PROGRAMMING IN PYTHON II

Data Loading and Types of Data

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Outline

MOTIVATION

Recap

- Last Unit, we learned that we
  1. want our model to generalize to unseen data
  2. need i.i.d. data to get an estimate for the generalization of our model (testset)
  3. can use clustering methods to inspect our data and search for potential issues
  4. might have to preprocess and normalize our data before feeding it to our method

Goal

- We want to feed our dataset to our model
- For this, we will learn
  1. which types of (statistical) data exist
  2. what our data need to look like for gradient-based methods (e.g. neural networks (NNs))
  3. about bottlenecks for loading data
  4. PyTorch Dataset and DataLoader

TYPES OF DATA

Typical ML point-of-view

- In ML we can represent our samples by vectors of feature values (=feature vectors) of length d

$$\mathbf{x} = (x_1, \ldots, x_d)T$$

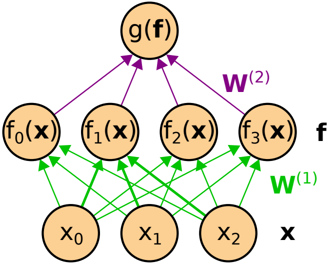
  - E.g.: Representing dogs by their height and weight would require 2 feature values (i.e. $d = 2$)
- We assume our feature vectors to be from a set/space X

$$\mathbf{x} = (x_1, \ldots, x_d)^T \in X$$

- If X is finite set of labels, we speak of *categorical variables/features*
- If $X = \mathbb{R}$, real interval, etc., we speak of *numerical variables/features*

Fully-connected feed-forward NN

- Standard fully-connected feed-forward NN (FFNN)



$$\mathbf{W}^{(1)} = W^{(1)}_{0\ldots3,0\ldots2}$$

$$f_1(x) = a(W^{(1)}_{1,0} * x_0 + W^{(1)}_{1,1} * x_1 + W^{(1)}_{1,2} * x_2) = a(\sum_j^n (W^{(1)}_{1,j} \cdot x_j))$$

- Weights $\mathbf{W}$ are adjusted such that $g(\mathbf{x};\mathbf{W}) \xrightarrow{training} target$
- a is an activation function, e.g. sigmoid, relu, selu, ...

Types of data

- We have 3 different types of data (in the statistical sense)
  1. Numerical data
  2. Categorical data
  3. Ordinal data
- In practice, we (usually) use the `float` datatype for our NN computations

$\rightarrow$ We need to represent our data as `float`

NUMERICAL DATA

Numerical data – Theory

- Data with quantitative meaning
- Continuous data
  - Measurements that cannot be counted (uncountably infinite)
  - Described using intervals on real number line
  - Example: Any real number in range $[0, 10]$
  - E.g. size of a leaf on a plant
- Discrete data
  - Countable data (countably finite or infinite)
  - Example (finite): $0, 1, 2, \ldots, 10$
  - Example (infinite): $0, 1, 2, \ldots, \infty$
  - E.g. number of leafs on a plant

Numerical data – Practice (1)

- We want to represent a numerical data value as a `float` value
- Problem: `float` values have limited number of bits

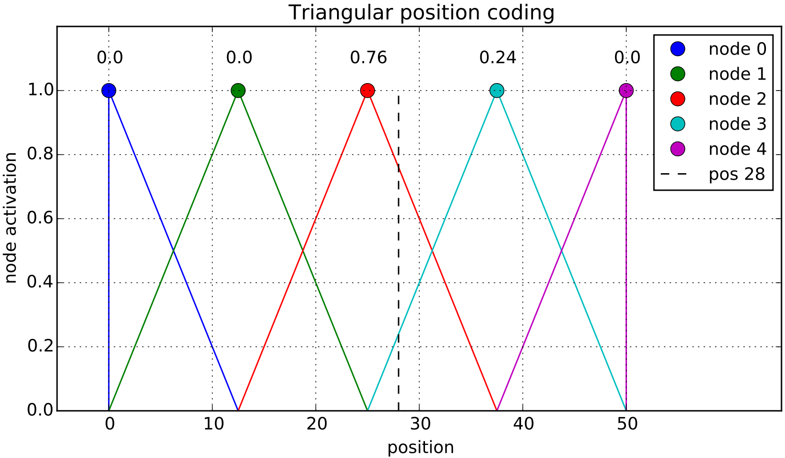
Numerical data – Practice (1)

- We want to represent a numerical data value as a `float` value
- Problem: `float` values have limited number of bits
- Approximate (quantize) numerical data:
  - Cap value ranges (to finite)
  - Lose precision (limited number of bits)
  - Focus on value ranges that are important for task
    - Common: Clip, square, logarithm, square root, sigmoid, tanh
    - Requires prior knowledge

Numerical data – Practice (2)

