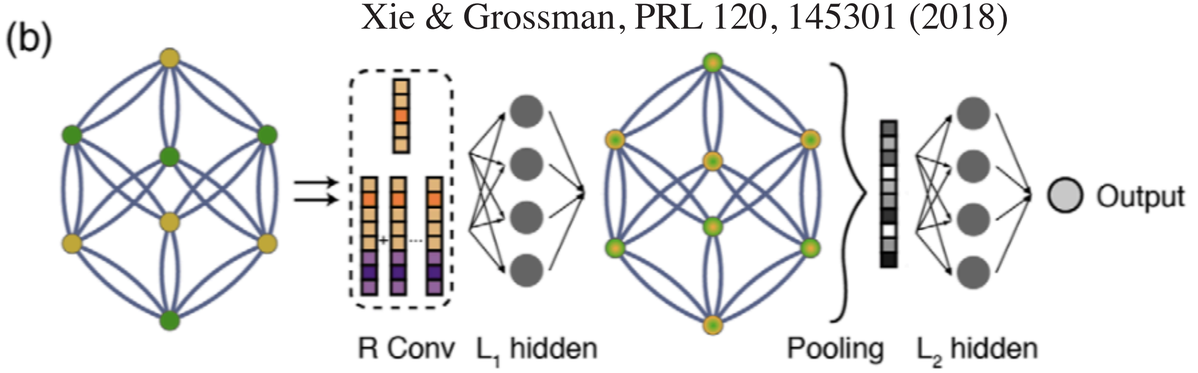
arXiv:1711.06385v2

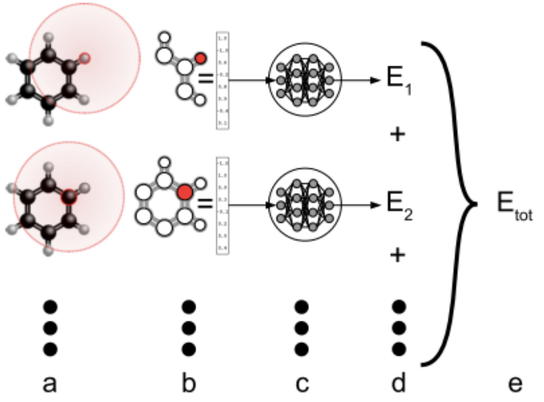


TensorMol



Xie & Grossman, PRL 120, 145301 (2018)



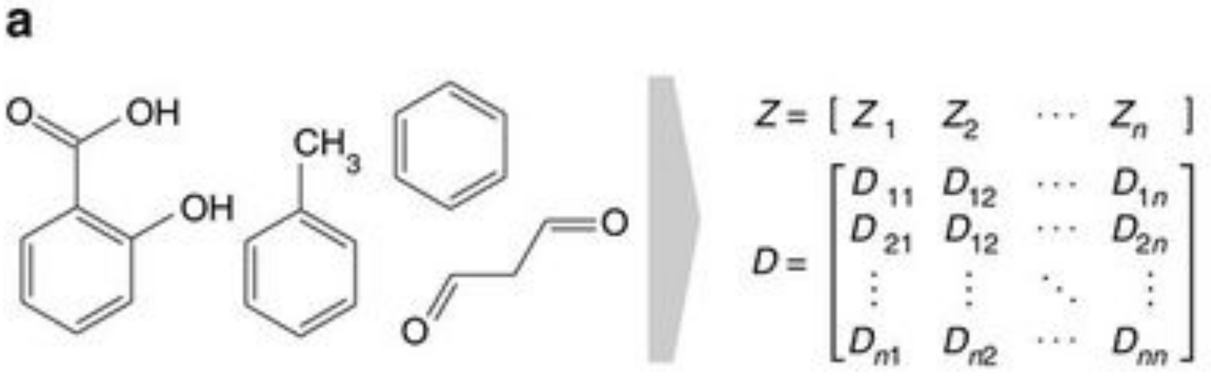


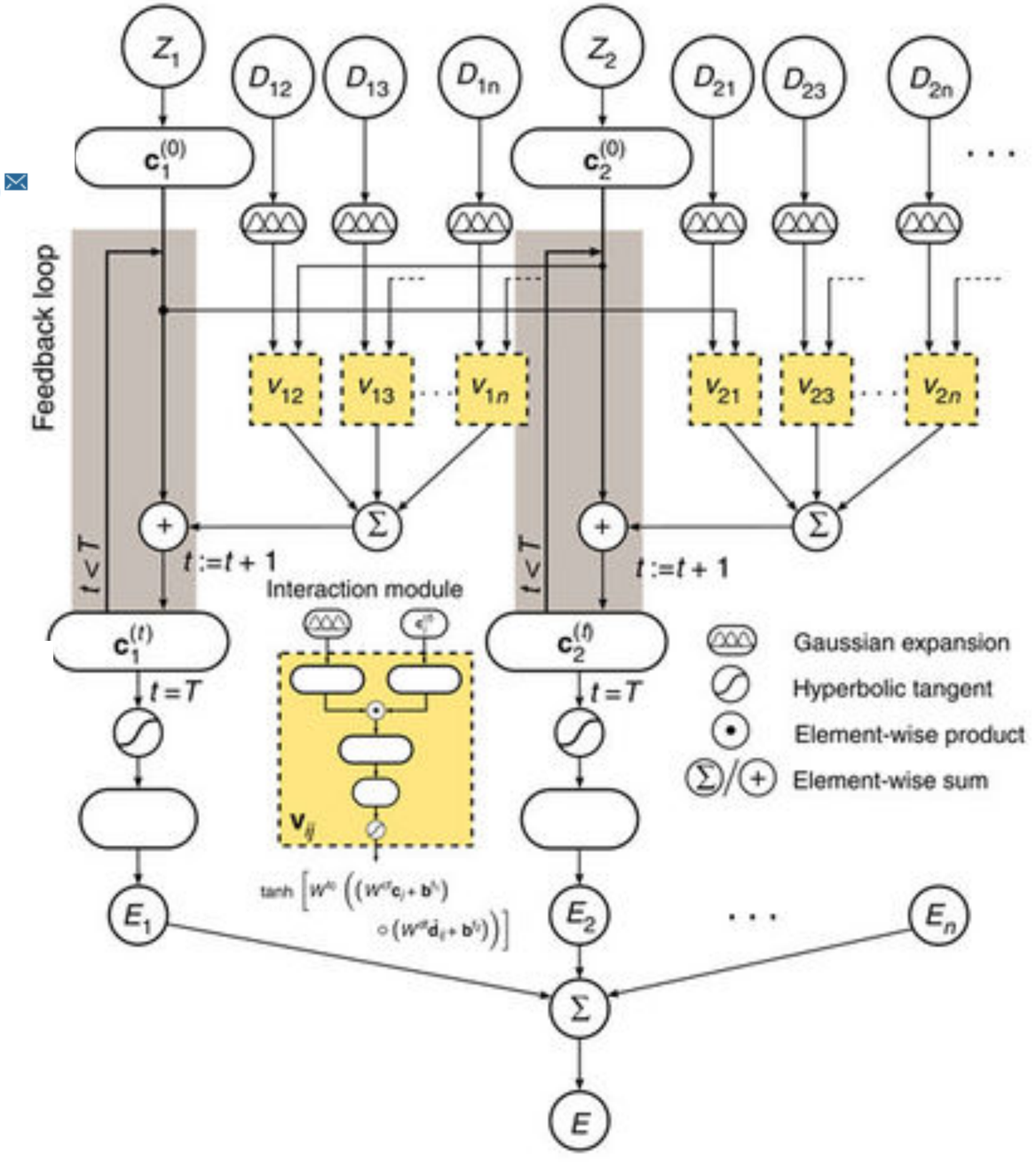
JCP148, 241708 (2018)

