



1



2

“If I can’t compute it, I
don’t understand it.”

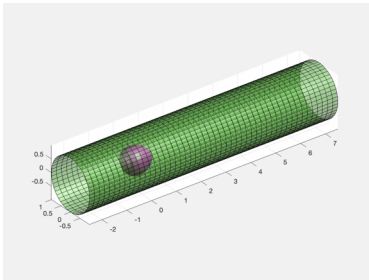
–John von Neumann

3

Mechanistic models build
on previous knowledge
and have meaningful
parameters

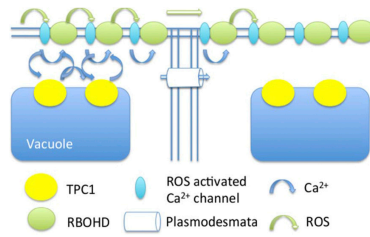
4

Fluid dynamics simulations of fluid flow in the xylem



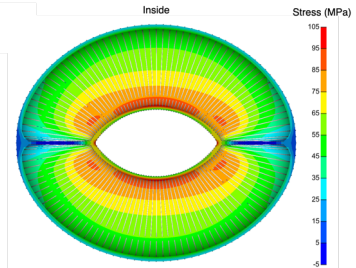
Evans and Morris (2016) The Plant Journal
 Blyth and Morris (2018) Mathematical Modelling in Plant Biology
 Blyth and Morris (2019) Frontiers in Plant Science

Fire-diffuse-fire modelling of spatio-temporal calcium waves



Evans et al. (2016) Plant Physiology
 Capoen et al (2011) PNAS
 Vaz Martins et al (2016) BMC Systems Biology

Finite Element Method modelling of guard cell dynamics

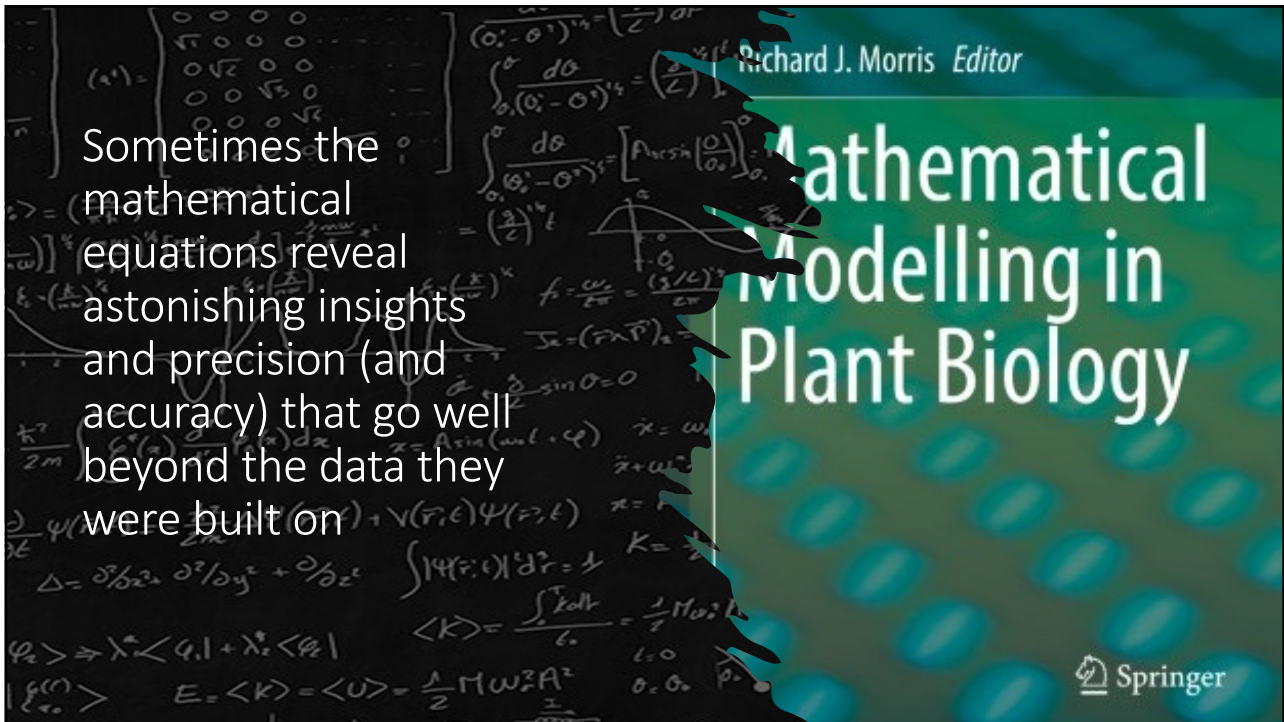


Woolfenden et al. (2017) The Plant Journal
 Carter et al. (2017) Current Biology
 Woolfenden et al. (2018) Trends in Plant Science

