Carnegie Mellon University
Heinz College

Unstructured Data Analysis

Lecture 14: Time series analysis with recurrent neural nets; some other deep learning topics; course wrap-up

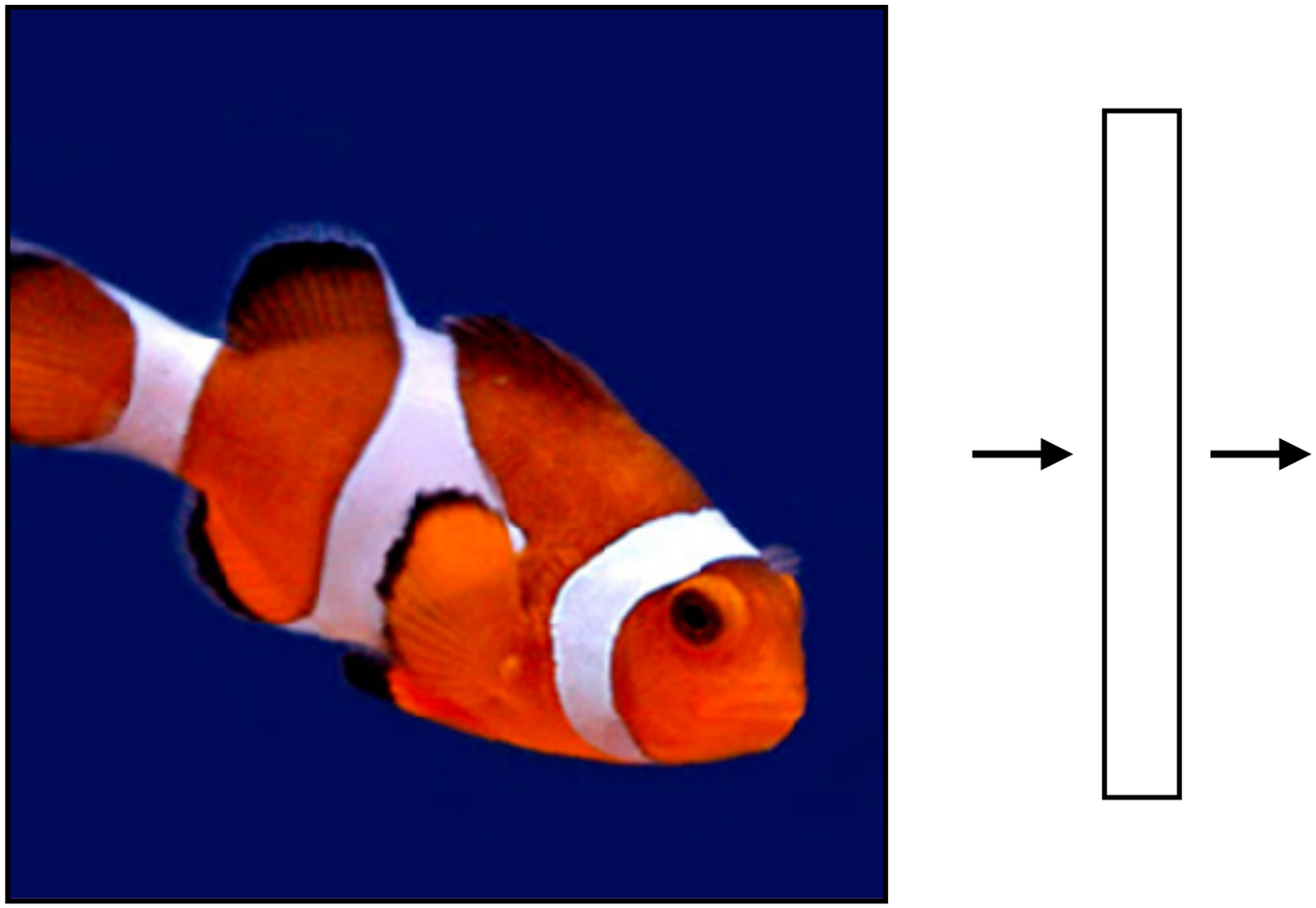
George Chen

Last Lecture!

- More on deep learning:
  - Time series analysis with recurrent neural nets
    - The demo is shifted to recitation
  - Extremely important concept we use: “word embeddings”
    - High-level idea shifted to recitation
  - I’ll also talk about some other deep learning topics
    - Roughly how learning a neural net works
    - How to deal with small datasets
    - Generating fake data that look real
    - AI agents that interact with environments
- I’ll end with a course wrap-up

Sequence Data

What we've seen so far are "feedforward" NNs



Sequence Data

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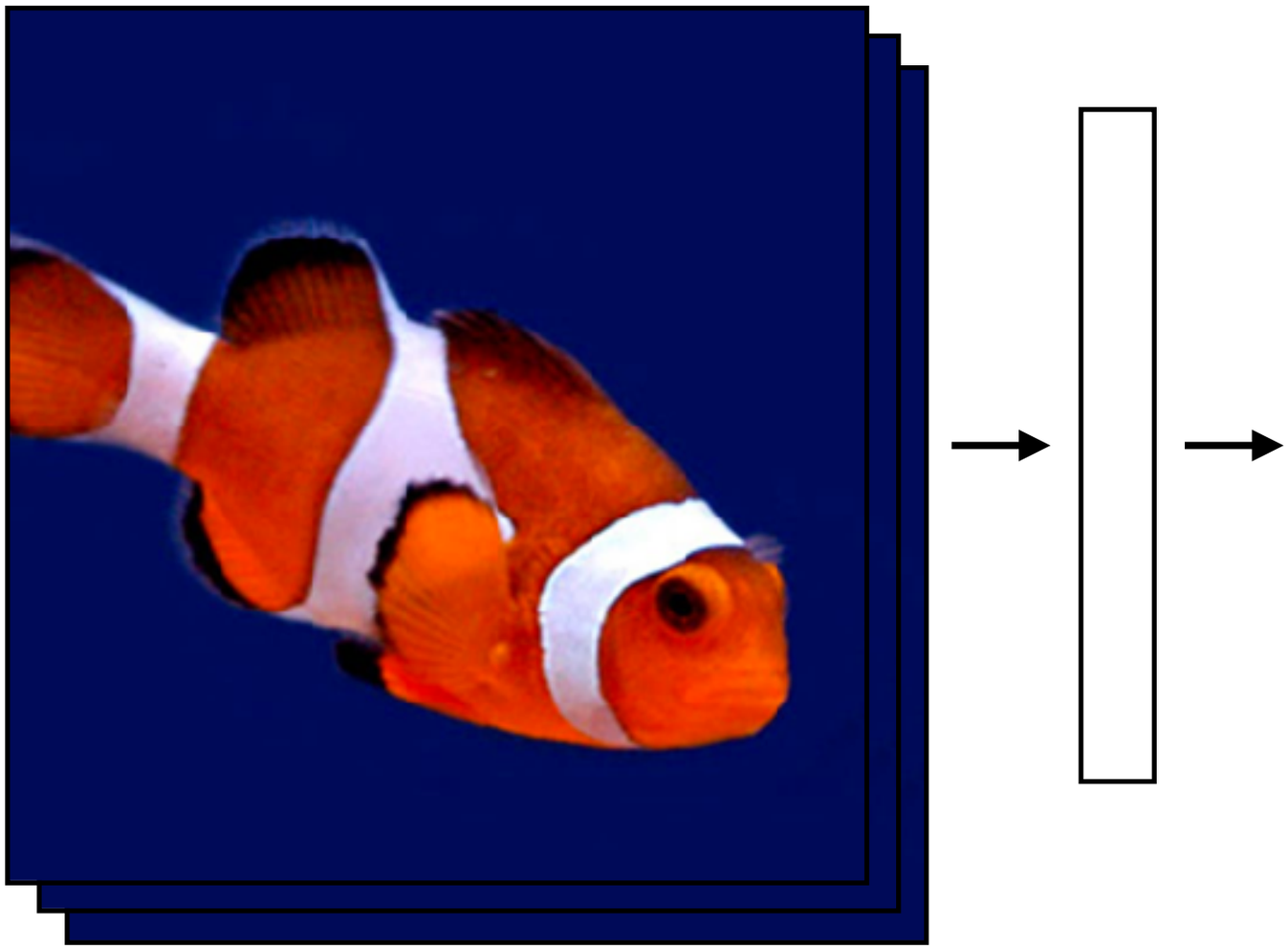


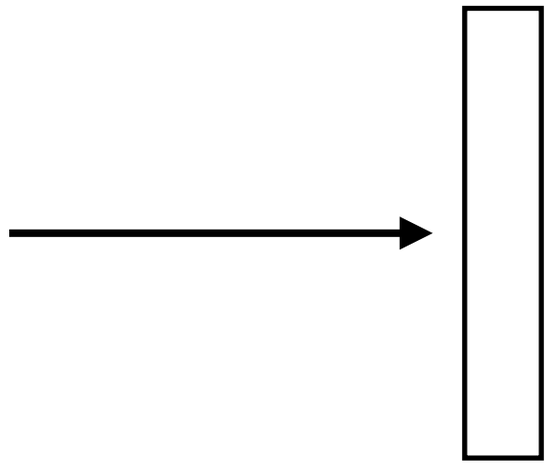
What if we had a video?

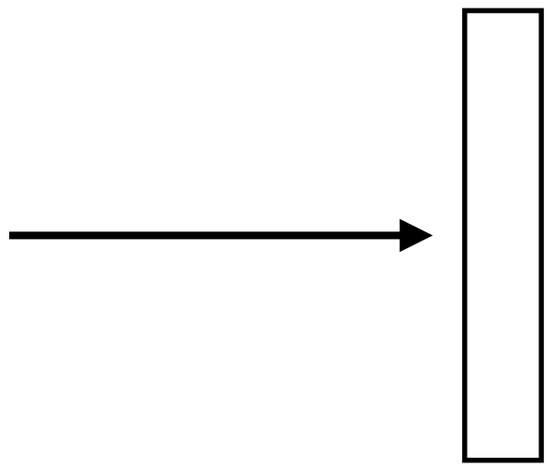
Recurrent Neural Nets

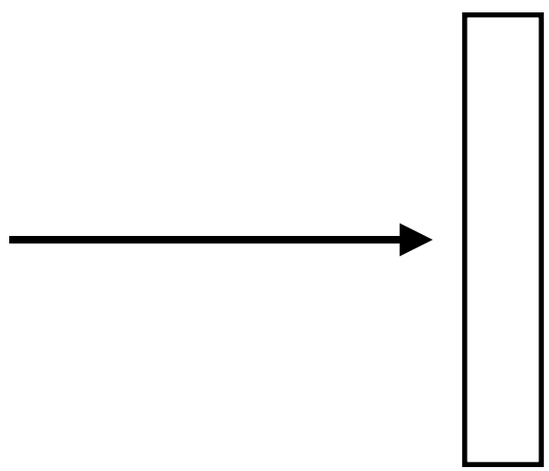
Time 0

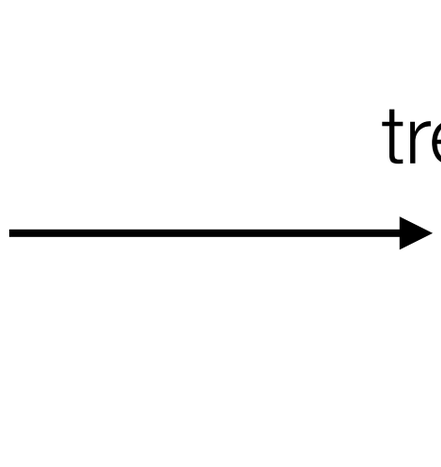
Time 1

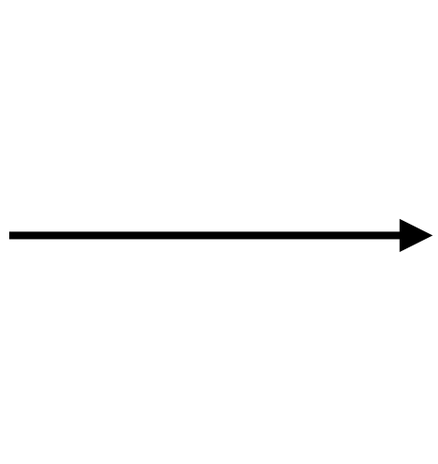
Time 2

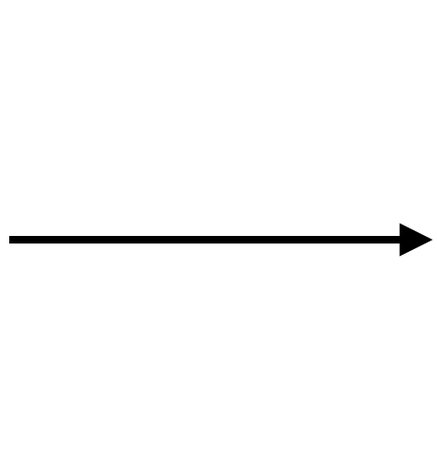








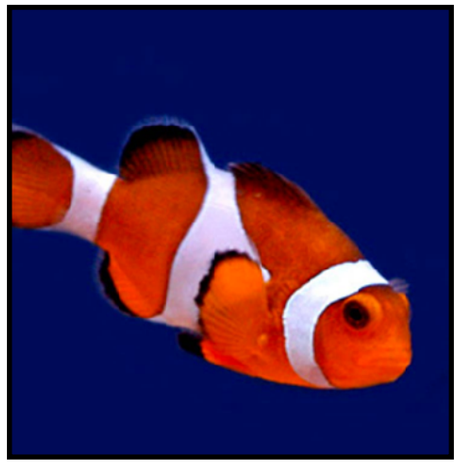




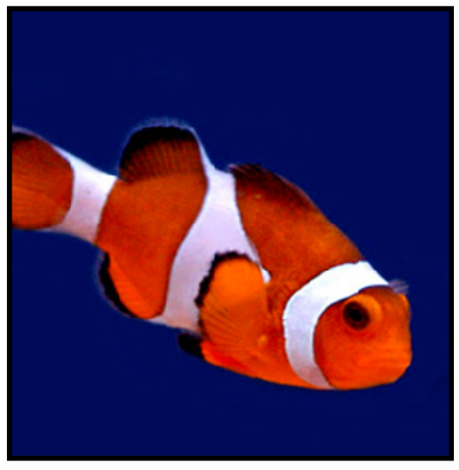
Feedforward NN's: treat each video frame separately

Recurrent Neural Nets

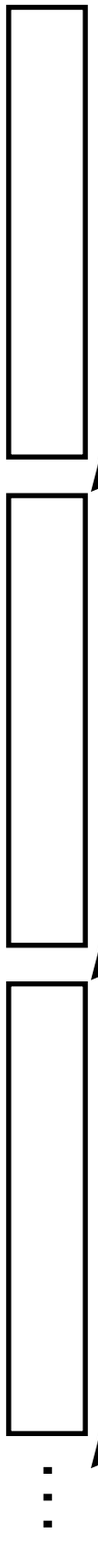
Time 0



Time 1



Time 2

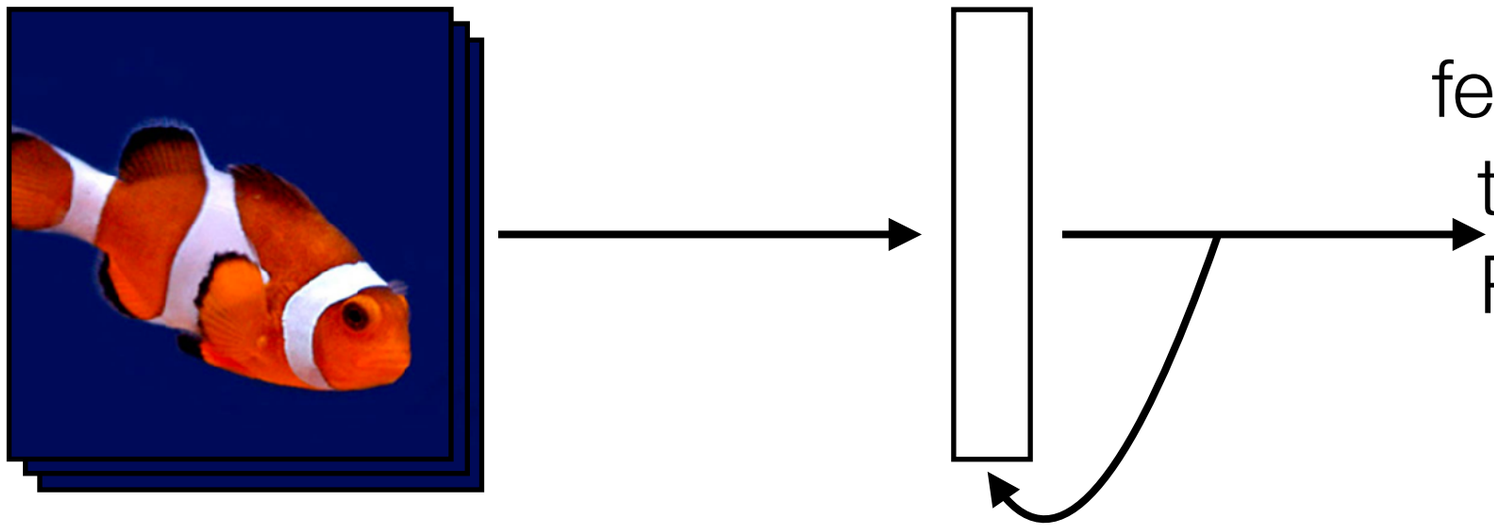


Feedforward NN's:
treat each video frame separately

RNNs:
feed output at previous time step as input to RNN layer at current time step

In PyTorch, different RNN options:
`RNN` (vanilla),
`LSTM`, `GRU`

Recurrent Neural Nets



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In PyTorch, different RNN options:
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Vanilla ReLU RNN

memory that evolves over time; we want to learn how it changes

```
current_state = np.zeros(num_nodes)

for input in input_sequence:

    linear = np.dot(input, W) \
           + np.dot(current_state, U) \
           + b

    output = np.maximum(0, linear) # ReLU

    current_state = output
```

`W` is a 2D table: # rows: (length of single time step's `input`), # cols: `num_nodes`