Quantum-chemical insights from deep tensor neural networks

Kristof T. Schütt, Farhad Arbabzadah, Stefan Chmiela, Klaus R. Müller & Alexandre Tkatchenko

Nature Communications **8**,
Article number: 13890 (2017)
doi:10.1038/ncomms13890





DTNN

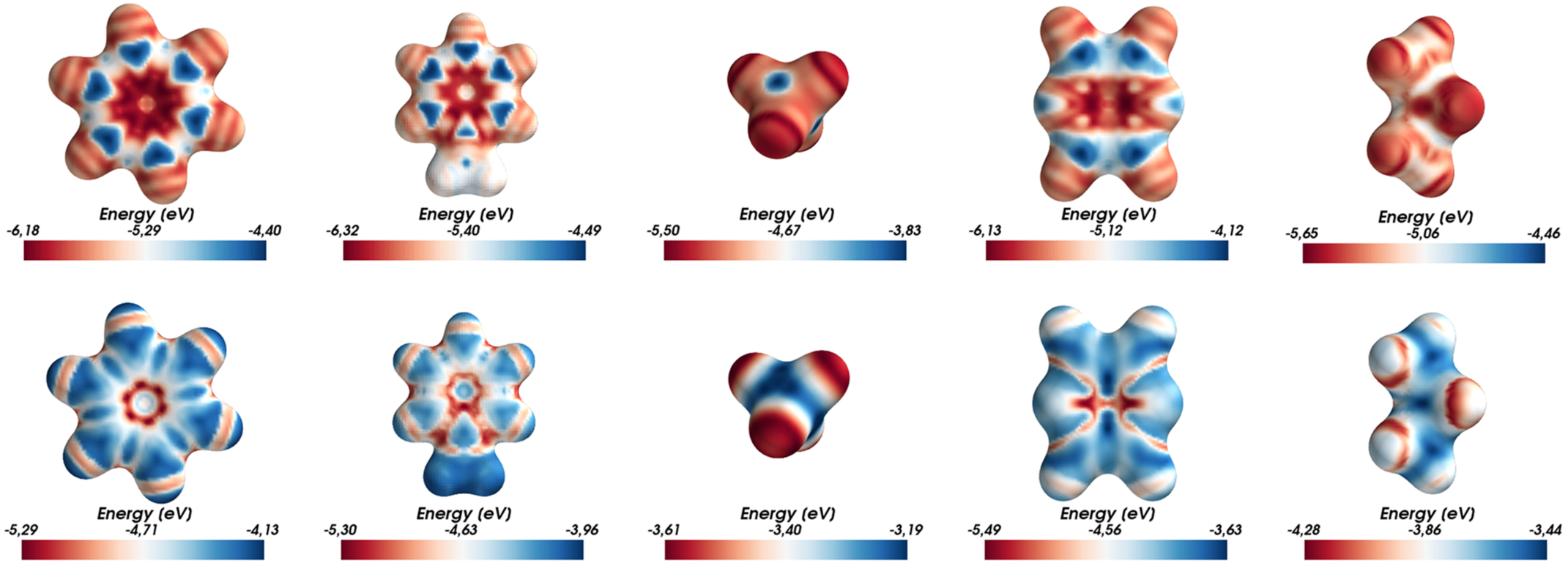


FIG. 5. Local chemical potentials $\Omega_C(\mathbf{r})$ of DTNN (top) and SchNet (bottom) using a carbon test charge on a $\sum_i \|\mathbf{r} - \mathbf{r}_i\| = 3.7$ Å isosurface are shown for benzene, toluene, methane, pyrazine, and propane.

…and materials!

