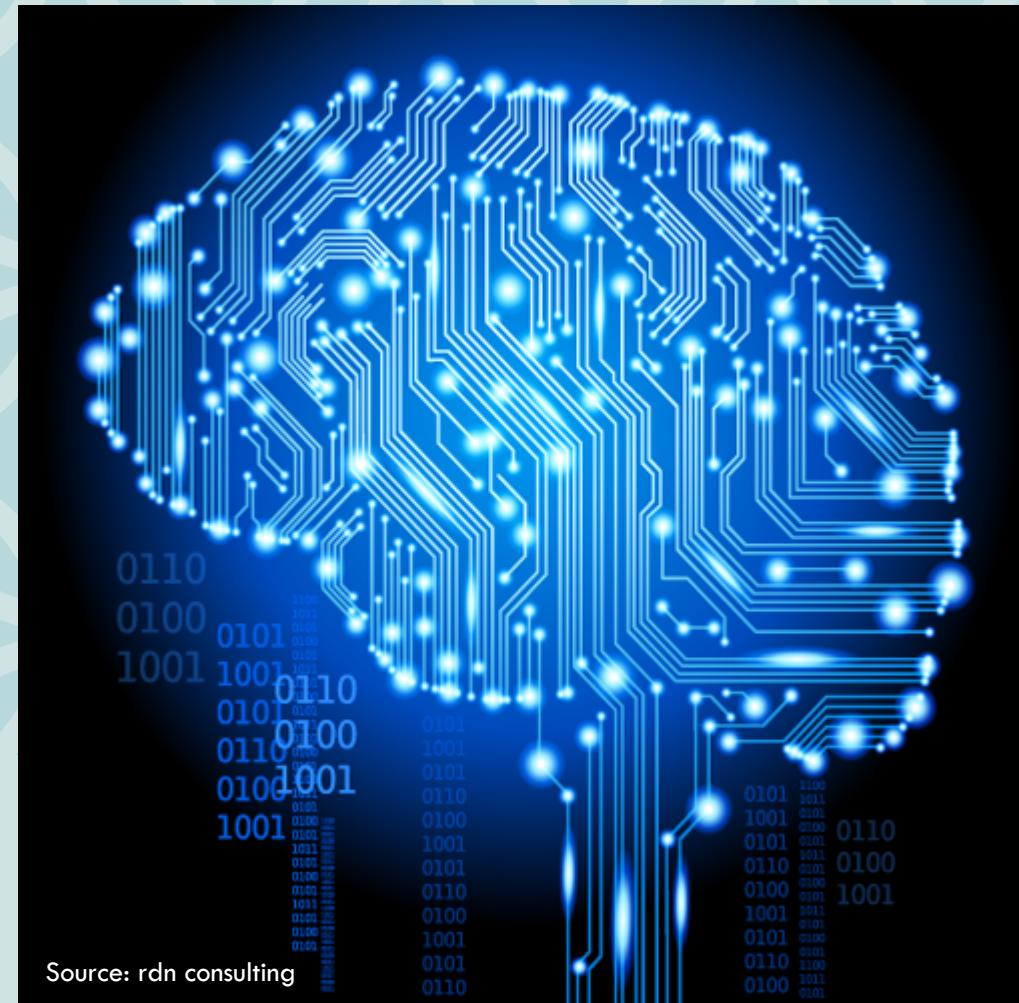


# DEEP LEARNING & APPLICATIONS IN NON-COGNITIVE DOMAINS

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[prada-research.net/~truyen](http://prada-research.net/~truyen)

AI'16, Hobart, Dec 5<sup>th</sup> 2016



# PRADA @ DEAKIN, GEELONG CAMPUS



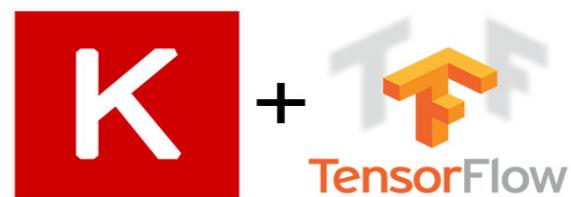
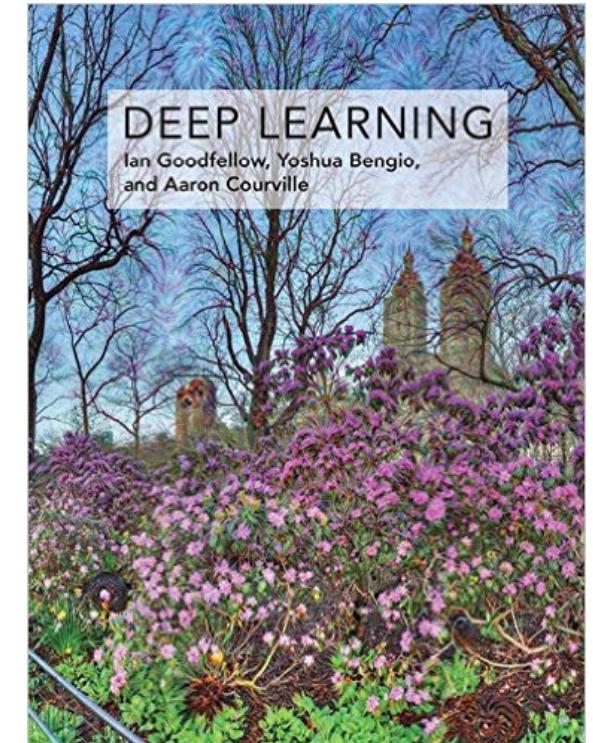
PRaDA@You Yangs, 2016

# RESOURCES

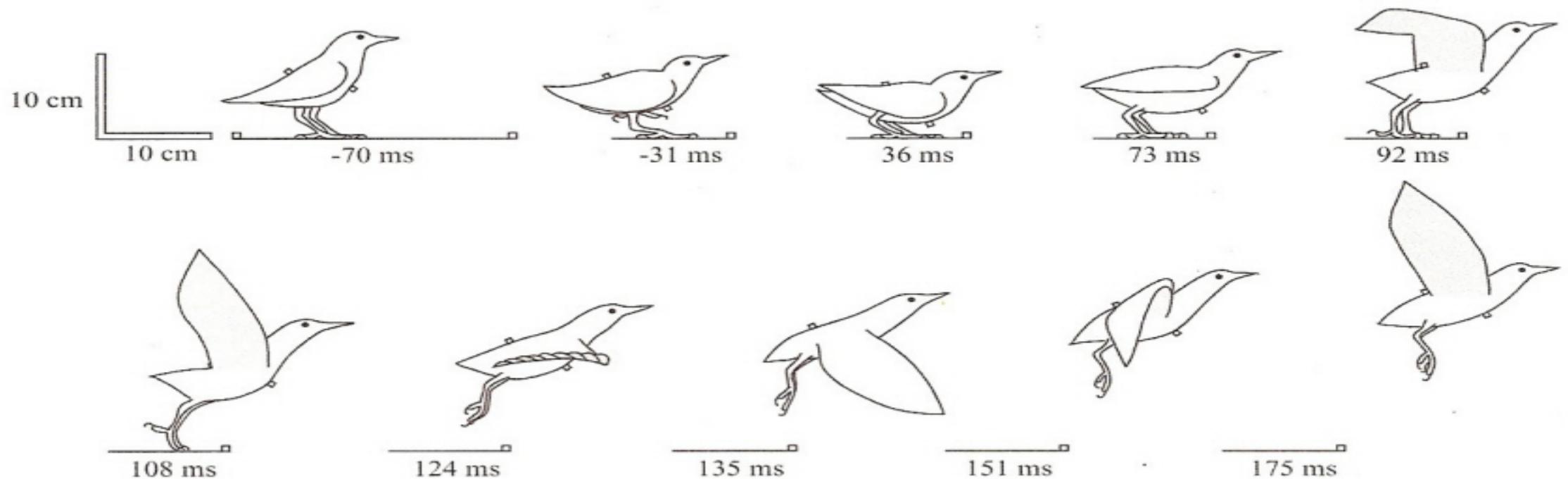
Tutorial page:

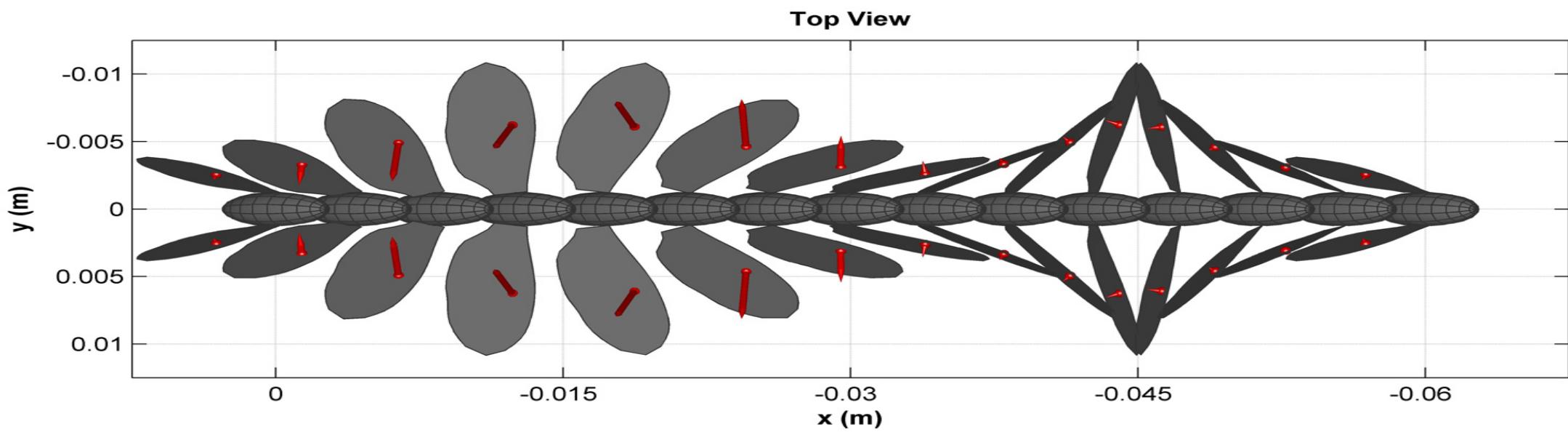
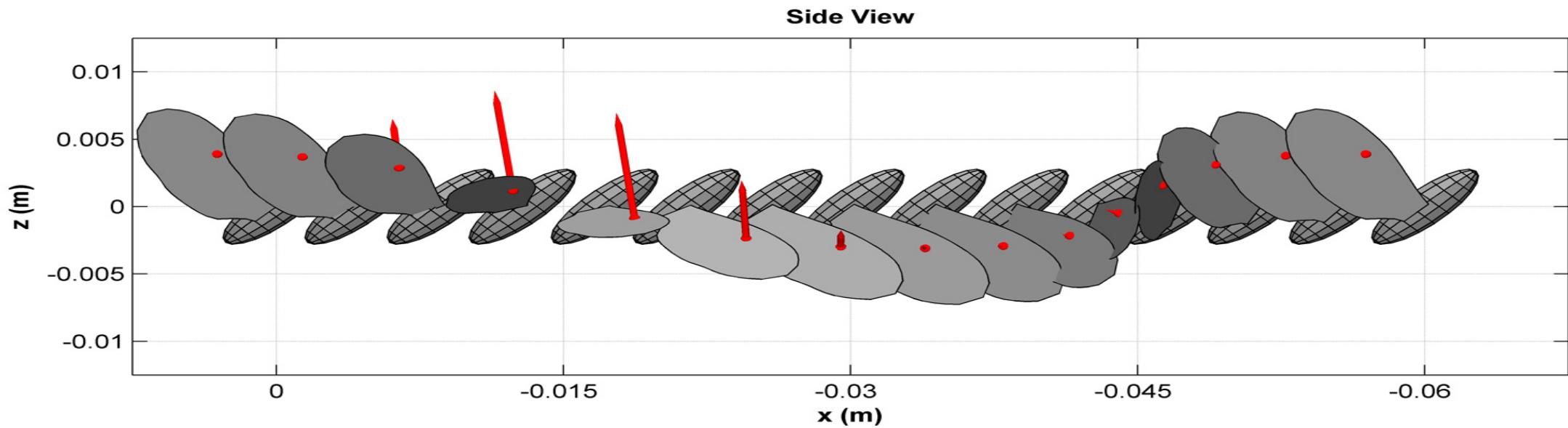
<http://prada-research.net/~truyen/ai16-tute.html>

Thanks to many people who have created beautiful graphics & open-source programming frameworks.

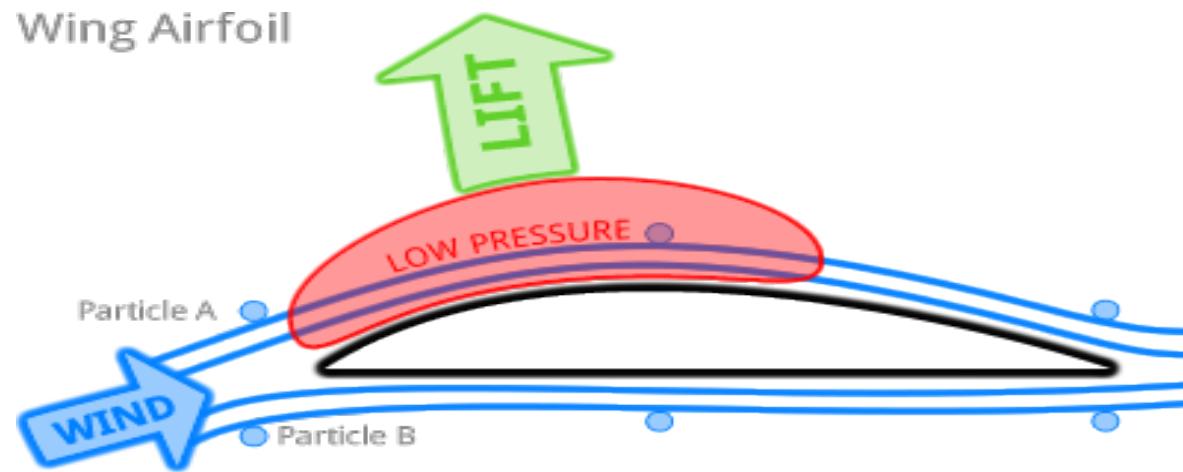


# Early approach to heavier-than-air flight





# A FASTER WAY



## Enabling factors

- ✓ Aerodynamics
- ✓ Powerful engines
- ✓ Light materials
- ✓ Advances in control
- ✓ Established safety practices

Sources:

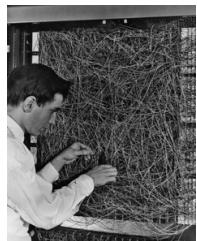
<http://aero.konelek.com/aerodynamics/aerodynamic-analysis-and-design>  
<http://www.foolishsailor.com/Sail-Trim-For-Cruisers-work-in-progress/Sail-Aerodynamics.html>

