Deep Learning I

Itthi Chatnuntawech
Nanoinformatics and Artificial Intelligence (NAI)
National Nanotechnology Center (NANOTEC)
National Science and Technology Development Agency (NSTDA)
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Outline

- Introduction to Supervised Machine Learning
  - AI vs ML vs DL
  - Traditional Machine Learning
  - Training, Validation, and Test Data
  - Overfitting and Underfitting
- Introduction to Supervised Deep Learning
  - Traditional ML vs Deep Learning
  - Artificial Neuron and Neural Network
  - Supervised Learning
- Deep Learning as a Function Approximator
- Deep Learning Components
  - Fully Connected Layers
  - Activation Functions
  - Optimization

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Artificial Intelligence

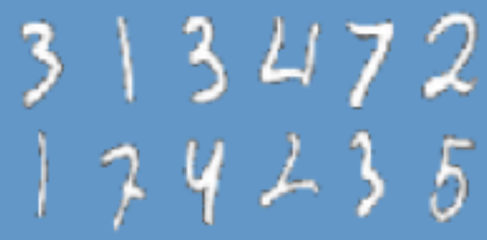
Any technique that enables computers to mimic human behavior

Machine Learning

Ability to learn without explicitly being programmed

Deep Learning

Learn underlying features in data using neural networks



1950's 1960's 1970's 1980's 1990's 2000's 2010's

Fasting blood sugar test

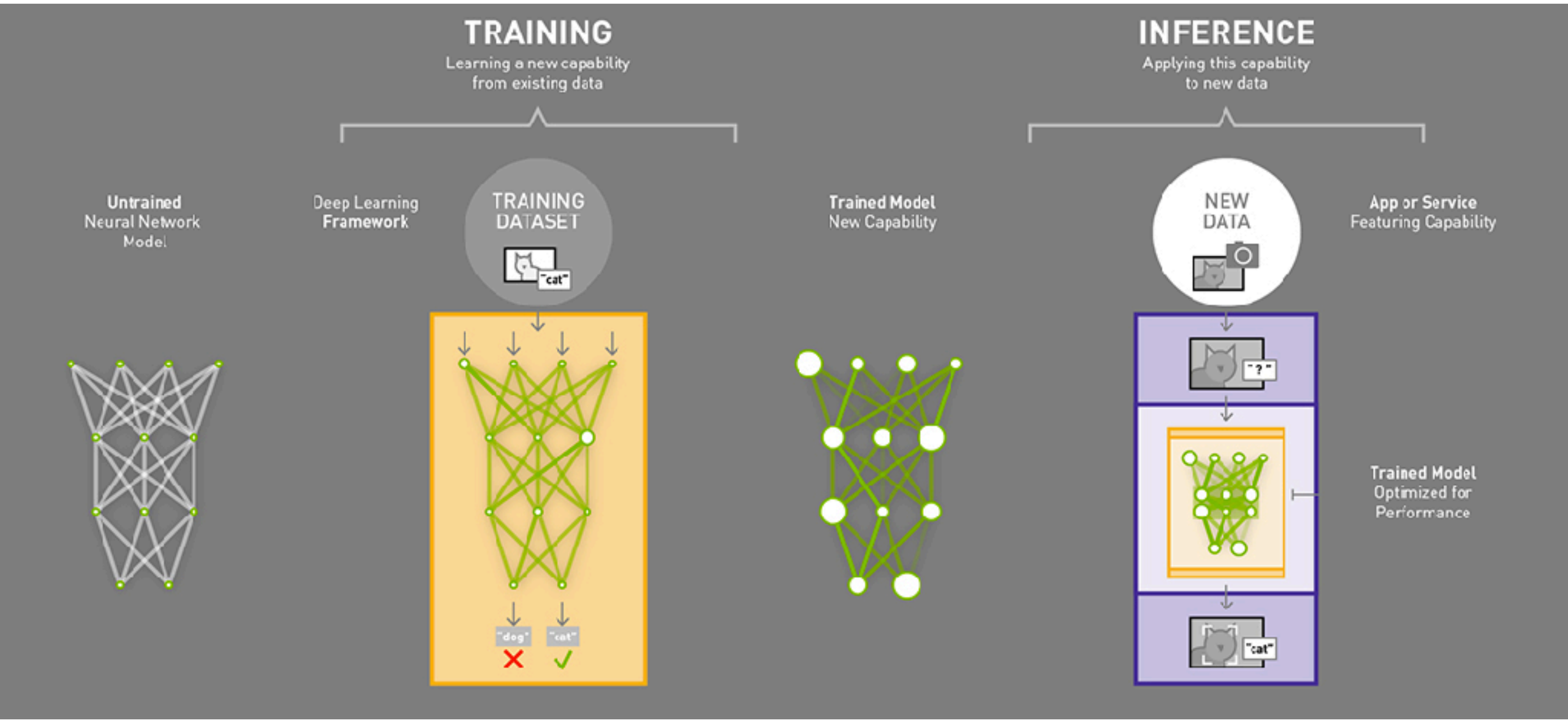
x mg/dL

normal if $x < 100$

prediabetes if $100 \leq x \leq 125$

diabetes if $125 < x$

Overview: Machine Learning



Create a model

Train the model with training data

Test the trained model with test data

Source: NVIDIA

keywords: feature extraction, classification task, classifier

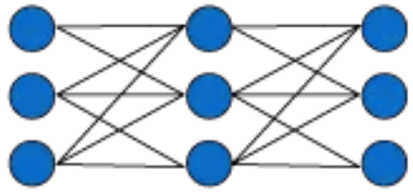
Example: Watermelon or Orange?

Traditional Machine Learning

Input image

Feature extraction

random forest, SVM, kNN, XGBoost, LGBM



Classification

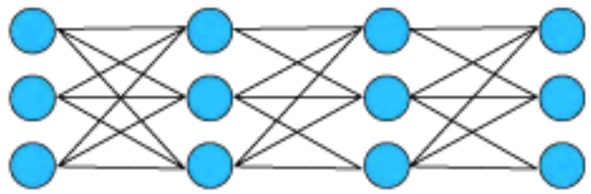
Output

watermelon

Deep Learning

Input image

deep neural network



Feature extraction + Classification

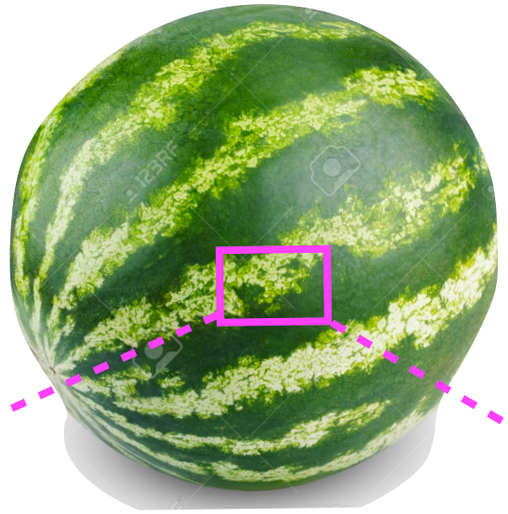
Output

watermelon

Some parts taken from: Azua Tech

keywords: vector, matrix, tensor, pixel

What we see



orange: 0

watermelon: 1

What computers see

Red

Green

Blue

52	55	56	50	50	60	54	48	50	61	57	66	68	113	117	86	129	153	181	206	205	207	203	203	217	209
55	75	97	70	94	64	55	52	57	55	71	87	72	97	133	148	190	204	204	209	204	200	204	194	153	204
82	111	121	97	107	90	54	77	68	58	134	179	113	119	163	205	203	180	203	206	194	184	187	149	144	198
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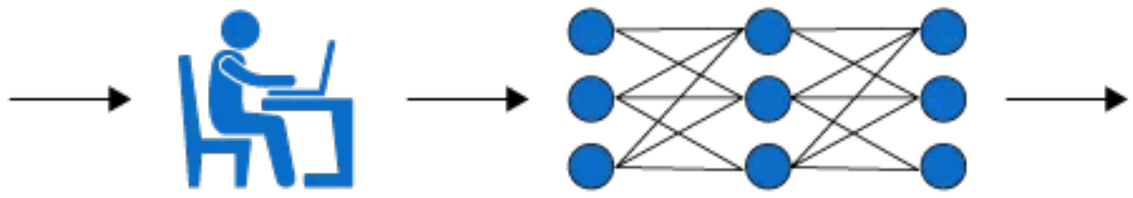
29	42	36	25	33	41	58	35	27	28	25	27	27	35	30	36	31	35	31	31	33	39	37	39	37	40
25	33	26	24	37	34	26	29	30	28	26	36	29	32	27	28	31	34	30	34	32	36	37	38	40	45

Watermelon or Orange?

Traditional Machine Learning

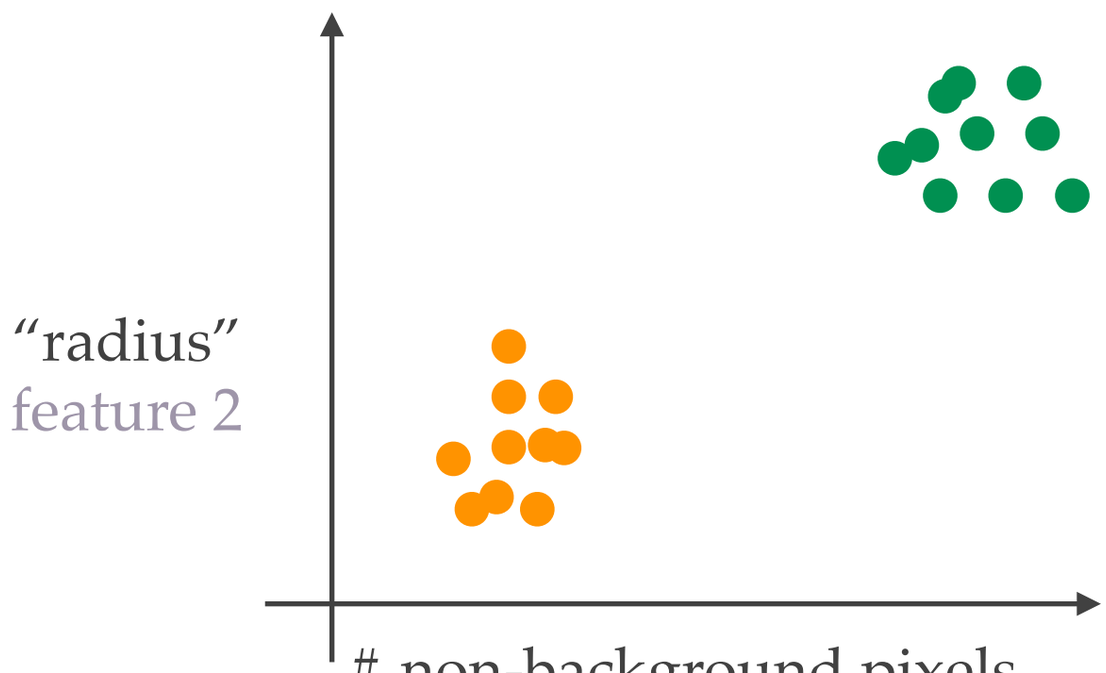
Input image



Output

watermelon

Phase: Training



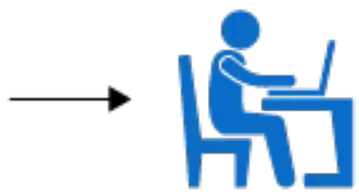
current sample

keywords: feature extraction, feature engineering, handcrafted/hand-designed features, feature space, descriptors

Watermelon or Orange?

Traditional Machine Learning

Input image

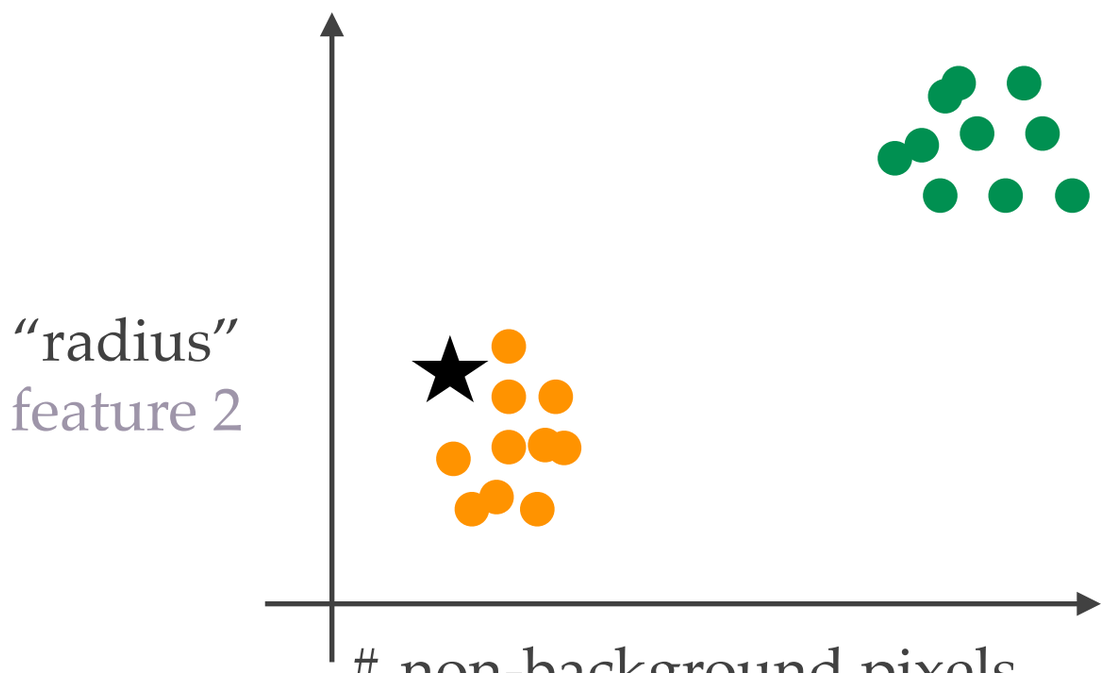


Output

watermelon

Phase: Testing

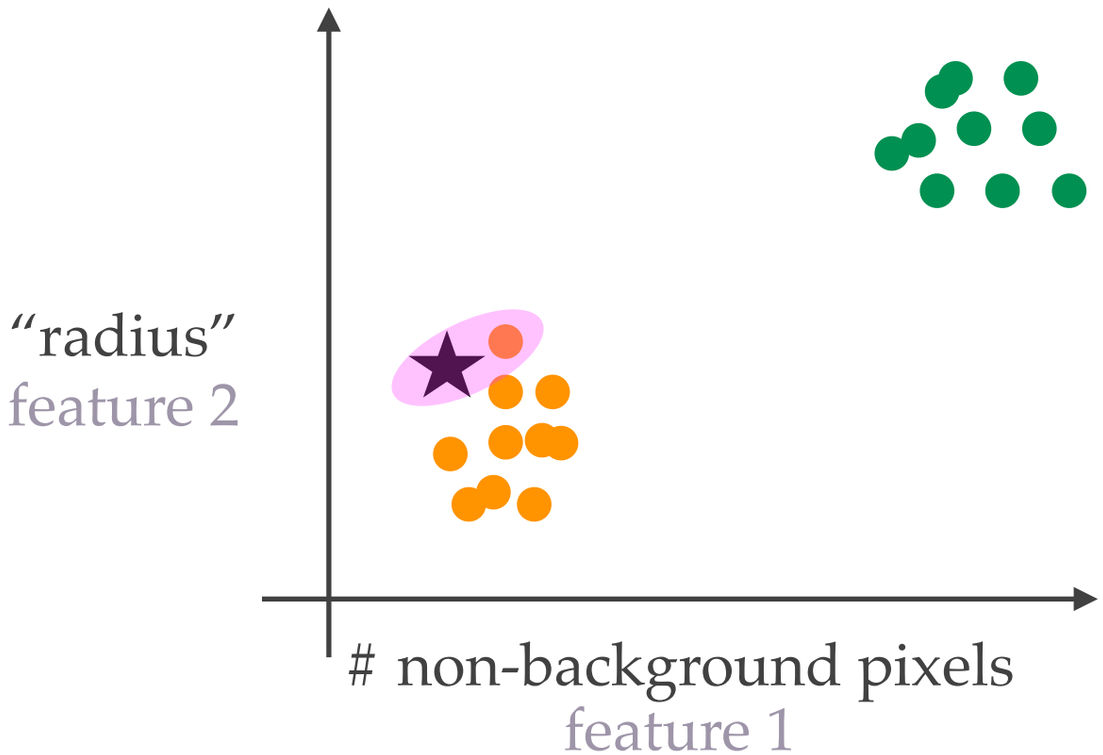
current sample



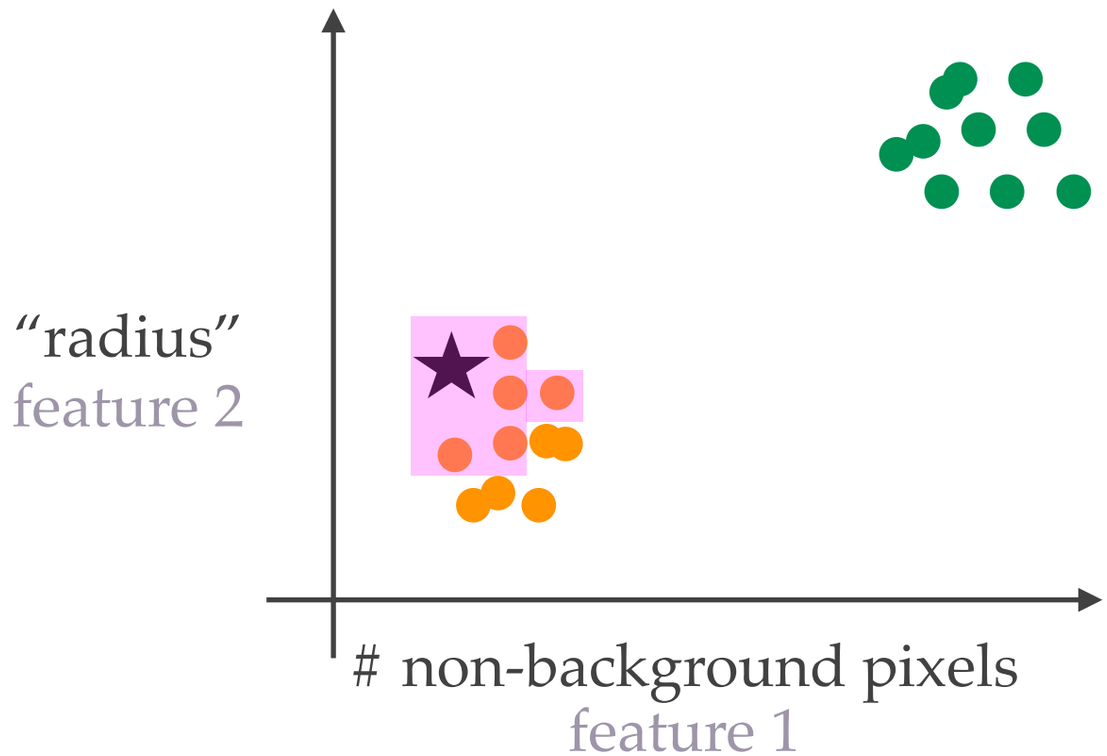
Orange!

keyword: decision boundary

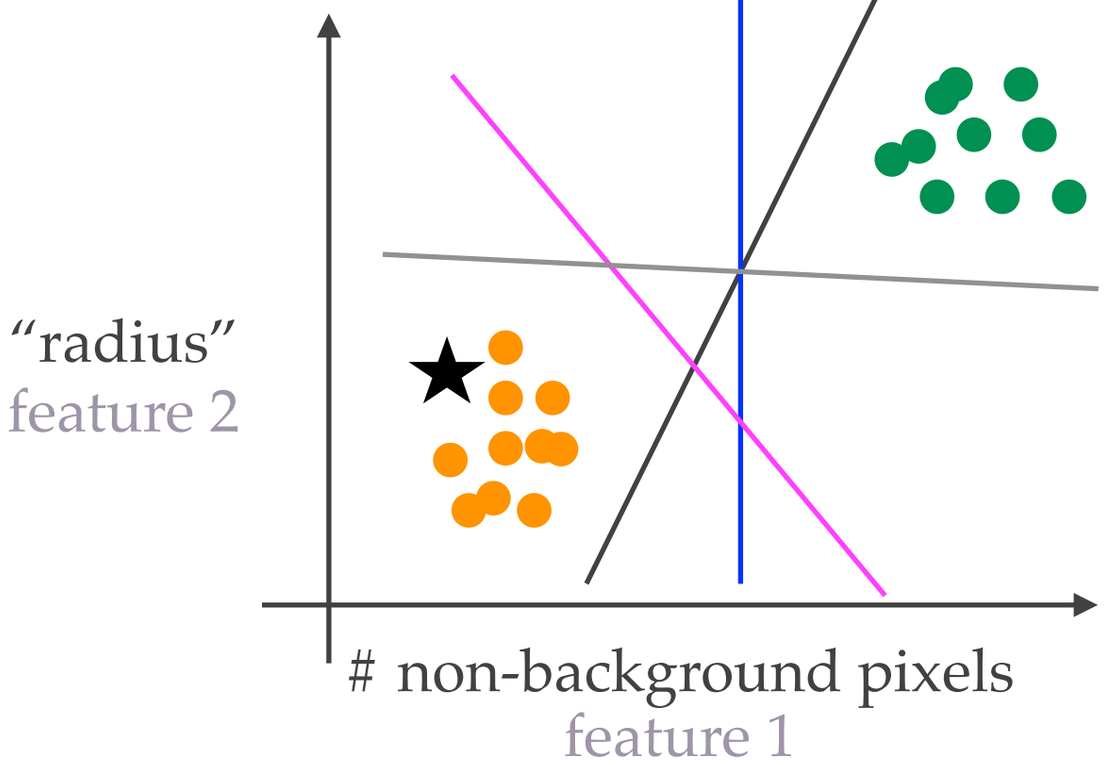
Nearest Neighbor



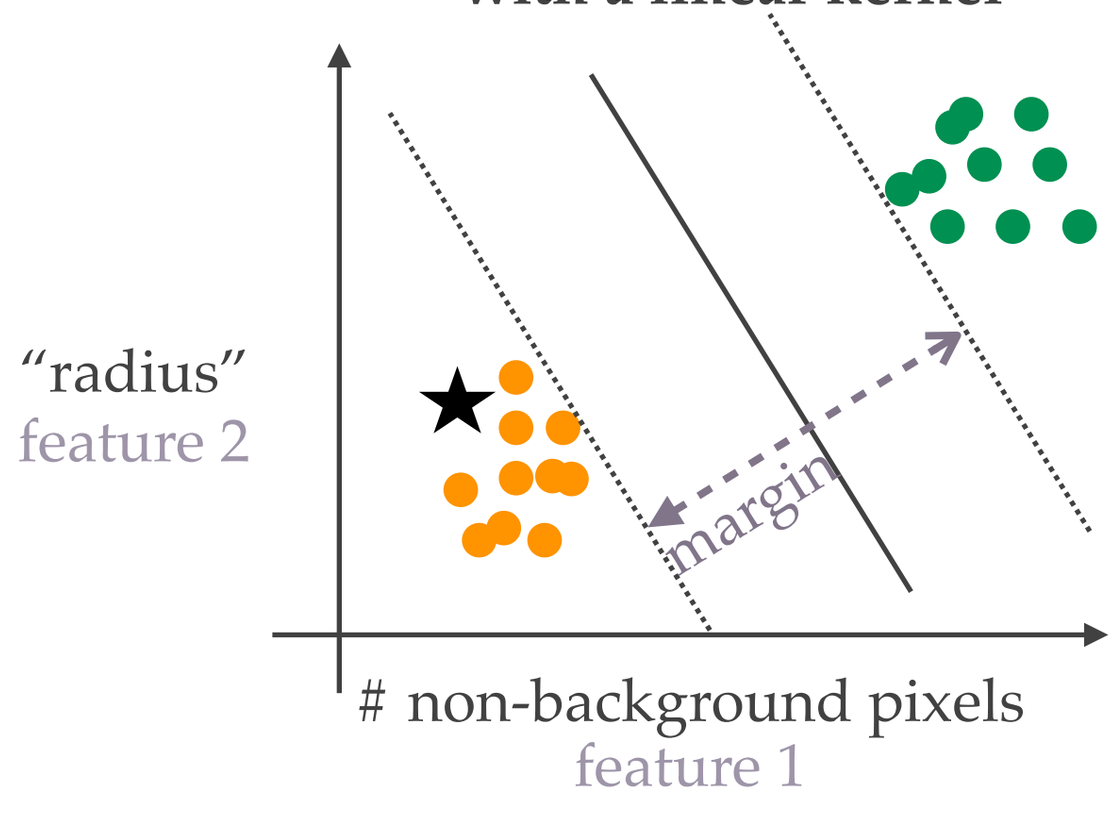
k-Nearest Neighbors (kNN)