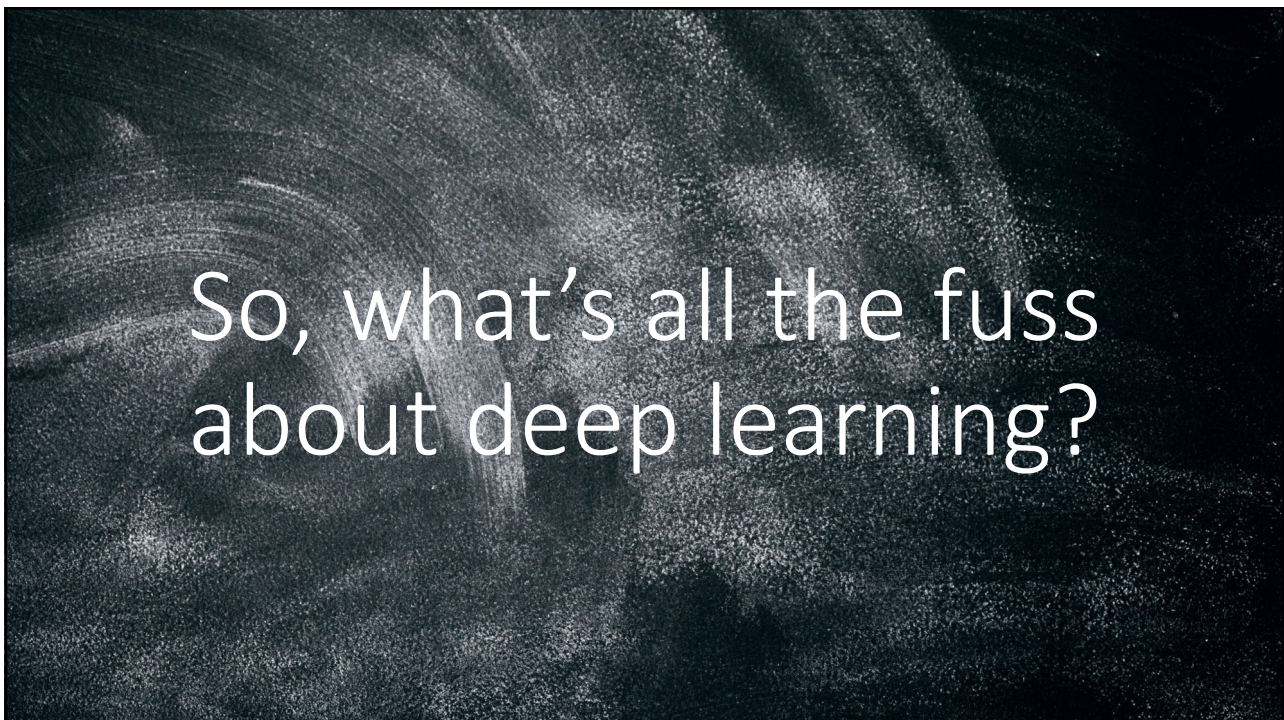
5

Sometimes the mathematical equations reveal astonishing insights and precision (and accuracy) that go well beyond the data they were built on

6



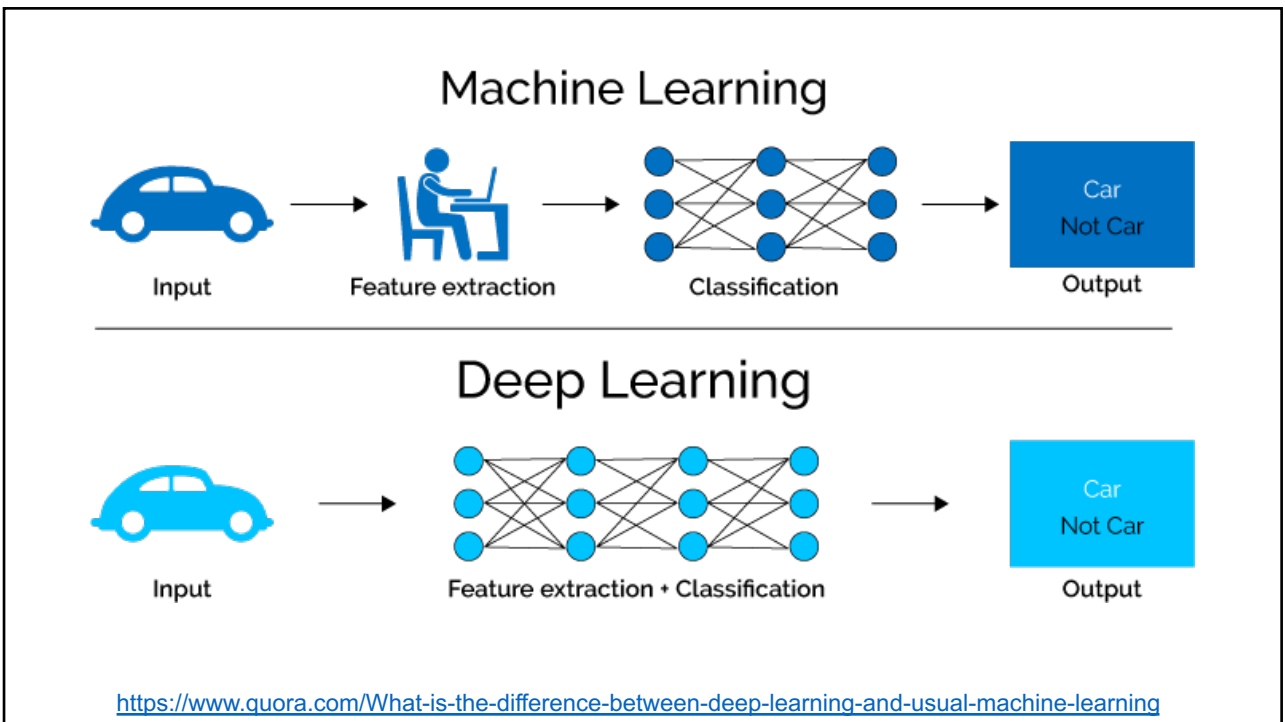
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The few extra layers are game changing!