HISTORY MAY BE REPEATING IN THE DEEP  
LEARNING APPROACH TO AI



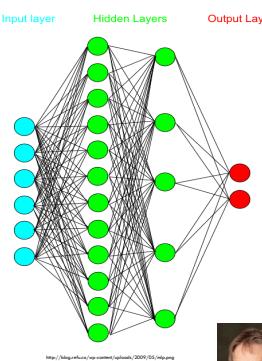
Yann LeCun

1988



Rosenblatt's  
perceptron

1958



1986

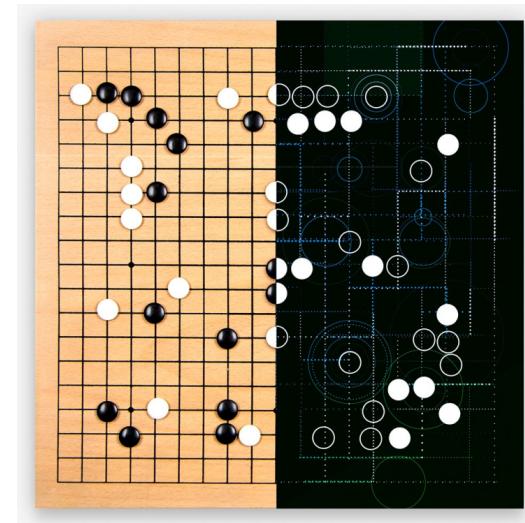


Geoff Hinton

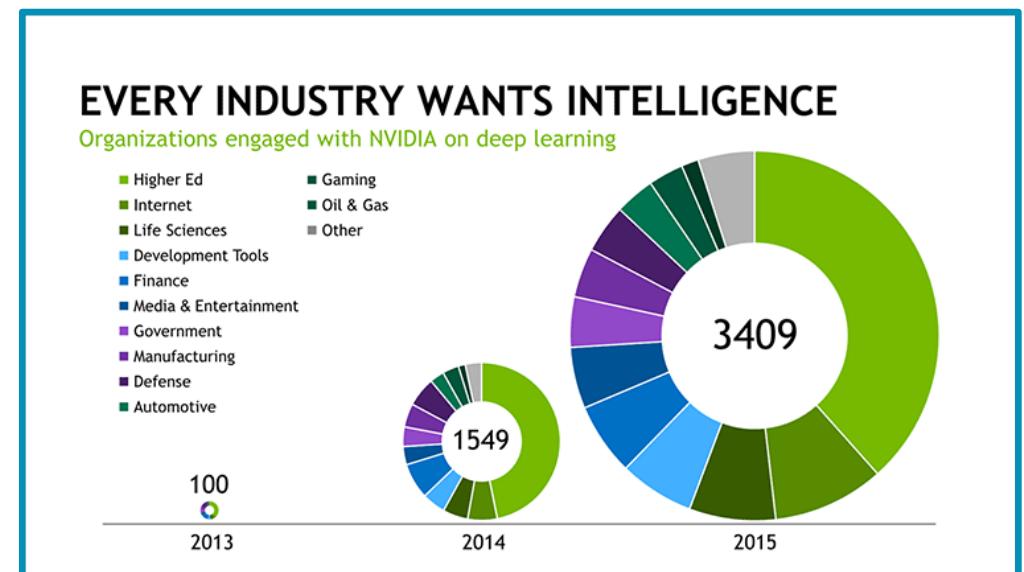
2006



2012



2016



# MORE ON HISTORY

J. Schmidhuber. Deep Learning in Neural Networks: An Overview. *Neural Networks*, Volume 61, January 2015, Pages 85-117 (DOI: 10.1016/j.neunet.2014.09.003)



Juergen Schmidhuber



Yann LeCun



Geoff Hinton



Yoshua Bengio



- Group theory (Lie algebra, renormalisation group, spin-class)

- Differential Turing machines
- Memory, attention & reasoning
- Reinforcement learning & planning
- Lifelong learning

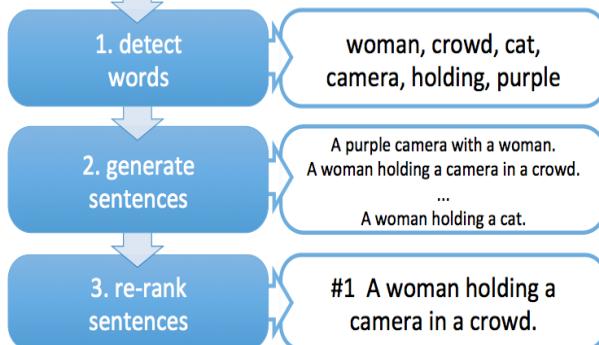
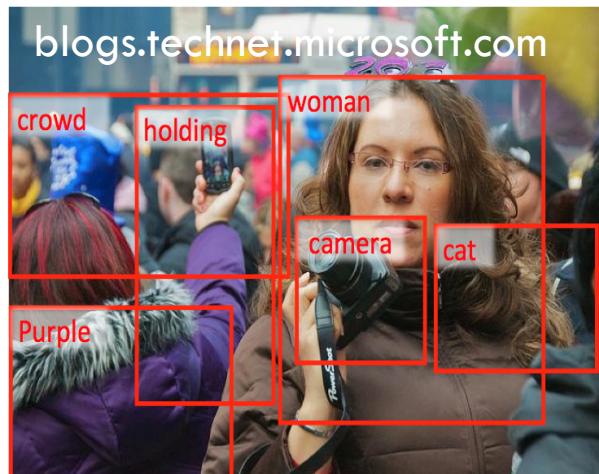
- Dropouts
- Rectifier linear transforms & skip-connections
- Highway nets, LSTM & CNN

- Representation learning (RBM, DBN, DBM, DDAE)
- Ensemble
- Back-propagation
- Stochastic gradient

# DEEP LEARNING IN COGNITIVE DOMAINS



Where human can  
recognise, act or answer  
accurately within seconds



A → B

(ANDREW NG, BAIDU)

# DEEP LEARNING IN NON-COGNITIVE DOMAINS

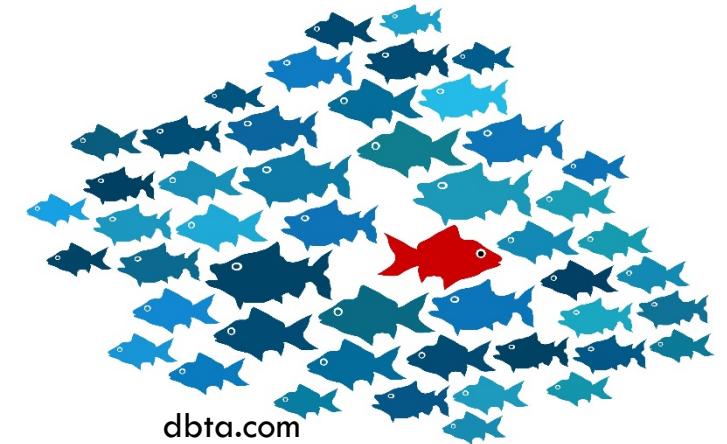
- Where humans need extensive training to do well
- Domains with great diversity but may be small in size
- Domains with great uncertainty, low-quality/missing data
- Domains that demand transparency & interpretability.



... healthcare

... security

... genetics, foods, water ...



# AGENDA

## Part I: Theory

Introduction to (mostly supervised) deep learning

## Part II: Practice

Applying deep learning to non-cognitive domains

## Part III: Advanced topics

Position yourself

# PART I: THEORY

## INTRODUCTION TO (MOSTLY SUPERVISED) DEEP LEARNING

Neural net as function approximation & feature detector

Three architectures: FFN → RNN → CNN

**Bag of tricks:** dropout → piece-wise linear units → skip-connections  
→ adaptive stochastic gradient → data augmentation

**Two principles:** distributed representation can be learnt → depth as prior

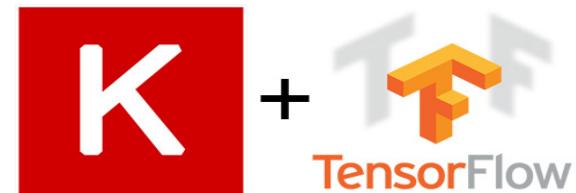
## PART II: PRACTICE APPLYING DEEP LEARNING TO NON-COGNITIVE DOMAINS

Hand-on:

- Introducing programming frameworks  
(Theano, TensorFlow, Keras, Mxnet)

Domains how-to:

- Healthcare
- Software engineering
- Web search
- Anomaly detection



# PART III: ADVANCED TOPICS

## POSITION YOURSELF

Unsupervised learning

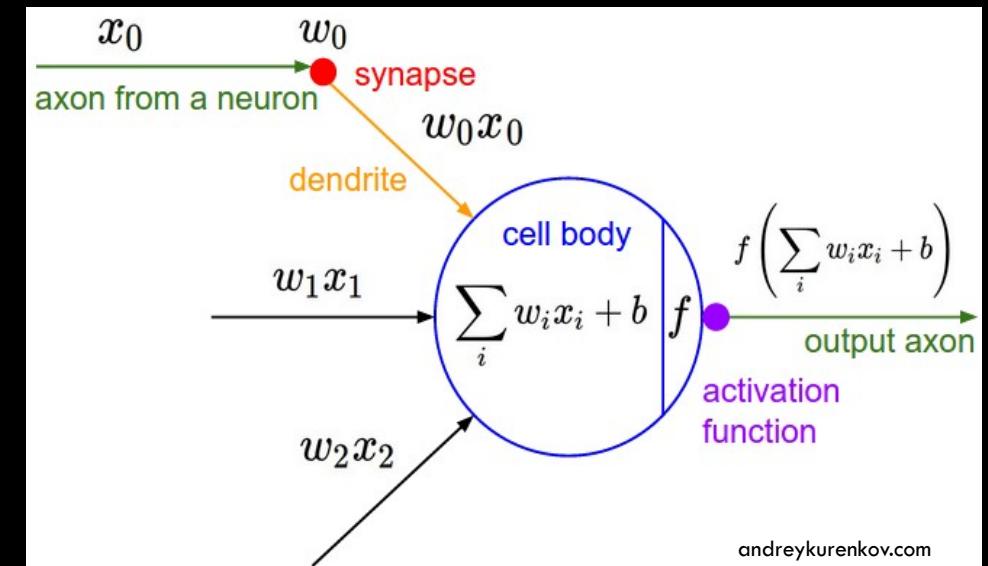
Relational data & structured outputs

Memory, attention & execution

Learning to learn

How to position ourselves

# PART I: THEORY

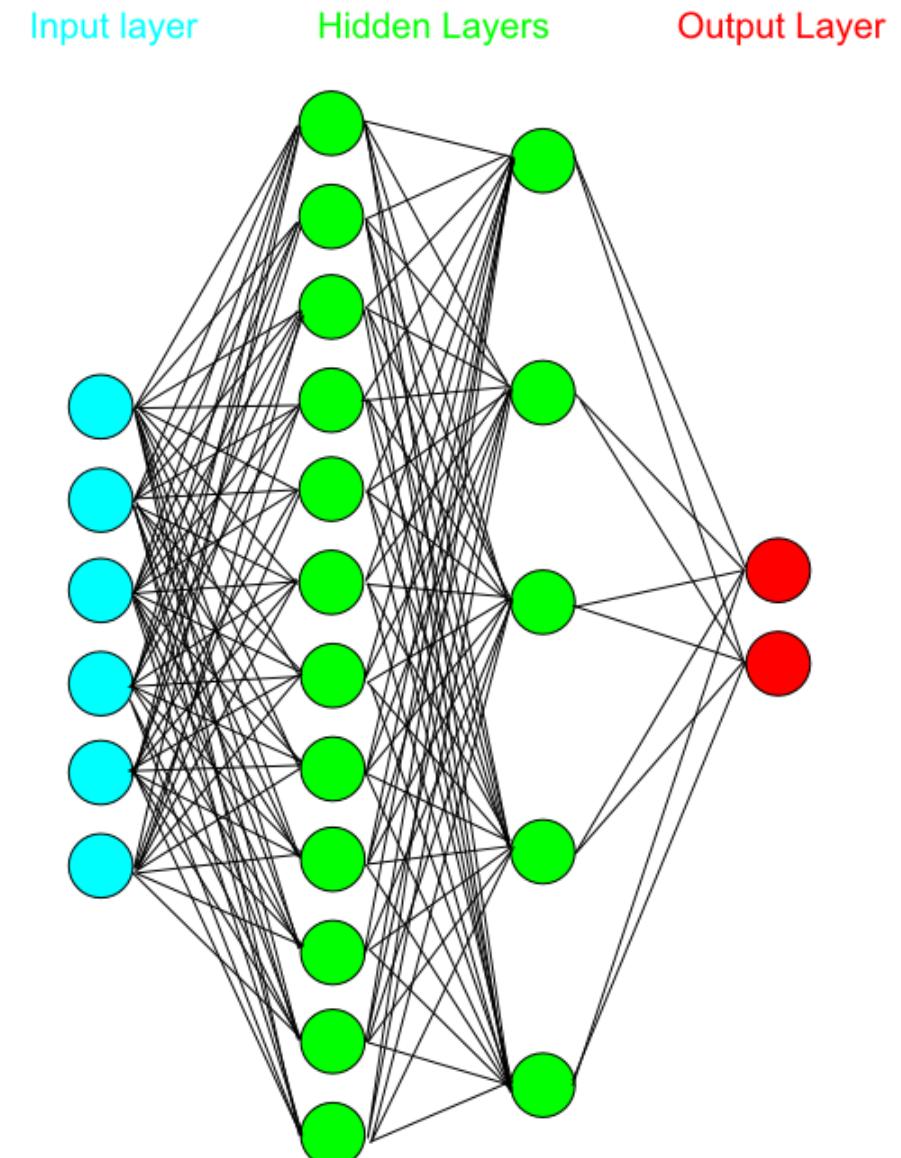


# WHAT IS DEEP LEARNING?

**Fast answer:** multilayer perceptrons (aka deep neural networks) of the 1980s rebranded in 2006.

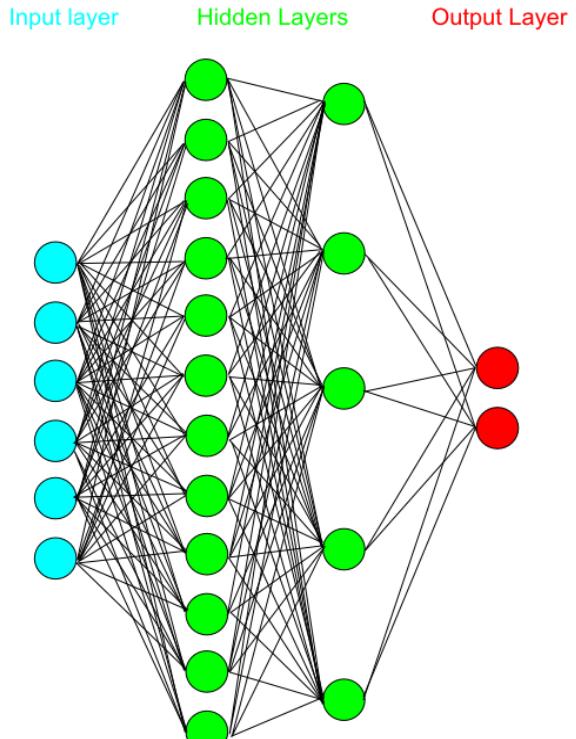
- But early nets go stuck at 1-2 hidden layers.

**Slow answer:** distributed representation, multiple steps of computation, modelling the compositionality of the world, a better prior, advances in **compute, data & optimization, neural architectures**, etc.