Schutt et al, JCP **148**, 241722 (2018)

ARTICLE

doi:10.1038/nature25978

Planning chemical syntheses with deep neural networks and symbolic AI

Marwin H. S. Segler[1,2], Mike Preuss[3] & Mark P. Waller[4]

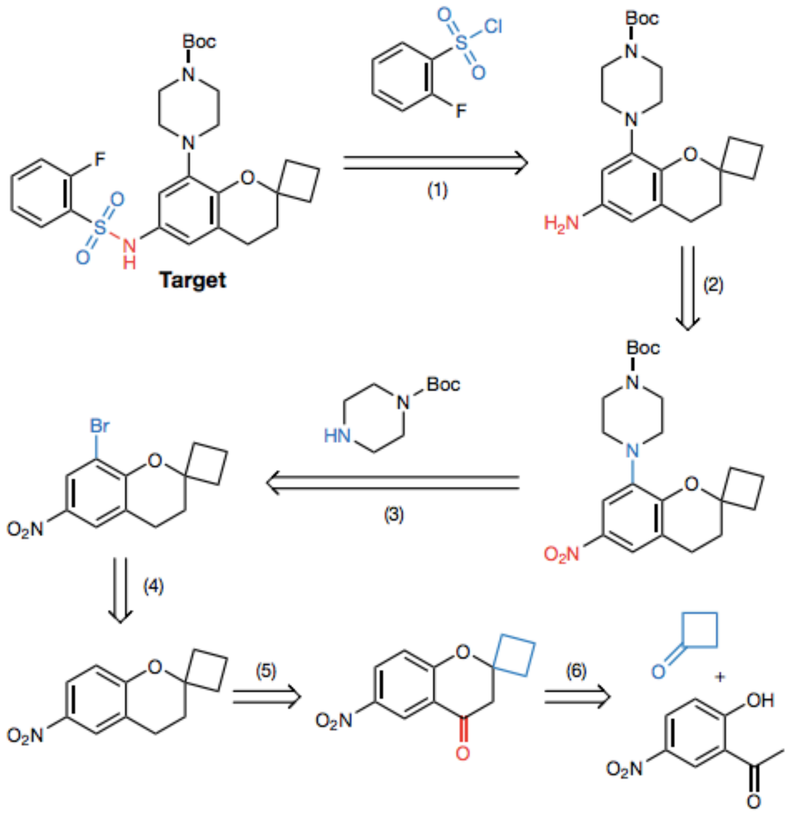


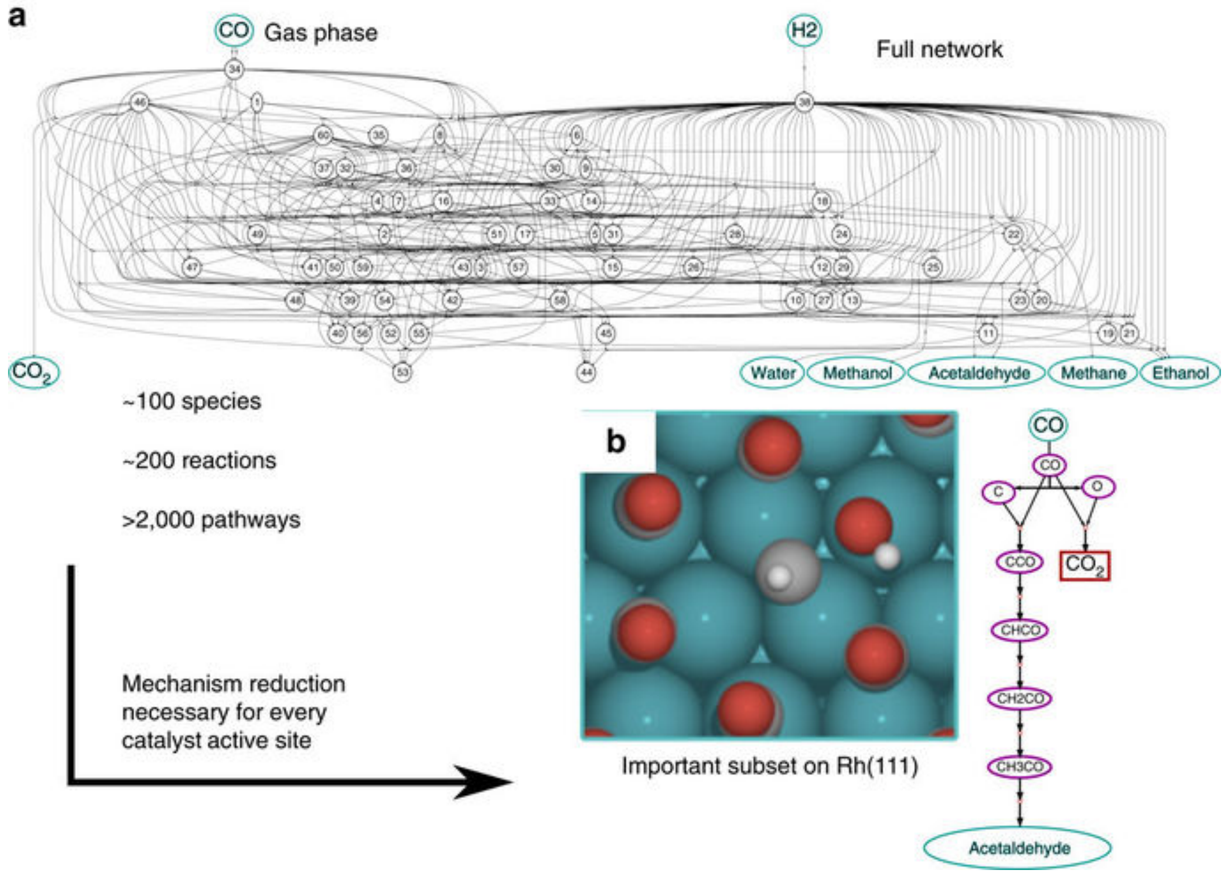
Figure 3 | An exemplary six-step synthesis route for an intermediate in a drug candidate synthesis. This route is identical to the published one[44] and was found by our algorithm autonomously within 5.4 s. The affected functional groups in each step are marked blue or red.