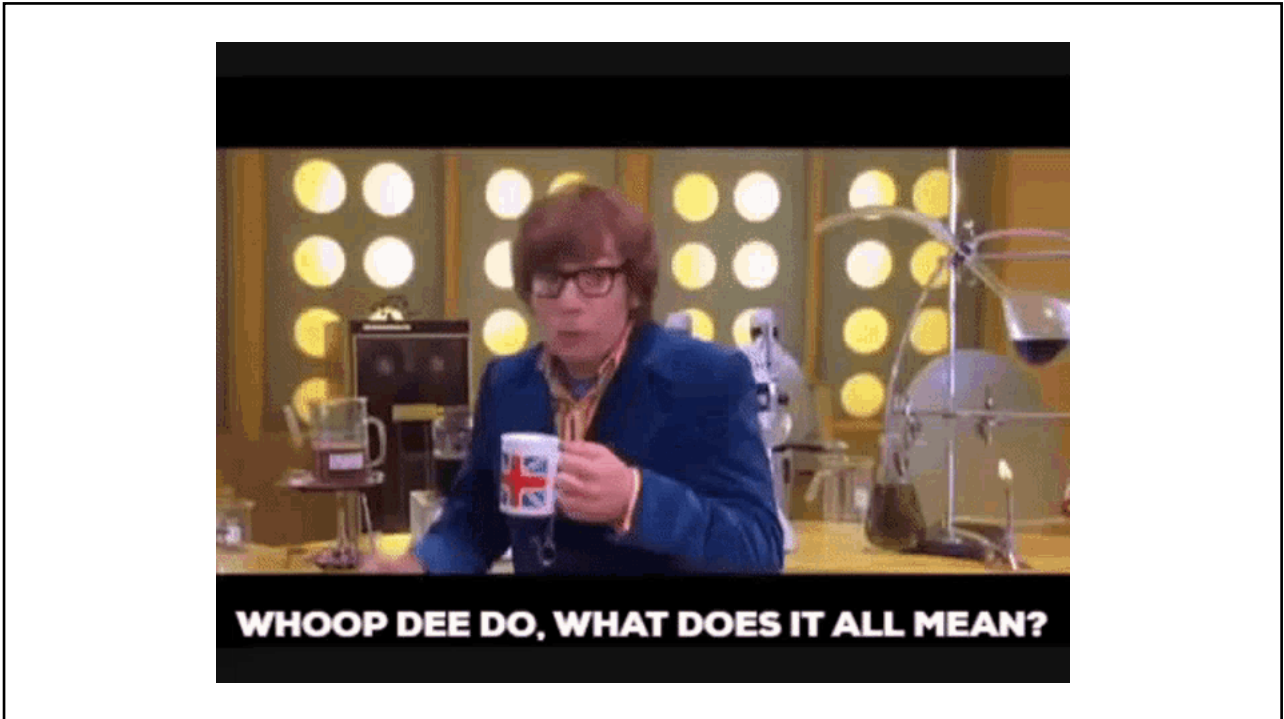
- Breaks the 80:20 rule for feature selection:training
- No longer requires expert domain knowledge
- Computer scientists are taking over

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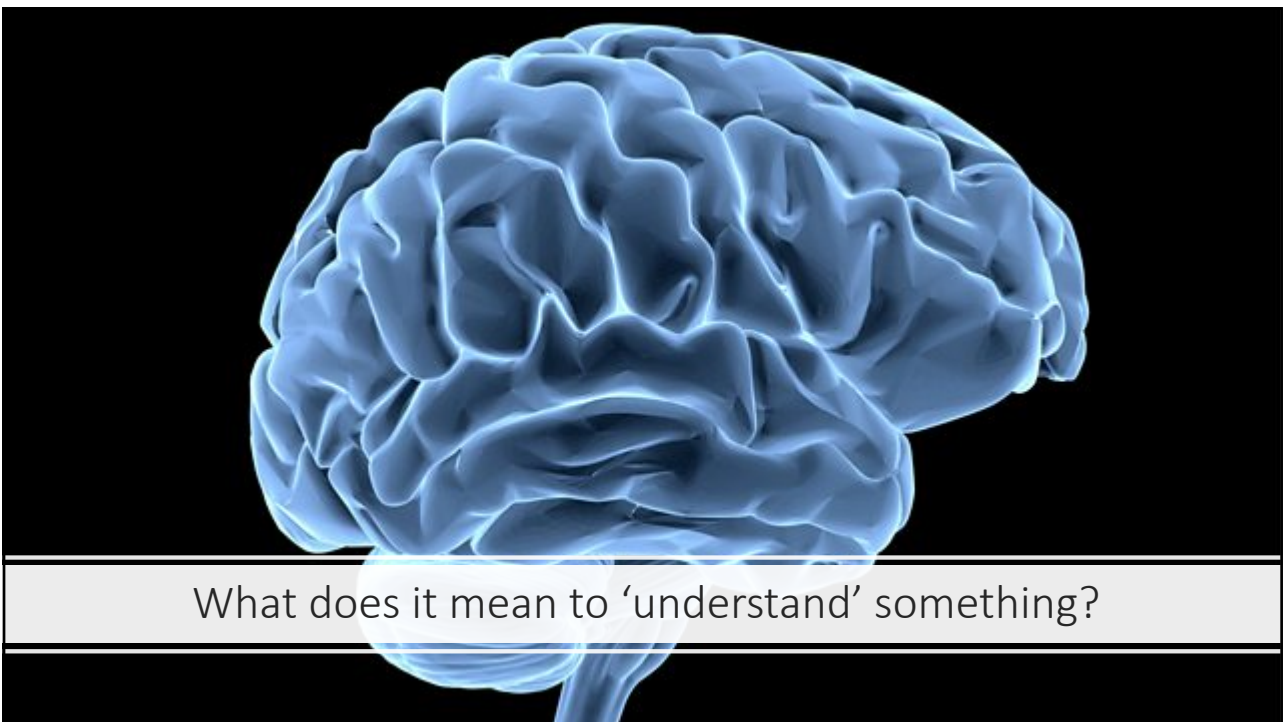
Deep learning approaches are not restricted by the imagination of the modeller but are currently difficult to 'understand'