Linear Classifier

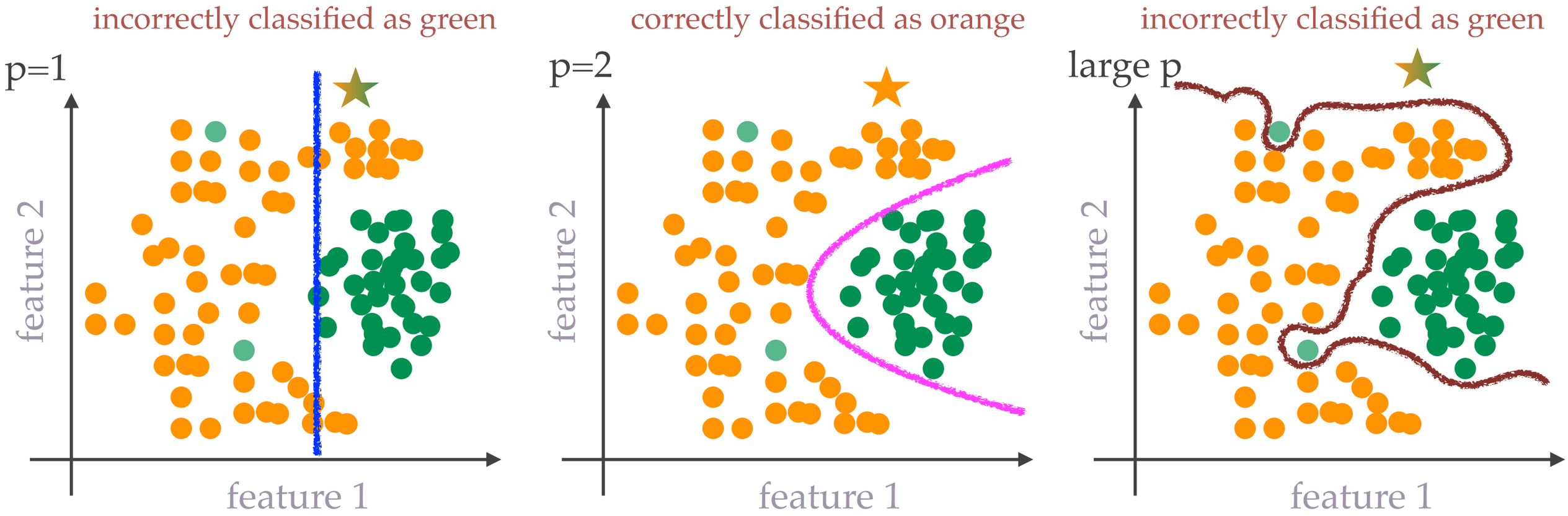


Support Vector Machine (SVM) with a linear kernel



What should we pick as our model?

If we use a p^{th} order polynomial to separate the classes, what happens when p=1? p=2? large p?



Underfit

Doesn't perform well for both seen (training) and unseen (test) data

- High training error
- High test error

Overfit

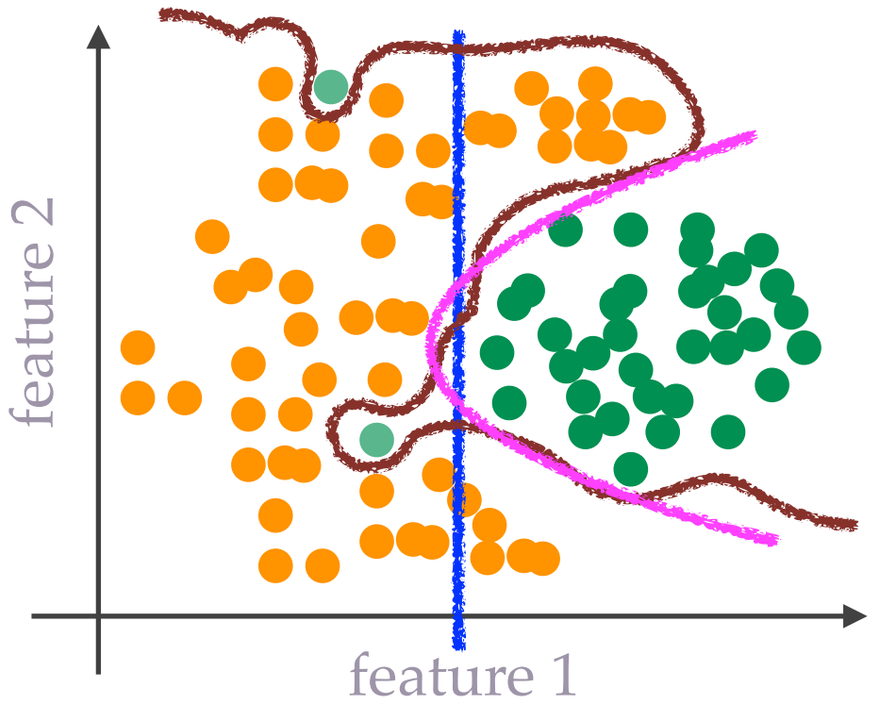
Perform well for training data, but not test data

- Low training error
- High test error

keywords: model selection, hyper-parameter tuning, training/validation/test data

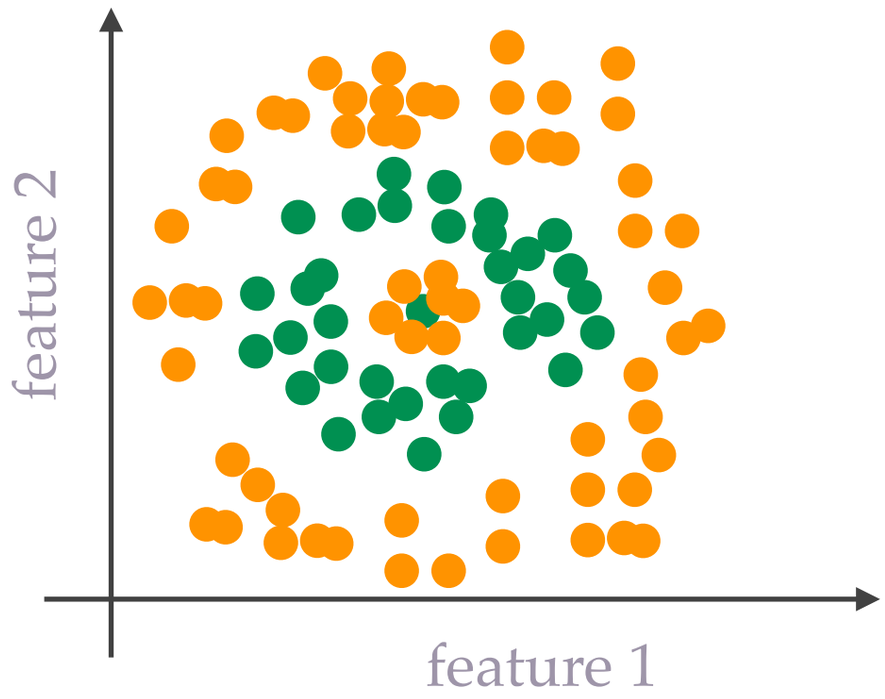
What should we pick as our model?

Polynomial order: p = ?



If we use a p^{th} order polynomial to separate the classes, what happens when p=1? p=2? p=1000?

k-Nearest Neighbors: k = ?



What happens when k is large (e.g., k=1000)?

What happens when k=1?

How do we pick a model (e.g., simple linear classifier, p^{th} order polynomial, k-nearest neighbors, logistic regressor)? How do we pick p and k?

Validation data (in addition to training and test data, which we have seen earlier)!

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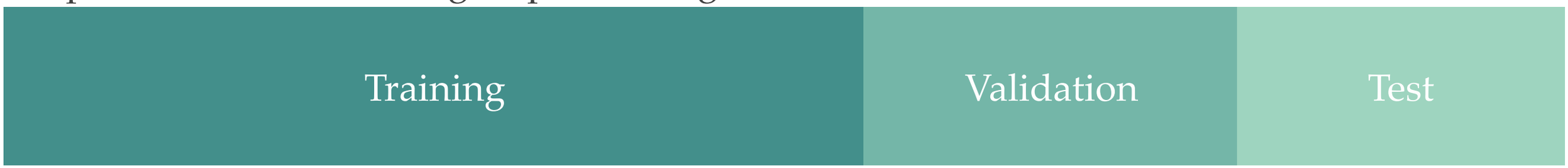
Simplified Pipeline & Training, Validation, and Test Data

1. Given a task, pick a model linear vs nonlinear? Polynomial of order p = 3 vs p = 21?

2. Split the data into three groups: training, validation, and test



3. Optimize the selected model using the training data

4. Evaluate the trained model using the validation data

5. Pick more models, optimize the models, and evaluate the trained models on the validation data

Ex. Pick the model with the smallest validation error (out of the 30 models)

6. Use the model with the lowest validation error as your final model

Ex. Try a linear model, 8 kNNs with different k, and 20 polynomials with p = 2, 3, …, 21

7. Evaluate the final model on the test data

Example: Training, Validation, and Test Data

Scenario: A time-limited, two-choice materials science exam will be held next month. We have come up with four strategies (i.e., 4 models) for acing the upcoming exam

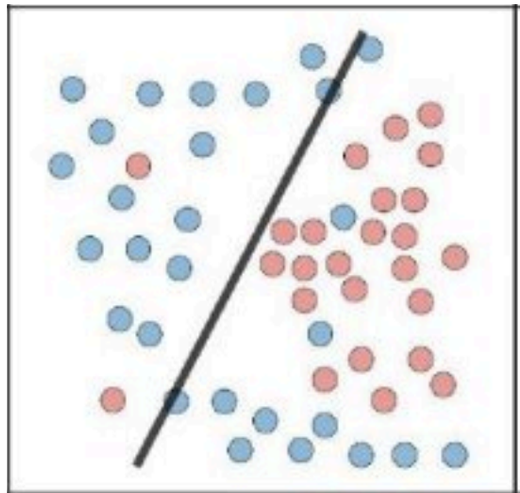
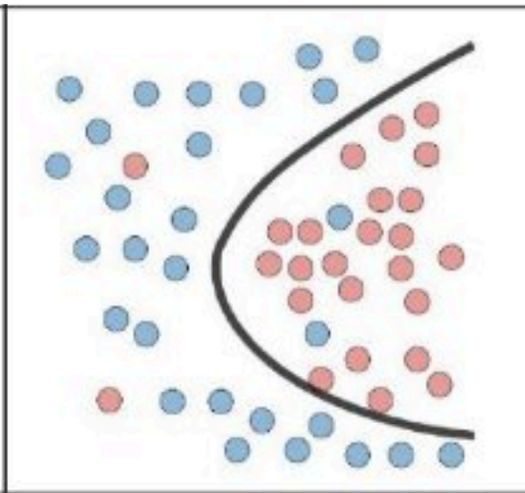
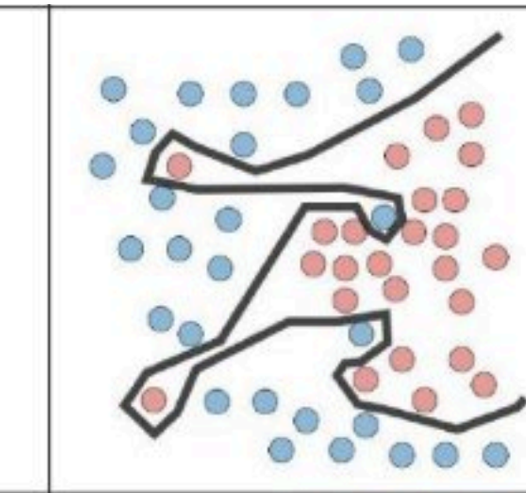
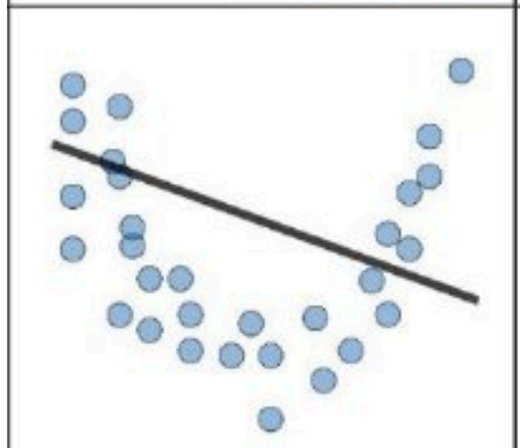
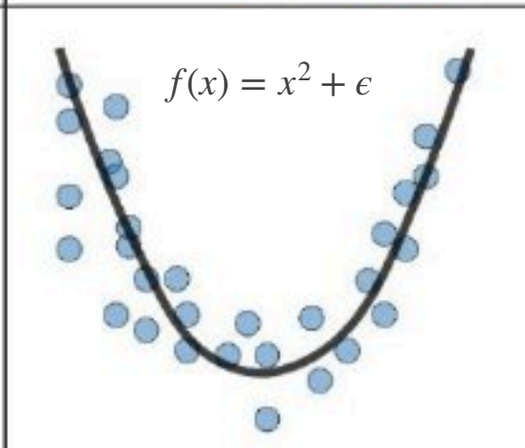
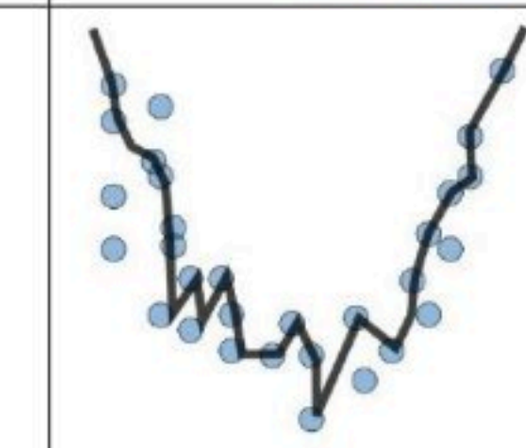
- AI #1: Always pick choice 1 ☐ choice 1 ☐ choice 2
- AI #2: Pick choice 1 for the first half of the exam and learn what to answer for the rest
- AI #3: Pick choice 2 for the first half of the exam and learn what to answer for the rest
- AI #4: Learn what to answer for all questions

Training	Validation	Test
Practice problems and previous exams from the last decade (except 2018-2021)	2018-2021 exams	The upcoming exam (unseen)

Steps

1. Use the training problems and exams to teach all the AI models.
2. Use the validation exams to see how the trained models perform.
3. Select the AI model that achieves the highest score on the validation exams to take the upcoming exam (test exam) for you

Overfitting and Underfitting

	Underfitting		Overfitting
Classification			
Regression			
Likely symptoms	• High training error • Training error close to test error	• Training error slightly lower than test error	• Low training error • Test error much higher than training error

https://i.pinimg.com/originals/72/e2/22/72e222c1542539754df1d914cb671bd7.png

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Watermelon or Orange?

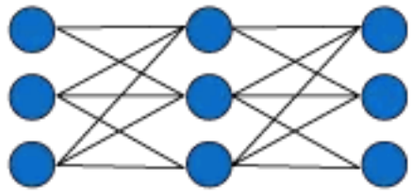
Traditional Machine Learning

Input image

hand-engineered / hand-crafted features

Feature extraction

random forest, SVM, kNN, XGBoost, LGBM



Classification

Output

watermelon

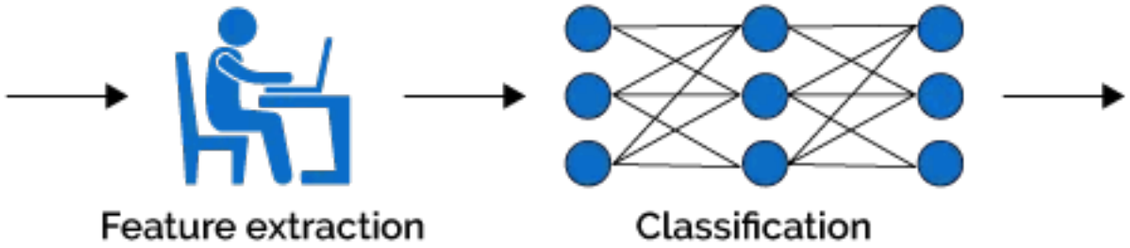
Problem with feature engineering?

Some parts taken from: Azua Tech

Watermelon or Orange?

Traditional Machine Learning

Input image

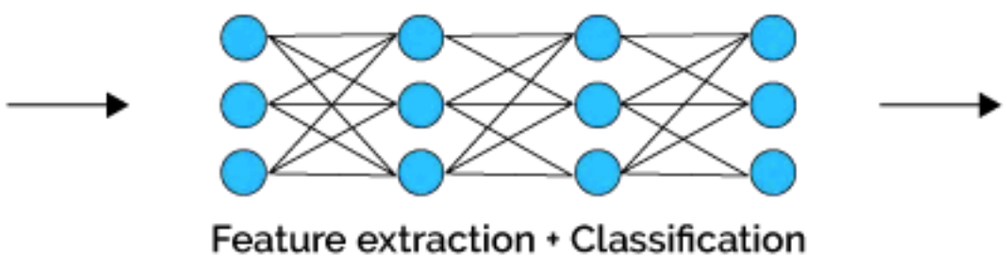


Output

watermelon

Deep Learning

Input image



Output

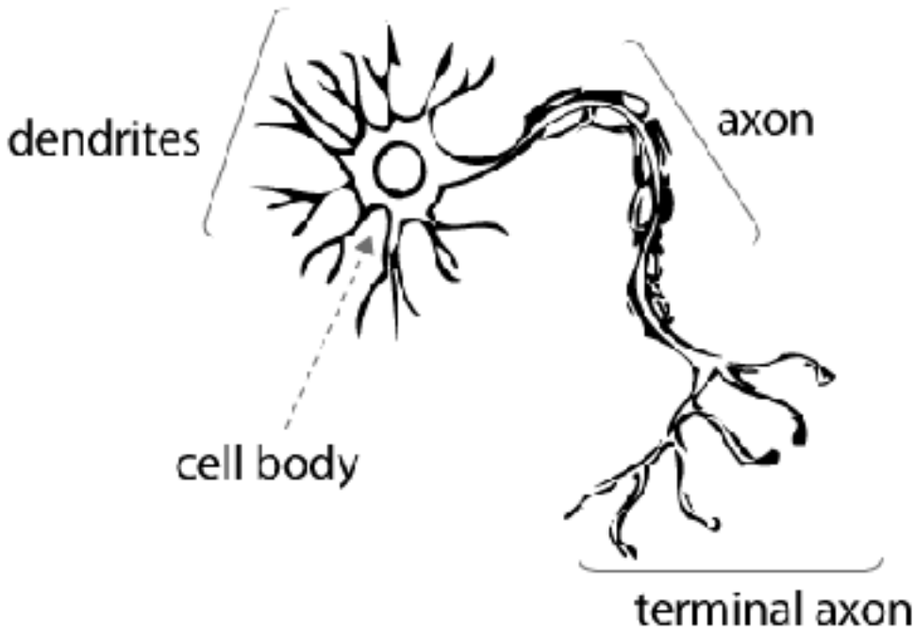
watermelon

Some parts taken from: Azua Tech

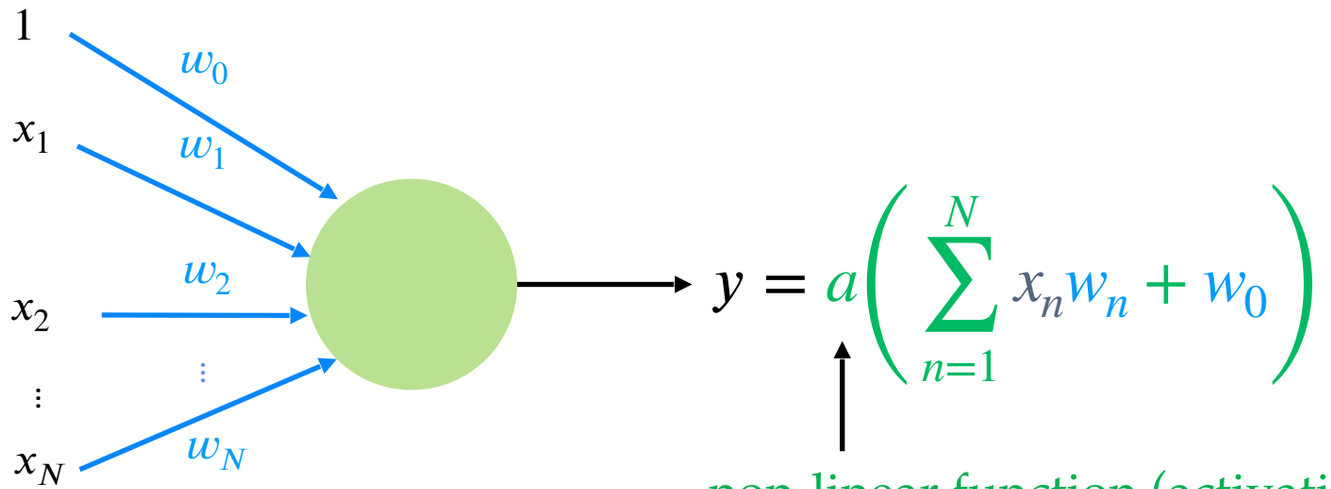
Deep Learning

- Deep learning is a subfield of machine learning that stems from artificial neural networks (ANN)