`U` is a 2D table: `num_nodes` by `num_nodes`

`b` is a 1D table: `num_nodes` entries

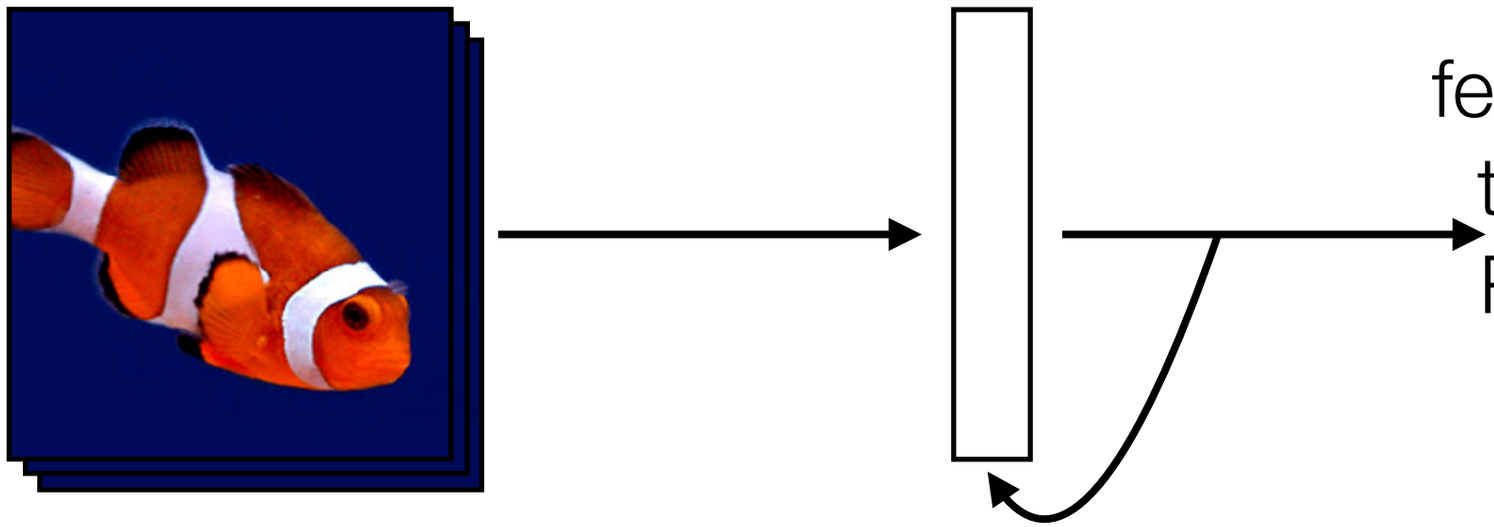
Parameters: weight matrices `W` & `U`, and bias vector `b`

Key idea: **it's like a linear layer in a `for` loop that tracks how memory changes over time**

Recurrent Neural Nets

Feedforward NN's:
treat each video frame separately

readily chains together with other neural net layers



Time series

RNN layer

like a linear layer that has memory

does not incorporate image structure!!!

RNNs:
feed output at previous time step as input to RNN layer at current time step

In PyTorch, different RNN options:
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Recurrent Neural Nets

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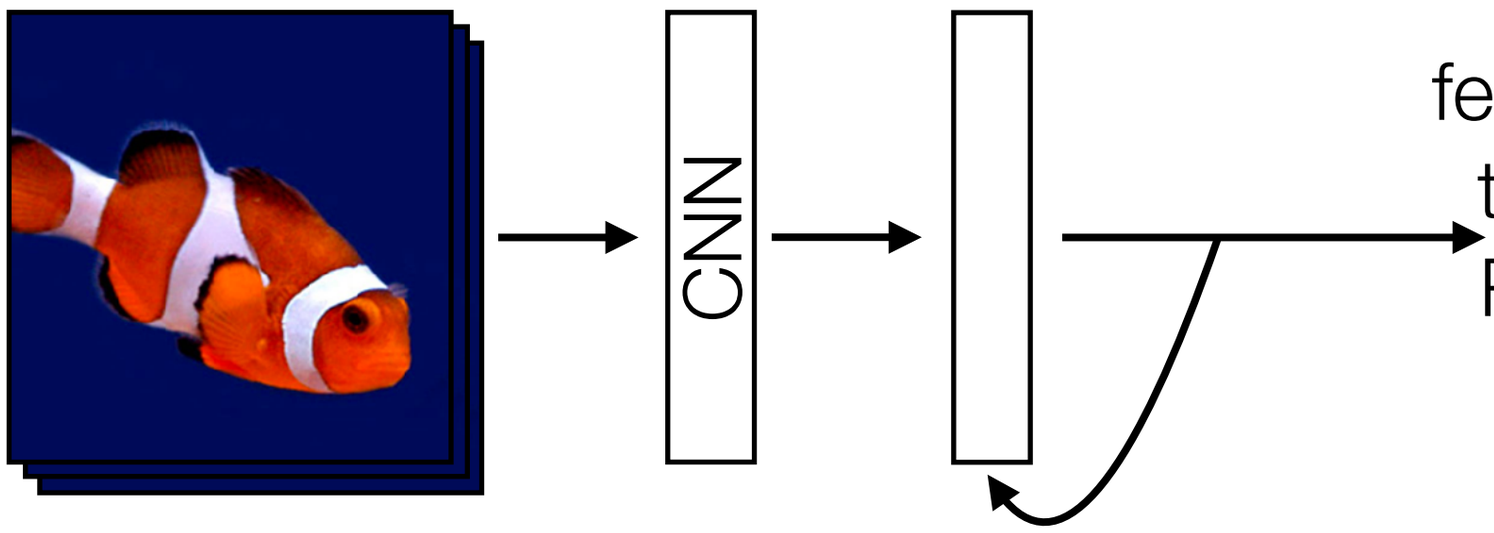

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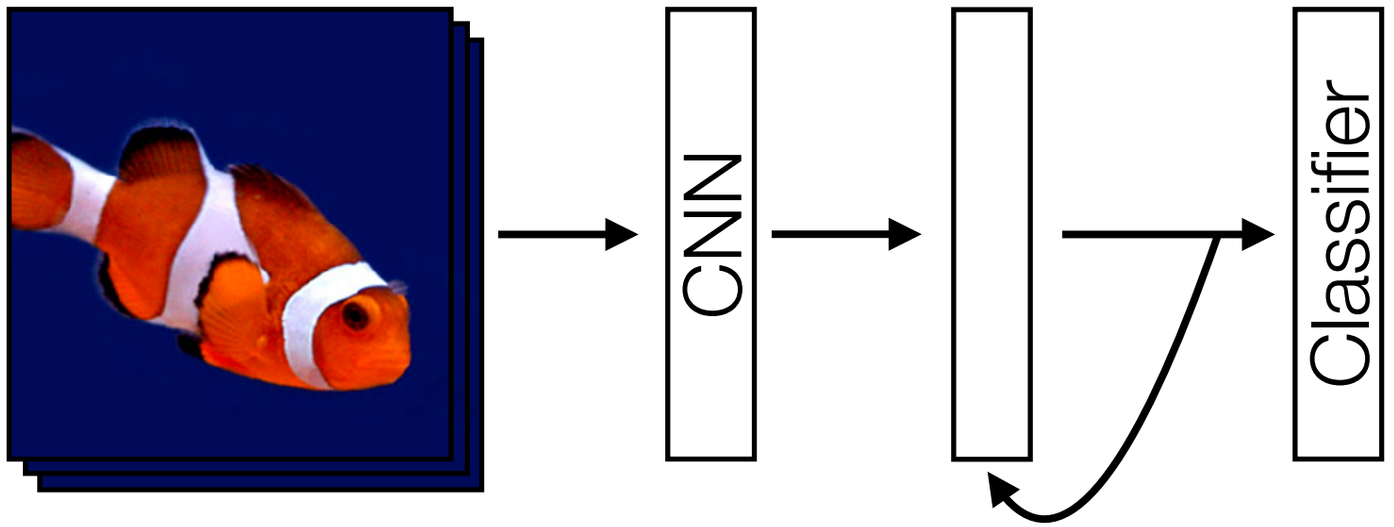

Time series

RNN layer

Use CNN to incorporate image structure!

like a linear layer that has memory

does not incorporate image structure!!!

In PyTorch, different RNN options:
`RNN` (vanilla),
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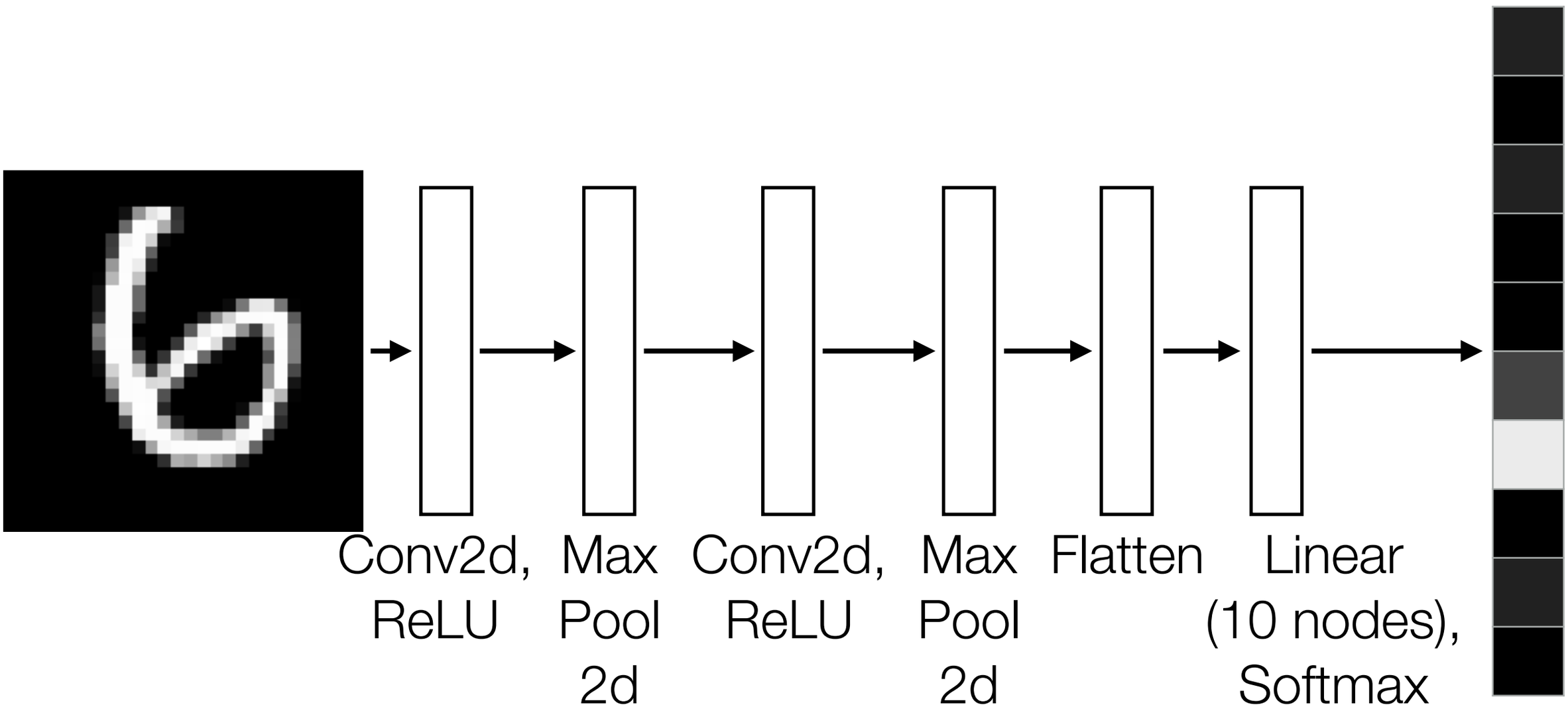
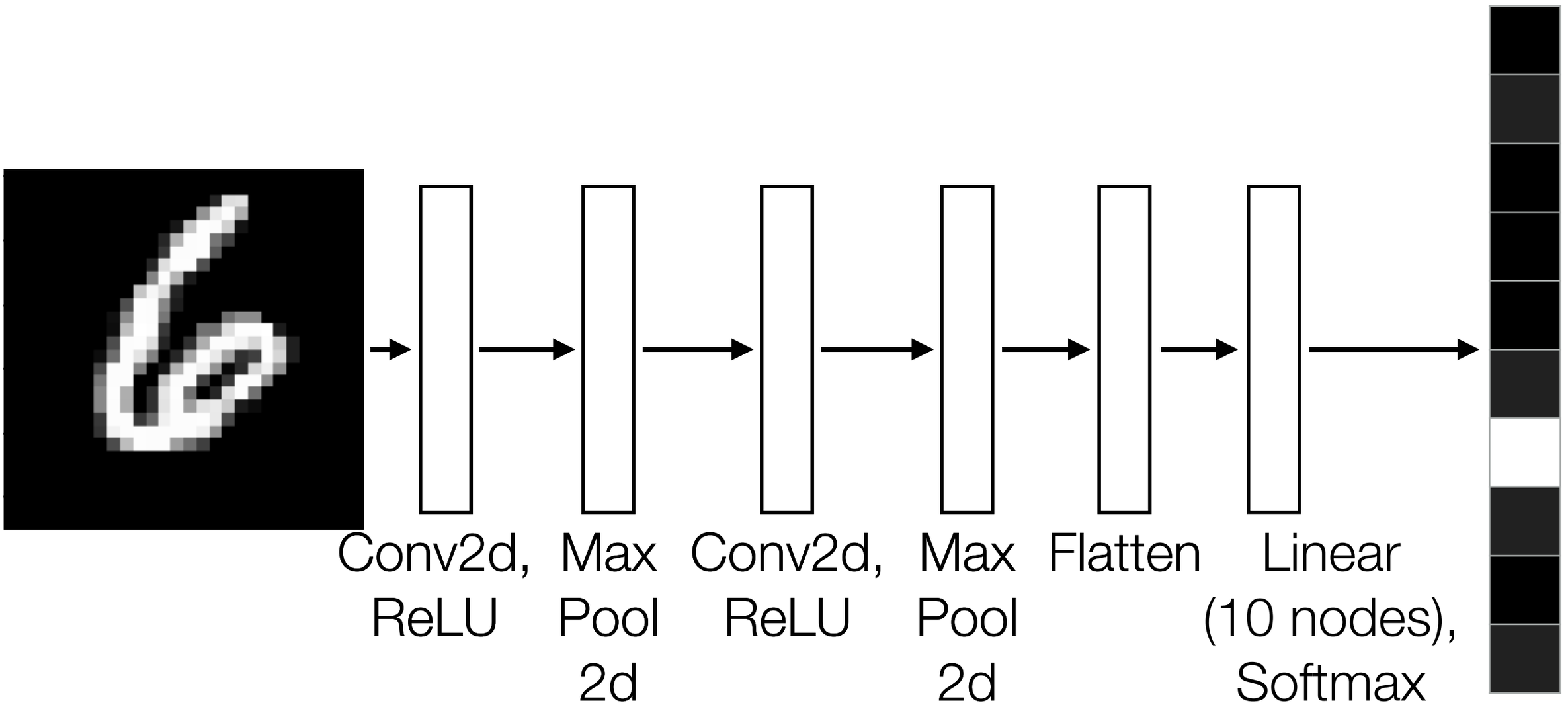
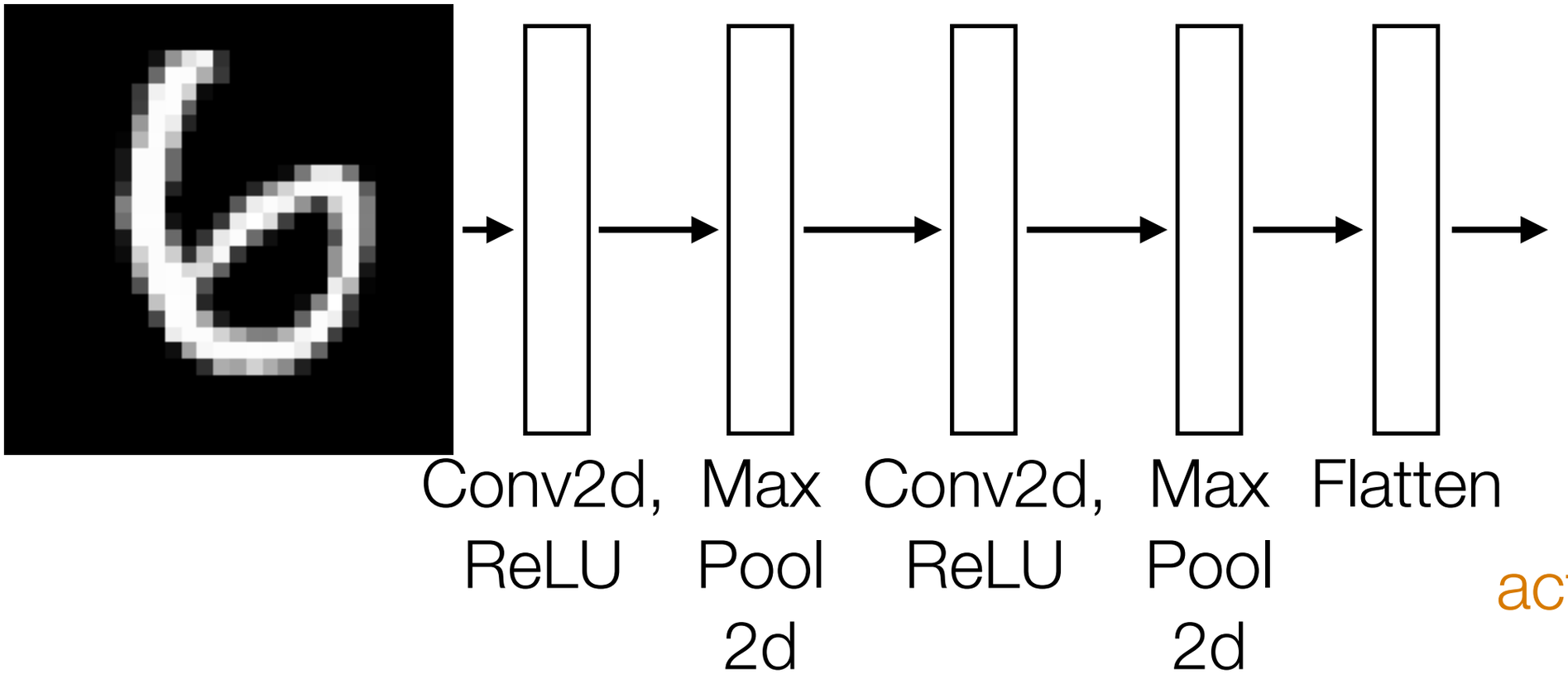
Intuition: CNNs Encode Semantic Structure for Images