# POWERFUL ARCHITECTURE: RESNET

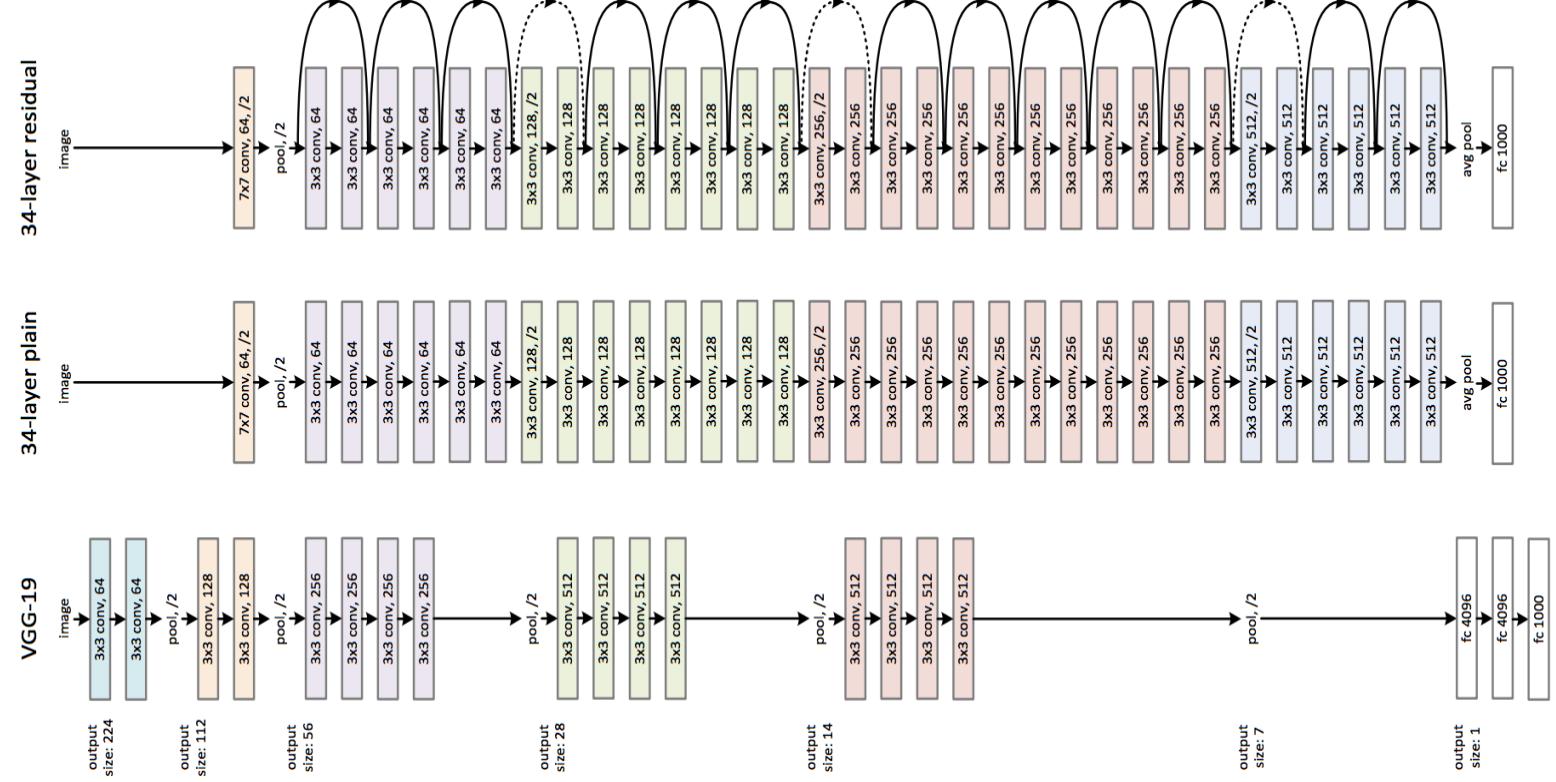
1986



<http://blog.refu.co/wp-content/uploads/2009/05/mlp.png>

3/12/16

2015



<http://felixlaumon.github.io/2015/01/08/kaggle-right-whale.html>

# WHY DEEP LEARNING?

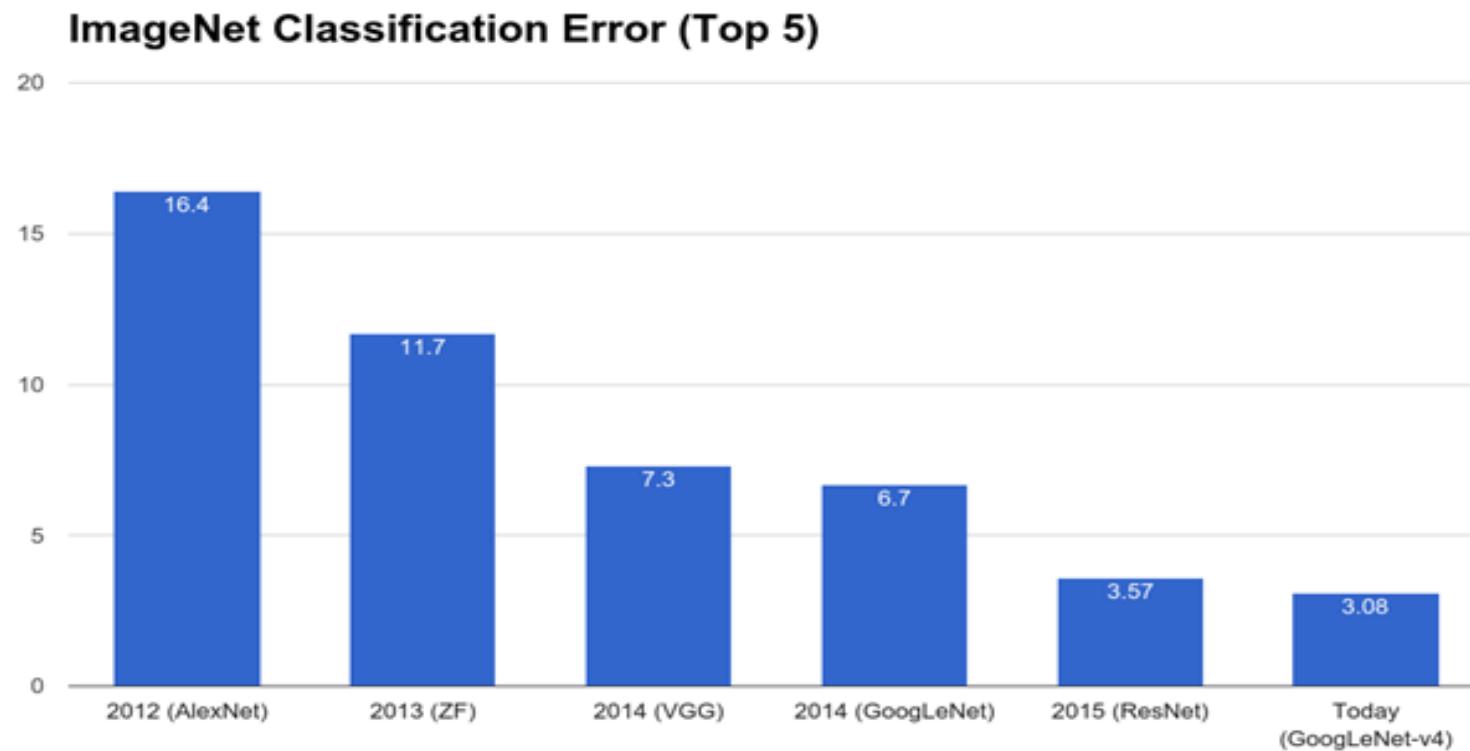
Because it works!

- Mostly performance-driven

But why does it work?

- Theory under-developed

Let's examine learning principles first.



<https://www.quora.com/What-is-the-state-of-the-art-today-on-ImageNet-classification-In-other-words-has-anybody-beaten-Deep-Residual-Learning>

# RECAP: THE BEST OF MACHINE LEARNING

## Strong/flexible priors:

- Good features → Feature engineering
- Data structure → HMM, CRF, MRF, Bayesian nets
- Model structure, VC-dimension, regularisation, sparsity → SVM, compressed sensing
- Manifold assumption, class/region separation → Metric + semi-supervised learning
- Factors of variation → PCA, ICA, FA

Uncertainty quantification: Bayesian, ensemble → RF, GBM

Sharing statistical strength: model reuse → transfer learning, domain adaption, multitask learning, lifelong learning

# PRACTICAL REALISATION

More data

More GPUs

Bigger models

Better models

Faster iterations

Pushing the limit of priors

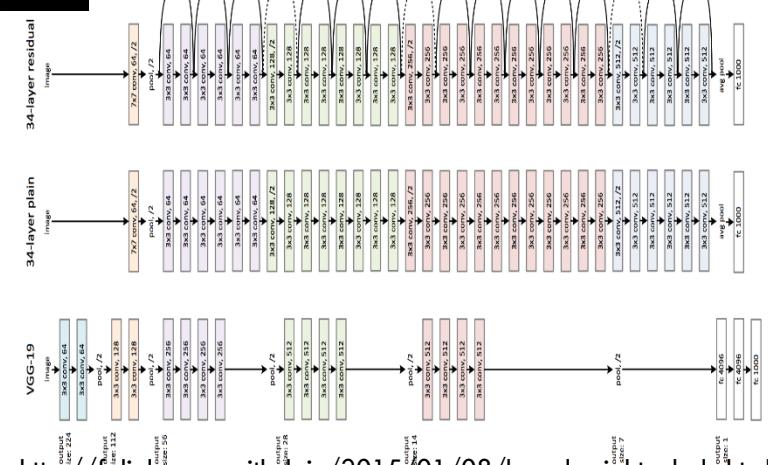
Pushing the limit of patience (best models take 2-3 weeks to run)

A LOT OF NEW TRICKS



© Getty Images/Universal Images Group

Data as new fuel



# STARTING POINT: FEATURE LEARNING

In typical machine learning projects, 80-90% effort is on feature engineering

- A right feature representation doesn't need much work. Simple linear methods often work well.

**Vision:** Gabor filter banks, SIFT, HOG, BLP, BOW, etc.

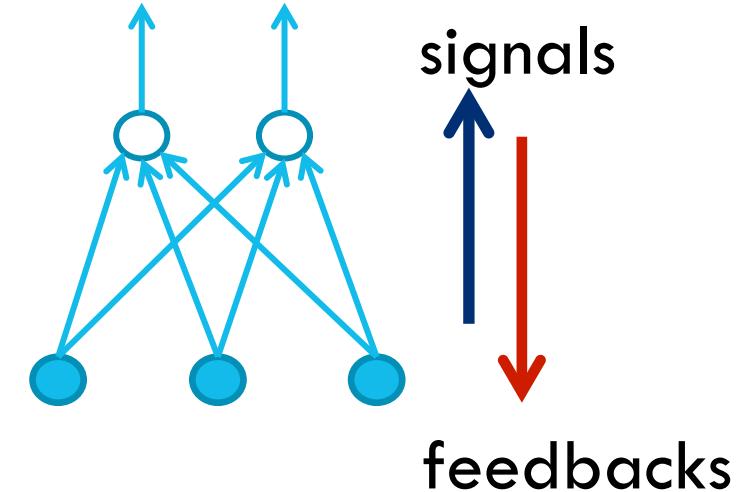
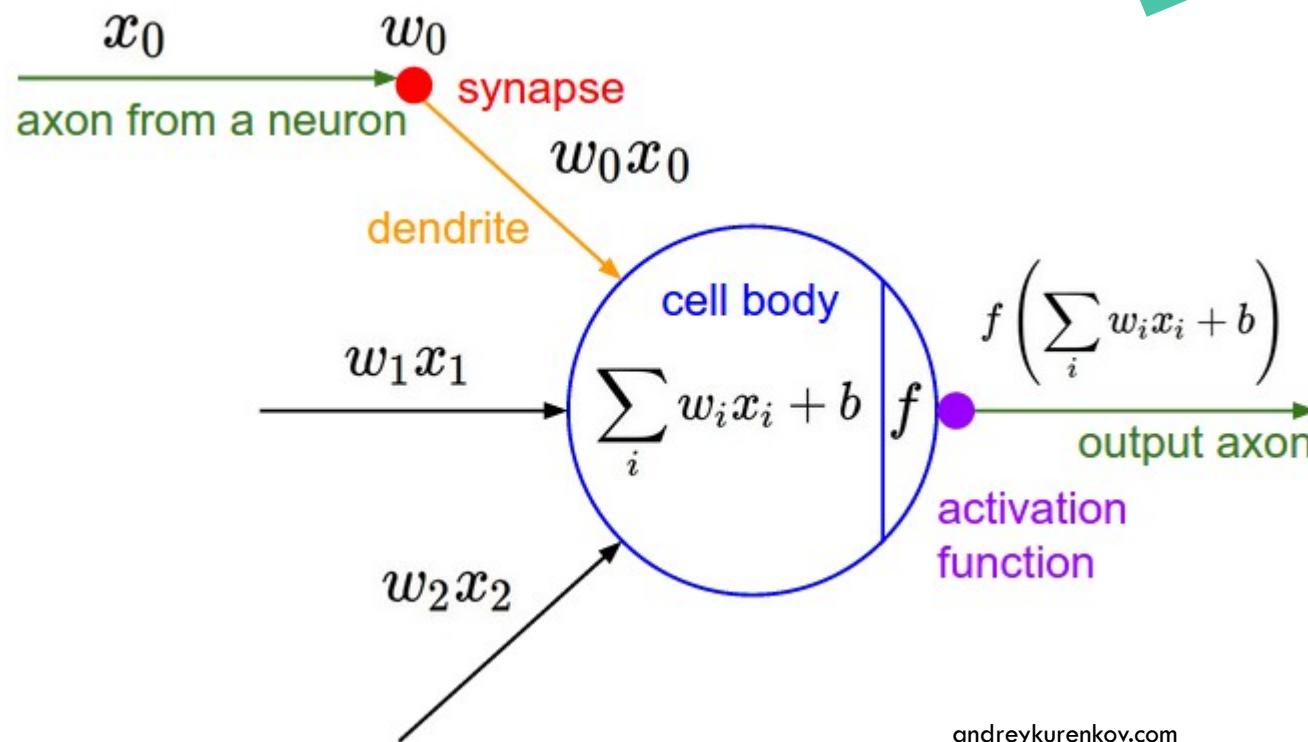
**Text:** BOW, n-gram, POS, topics, stemming, tf-idf, etc.

**SW:** token, LOC, API calls, #loops, developer reputation, team complexity, report readability, discussion length, etc.

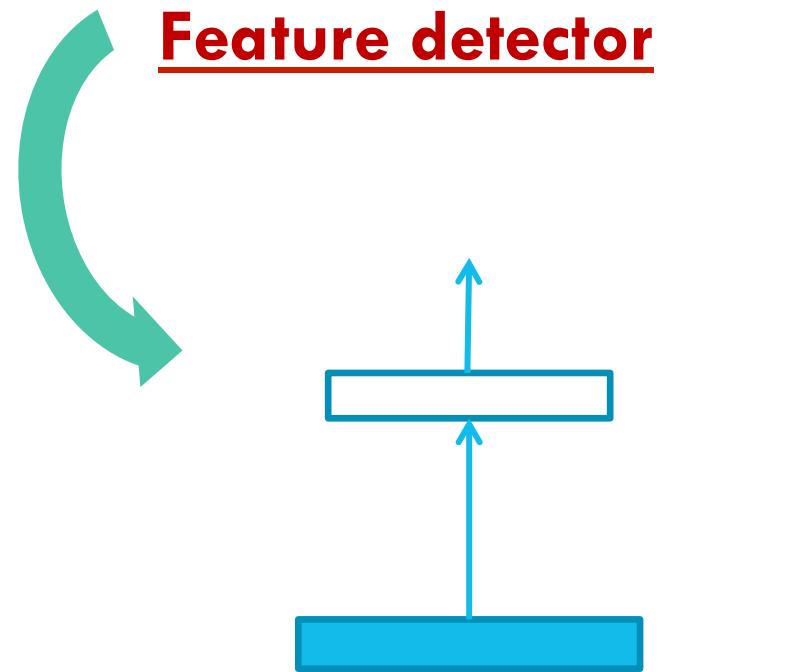
Try yourself on [Kaggle.com!](https://www.kaggle.com)

# THE BUILDING BLOCKS: FEATURE DETECTOR

## Integrate-and-fire neuron



## Feature detector



## Block representation

# THREE MAIN ARCHITECTURES: FNN, RNN & CNN

**Feed-forward (FFN):** Function approximator (Vector to vector)

- Most existing ML/statistics fall into this category

**Recurrent (RNN):** Sequence to sequence

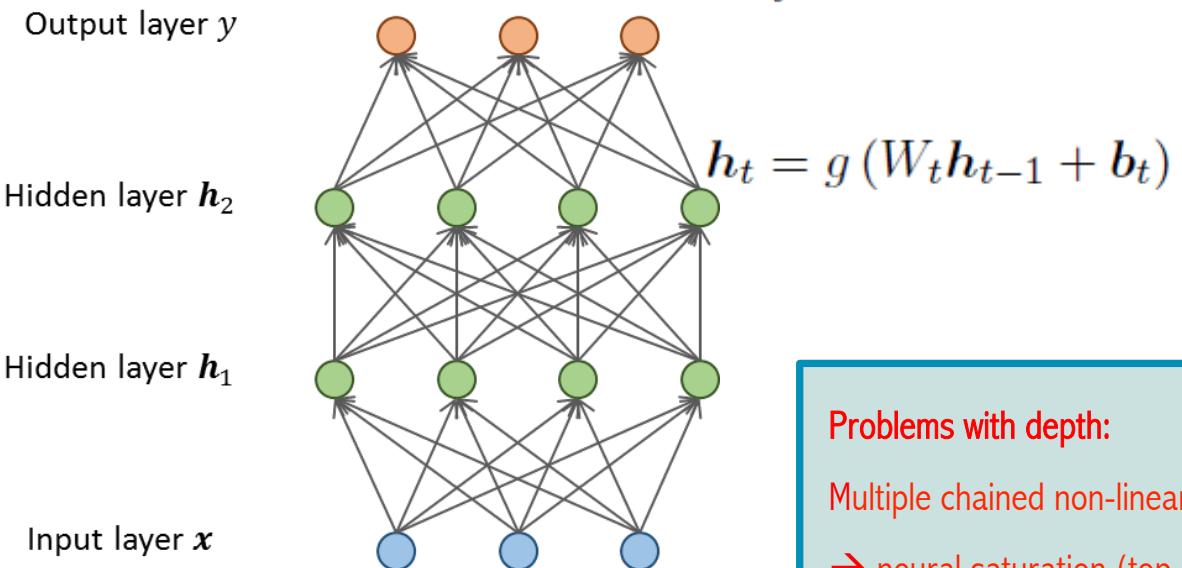
- Temporal, sequential. E.g., sentence, actions, DNA, EMR
- Program evaluation/execution. E.g., sort, traveling salesman problem

