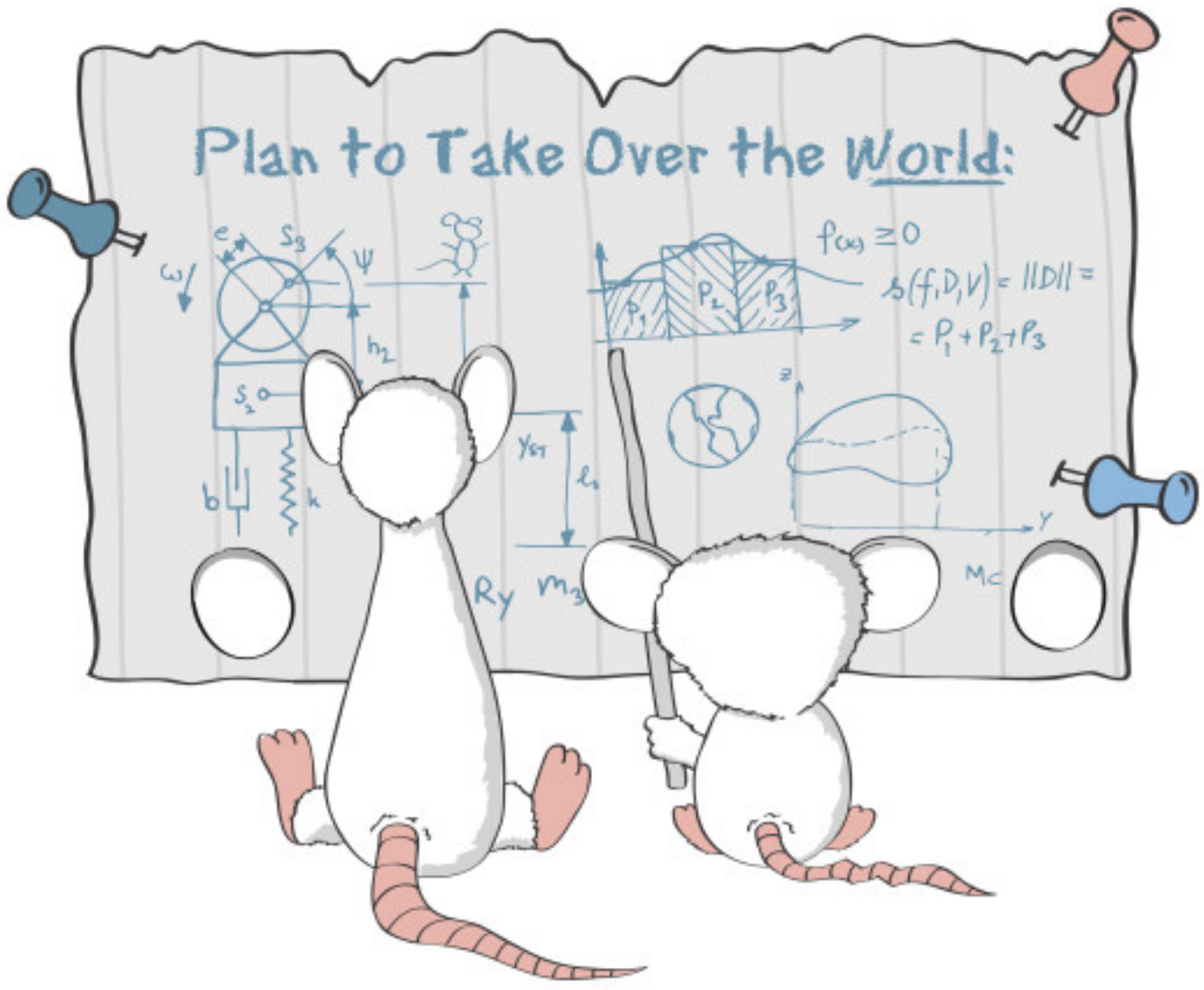


Lecture #5

F5611 Machine Learning for Astronomers
by Martin Topinka

https://github.com/toastmaker/f5611-ML4A

*Lecture by **Ashish Mahabal** (Caltech)*

15 Dec 2020

Classification of transients at Zwicky Transient Factory
&
Hands-On-Session

Let's get ready (colab)

Python modules python 3
tensorflow
numpy
matplotlib
scikit-learn

Additional Resources

http://cs231n.stanford.edu

Outline

- Introduction to **N**eural **N**etwork: the idea behind, SGD, back-propagation, vanishing gradient, fighting over-fitting)

- **C**onvolutional **N**eural **N**etwork — next regular lecture by Matej!

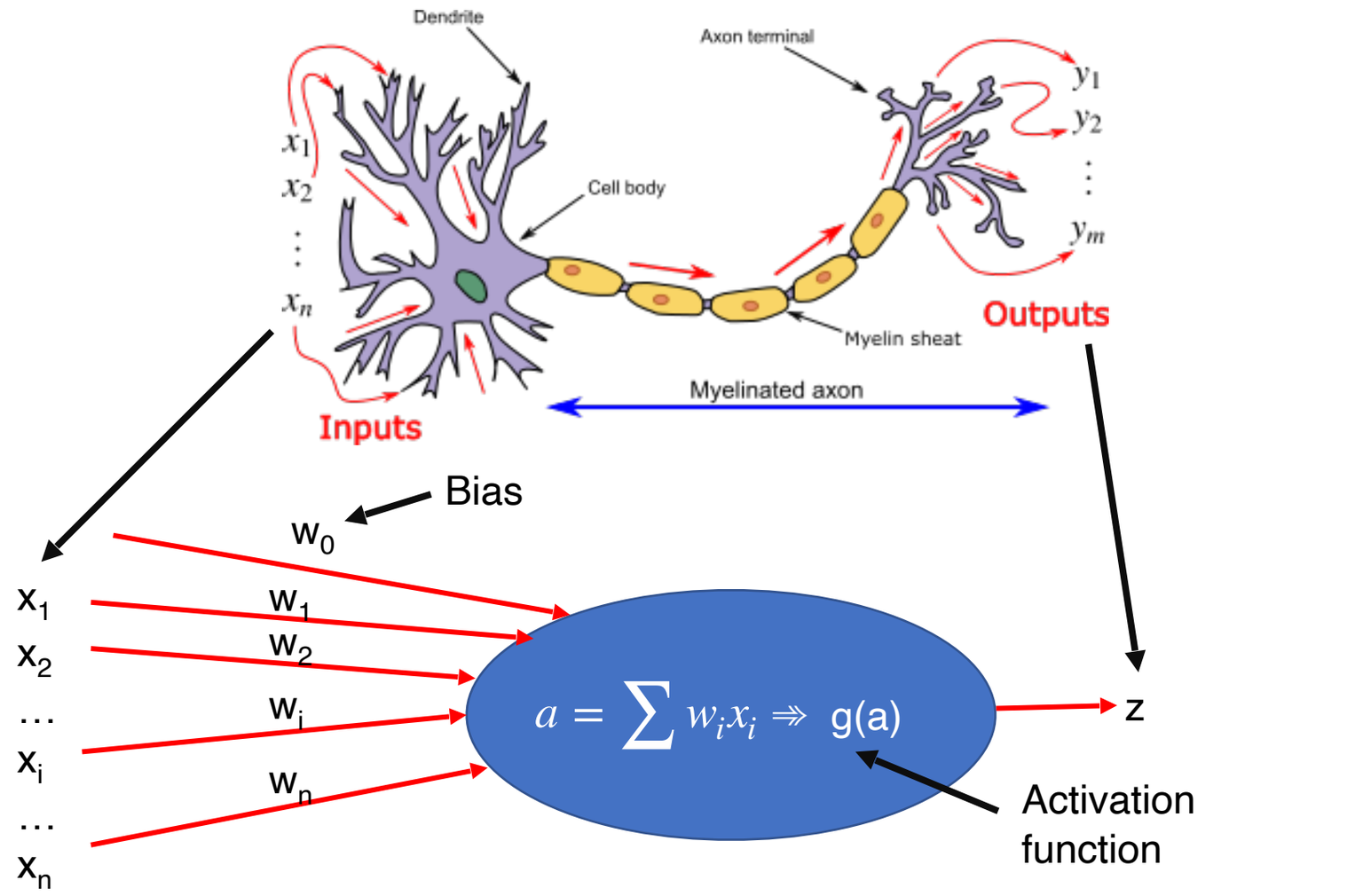
- Encoder-decoders, **A**uto-**E**ncoders, **V**ariational **A**uto-**E**ncoders

- **R**ecurrent **N**eural **N**etworks, **G**enerative **A**dversarial **N**etworks

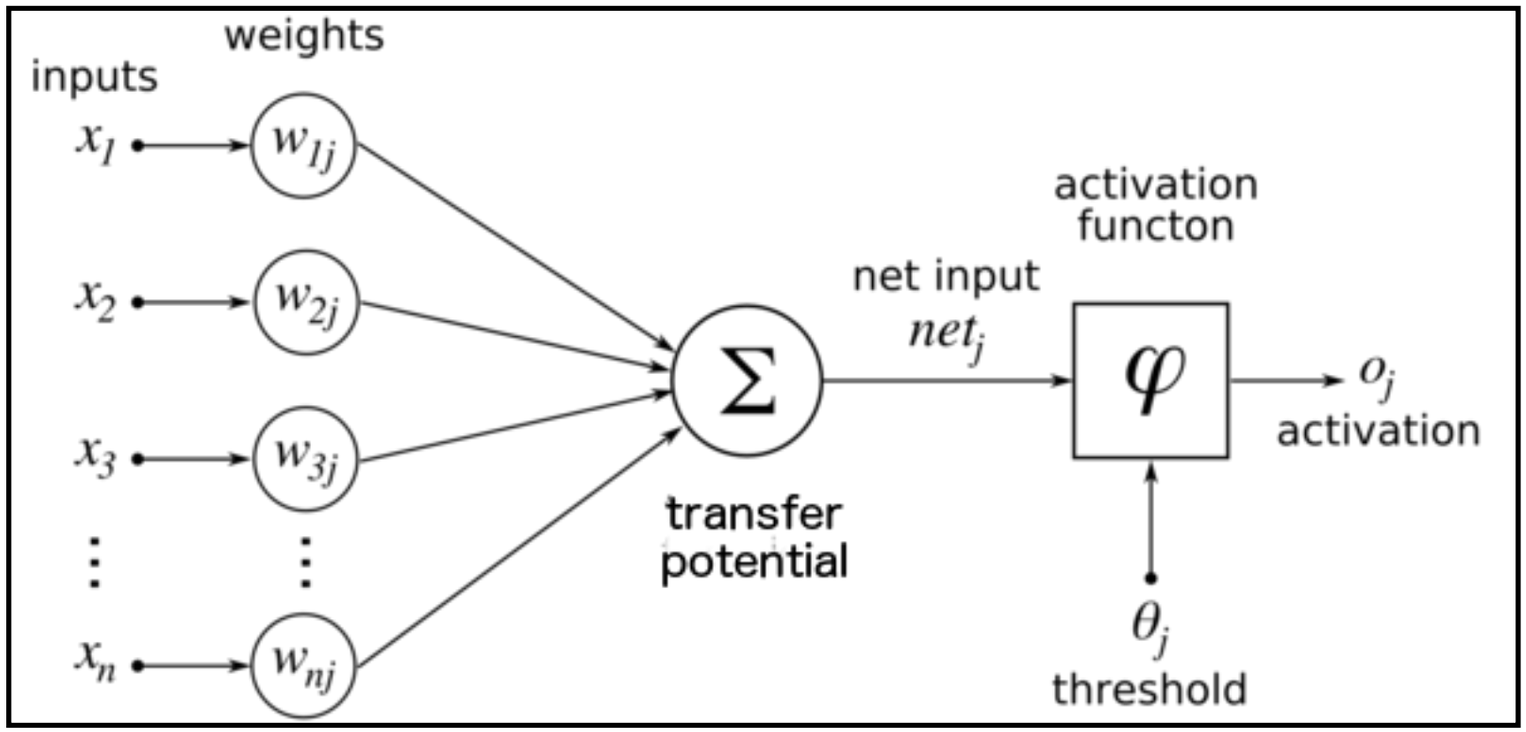
- TensorFlow/Keras

- Hands-on session: NN star/quasar classification, NN Fourier Transform, ConvNN source finding/denoising

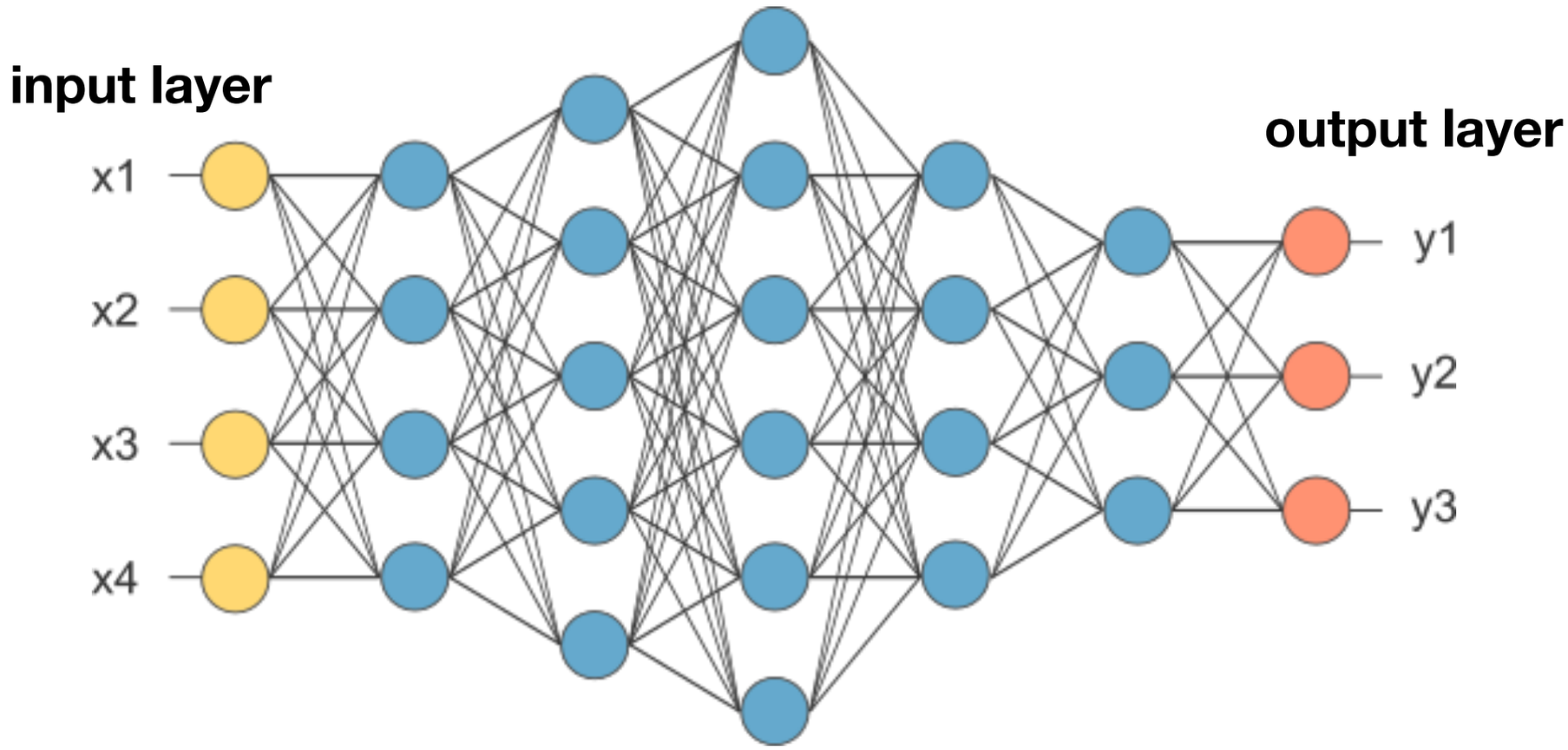
Boom of species 543 million years ago due to enhanced vision



g = identity or sigmoid
Linear/logistic regression



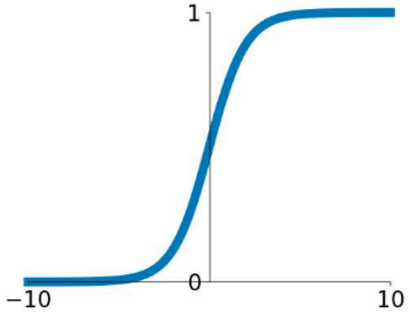
hidden layers



Activation functions

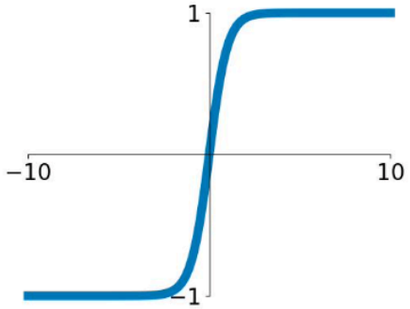
Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



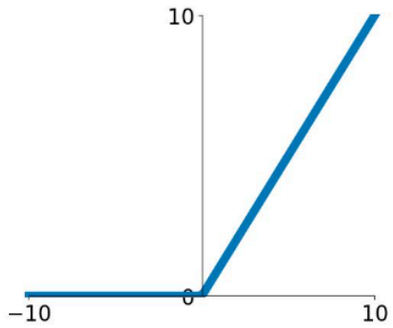
tanh

$$\tanh(x)$$



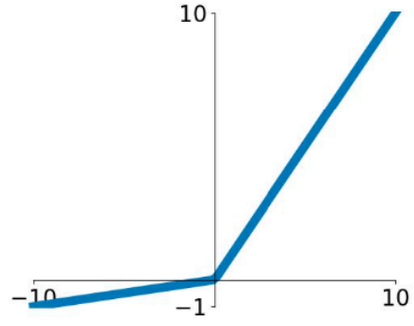
ReLU

$$\max(0, x)$$



Leaky ReLU

$$\max(0.1x, x)$$

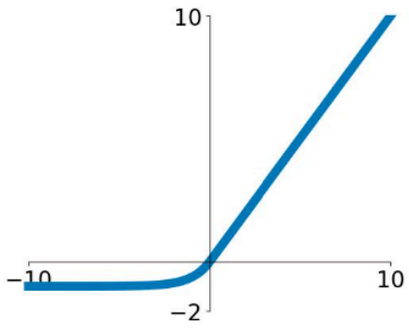


Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

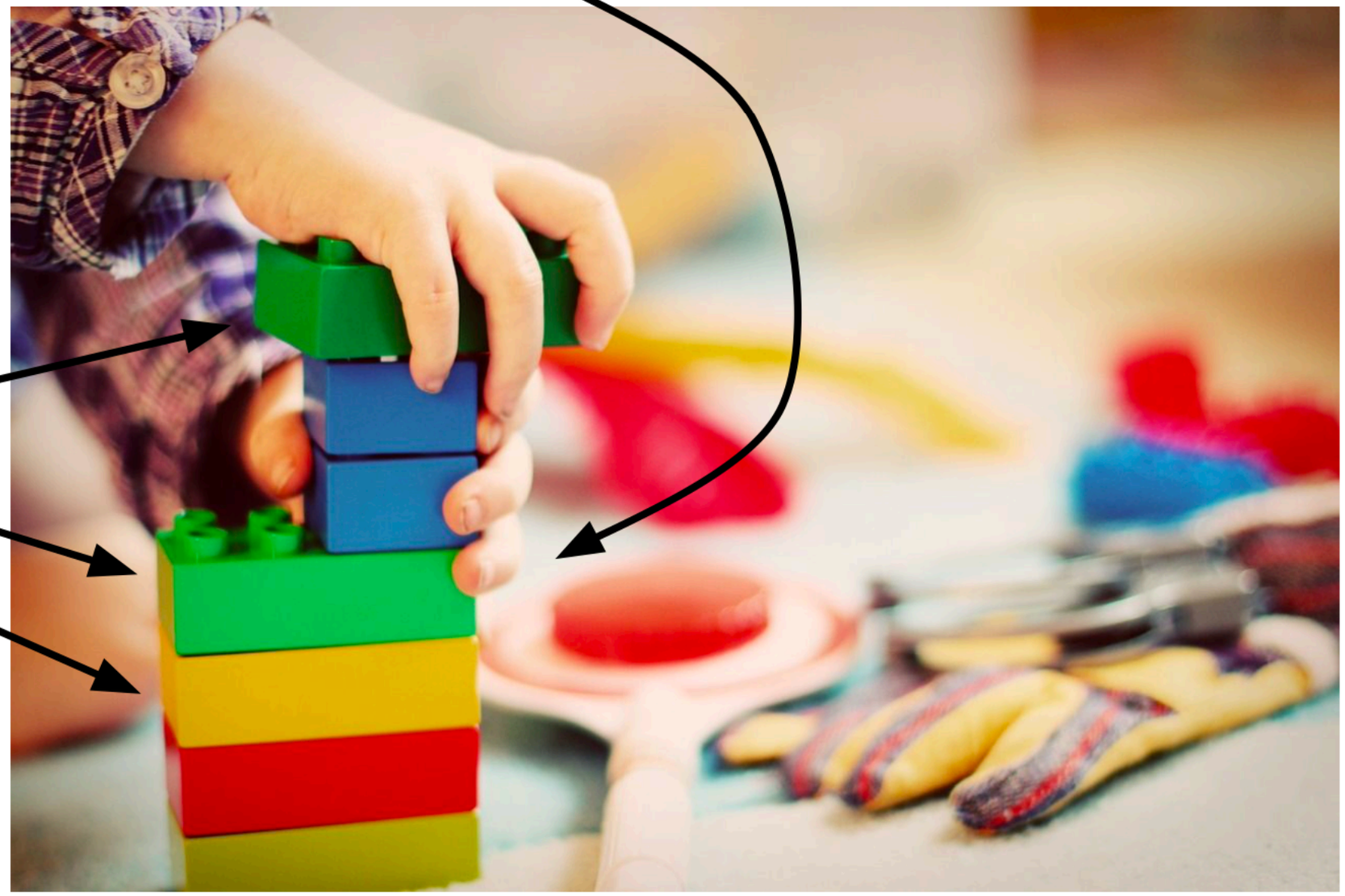
ELU

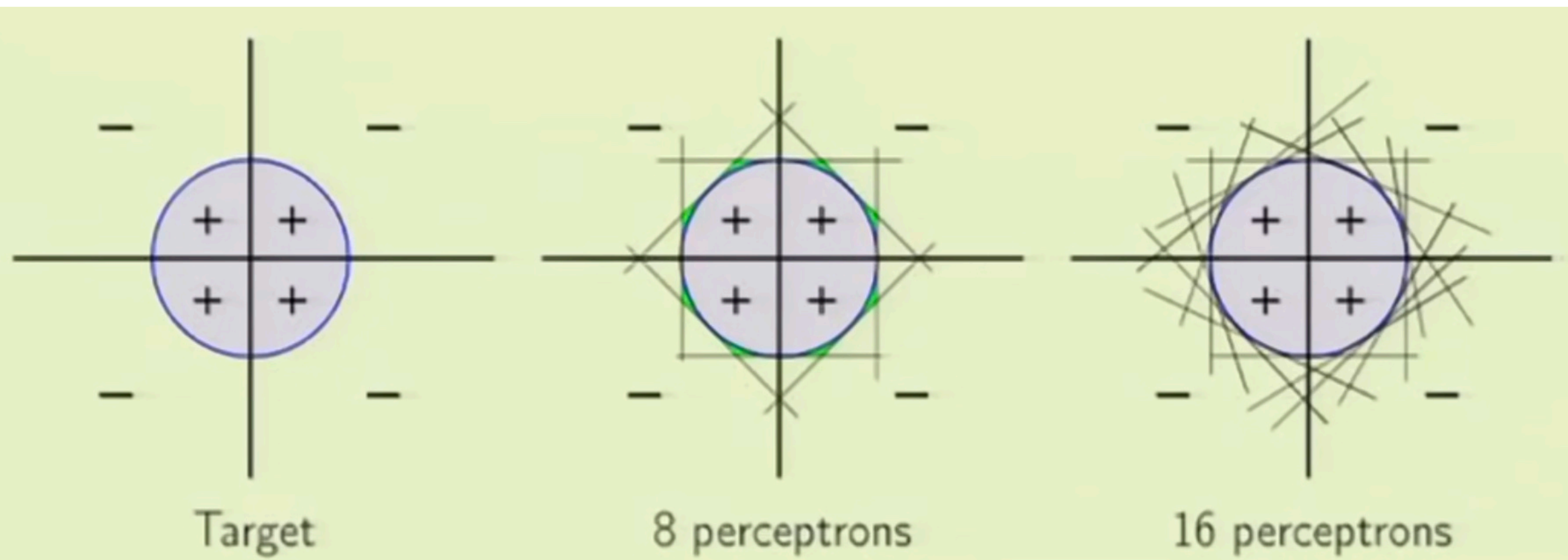
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