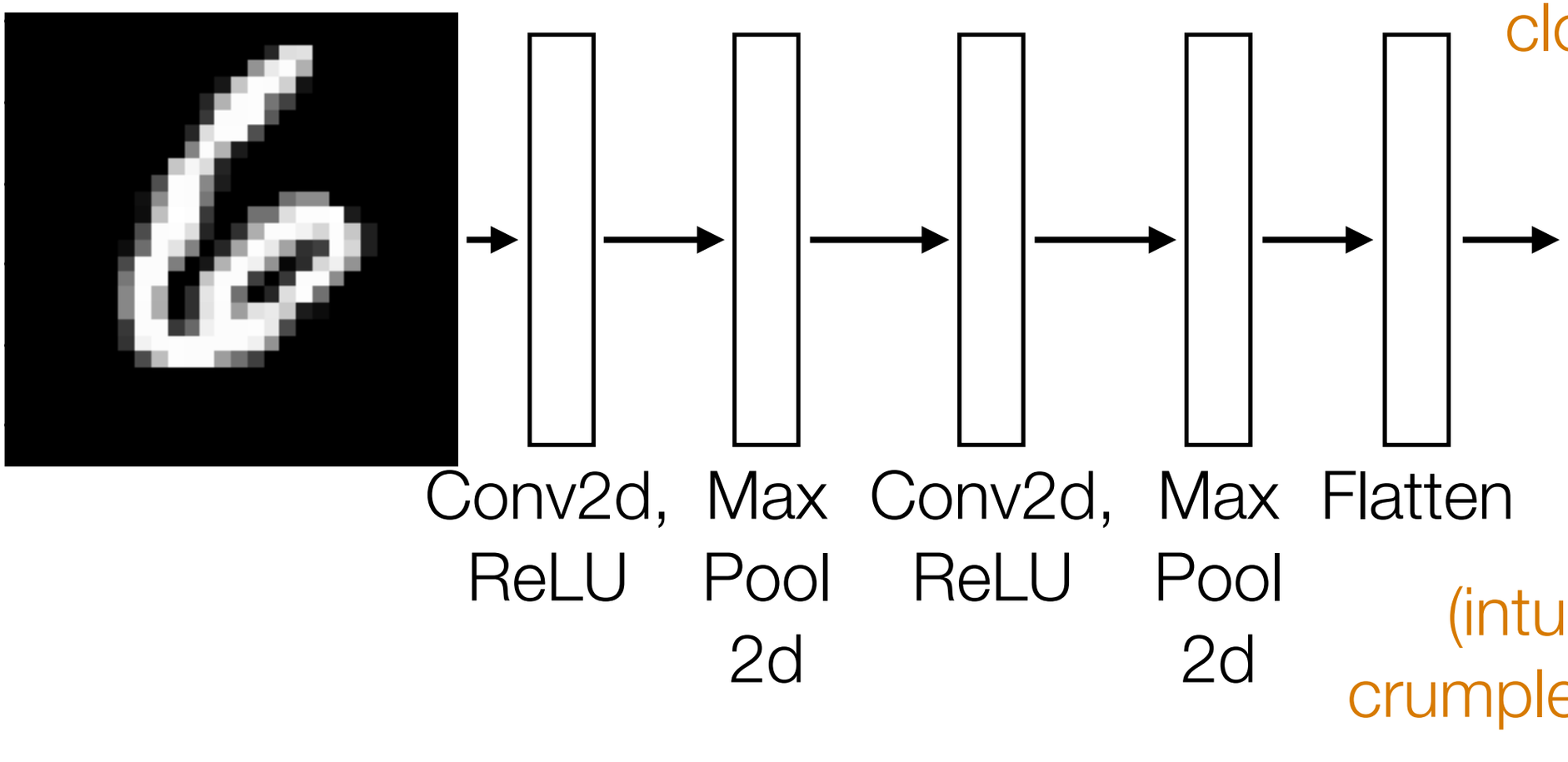
Intuition: CNNs Encode Semantic Structure for Images



final output for different input 6's is similar



actually, intermediate representations



close to the last layer are also similar!

(intuition: recall the crumpled paper analogy!)

Recurrent Neural Nets

Feedforward NN's:
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readily chains together with other neural net layers

RNNs:
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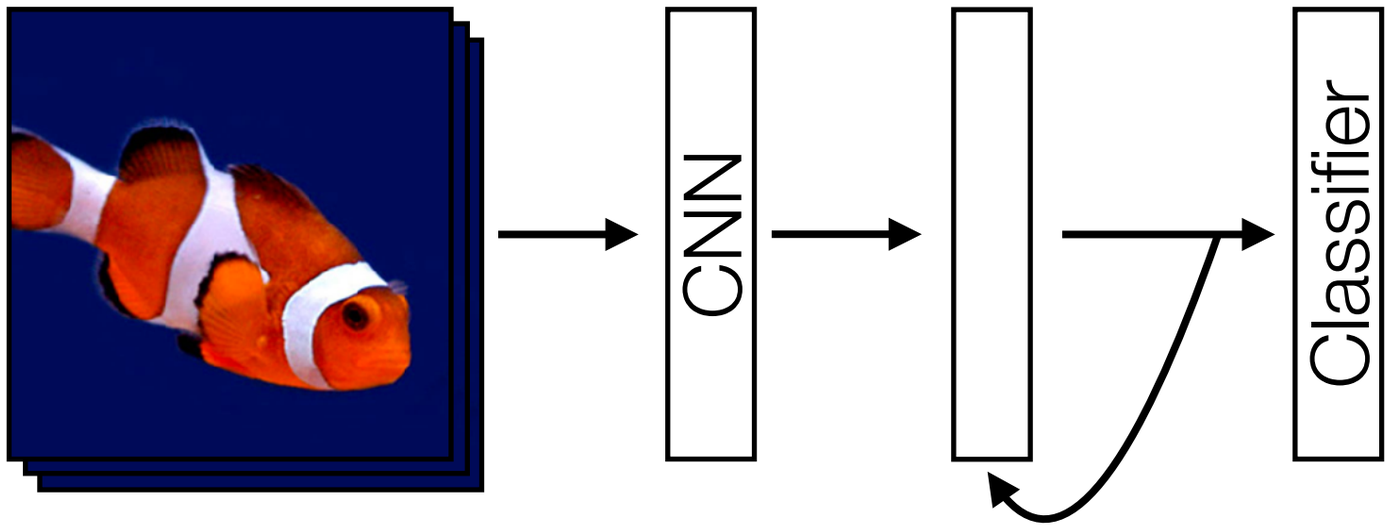

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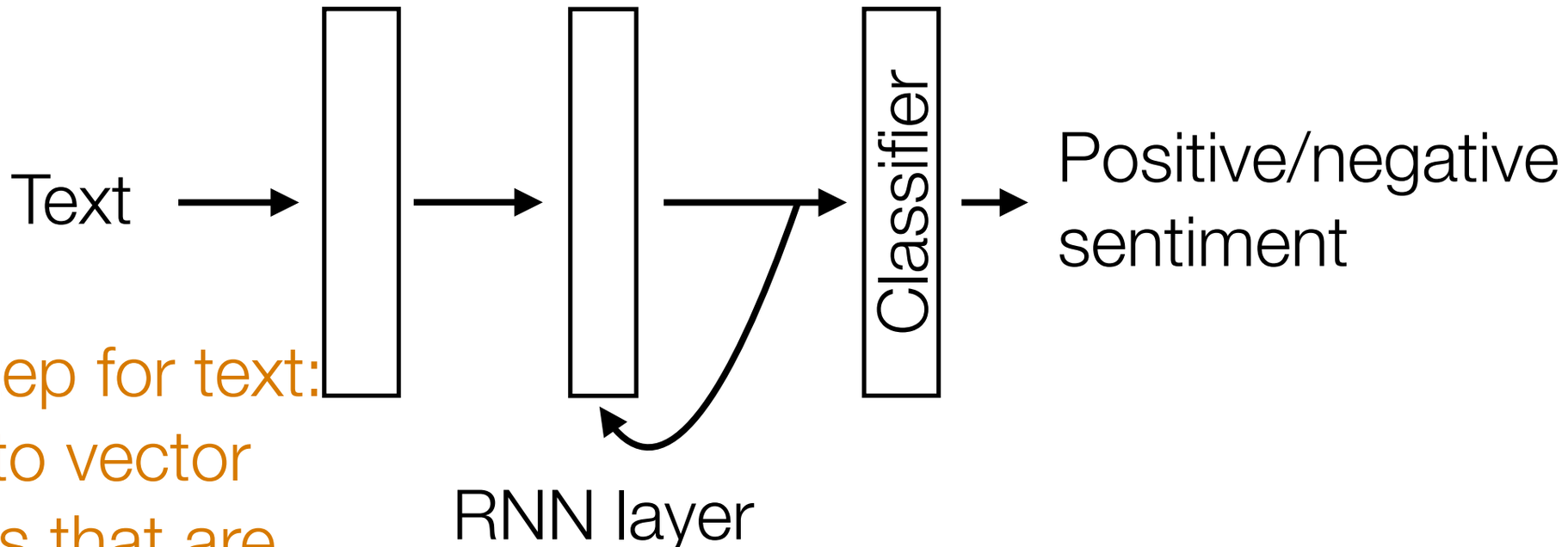
Recurrent Neural Nets

Example: Given text (e.g., movie review, Tweet), figure out whether it has positive or negative sentiment (binary classification)



Common first step for text: turn words into vector representations that are semantically meaningful

(Flashback) Do Data Actually Live on Manifolds?

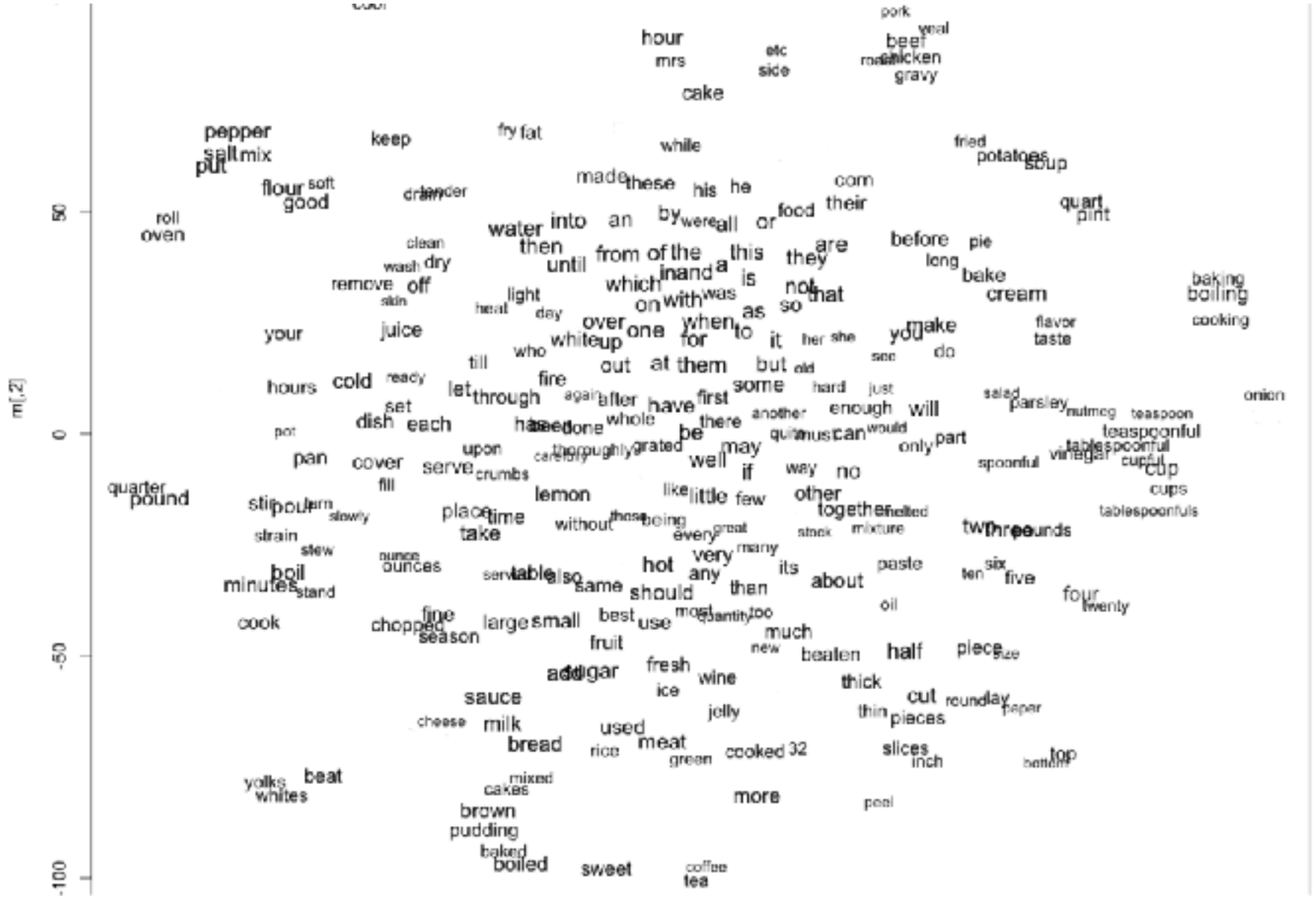


Image source: http://www.adityathakker.com/wp-content/uploads/2017/06/word-embeddings-994x675.png

Recurrent Neural Nets

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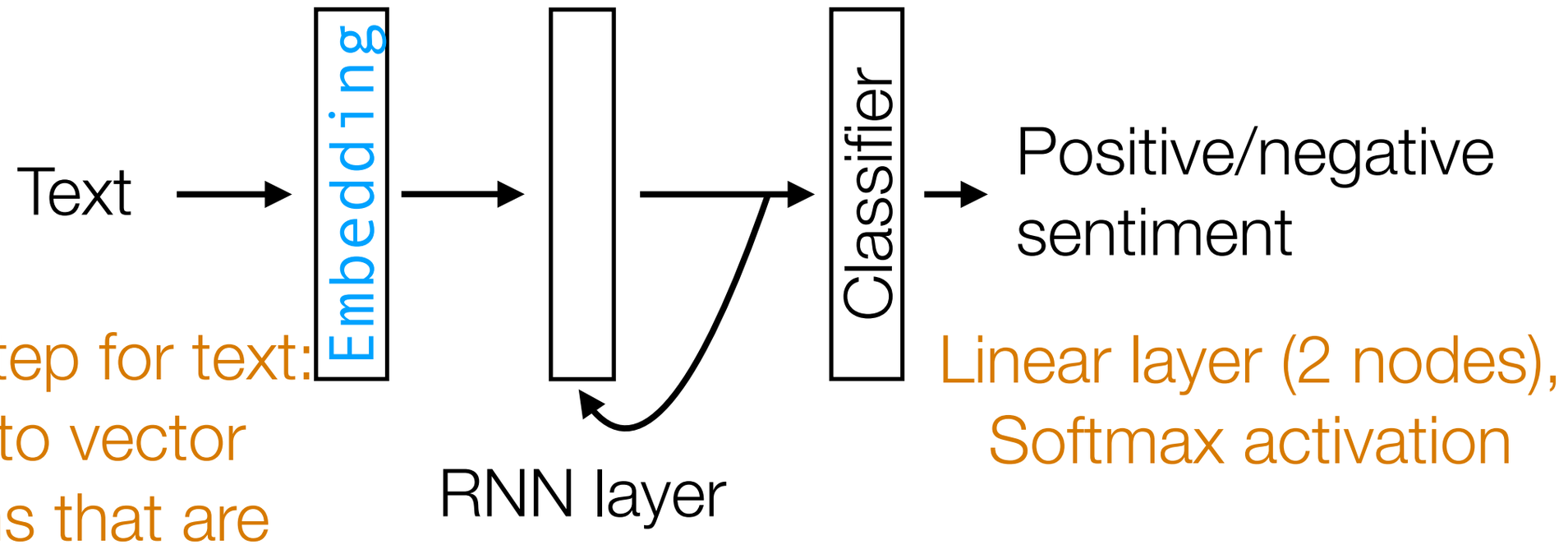
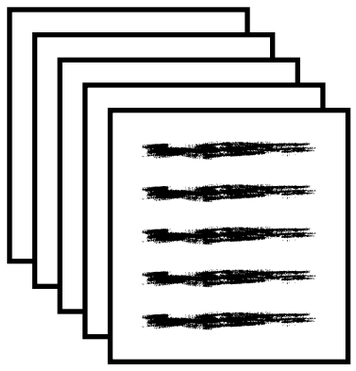


Common first step for text: turn words into vector representations that are semantically meaningful

Linear layer (2 nodes), Softmax activation

In PyTorch, use the `Embedding` layer

Sentiment Analysis with IMDb Reviews



Training reviews

Step 1: Tokenize & build vocabulary

Word index	Word	2D Embedding
0	this	[-0.57, 0.44]
1	movie	[0.38, 0.15]
2	rocks	[-0.85, 0.70]
3	sucks	[-0.26, 0.66]