Single neuron



Artificial neuron



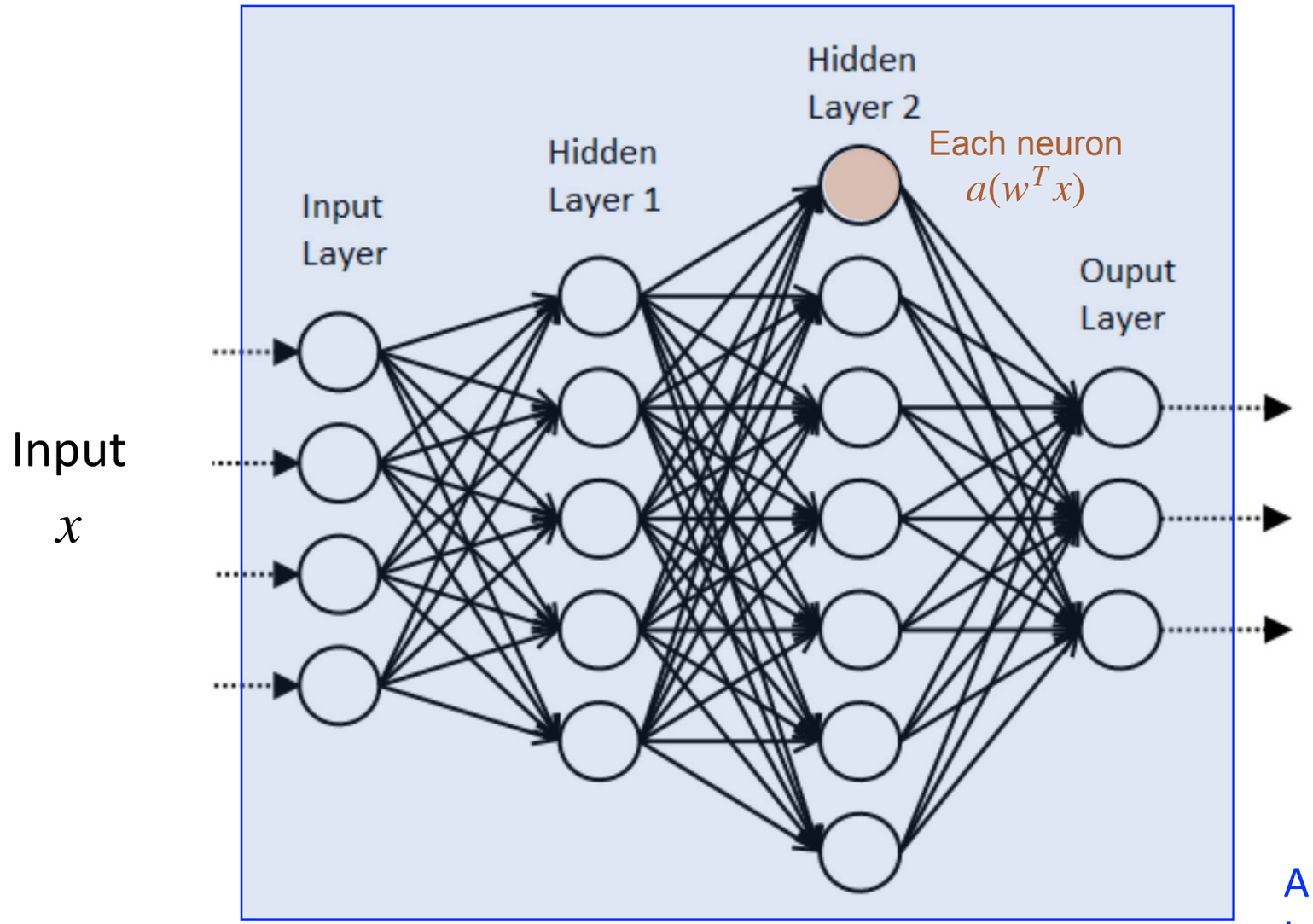
If we set all the weights to 0, then $y = 0$.
If we set $w_1 = 1$ and the rest to 0, then $y = a(x_1)$.
If we set $w_0 = 0$ and the rest to 1, then $y = a(x_1 + x_2 + \ldots + x_N)$.

Different weights give rise to different behavior

Source: The Essense of Artificial Neural Networks by Ivan Liljeqvist (Medium)

Deep Learning

- An artificial neural network with many hidden layers is called a deep artificial neural network (ANN)



$$y = f_W(x)$$

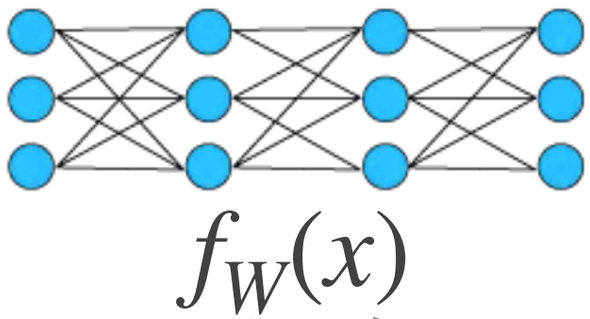
A function that can change behavior depending on the current value of W

Deep Learning

- Think of a deep NN as a universal function approximator

Image classification

Input image

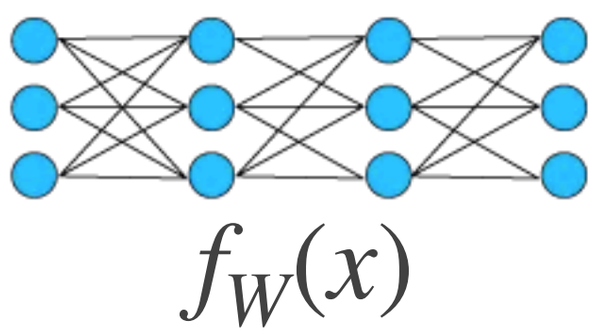


Output: Label

1 (watermelon)

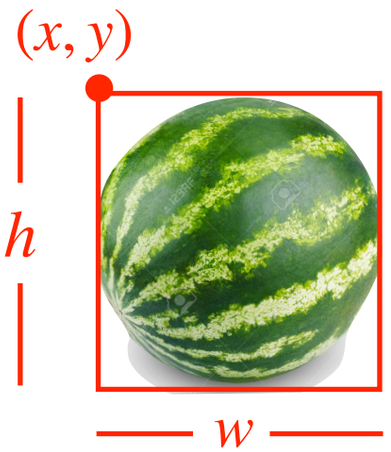
Object detection

Input image



Output: rectangular box

$$\begin{bmatrix} x \\ y \\ w \\ h \end{bmatrix}$$



Fully connected layer
(Dense)

Optimizer

SGD
Adam
RMSprop

Convolutional layer

Conv1D, 2D, 3D, …
separable Conv

Deep Learning

Evaluation metric

accuracy
F1-score
AUC
confusion matrix

Pooling layer

max-pooling
average-pooling

Activation function

sigmoid
softmax
ESP (swish)
ReLU

Loss function

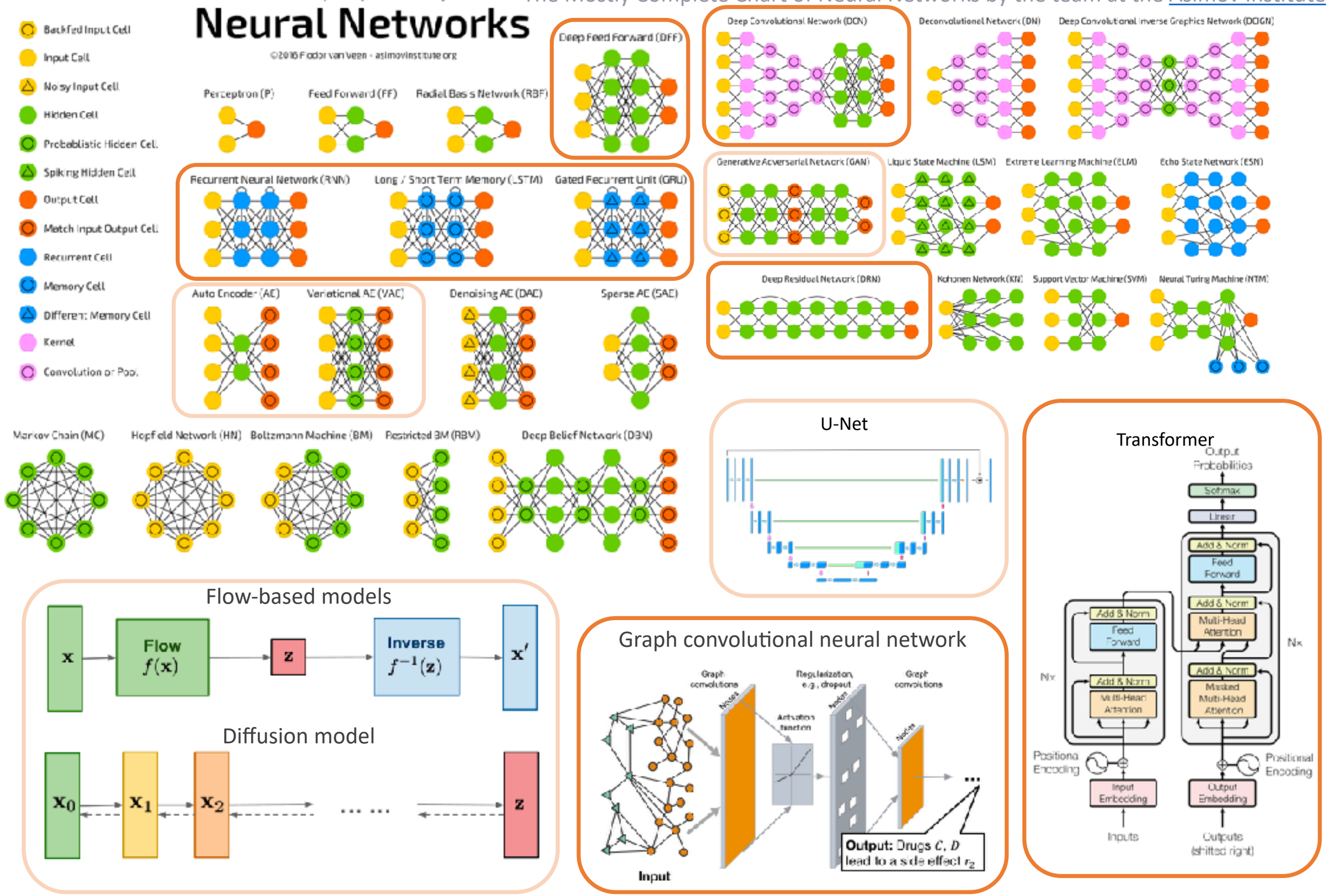
categorical crossentropy
binary crossentropy
mean squared error
mean absolute error

Regularization

Dropout
Data augmentation
l_1, l_2 regularizations

- Combine basic components to build a neural network
  - More components → "More" representative power

The Mostly Complete Chart of Neural Networks by the team at the Asimov Institute



U-Net

Transformer

Flow-based models

Diffusion model

What are Diffusion Models?

Graph convolutional neural network

Graph Neural Networks for Multirelational Link Prediction

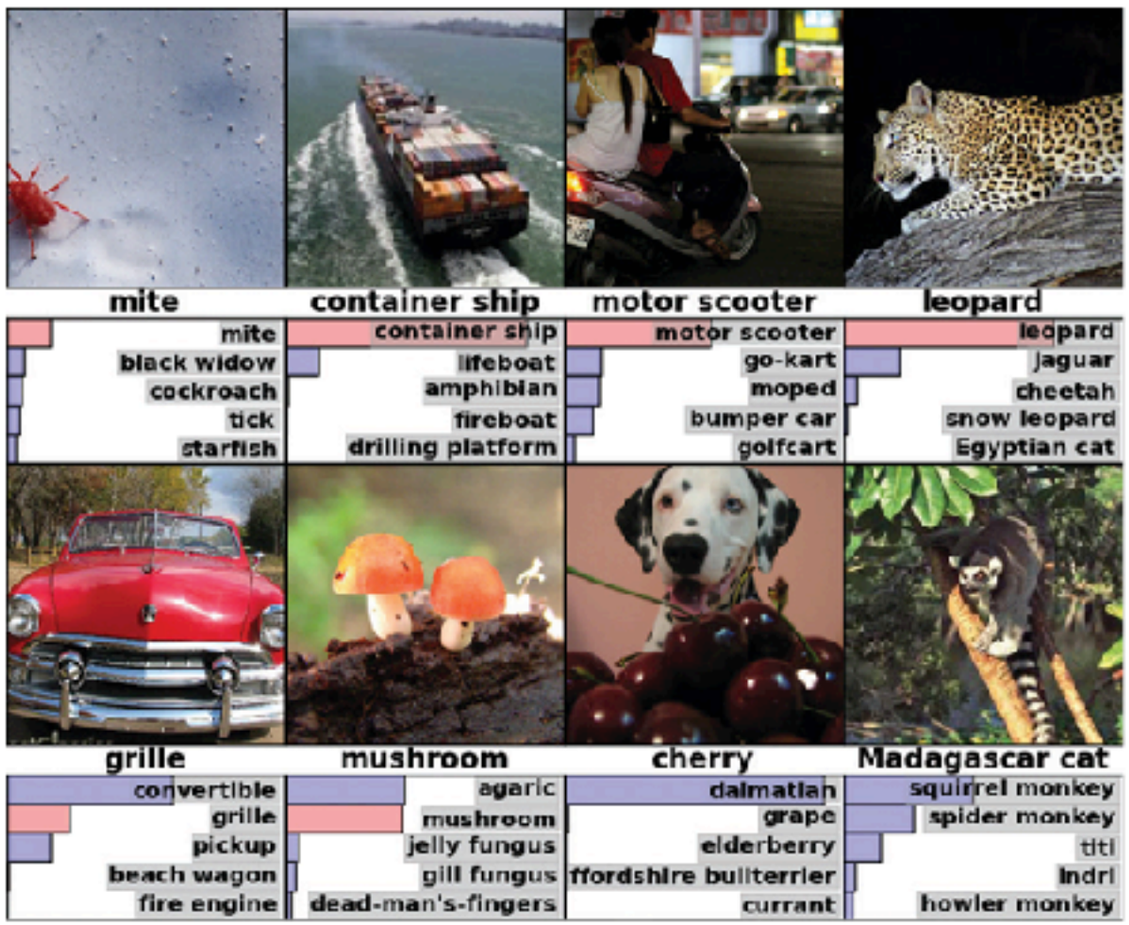
Vaswani, Ashish, et al. "Attention is all you need." Advances in neural information processing systems 30 (2017).

ImageNet

IMAGENET

1000 classes, 14,197,122 images

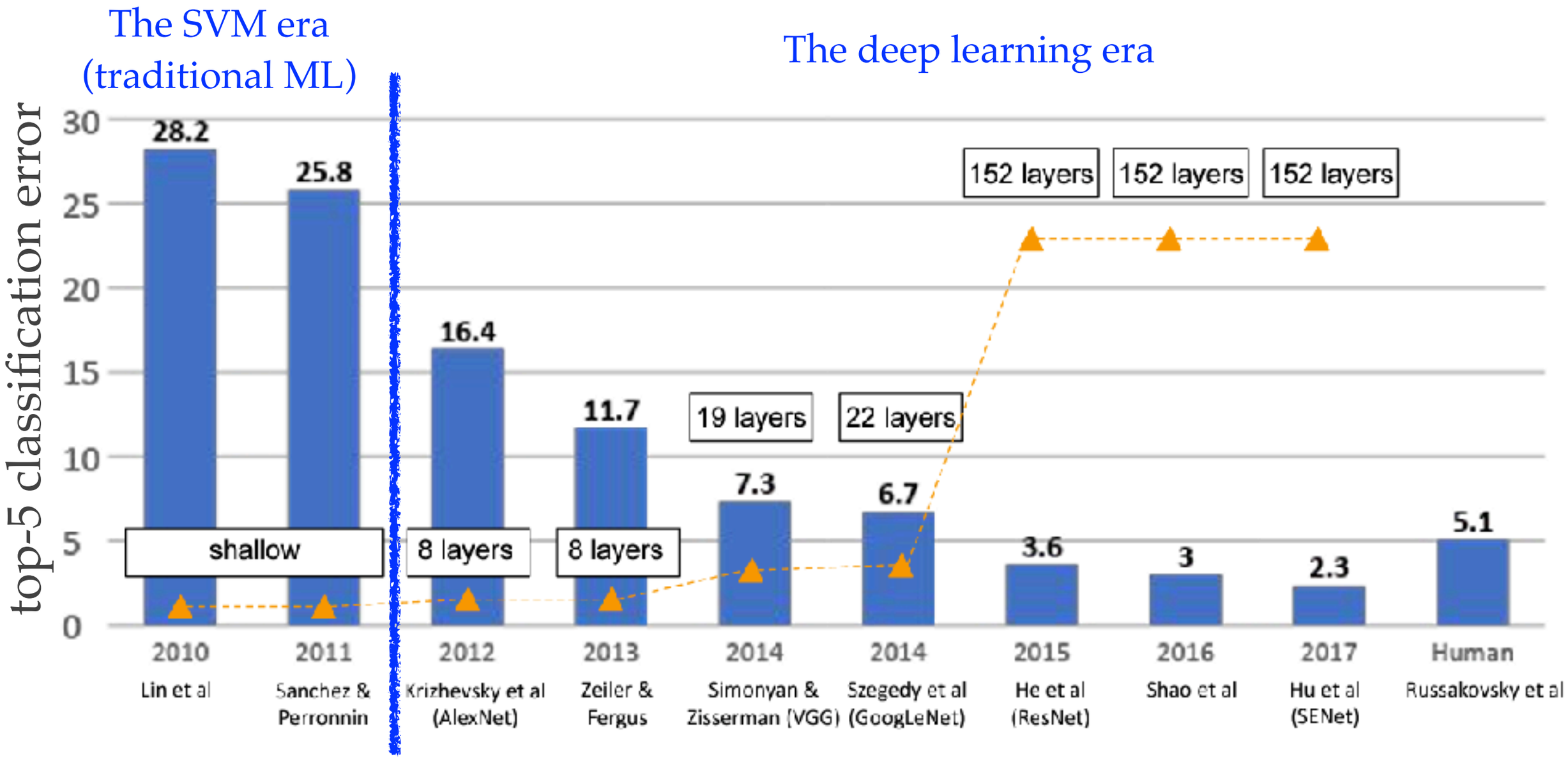
Figure 4. (Left) Eight ILSVRC-2010 test images and the five labels considered most probable by our model. The correct label is written under each image, and the probability assigned to the correct label is also shown with a red bar (if it happens to be in the top 5). (Right) Five ILSVRC-2010 test images in the first column. The remaining columns show the six training images that produce feature vectors in the last hidden layer with the smallest Euclidean distance from the feature vector for the test image.



Krizhevsky, Alex, Ilya Sutskever, and Geoffrey E. Hinton. "Imagenet classification with deep convolutional neural networks." Advances in neural information processing systems 25 (2012).

ImageNet

ImageNet Large Scale Visual Recognition Challenge (ILSVRC) winners



Outline

- Introduction to Supervised Machine Learning
  - AI vs ML vs DL
  - Traditional Machine Learning
  - Training, Validation, and Test Data
  - Overfitting and Underfitting
- Introduction to Supervised Deep Learning
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  - Fully Connected Layers
  - Activation Functions
  - Optimization

Supervised Model Training

Step 1: Create a neural network with some initial weight f_{W_0}

Neural network

Training iteration 0

f_{W_0}

Supervised Model Training

Step 2: Prepare a dataset which is a collection of input-output pairs

Prepared inputs
x

Prepared outputs
(true labels)
y

1

0

0

1

Neural network

Training iteration 0
f_{W_0}

orange: 0
watermelon: 1

Supervised Model Training

Step 3: Pass the prepared inputs to the network

Prepared inputs
x

Neural network

Training iteration 0
f_{W_0}

Estimated outputs
$\hat{y} = f_{W_0}(x)$

Prepared outputs (true labels)
y

Estimated outputs $\hat{y} = f_{W_0}(x)$	Prepared outputs (true labels) y
0.6	1
0.6	0
0.5	0
0.5	1

orange: 0

watermelon: 1

Supervised Model Training

Step 4: Compare $\hat{y}$ to y and modify the weights of the neural network to make $\hat{y}$ approach y using the backpropagation algorithm

Prepared inputs
x

A simple loss function: $L(y, \hat{y}) = \sum_{i=1}^{N} (\hat{y}_i - y_i)^2$

$L(y, \hat{y}) = (0.6 - 1)^2 + (0.6 - 0)^2 + (0.5 - 0)^2 + (0.5 - 1)^2 = 1.02$

Estimated outputs
$\hat{y} = f_{W_0}(x)$

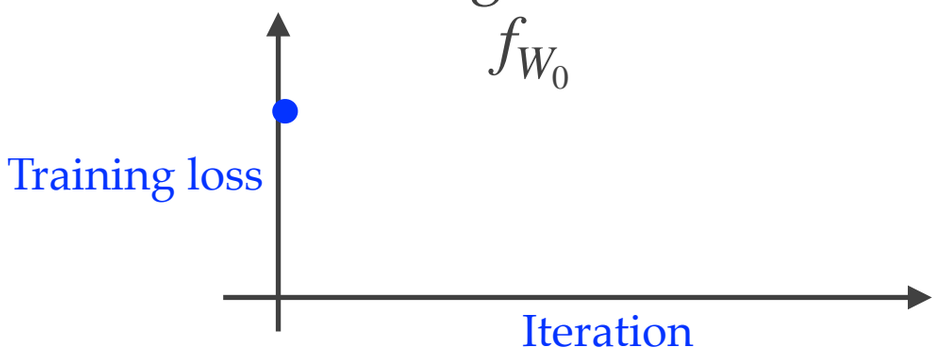
Prepared outputs (true labels)
y

0.6

1

Neural network

Training iteration 0
f_{W_0}



0.6 0

0.5 0

0.5 1

orange: 0

watermelon: 1

Supervised Model Training

Repeat steps 3 and 4 to continuously improve the weights of the neural network

Prepared inputs
x

A simple loss function: $L(y, \hat{y}) = \sum_{i=1}^{N} (\hat{y}_i - y_i)^2$

Estimated outputs
$\hat{y} = f_{W_1}(x)$

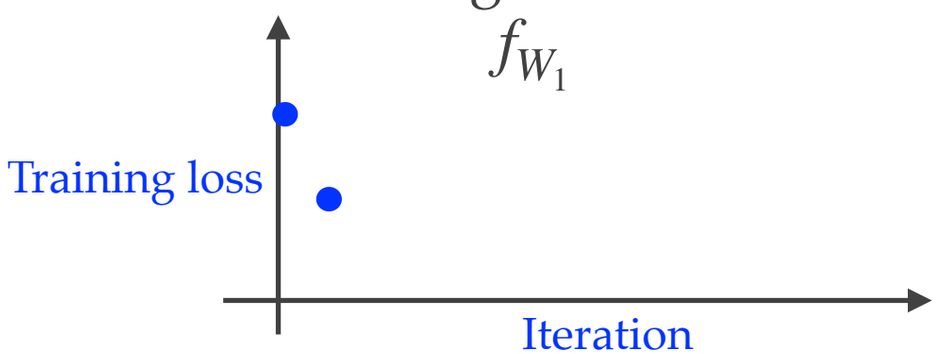
Prepared outputs (true labels)
y

$L(y, \hat{y}) = (0.6 - 1)^2 + (0.4 - 0)^2 + (0.4 - 0)^2 + (0.6 - 1)^2 = 0.64$

0.6 | 1

Neural network

Training iteration 1



0.4 | 0

0.4 | 0

0.6 | 1

orange: 0

watermelon: 1

Supervised Model Training

Repeat steps 3 and 4 to continuously improve the weights of the neural network

Prepared inputs
x

A simple loss function: $L(y, \hat{y}) = \sum_{i=1}^{N} (\hat{y}_i - y_i)^2$

Estimated outputs
$\hat{y} = f_{W_2}(x)$

Prepared outputs (true labels)
y

$L(y, \hat{y}) = (0.7 - 1)^2 + (0.35 - 0)^2 + (0.4 - 0)^2 + (0.6 - 1)^2 = 0.5325$