12

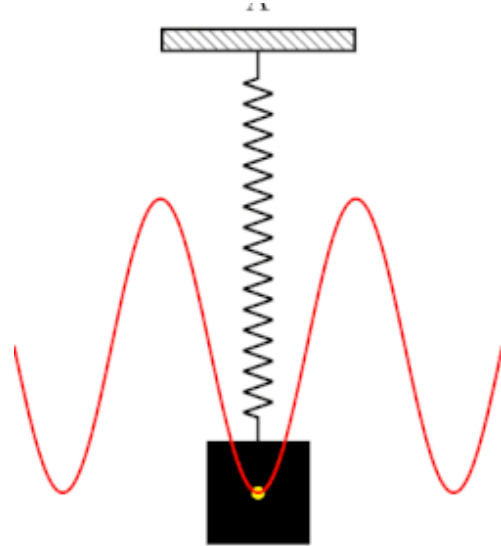


13

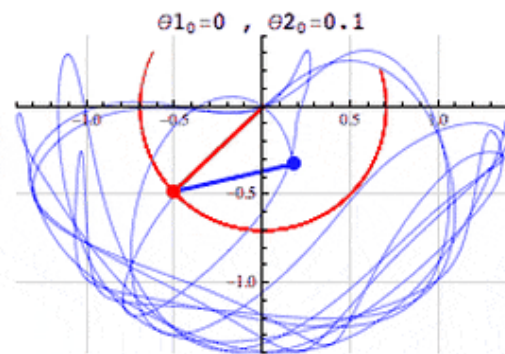
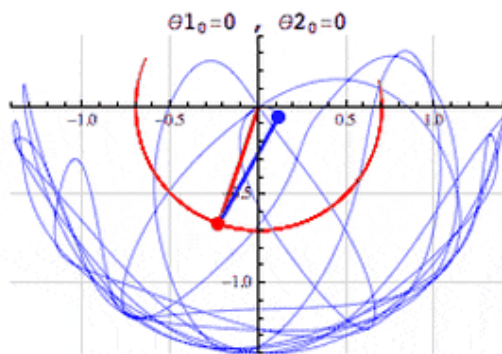


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To 'understand'
often means
relating it to
something else



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Even simple systems can show non-intuitive behaviour

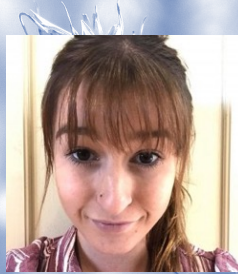
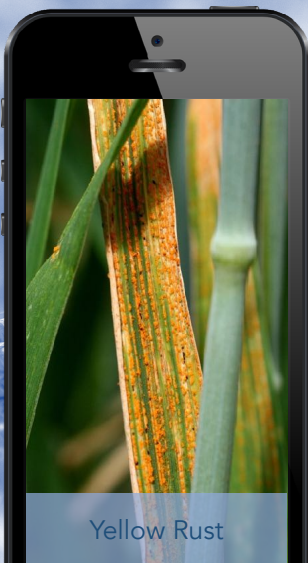
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“I think I can safely say that nobody really understands quantum mechanics.”

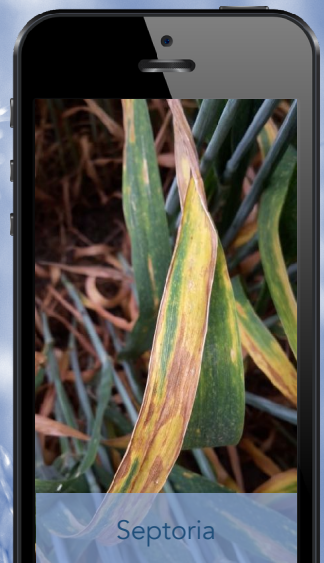
—Richard Feynman

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AI for plant disease detection in wheat



Megan Long



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From lab to field – getting real world data



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From lab to field – getting real world data



What?
Images of diseased (Septoria, yellow rust, brown rust, mildew) and healthy wheat leaves

Where?

Multiple sites across the UK, in England, Ireland and Scotland.

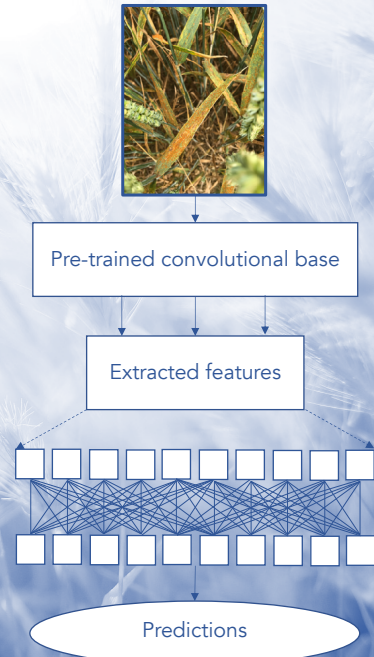
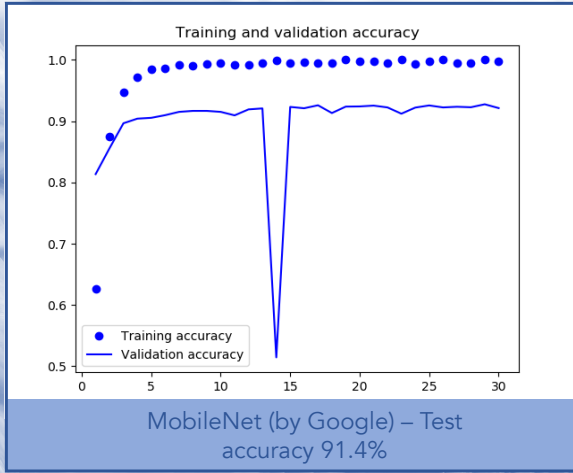
How?

Predominantly using smartphone cameras, some with a digital camera
With all possible conditions



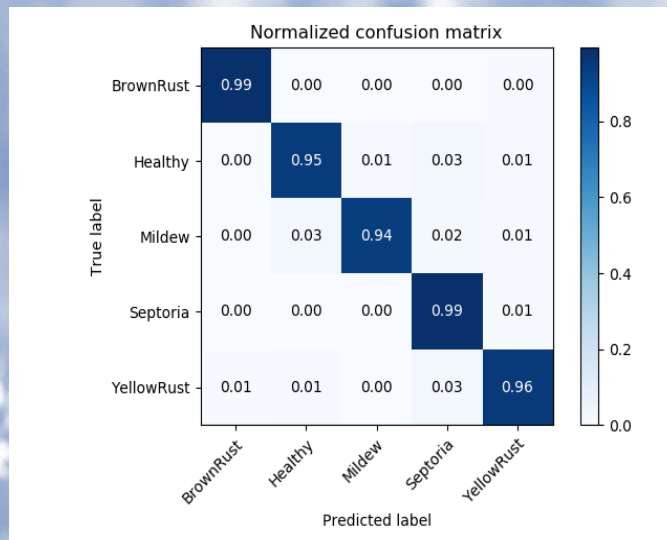
20

Networks – Pre-trained



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Megan's network performs astonishingly well