Ordering of words matters

Different reviews can have different lengths

Step 2: Encode each review as a sequence of word indices into the vocab

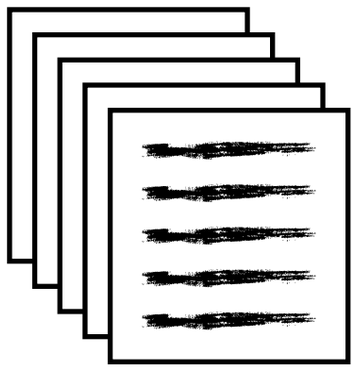
“this movie rocks” → 0 1 2

“this movie sucks” → 0 1 3

“this sucks” → 0 3

Step 3: Use word embeddings to represent each word

Sentiment Analysis with IMDb Reviews



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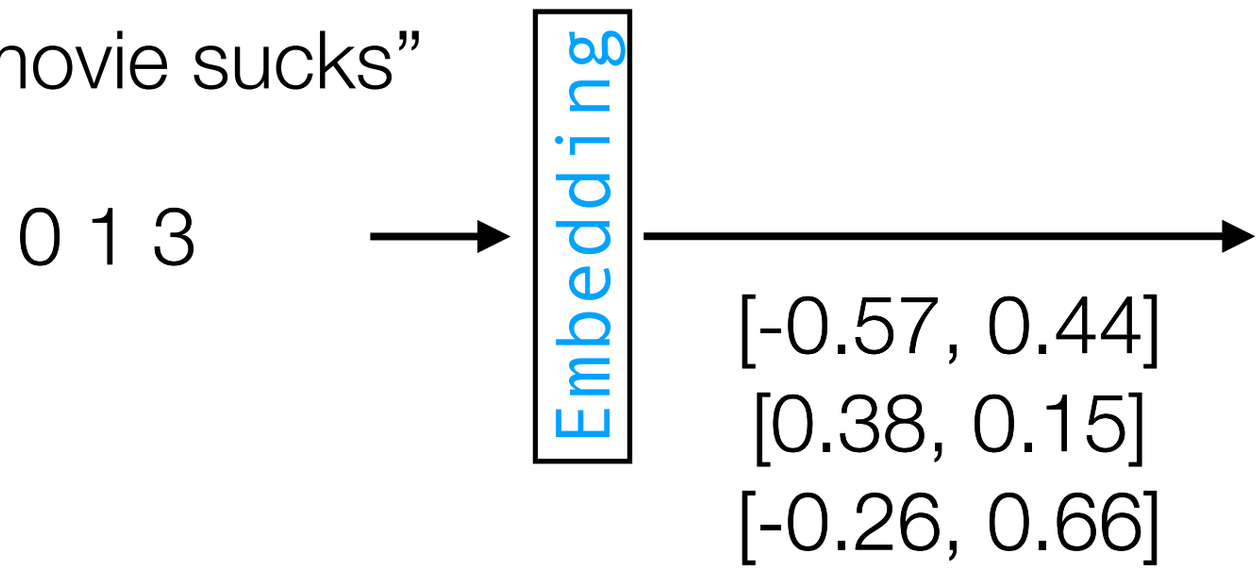
Sentiment Analysis with IMDb Reviews



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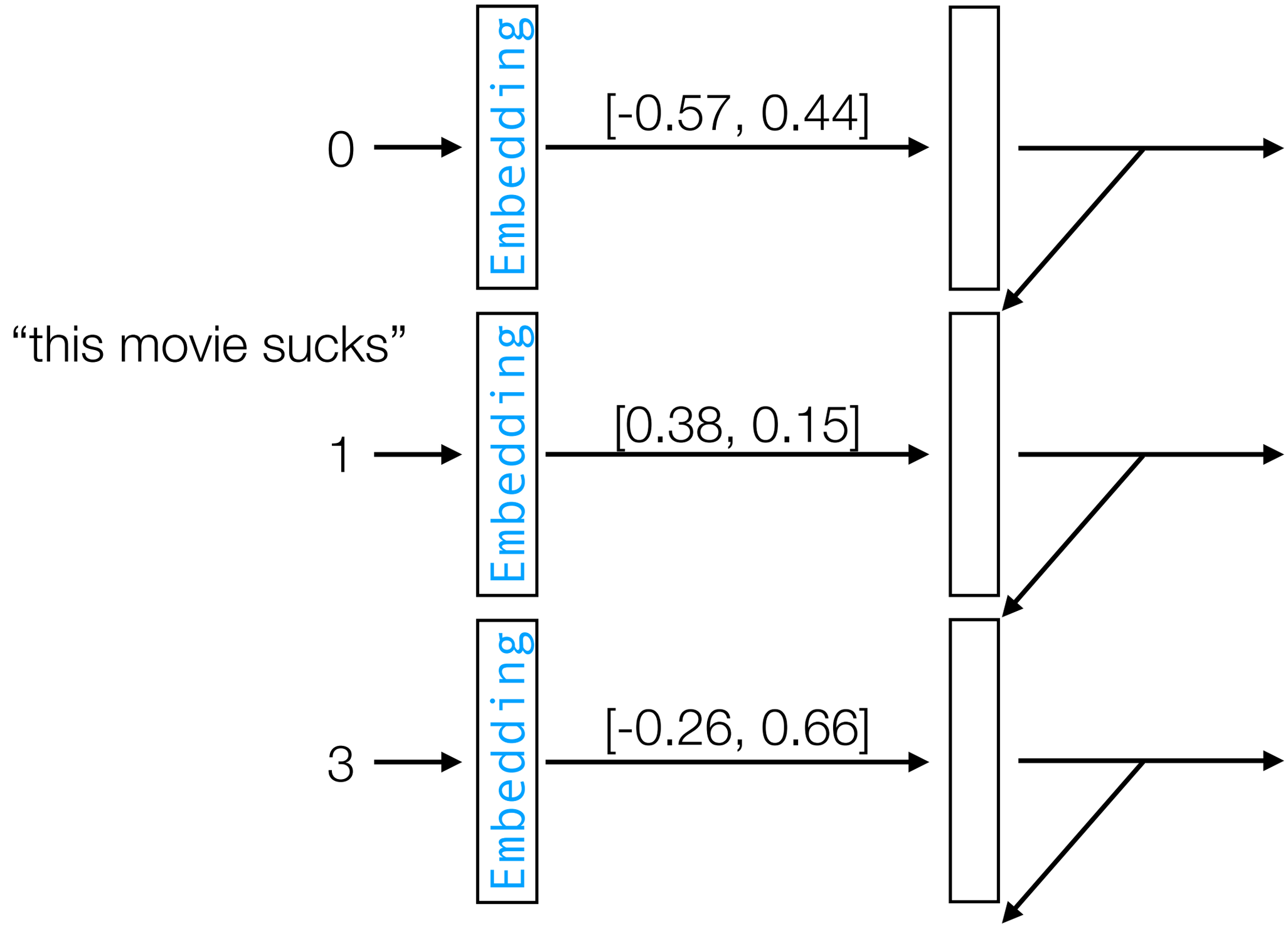

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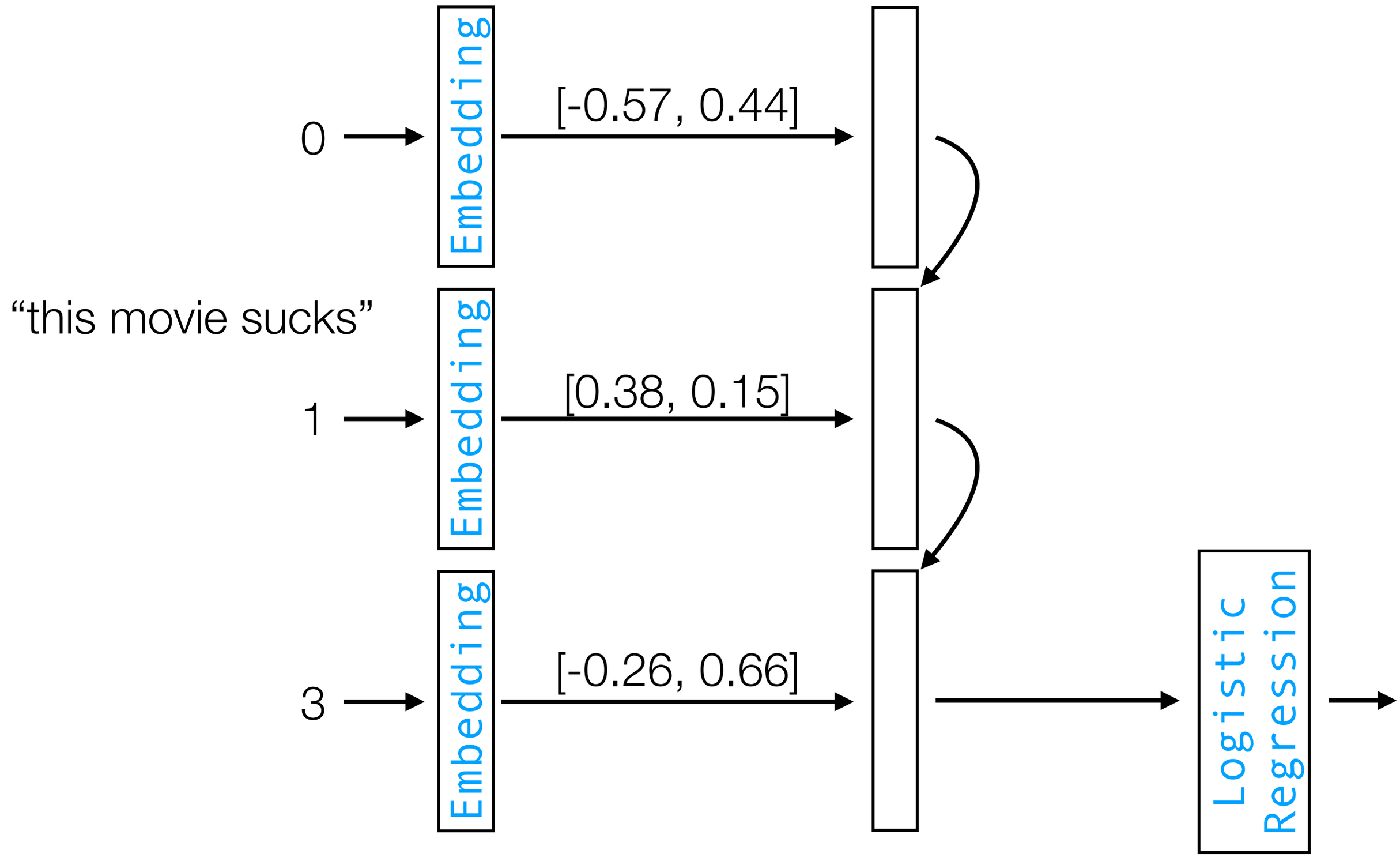

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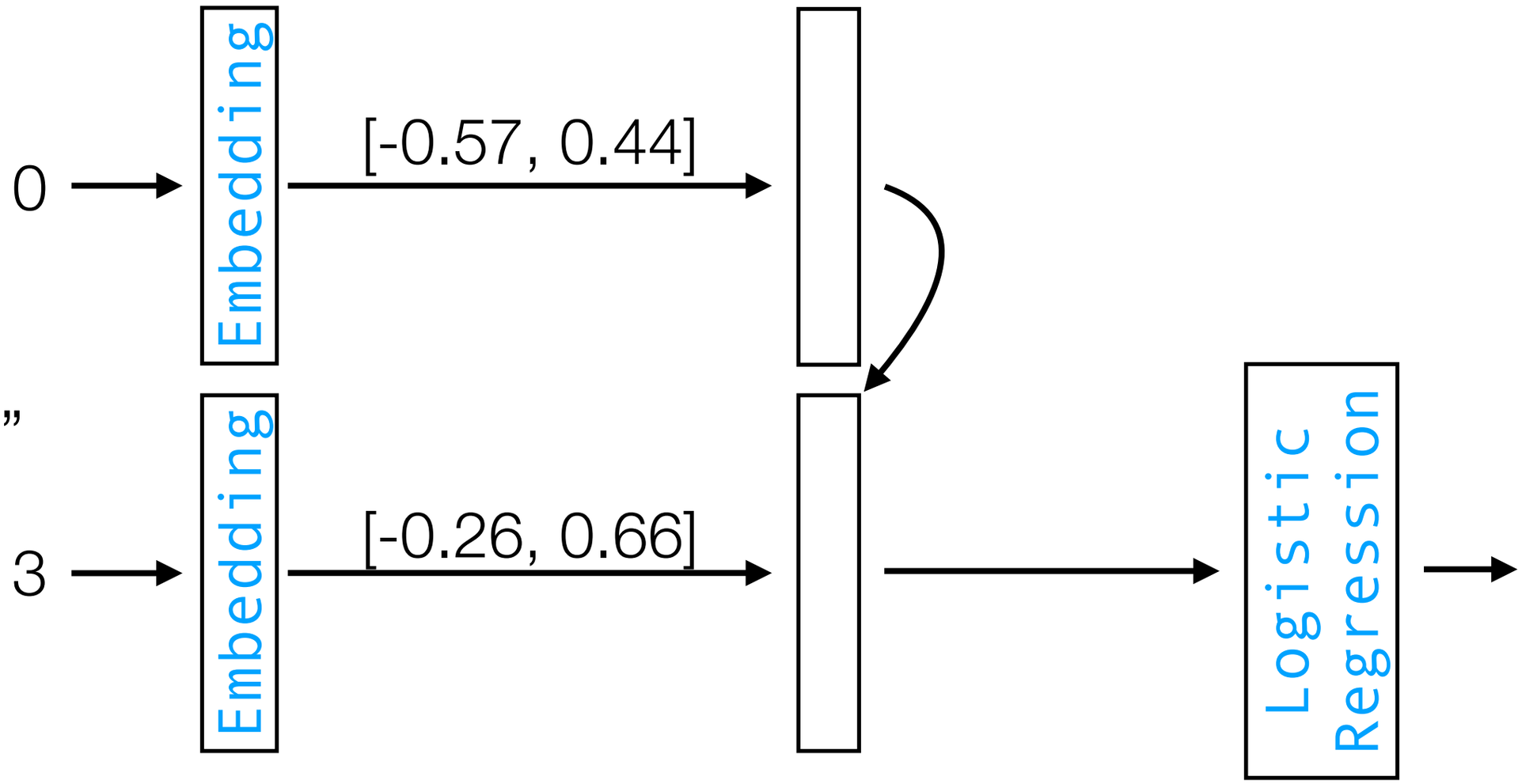
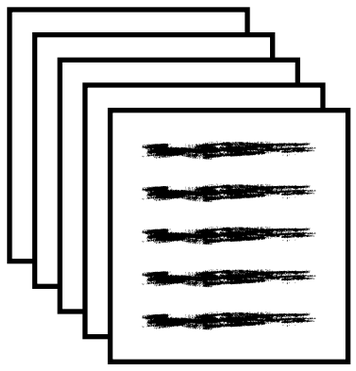


RNN's work with variable-length inputs

Note: Often in text analysis, the word embeddings are treated as fixed, so we do *not* update them during training

What if we didn’t use word embeddings?

Sentiment Analysis with IMDb Reviews



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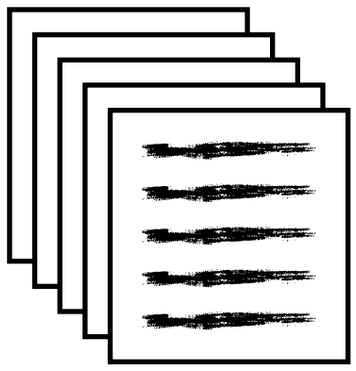
Step 2: Encode each review as a sequence of word indices into the vocab

“this movie sucks” → 0 1 3

Step 3: Use word embeddings to represent each word

[-0.57, 0.44]
[0.38, 0.15]
[-0.26, 0.66]

Bad Strategy: One-Hot Encoding



Training reviews

Step 1: Tokenize & build vocabulary

Word index	Word	One-hot encoding
0	this	[1, 0, 0, 0]
1	movie	[0, 1, 0, 0]
2	rocks	[0, 0, 1, 0]
3	sucks	[0, 0, 0, 1]

Step 2: Encode each review as a sequence of word indices into the vocab

“this movie sucks” → 0 1 3

Step 3: Use one-hot encoding to represent each word

[1, 0, 0, 0]
[0, 1, 0, 0]
[0, 0, 0, 1]

This strategy tends to work poorly in practice: distance between every pair of words is the same in one-hot encoding!

Recap/Important Reminder

- Neural nets are *not* doing magic; **incorporating structure is very important to state-of-the-art deep learning systems**

    - Word embeddings encode semantic structure—words with similar meaning are mapped to nearby Euclidean points

    - CNNs encode semantic structure for images—images that are “similar” are mapped to nearby Euclidean points

- An RNN tracks how what’s stored in memory changes over time — **an RNN’s job is made easier if the memory is a semantically meaningful representation**

Sentiment Analysis with IMDb Reviews

Demo will be in your recitation

A special kind of RNN: an “LSTM”

(Flashback) Vanilla ReLU RNN

```
current_state = np.zeros(num_nodes)

for input in input_sequence:

  linear = np.dot(input, W) \
           + np.dot(current_state, U) \
           + b

  output = np.maximum(0, linear) # ReLU

  current_state = output
```

Parameters: weight matrices `W` & `U`, and bias vector `b`

Key idea: **it's like a linear layer in a `for` loop that tracks how memory changes over time**

(Flashback) Vanilla ReLU RNN

```
current_state = np.zeros(num_nodes)

outputs = []

for input in input_sequence:

    linear = np.dot(input, W) \
           + np.dot(current_state, U) \
           + b

    output = np.maximum(0, linear)  # ReLU

    outputs.append(output)

    current_state = output
```

Time series

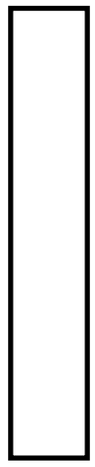
RNN layer

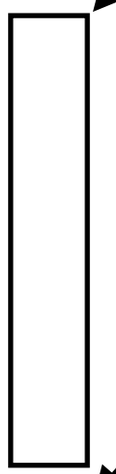
output prediction

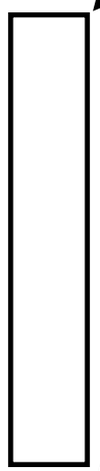
Time 0

Time 1

Time 2







output prediction 0

output prediction 1

output prediction 2

Time
$t - 1$

Time t

Time
$t + 1$

output $t - 1$

Vanilla RNN tends to
forget things quickly

output t

```
outputs[t]
= np.maximum(np.dot(input_sequence[t], W)
             + np.dot(outputs[t-1], U)
             + b, 0)
```

output $t + 1$

Long-term memory

Add explicit long-term memory!

Time $t - 1$

output $t - 1$

But need some way to update long-term memory!

Time t

output t

Time $t + 1$

output $t + 1$

Long-term memory

Add explicit long-term memory!

Time $t - 1$

output $t - 1$

But need some way to update long-term memory!