**Convolutional (CNN):** Image to vector/sequence/image

- In time: Speech, DNA, sentences
- In space: Image, video, relations

# FEED-FORWARD NET (FFN) VEC2VEC MAPPING

$$P(\tilde{y} = i \mid \mathbf{x}) = \text{softmax}(h_{T+1}^i) = \frac{e^{h_{T+1}^i}}{\sum_j e^{h_{T+1}^j}}$$



## Problems with depth:

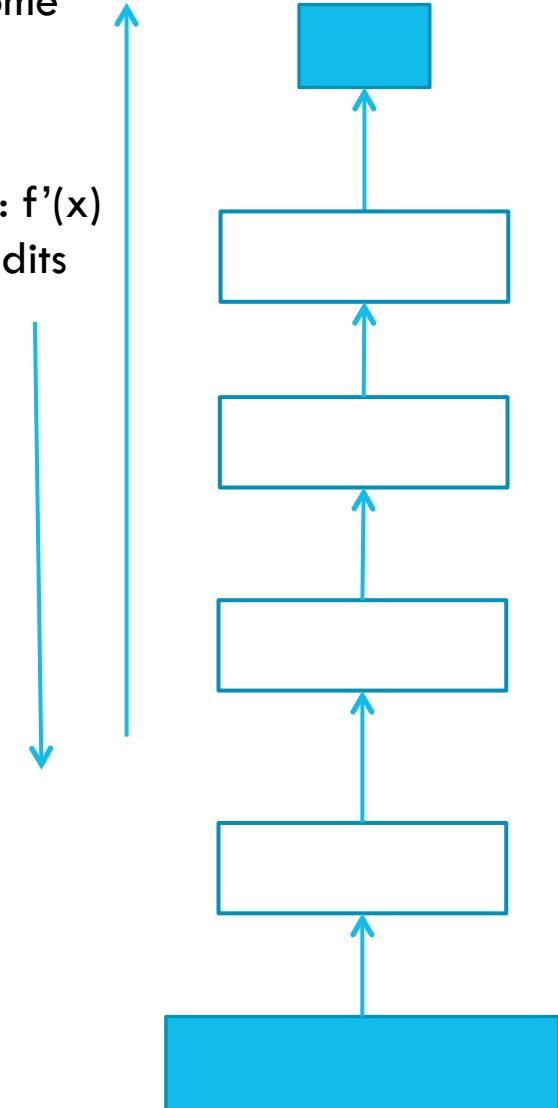
Multiple chained non-linearity steps

→ neural saturation (top units have little signal from the bottom)

→ vanishing gradient (bottom layers have much less training information from the label).

Forward pass:  $f(x)$  that carries units' contribution to outcome

Backward pass:  $f'(x)$  that assigns credits to units



# TWO VIEWS OF FNN

- ❖ The functional view: FNN as nested composition of functions

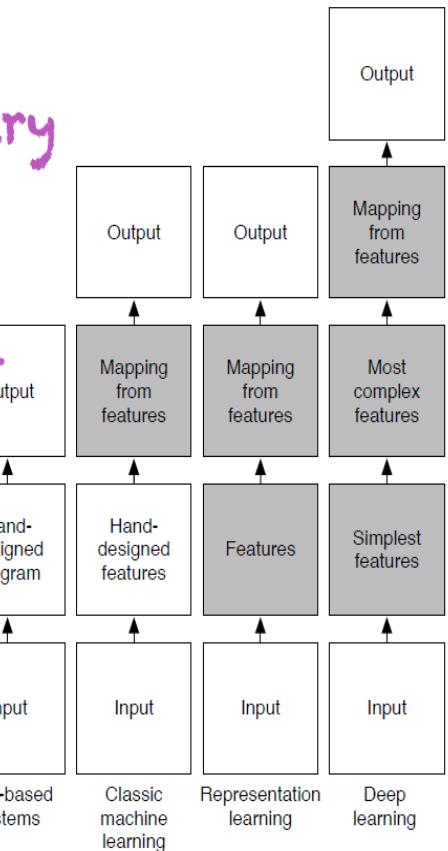
$$P(\tilde{y} = i \mid x) = \text{softmax}(h_{T+1}^i) = \frac{e^{h_{T+1}^i}}{\sum_j e^{h_{T+1}^j}}$$
$$h_t = g(W_t h_{t-1} + b_t)$$

- ❖ The representation view: FNN as staged abstraction of data

Automating Feature Discovery

Discovering and representing higher-level abstractions

(Bengio, DLSS 2015)



# SOLVING PROBLEM OF VANISHING GRADIENTS

Principle: Enlarging the channel to pass feature and gradient

Method 1: Removing saturation with piecewise linear units

- Rectifier linear unit (ReLU)

Method 2: Explicit copying through gating & skip-connection

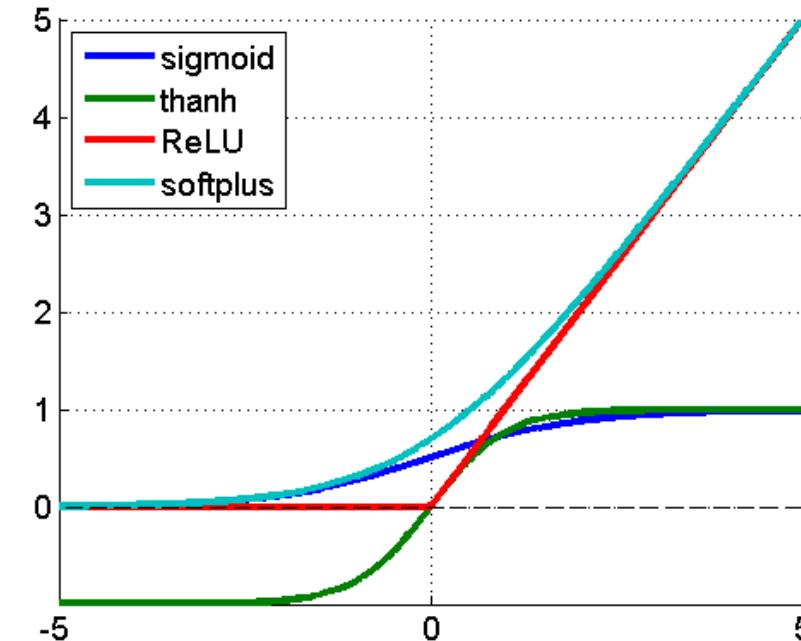
- Highway networks
- Skip-connection: ResNet

# METHOD 1: RECTIFIER LINEAR TRANSFORMATION

The usual logistic and tanh transforms are saturated at infinity

The gradient approaches zero, making learning impossible

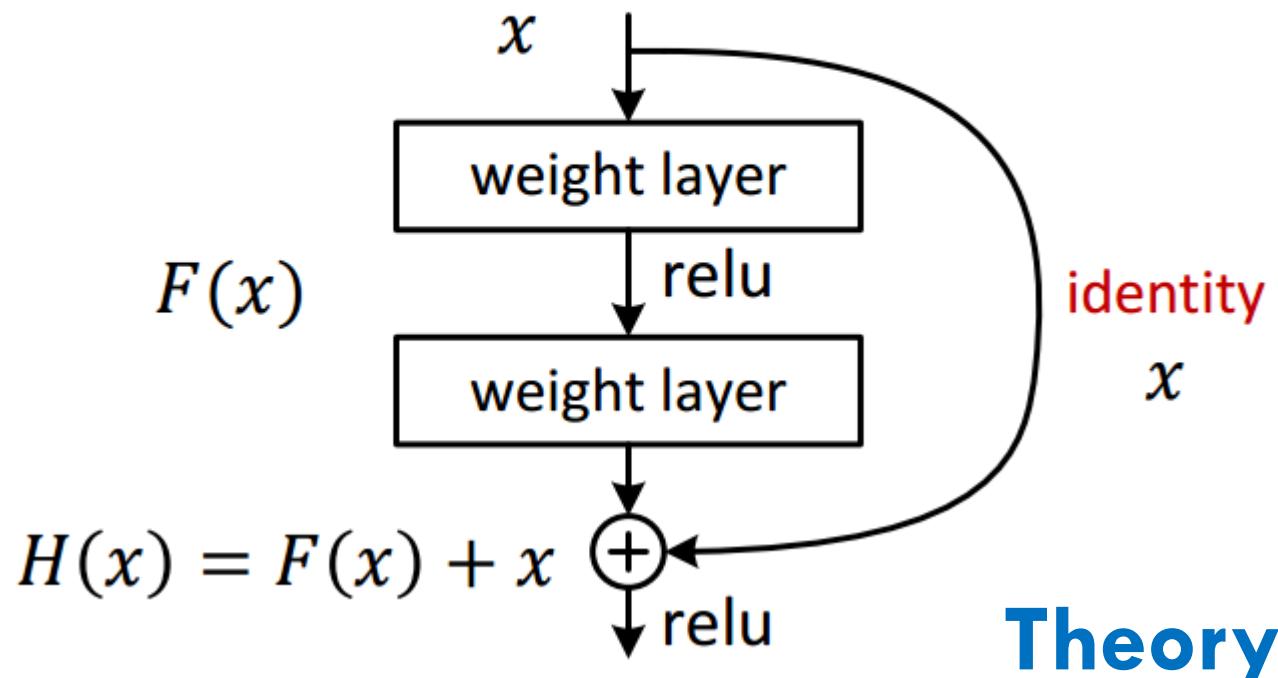
Rectifier linear function has constant gradient making information flows much better



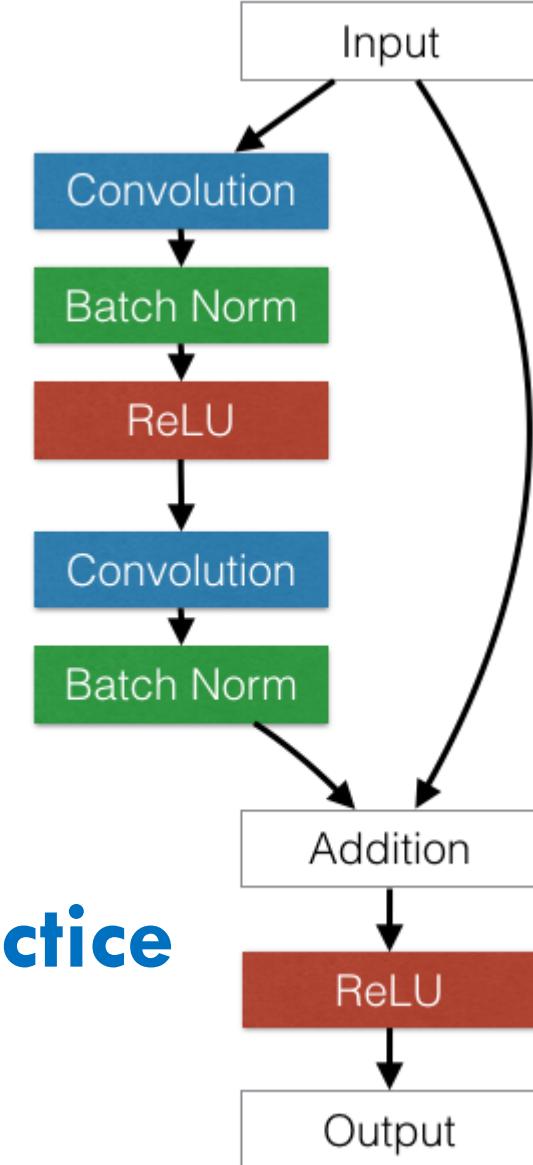
Source: <https://imiloinf.wordpress.com/2013/11/06/rectifier-nonlinearity/>

# METHOD 2: SKIP-CONNECTION WITH RESIDUAL NET

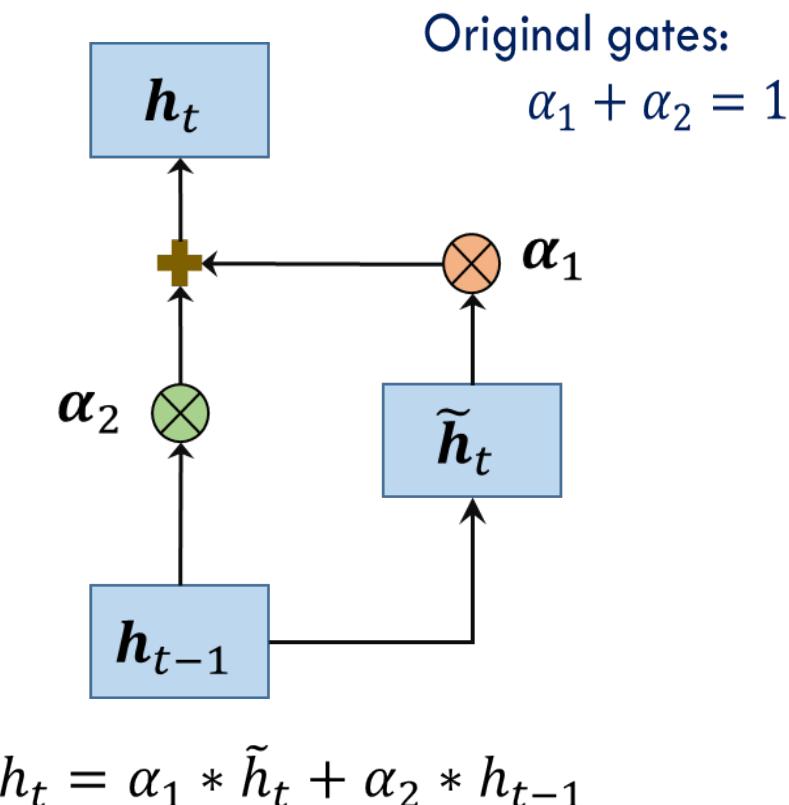
- Residual net



Practice



# METHOD 2: SKIP-CONNECTION WITH HIGHWAY NET & P-NORM



Original gates:

$$\alpha_1 + \alpha_2 = 1$$

**Flexible  $p$ -norm gates:**

$$(\alpha_1^p + \alpha_2^p)^{\frac{1}{p}} = 1$$

- $p > 1 \rightarrow \alpha_1 + \alpha_2 > 1$
- The gates are more open, letting more amount of information in the linear part passing through
- For example,  $\alpha_1 = 0.9$ 
  - $p = 1 \rightarrow \alpha_2 = 0.1$
  - $p = 2 \rightarrow \alpha_2 = 0.436$
  - $p = 5 \rightarrow \alpha_2 = 0.865$

# WHAT IF PARAMETERS ARE TIED ACROSS LAYERS?

Model size is compact, independent of depth → less overfitting

- Surprisingly: we found model capacity does not suffer!

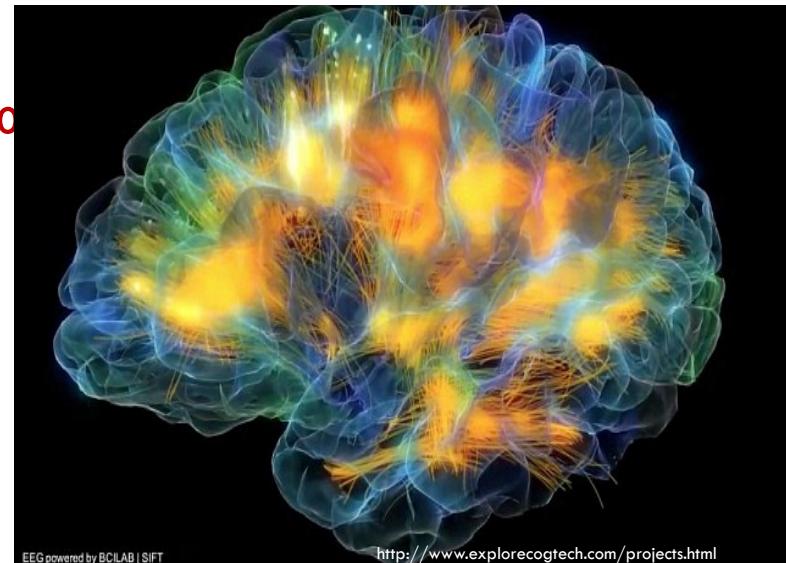
The functional view: FNN as nested composition of functions

The representation view: FNN as staged abstraction of data

**Third view of FNN: deep nets are essentially multiple steps of non-linear computation**

We have a **recurrent network** with null-input at each step!