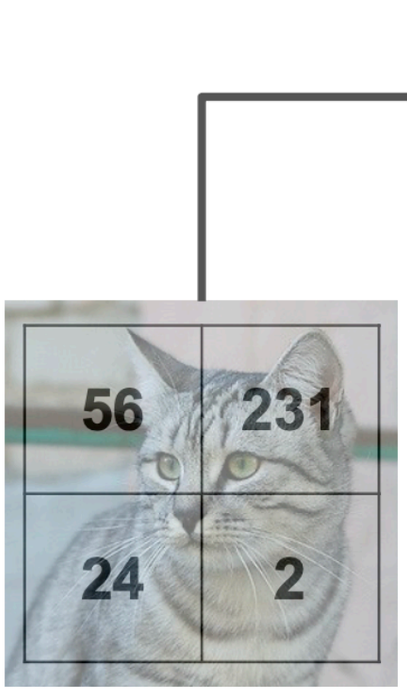
Neural Network

Linear classifiers

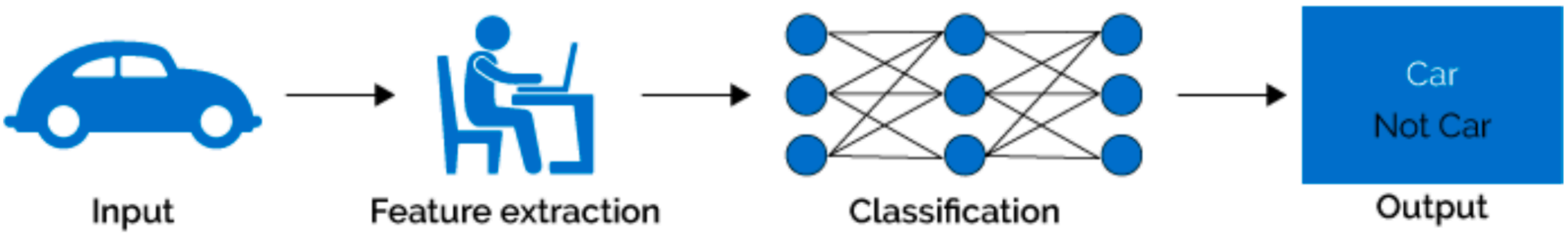



Target
8 perceptrons
16 perceptrons

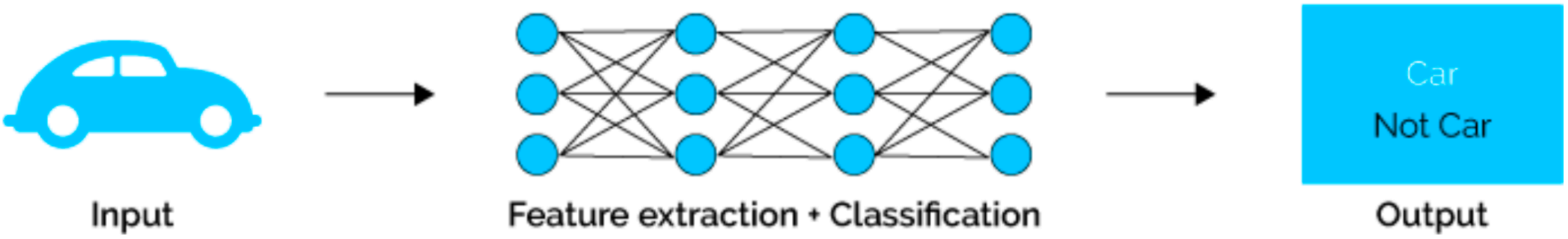
Example with an image with 4 pixels, and 3 classes (cat/dog/ship)



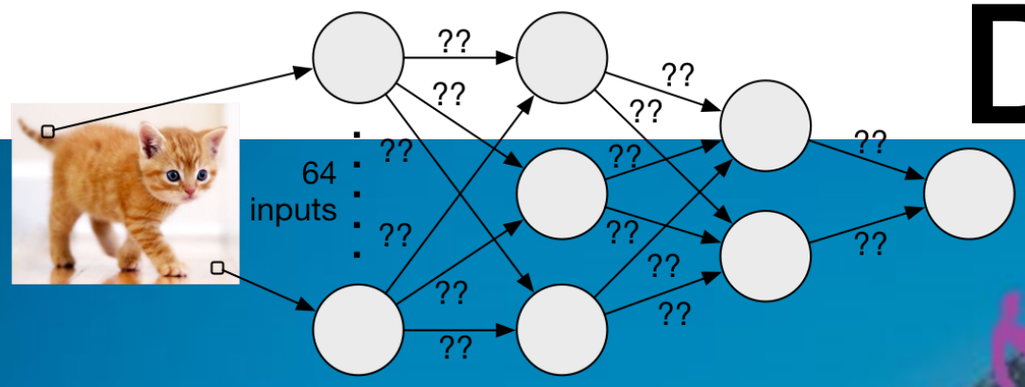
Machine Learning



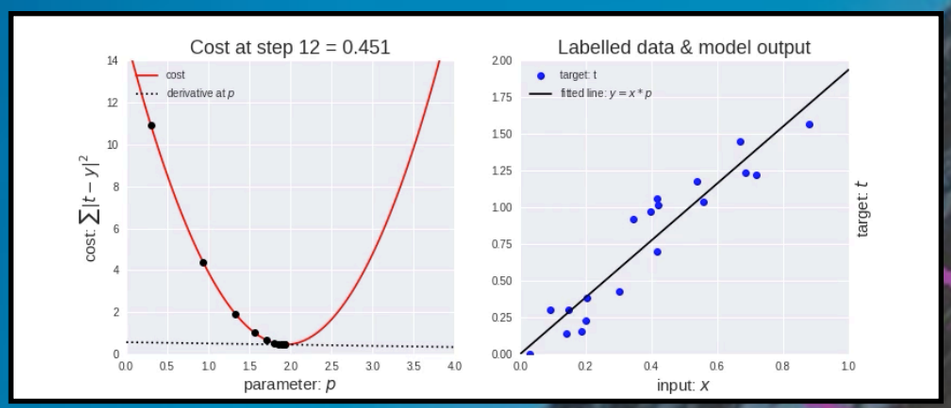
Deep Learning



(Stochastic) Gradient Descent



$$w = w - \alpha \nabla_w J(w)$$



Stochastic Gradient Descent (SGD)

$$L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(x_i, y_i, W) + \lambda R(W)$$

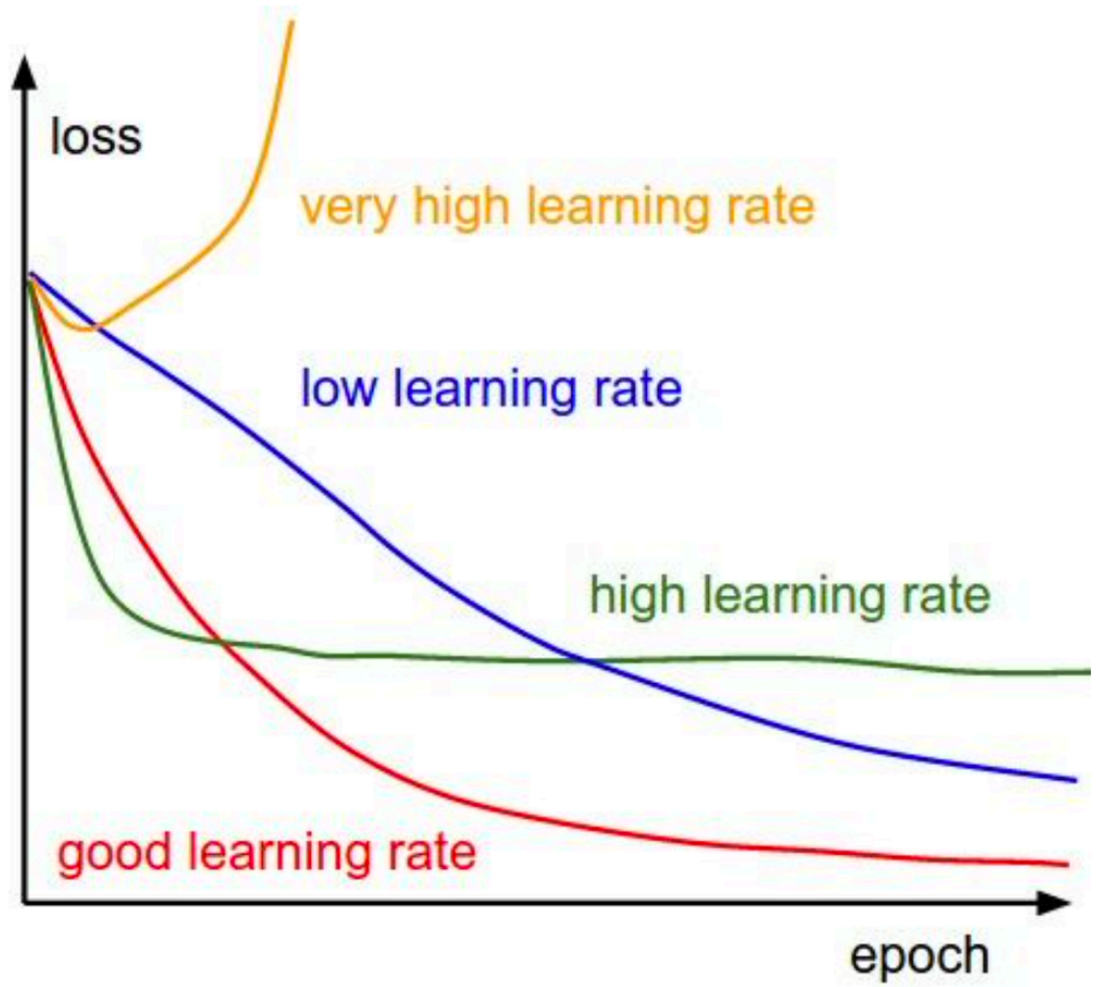
$$\nabla_W L(W) = \frac{1}{N}\sum_{i=1}^{N} \nabla_W L_i(x_i, y_i, W) + \lambda \nabla_W R(W)$$

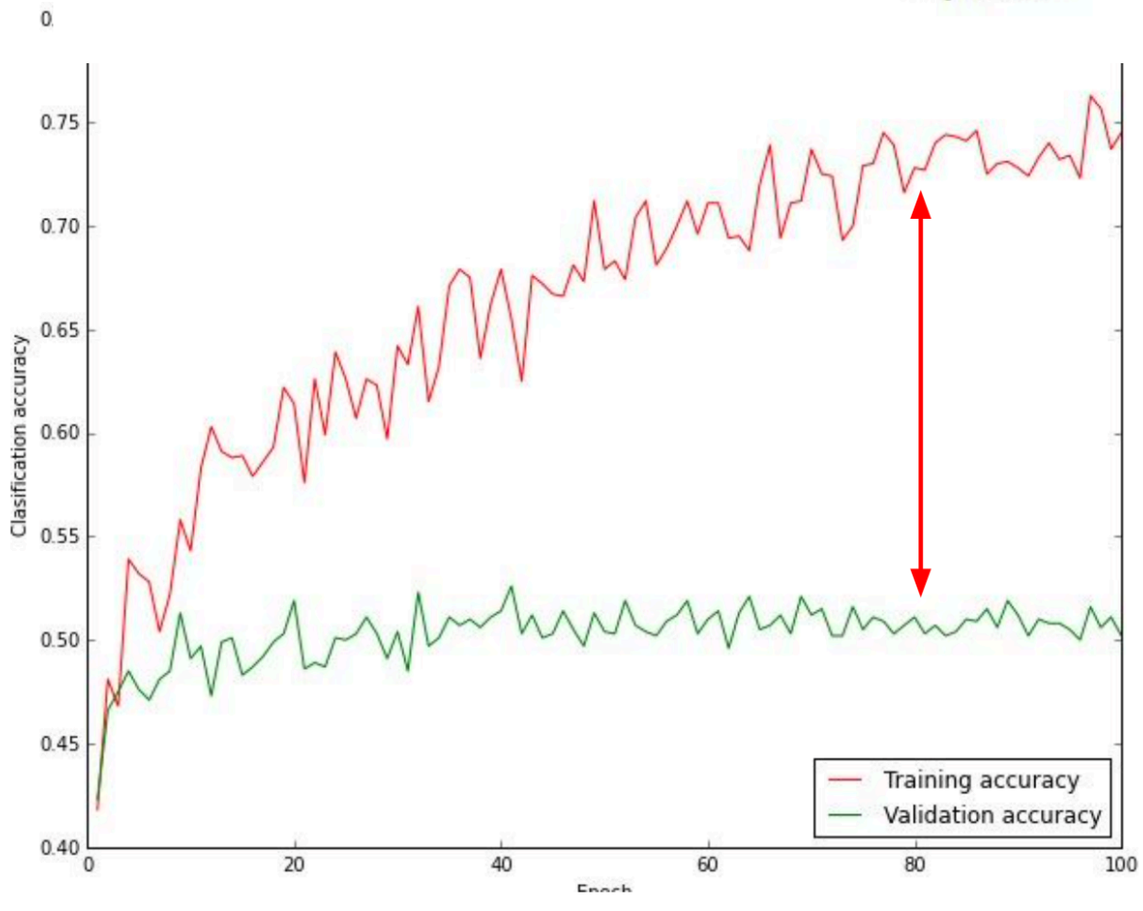
Full sum expensive when N is large!

Approximate sum using a **minibatch** of examples
32 / 64 / 128 common

```
# Vanilla Minibatch Gradient Descent

while True:
  data_batch = sample_training_data(data, 256) # sample 256 examples
  weights_grad = evaluate_gradient(loss_fun, data_batch, weights)
  weights += - step_size * weights_grad # perform parameter update
```





big gap = overfitting

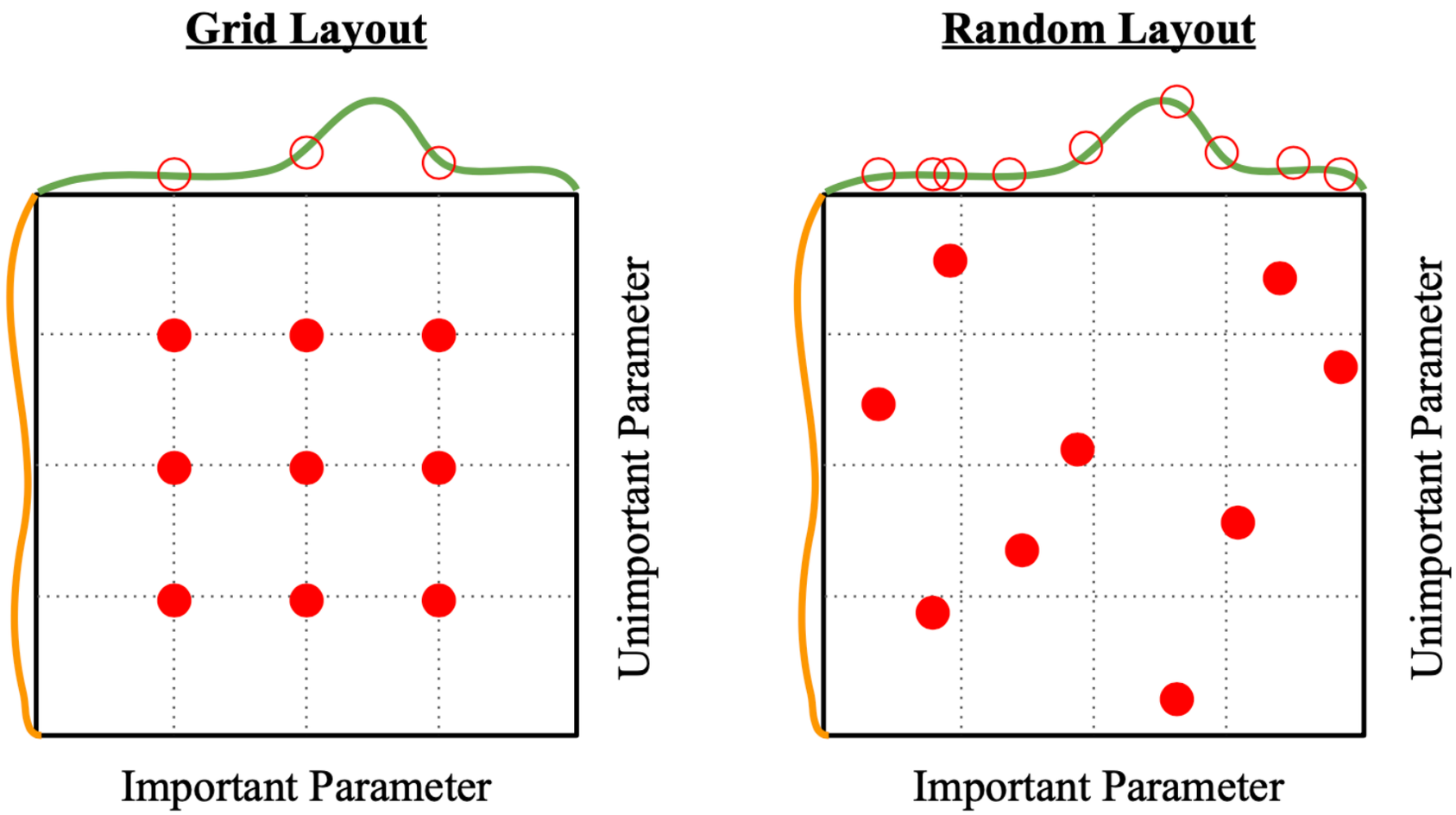
=> increase regularization strength?

no gap

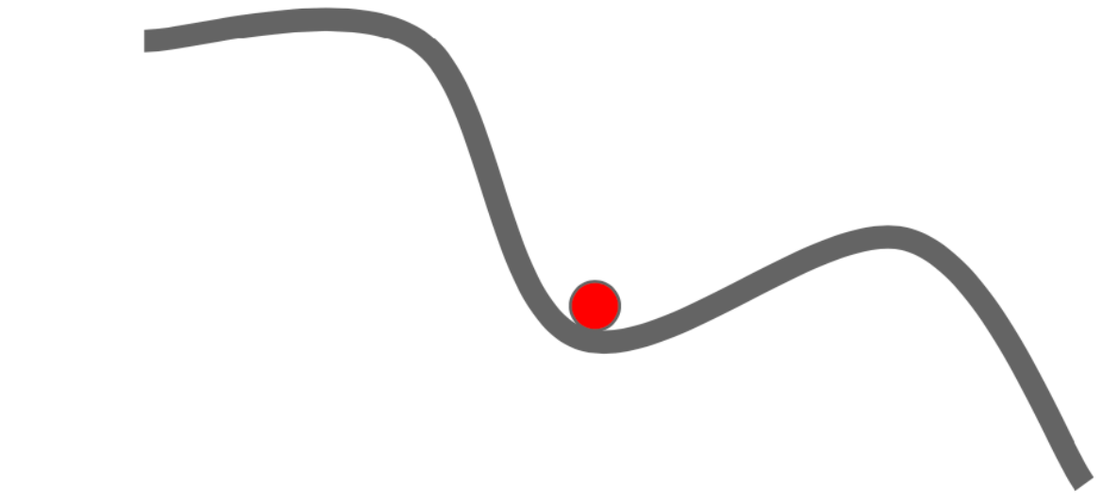
=> increase model capacity?