Time t

output t

Long-term memory

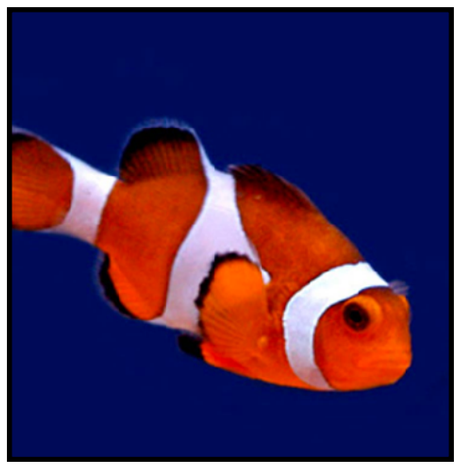
Add explicit long-term memory!

Time $t - 1$

output $t - 1$

But need some way to update long-term memory!

Time t



output t

Long-term memory

Time
$t - 1$

Long-term
memory updater

output $t - 1$

Add explicit long-term memory!

But need some way to update long-term memory!

Called a “long short-term memory” (LSTM) RNN

Remembers things longer than vanilla RNN

Time t

output t

Analyzing Times Series with CNNs

- Think about an image with 1 column, and where the rows index time steps: this is a time series!

- Think about a 2D image where rows index time steps, and the columns index features: this is a multivariate time series (feature vector that changes over time!)

- CNNs can be used to analyze time series *but inherently the size of the filters used say how far back in time we look*

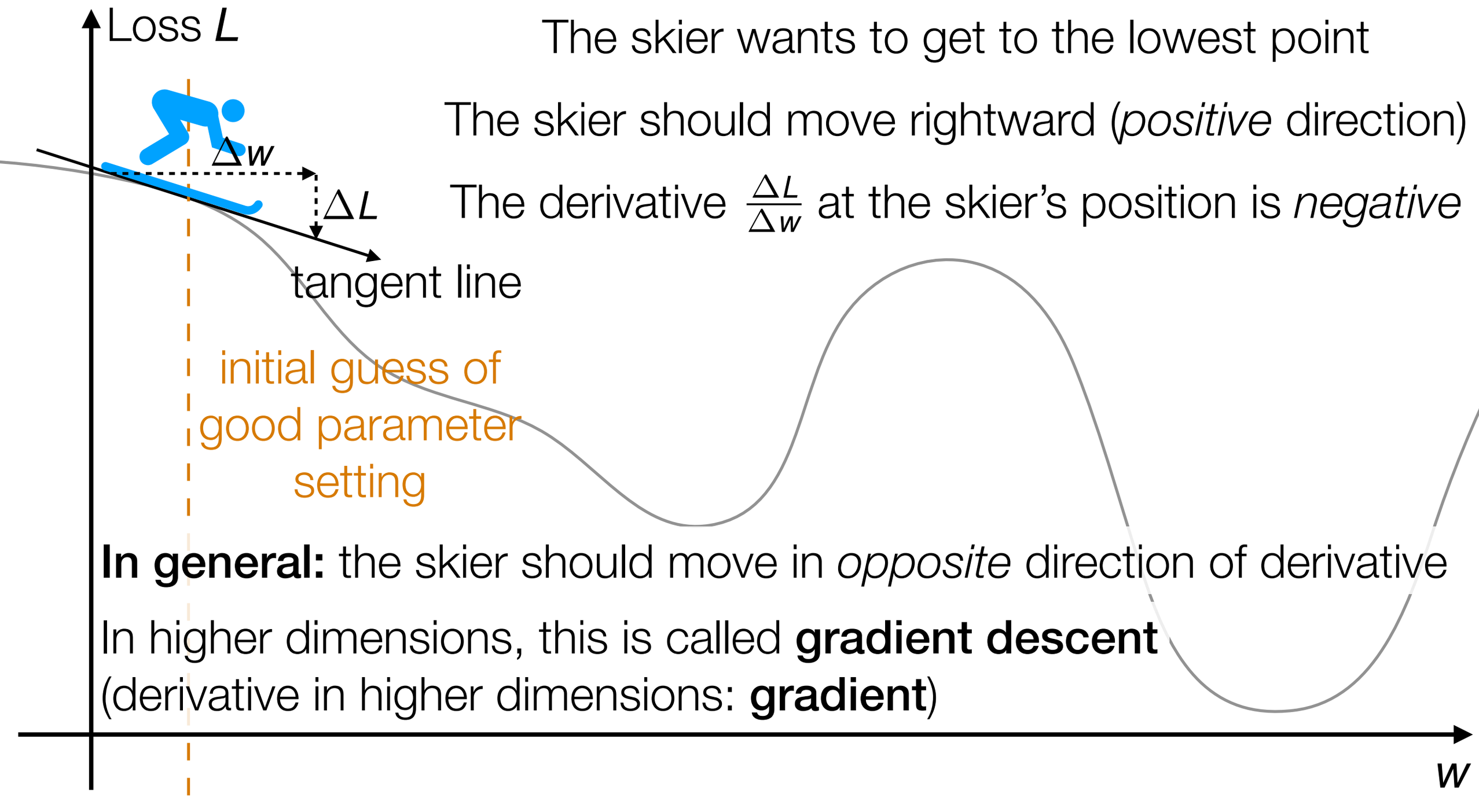
- If your time series does not have long-range dependencies that require long-term memory, CNNs can do well already!

    - If you need long-term memory, use RNNs

Some Other Deep Learning Topics

Learning a Deep Net

Suppose the neural network has a single real number parameter ***w***



The skier wants to get to the lowest point

The skier should move rightward (*positive* direction)

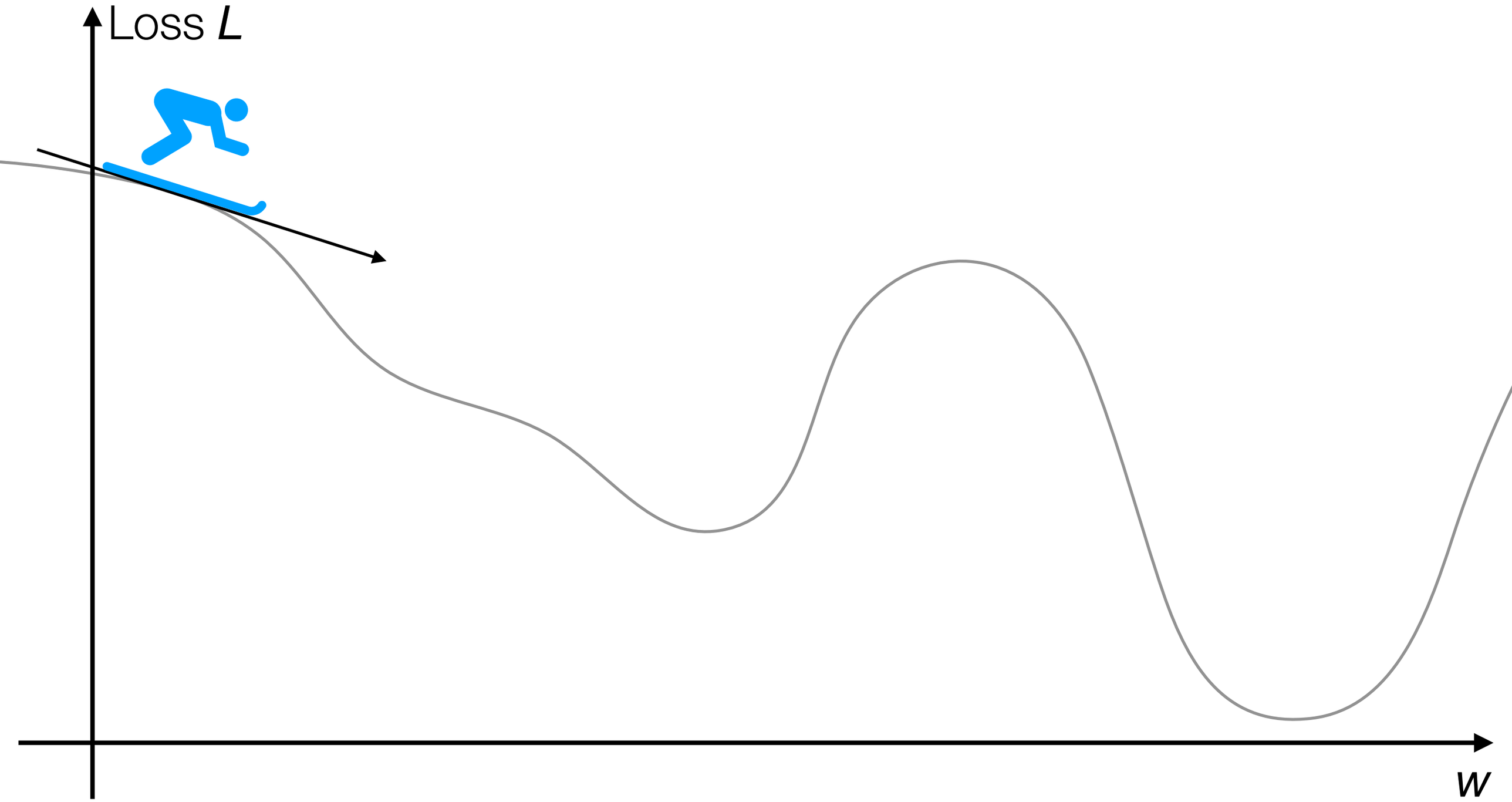
The derivative $\frac{\Delta L}{\Delta w}$ at the skier's position is *negative*

In general: the skier should move in *opposite* direction of derivative

In higher dimensions, this is called **gradient descent**
(derivative in higher dimensions: **gradient**)

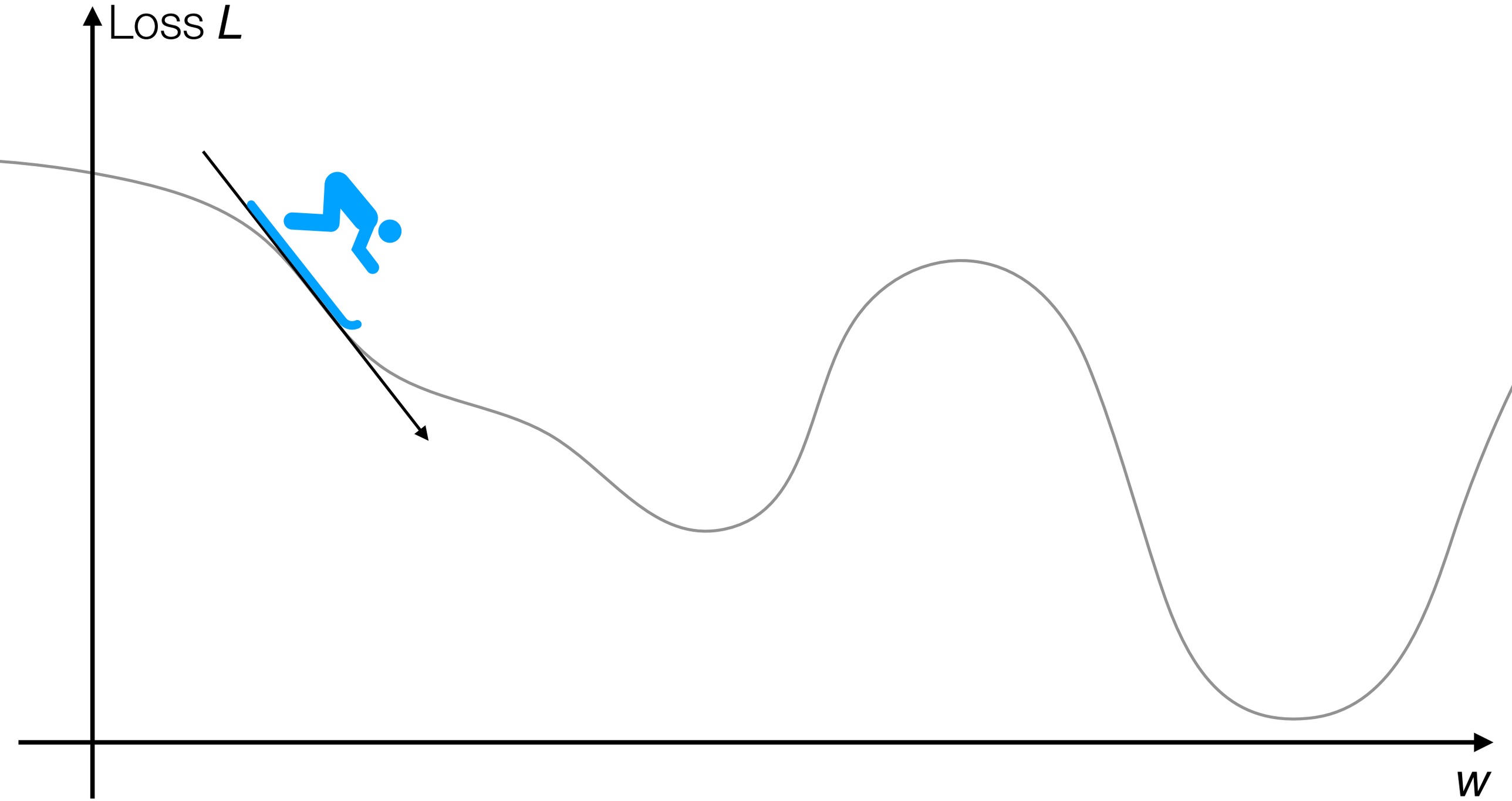
Learning a Deep Net

Suppose the neural network has a single real number parameter *w*



Learning a Deep Net

Suppose the neural network has a single real number parameter *w*



Learning a Deep Net

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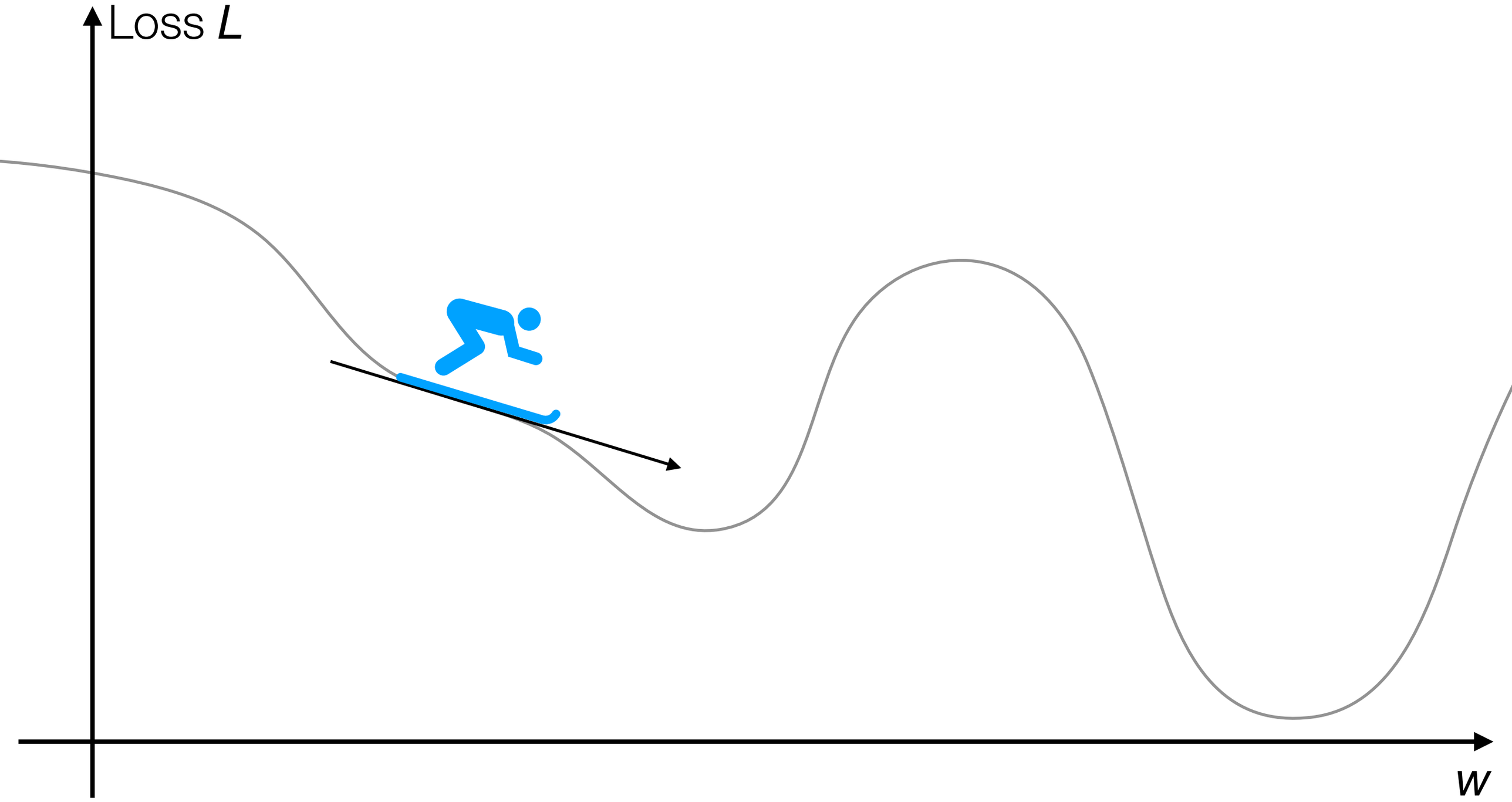


Learning a Deep Net

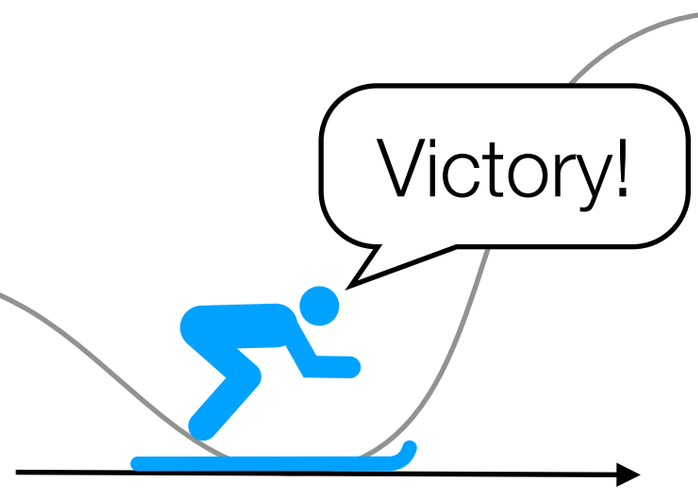
Suppose the neural network has a single real number parameter ***w***

Loss *L*

In general: not obvious what error landscape looks like!