0.7 1

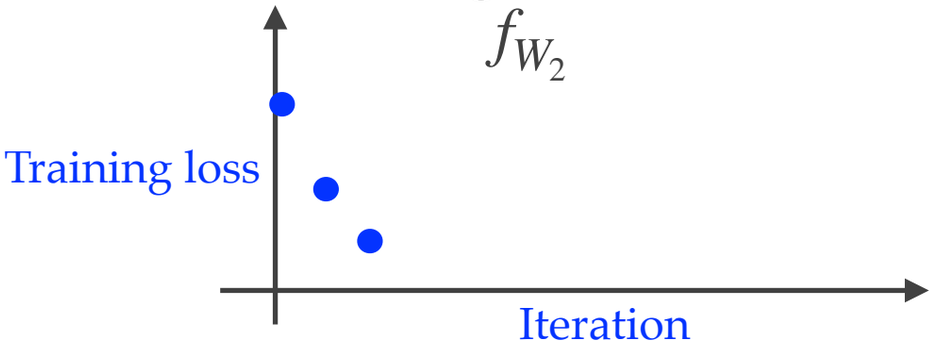
Neural network

0.35 0

0.4 0

Training iteration 2

f_{W_2}



0.6 1

orange: 0

watermelon: 1

Supervised Model Training

Repeat steps 3 and 4 to continuously improve the weights of the neural network

Prepared inputs
x

A simple loss function: $L(y, \hat{y}) = \sum_{i=1}^{N} (\hat{y}_i - y_i)^2$

Estimated outputs
$\hat{y} = f_{W_{50}}(x)$

Prepared outputs (true labels)
y

$L(y, \hat{y}) = (0.8 - 1)^2 + (0.15 - 0)^2 + (0.1 - 0)^2 + (0.9 - 1)^2 = 0.0825$

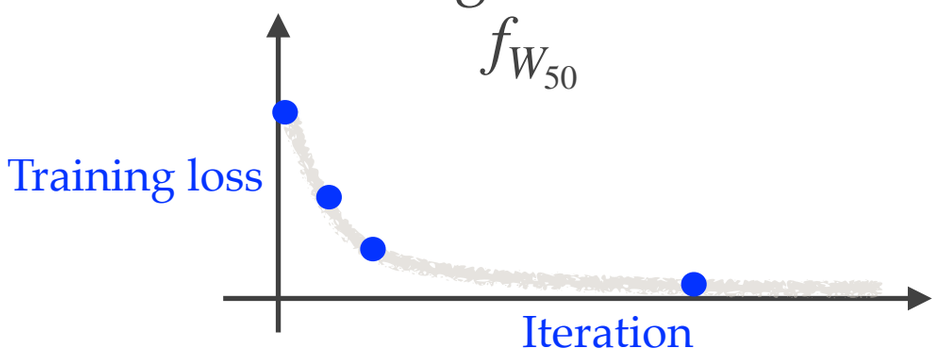
0.8 — 1

Neural network

0.15 — 0

0.1 — 0

Training iteration 50
$f_{W_{50}}$



0.9 — 1

orange: 0
watermelon: 1

Supervised Model Training

Repeat steps 3 and 4 to continuously improve the weights of the neural network

Prepared inputs

x

A simple loss function: $L(y, \hat{y}) = \sum_{i=1}^{N} (\hat{y}_i - y_i)^2$

Estimated outputs

$\hat{y} = f_{W_{1000}}(x)$

Prepared outputs (true labels)

y

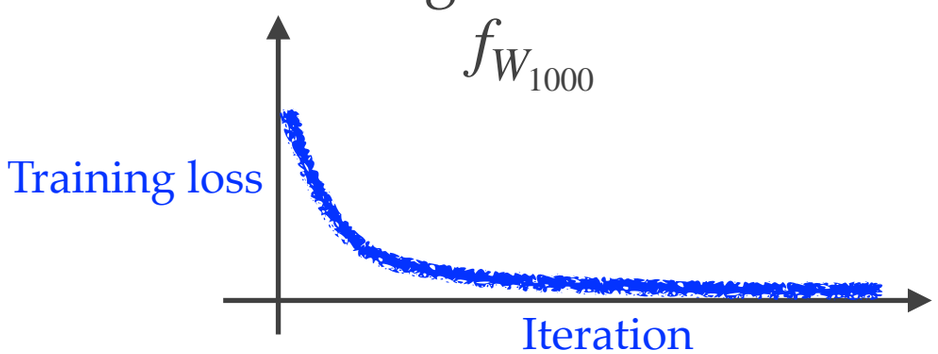
$L(y, \hat{y}) = (0.99 - 1)^2 + (0.05 - 0)^2 + (0.01 - 0)^2 + (0.97 - 1)^2 = 0.0036$

0.99 1

Neural network

Training iteration 1000

$f_{W_{1000}}$



0.05 0

0.01 0

0.97 1

orange: 0

watermelon: 1

keywords: overfitting, underfitting, regularization, early stopping, data augmentation, training/validation/test data

Test the Trained Model

Test image (unseen)

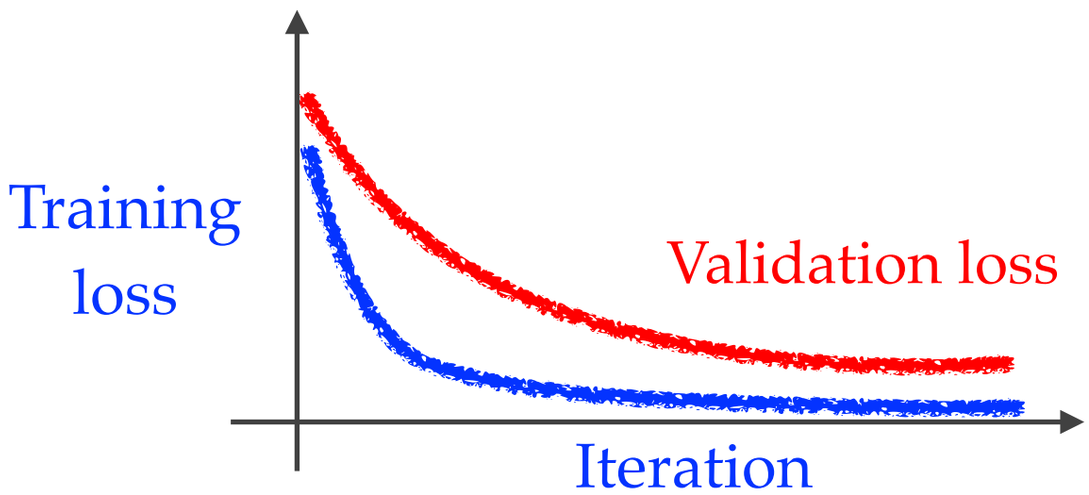
Trained neural network

Predicted Label

0.01

less than 0.5, so it is likely orange

orange: 0
watermelon: 1



https://i.pinimg.com/originals/72/e2/22/72e222c1542539754df1d914cb671bd7.png

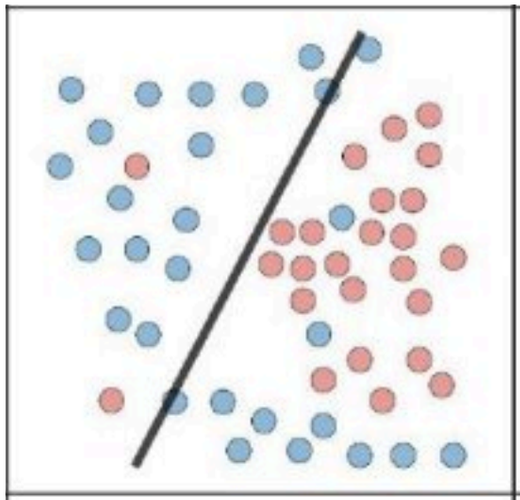
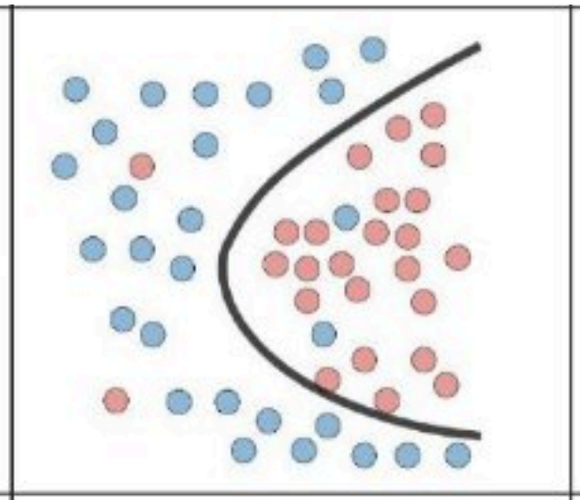
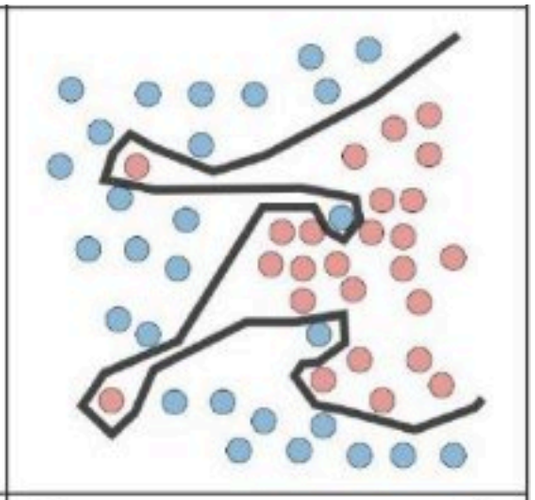
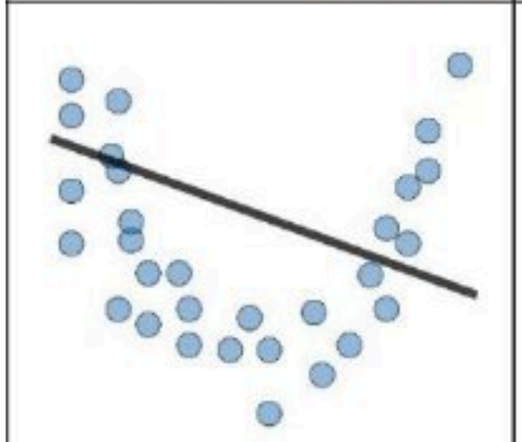
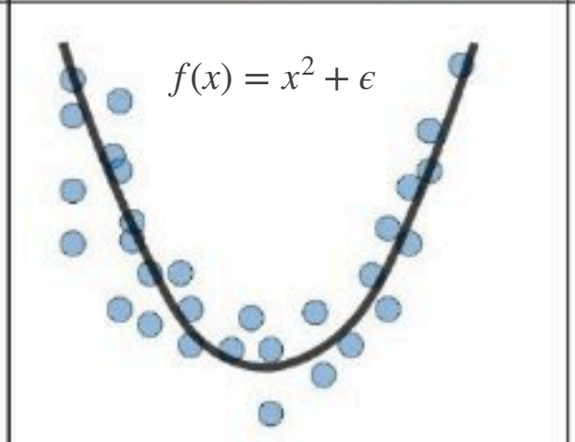
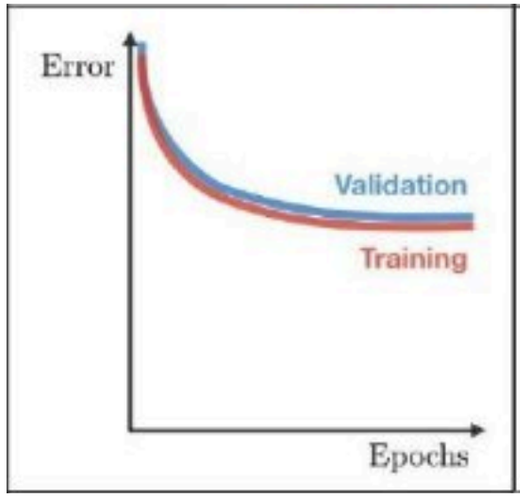
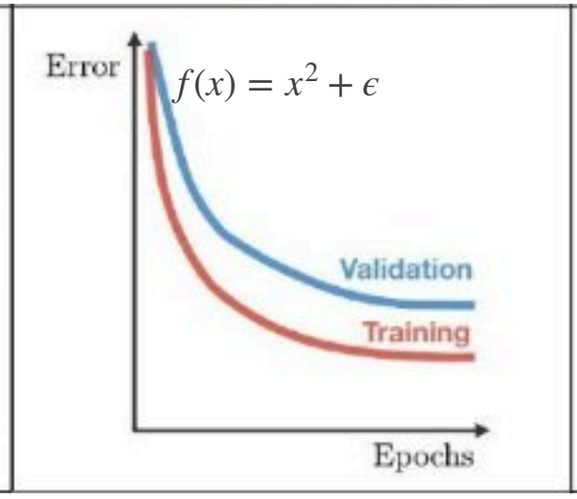
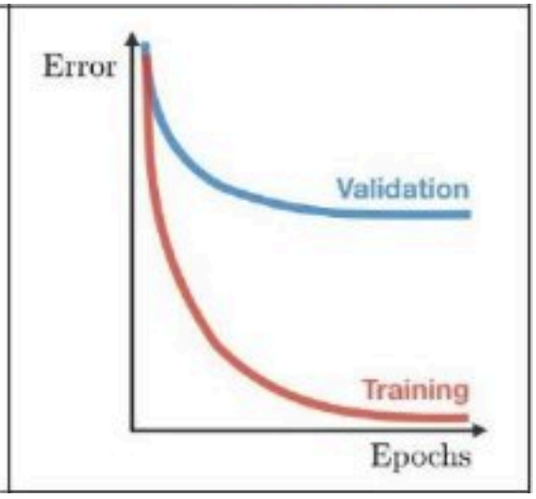
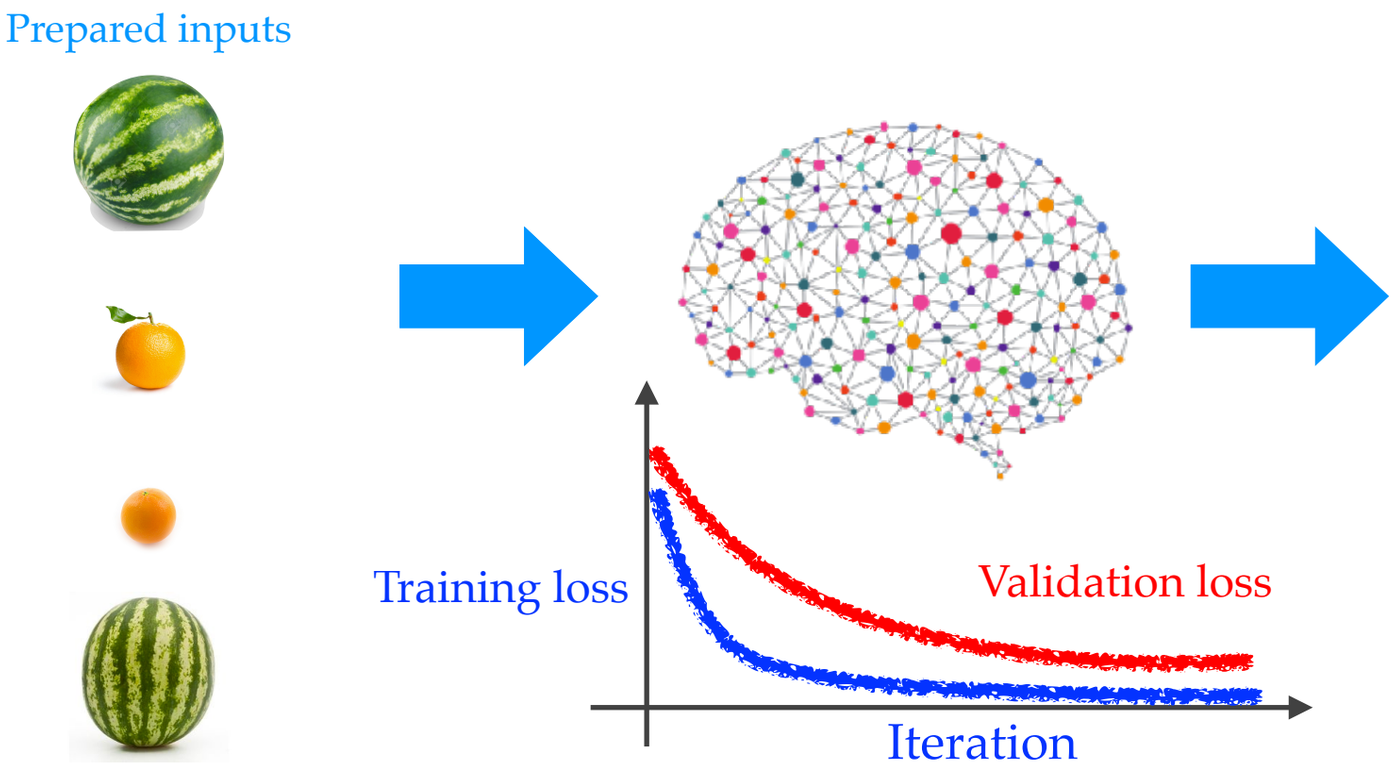
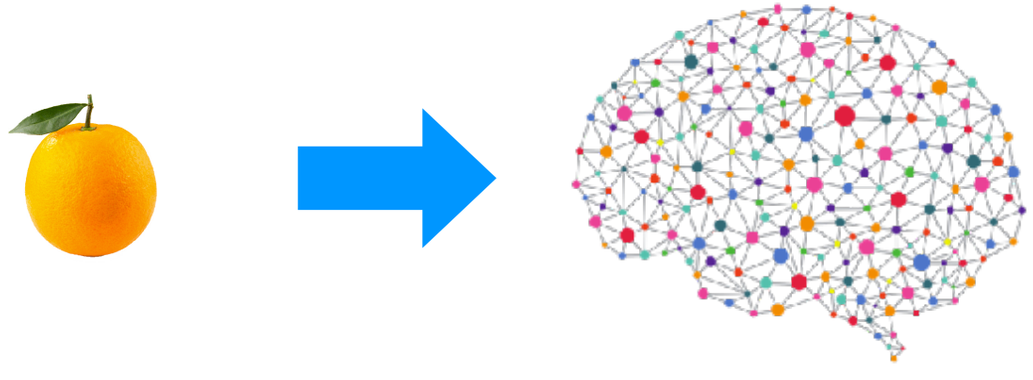
	Underfitting		Overfitting
Classification			
Regression			
Likely symptoms	• High training error • Training error close to test error	• Training error slightly lower than test error	• Low training error • Test error much higher than training error
A way to check for the deep-learning-based methods (both classification and regression)			

Image Classification Using Deep Learning

- Training phase: Optimize the weights of a deep neural network



- Test phase: Perform prediction using the trained neural network



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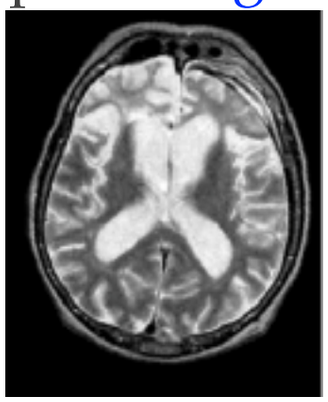
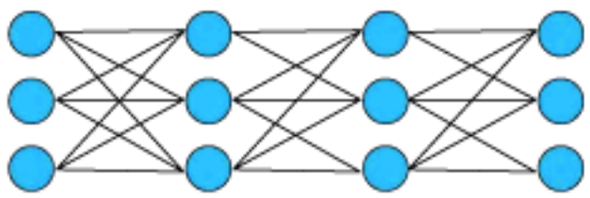
Deep Learning

- Train a deep neural network (NN) to perform some task from data
- Think of a deep NN as a universal function approximator

Image classification

Input: image



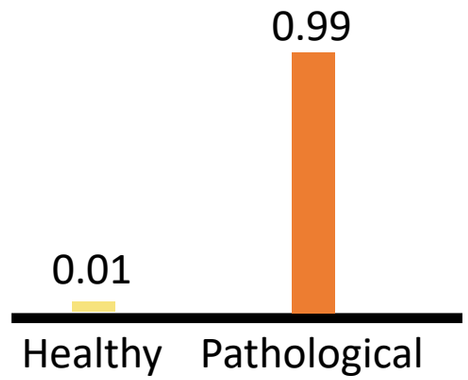


$f_W(x)$

Adjustable weight

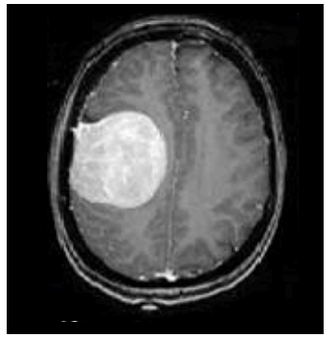
Input

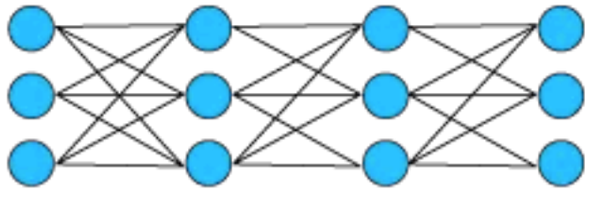
Output: Label



Defect detection

Input: image



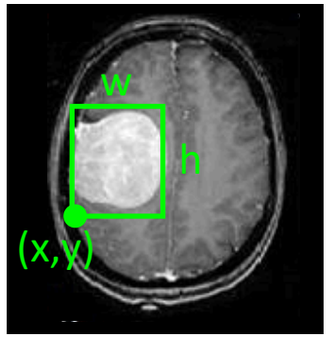


$f_W(x)$

Output: rectangular box(es) and the corresponding class(es)

$$\begin{bmatrix} x \\ y \\ w \\ h \end{bmatrix}$$

corresponding class

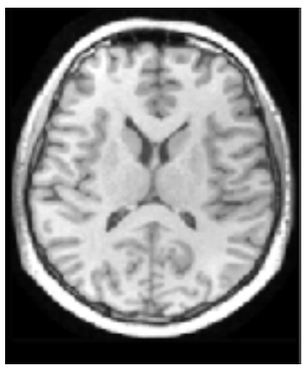


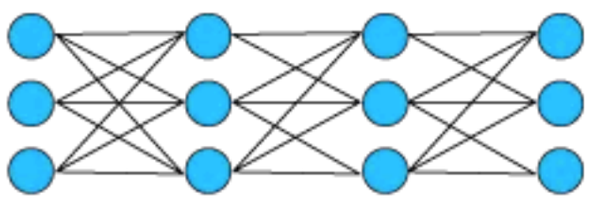
class: tumor

Segmentation

Input

image

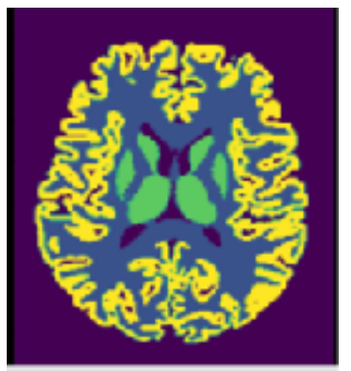




$f_W(x)$

Output

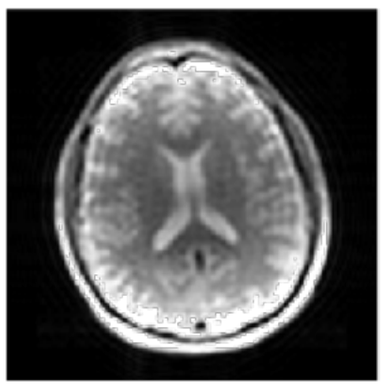
segmentation map

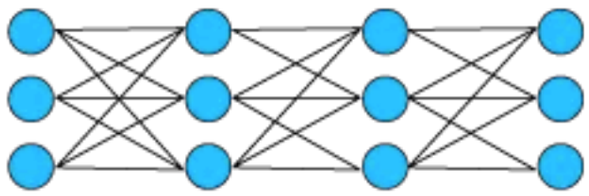


Super-resolution

Input

low-res image

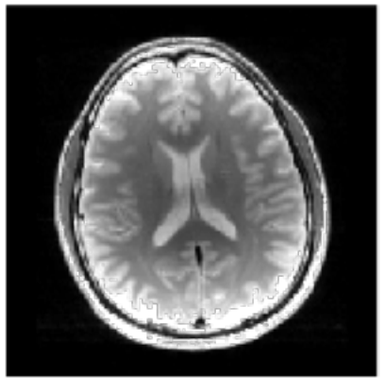




$f_W(x)$

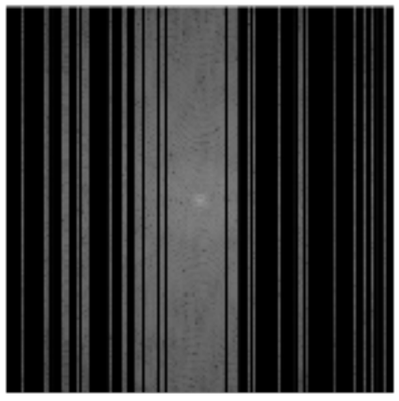
Output

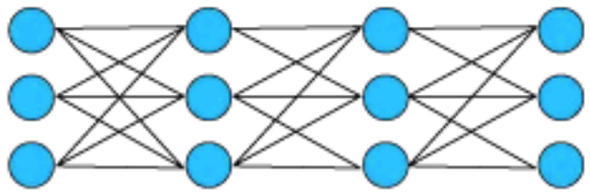
high-res image



MRI reconstruction function

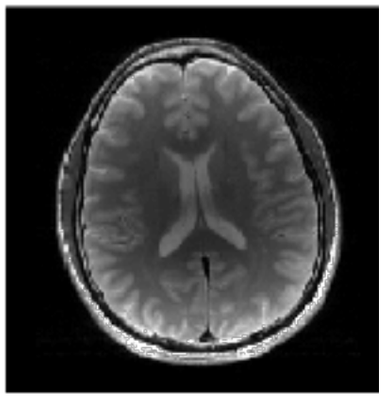
Input





$f_W(x)$

Output



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Fully connected layer
(Dense)