Random Search vs. Grid Search

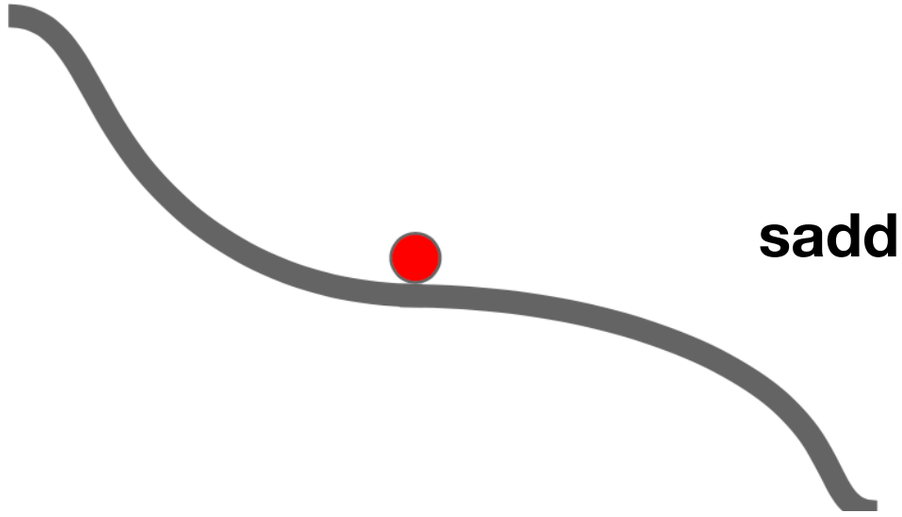
Random Search for Hyper-Parameter Optimization
Bergstra and Bengio, 2012



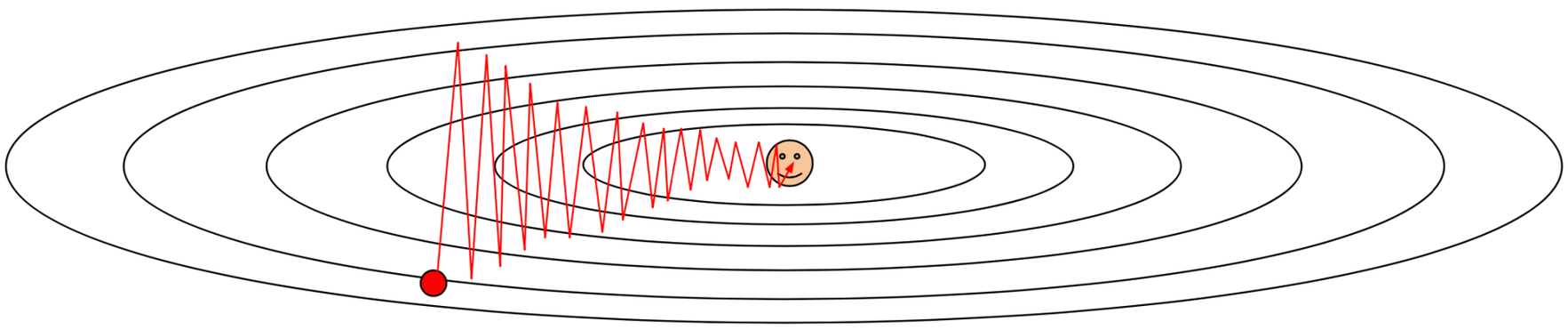
Problems with Gradient Descent



local minimum (rare in high dims)



saddle point (common in high dims)



loss changes quickly in one dim but slowly in other

SGD

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

```
while True:
  dx = compute_gradient(x)
  x += learning_rate * dx
```

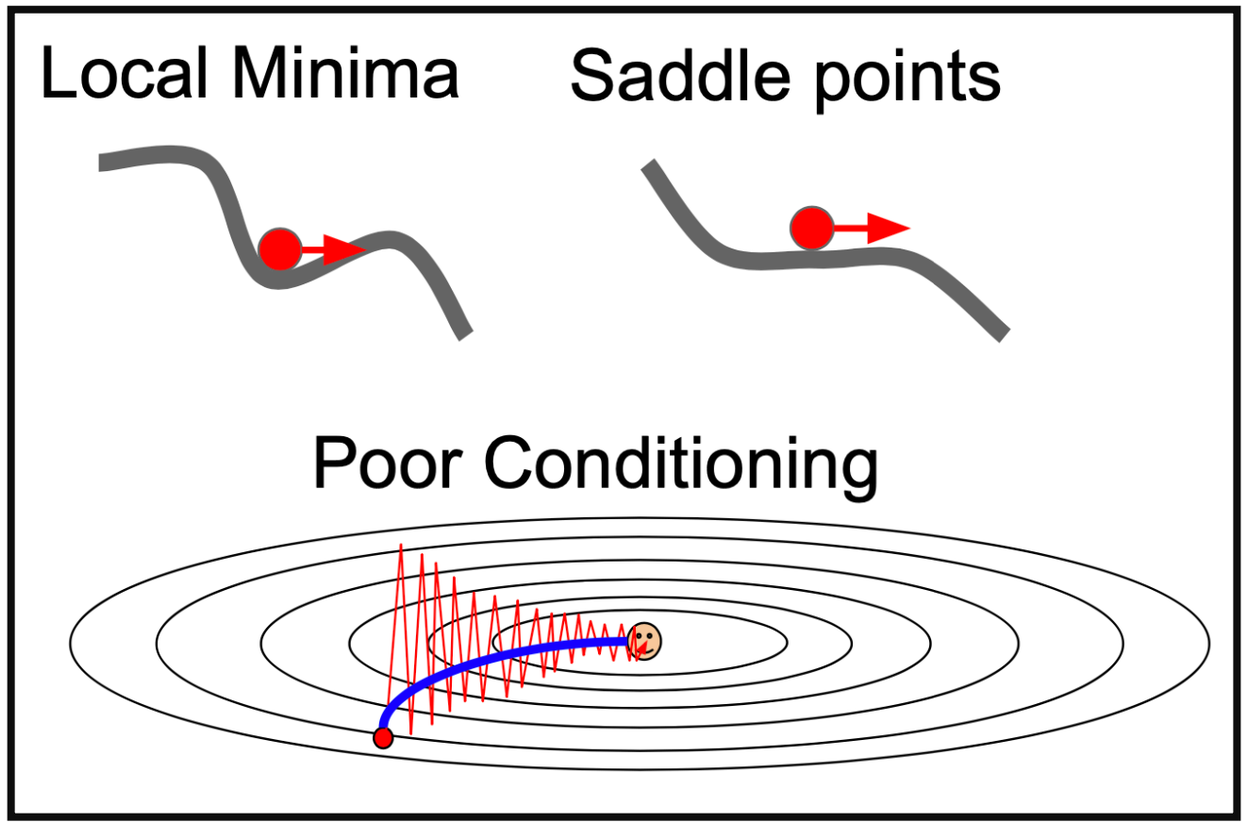
SGD+Momentum

$$v_{t+1} = \rho v_t + \nabla f(x_t)$$

$$x_{t+1} = x_t - \alpha v_{t+1}$$

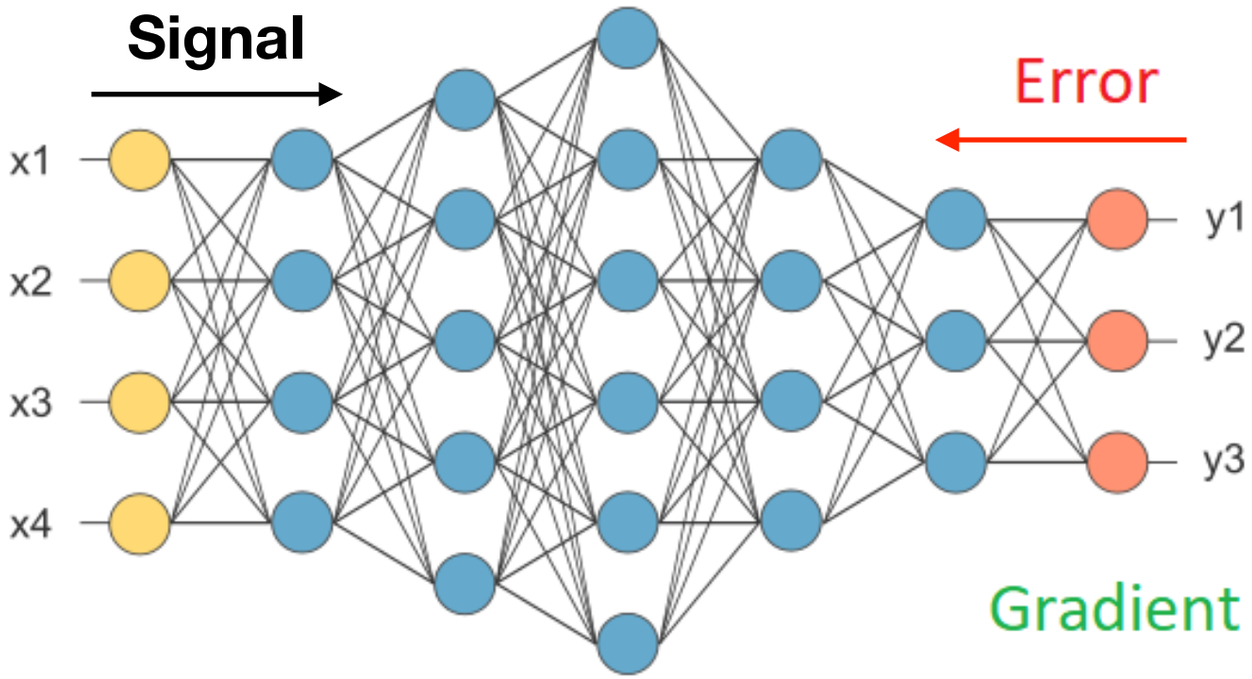
```
vx = 0
while True:
  dx = compute_gradient(x)
  vx = rho * vx + dx
  x += learning_rate * vx
```

- Build up “velocity” as a running mean of gradients
- Rho gives “friction”; typically rho=0.9 or 0.99



Back-propagation

Forward-propagation: get **estimates** during training and **predictions** then
Back-propagation: apply chain rule to gradient of loss function to **adjust weights/biases**



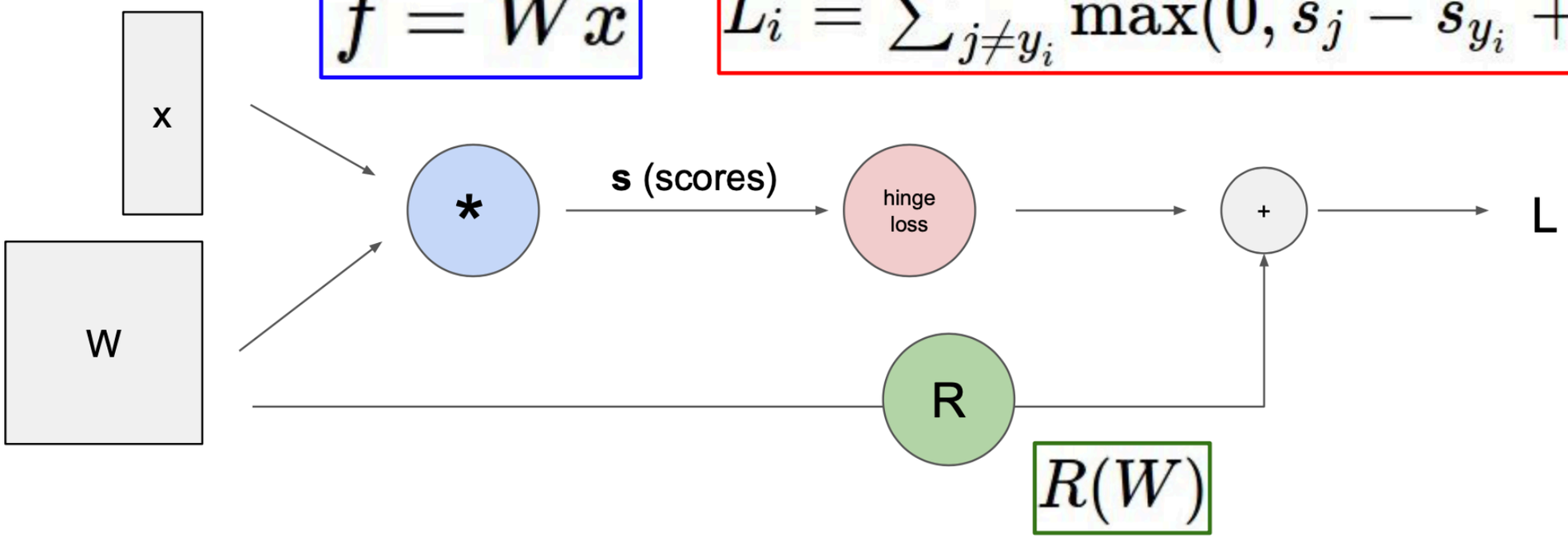
Remedies against vanishing gradient:

- ReLU
- Re-normalisation

Computational graphs

$$f = Wx$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$



Backpropagation: a simple example

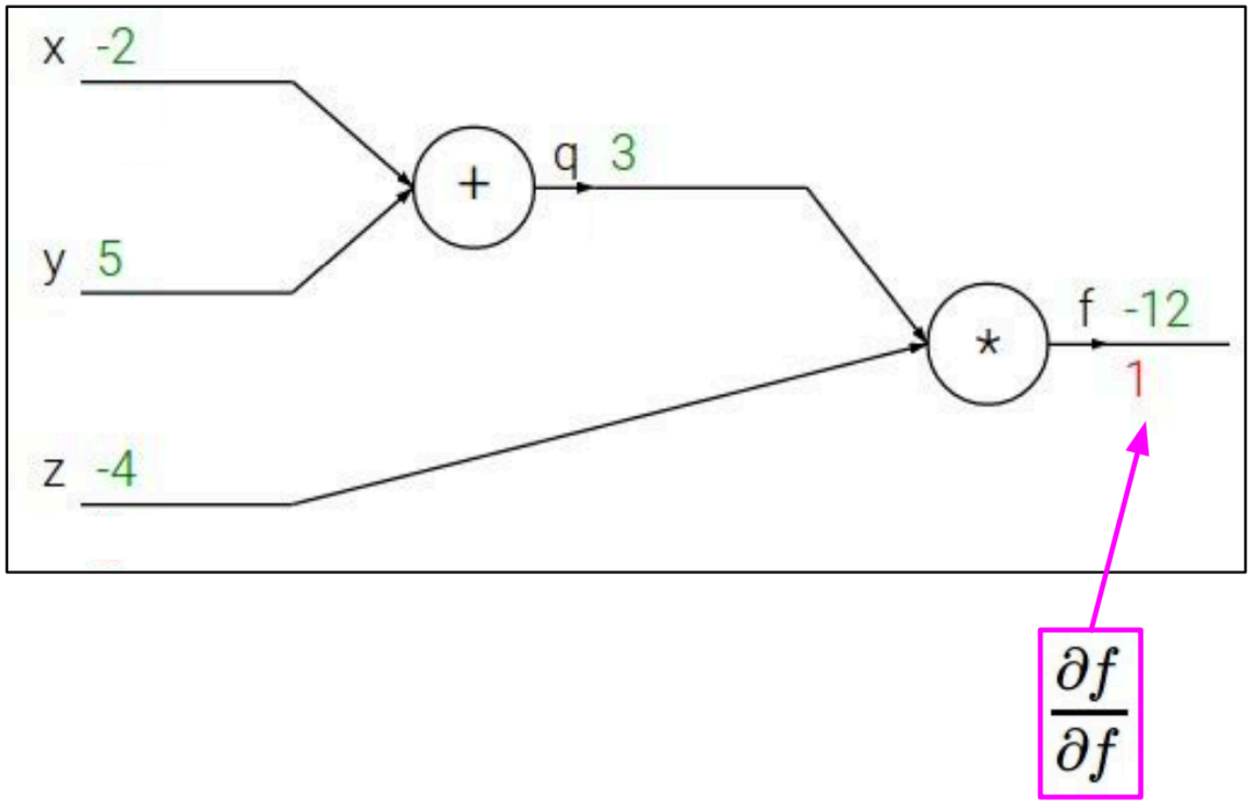
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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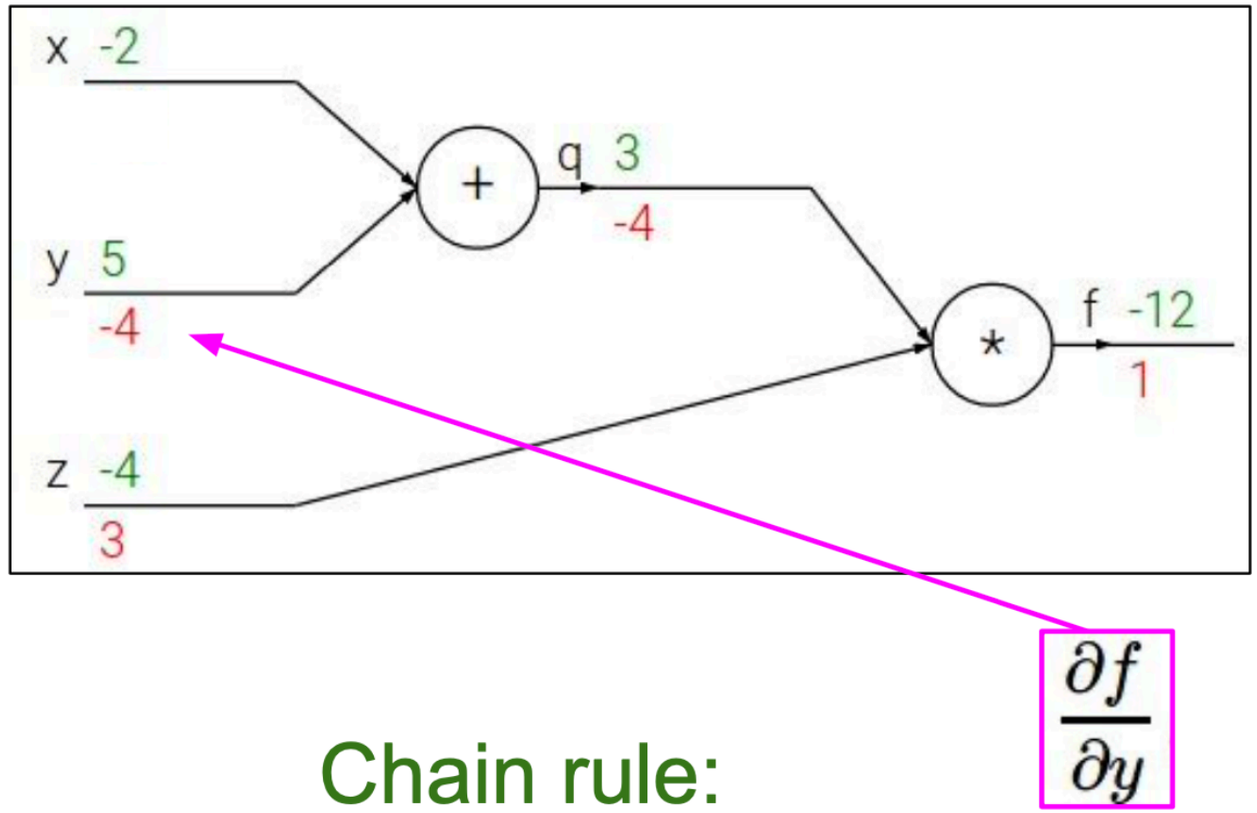
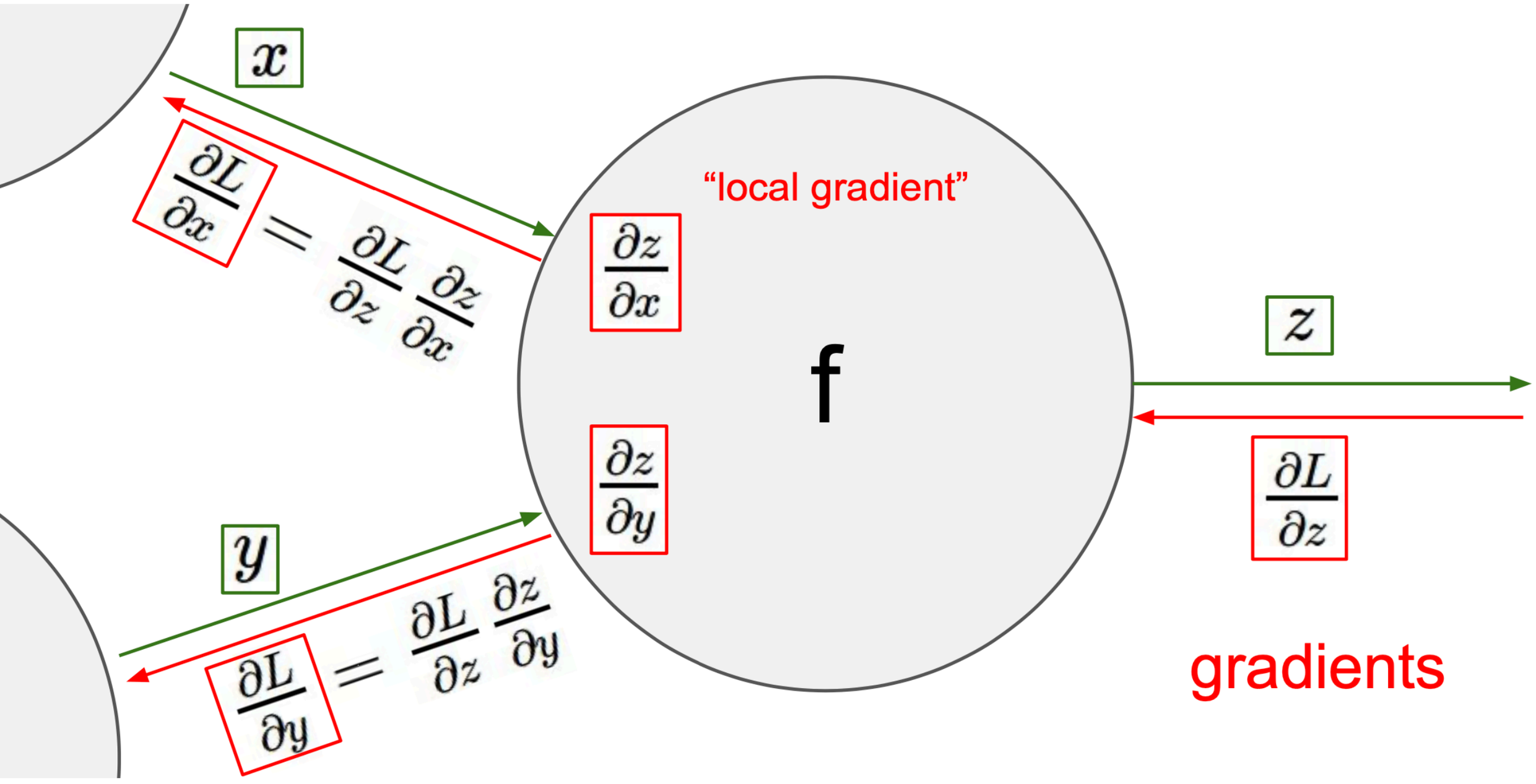
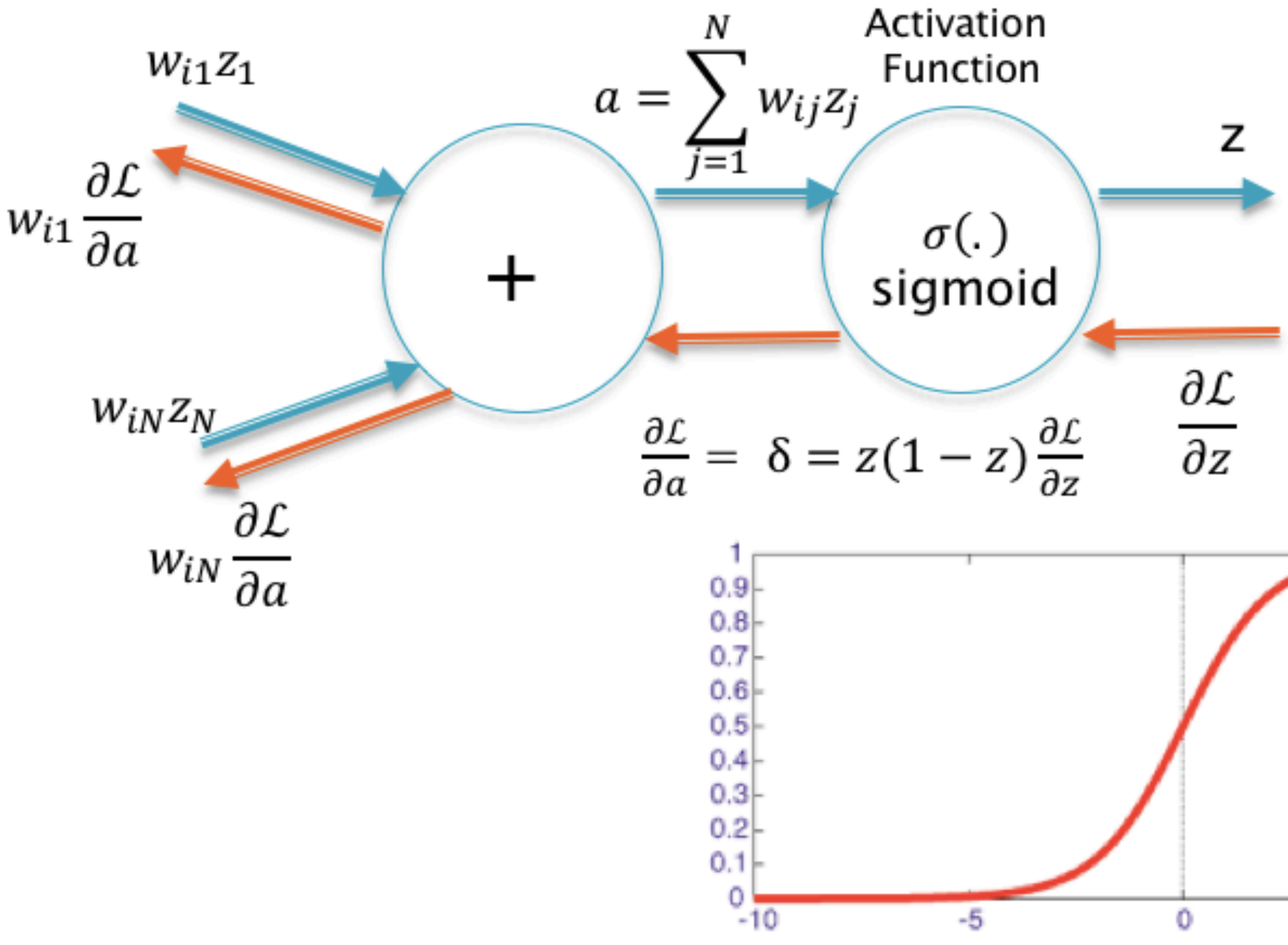
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