➔ we wouldn't know there's a better solution beyond the hill

Popular optimizers (e.g., RMSprop, Adam, LookAhead, RAdam) are variants of gradient descent



Local minimum

Better solution

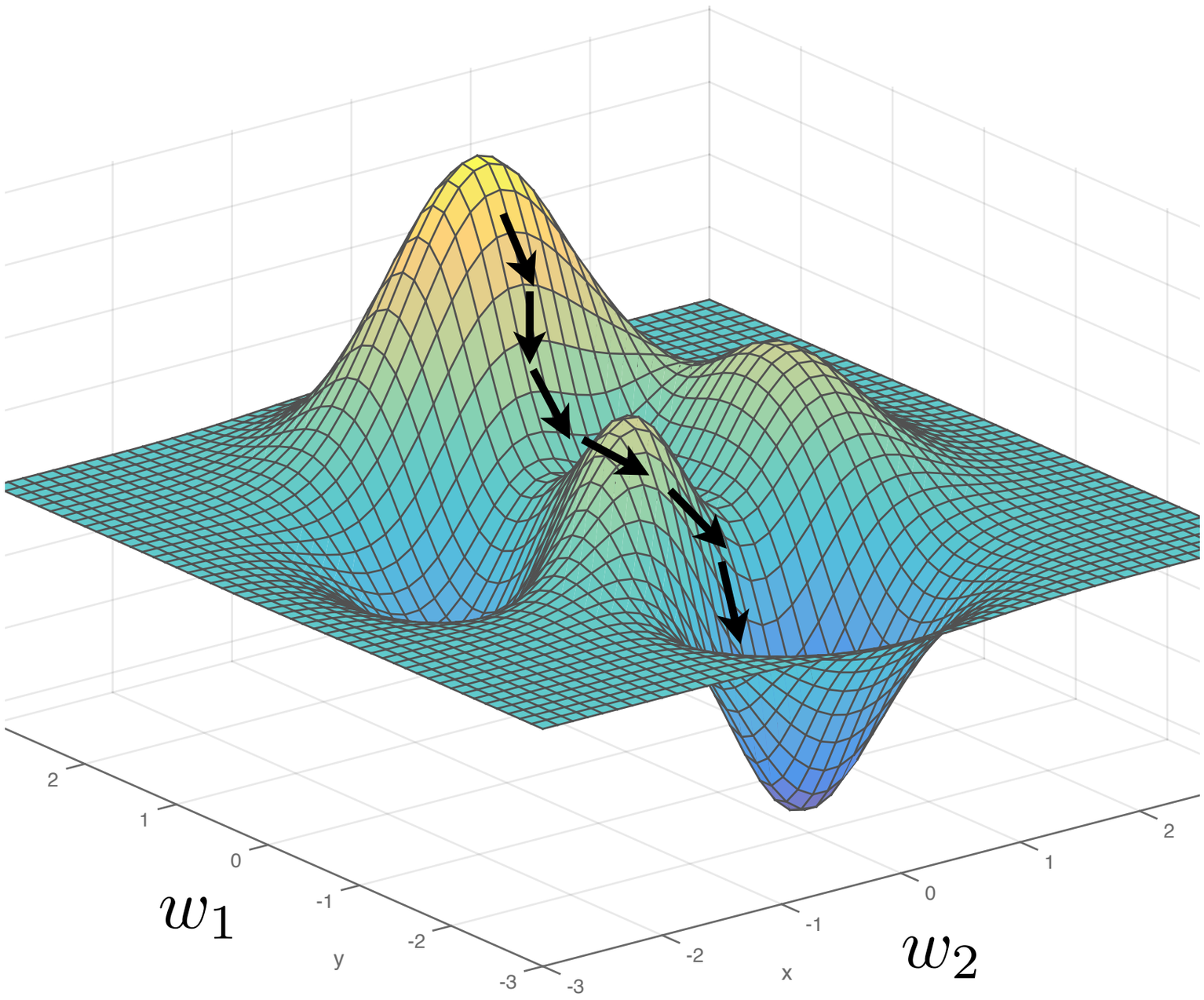
In practice: local minimum often good enough

w

Learning a Deep Net

2D example

$L(\mathbf{w})$



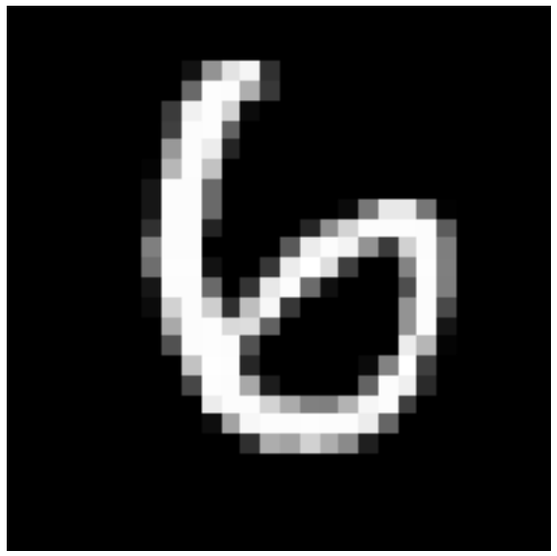
Slide by Phillip Isola

Remark: In practice, deep nets often have > *millions* of parameters, so *very* high-dimensional gradient descent

Handwritten Digit Recognition

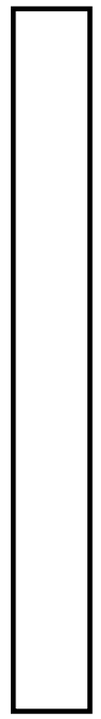
Training label: 6

y_i



28x28 image

x_i



f_1

$f_1(x_i)$

f_2

$f_2(f_1(x_i))$

Loss

L

error

$L(f_2(f_1(x_i)), y_i)$

A neural net is a function composition!

Overall loss:

$$\frac{1}{n}\sum_{i=1}^{n} L(f_2(f_1(x_i)), y_i)$$

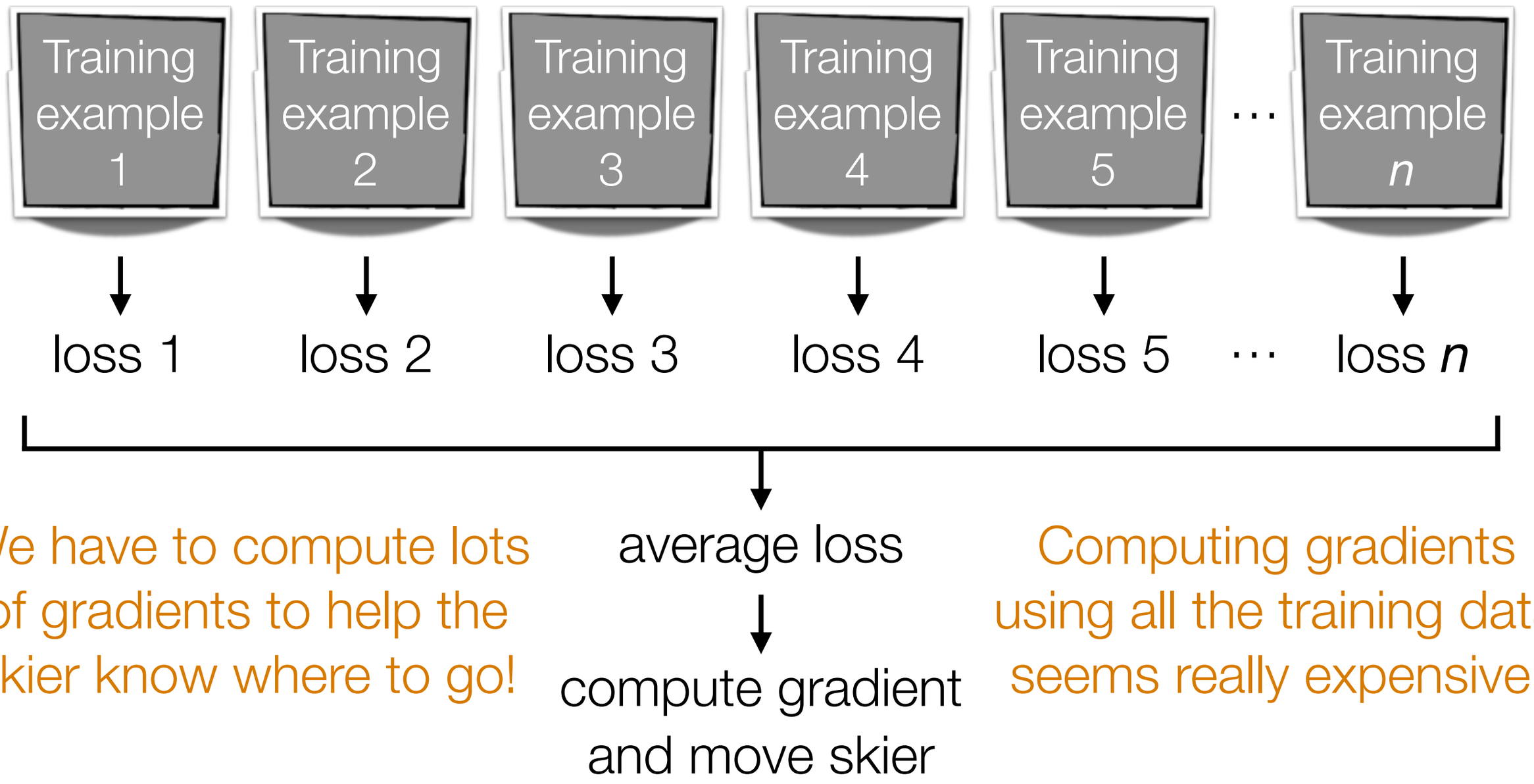
All parameters: θ

Gradient: $\frac{\partial \frac{1}{n}\sum_{i=1}^{n} L(f_2(f_1(x_i)), y_i)}{\partial \theta}$

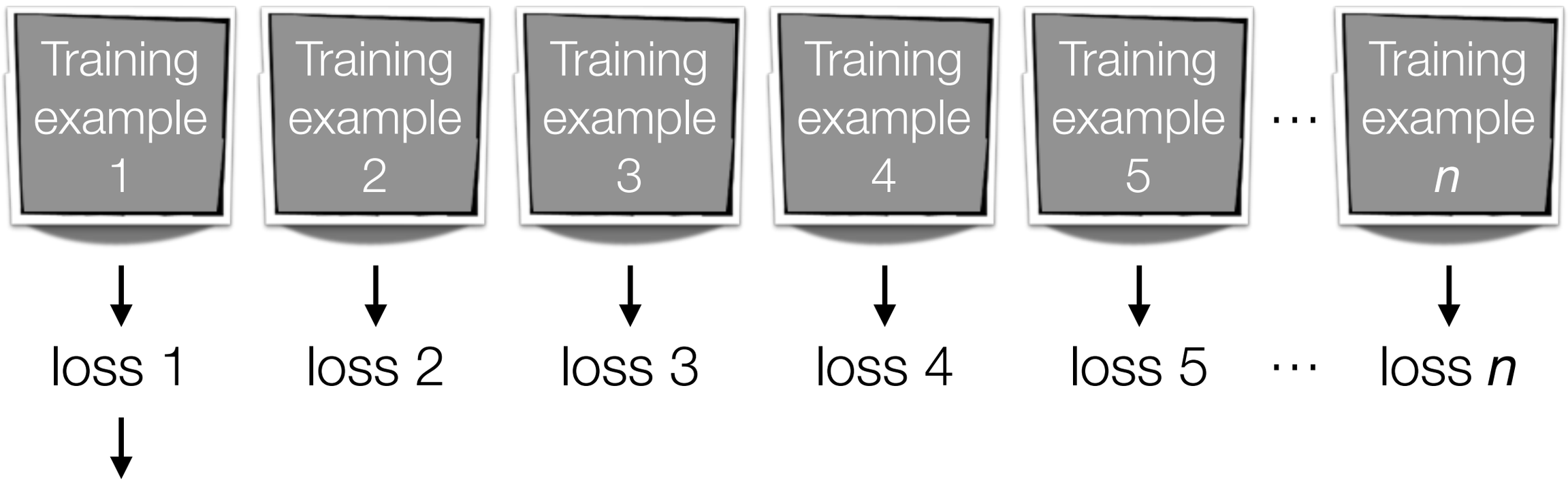
Automatic differentiation is crucial in learning deep nets!

Careful derivative chain rule calculation: **back-propagation**

Gradient Descent



Stochastic Gradient Descent (SGD)



SGD: compute gradient using only 1 training example at a time
(can think of this gradient as a noisy approximation of the “full” gradient)

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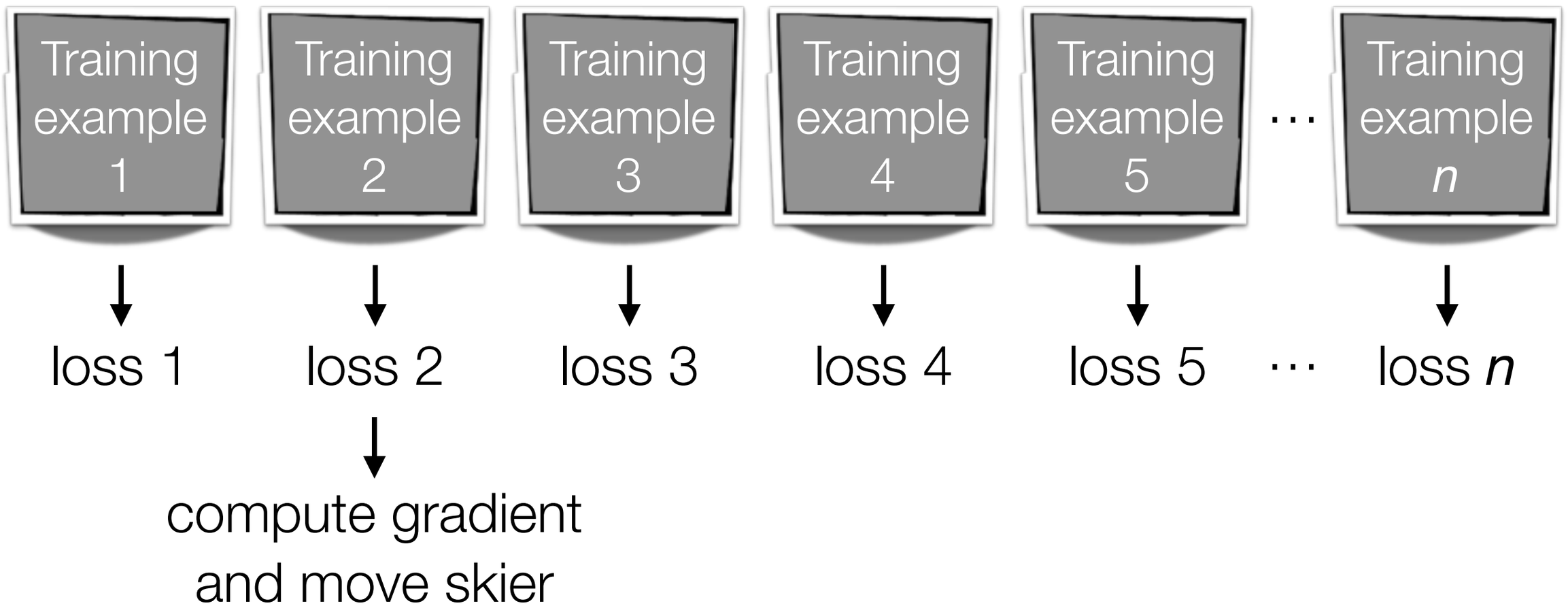

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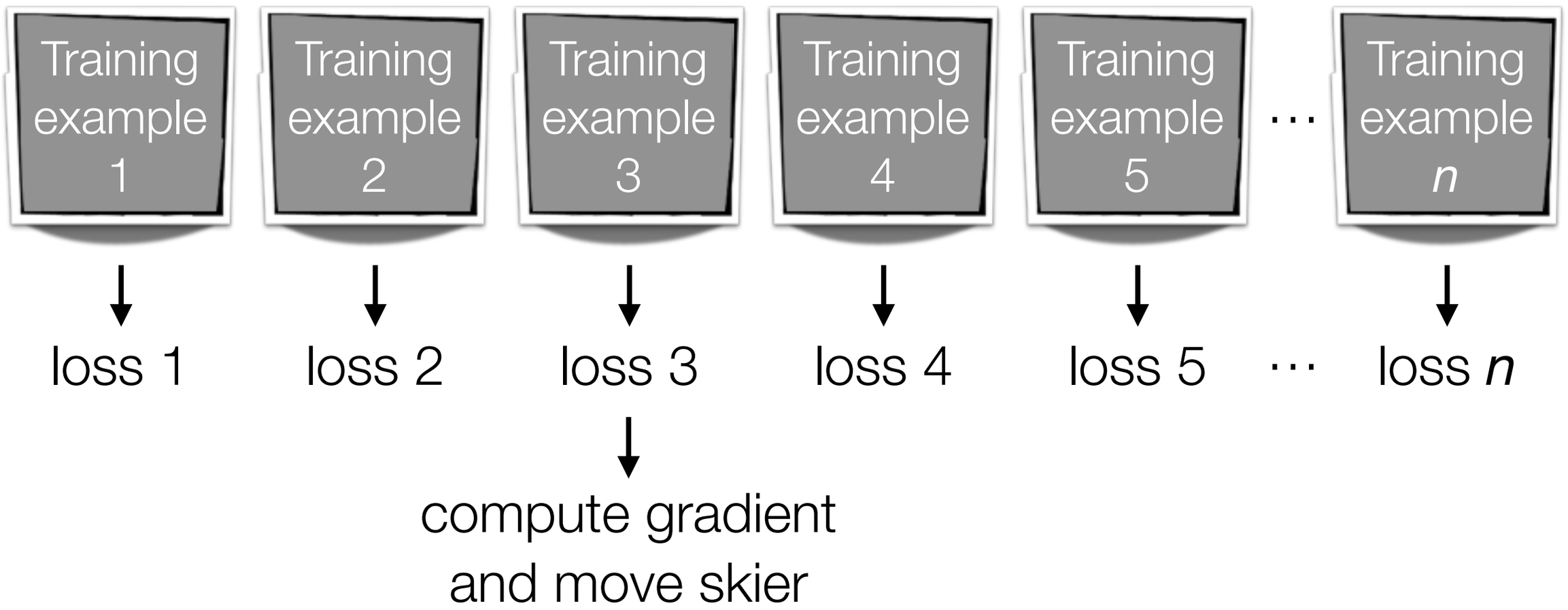