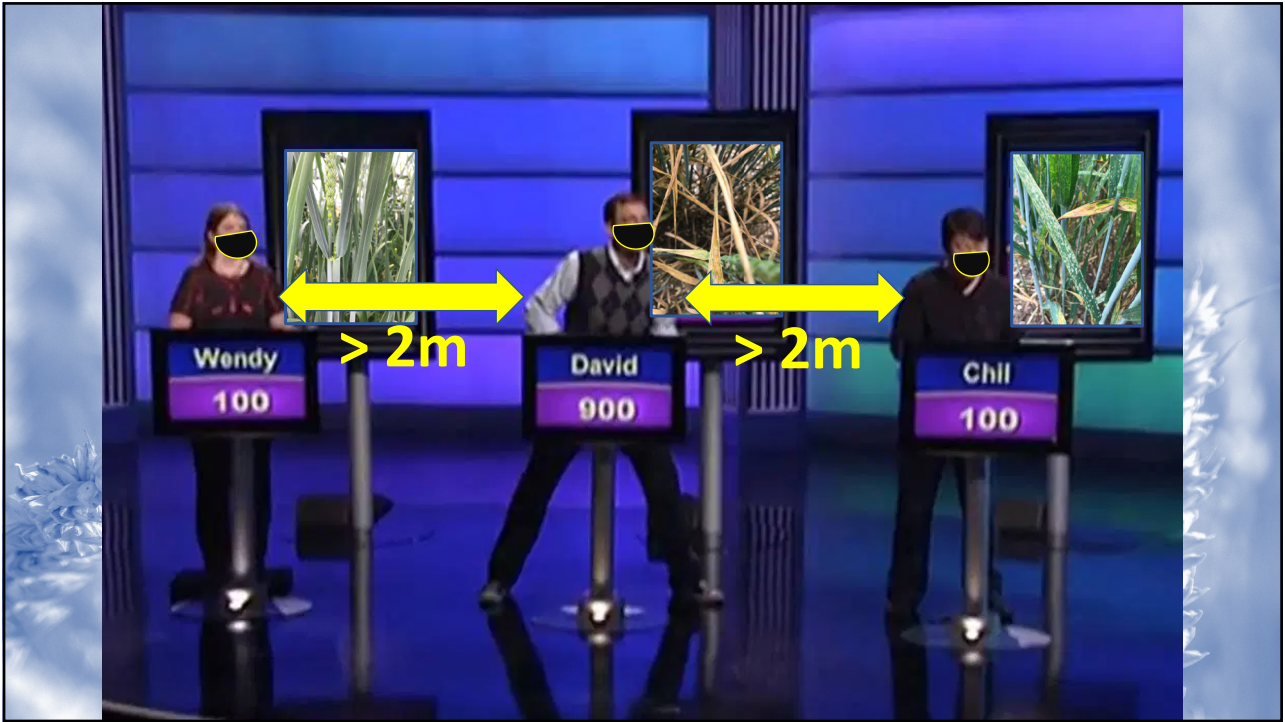
22



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Megan's network even outperforms expert crop pathologists!

	Participant 1		Participant 2		Participant 3		Participant 4		Participant 5		Network	
	Correct	Incorrect	Correct	Incorrect	Correct	Incorrect	Correct	Incorrect	Correct	Incorrect	Correct	Incorrect
Brown rust	103	25	120	8	121	7	121	7	116	12	125	3
Healthy	104	18	98	24	94	28	96	26	117	5	99	23
Mildew	151	10	152	9	151	10	153	8	152	9	128	33
Septoria	265	84	273	76	296	53	331	18	266	83	336	13
Yellow rust	215	24	217	22	204	35	167	72	207	32	200	39
Accuracy	83.88%		86.08%		86.68%		86.88%		85.88%		88.88%	

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Unravelling the control of developmental transitions in Brassicas




Alex Calderwood

Andrew Lloyd

Jo Hepworth

Eleri Tudor

Marc Jones

Shannon Woodhouse

Catherine Chinoy

Lorelie Bilham

Kevin Williams

Fiona Corke

John Doonan

Lars Ostergaard

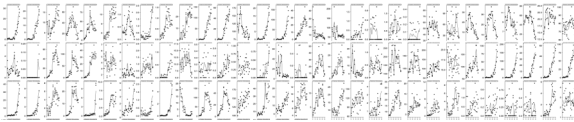
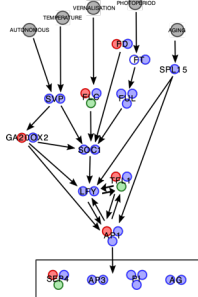
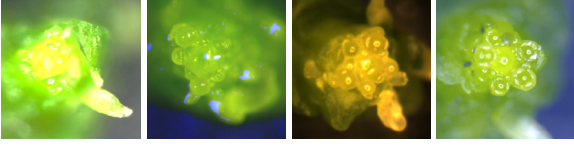
Judith Irwin

Rachel Wells

Richard J Morris

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Using modelling and machine learning to unravel developmental transitions in Brassica