Chain rule:

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial y}$$


x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"local gradient"
$\frac{\partial z}{\partial x}$
f
$\frac{\partial z}{\partial y}$
z
$\frac{\partial L}{\partial z}$
y
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
gradients


$w_{i1}z_1$
$w_{i1}\frac{\partial \mathcal{L}}{\partial a}$
$w_{iN}z_N$
$w_{iN}\frac{\partial \mathcal{L}}{\partial a}$
+
$a = \sum_{j=1}^{N} w_{ij}z_j$
Activation Function
$\sigma(.)$ sigmoid
z
$\frac{\partial \mathcal{L}}{\partial z}$
$\frac{\partial \mathcal{L}}{\partial a} = \delta = z(1-z)\frac{\partial \mathcal{L}}{\partial z}$
$\frac{1}{1+e^{-x}}$
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-10
-5
0
5
10

$$\frac{\partial E_p}{\partial w_{ji}} = \frac{\partial E_p}{\partial o_{pj}} \frac{\partial o_{pj}}{\partial w_{ji}}$$

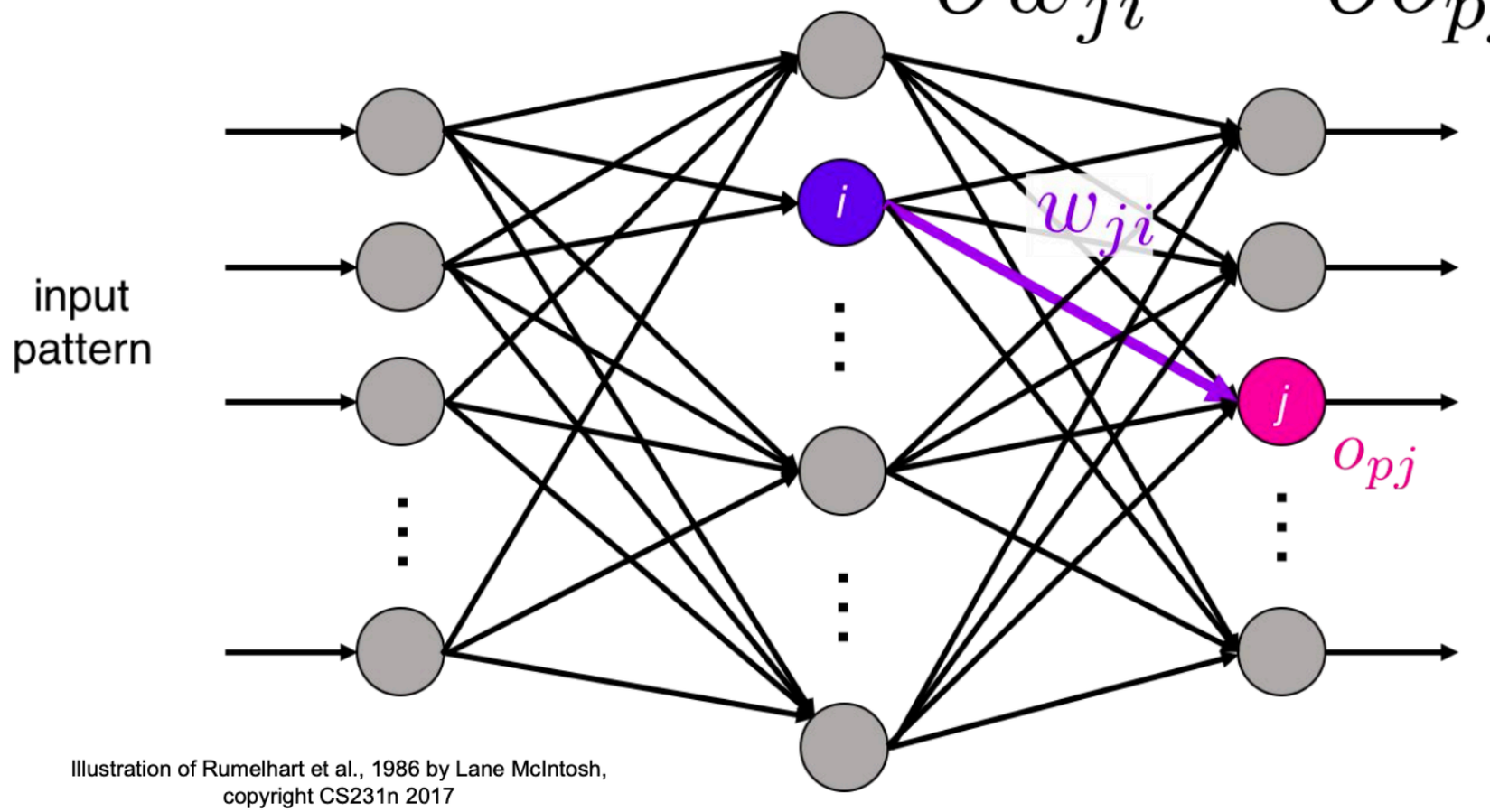
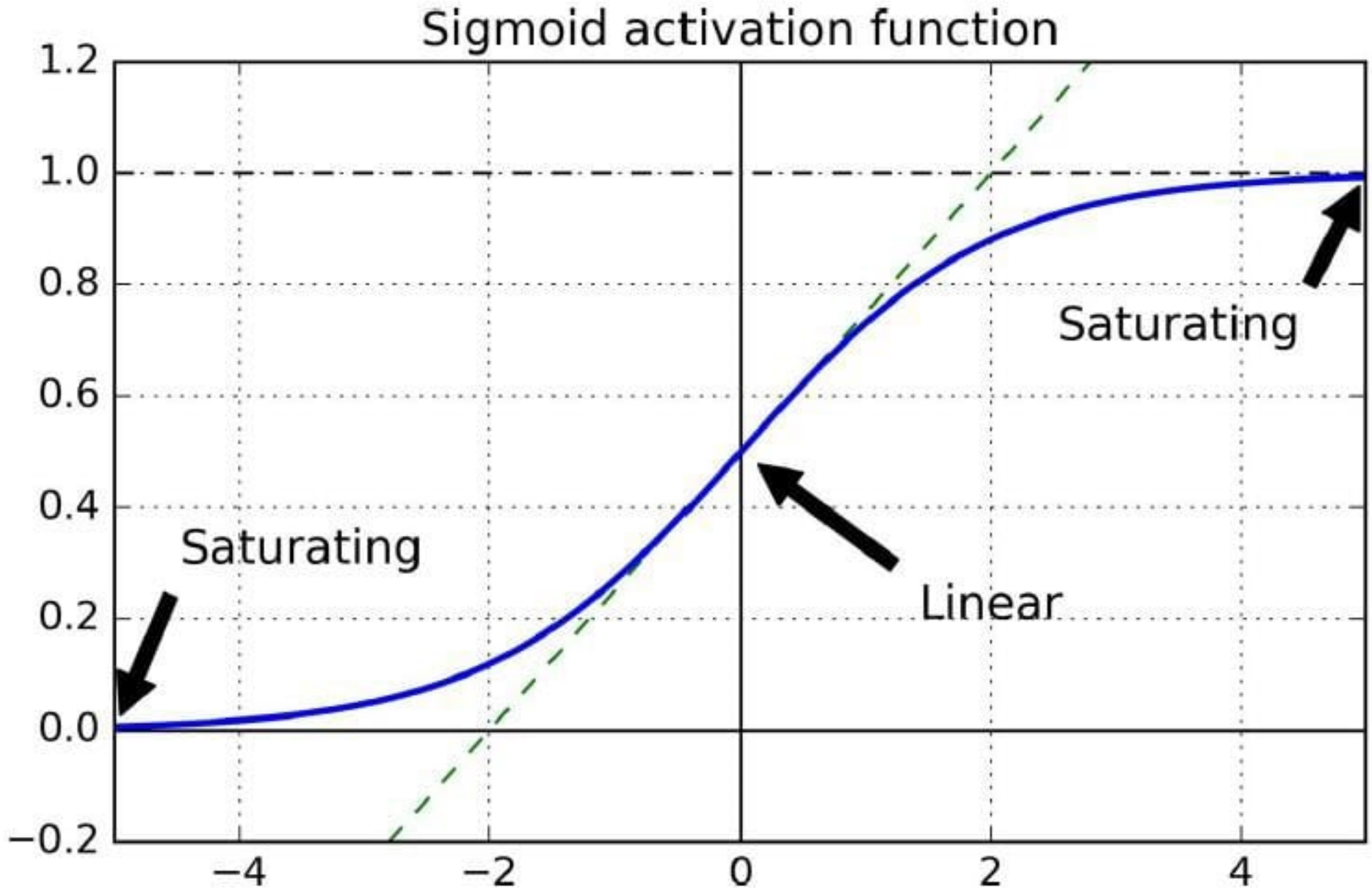
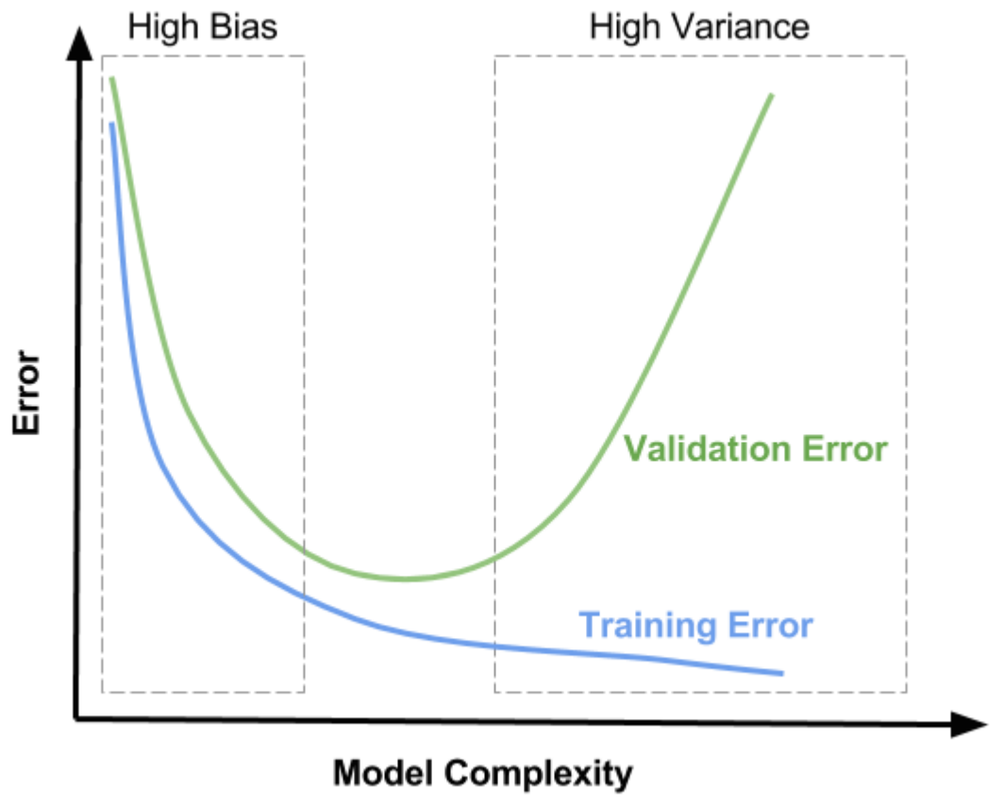


Illustration of Rumelhart et al., 1986 by Lane McIntosh,
copyright CS231n 2017


Sigmoid activation function
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−4
−2
0
2
4
Saturating
Saturating
Linear

Fighting over-fitting

- Regularisation
- Dropout
- Early stopping
- Simplify the architecture

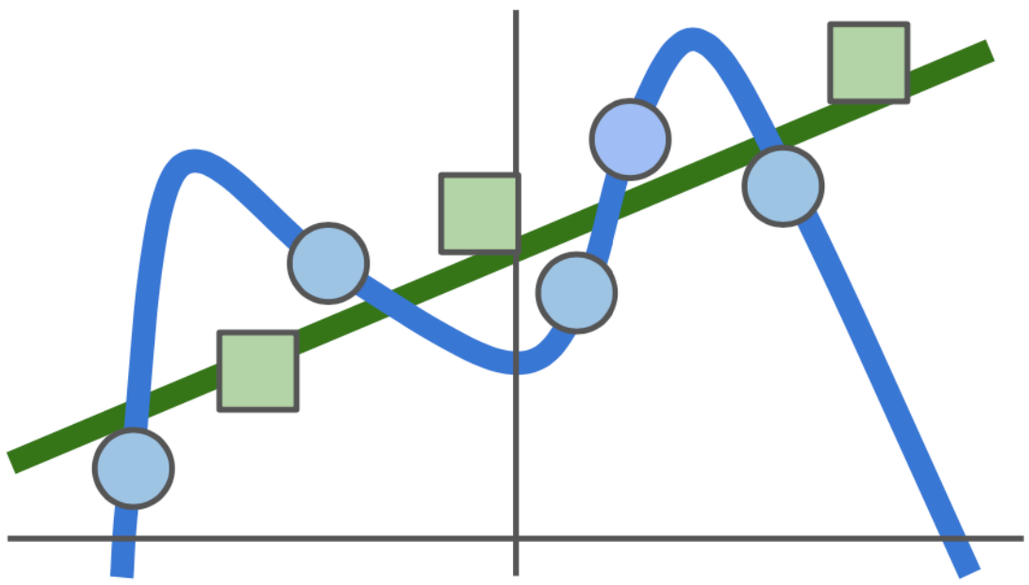


- More data (even if you have to make it up: translate, rotate, flip, crop, lighten/darken, add noise)

# of weights ~ VC dimension ~ # degrees of freedom

$$L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i) + \lambda R(W)$$

Data loss: Model predictions should match training data



Regularization: Model should be “simple”, so it works on test data

Occam’s Razor:
“Among competing hypotheses, the simplest is the best”
William of Ockham, 1285 - 1347

Regularization

λ = regularization strength (hyperparameter)

$$L = \frac{1}{N}\sum_{i=1}^{N}\sum_{j\neq y_i}\max(0, f(x_i; W)_j - f(x_i; W)_{y_i} + 1) + \lambda R(W)$$

In common use:

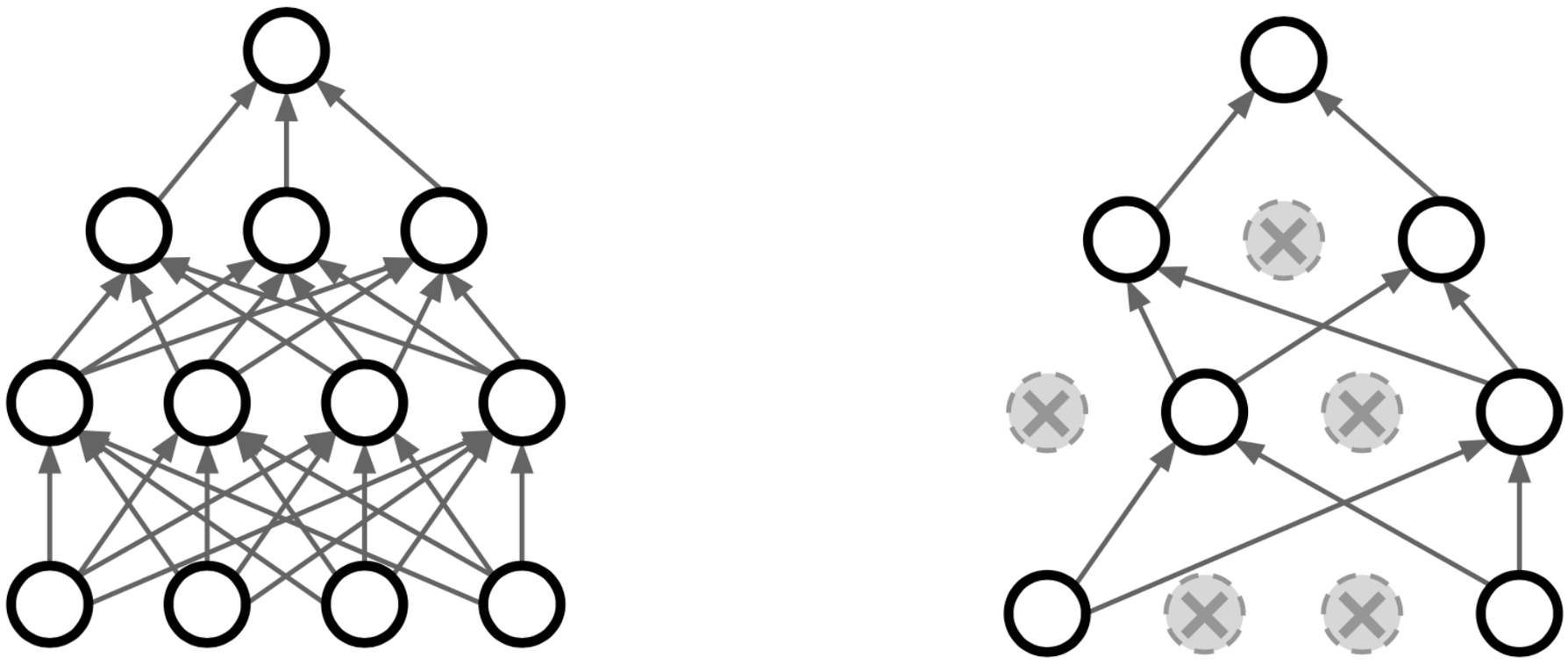
L2 regularization $R(W) = \sum_k \sum_l W_{k,l}^2$ "weight decay"

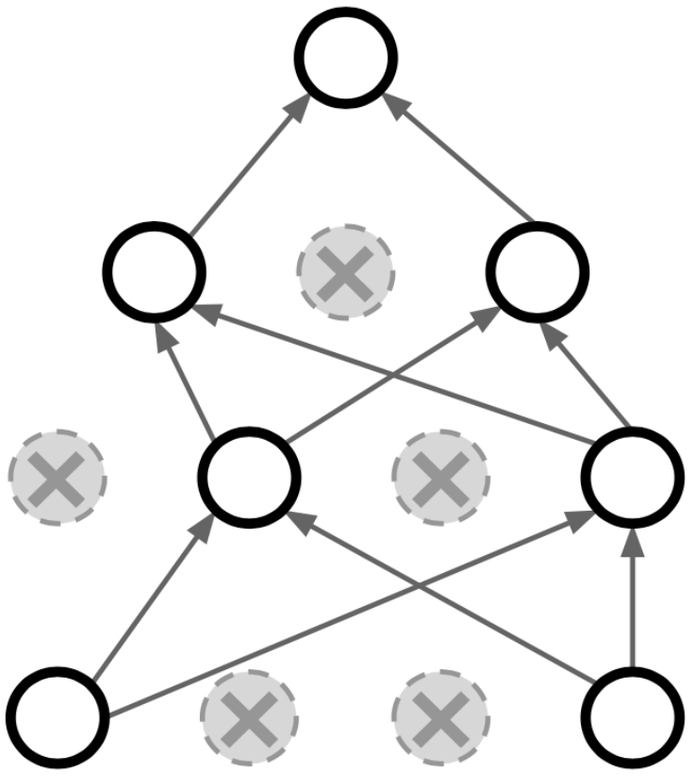
L1 regularization $R(W) = \sum_k \sum_l |W_{k,l}|$