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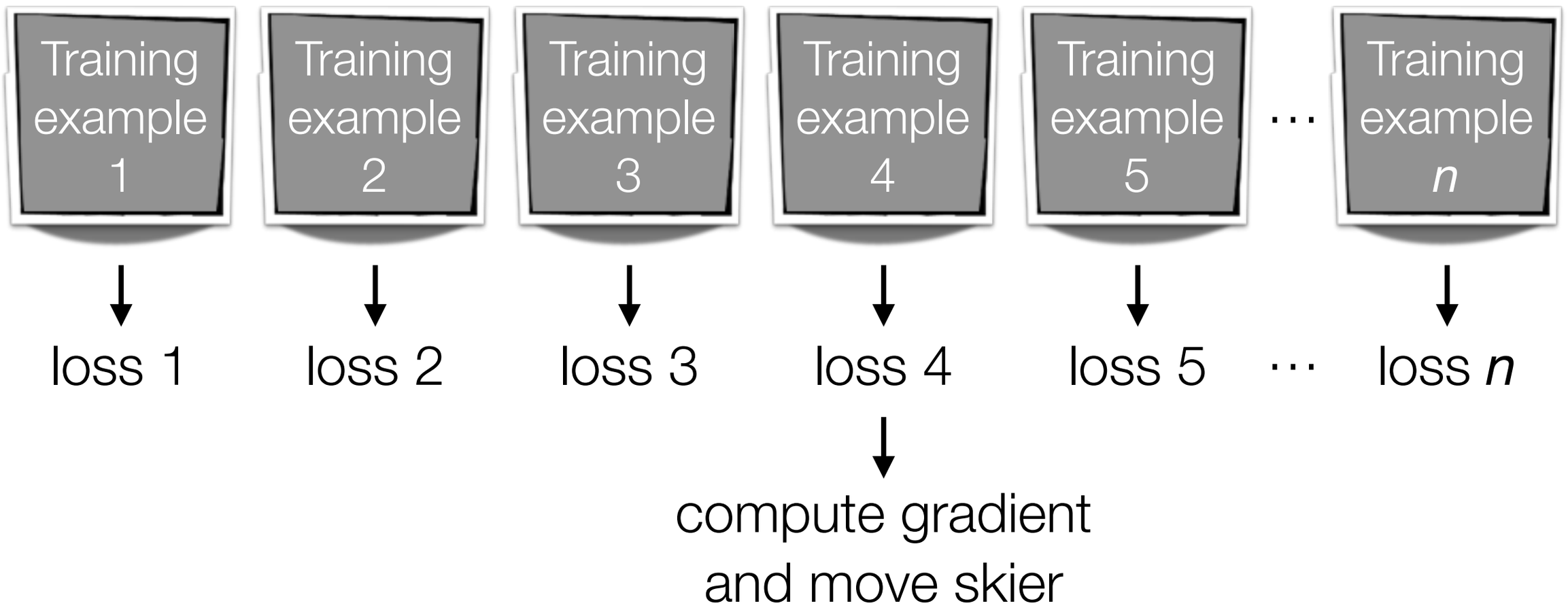

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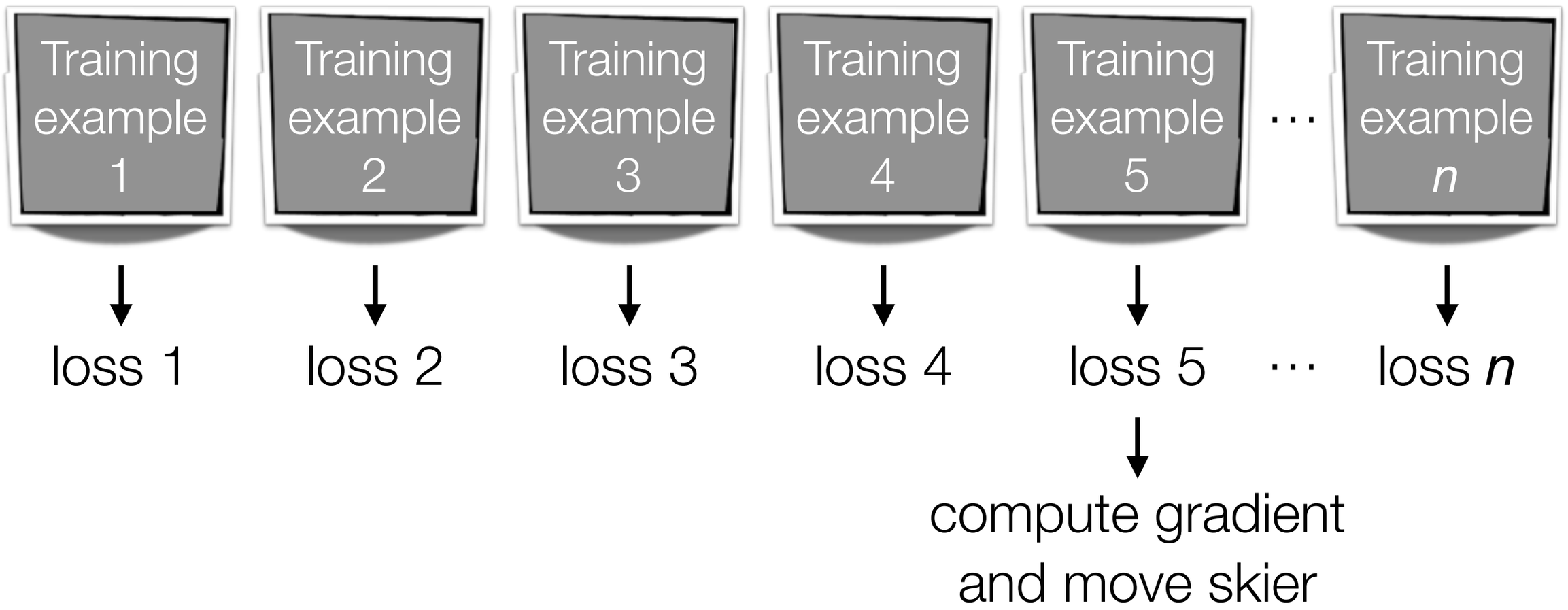

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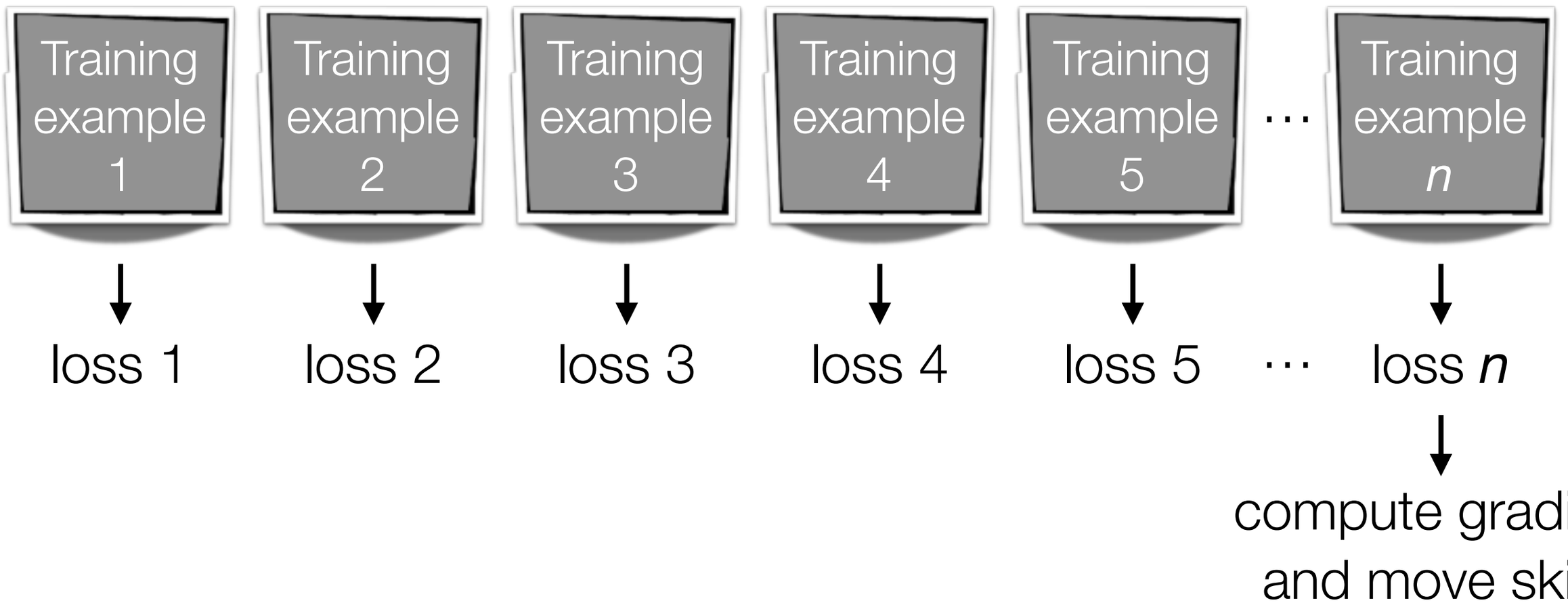

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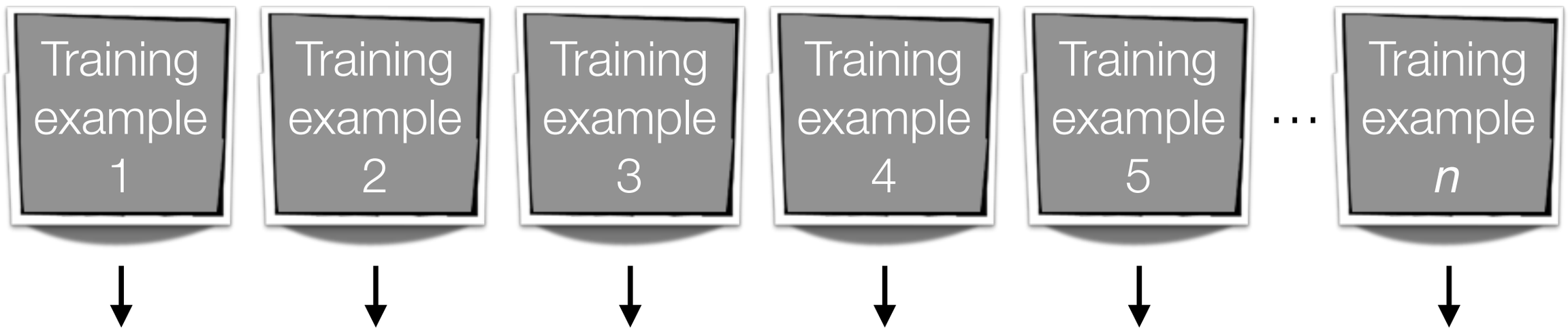

An epoch refers to 1 full pass through all the training data

SGD: compute gradient using only 1 training example at a time
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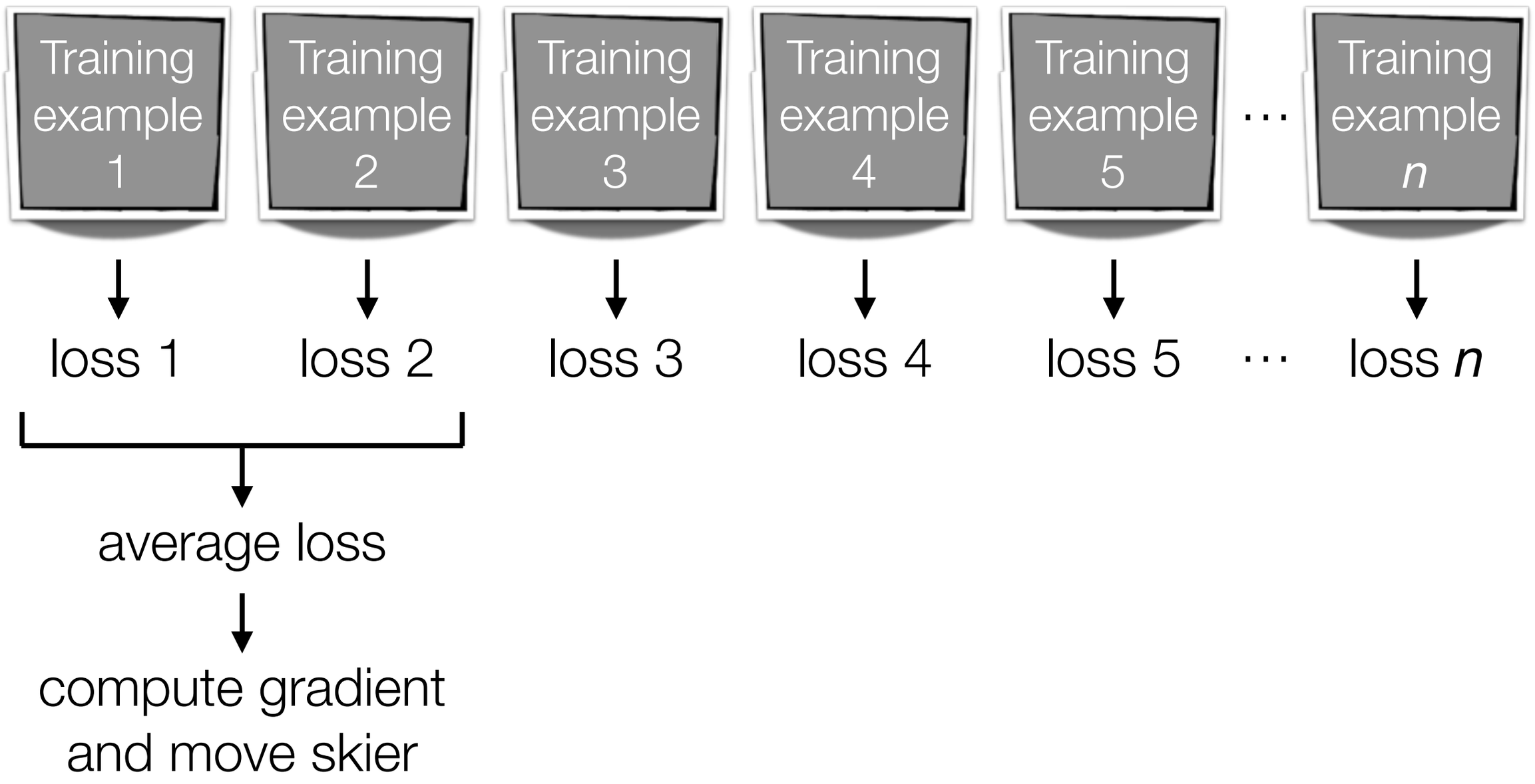
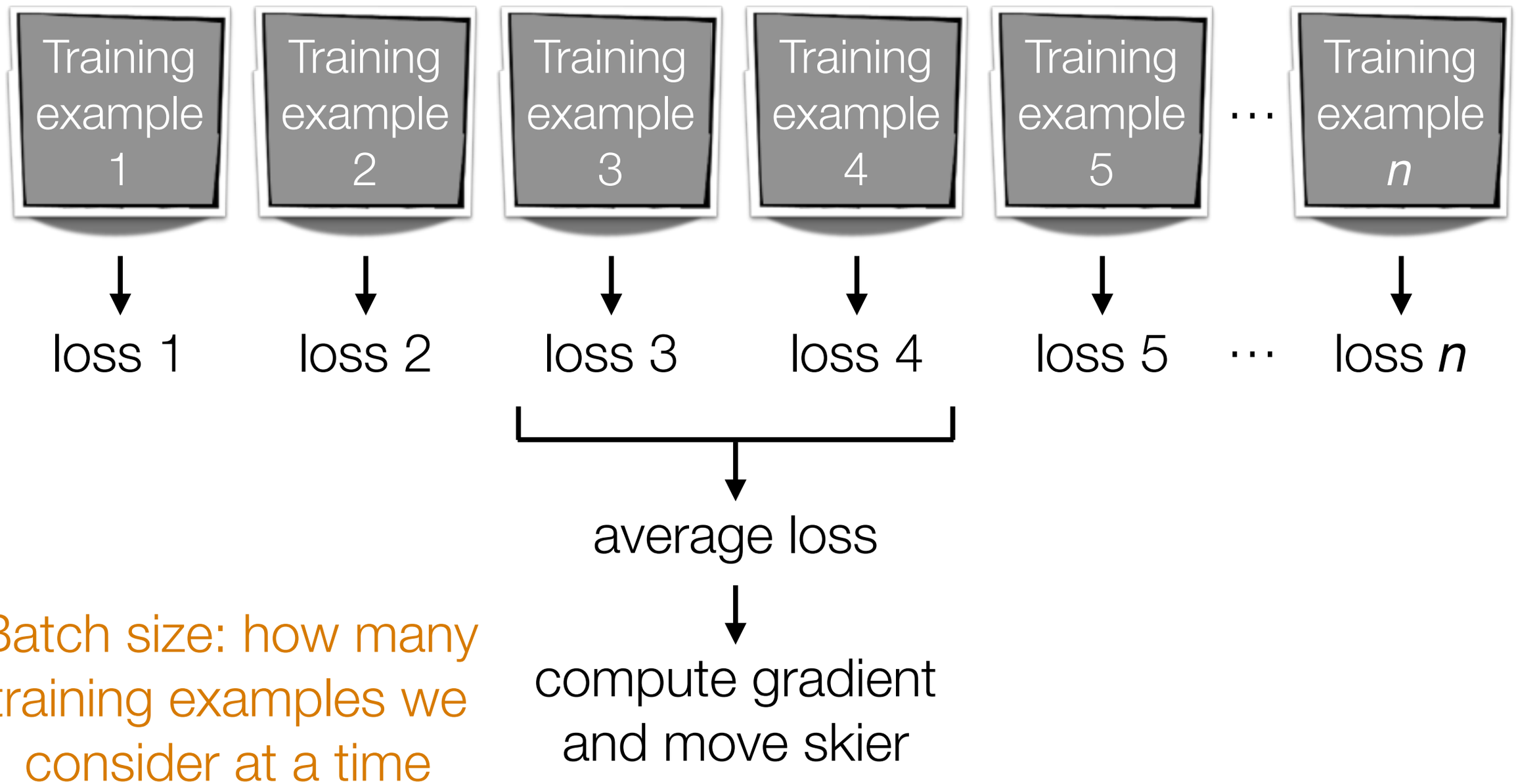
Minibatch Gradient Descent



Minibatch Gradient Descent



Batch size: how many training examples we consider at a time (in this example: 2)

Best optimizer? Best learning rate?