log₂ norm. rpm. sc

diff. lu

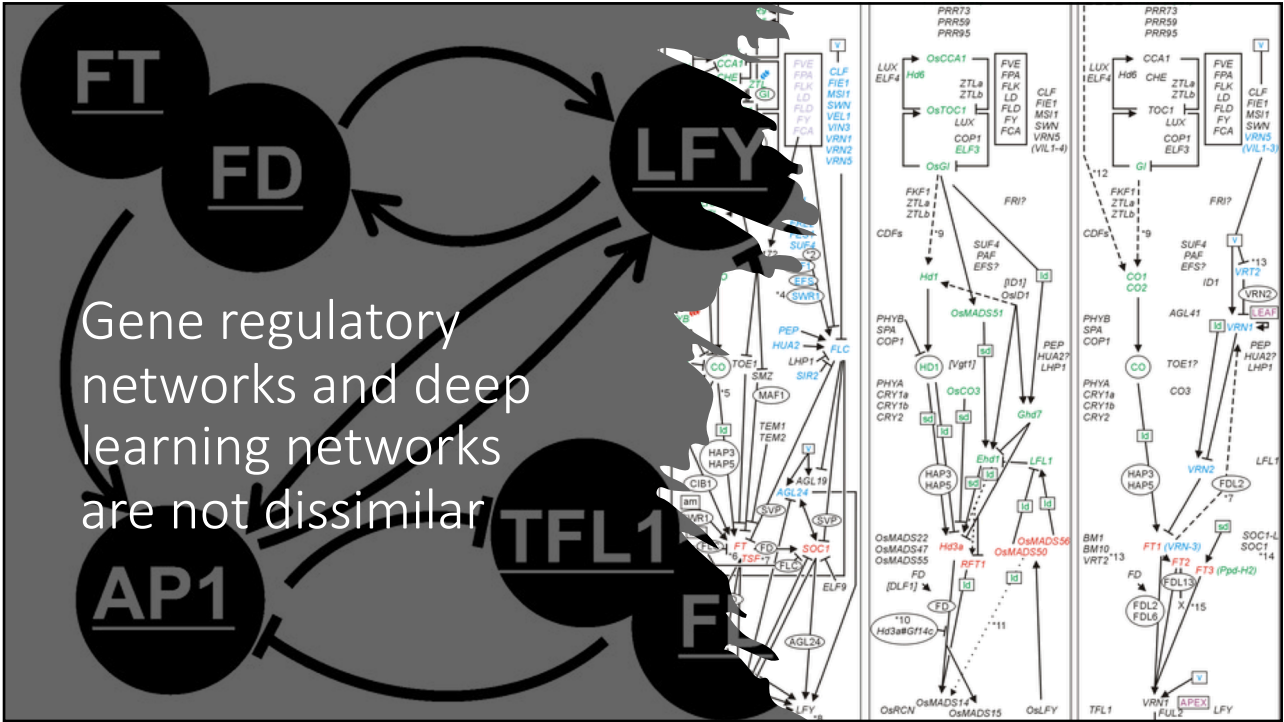
timepoint

diff. timepoint

SUBFUNCTIONALISED!

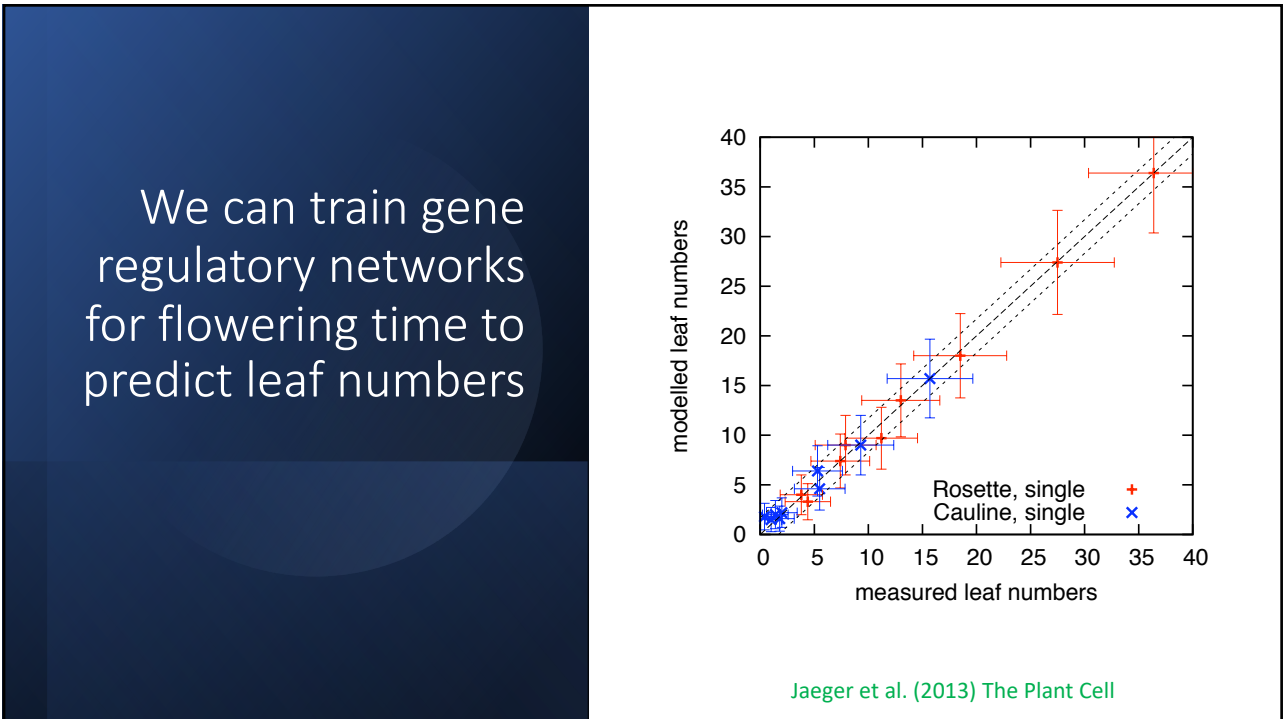
Calderwood et al. (2021) QPB (accepted)

28



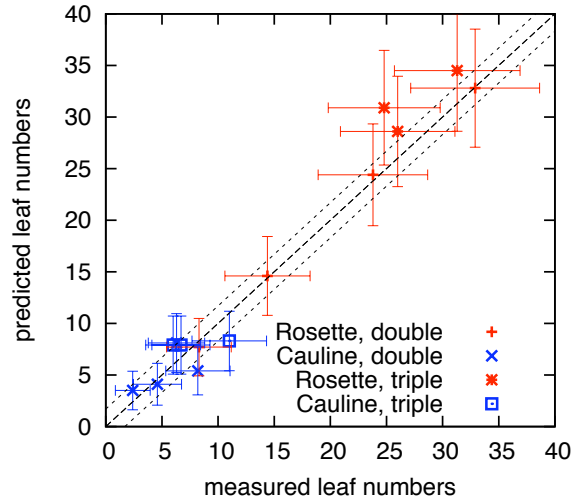
Gene regulatory networks and deep learning networks are not dissimilar