- Neuroscience: self-sustained neural activity.



# THREE MAIN ARCHITECTURES: FNN, RNN & CNN

**Feed-forward (FFN):** Function approximator (Vector to vector)

- Most existing ML/statistics fall into this category

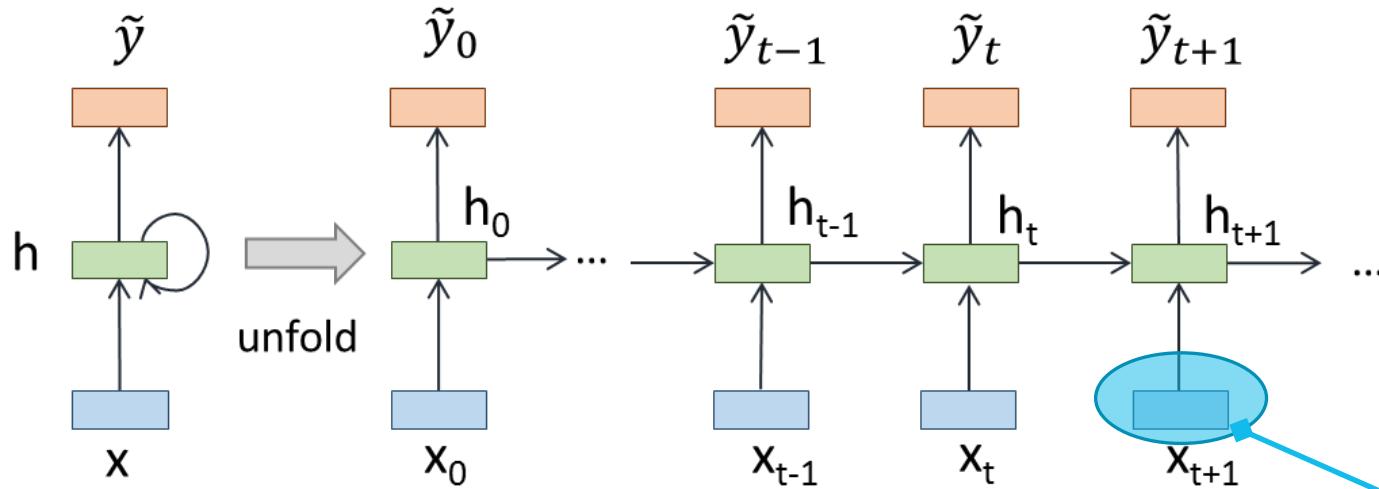
**Recurrent (RNN):** Sequence to sequence

- Temporal, sequential. E.g., sentence, actions, DNA, EMR
- Program evaluation/execution. E.g., sort, traveling salesman problem

**Convolutional (CNN):** Image to vector/sequence/image

- In time: Speech, DNA, sentences
- In space: Image, video, relations

# RECURRENT NET (RNN)



$$h_t = g(b + Wh_{t-1} + Ux_t)$$

$$a_t = c + Vh_t$$

$$P(\tilde{y}_t) = f_{prob}(a_t)$$

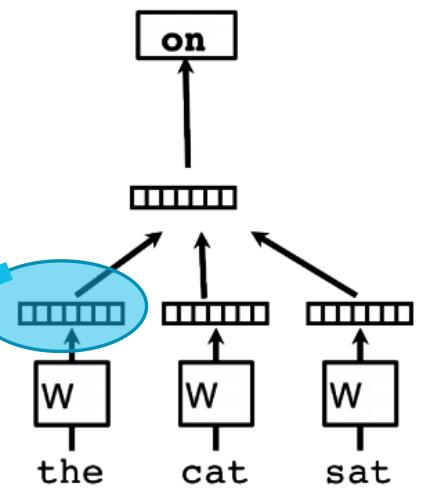
**Example application:** Language model which is essentially to predict the next word given previous words in the sentence.

**Embedding** is often used to convert a word into a vector, which can be initialized from **word2vec**.

Classifier

Average/Concatenate

Word Matrix



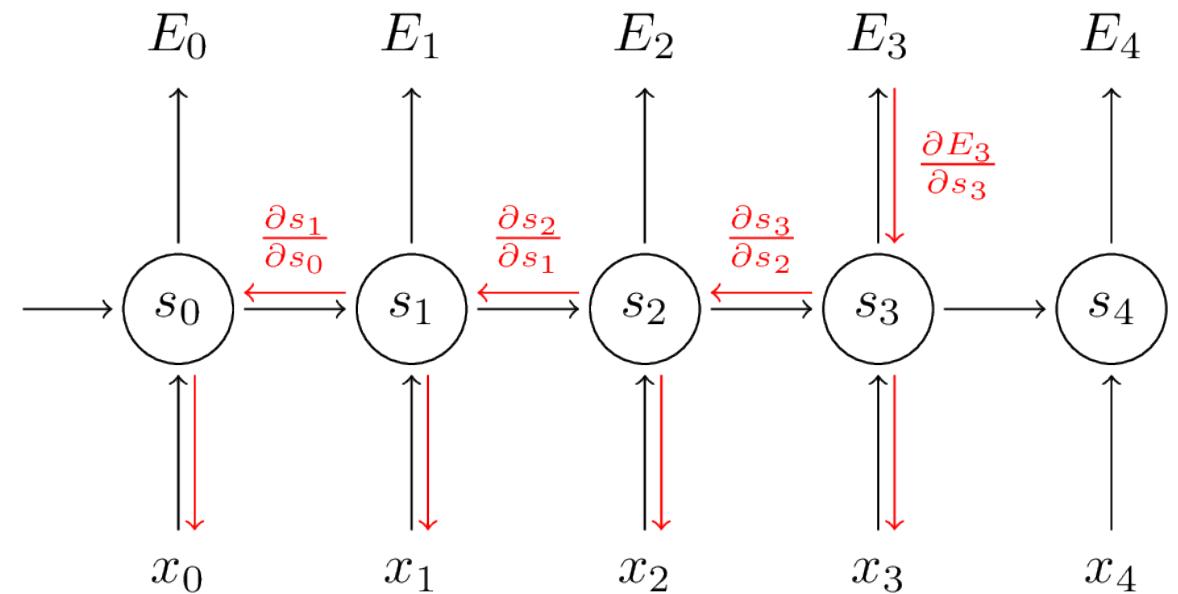
# RNN IS POWERFUL BUT ...

RNN is Turing-complete (Hava T. Siegelmann and Eduardo D. Sontag, 1991).

Brain can be thought of as a giant RNN over discrete time steps.

But training is very difficult for long sequences (more than 10 steps), due to:

- Vanishing gradient
- Exploding gradient



<http://www.wildml.com/>

# SOLVING PROBLEM OF VANISHING/EXPLODING GRADIENTS

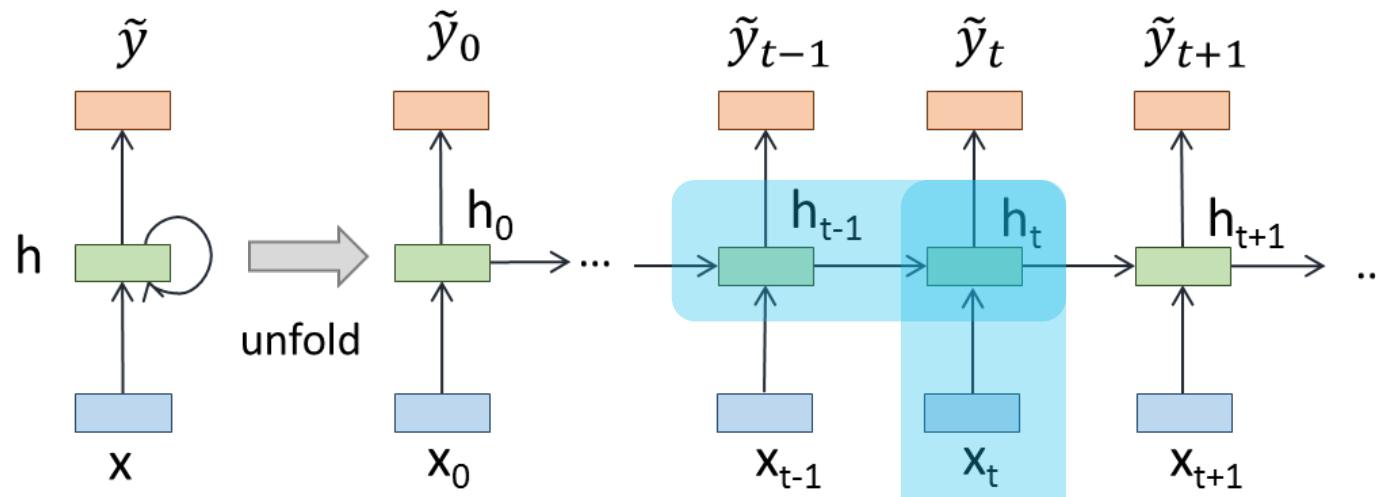
Trick 1: modifying the gradient, e.g., truncation for exploding gradient ([not always works](#))

Trick 2: changing learning dynamics, e.g., adaptive gradient descent partly solves the problem ([will see later](#))

Trick 3: modifying the information flow:

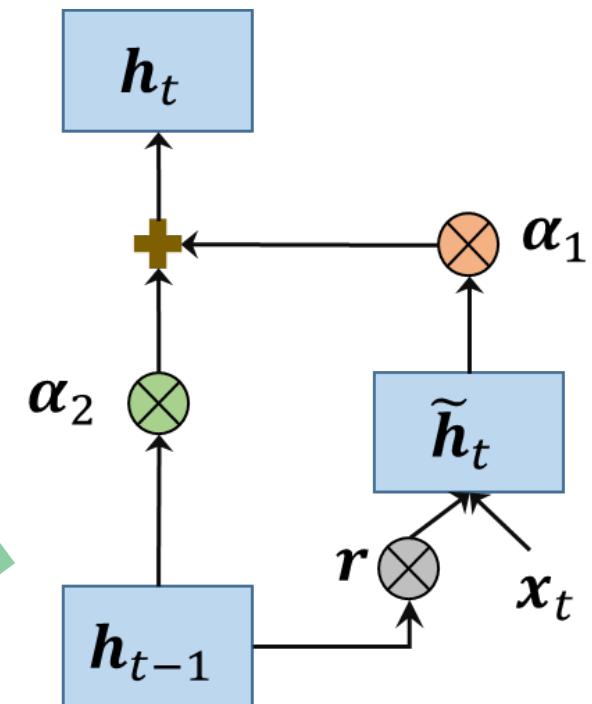
- Explicit copying through gating: Gated Recurrent Unit (GRU, 2014)
- Explicit memory: Long Short-Term Memory (LSTM, 1997)

# GATED RECURRENT UNITS (GRU)



$$h_t = \alpha_1 * \tilde{h}_t + \alpha_2 * h_{t-1}$$

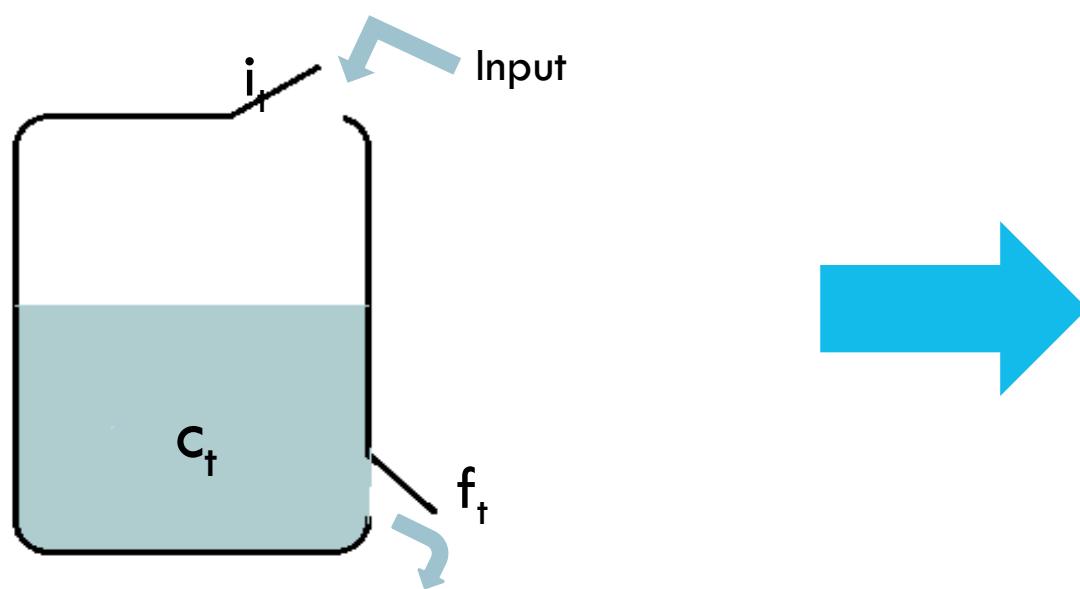
$$1 = \alpha_1 + \alpha_2$$



$$r_t = \sigma (W_r x_t + U_r h_{t-1} + b_r)$$

$$\tilde{h}_t = \tanh (W_h x_t + U_h (r_t * h_{t-1}) + b_h)$$

# LONG SHORT-TERM MEMORY (LSTM)



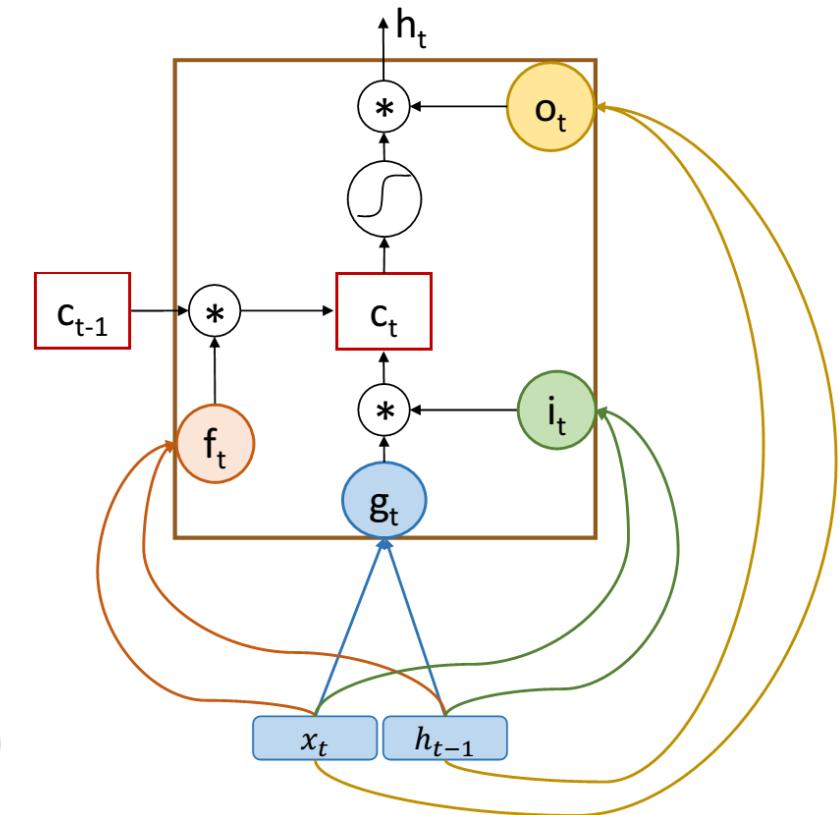
$$i_t = \sigma(W_i x_t + U_i h_{t-1} + b_i)$$