Elastic net (L1 + L2) $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$

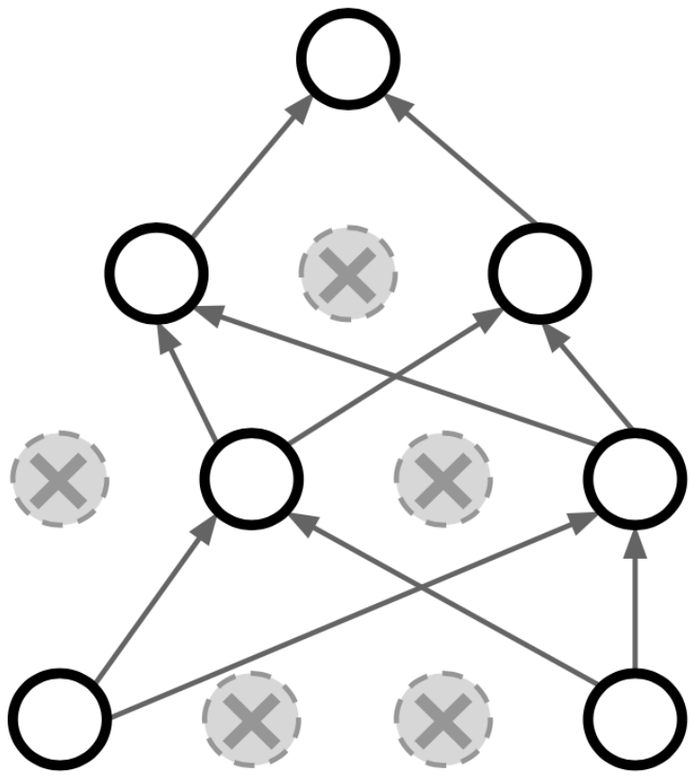
Regularization: Dropout

In each forward pass, randomly set some neurons to zero
Probability of dropping is a hyperparameter; 0.5 is common





Forces the network to have a redundant representation;
Prevents co-adaptation of features



Another interpretation:

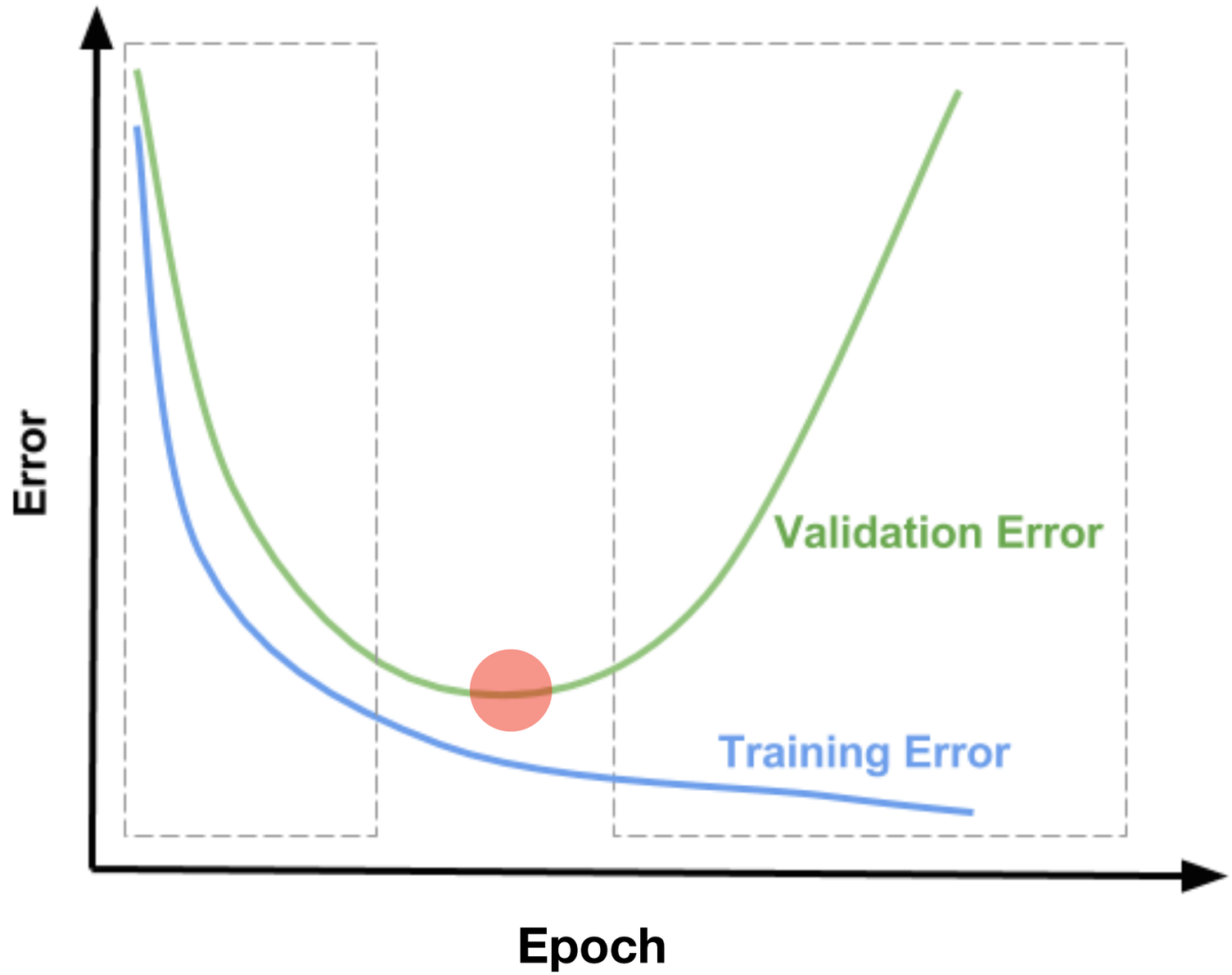
Dropout is training a large **ensemble** of models (that share parameters).

Each binary mask is one model

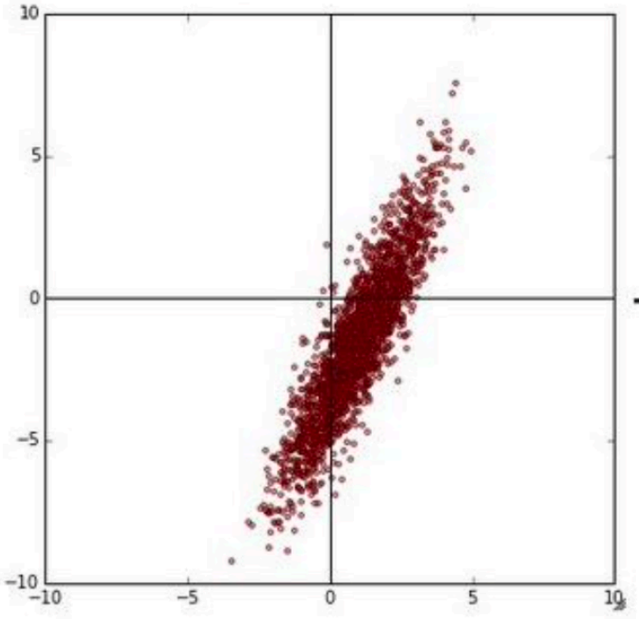
An FC layer with 4096 units has
$2^{4096} \sim 10^{1233}$ possible masks!
Only $\sim 10^{82}$ atoms in the universe...

Early Stopping

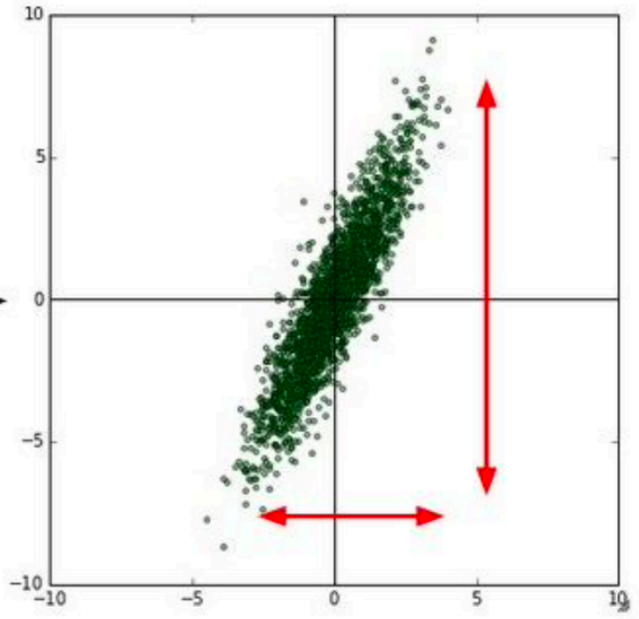
@best or @plateau



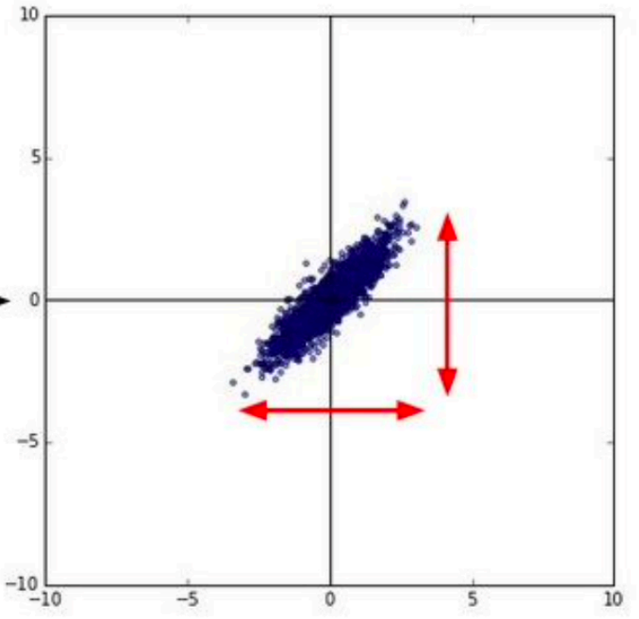
original data



zero-centered data



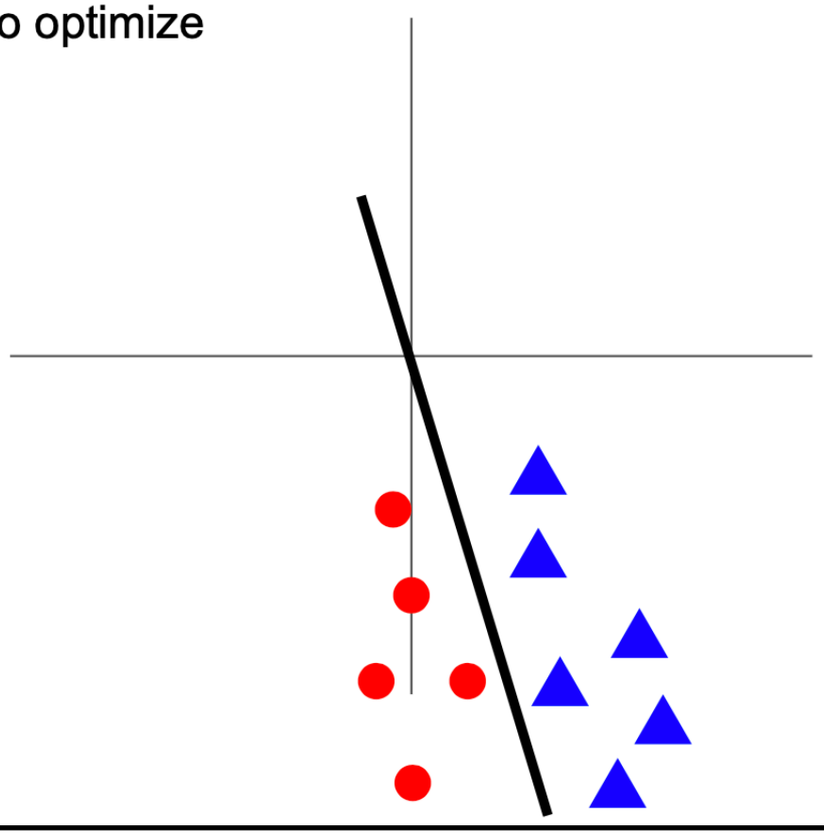
normalized data



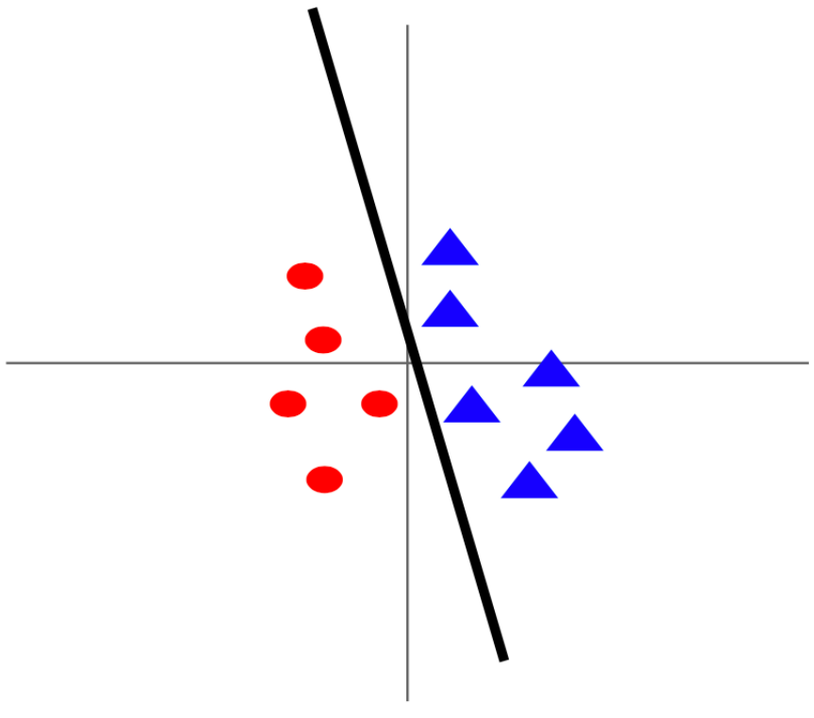
```
X -= np.mean(X, axis = 0)
```

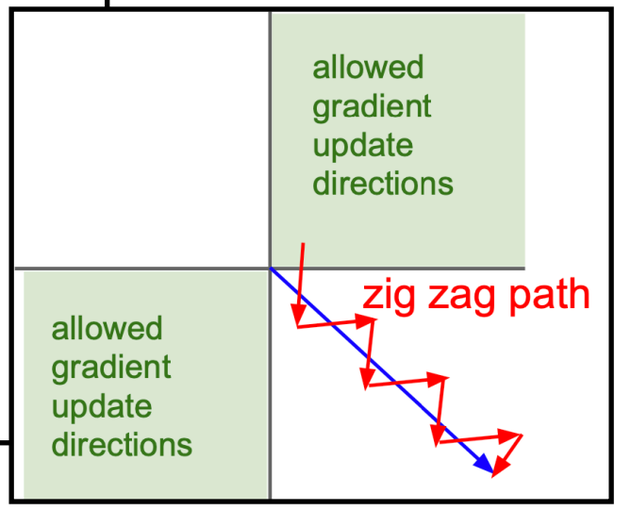
```
X /= np.std(X, axis = 0)
```

Before normalization: classification loss very sensitive to changes in weight matrix; hard to optimize

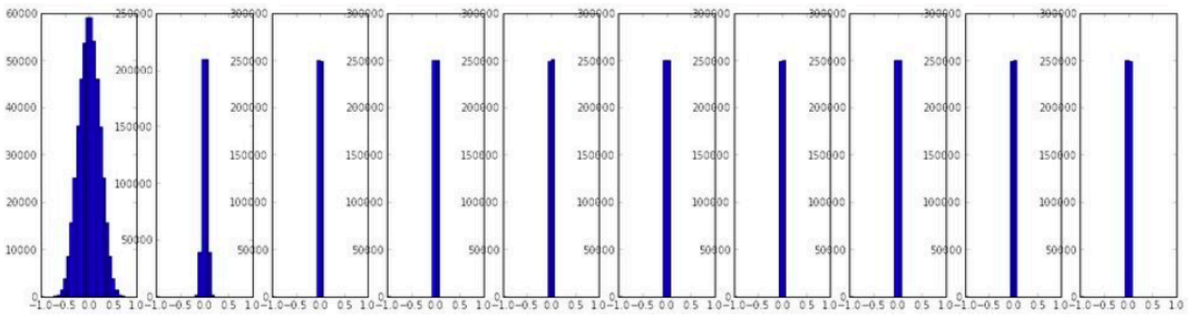


After normalization: less sensitive to small changes in weights; easier to optimize

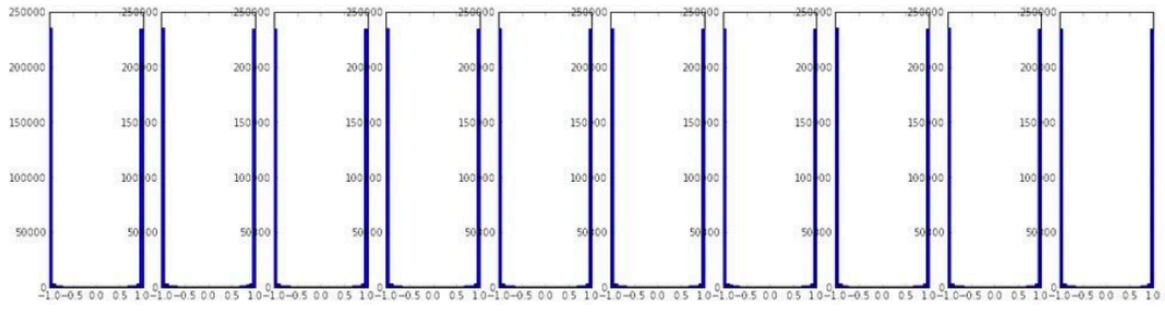




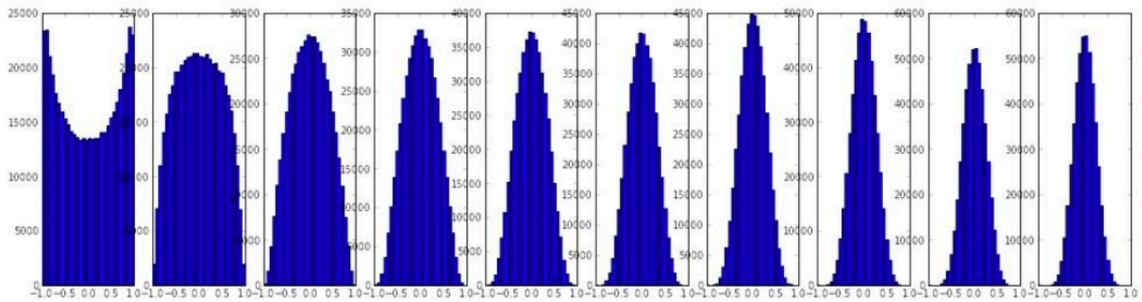
Weight initialisation



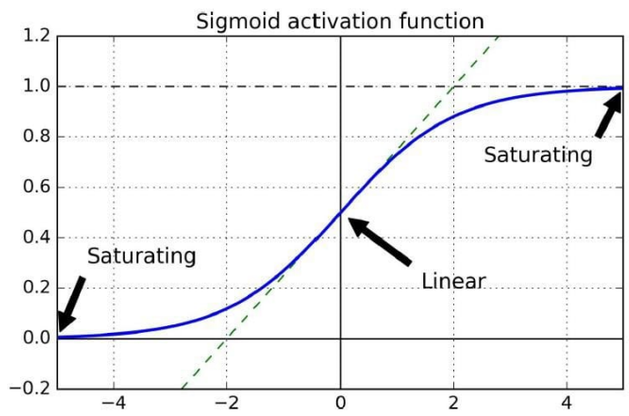
Initialization too small:
Activations go to zero, gradients also zero,
No learning

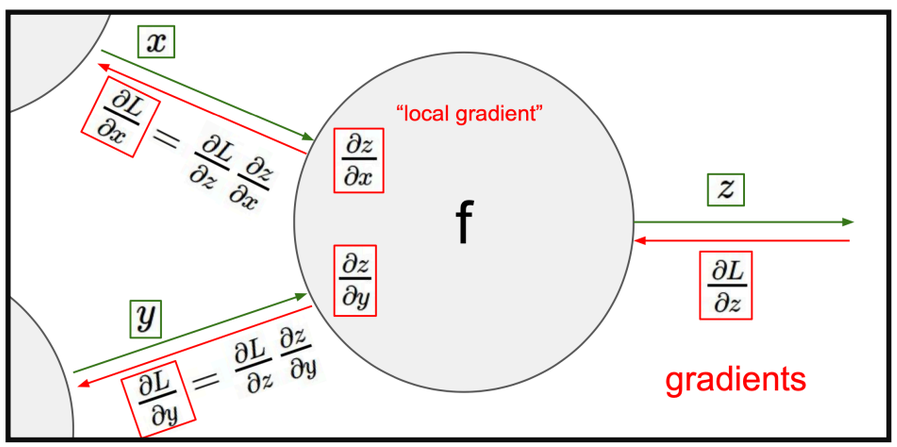


Initialization too big:
Activations saturate (for tanh),
Gradients zero, no learning



Initialization just right:
Nice distribution of activations at all layers,
Learning proceeds nicely





Batch Normalization

[Ioffe and Szegedy, 2015]

Normalize:

$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

And then allow the network to squash the range if it wants to:

$$y^{(k)} = \gamma^{(k)}\widehat{x}^{(k)} + \beta^{(k)}$$

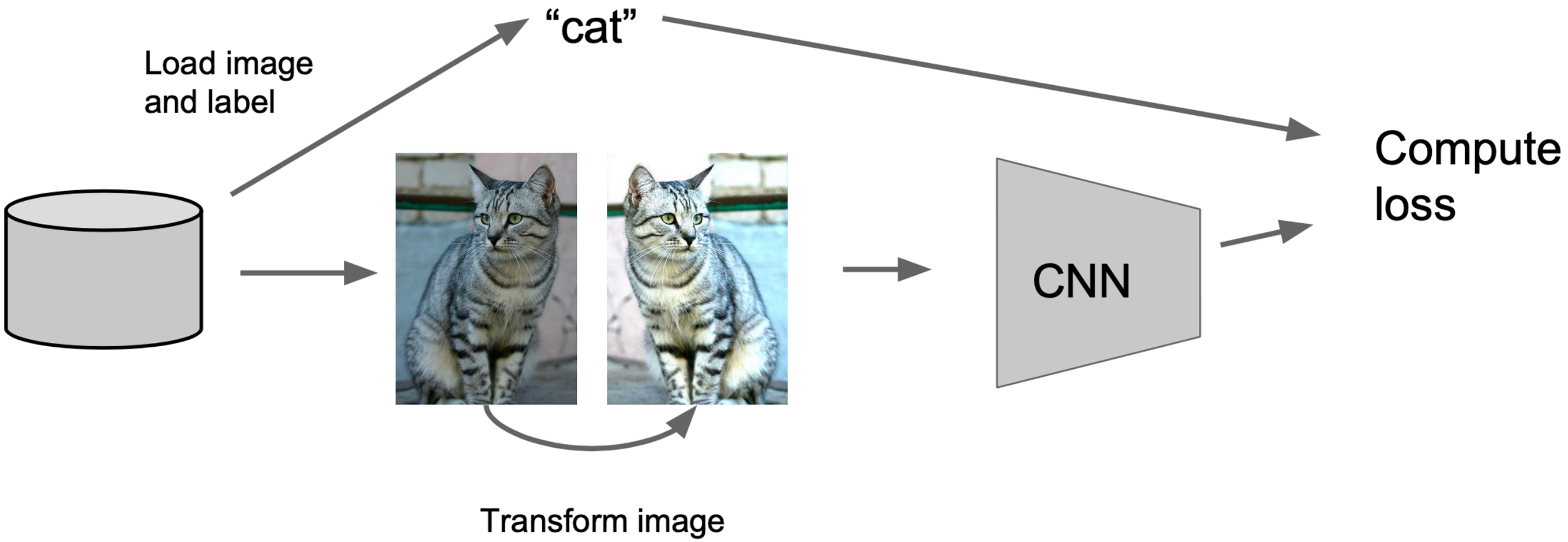
Note, the network can learn:

$$\gamma^{(k)} = \sqrt{\mathrm{Var}[x^{(k)}]}$$

$$\beta^{(k)} = \mathrm{E}[x^{(k)}]$$

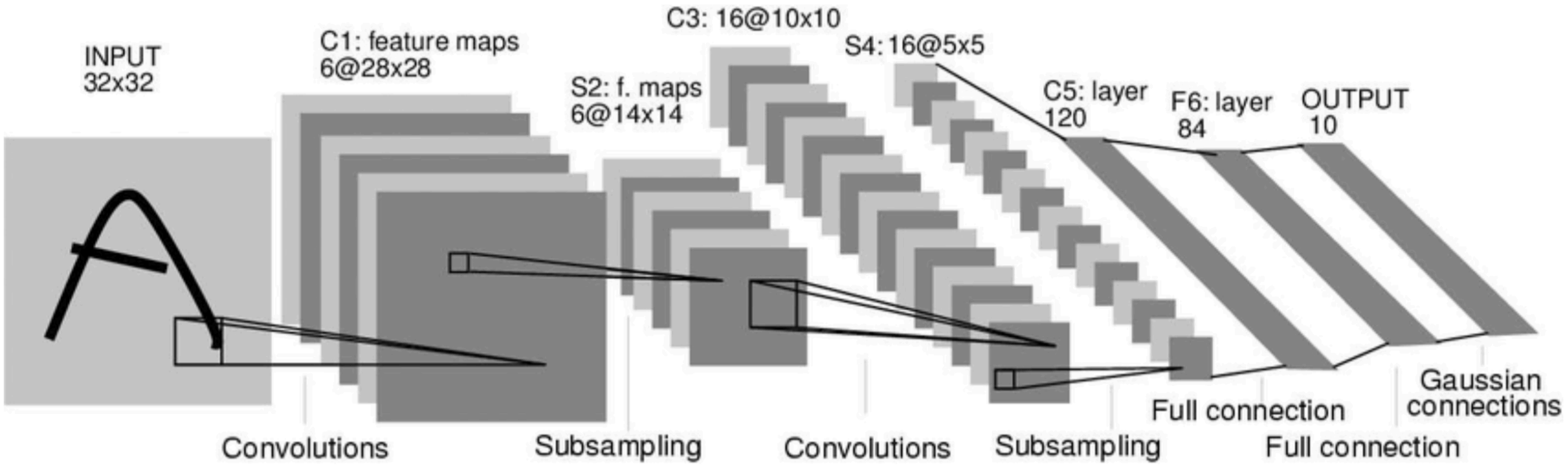
to recover the identity mapping.

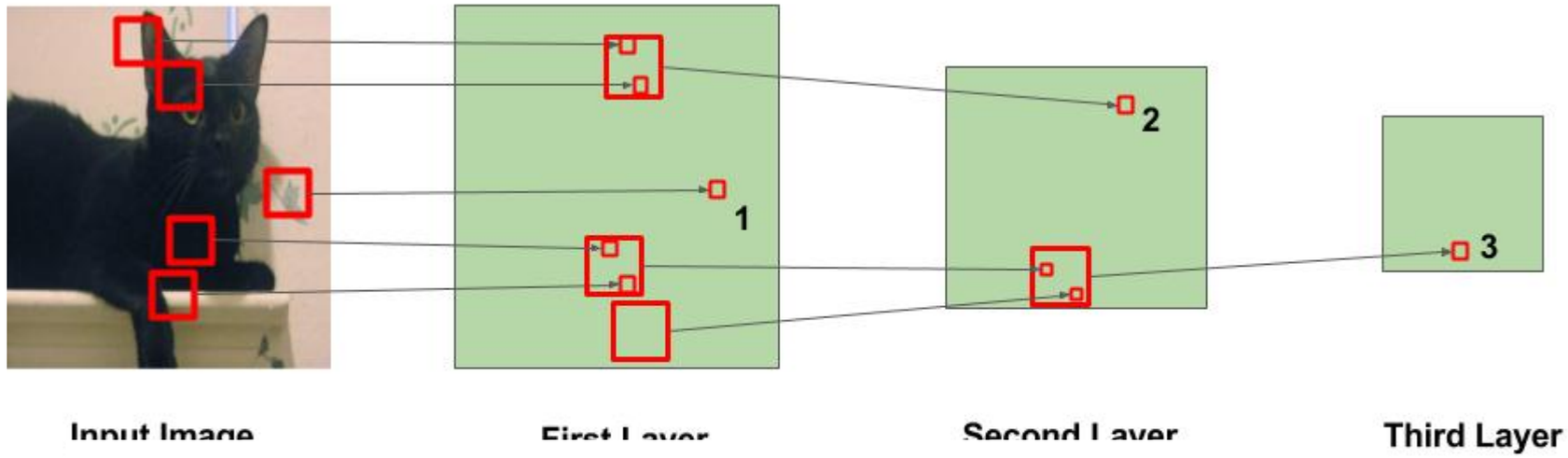
Regularization: Data Augmentation



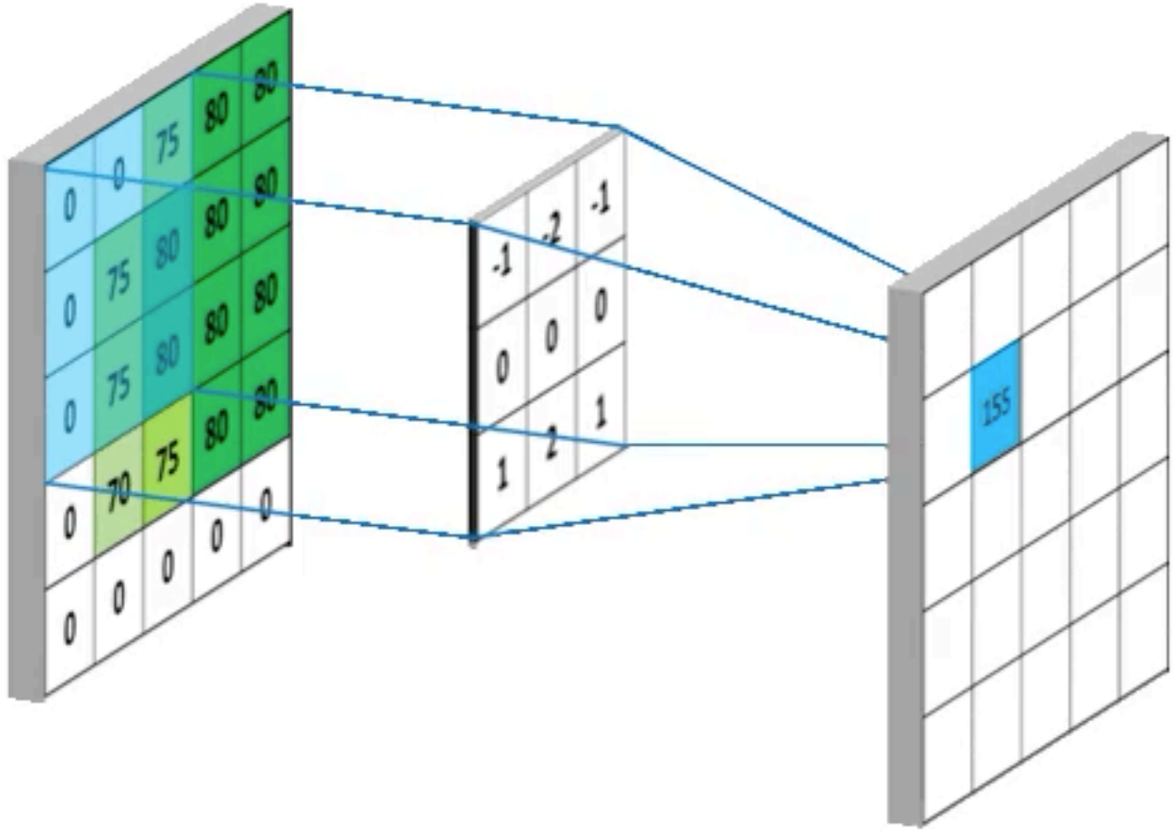
translate, rotate, flip, crop, lighten/darken, mask, add noise, …
use your fantasy…

Convolutional Neural Networks

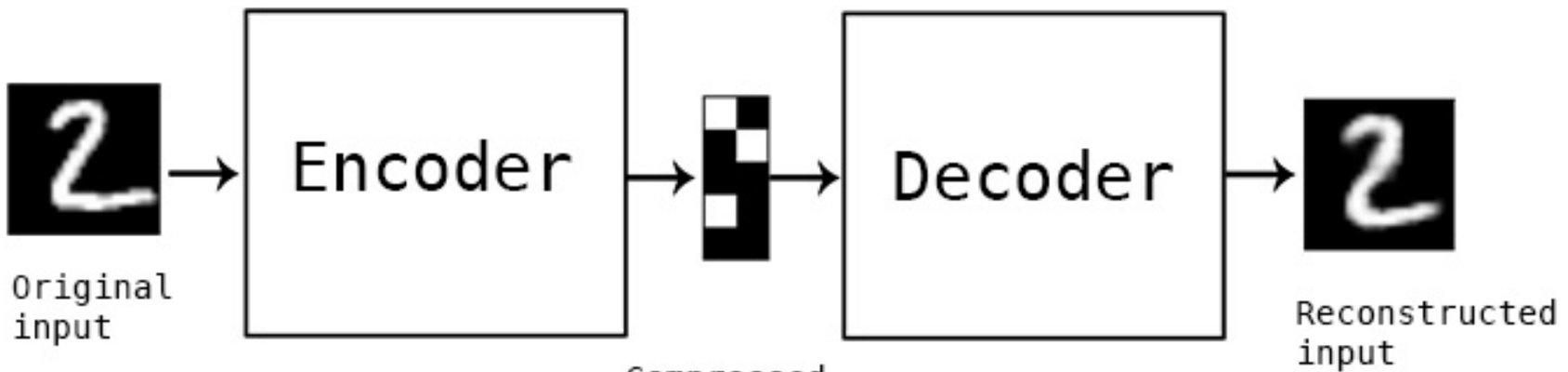


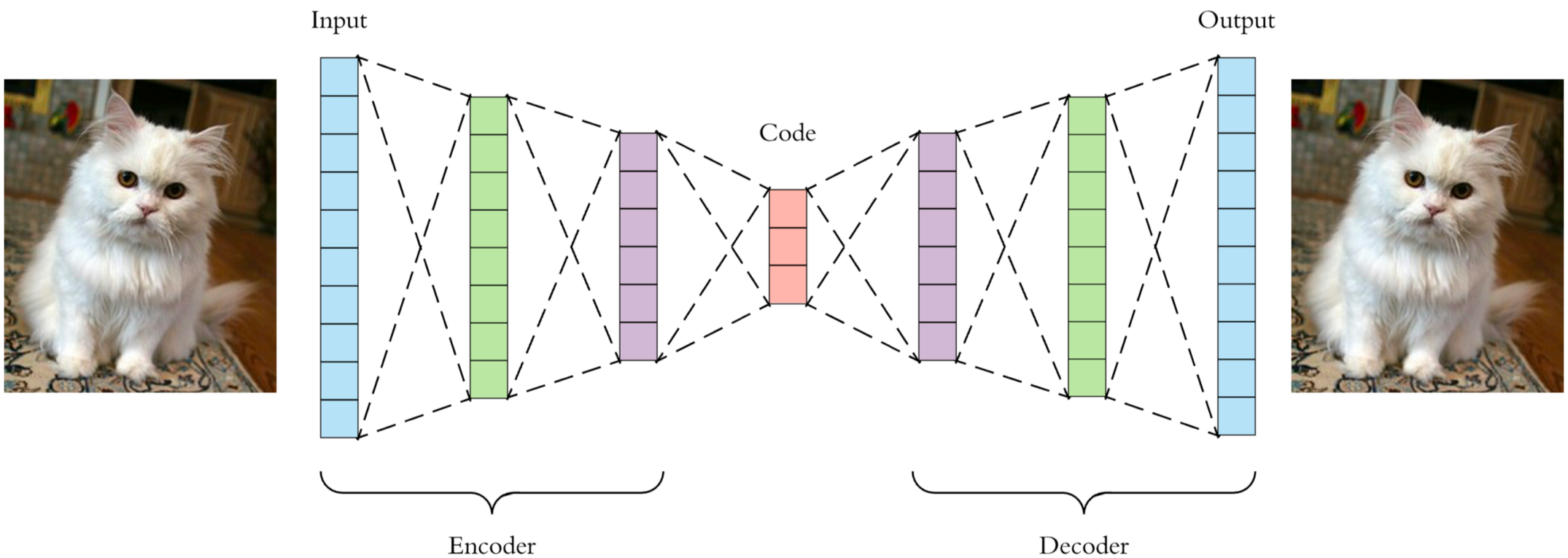


Convolution (with a kernel values that are parameters to be fit)

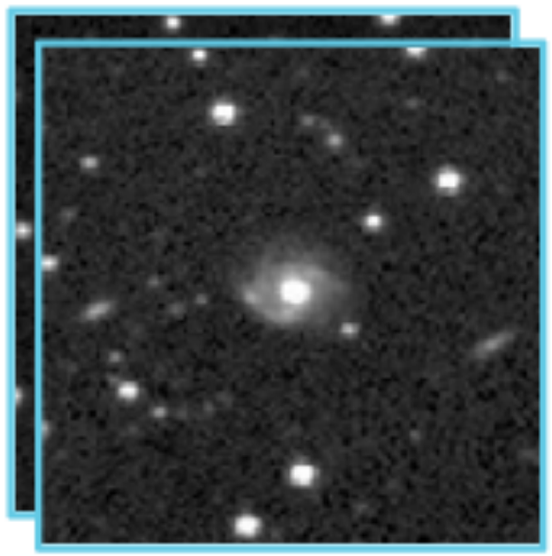


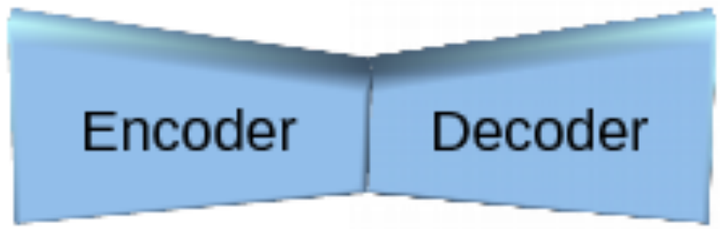
Encoder-decoders (Autoencoders)





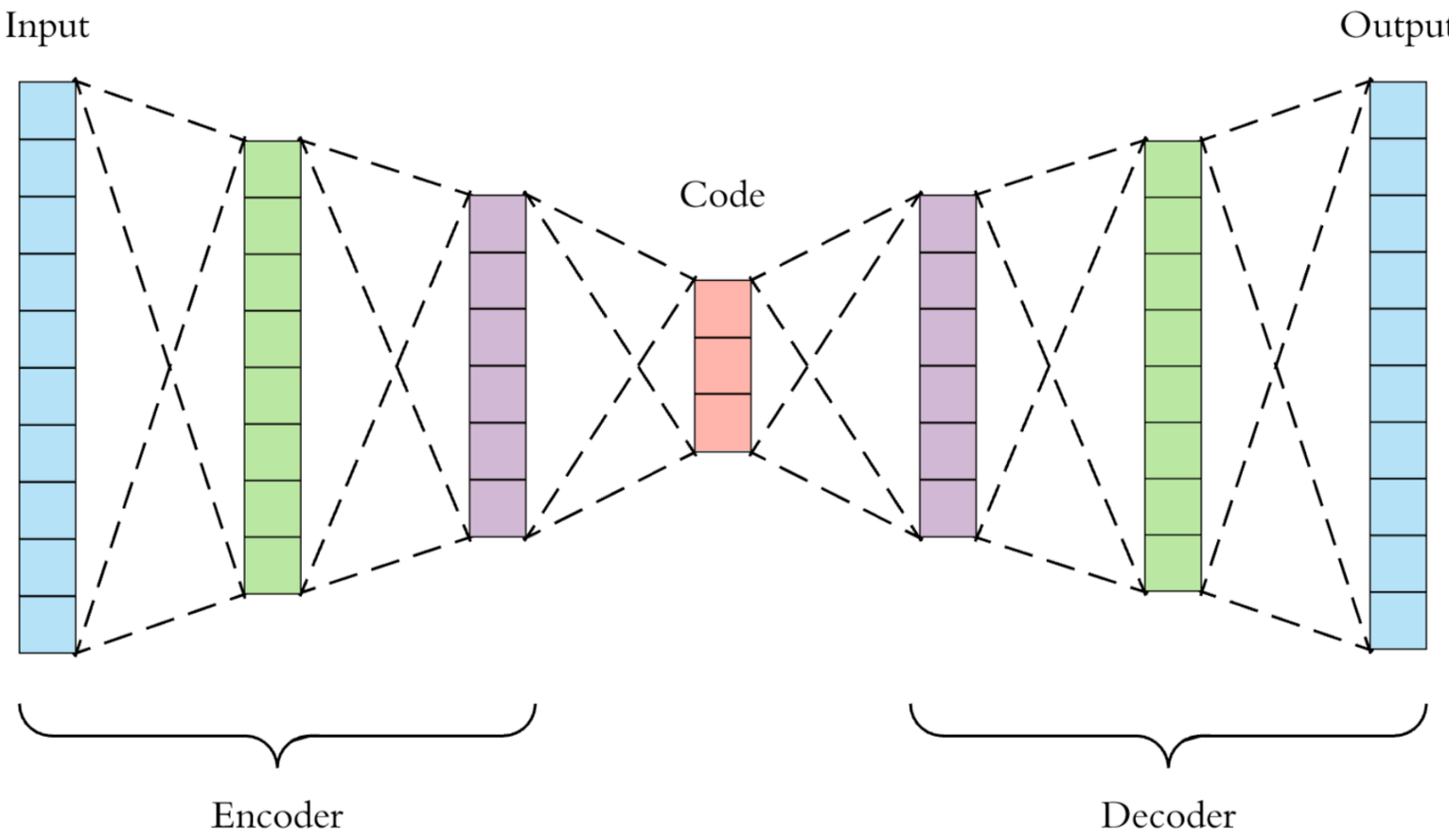
TransiNet



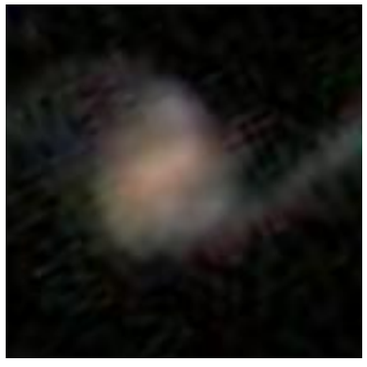

Encoder
Decoder

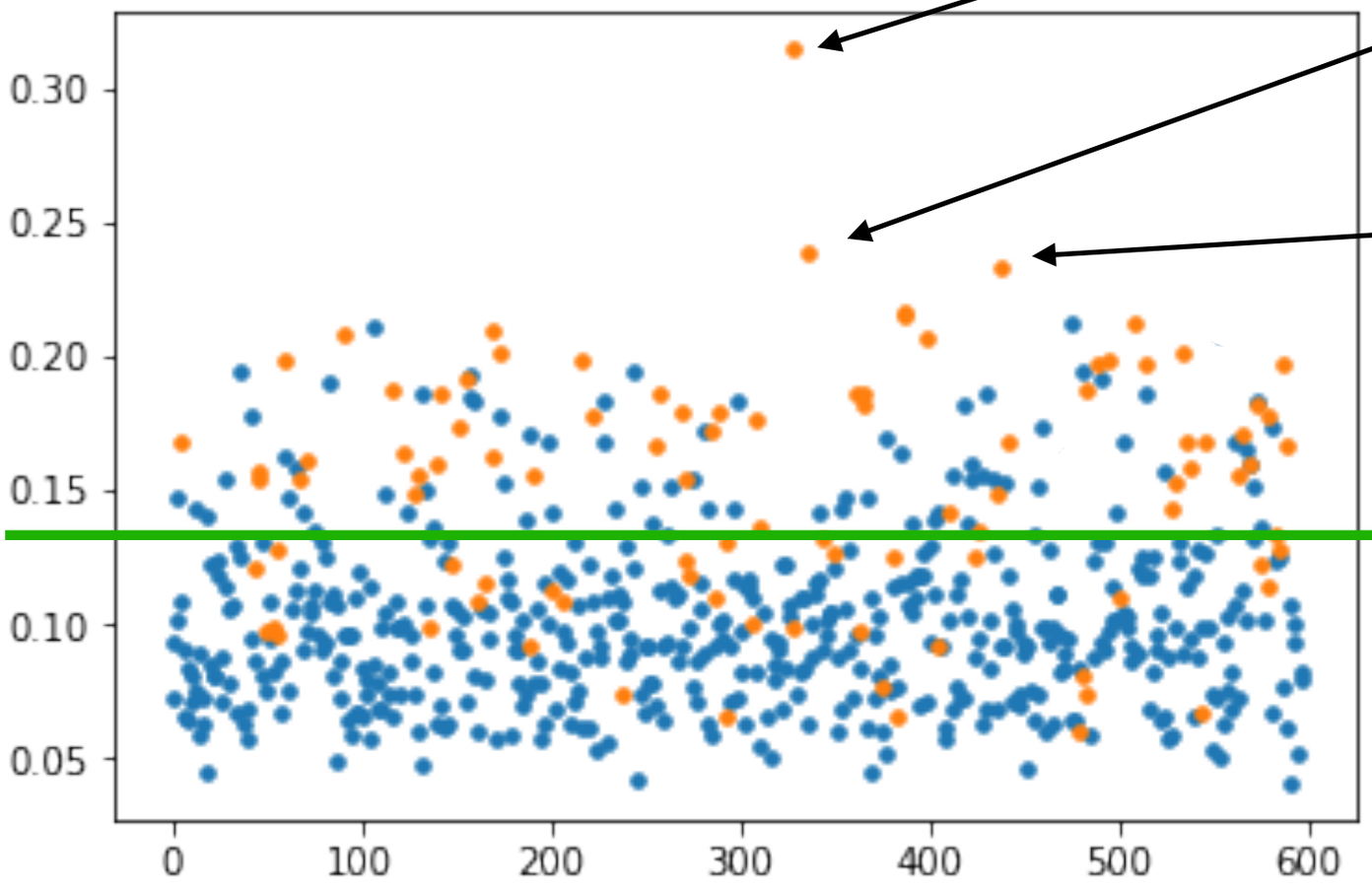
Input
Conv1
7x7 : 128
Conv2
5x5 : 256
Conv3
5x5 : 512
Conv3_1
3x3 : 512
Conv4
3x3 : 1024
Conv4_1
3x3 : 1024
Conv5
3x3 : 1024
Conv5_1
3x3 : 1024
Conv6
3x3 : 2048
Conv6_1
3x3 : 2048
L1 Loss
Output
Upconv0
4x4 : 32
Upconv1
4x4 : 64
Upconv2
4x4 : 128
Upconv3
4x4 : 256
Upconv4
4x4 : 512
Upconv5
4x4 : 1024