To address surface reaction network complexity using scaling relations machine learning and DFT calculations

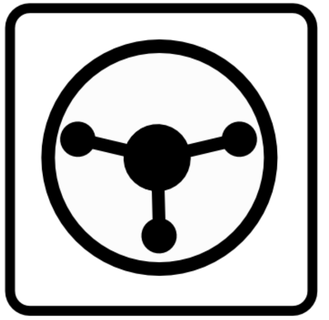
Zachary W. Ulissi, Andrew J. Medford, Thomas Bligaard ✉ & Jens K. Nørskov ✉

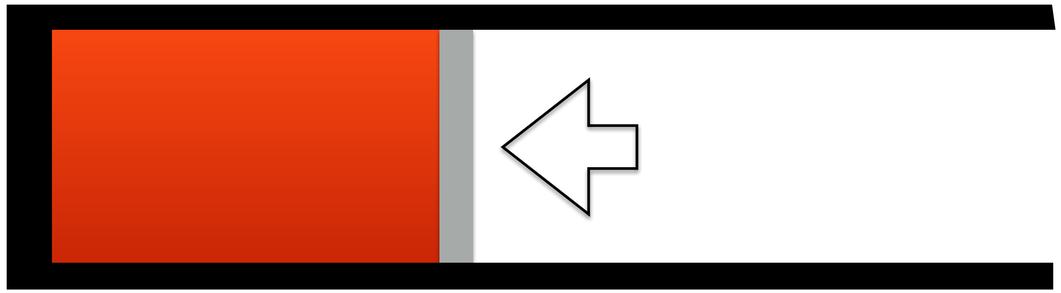
Nature Communications **8**,
Article number: 14621 (2017)
doi:10.1038/ncomms14621

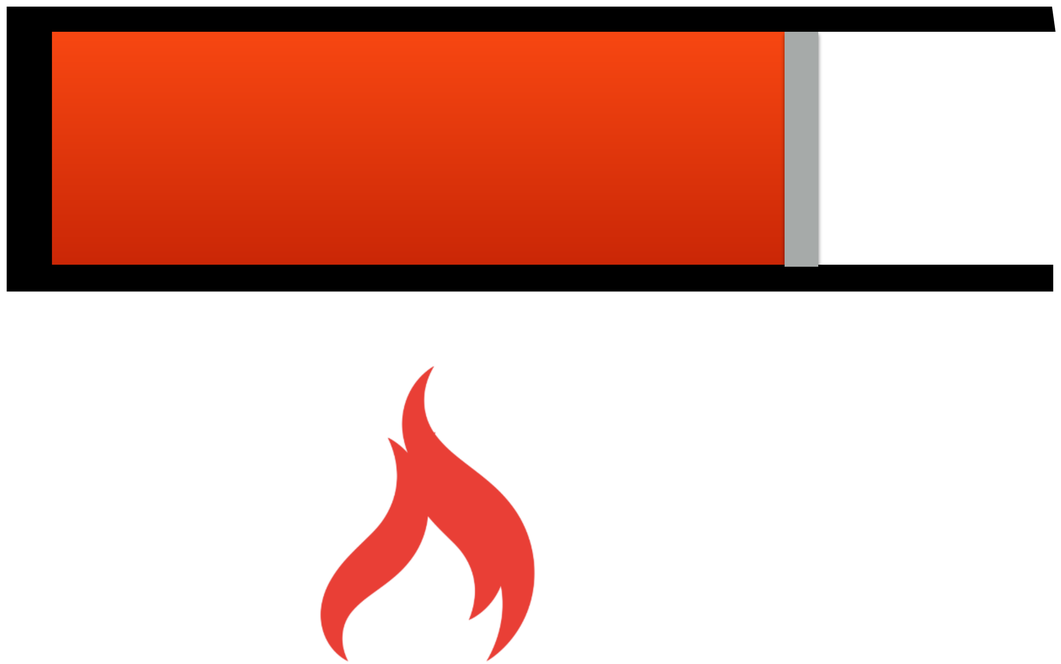
Received: 11 October 2016
Accepted: 03 January 2017
Published: 06 March 2017