Optimizer

SGD
Adam
RMSprop

Convolutional layer

Conv1D, 2D, 3D, …
separable Conv

Deep Learning

Evaluation metric

accuracy
F1-score
AUC
confusion matrix

Pooling layer

max-pooling
average-pooling

Activation function

sigmoid
softmax
ESP (swish)
ReLU

Loss function

categorical crossentropy
binary crossentropy
mean squared error
mean absolute error

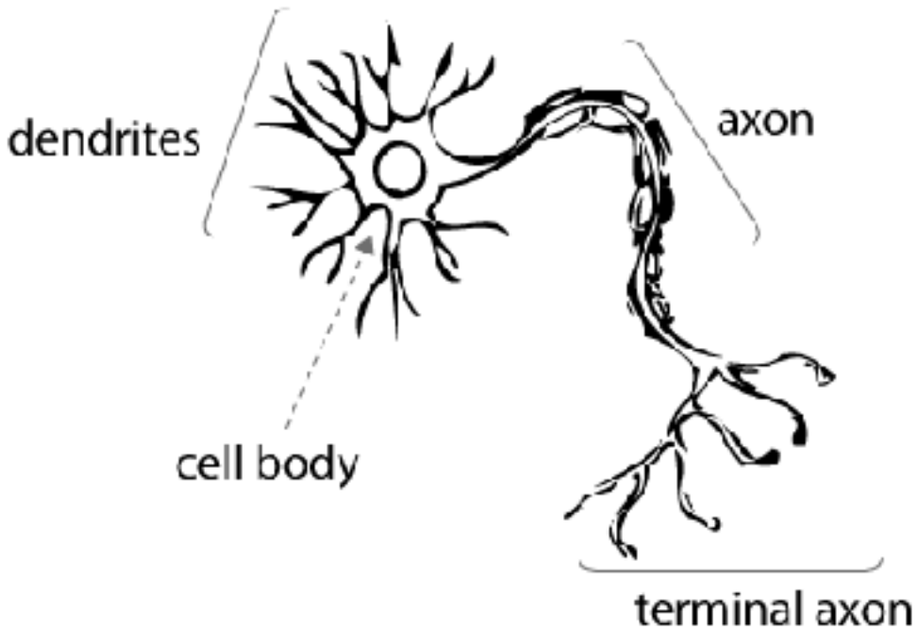
Regularization

Dropout
Data augmentation
l_1, l_2 regularizations

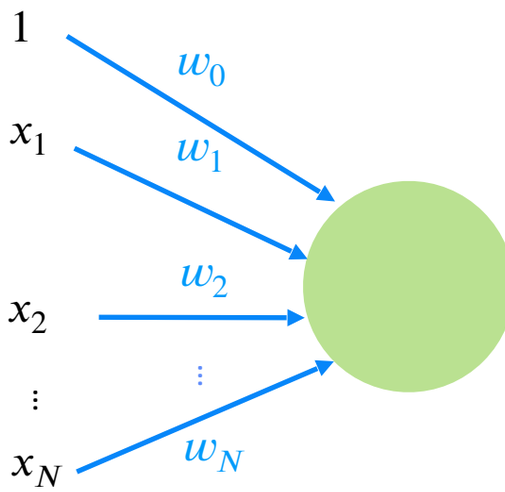
- Combine basic components to build a neural network
  - More components → "More" representative power

Artificial Neuron

Single neuron

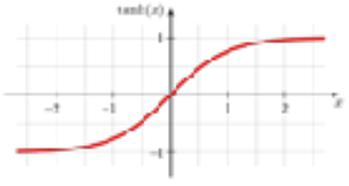


Artificial neuron



$$y = a\left(\sum_{n=1}^{N} x_n w_n + w_0\right)$$

non-linear function (activation)

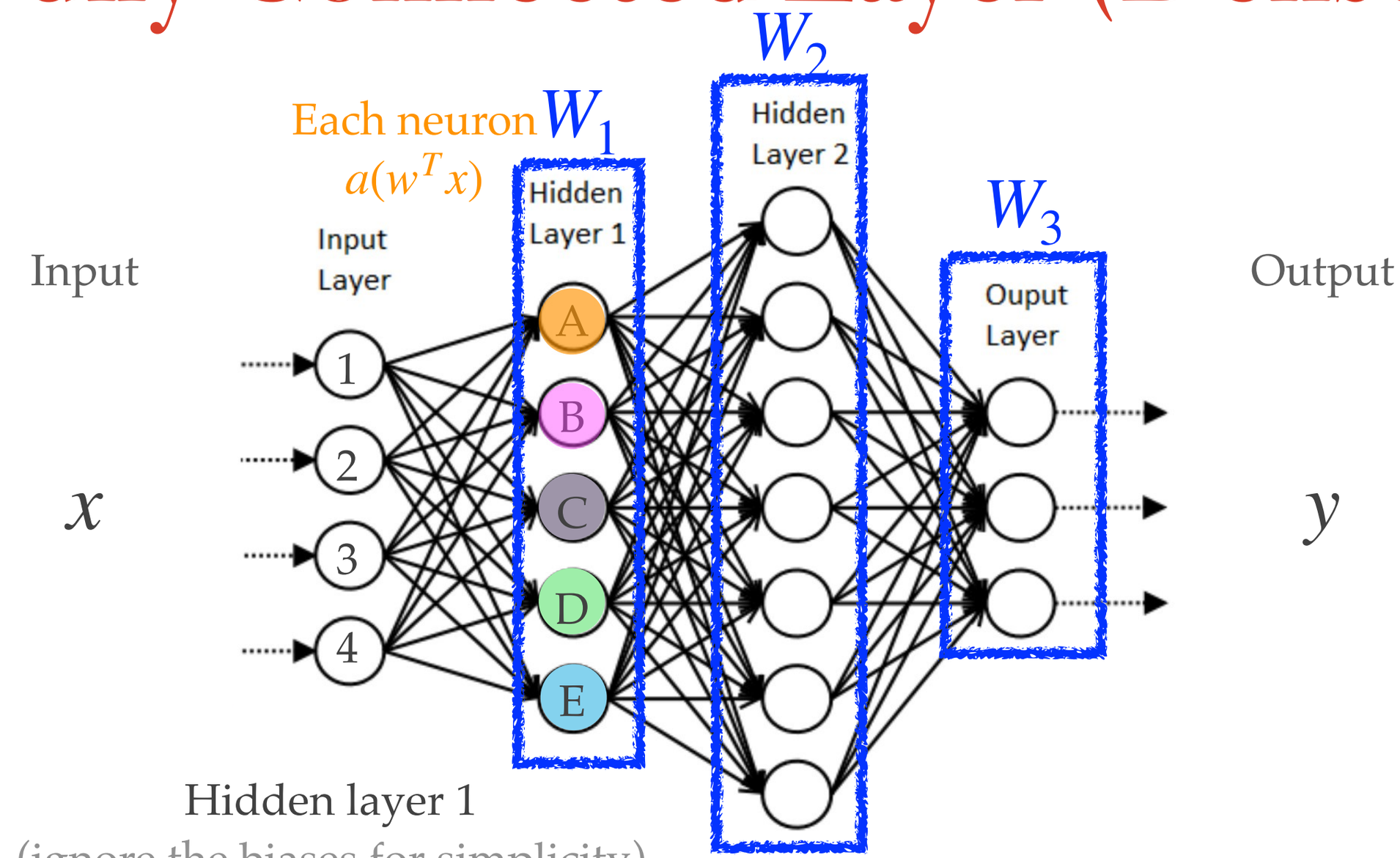


If we set all the weights to 0, then $y = 0$.
If we set $w_1 = 1$ and the rest to 0, then $y = a(x_1)$.
If we set $w_0 = 0$ and the rest to 1, then $y = a(x_1 + x_2 + \ldots + x_N)$.

Different weights give rise to different behavior

The Essense of Artificial Neural Networks by Ivan Liljeqvist (Medium)

Fully Connected Layer (Dense)



Hidden layer 1

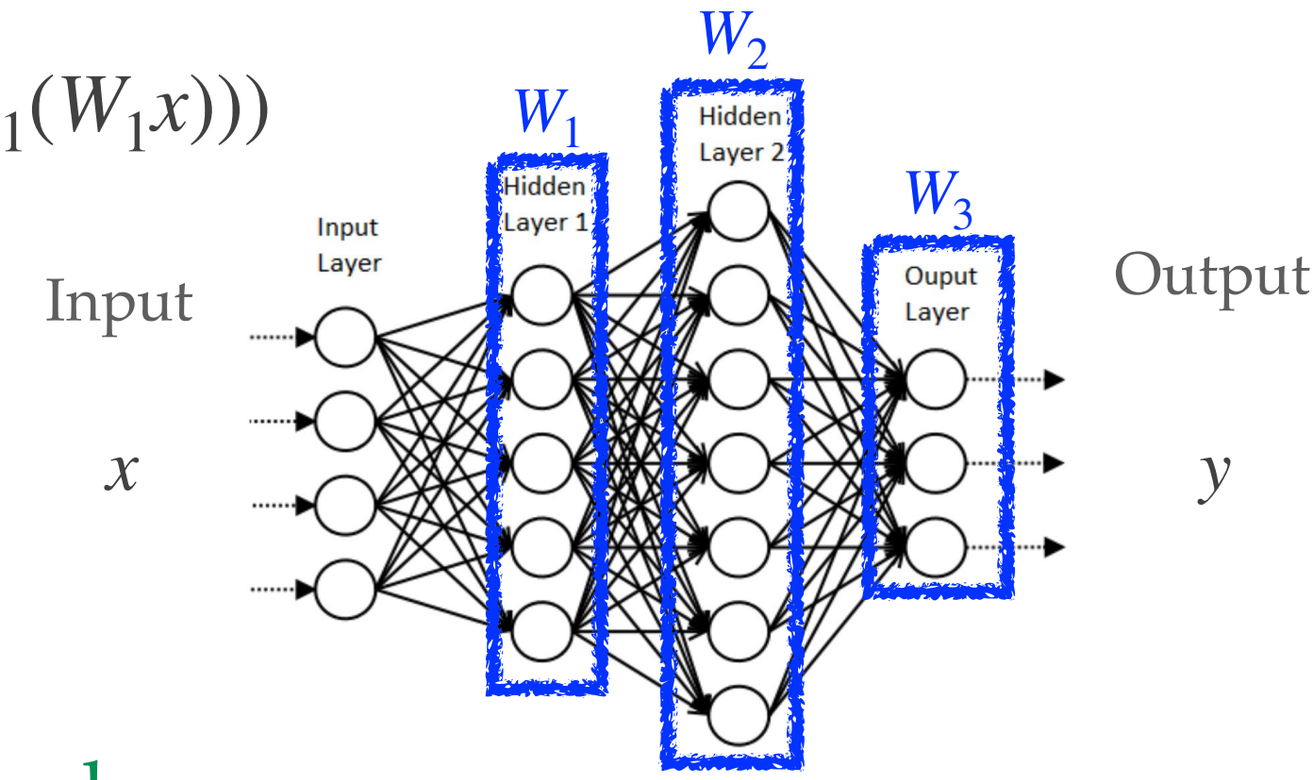
(ignore the biases for simplicity)

$$\begin{bmatrix} out_A \\ out_B \\ out_C \\ out_D \\ out_E \end{bmatrix} = a_1(W_1 x) = a_1\left(\begin{bmatrix} w_{A,1} & w_{A,2} & w_{A,3} & w_{A,4} \\ w_{B,1} & w_{B,2} & w_{B,3} & w_{B,4} \\ w_{C,1} & w_{C,2} & w_{C,3} & w_{C,4} \\ w_{D,1} & w_{D,2} & w_{D,3} & w_{D,4} \\ w_{E,1} & w_{E,2} & w_{E,3} & w_{E,4} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \right)$$

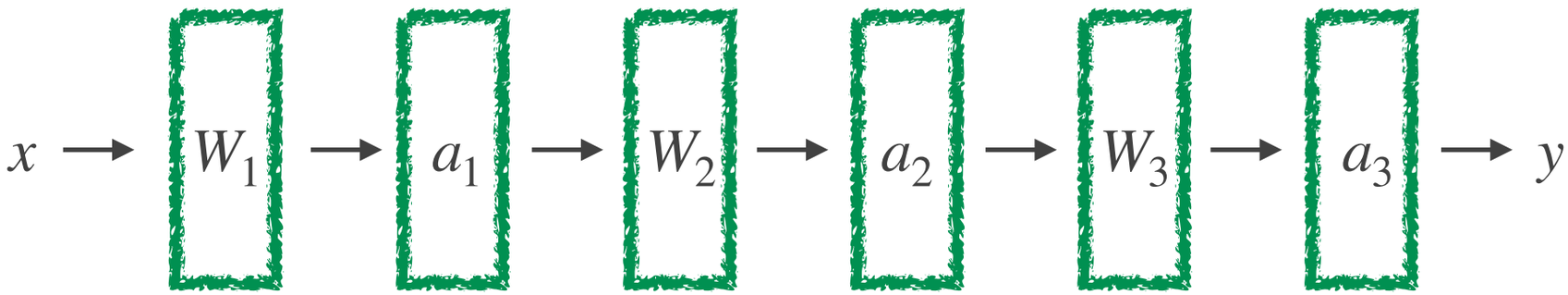
$$y = a_3(W_3 a_2(W_2 a_1(W_1 x)))$$

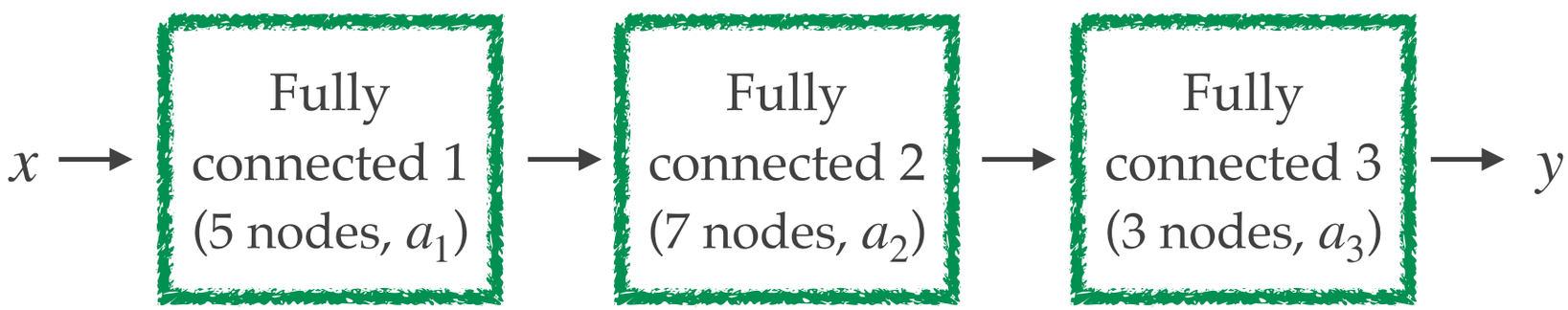
Representing Neural Network

$$y = a_3(W_3 a_2(W_2 a_1(W_1 x)))$$



Computation graph

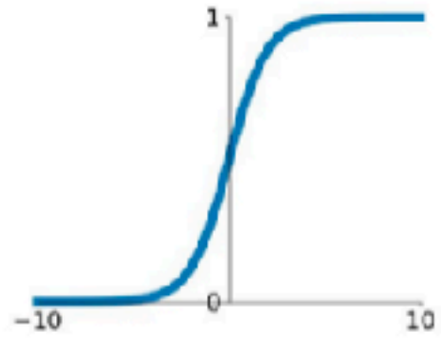




Activation Functions

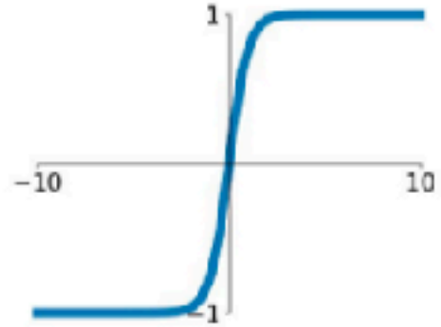
Sigmoid

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



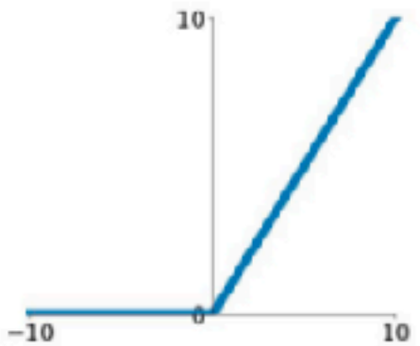
tanh

$$\tanh(x)$$



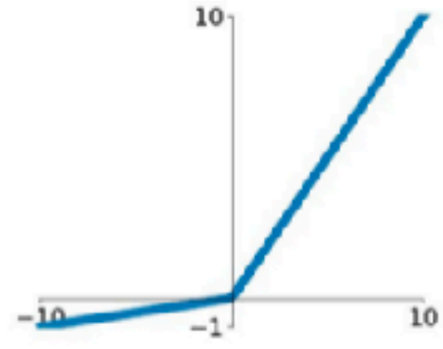
ReLU

$$\max(0, x)$$



Leaky ReLU

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

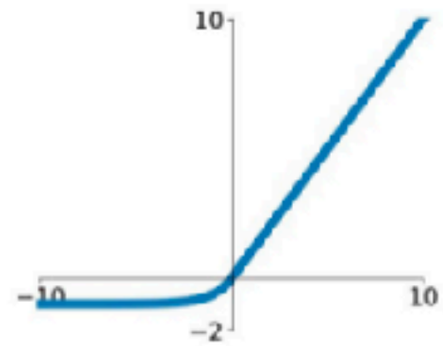


Maxout

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

ELU

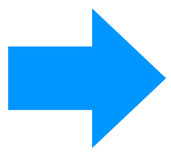
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$