29



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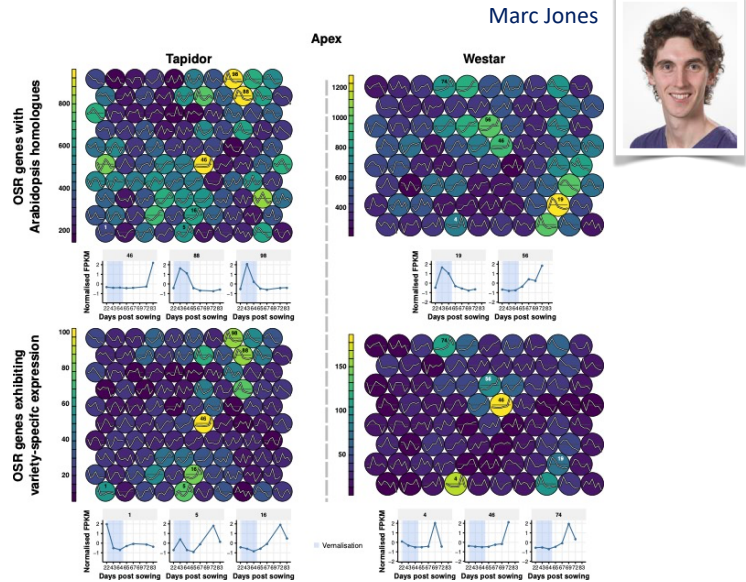
We can train gene regulatory networks for flowering time to predict leaf numbers



Jaeger et al. (2013) *The Plant Cell*

31

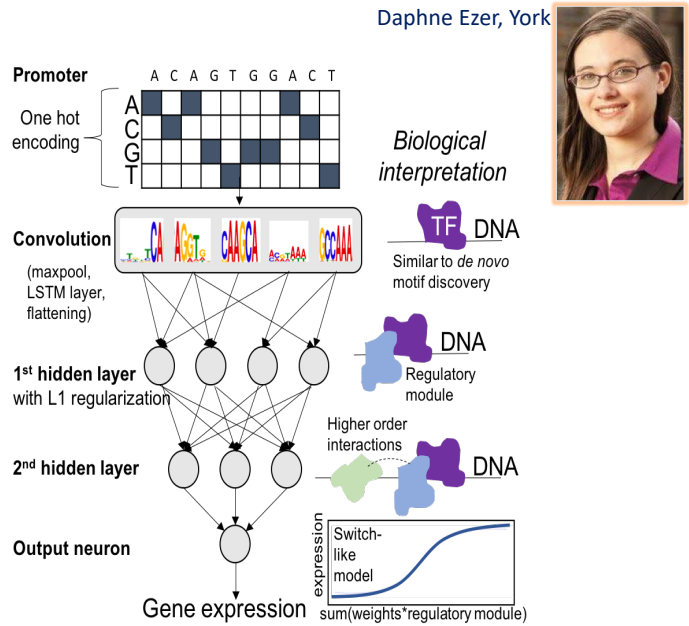
Self-organizing maps reveal patterns in transcript dynamics



Jones et al. (2018) *The Plant Journal* Jones et al. (2020) *BMC Plant Biology*
 Jones et al. (2021) *In preparation*

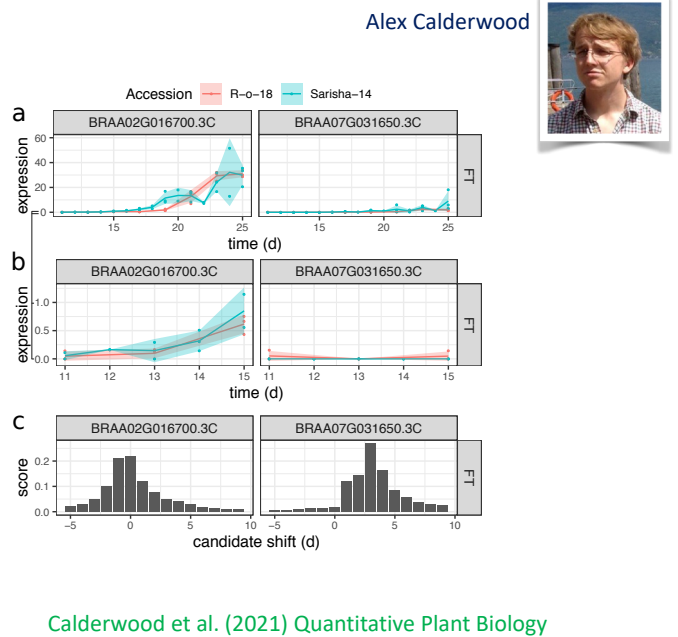
32

Convolutional Neural Networks can predict expression in *Brassica rapa*



33

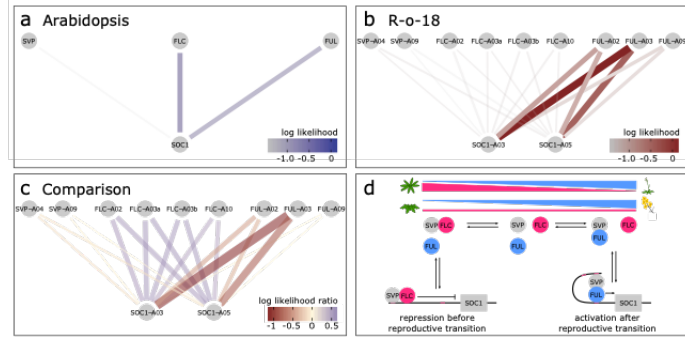
Dynamic time warping of gene expression reveals key differences in flowering in *Brassica rapa*



34

Gaussian Process network inference reveals key differences in flowering in *Brassica rapa*