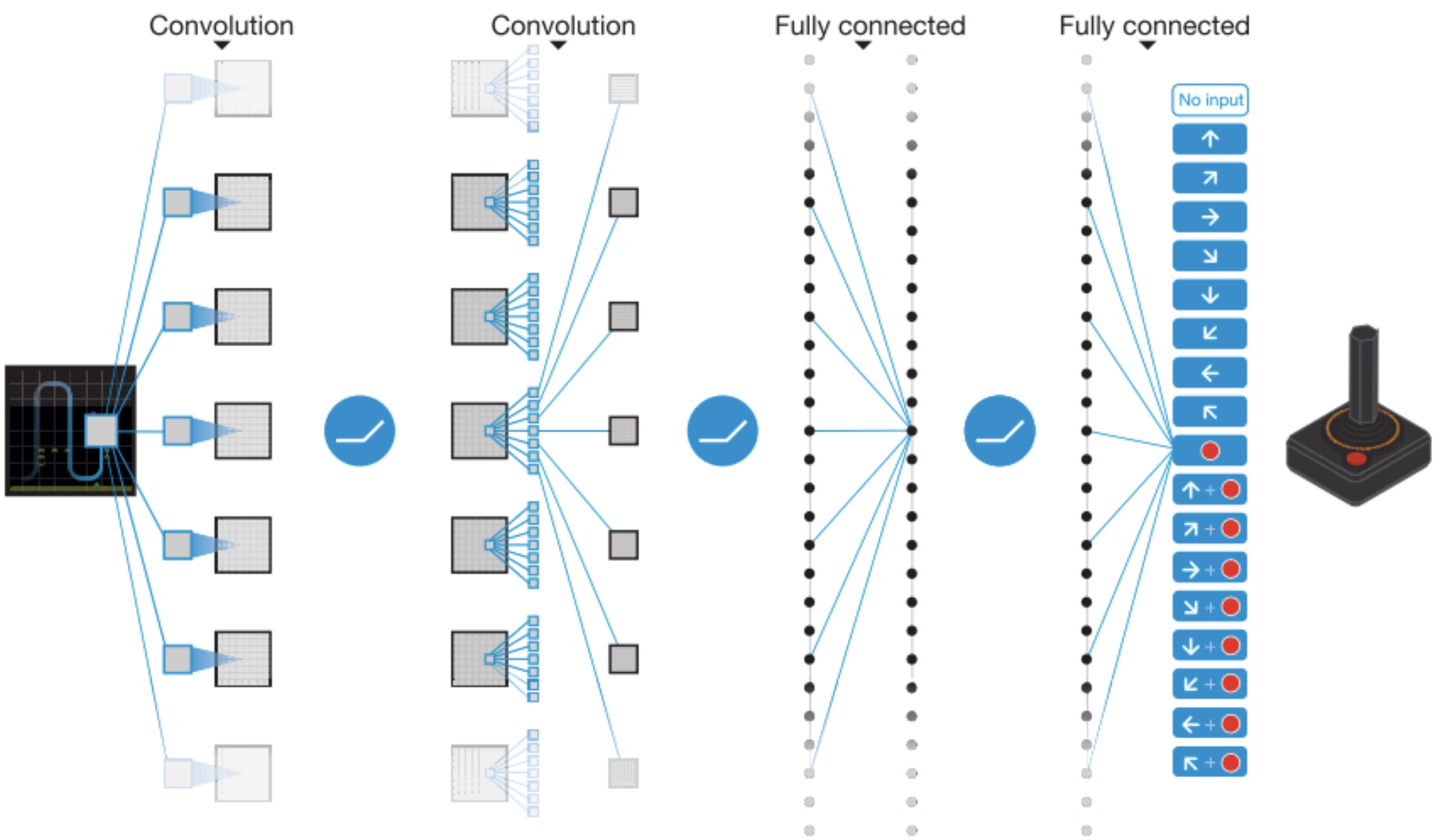



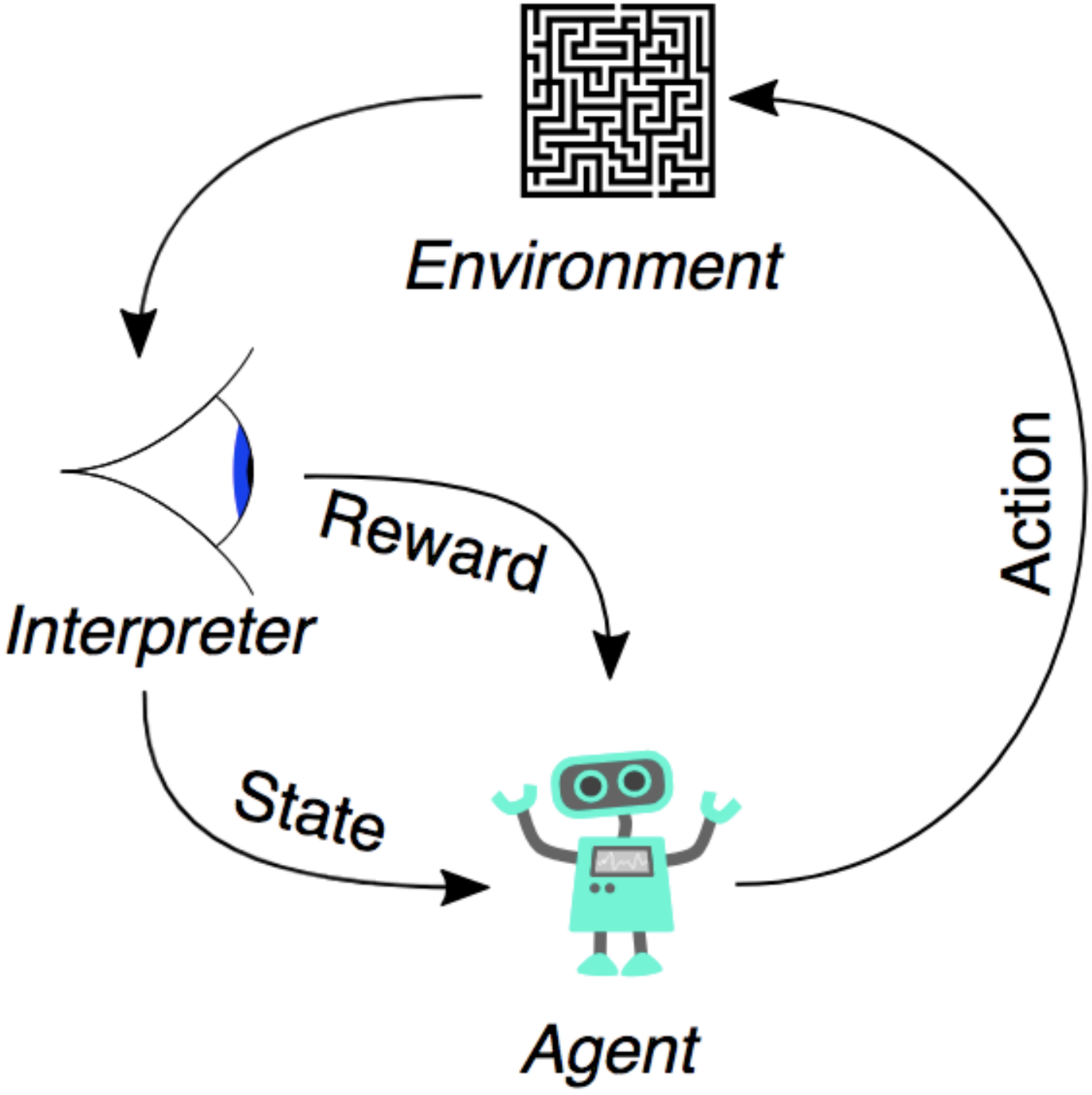





Energy

How do I extract work?