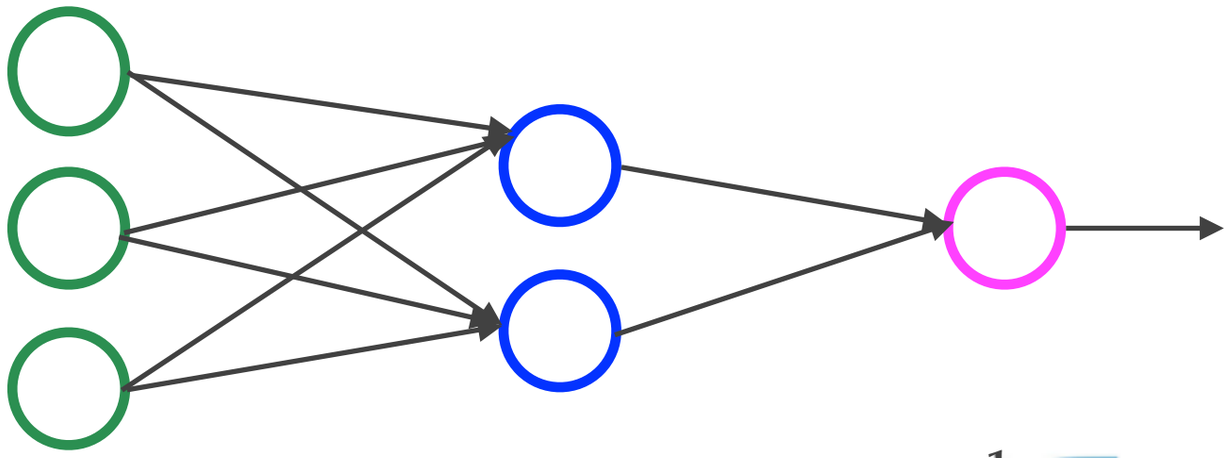


Introduction to Exponential Linear Unit

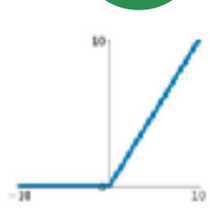
class 1 class 2

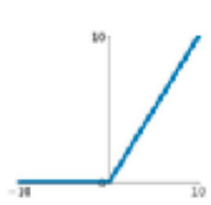
Two-class Classification

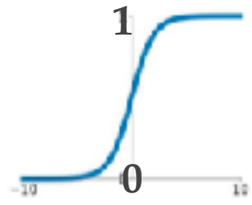




activation functions







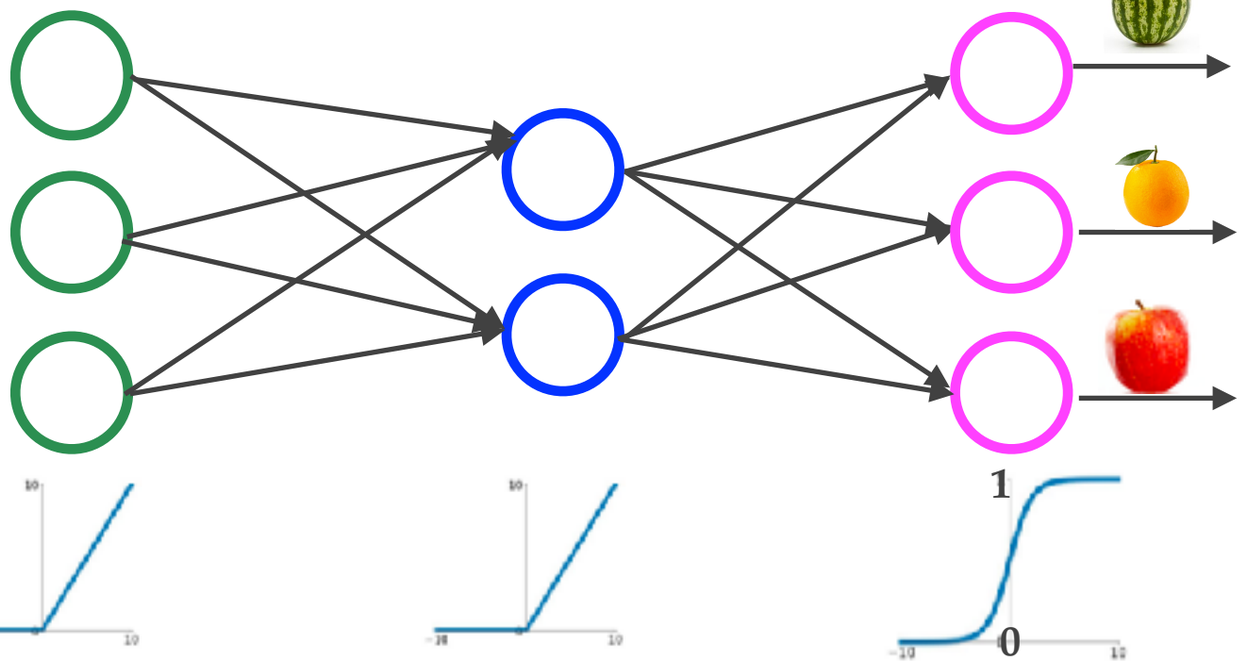
Fully connected 1 (3 nodes, ReLU) → Fully connected 2 (2 nodes, ReLU) → Fully connected 3 (1 nodes, sigmoid) → 0.99

```
model.add(tf.keras.layers.Dense(3, activation='relu'))
model.add(tf.keras.layers.Dense(2, activation='relu'))
model.add(tf.keras.layers.Dense(1, activation='sigmoid'))
```

class 1 class 2 class 3



Three-class Classification



probability of being class 1

probability of being class 2

probability of being class 3

activation functions

Fully connected 1 (3 nodes, ReLU) → Fully connected 2 (2 nodes, ReLU) → Fully connected 3 (**3 nodes**, sigmoid)



0.99

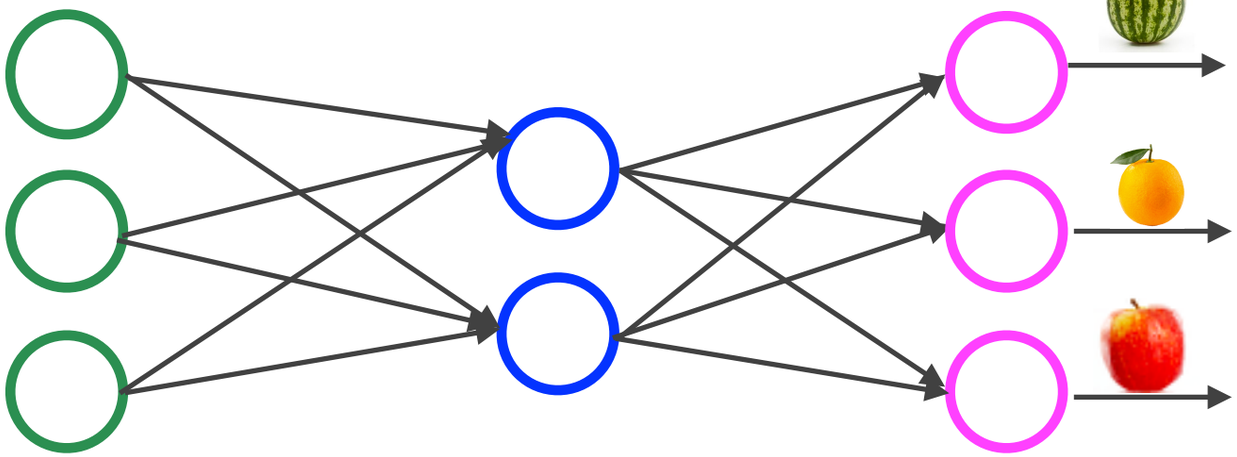
0.1

0.02

What if our model output something like 0.99 0.99 0.99 ? Not good

class 1 class 2 class 3

Three-class Classification



probability of being class 1

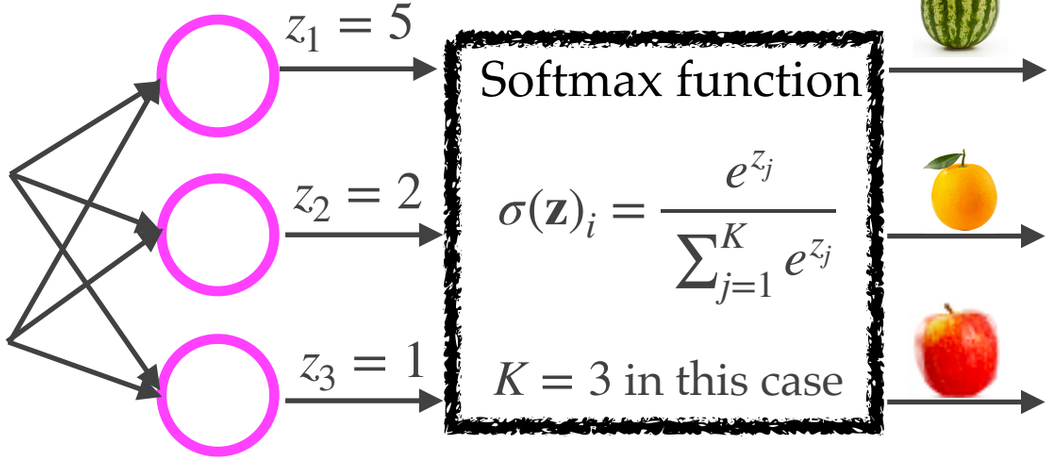
probability of being class 2

probability of being class 3

activation functions

Softmax function

…



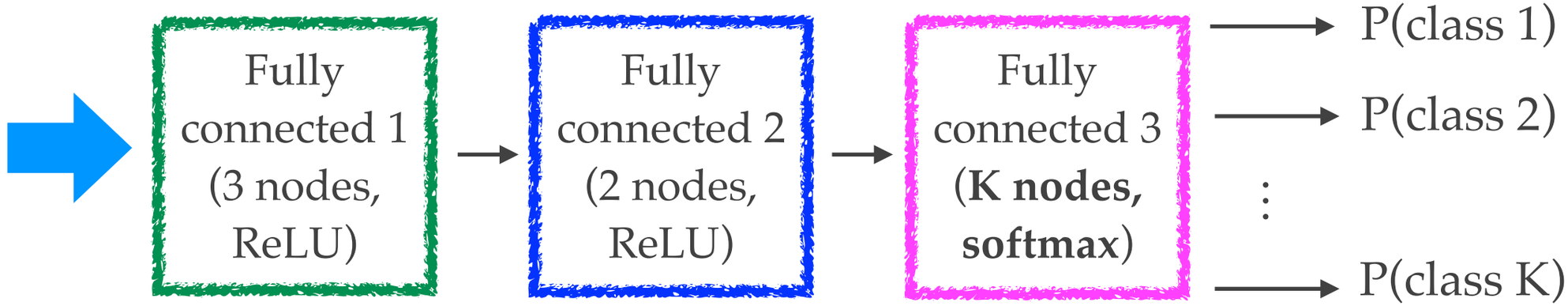
$$\frac{e^{z_1}}{e^{z_1}+e^{z_2}+e^{z_3}} = \frac{e^{5}}{e^{5}+e^{2}+e^{1}} = 0.936$$

$$\frac{e^{z_2}}{e^{z_1}+e^{z_2}+e^{z_3}} = \frac{e^{2}}{e^{5}+e^{2}+e^{1}} = 0.047$$

$$\frac{e^{z_3}}{e^{z_1}+e^{z_2}+e^{z_3}} = \frac{e^{1}}{e^{5}+e^{2}+e^{1}} = 0.017$$

$$0.936 + 0.047 + 0.017 = 1$$

Extend the model to K-class Classification




```
model.add(tf.keras.layers.Dense(3, activation='relu'))
model.add(tf.keras.layers.Dense(2, activation='relu'))
model.add(tf.keras.layers.Dense(K, activation='softmax'))
```

Fully connected layer
(Dense)

Convolutional layer

Conv1D, 2D, 3D, …
separable Conv

Optimizer

SGD
Adam
RMSprop

Pooling layer

max-pooling
average-pooling

Evaluation metric

accuracy
F1-score
AUC
confusion matrix

Activation function

sigmoid
softmax
ESP (swish)
ReLU

Loss function

categorical crossentropy
binary crossentropy
mean squared error
mean absolute error

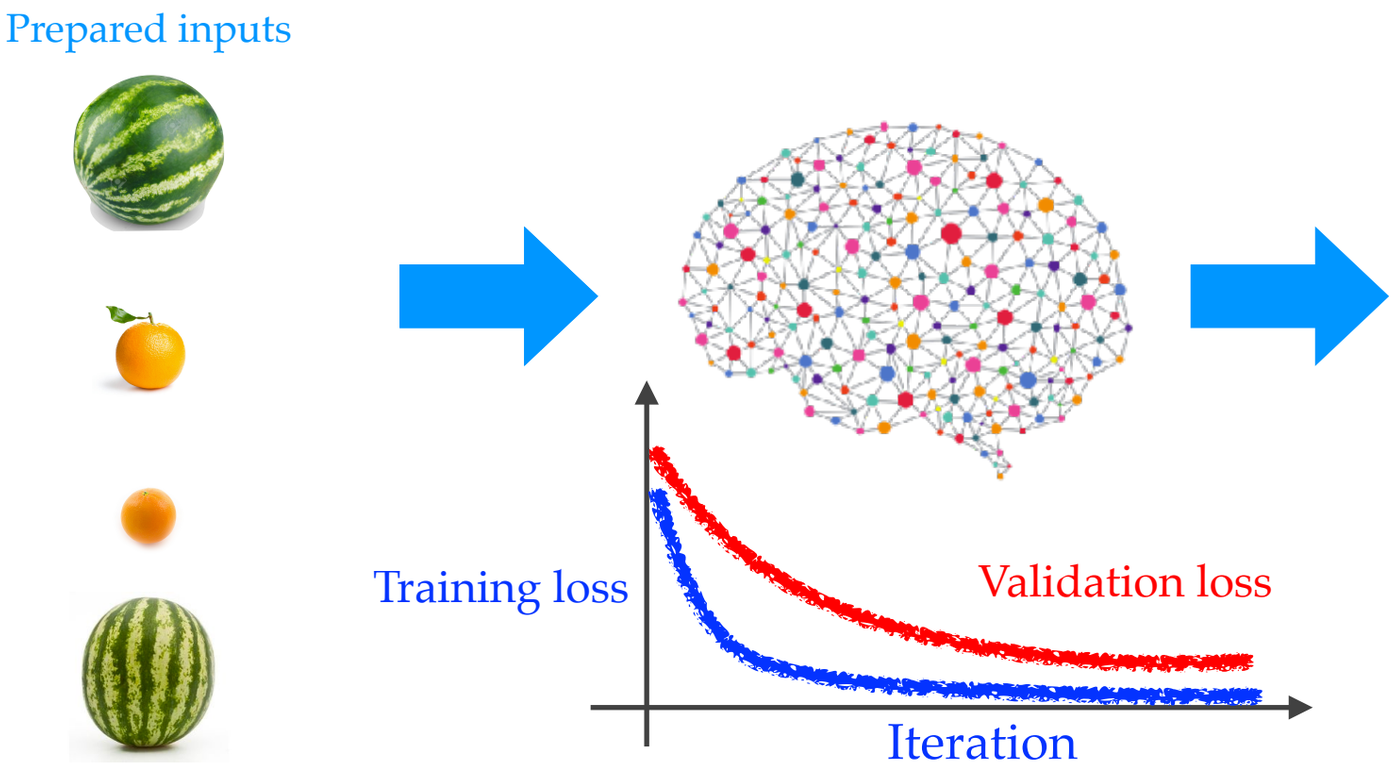
Regularization

Dropout
Data augmentation
l_1, l_2 regularizations

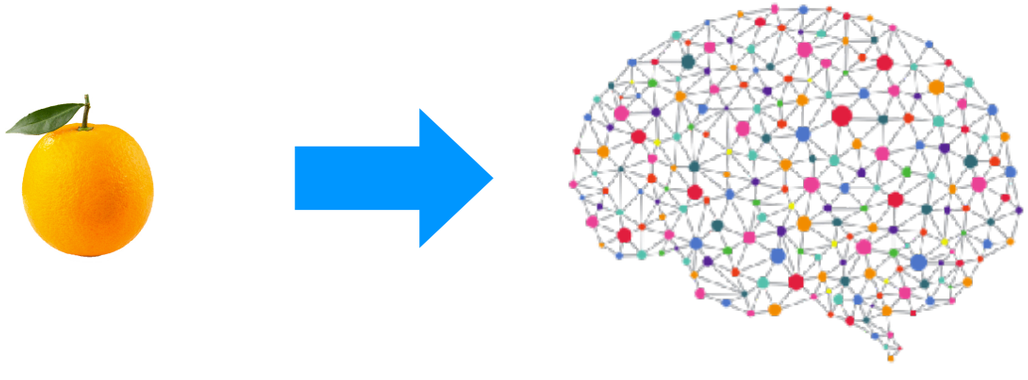
- Combine basic components to build a neural network
  - More components → "More" representative power

Image Classification Using Deep Learning

- Training phase: Optimize the weights of a deep neural network



- Test phase: Perform prediction using the trained neural network



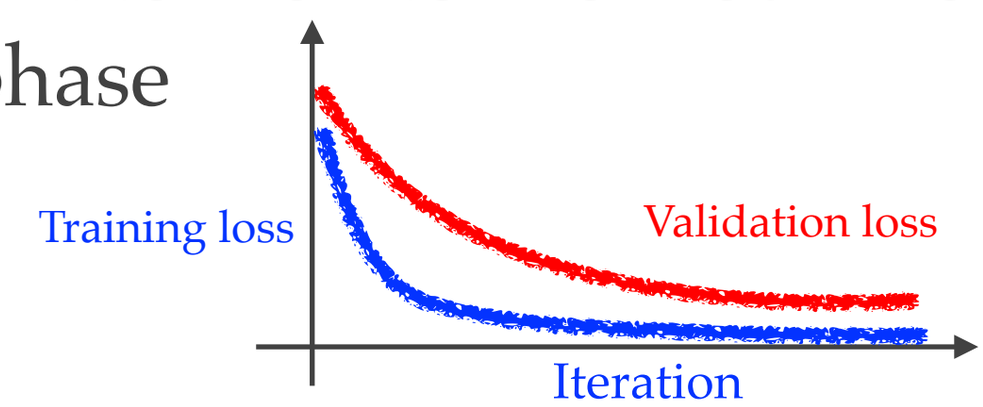
Loss function

(cost function and error function)

- A function L that maps values of variable(s) onto a real number

  For example, $L(y, \hat{y})$ gives us a number that tell us how "different" y and $\hat{y}$ are

- We have used it to monitor how our model performs during the training phase



$$L(y, \hat{y}) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

$$L(y, \hat{y}) = \frac{1}{N}\sum_{i=1}^{N}|y_i - \hat{y}_i|$$

- Mean squared error (MSE) and mean absolute error (MAE) are two popular choices for regression

- Cross-entropy is the most common choice for a classification task

Cross-entropy

- Well suited to comparing probability distributions

3-class classification

deep learning layers → Fully connected (**3 nodes, softmax**)

	predicted prob. dist. $\hat{y}$	true prob. dist. y
	0.7	1
	0.1	0
	0.2	0

One-hot encoding

$$L(y,\hat{y}) = -\sum_{k=1}^{K} y_k log\hat{y}_k \quad \text{by definition } (K=3)$$

$$= -(1 \times log(0.7) + 0 \times log(0.1) + 0 \times log(0.2)) = -1 \times log(0.7) = 0.15$$

Assume that we have updated the weights of our model and got $\hat{y} = [0.9, 0.1, 0]$, then $L(y,\hat{y}) = -1 \times log(0.9) + 0 + 0 = 0.046$

Lower loss. $\hat{y}$ has become more similar to y than the previous case.
Our model performs better!

Optimizing Our Model

- To train our model f_W, we adjust its weights W in a way that decreases your loss function
- Particularly, we are minimizing our loss function with respect to W

prepared output/ labels/targets — prepared input

$$L(y, \hat{y}) = L(y, f_W(x))$$

predicted output — Weights

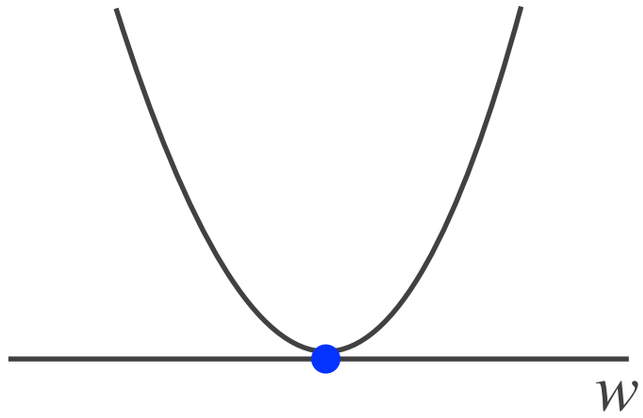
Calculus!

Compute the derivative of $L(y, f_W(x))$ with respect to W and set it to 0.

Example: Optimization

- Goal: Find w that minimizes the following loss function

$$L(w) = w^2$$



Method 1: Compute the derivative and set it to 0

Gradient $\dfrac{dL(w)}{dw} = \dfrac{dw^2}{dw} = 2w \quad = 0 \quad \Rightarrow \quad w = 0$

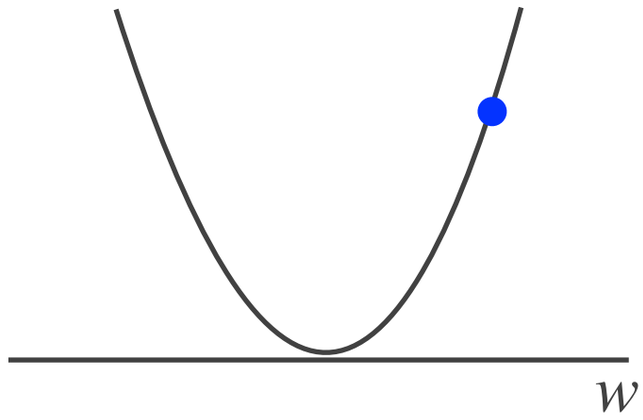
In our case, we have $L(y, f_W(x))$. Not simple to compute the gradient with respect to W.

Even when we have a way to compute the gradient and manage to set it to zero, we might not be able to get a closed-form solution for it.

Example: Optimization

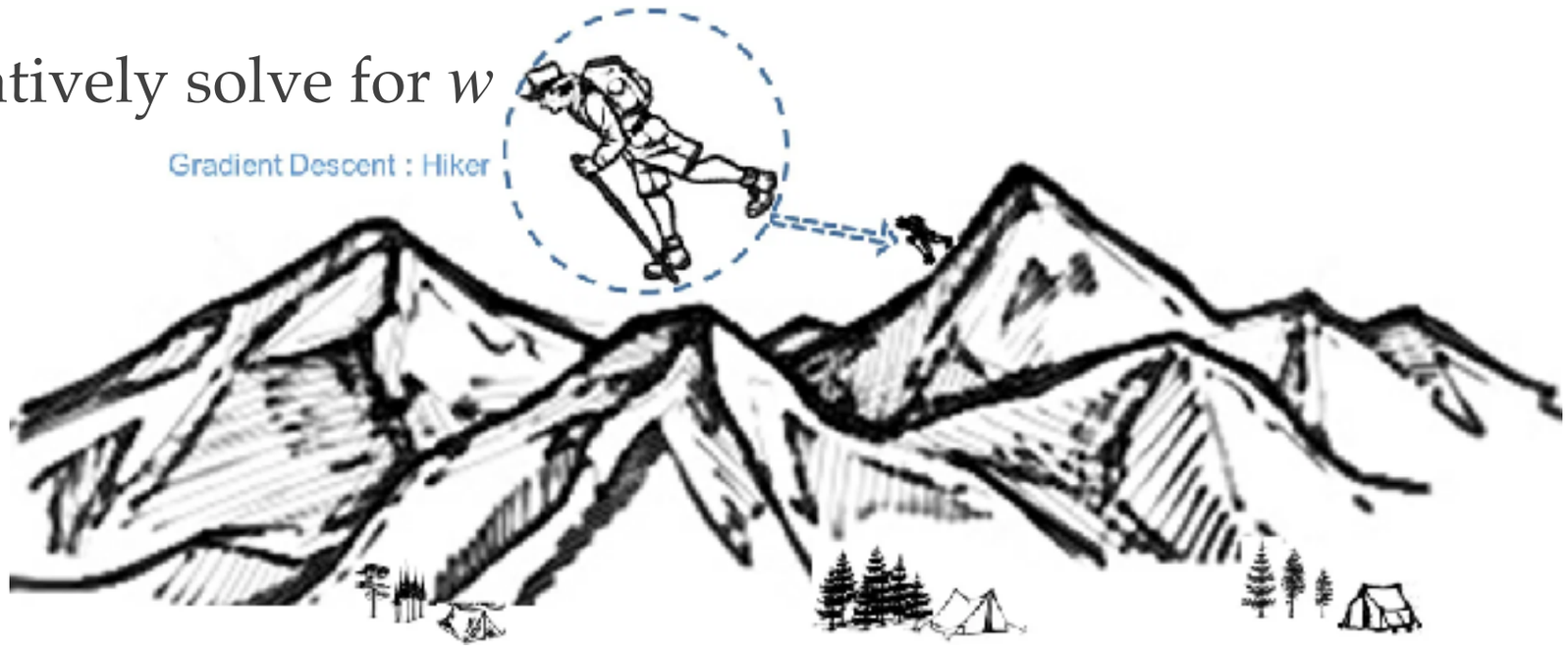
- Goal: Find w that minimizes the following loss function

$$L(w) = w^2$$



- Randomly start somewhere
- Gradually move to the minimum of the function

Method 2: Iteratively solve for w

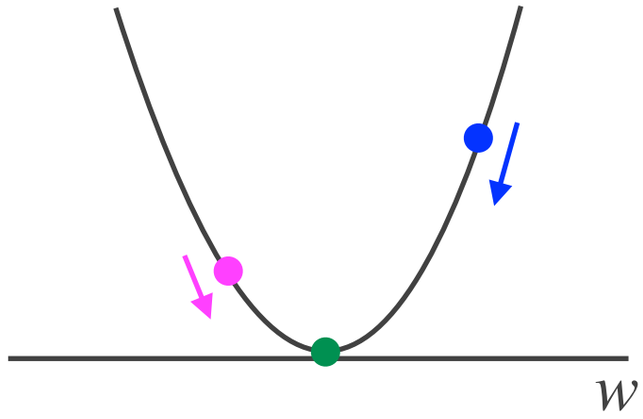


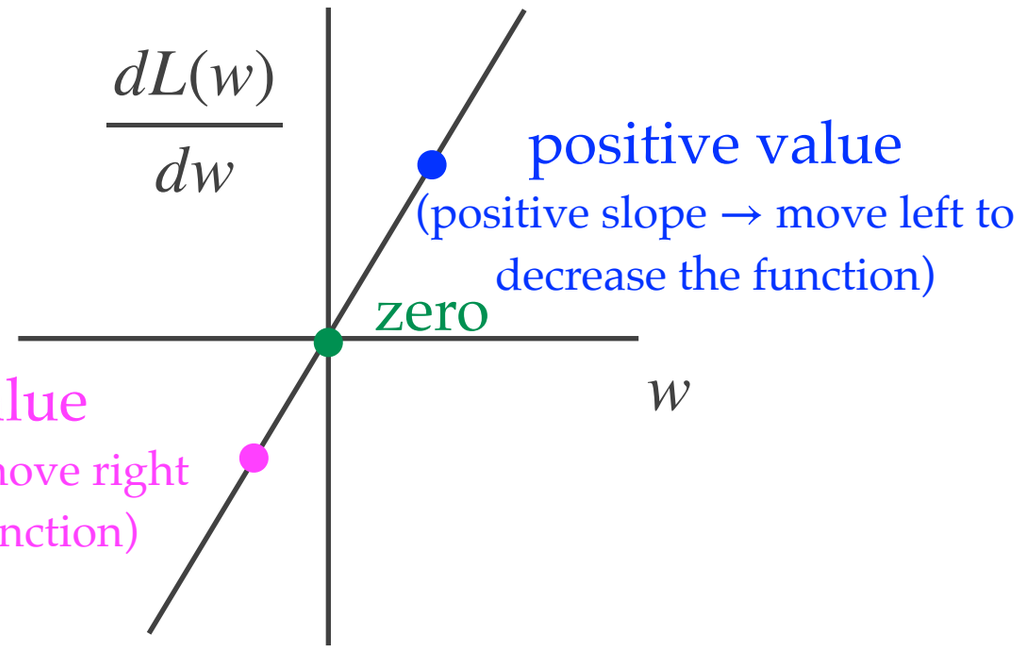
Gradient Descent for Logistic Regression Simplified – Step by Step Visual Guide