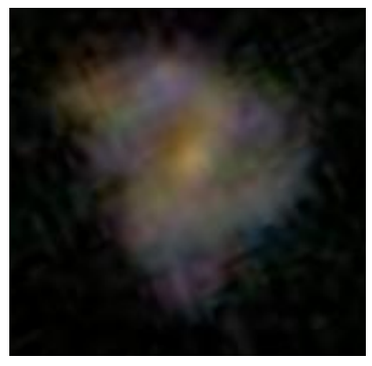
E.g. De-noising



Anomaly detection

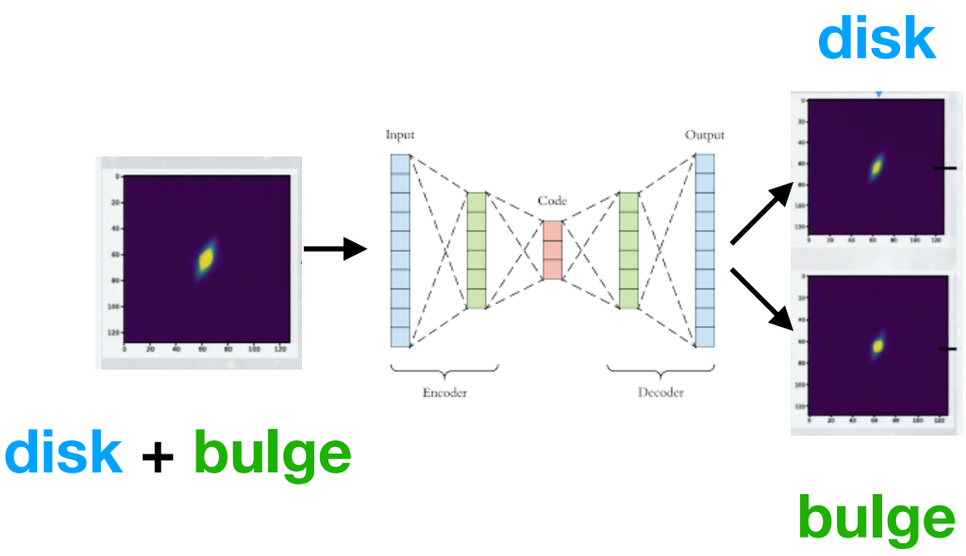






Encoder/decoder usage

- Dimensionality reduction
- Denoising
- Outlier detection (measure of reconstruction error)
- Image segmentation
- Deblending
- Predicting next move
- Many others…
- (Can be considered as an unsupervised learning)



- Distance metrics on pixels are not informative

Original

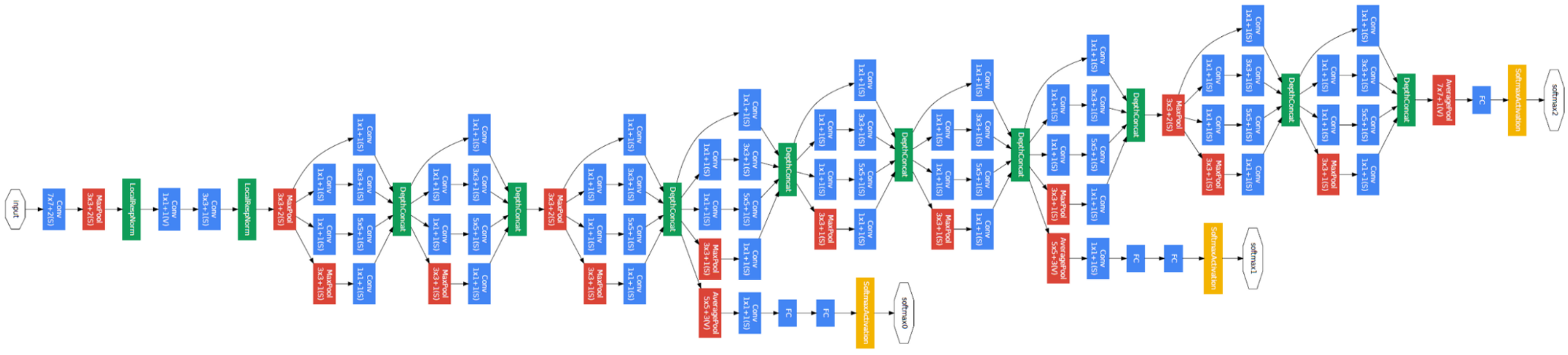
Boxed

Shifted

Tinted

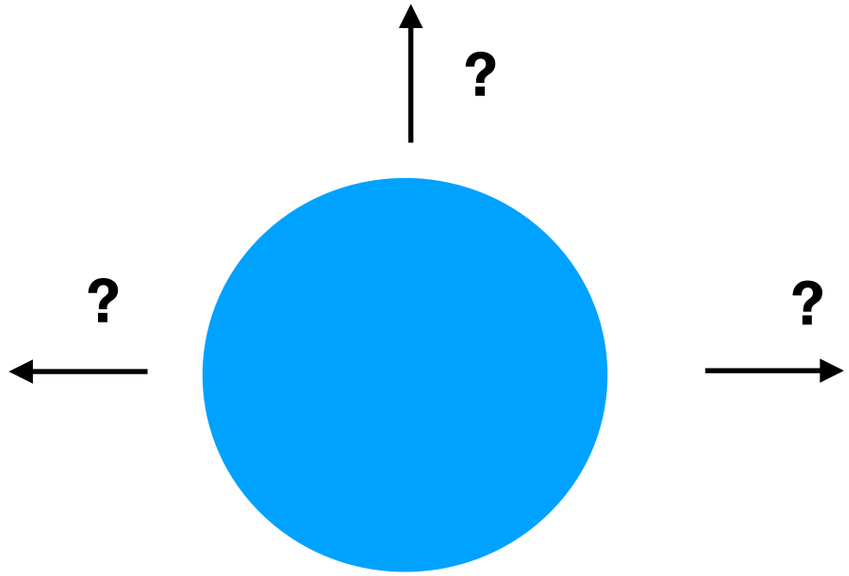
(all 3 images have same L2 distance to the one on the left)

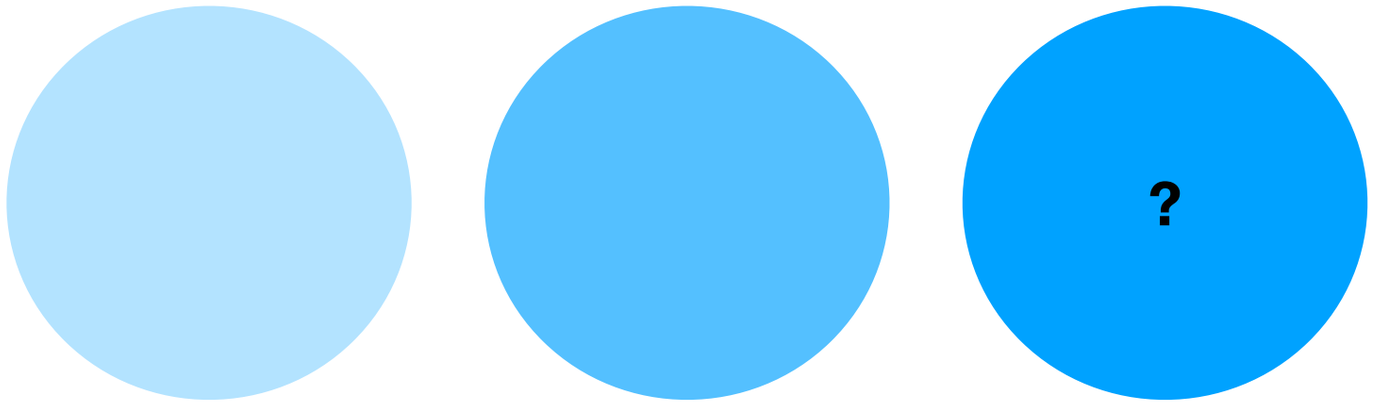
Transfer Learning



https://keras.io/api/applications/

Recurrent Neural Network





Recurrent Neural Network

We can process a sequence of vectors **x** by applying a **recurrence formula** at every time step:

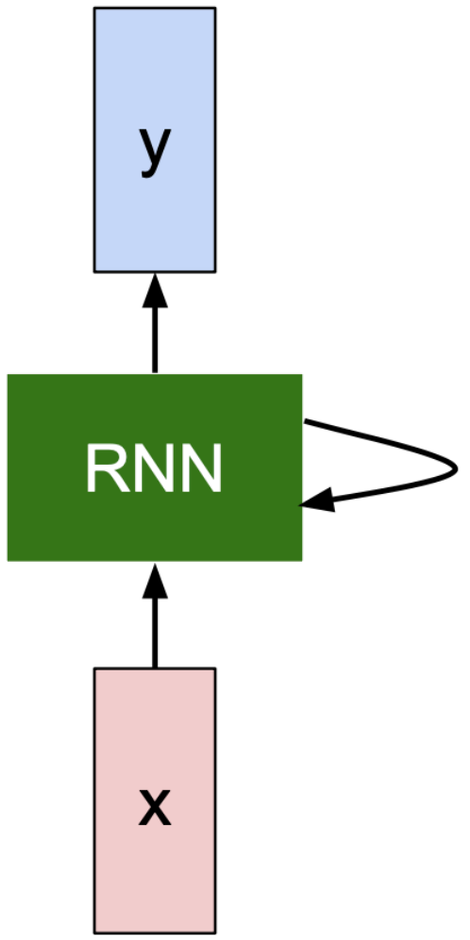
$$h_t = f_W(h_{t-1}, x_t)$$

new state

some function with parameters W

old state

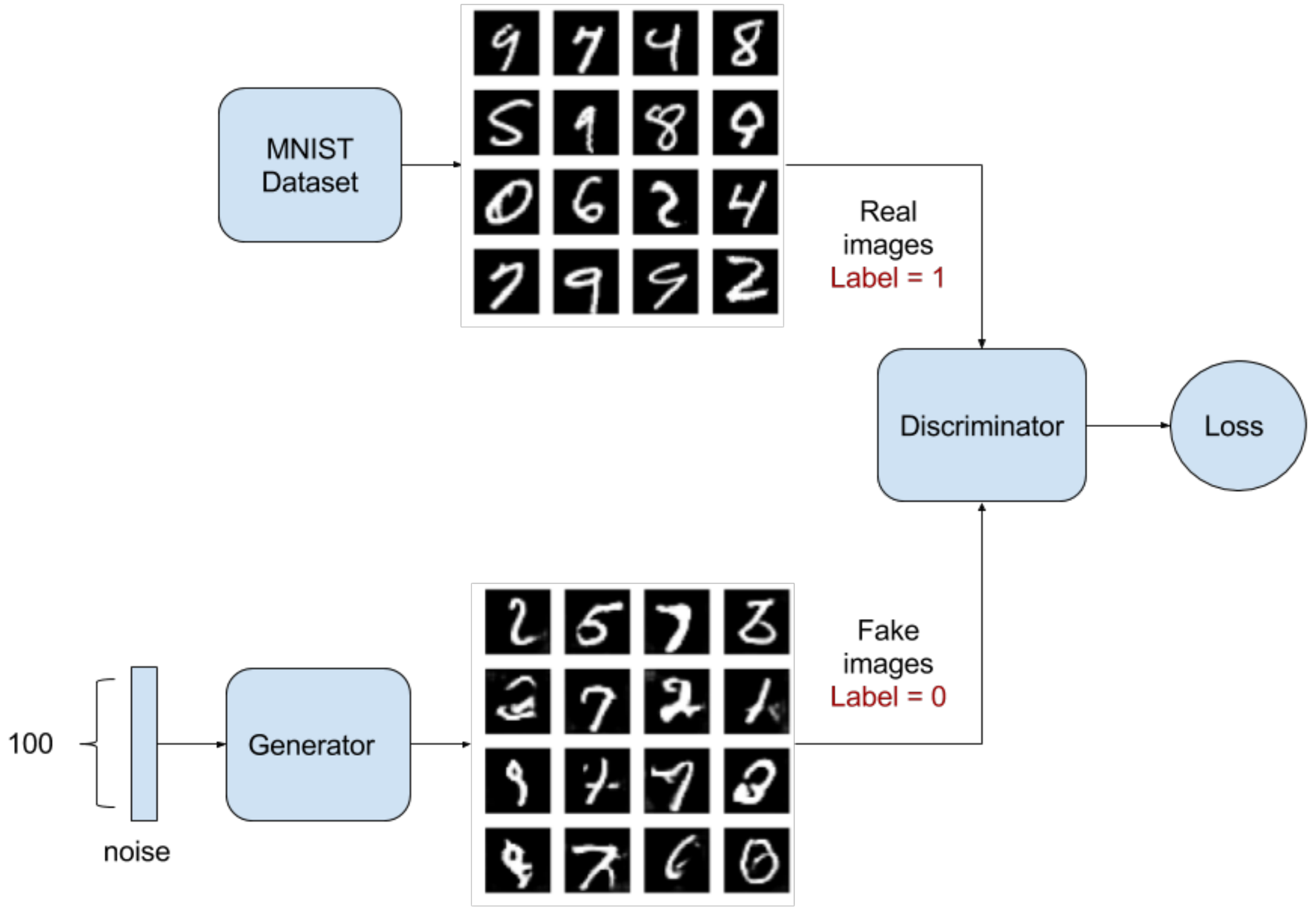
input vector at some time step

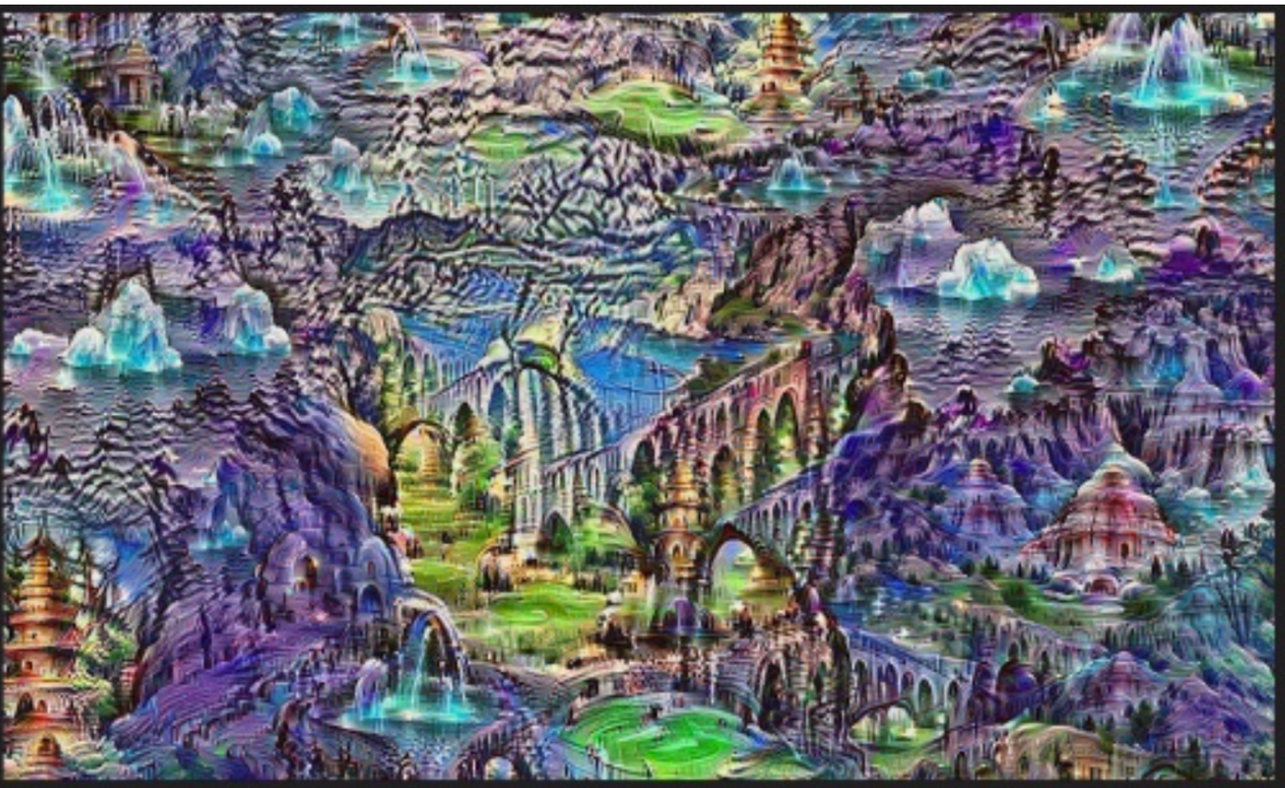
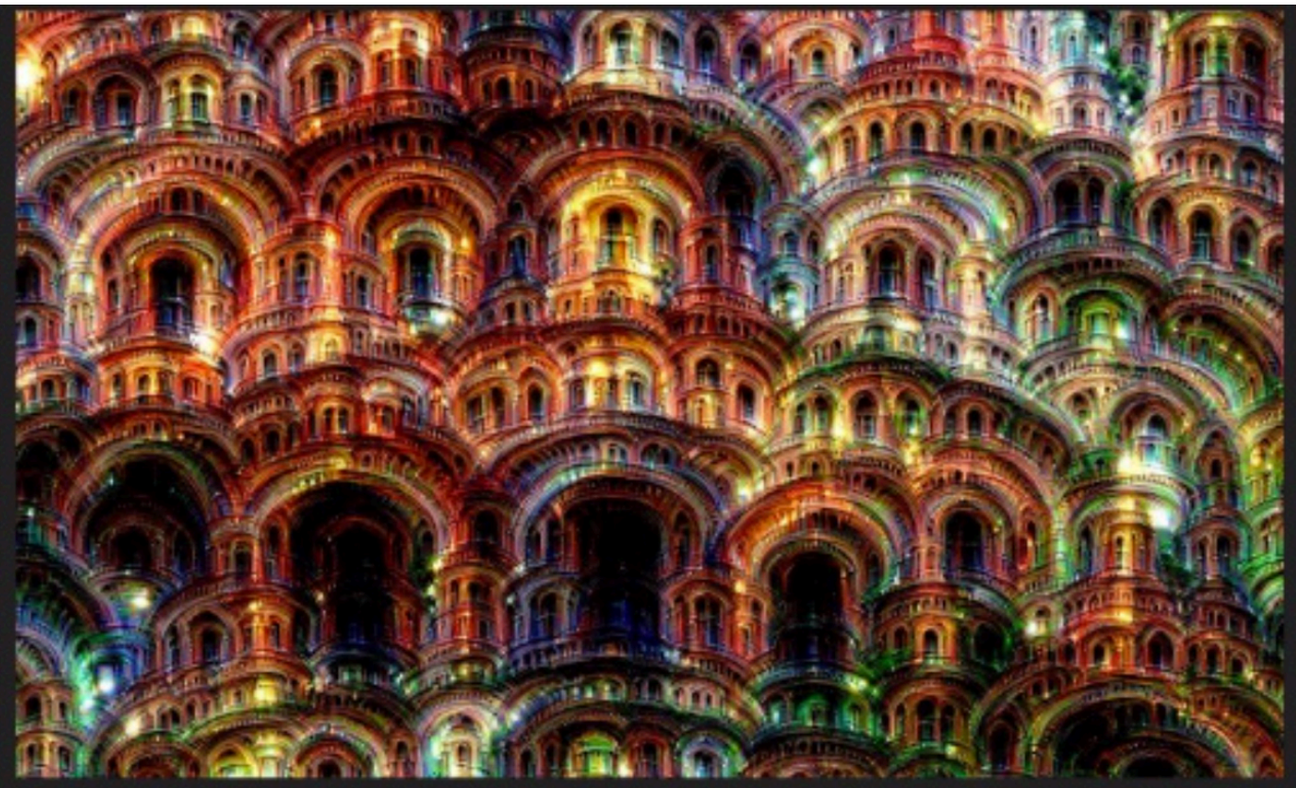
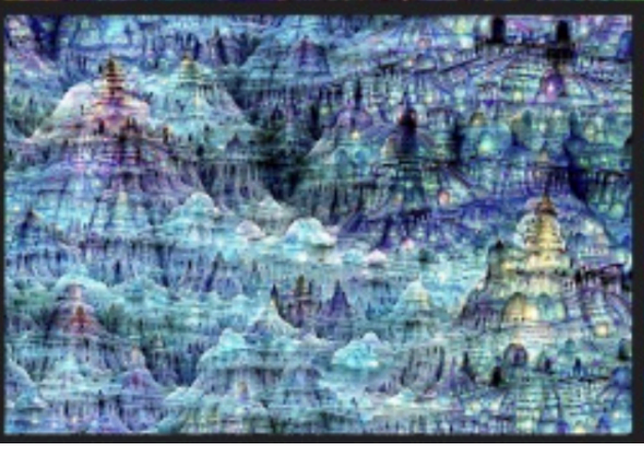
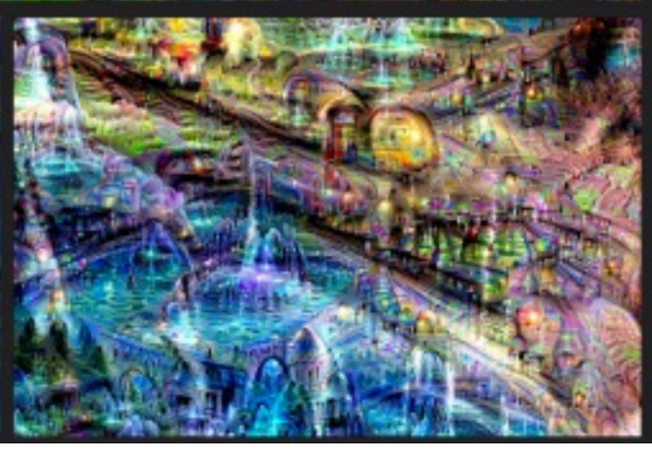
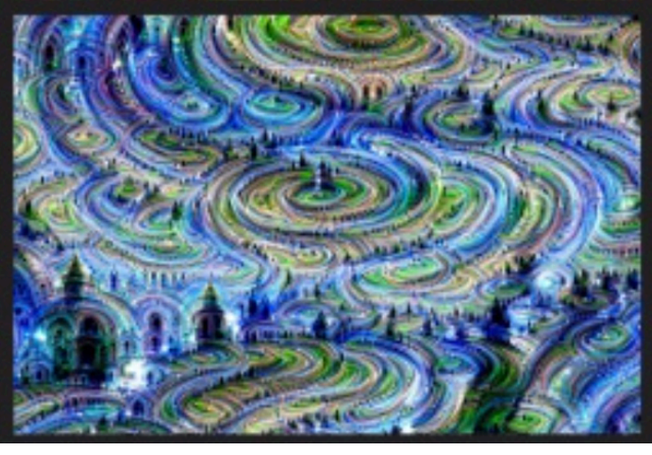