Convolution
Convolution
Fully connected
Fully connected
No input


Environment
Reward
Interpreter
State
Action
Agent

- isothermal compression

- isothermal expansion

- adiabatic compression

- adiabatic expansion

- isochoric heating

- isochoric cooling

$$\pi(\vec{S}) \rightarrow \vec{a}$$

state of system (T,V) action

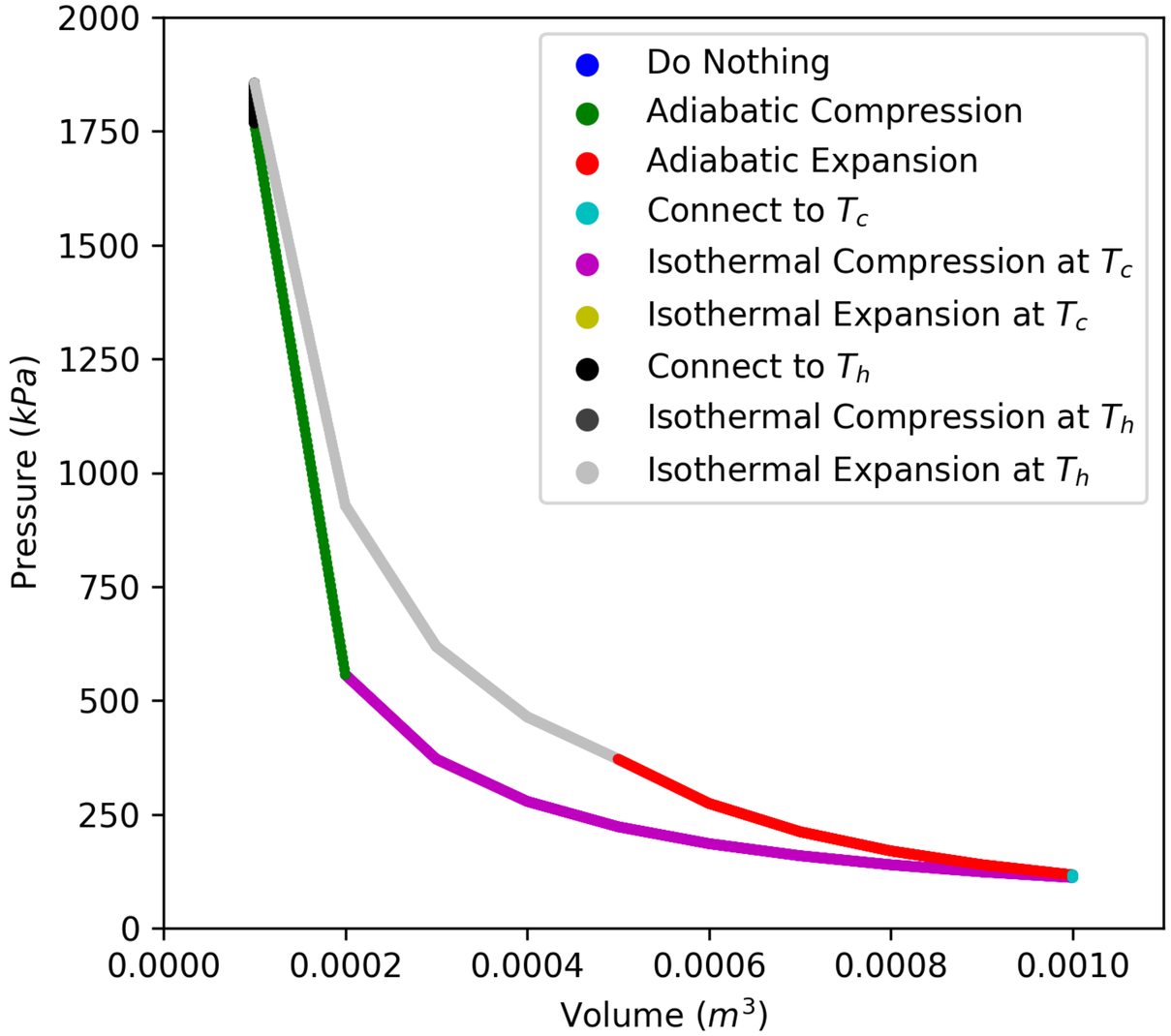
$$\vec{a} = \begin{bmatrix} \text{- isothermal compression} \\ \text{- isothermal expansion} \\ \text{- adiabatic compression} \\ \text{- adiabatic expansion} \\ \text{- isochoric heating} \\ \text{- isochoric cooling} \end{bmatrix}$$