$$f_t = \sigma(W_f x_t + U_f h_{t-1} + b_f)$$

$$o_t = \sigma(W_o x_t + U_o h_{t-1} + b_o)$$

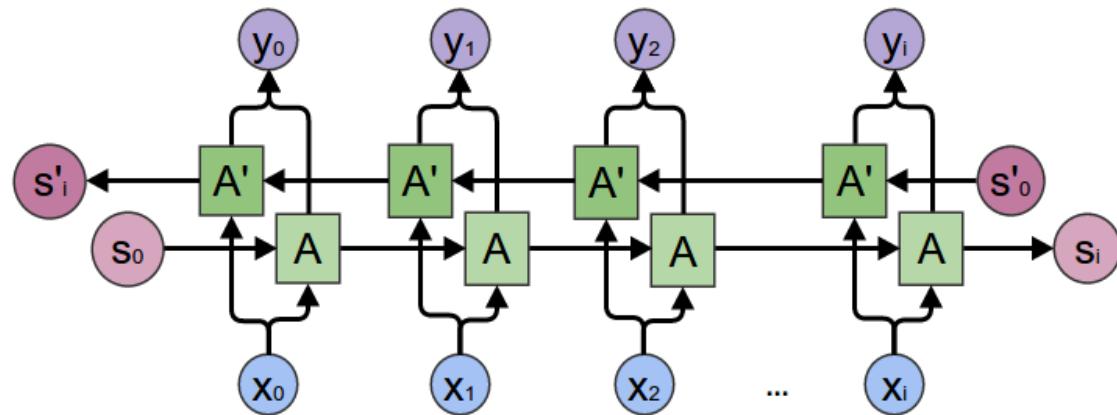
$$c_t = f_t * c_{t-1} + i_t * \tanh(W_c x_t + U_c h_{t-1} + b_c)$$

$$h_t = o_t * \tanh(c_t)$$

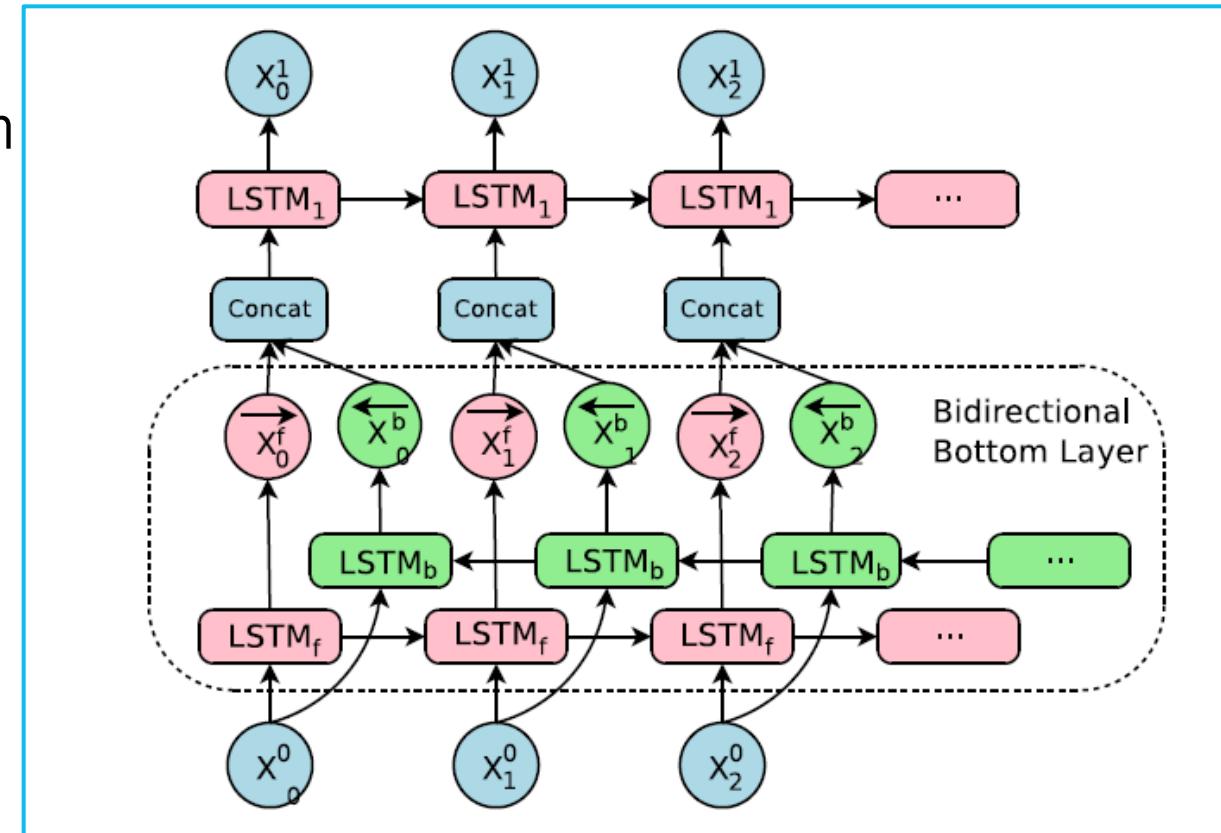


# BI-DIRECTIONAL RNNs

Bi-directional RNNs are often more powerful than uni-directional RNNs.

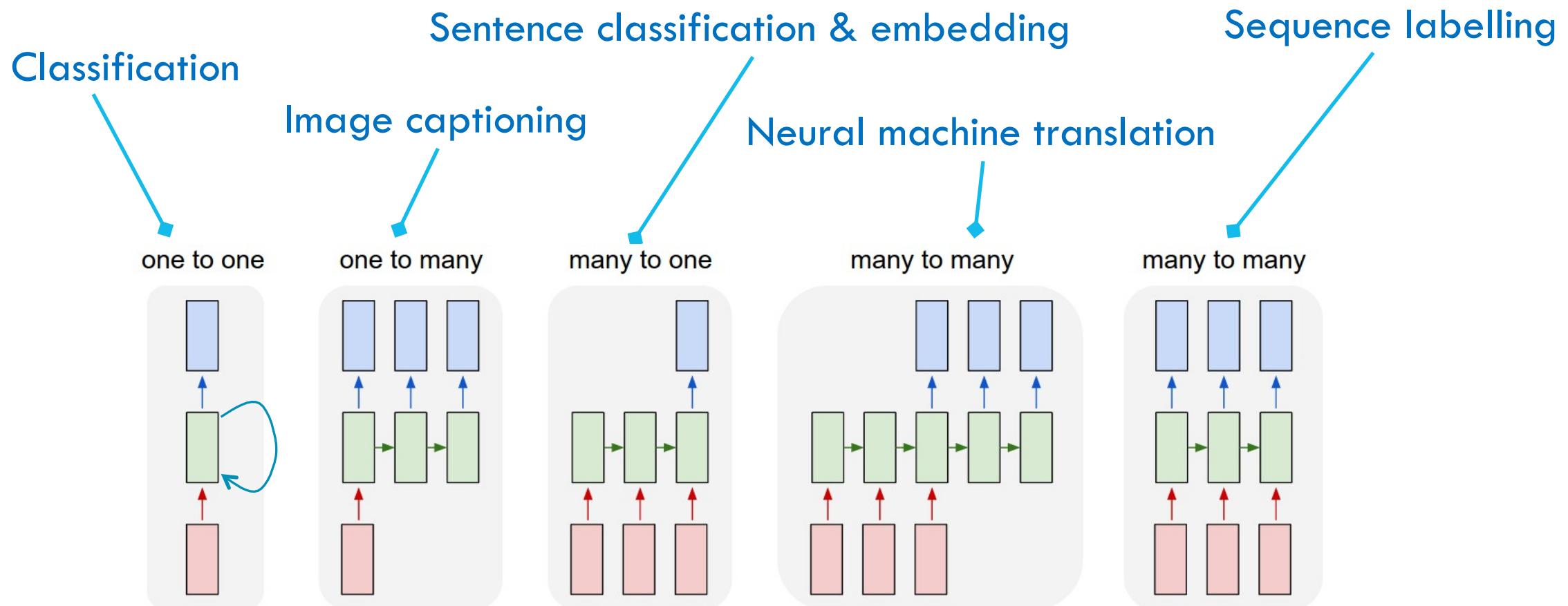


<http://colah.github.io/posts/2015-09-NN-Types-FP/>



Encoder (Wu et al, 2016, Google's NMT)

# RNN: WHERE IT WORKS



Source: <http://karpathy.github.io/assets/rnn/diags.jpeg>

# THREE MAIN ARCHITECTURES: FNN, RNN & CNN

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- Most existing ML/statistics fall into this category

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- Temporal, sequential. E.g., sentence, actions, DNA, EMR
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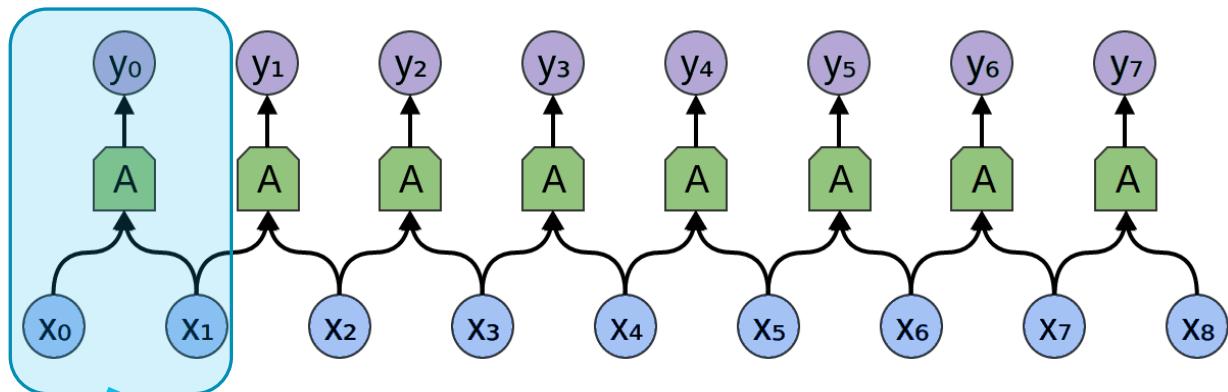
**Convolutional (CNN):** Image to vector/sequence/image

- In time: Speech, DNA, sentences
- In space: Image, video, relations

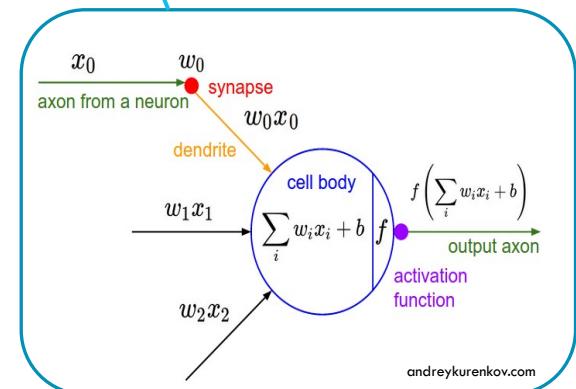
# LEARNABLE CONVOLUTION AS FEATURE DETECTOR (TRANSLATION INVARIANCE)