Example: Optimization

- Goal: Find w that minimizes the following loss function

$$L(w) = w^2$$





Method 2: Iteratively solve for w

1. Guess an initial solution w_0 and pick α

For $k = 0,1,2,...$

2. Compute $\frac{dL(w)}{dw}|_{w=w_{(k)}} = 2w|_{w=w_{(k)}} = 2w_{(k)}$

Iteration k

The negative of the gradient $-\frac{dL(w)}{dw}$ tells us the direction we should move to decrease the function

3. Compute a new solution $w_{(k+1)} := w_{(k)} - \alpha \frac{dL(w)}{dw}|_{w=w_{(k)}} = w_{(k)} - \alpha * 2w_{(k)}$

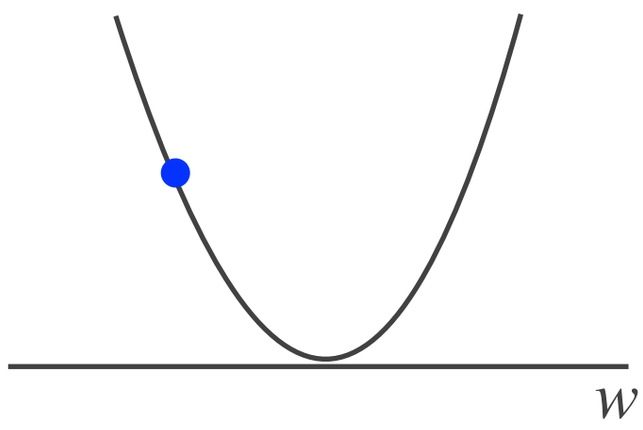
step size/learning rate α indicates how far we want to move

4. Repeat step 2 and 3 until converge

Example: Optimization

- Goal: Find w that minimizes the following loss function

$$L(w) = w^2$$



$$w_{(0)} = -2, \alpha = 0.5$$

$$w_{(1)} = w_{(0)} - \alpha * 2w_{(0)} = -2 - 0.5 * 2 * -2 = 0$$

$$w_{(2)} = w_{(1)} - \alpha * 2w_{(1)} = 0$$

$$w_{(3)} = w_{(2)} - \alpha * 2w_{(2)} = 0$$

Method 2: Iteratively solve for w

1. Guess an initial solution w_0 and pick α

For $k = 0,1,2,...$

2. Compute $\frac{dL(w)}{dw}|_{w=w_{(k)}} = 2w|_{w=w_{(k)}} = 2w_{(k)}$

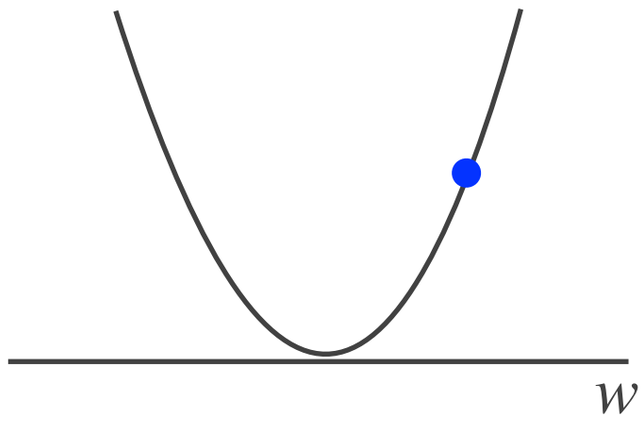
3. Compute a new solution $w_{(k+1)} := w_{(k)} - \alpha \frac{dL(w)}{dw}|_{w=w_{(k)}} = w_{(k)} - \alpha * 2w_{(k)}$

4. Repeat step 2 and 3 until converge

Example: Optimization

- Goal: Find w that minimizes the following loss function

$$L(w) = w^2$$



$$w_{(0)} = 2, \alpha = 0.5$$

$$w_{(1)} = w_{(0)} - \alpha * 2w_{(0)} = 2 - 0.5 * 2 * 2 = 0$$

$$w_{(2)} = w_{(1)} - \alpha * 2w_{(1)} = 0$$

$$w_{(3)} = w_{(2)} - \alpha * 2w_{(2)} = 0$$

Method 2: Iteratively solve for w

1. Guess an initial solution w_0 and pick α

For $k = 0,1,2,...$

2. Compute $\frac{dL(w)}{dw}|_{w=w_{(k)}} = 2w|_{w=w_{(k)}} = 2w_{(k)}$

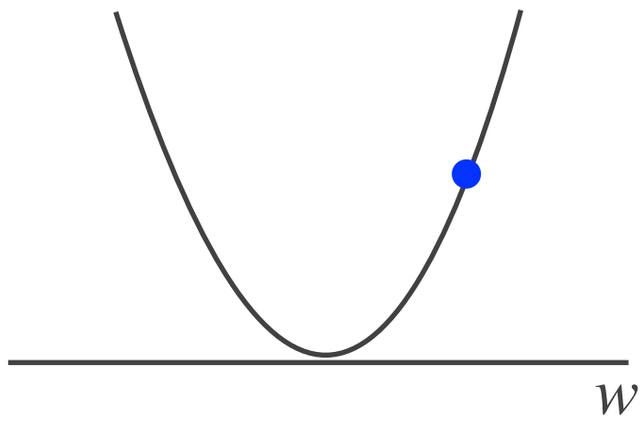
3. Compute a new solution $w_{(k+1)} := w_{(k)} - \alpha \frac{dL(w)}{dw}|_{w=w_{(k)}} = w_{(k)} - \alpha * 2w_{(k)}$

4. Repeat step 2 and 3 until converge

Example: Optimization

- Goal: Find w that minimizes the following loss function

$$L(w) = w^2$$



$$w_{(0)} = 2, \alpha = 0.25$$

$$w_{(1)} = w_{(0)} - \alpha * 2w_{(0)} = 2 - 0.25 * 2 * 2 = 1$$

$$w_{(2)} = w_{(1)} - \alpha * 2w_{(1)} = 1 - 0.25 * 2 * 1 = 0.5$$

$$w_{(3)} = w_{(2)} - \alpha * 2w_{(2)} = 0.5 - 0.25 * 2 * 0.5 = 0.25$$

$$w_{(4)} = w_{(3)} - \alpha * 2w_{(3)} = 0.125$$

$$w_{(5)} = w_{(4)} - \alpha * 2w_{(4)} = 0.0625$$

Method 2: Iteratively solve for w

1. Guess an initial solution w_0 and pick α

For $k = 0,1,2,...$

2. Compute $\frac{dL(w)}{dw}|_{w=w_{(k)}} = 2w|_{w=w_{(k)}} = 2w_{(k)}$

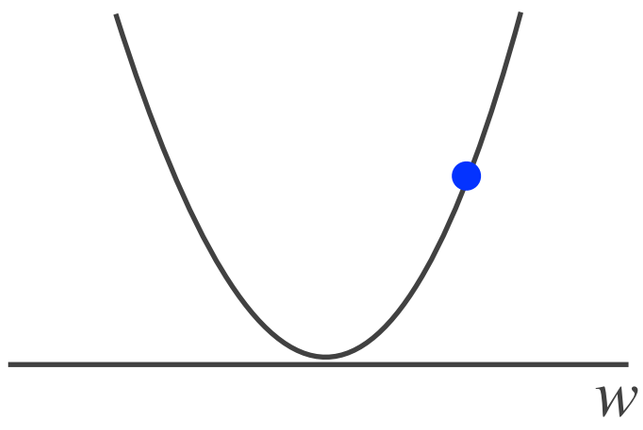
3. Compute a new solution $w_{(k+1)} := w_{(k)} - \alpha \frac{dL(w)}{dw}|_{w=w_{(k)}} = w_{(k)} - \alpha * 2w_{(k)}$

4. Repeat step 2 and 3 until converge

Example: Optimization

- Goal: Find w that minimizes the following loss function

$$L(w) = w^2$$



$$w_{(0)} = 2, \alpha = 1$$

$$w_{(1)} = w_{(0)} - \alpha * 2w_{(0)} = 2 - 1 * 2 * 2 = -2$$

$$w_{(2)} = w_{(1)} - \alpha * 2w_{(1)} = -2 - 1 * 2 * -2 = 2$$

$$w_{(3)} = w_{(2)} - \alpha * 2w_{(2)} = -2$$

$$w_{(4)} = w_{(3)} - \alpha * 2w_{(3)} = 2$$

$$w_{(5)} = w_{(4)} - \alpha * 2w_{(4)} = -2$$

Method 2: Iteratively solve for w

1. Guess an initial solution w_0 and pick α

For $k = 0,1,2,...$

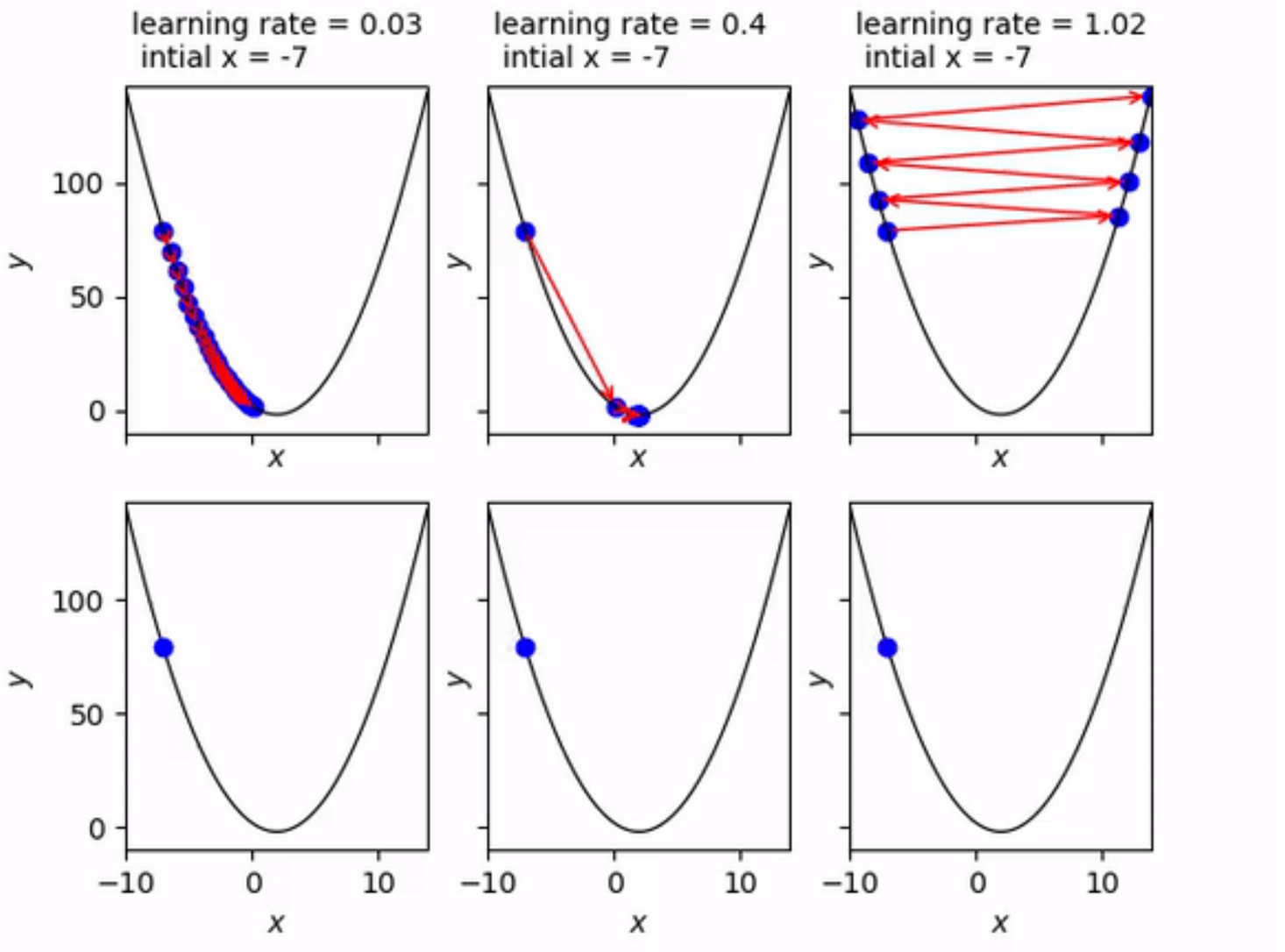
2. Compute $\frac{dL(w)}{dw}|_{w=w_{(k)}} = 2w|_{w=w_{(k)}} = 2w_{(k)}$

3. Compute a new solution $w_{(k+1)} := w_{(k)} - \alpha \frac{dL(w)}{dw}|_{w=w_{(k)}} = w_{(k)} - \alpha * 2w_{(k)}$

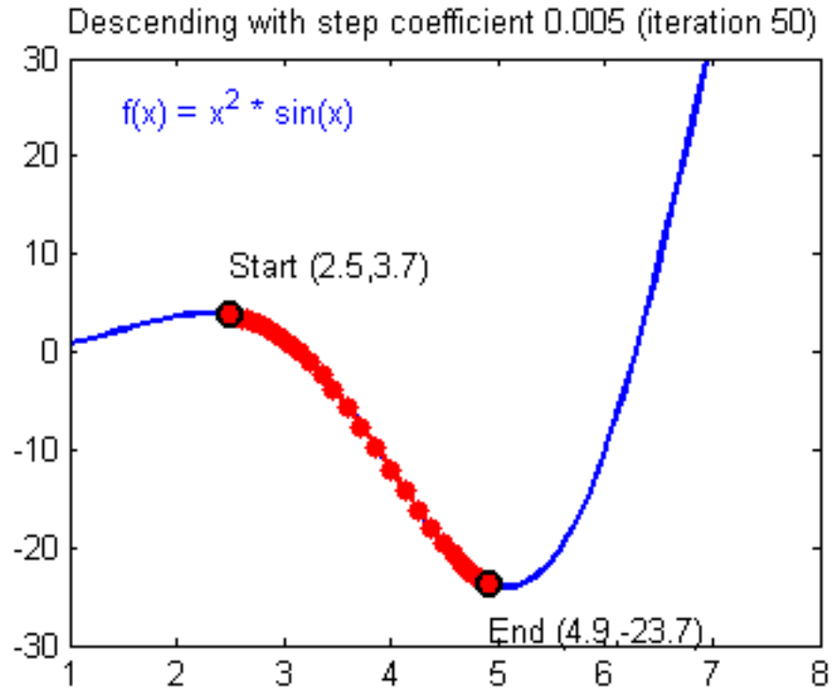
4. Repeat step 2 and 3 until converge

α: learning rate

Optimization: Learning Rate



Fixed learning rate

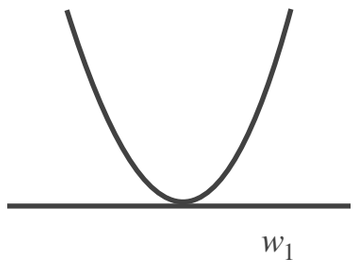


Adaptive learning rate

Gradient

1-dimensional case

$$L(w_1) = w_1^2$$



Derivative of $L(w_1)$

$$\frac{dL(w_1)}{dw_1} = \frac{dw_1^2}{dw_1} = 2w_1$$

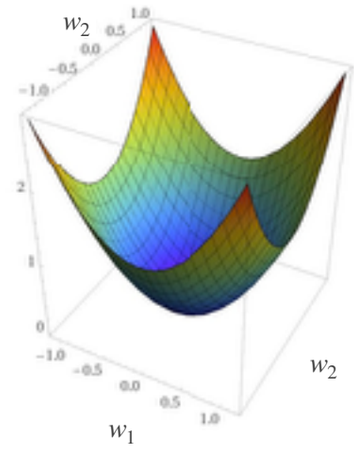
Weight update

$$w_{1,(k+1)} := w_{1,(k)} - \alpha \frac{dL(w_1)}{dw_1}\Big|_{w_1=w_{1,(k)}}$$

$$= w_{1,(k)} - 2w_{1,(k)}$$

2-dimensional case

$$L(w_1, w_2) = w_1^2 + w_2^2$$



Partial derivatives of $L(w_1, w_2)$

$$\frac{\partial L(w_1, w_2)}{\partial w_1} = \frac{\partial}{\partial w_1}(w_1^2 + w_2^2) = 2w_1$$

$$\frac{\partial L(w_1, w_2)}{\partial w_2} = \frac{\partial}{\partial w_2}(w_1^2 + w_2^2) = 2w_2$$

Gradient $\nabla_w L(w_1, w_2)$

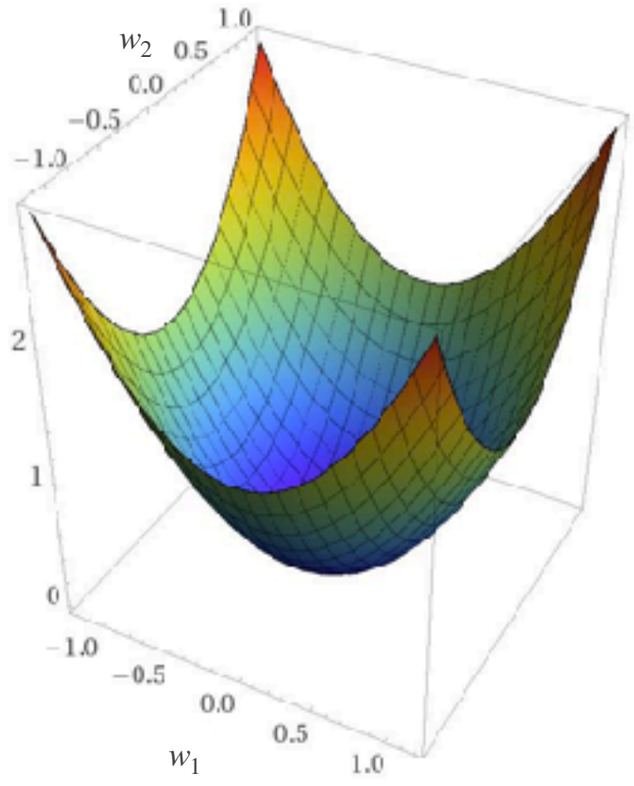
Weight update

$$\begin{bmatrix} w_{1,(k+1)} \\ w_{2,(k+1)} \end{bmatrix} = \begin{bmatrix} w_{1,(k)} \\ w_{2,(k)} \end{bmatrix} - \alpha \begin{bmatrix} \frac{\partial L(w_1, w_2)}{\partial w_1}\Big|_{w_1=w_{1,(k)}} \\ \frac{\partial L(w_1, w_2)}{\partial w_2}\Big|_{w_2=w_{2,(k)}} \end{bmatrix}$$

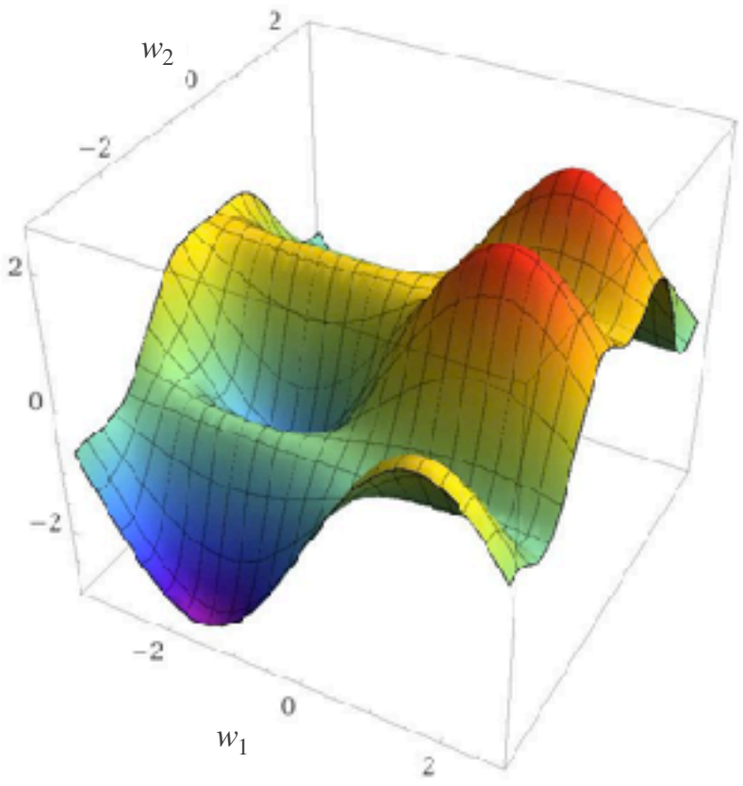
$$= \begin{bmatrix} w_{1,(k)} \\ w_{2,(k)} \end{bmatrix} - \alpha \begin{bmatrix} 2w_{1,(k)} \\ 2w_{2,(k)} \end{bmatrix}$$

Optimization

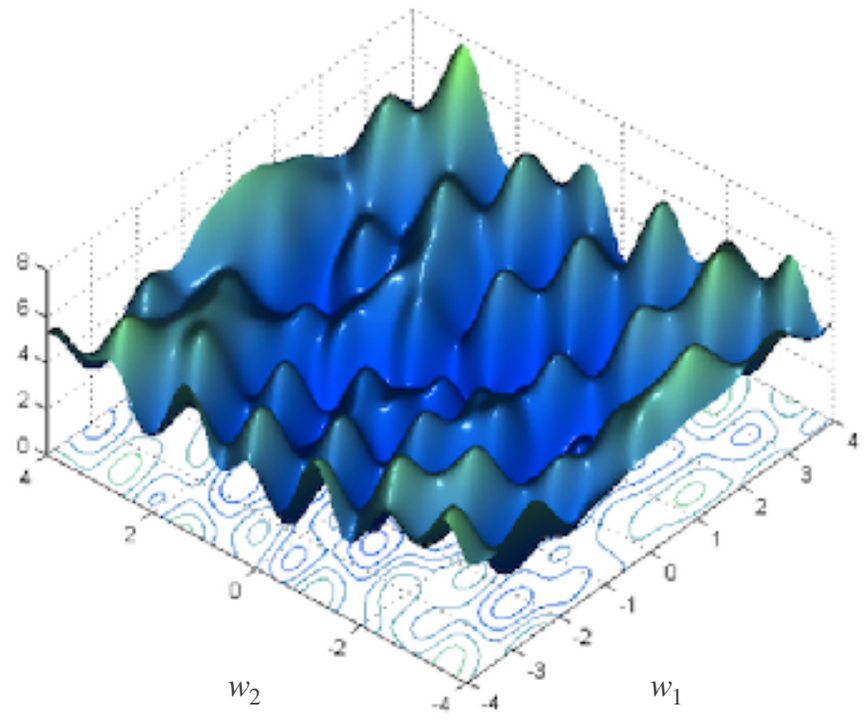
Real Life



No local minima problem (global minimum = local minimum)



Could get stuck in local minima



@#Q#@%!!!!!!