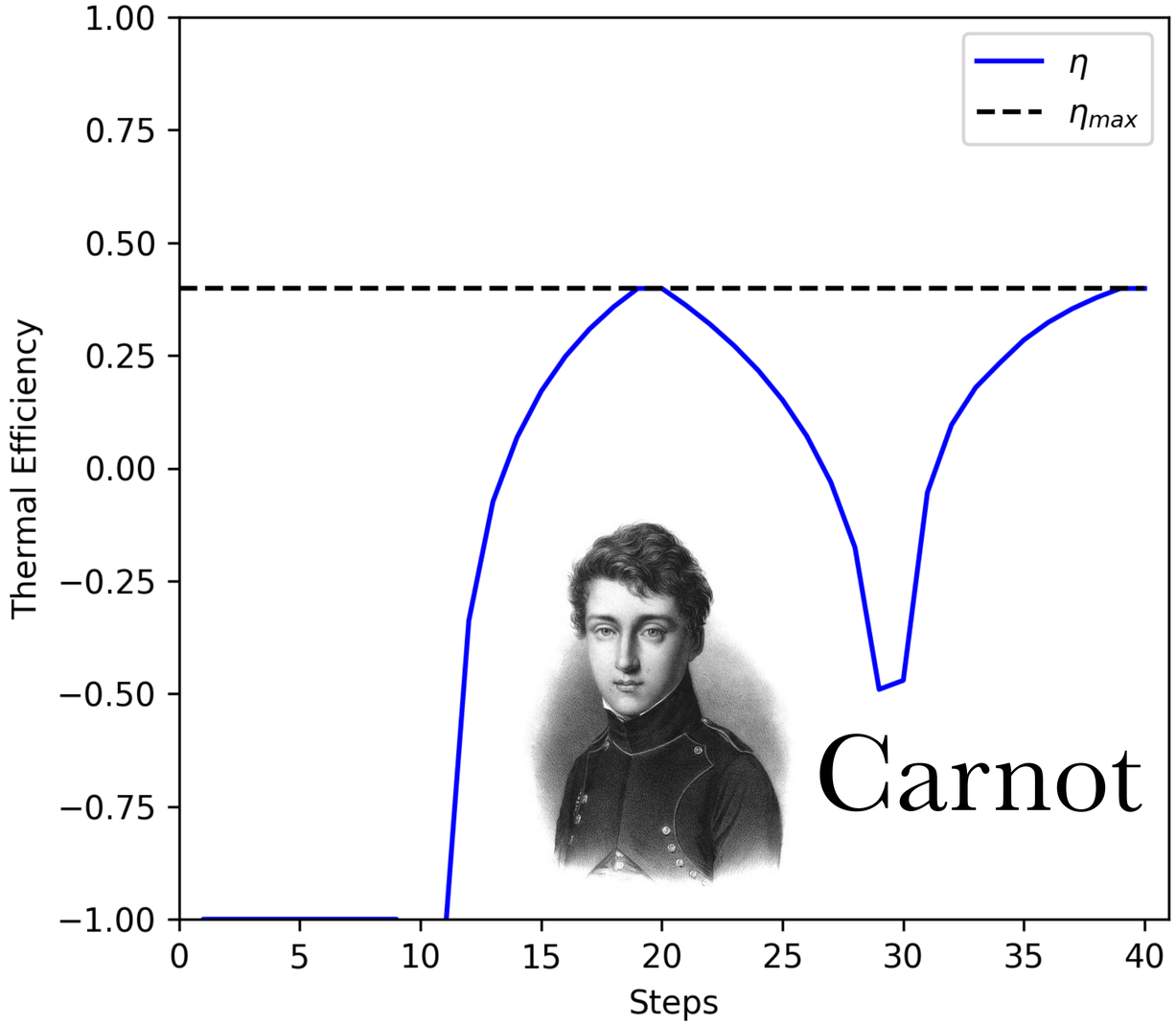
$\pi =$ deep neural network

optimize with genetic algorithm[1]
to maximize efficiency, η

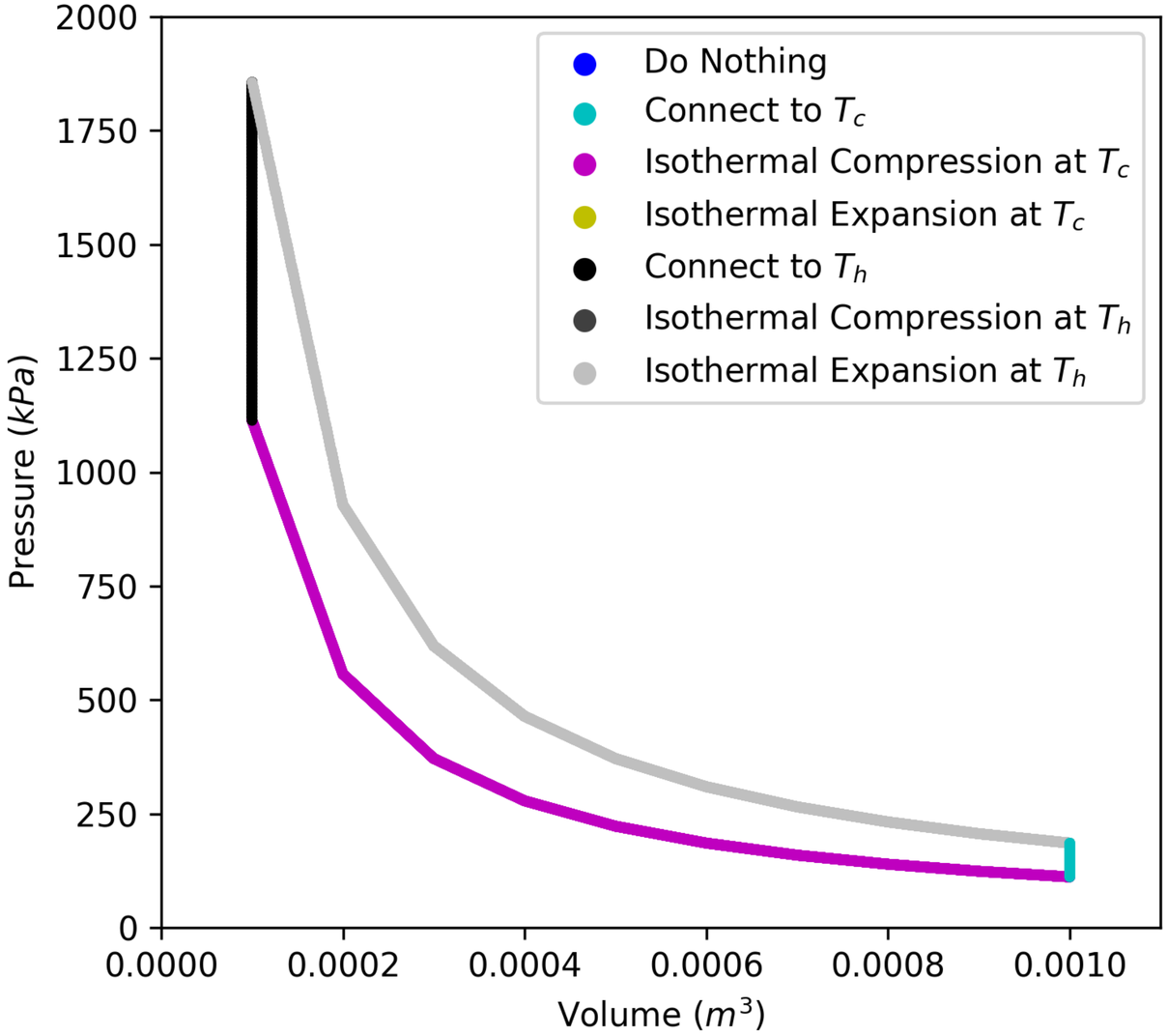
[1] https://eng.uber.com/deep-neuroevolution