$$y_i = \sum_c K(c) x_{i+c}$$

Learnable kernels

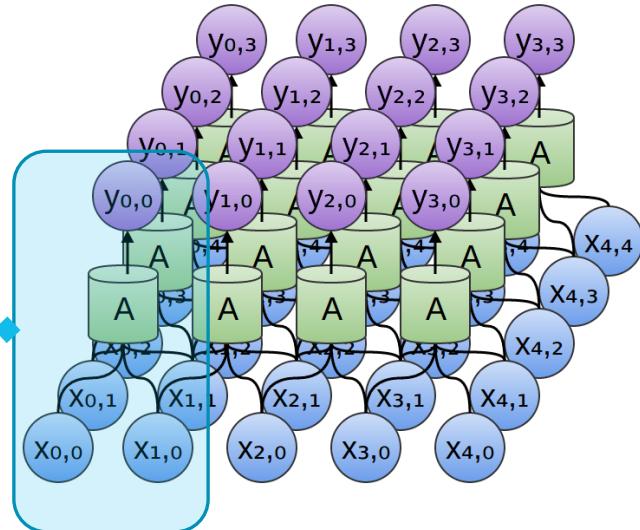


<http://colah.github.io/posts/2015-09-NN-Types-FP/>



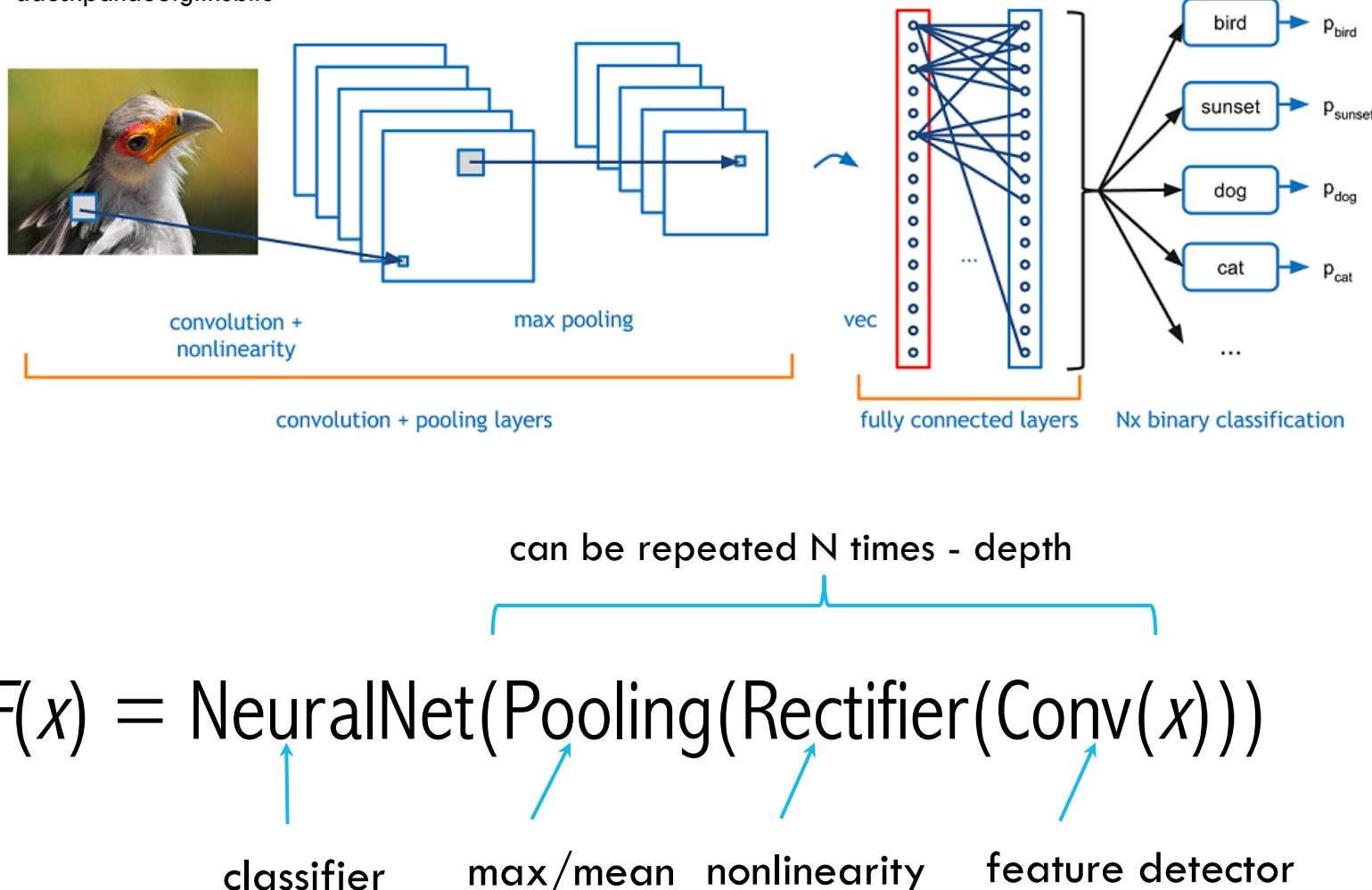
Feature detector,  
often many

$$y_{ij} = \sum_{c,d} K(c, d) x_{i+c, j+d}$$



# CNN IS (CONVOLUTION → POOLING) REPEATED

adeshpande3.github.io



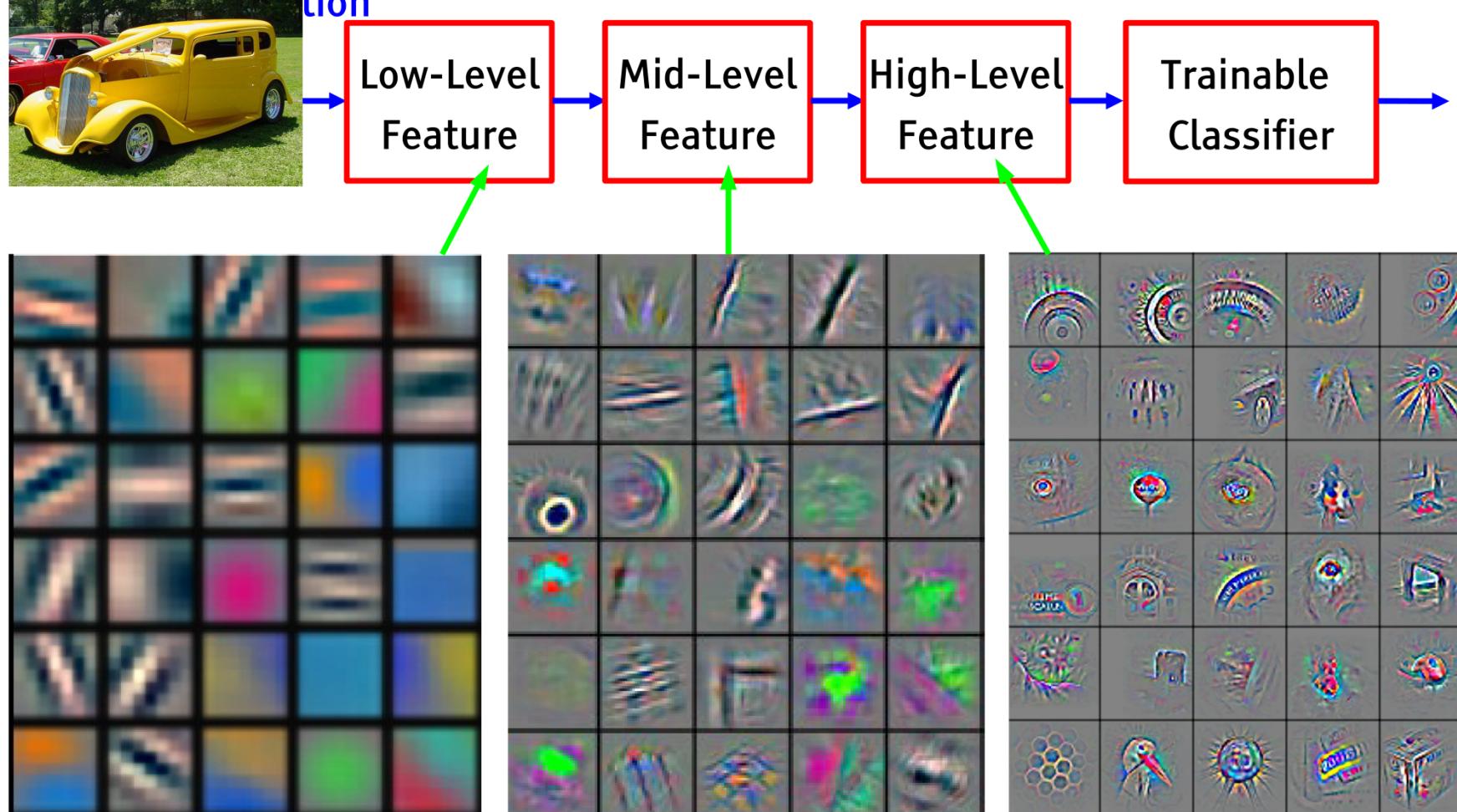
- Design parameters:**
- Padding
  - Stride
  - #Filters (maps)
  - Filter size
  - Pooling size
  - #Layers
  - Activation function



# Deep Learning = Learning Hierarchical Representations

Y LeCun  
MA Ranzato

- It's deep if it has more than one stage of non-linear feature transformation



# CNN: WHY IT WORKS

Learn instead of hand-pick the convolution operators in vision, like Gabor filter bank

Parameter sharing for translation invariance

Pooling and subsampling for higher-semantics

But not clear on sub-images modelling

- Pooling/subsampling destroys locations and views
- It suggests combination with RNNs.

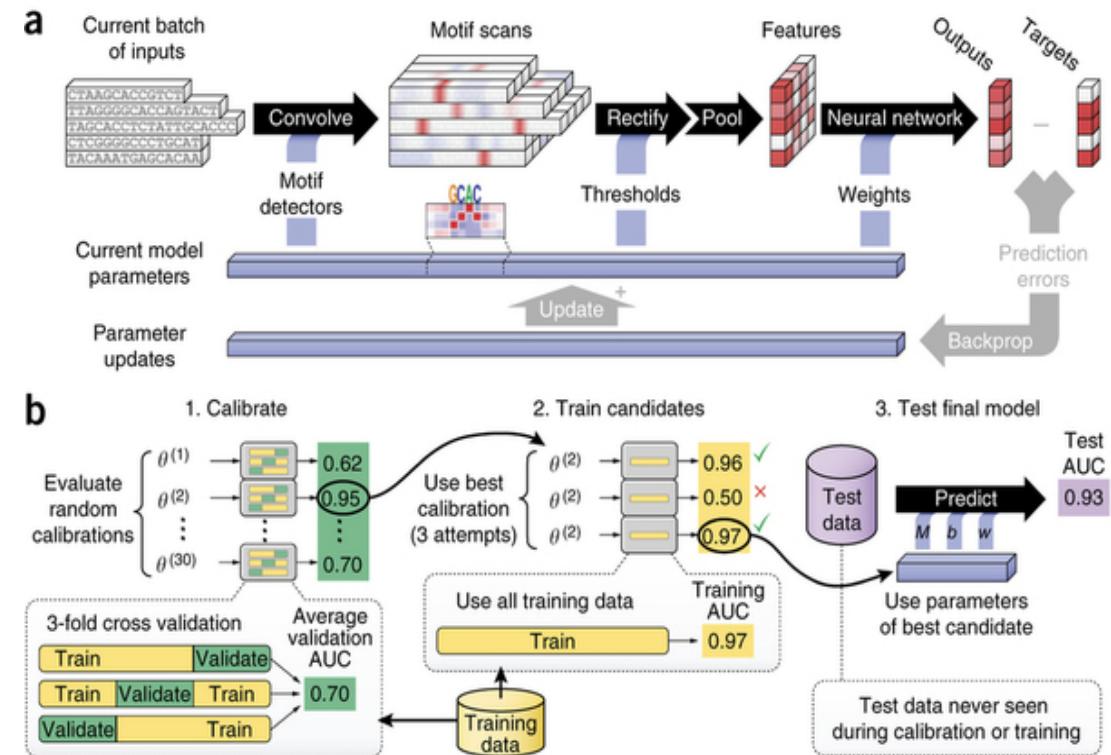
# CNN: WHERE IT WORKS

Translation invariance: Image, video, repeated motifs

Examples:

- Sentence – a sequence of words (used on conjunction with word embedding)
- Sentence – a sequence of characters
- DNA sequence of {A,C,T,G}
- Relations (e.g., right-to, left-to, father-of, etc)

**DeepBind, Nature 2015**



<http://www.nature.com/nbt/journal/v33/n8/full/nbt.3300.html>

# CURRENT WORK: COMBINATIONS OF {FFN,RNN,CNN}

Image classification: CNN + FFN

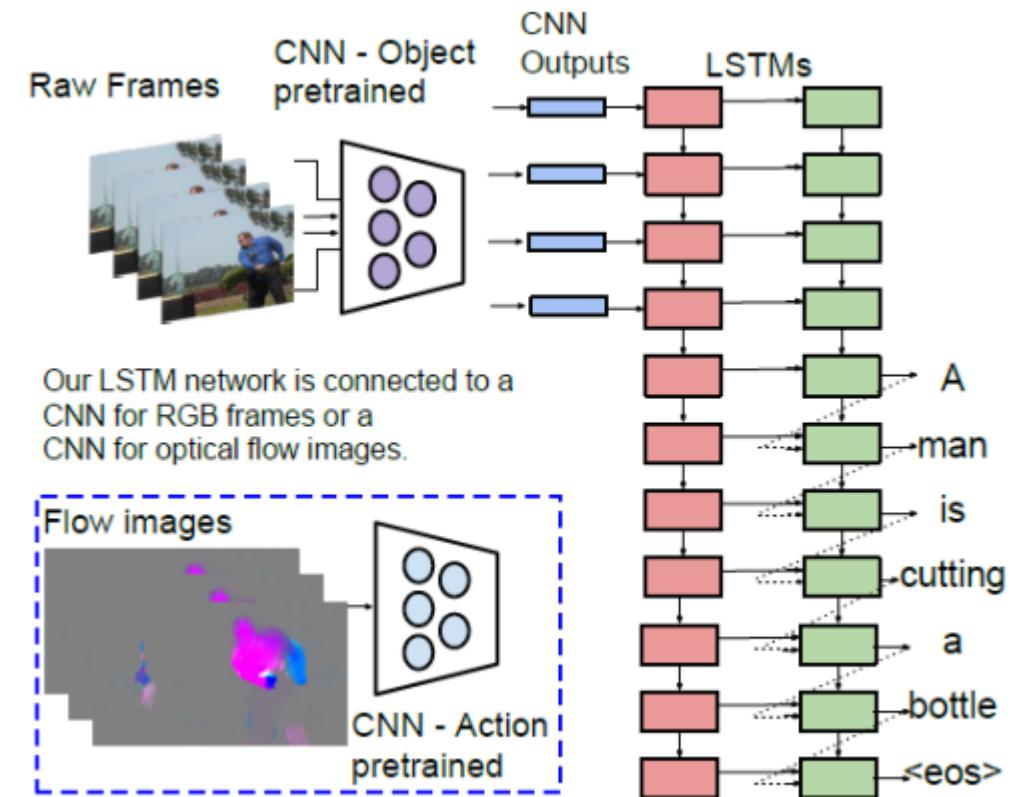
Video modelling: CNN + RNN

Image caption generation: CNN + RNN

Sentence classification: CNN + FFN

Sentence classification: RNN + FFN

Regular shapes (chain, tree, grid): CNN | RNN



# PRACTICAL REALISATION

More data

More GPUs

Bigger models

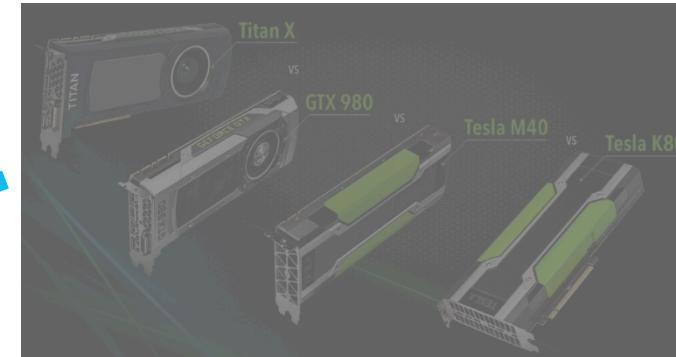
Better models

Faster iterations

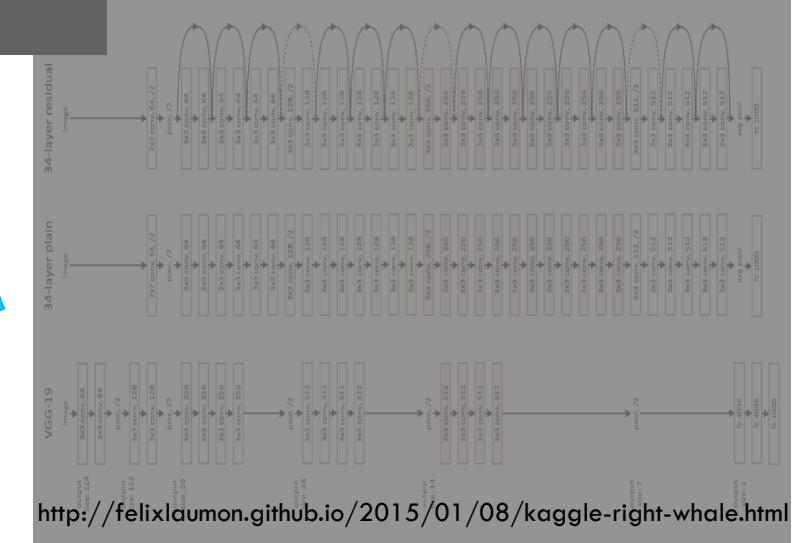
Pushing the limit of priors

Pushing the limit of patience (best models take 2-3 weeks to run)

A LOT OF NEW TRICKS



Data as new fuel



<http://felixlaumon.github.io/2015/01/08/kaggle-right-whale.html>

# TWO ISSUES IN LEARNING

## 1. Slow learning and local traps

- Very deep nets make gradients uninformative
- Model uncertainty leads to rugged objective functions with exponentially many local minima

## 2. Data/model uncertainty and overfitting

- Many models possible
- Models are currently very big with hundreds of millions parameters
- Deeper is more powerful, but more parameters.

# SOLVING ISSUE OF SLOW LEARNING AND LOCAL TRAPS

Redesign model, e.g., using skip-connections

Sensible initialisation

Adaptive stochastic gradient descent

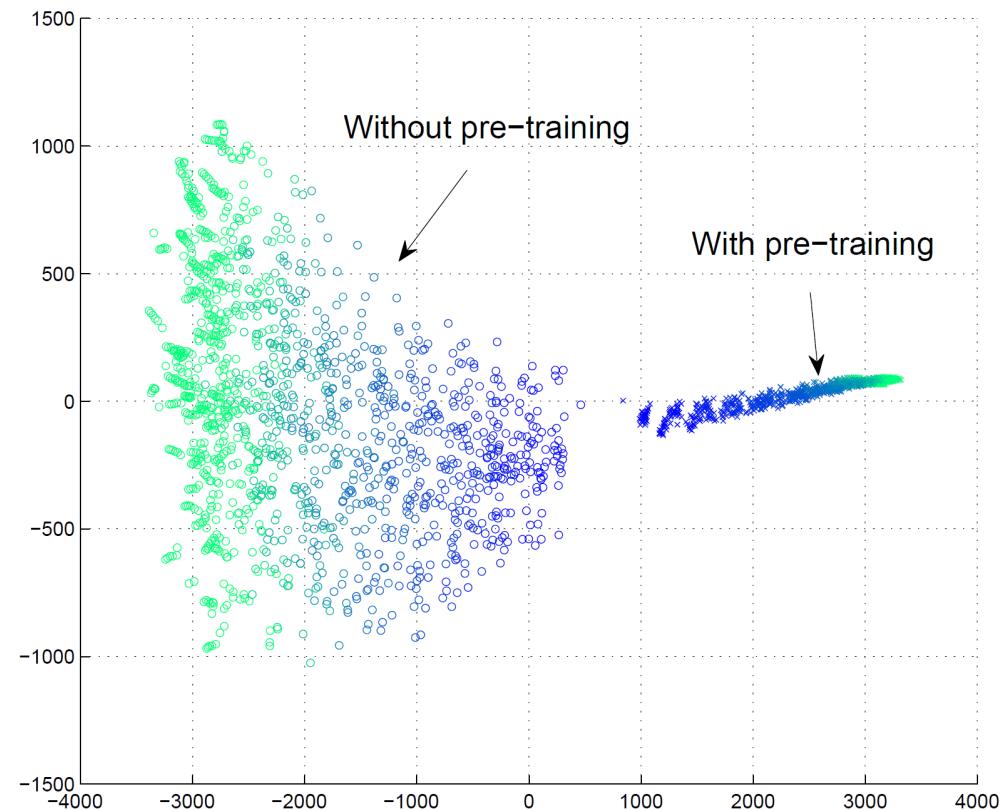
# SENSIBLE INITIALISATION

Random Gaussian initialisation often works well

- TIP: Control the fan-in/fan-out norms

If not, use pre-training

- When no existing models: Unsupervised learning (e.g., word2vec, language models, autoencoders)
- Transfer from other models, e.g., popular in vision with AlexNet, Inception, ResNet, etc.