Furthermore, how do we compute a complicated loss function such as the one in our example $L(y, f_W(x))$?

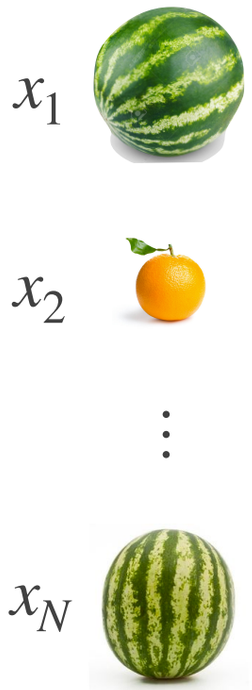
Backpropagation!

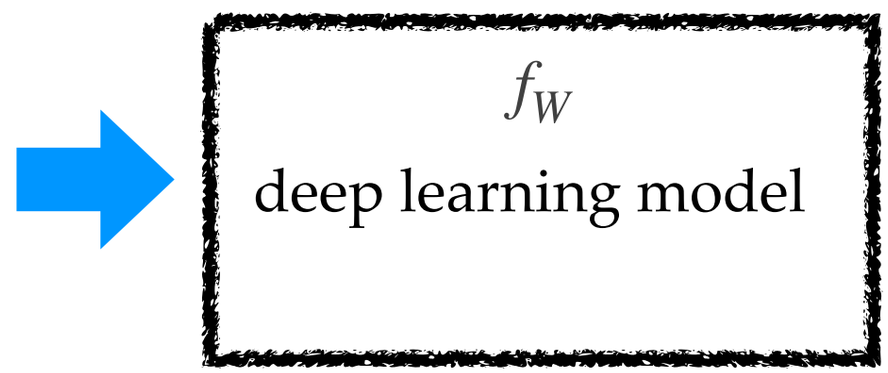
O'Reilly Media

Yoshua Bengio

Training Our Model

prepared inputs





predicted outputs	prepared outputs	loss values
$\hat{y}_1$	y_1	$L(y_1, \hat{y}_1)$
$\hat{y}_2$	y_2	$L(y_2, \hat{y}_2)$
$\vdots$	$\vdots$	$\vdots$
$\hat{y}_N$	y_N	$L(y_N, \hat{y}_N)$

Total loss $L(y, \hat{y}) = \sum_{i=1}^{N} L(y_i, \hat{y}_i) = \sum_{i=1}^{N} L(y_i, f_W(x_i))$

Update the weights

Compute the gradient of the total loss w.r.t. to W using backpropagation

$$\nabla_W L = \sum_{i=1}^{N} \nabla_W L(y_i, f_W(x_i))$$

Assign the new weights $W \leftarrow W - \alpha \nabla_W L$

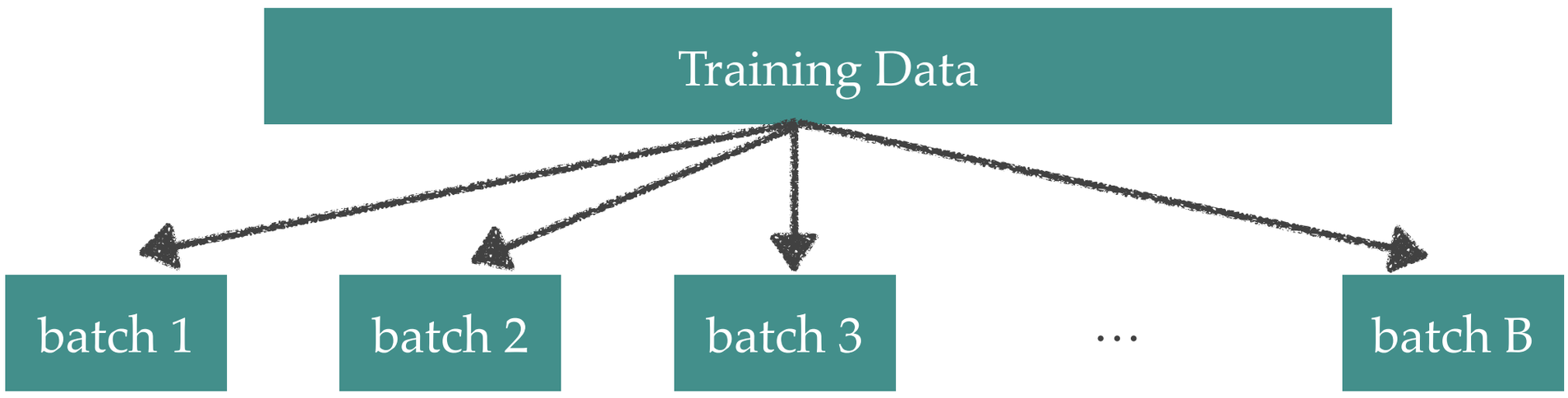
Stochastic Gradient Descent

- Every time we want to update W, we need to compute the loss functions and their gradients of all samples

$$\nabla_W L = \sum_{i=1}^{N} \nabla_W L(y_i, f_W(x_i))$$

  - For very large N, we might not be able to do it due to both the time and memory constraints 14,000,000 images?

  - For stochastic gradient descent (SGD), we update W based on subsets of samples called a mini-batch



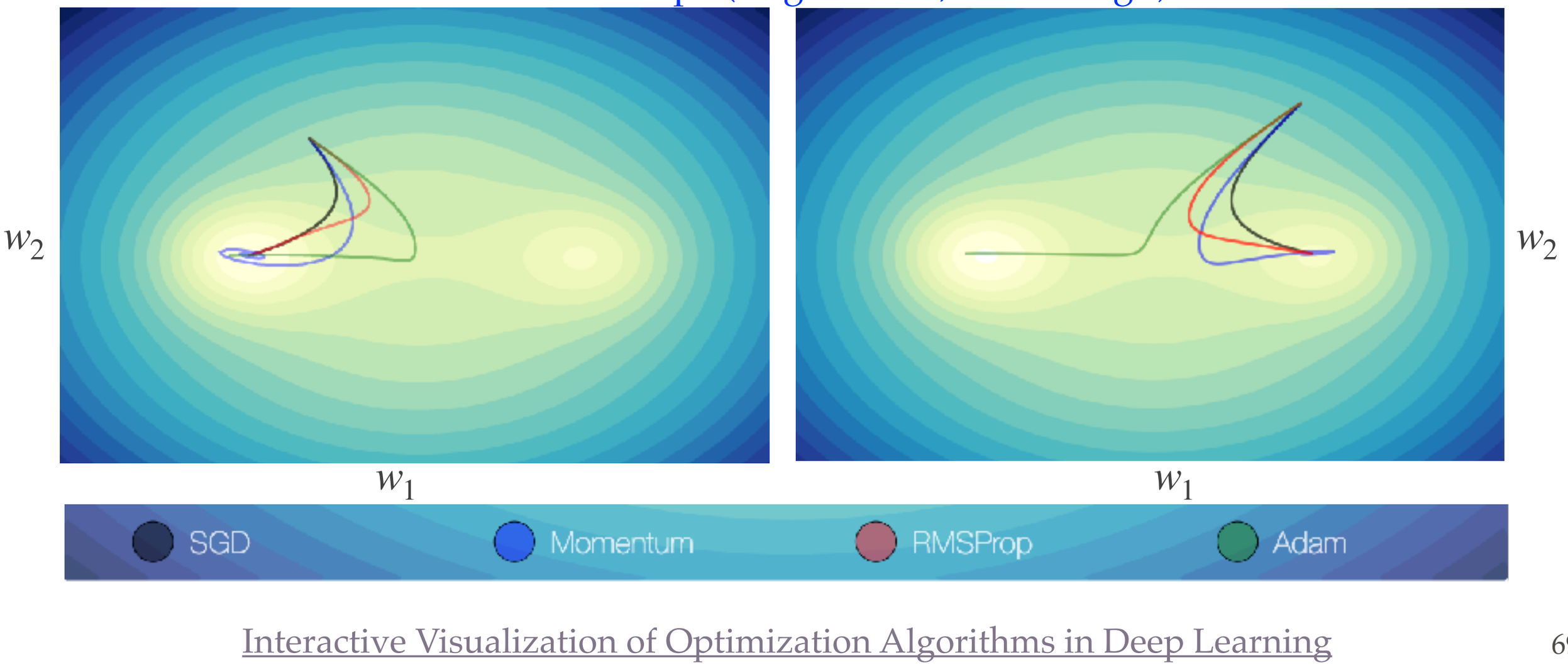
1 epoch = the model has seen the whole training data once (i.e., B batches in this case)

In this example, the weight matrix W is updated B times per epoch.

Optimizers

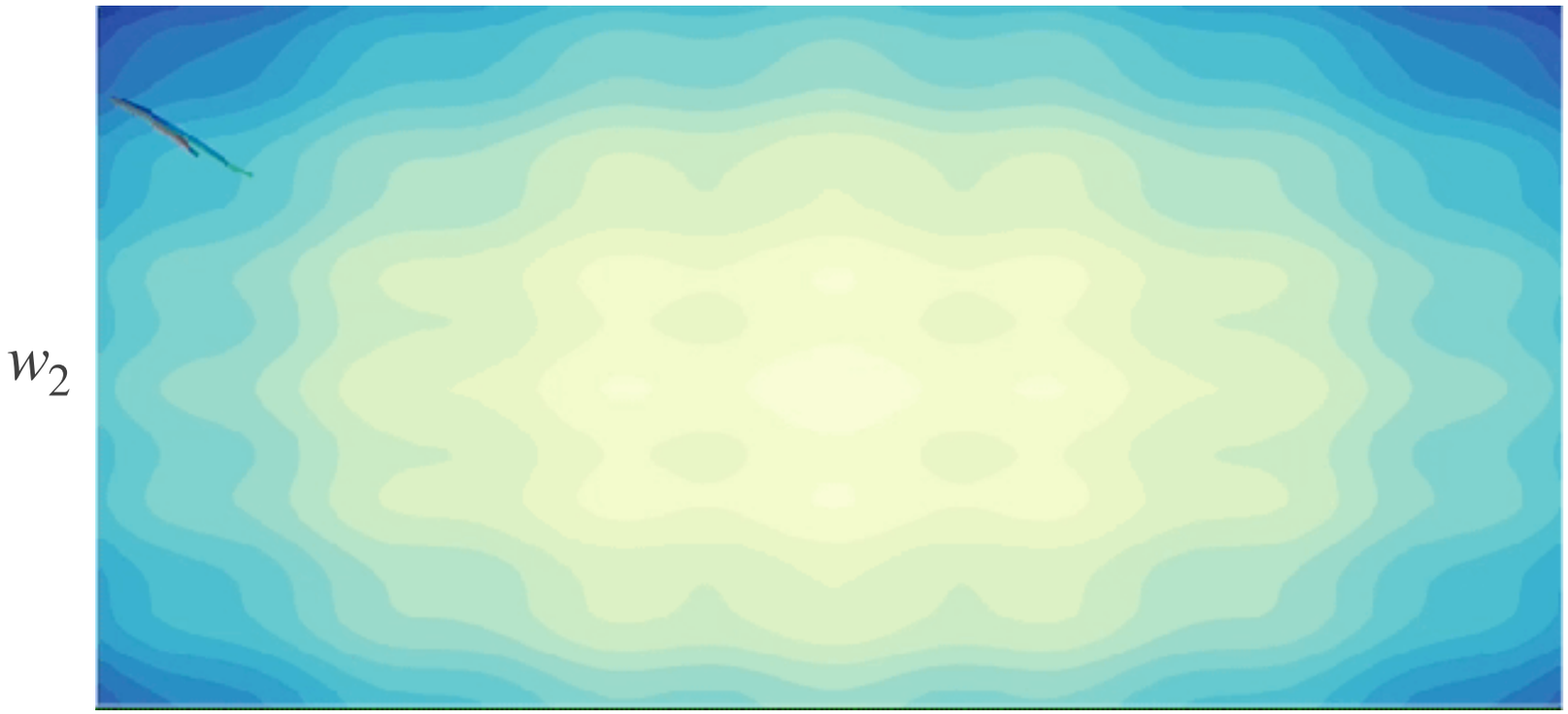
- Popular choices are
  - Stochastic gradient descent (SGD)
  - SGD with momentum
  - RMSprop
  - Adam
  - ADADELTA
  - AdaGrad

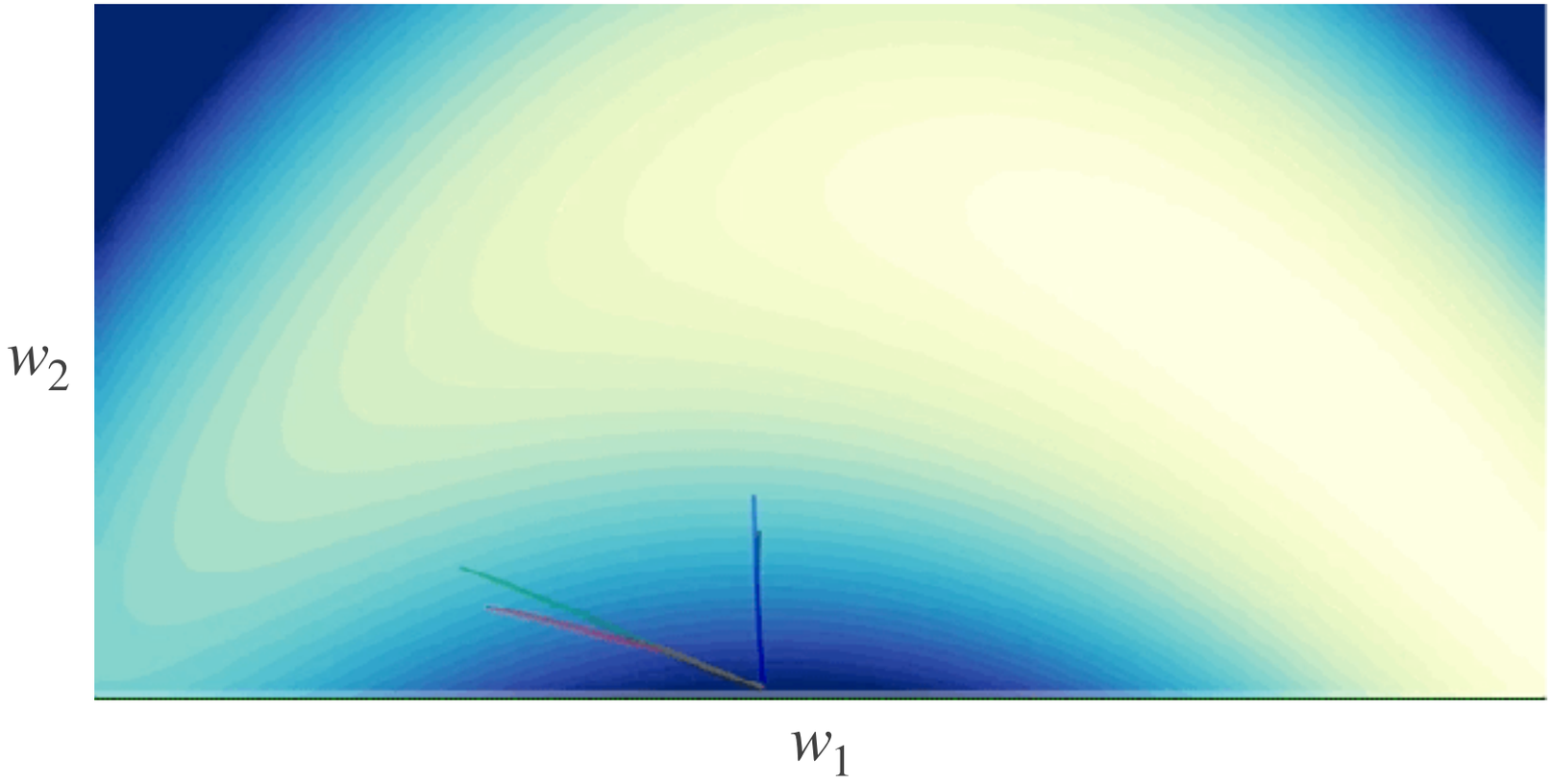
Loss landscape (bright = low, dark = high)



Interactive Visualization of Optimization Algorithms in Deep Learning

Loss landscape (bright = low, dark = high)





Interactive Visualization of Optimization Algorithms in Deep Learning

Fully connected layer
(Dense)

Convolutional layer

Conv1D, 2D, 3D, …
separable Conv

Optimizer

SGD
Adam
RMSprop

Deep Learning

Pooling layer

max-pooling
average-pooling

Evaluation metric

accuracy
F1-score
AUC
confusion matrix

Activation function

sigmoid
softmax
ESP (swish)
ReLU

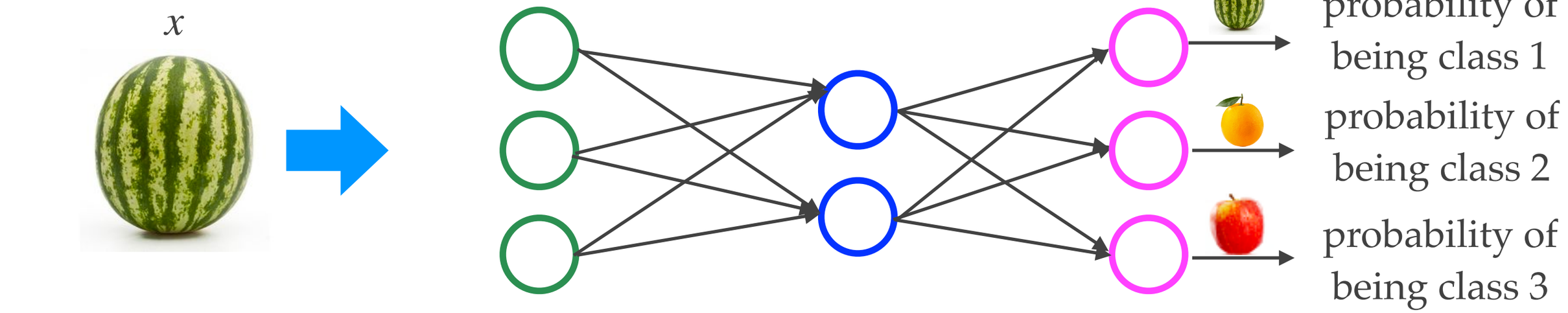
Loss function

categorical crossentropy
binary crossentropy
mean squared error
mean absolute error

Regularization

Dropout
Data augmentation
l_1, l_2 regularizations

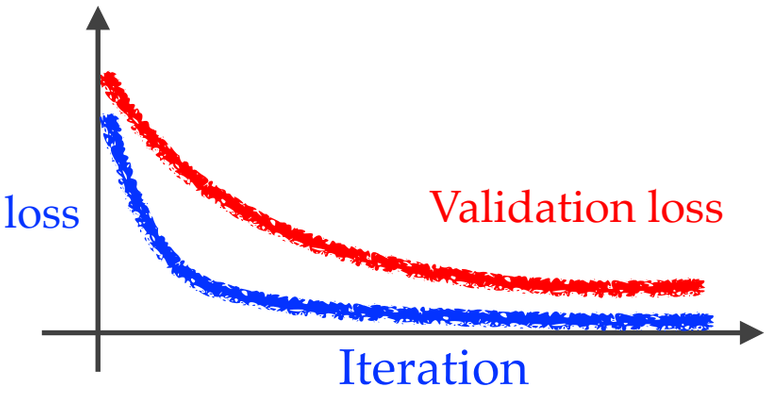
- Combine basic components to build a neural network
  - More components → "More" representative power




```
# Import necessary modules
import tensorflow as tf
from tensorflow import keras
from tensorflow.keras import layers

# Create the model
model = keras.Sequential()
model.add(layers.Dense(3, activation="relu"))
model.add(layers.Dense(2, activation="relu"))
model.add(layers.Dense(3, activation="softmax"))

# Compile the model
model.compile(
    optimizer='adam',
    loss=tf.keras.losses.CategoricalCrossentropy(),
)

# Train the model for 100 epochs with a batch size of 32
model.fit(x_train, y_train, batch_size=32, epochs=100, validation_data=(x_val,y_val))
```

Model

Loss function and optimizer



Outline

- Introduction to Supervised Machine Learning
  - AI vs ML vs DL
  - Traditional Machine Learning
  - Training, Validation, and Test Data
  - Overfitting and Underfitting
- Introduction to Supervised Deep Learning
  - Traditional ML vs Deep Learning
  - Artificial Neuron and Neural Network
  - Supervised Learning
- Deep Learning as a Function Approximator
- Deep Learning Components
  - Fully Connected Layers
  - Activation Functions
  - Optimization

Next Lecture

- Deep Learning Components
  - Regularization
    - ℓ_2 and ℓ_1 regularization
    - Dropout
    - Batch normalization
    - Convolutional layer
    - Pooling layer
- Convolutional Neural Network (CNN)
- Hands-on: MRI Tumor Classification Using CNN
  - https://github.com/ichatnun/CMU-medical-imaging-deep-learning