RNN pseudo-code

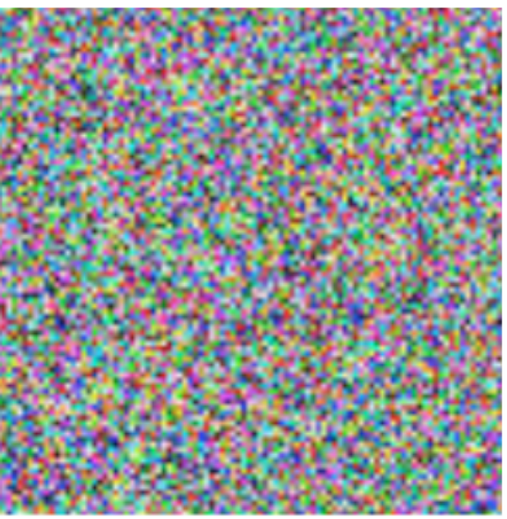
```
rnn = RNN()
ff = FeedForwardNN()
hidden_states = [0,0,0,0]

for word in input:
  output, hidden_state = rnn(word, hidden_state)

prediction = ff(output)
```

GAN (Generative Adversarial Network)




Noise ~ N(0,1)

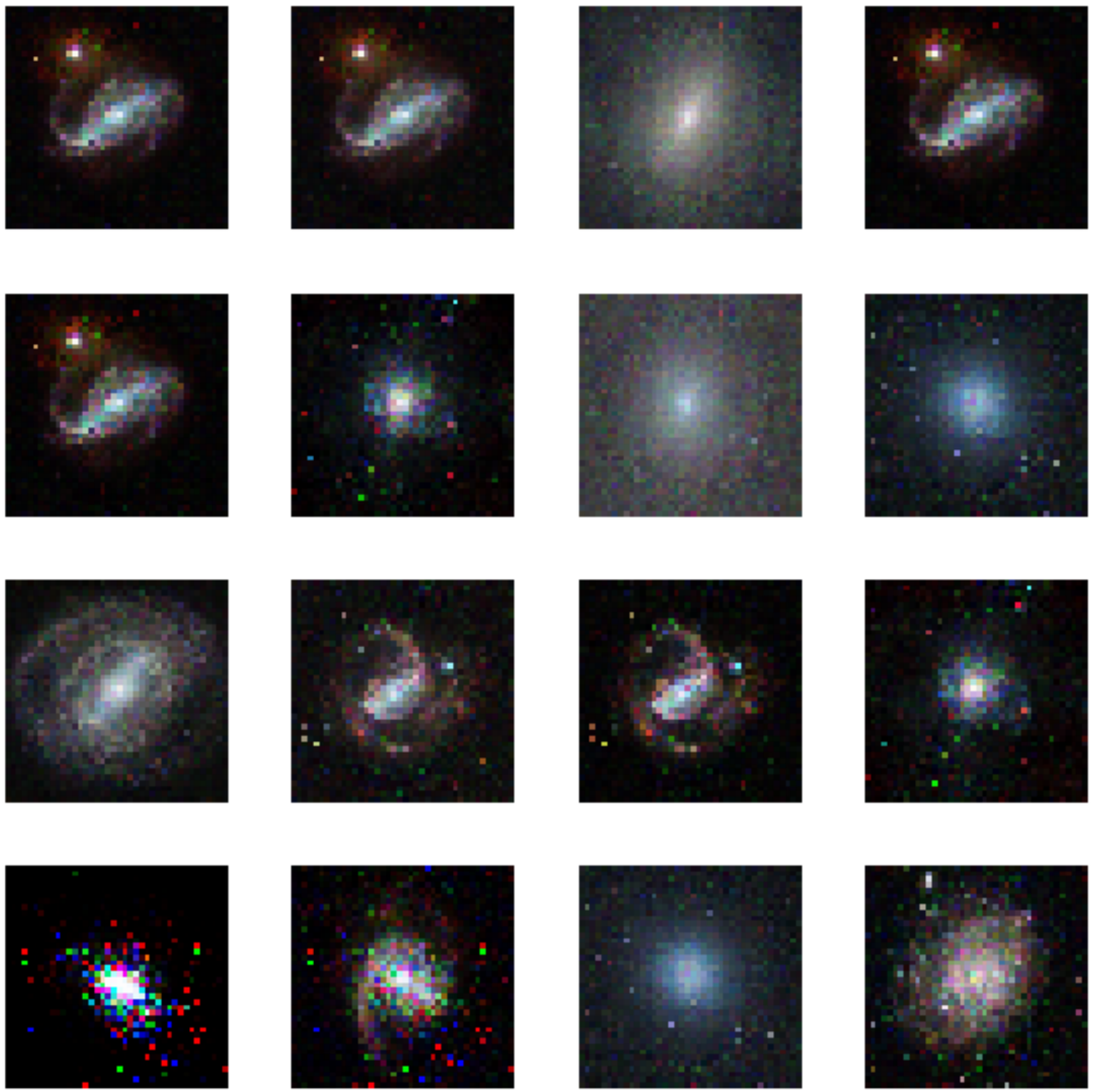


Generative Model

Elliptical

Barred Spiral

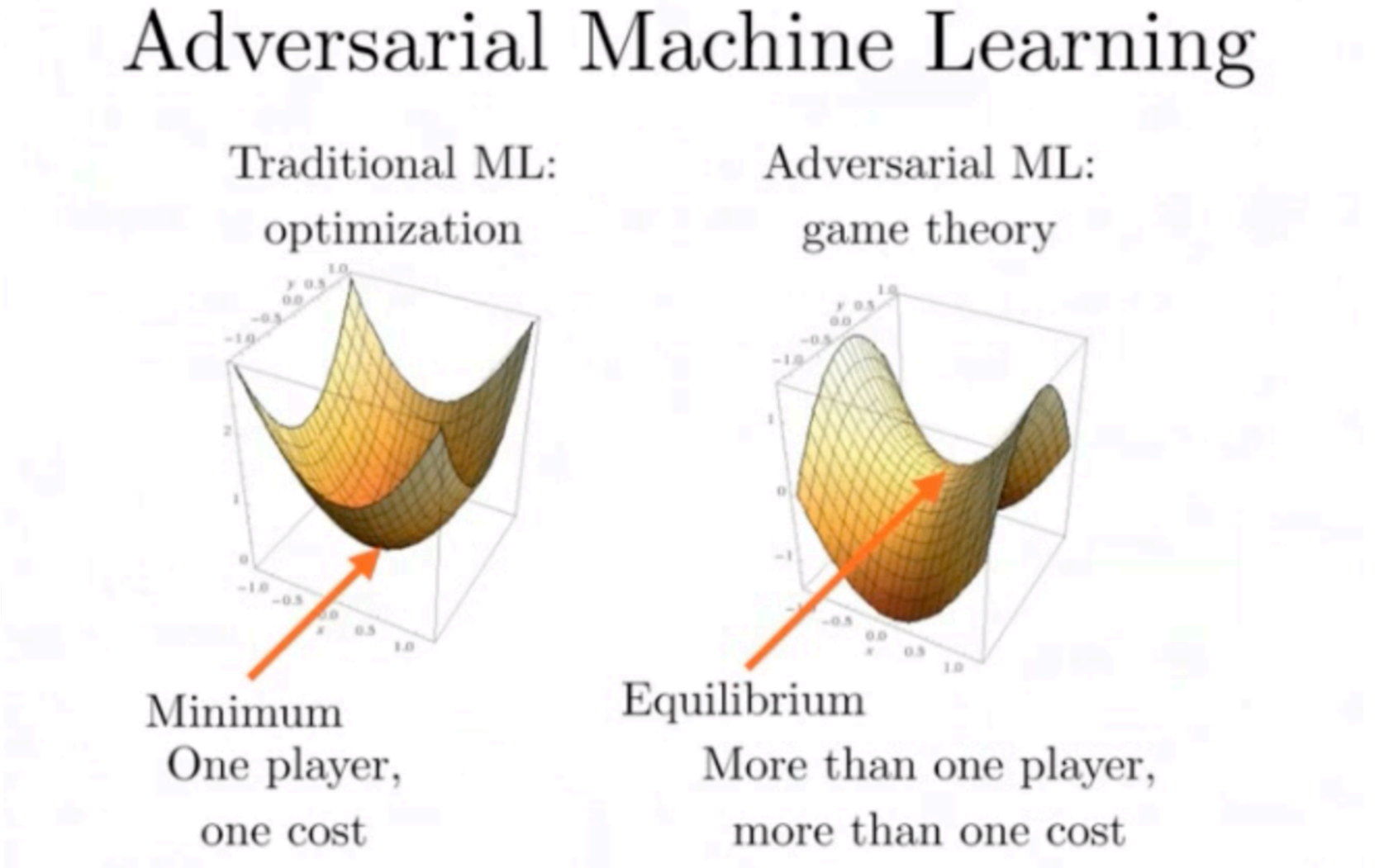
Spiral

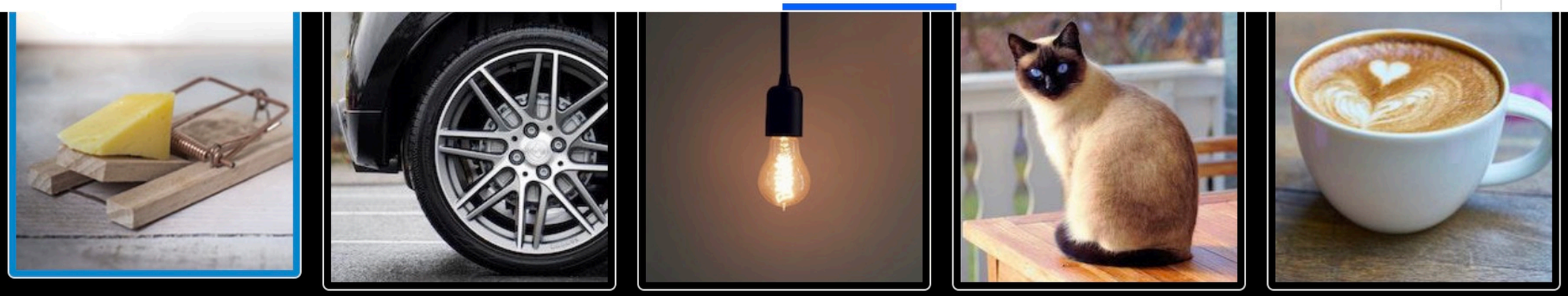


GAN usage

- Mock catalogs
- Denoising
- Compete gaming

Warning: Hard to train





2. Simulate Attack

Adversarial noise type

C&W Attack

Determine strength

None low med high

3. Defend attack

Gaussian Noise

None low med high

Spatial Smoothing

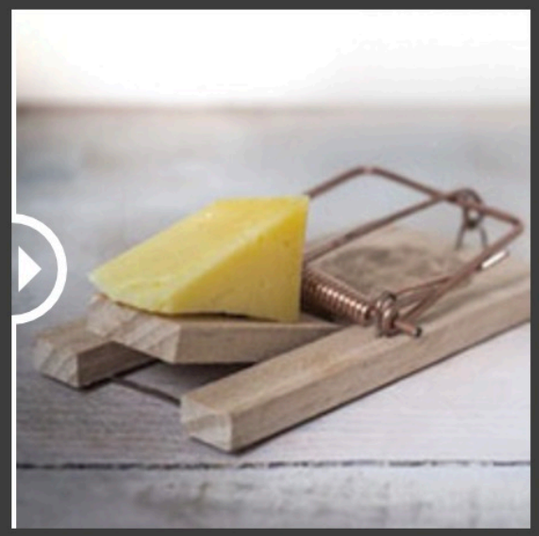
None low med high

Feature Squeezing

None low med high

Visual Code

Original Modified



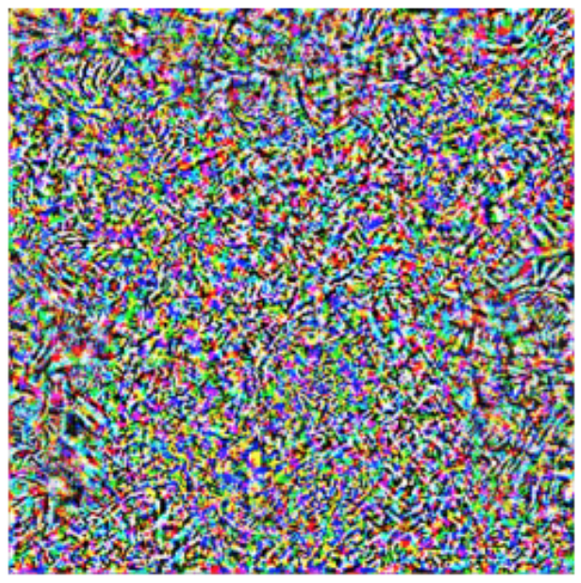
94%

scorpion

“pig” (91%)

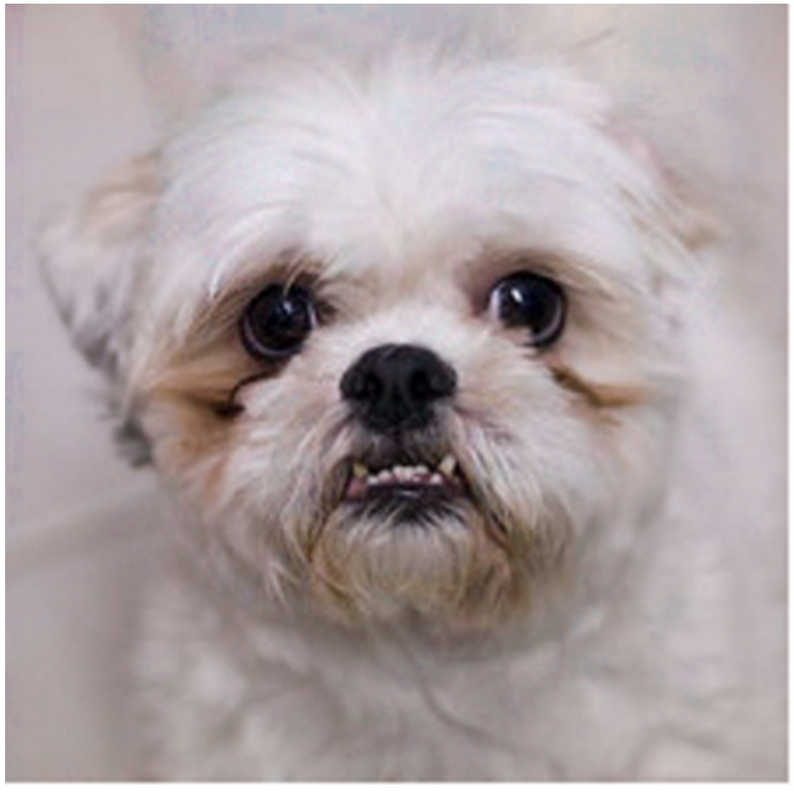
+ 0.005 x

noise (NOT random)

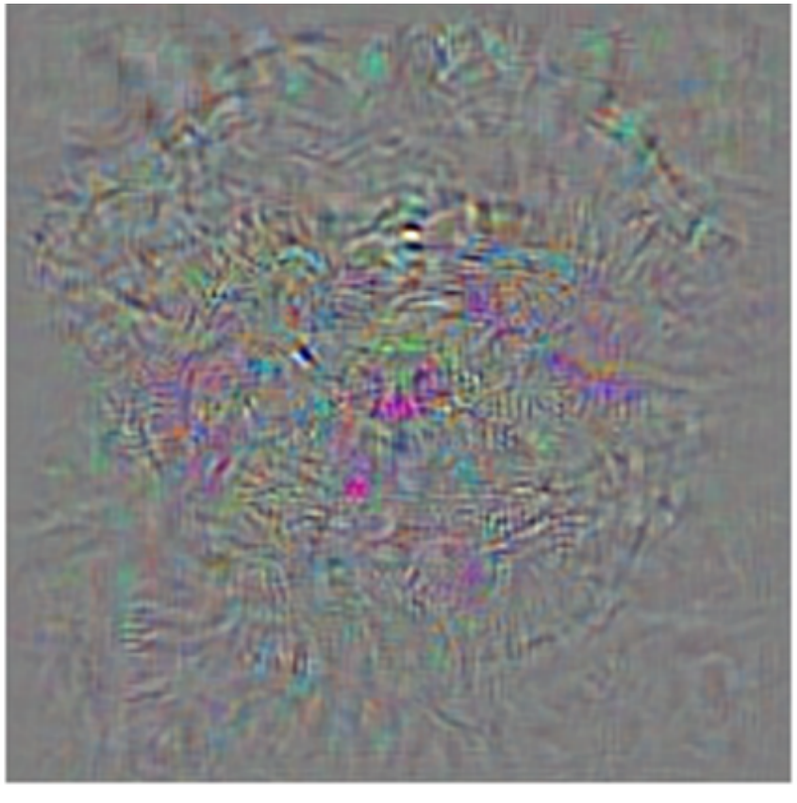


=

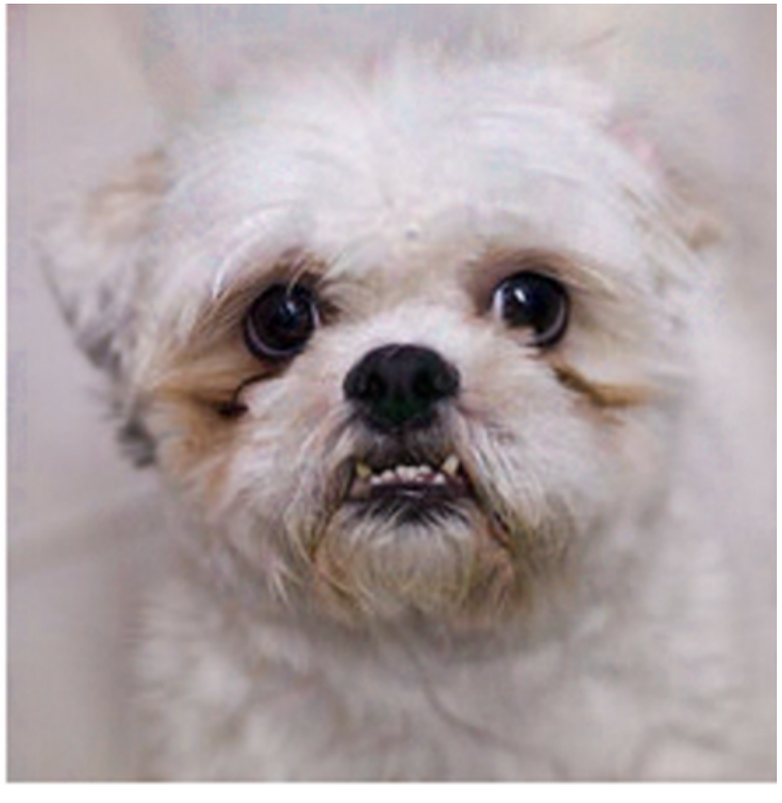
“airliner” (99%)



dog



+noise



ostrich

Logic behind  Keras

1- **Import** model class

from keras.models import **Sequential**

2 - **Instantiate** model class

model = Sequential()

3 - **Add layers** with the add() method specifying input_dim or input_shape

model.**add**(Dense(32, input_dim=784))

4 - Add activation functions

model.add(**Activation**('relu'))

5 - Configure **training** with compile(loss=,optimizer=, metrics[])

model.**compile**(optimizer='rmsprop', loss='binary_crossentropy',
metrics=['accuracy'])

6 - **Train** with the fit() method

model.**fit**(data, labels, epochs=10, batch_size=32)

7- **Evaluate** the model performance with the evaluate() method:

score = model.**evaluate**(x_test, y_test, verbose=0)

8 – Make **predictions** with predict():

predictions = model.**predict**(x_test)

in TensorFlow
in anaconda for python 3.6

```python
# import tensorflow and keras (tf.keras not "vanilla" Keras)
import tensorflow as tf
from tensorflow import keras

# get data
(train_images, train_labels), (test_images, test_labels) = \
keras.datasets.mnist.load_data()

# setup model
model = keras.Sequential([
    keras.layers.Flatten(input_shape=(28, 28)),
    keras.layers.Dense(128, activation=tf.nn.relu),
    keras.layers.Dense(10, activation=tf.nn.softmax)
])

model.compile(optimizer=tf.train.AdamOptimizer(),
              loss='sparse_categorical_crossentropy',
              metrics=['accuracy'])

# train model
model.fit(train_images, train_labels, epochs=5)

# evaluate
test_loss, test_acc = model.evaluate(test_images, test_labels)
print('test accuracy:', test_acc)

# make predictions
predictions = model.predict(test_images)
```

Top 5 (supervised)

Algorithm	Comments
Neural Networks	• Take long to train - lot of CPU • Overfits • Requires lot of data
Gradient Boosted Trees	• Fast • Overfit danger
Random Forest	• Robust to overfitting
SVM w/non-linear kernel	• Pretty good
Gaussian Processes	• non-parametric fitting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