Source: (Erhan et al, JMLR'10, Fig 6)

# STOCHASTIC GRADIENT DESCENT (SGD)

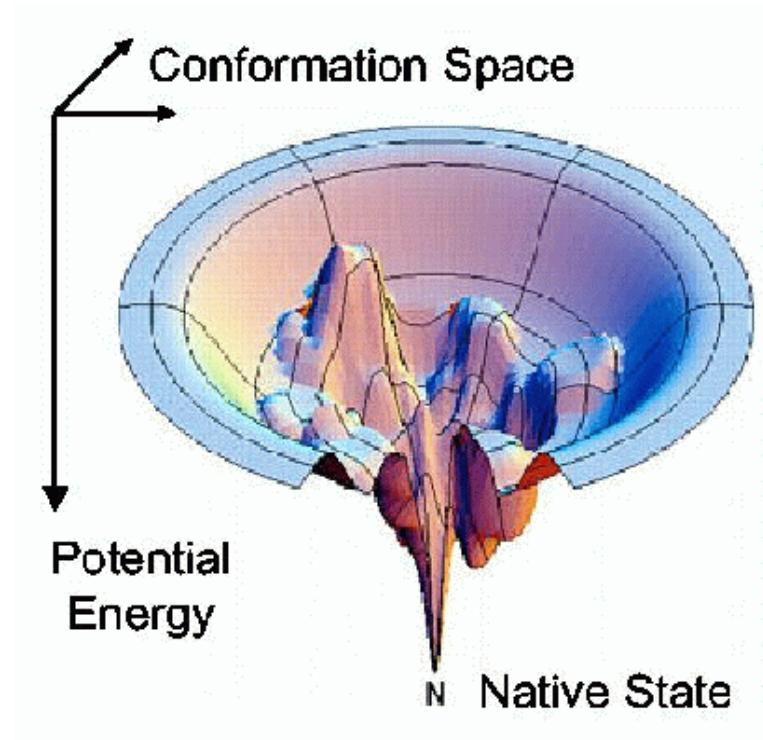
Using mini-batch to smooth out gradient

Use large enough learning rate to get over poor local minima

Periodically reduce the learning rate to land into a good local minima

It sounds like simulated annealing, but without proven global minima

Works well in practice since the energy landscape is a funnel



# ADAPTIVE SGDS

## Problems with SGD

- Poor gradient information, ill-conditioning, slow convergence rate
- Scheduling learning rate is an art
- Pathological curvature

Speed search: Exploiting local search direction with **momentum**

Rescaling gradient with **Adagrad**

A smoother version of Adagrad: **RMSProp** (usually good for RNNs)

All tricks combined: **Adam** (usually good for most jobs)

## Adagrad (Duchi et al, 2011)

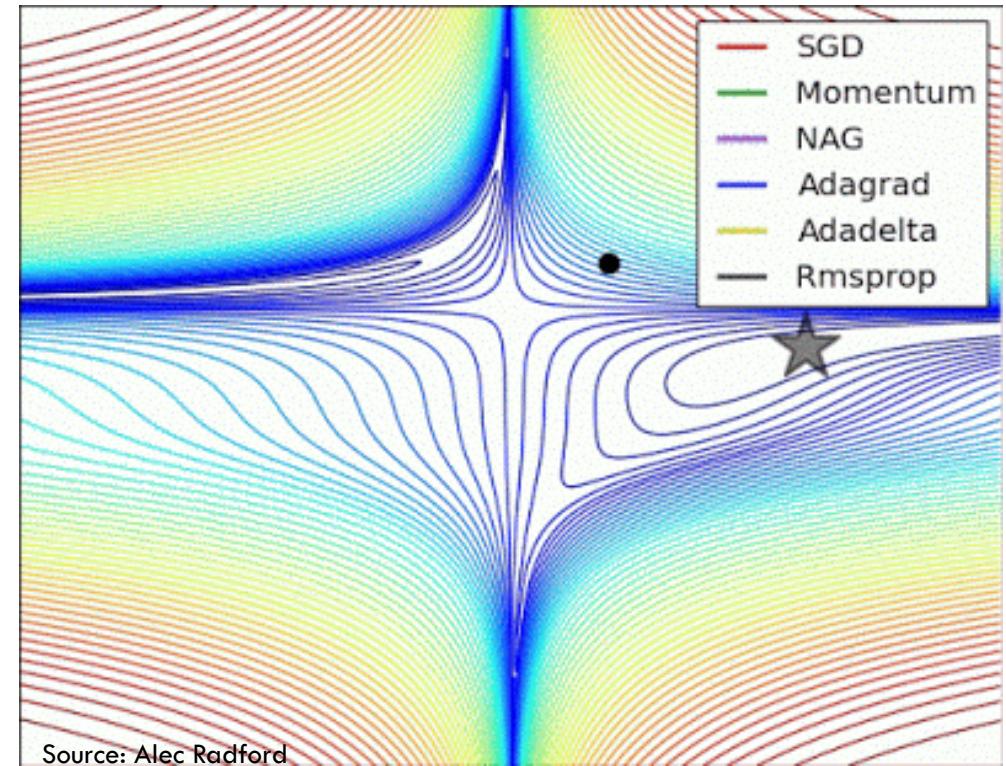
$$w_t \leftarrow w_{t-1} - \eta \frac{g_t}{\sqrt{\epsilon + \sum_{j=1}^{t-1} g_j * g_j}}$$

Init learning rate

Gradient

Smoothing factor

Previous gradients



# SOLVING ISSUE OF DATA/MODEL UNCERTAINTY AND OVERFITTING

Dropouts as fast ensemble/Bayesian

Data augmentation

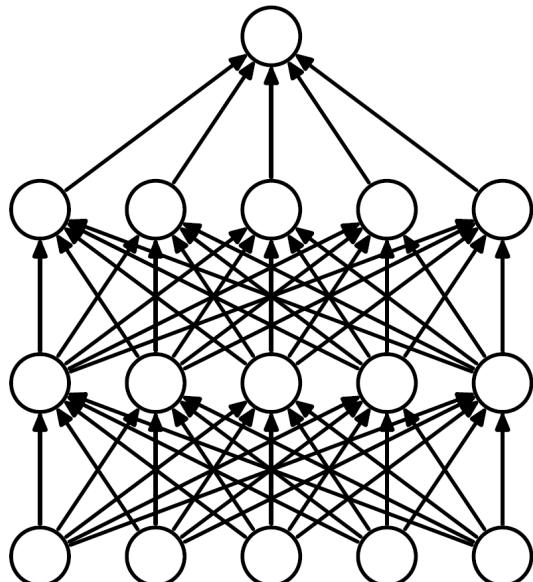
Max-norm: hidden units, channel and path

Dropout is known as the best trick in the past 10 years

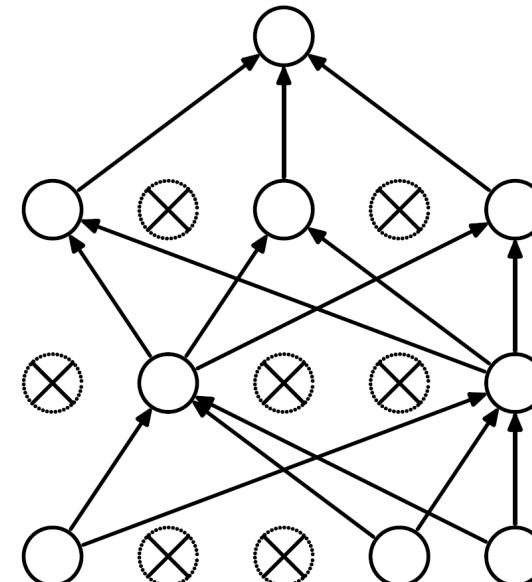
# DROPOUTS

A method to build ensemble of neural nets at zero cost

- For each param update, for each data point, randomly remove part of hidden units

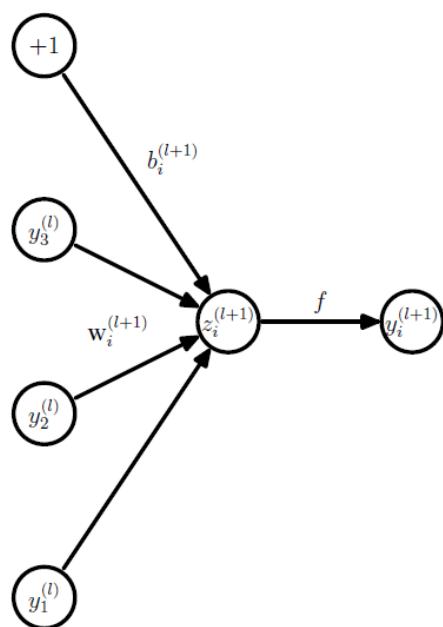


(a) Standard Neural Net

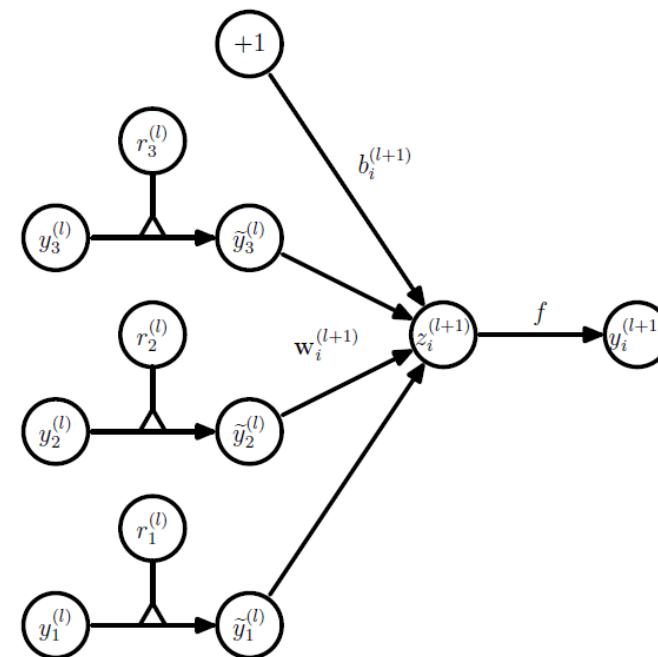


(b) After applying dropout.

# DROPOUTS AS LATENT BINARY VARIABLES



(a) Standard network



(b) Dropout network

# DROPOUTS AS ENSEMBLE

A method to build ensemble of neural nets at zero cost

- There are  $2^K$  such options for  $K$  units
- At the end, adjust the param with the same proportion

Only one model reported, but with the effect of  $n$  models, where  $n$  is number of data points.

Can be extended easily to:

- Drop features
- Drop connections
- Drop any components

# WHY DROPOUTS WORK WITH NEURAL NETS?

Hidden units are feature detectors

Dropouts force them to be less correlated

Learning is stochastic, so you can learn as many models as you like, but all models share parameters, so the statistical strength is maintained.

# DROPOUTS ARE NOT MAGIC

Can be formulated as marginalisation over corrupted features (Wager et al., NIPS 2013; Maaten et al., ICML 2013)

- True features are treated as latent variables

It has been proved (in simple cases) that dropouts are **data-dependent regularisation**

- Standard regularisation is independent of data (think about the prior!)

Dropouts as approximate Bayesian inference (Yarin Gal, Zoubin Ghahramani and others, 2014-2015)

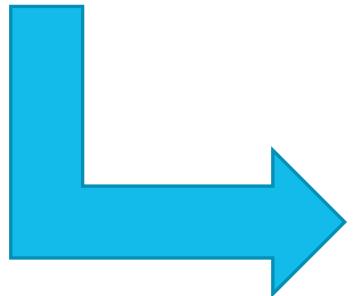
# DATA AUGMENTATION

This is not specific to deep learning

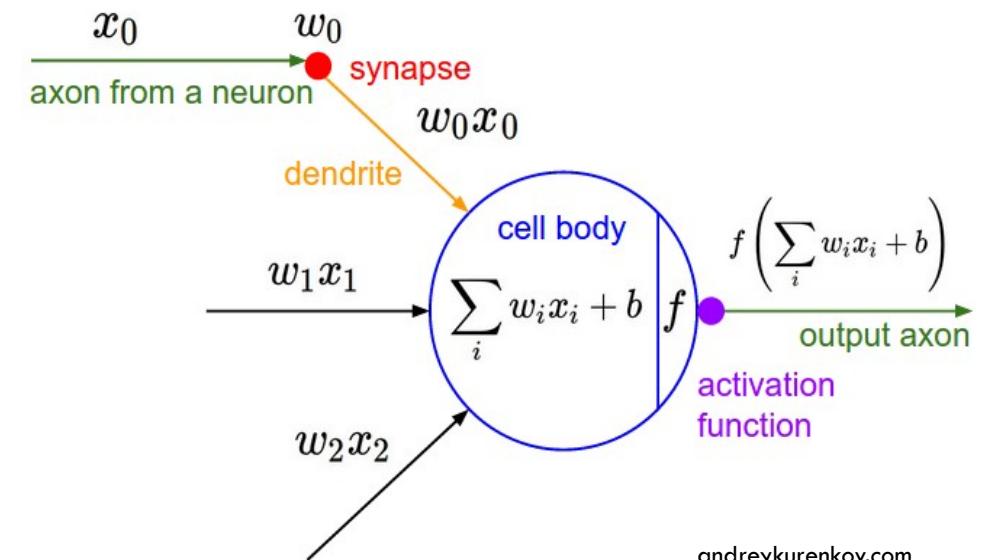
Guess/simulate variance structure → building invariance

Tried methods

- **Vision:** Translation, rotation, stretching, views, lighting condition, occlusion
- **Non-vision:** Local transformations, linear transformations, random projections



# PART I: WRAPPING UP



[andreykurenkov.com](http://andreykurenkov.com)

# TWO MAJOR VIEWS OF “DEPTH” IN DEEP LEARNING

- [2006-2012] Learning layered representations, from raw data to abstracted goal (DBN, DBM, SDAE, GSN).
  - Typically 2-3 layers.
  - High hope for unsupervised learning. A conference set up for this: ICLR, starting in 2013.
  - **We will return in Part III.**
- [1991-1997] & [2012-2016] Learning using multiple steps, from data to goal (LSTM/GRU, NTM/DNC, N2N Mem, HWN, CLN).
  - Reach hundreds if not thousands layers.
  - Learning as credit-assignment.
  - Supervised learning won.
  - Unsupervised learning took a detour (VAE, GAN, NADE/MADE).

# WHEN DOES DEEP LEARNING WORK?

Lots of data (e.g., millions)

Strong, clean training signals (e.g., when human can provide correct labels – cognitive domains).

- Andrew Ng of Baidu: When humans do well within sub-second.

Data structures are well-defined (e.g., image, speech, NLP, video)

Data is compositional (luckily, most data are like this)

The more primitive (raw) the data, the more benefit of using deep learning.

# DEEP LEARNING: MACHINE THAT LEARNS EVERYTHING

End-to-end machine learning – no human involved.

Models are **compositional**, e.g., object is composed of parts.

- → Models can be complex, but building block is simple and universal!
- → Learning is more efficient in multiple steps

Things can be learn: **Feature** | Selectivity | Invariance | Dynamics | Memory  
encoding and forgetting | Attention | Planning

# WHY DEPTH?

*Depth as multiple steps of computation.*

Deep nets are cheap way to achieve similar capacity to wide nets

- Minimum extra parameters – think about multiple orders of derivatives
- Recursion of transformation → easier non-linearity
- Easy to share feature detectors between tasks
  - Vision seems to organise this way.
- Multiple specialised deep nets (columns) are good for complex, loosely decomposable tasks

# DEPTH AS PRIORS

Depth is a hyper-parameter

Deep hidden variables govern prior belief of data structures

Ability to generalise far from training samples

The interplay between distributed representation and hierarchy

- Bengio's theory: (nearly independent) factors of variation in a generative manner (e.g., age, gender, glass, cloth colour). Can learn a factor from just few examples.
- Easy to deal with multimodality with diverse variance structures

# DEPTH CAN BE THEORETICALLY CHARACTERISED

Deep narrow Boltzmann machines are universal approximator (Montúfar, 2014).

Deep narrow belief networks are universal approximator (Sutskever and Hinton, 2008; Le Roux and Bengio, 2008, 2010; Montufar and Ay, 2011).

Modern CNN are essentially hierarchy of radial basis functions (RBFs) (Poggio, 2015).

FNN as recursive GLMs.

FNN with rectified linear units learn polynomials with depth as degree (Choromanska et al, 2015)

# IN CASE YOU FORGOT, DEEP LEARNING MODELS ARE COMBINATIONS OF

Three models:

- FFN (layered vectors)
- RNN (recurrence for sequences)
- CNN (translation invariance + pooling)

→ Architecture engineering!

A bag of tricks:

- dropout
- piece-wise linear units (i.e., ReLU)
- adaptive stochastic gradient descent
- data augmentation
- skip-connections

END OF PART I