Alex Calderwood

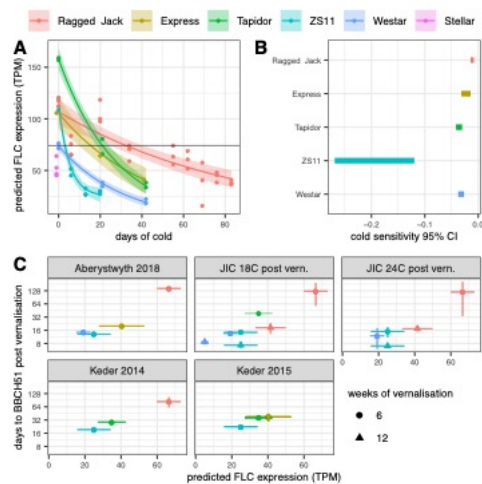


Calderwood et al. (2021) biorxiv

35

Unsupervised learning leads to a mathematical model that explains phenotypic diversity in *Brassica napus*


Alex Calderwood




Calderwood et al. (2021) New Phytologist

36


Trans-Learn – Multivariate Gene Patterns



Josh Colmer



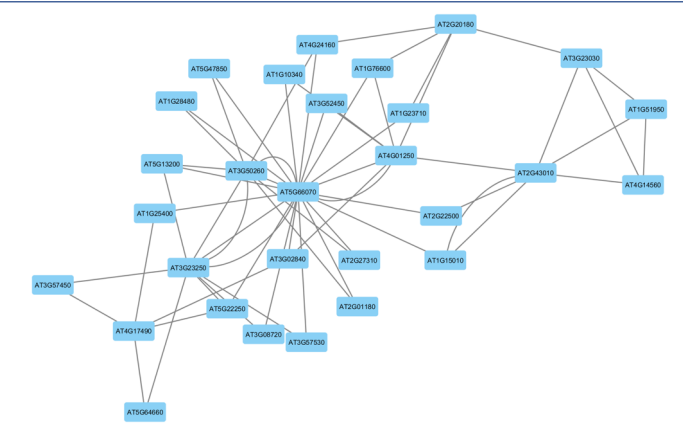
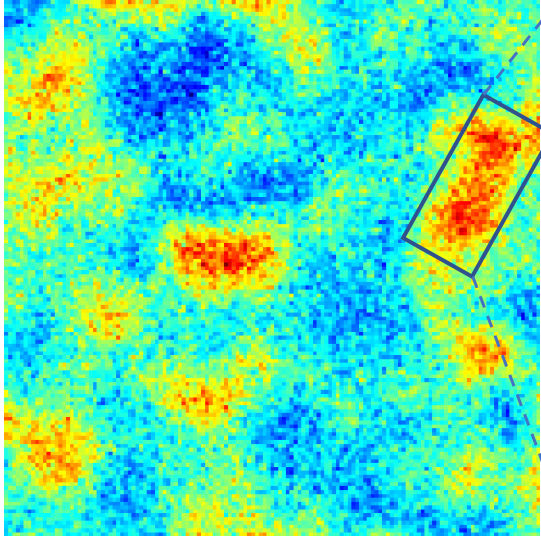
KYOTO UNIVERSITY
FOUNDED 1867



Earlham Institute

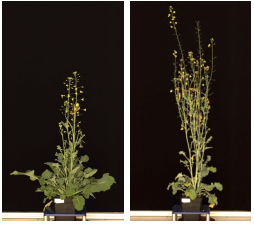


Decoding Living Systems

71x71 gene matrix



The orange/red clusters found in a heatmap contain subsets of genes that collectively possess non-linear joint dependencies with the infection status/severity

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From genotype to phenotype and back

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Challenges and thoughts

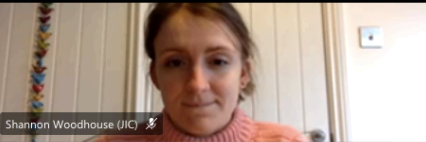

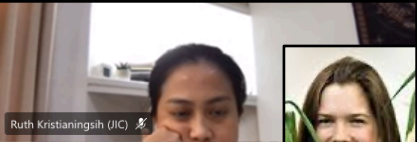

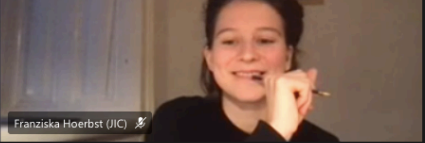
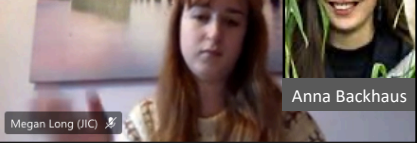
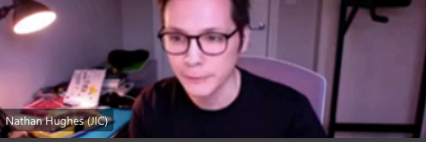
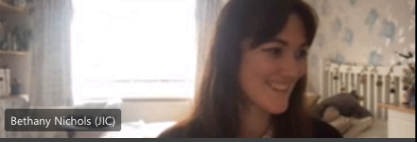
-  Annotated balanced data sets
-  Easy ways of sharing trained networks and retraining them (transfer learning)
-  Better ways of accounting for uncertainties in the data
-  Wishlist for linking to mechanistic models:
The ability to enforce thermodynamically consistent models
Better ways of extracting information from trained networks

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Sometimes our understanding of the physics is outperformed by Deep Learning approaches



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 <p>Shannon Woodhouse (JIC)</p>	 <p>Clinton Durney (JIC)</p>	 <p>Ruth Kristianingsih (JIC)</p>
 <p>Hugh Woolfenden (JIC)</p>	 <p>Franziska Hoerbst (JIC)</p>	 <p>Megan Long (JIC)</p>
 <p>Nathan Hughes (JIC)</p>	 <p>Melissa Tomkins (JIC)</p>	 <p>Bethany Nichols (JIC)</p>

Anna Backhaus

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The Alan Turing Institute

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