Best # of epochs? Best batch size?

Active area of research

Depends on problem, data, hardware, etc

Example: even with a GPU, you can get slow learning (slower than CPU!) if you choose # epochs/batch size poorly!!!

Dealing with Small Datasets

Fine Tuning

If there's an existing pre-trained neural net, you could modify it for your problem that has a small dataset

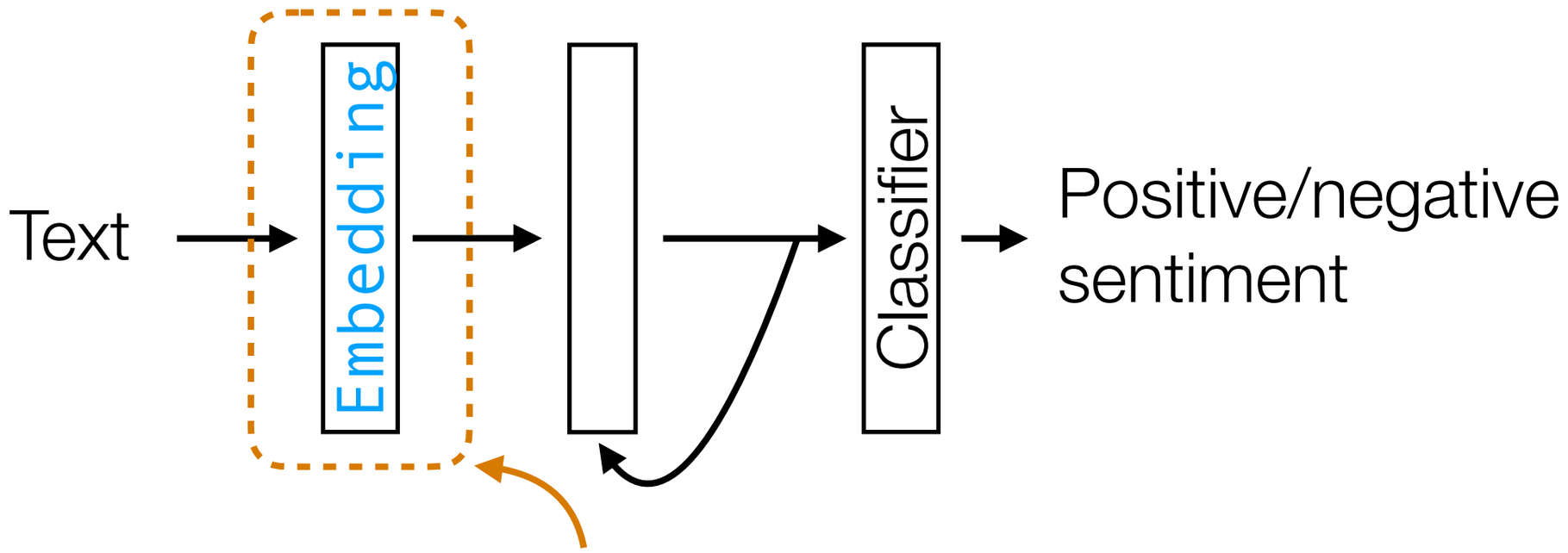
Example: classify between Tesla's and Toyota's

You collect photos from the internet of both, but your dataset size is small, on the order of 1000 images

Strategy: take pre-trained convnet (such as the state-of-the-art ResNet) for ImageNet classification and change final layers to do classification between Tesla's and Toyota's instead of classifying 1000 objects

Fine Tuning

Sentiment analysis RNN demo



GloVe vectors pre-trained on massive dataset (Wikipedia + Gigaword)

IMDb review dataset is small in comparison

Data Augmentation

Another way of dealing with small datasets: generate perturbed versions of your training data to get a larger training dataset

Training image

Training label: cat

Mirrored

Still a cat!

Rotated & translated

Still a cat!

We just turned 1 training example in 3 training examples

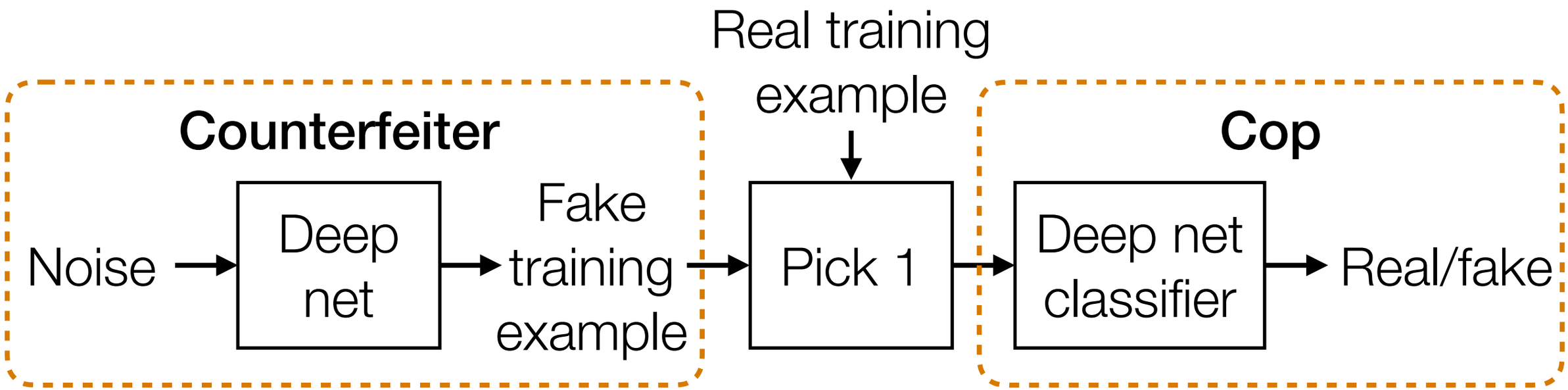
Allowable perturbations depend on data
(e.g., for handwritten digits, rotating by 180 degrees would be bad: confuse 6's and 9's)

Generating Fake Data That Look Real

Generate Fake Data that Look Real

Unsupervised approach: generate data that look like training data

Example: Generative Adversarial Network (GAN)



Counterfeiter tries to get better at tricking the cop

Cop tries to get better at telling which examples are real vs fake

Terminology: counterfeiter is the **generator**, cop is the **discriminator**

Other approaches: variational autoencoders, pixelRNNs/pixelCNNs

Generate Fake Data that Look Real

Fake celebrities generated by NVIDIA using GANs
(Karras et al Oct 27, 2017)

Google DeepMind's WaveNet makes fake audio that sounds like whoever you want using pixelRNNs (Oord et al 2016)

Generate Fake Data that Look Real

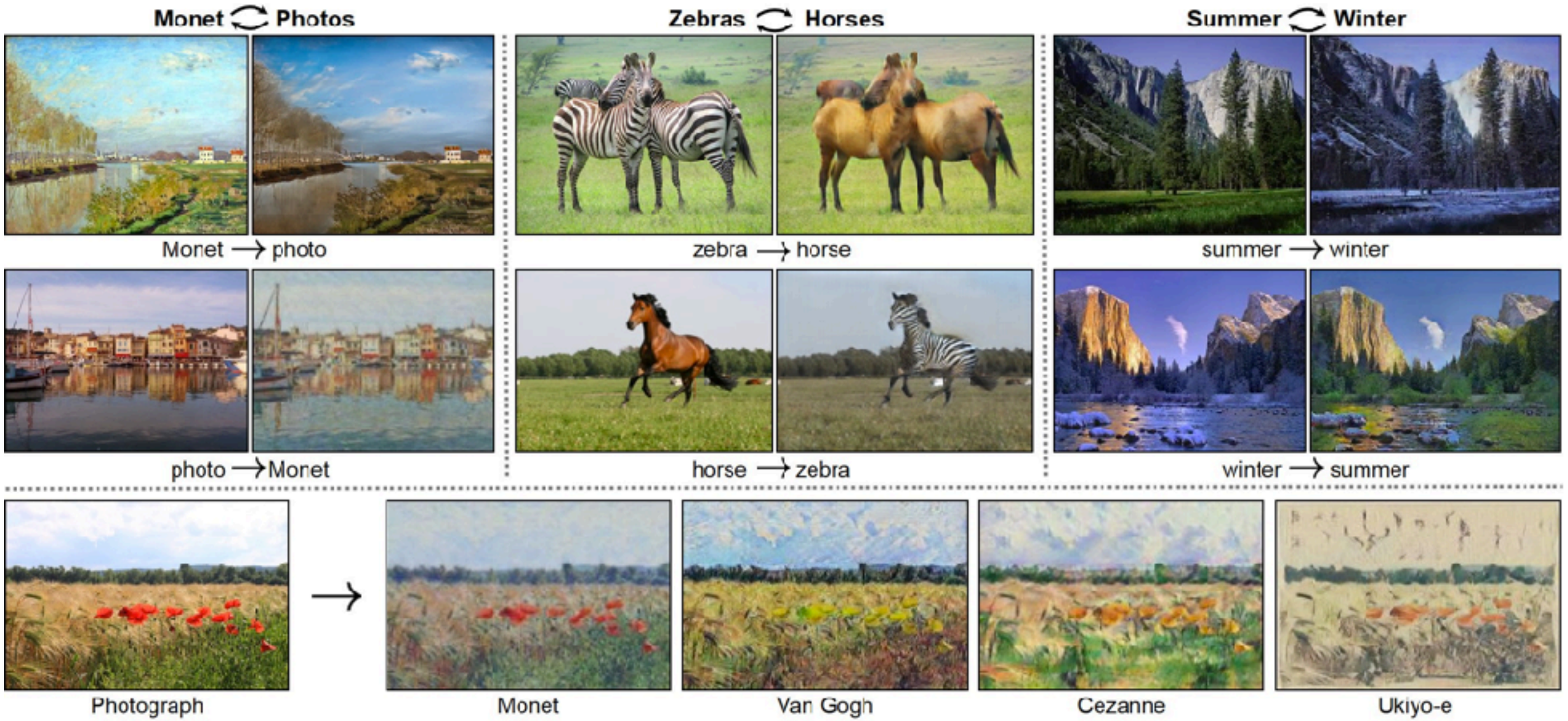


Image-to-image translation results from UC Berkeley using GANs (Isola et al 2017, Zhu et al 2017)

AI News Anchor

China's Xinhua agency unveils AI news presenter

By Chris Baraniuk
Technology reporter

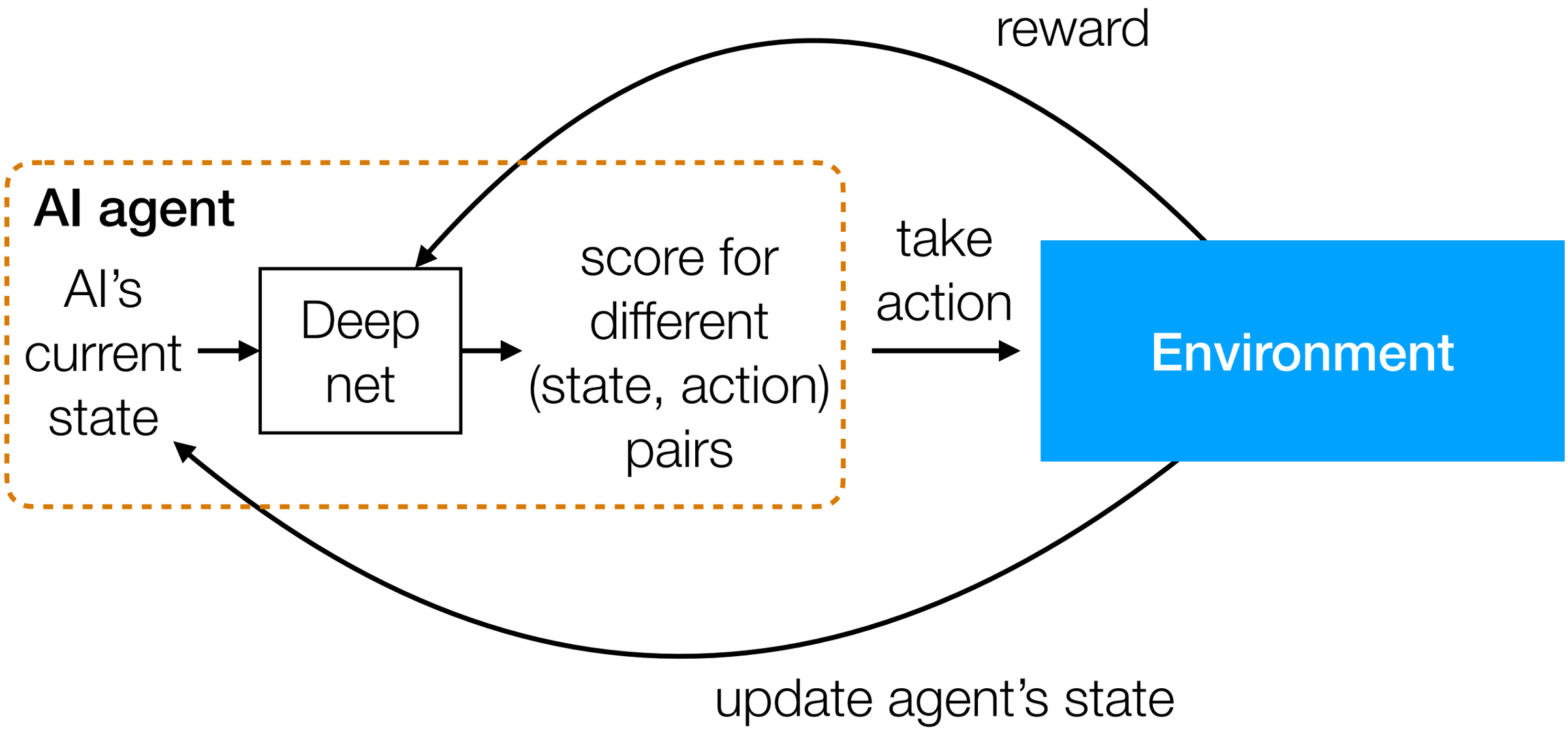
8 November 2018

Share

Source: https://www.bbc.com/news/technology-46136504

Deep Reinforcement Learning

The machinery behind AlphaGo and similar systems

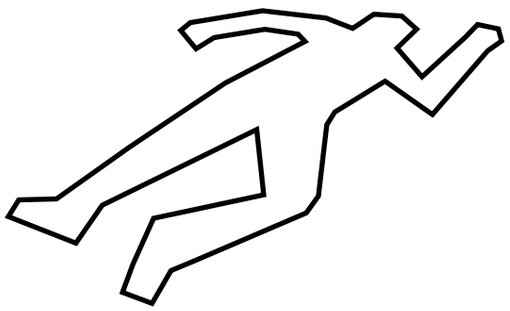


The Future of Deep Learning

- Deep learning currently is still very limited in what it can do
  - Learns simple computer programs (functions) comprised of a series of basic operations — need to be able to compute derivatives of these basic operations
- Adversarial examples at test time remain a problem
- Pretty much all the best ideas that lead to amazing prediction results incorporate problem-specific structure
  - For example, think about how CNNs and RNNs incorporate structure of images/time series
  - How do we get away with using less expert knowledge?
- How do we do lifelong learning?
- How do we reason about causality?

Unstructured Data Analysis

Question



The dead body

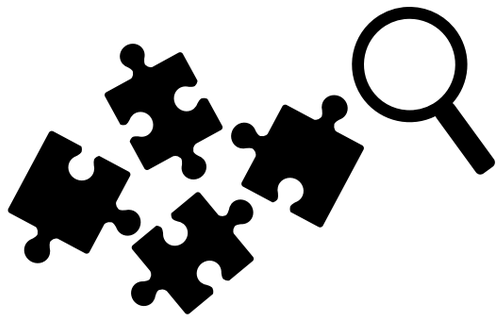
This is provided by a practitioner

Data

The evidence

Some times you have to collect more evidence!

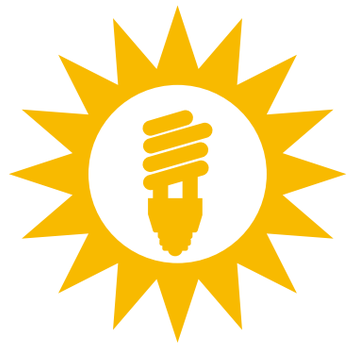
Finding Structure



Puzzle solving, careful analysis

Exploratory data analysis

Insights



When? Where? Why? How? Perpetrator catchable?

Answer original question

<u>There isn't always a follow-up prediction problem to solve</u>

Some Parting Thoughts

- Remember to **visualize steps of your data analysis pipeline**
  - Helpful in debugging & interpreting intermediate/final outputs
- Very often there are *tons* of models/design choices to try
  - Come up with **quantitative metrics** that make sense for your problem, and use these metrics to **evaluate models (think about how we chose hyperparameters!)**
  - But don't blindly rely on metrics without **interpreting results in the context of your original problem!**
- Often times you won't have labels! If you really want labels:
  - Manually obtain labels (either you do it or crowdsource)
  - Set up "self-supervised" learning task
- There is a *lot* we did not cover — **keep learning!**

Want to Learn More?

- Some courses at CMU:
  - Natural language processing (analyze text): 11-611
  - Computer vision (analyze images): 16-720
  - Deep learning: 11-785, 10-707
  - Deep reinforcement learning: 10-703
  - Math for machine learning: 10-606, 10-607
  - Intro to machine learning at different levels of math: 10-601, 10-701, 10-715
  - Machine learning with large datasets: 10-605

- One of the best ways to learn material is to teach it!

  Apply to be a TA for me next term!