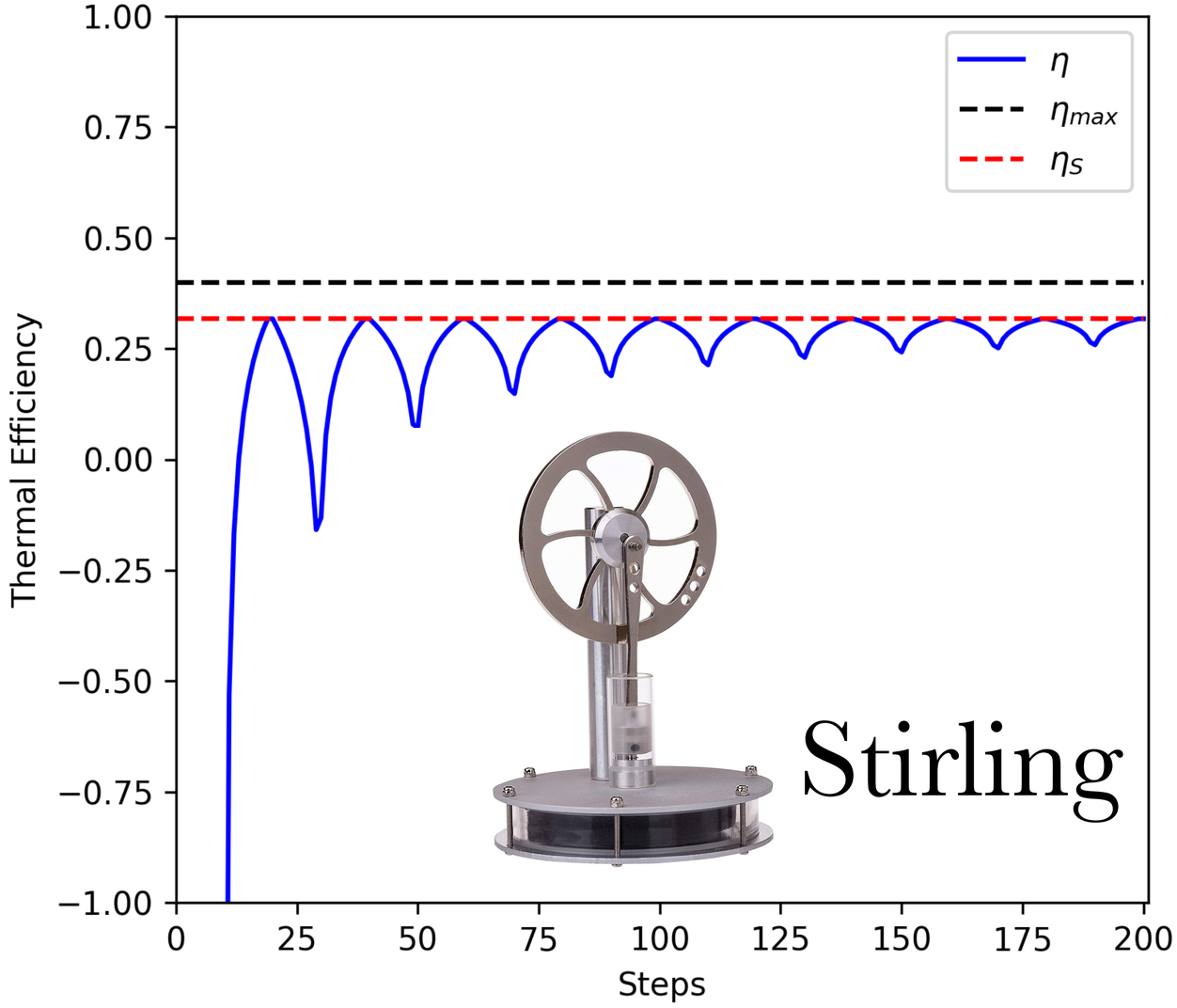
Agent is only told final efficiency





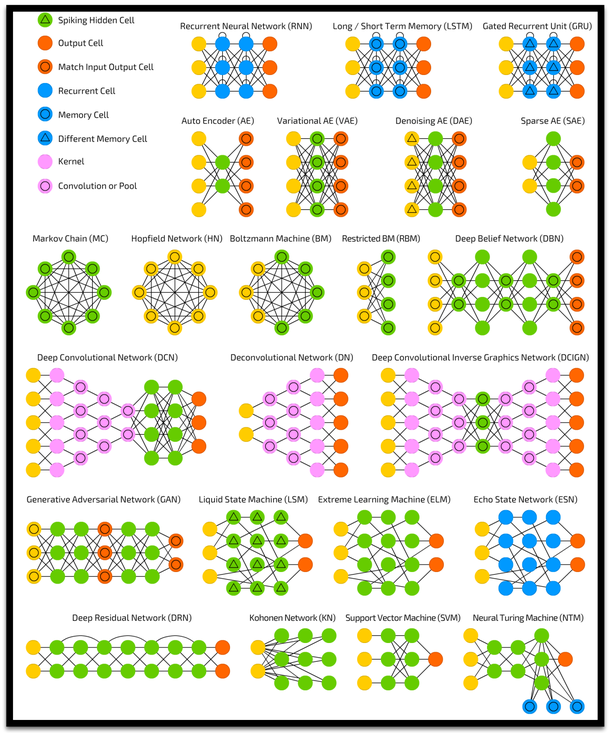
Restricted move set gives a different cycle



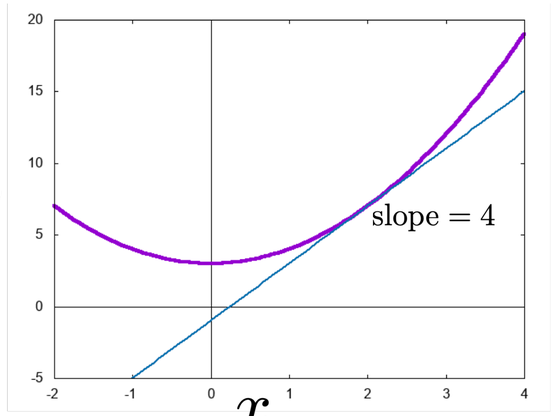


The definition of difficult is changing

Architectures



Optimization



$$\frac{dy}{dx}$$

$$\frac{df}{dt} = \frac{\partial f}{\partial x} \cdot \frac{dx}{dt} + \frac{\partial f}{\partial y} \cdot \frac{dy}{dt} + \frac{\partial f}{\partial z} \cdot \frac{dz}{dt} + \frac{\partial f}{\partial t}$$

Active research problems

- drug design
- categorizing experimental data
- controlling chemical synthesis
- multi-scale simulation
- materials discovery
- detecting new quantum phases

Hardware

NVIDIA intel Google IBM SYNOPSYS® QUALCOMM®