- Problem: Especially for discrete data with large value ranges:
  - Loss of precision makes task unsolvable
  - Learning to focus on precise values is difficult for NN
    - Has to adjust bias weights very precisely
- Solution: Encode the numerical value in multiple input units
  - Each unit spans a range of values (e.g. triangles, gaussians)
  - Common: Encoding of position or time

Discrete data – Triangle encoding



CATEGORICAL DATA

Categorical data – Theory

- Qualitative data
- No mathematical meaning
- Mathematical operations (e.g. $\sum$) do not make sense
  - Example: “Dog”, “Rat”, “Cat”

Categorical data – Practice (1)

- Assume we consider n different categories
- We could represent each category as integer value
  - Requires n different integer values, one for each category
  - We could encode these integer values as `float`
  - Example: “Dog”$= 0$, “Rat”$= 1$, “Cat”$= 2$

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  - Example: "Dog"$= 0$, "Rat"$= 1$, "Cat"$= 2$
- Problem: Our method (e.g. NN) performs mathematical operations on the input values!
  - We would introduce new (probably false) information
  - The NN would first have to learn to ignore this false information
  - Example: In our ranking, "Dog" $<$ "Rat' and "Rat" $\cdot 2 =$ "Cat"

  → Not suitable for us

Categorical data – Practice (2)

- Solution: Represent a categorical feature as binary vector $\mathbf{v}_{0 \ldots n}$
  - Categorical data with n different values is enumerated from $0 \ldots n$
  - $v_i = 1$ if category i is true, otherwise $v_i = 0$
  - Each element in the vector represents one category $\rightarrow$no false information!*
- Example:
  - Possible values: “Dog”, “Rat”, “Cat” ($n = 3$)
  - Sample is “Dog” $\rightarrow \mathbf{v} = (1, 0, 0)^T$
  - Sample is “Cat” $\rightarrow \mathbf{v} = (0, 0, 1)^T$

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- *) Only applies if information about order in feature vector is not used

Categorical data – Practice (3)

- Mutually-exclusive categories:
  - One-hot feature vector
  - Only one element in feature vector is 1, others are 0
  - Feature vectors are typically sparse
- Categories include combinations (e.g. “Dog” and “Cat”):
  - Can be encoded/embedded in binary feature vector with multiple 1-entries per sample
  - NN does not have to learn that e.g. feature 5 is a combination of feature 2 and feature 26
- Additional information (e.g. measurement certainty)
  - Values in binary feature vector can be scaled to increase/decrease signal strength of input

ORDINAL DATA

Ordinal data – Theory

- Mix of numerical and categorical data
- Ranking between categories exist but distance is unknown
- Example: “small”, “medium”, “large”
  - Ranking “small” $<$ “medium” $<$ “large” exists
  - Distance is unclear (“small”$+$“small”$=$“medium”?)

Ordinal data – Practice (1)

- Apply our approach from categorical data
- Sort features in $\mathbf{v}$ according to ranking
- Fully-connected feed-forward NN
  - No initial awareness about order of features in $\mathbf{x}$
  - FFNN has to learn ranking by itself
  - Possible but not efficient
- Better: Use methods that naturally take ranking/hierarchy in feature vector into account
  - FFNN vs. CNN, RNN, attention, graph-NNs, ...
  - Allows for additional information via 1D, 2D, 3D, nD feature matrices or graph representations

Ordinal data – Practice (2)

- Especially in natural language processing (NLP):
  Use learned or fixed embedding of features
- Features are projected to feature space with better properties for NN training
- Simple approach: Random combinations of existing features as new features
- Better: Include prior knowledge of relationships within categories
  - Good combinations of categories easier accessible for NN
  - Example: Handcrafted embedding, pre-trained embeddings (NLP), dynamically learned embeddings

OPTIONAL: FEATURE DESIGN FOR NN

Feature design for NNs (1)

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  - I.e. with enough units you can build any function

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Feature design for NNs (1)

- NNs are universal function approximators
  - I.e. with enough units you can build any function
- Problem: You need to train it first to get there
  - . . . and there is not guarantee that this will work
- NN are typically trained with gradient-based methods
  - Weights will move across error surface to suitable values
- We need a (smooth) path from our initial weights to our target weights
  - Otherwise we will get stuck in local minima and/or need more samples

  $\rightarrow$ Bad feature design can make your training fail

Feature design for NNs (2)

- How complex does the function have to be to create the target outputs from the inputs?
  - Do weights need to be very precise to separate good from bad output?
  - Example: hash value space vs. pixel space

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  - Example: hash value space vs. pixel space
- Can the network change from initial output to target output smoothly?
  - Need to flip signs of weights or make large jumps to overcome worse outputs?
  - Need to set weights to 0 to quickly down-weight large inputs? (0 activation $\rightarrow$no gradient/path)
- Which information does the NN have to unecessarily encode from the inputs?
  - E.g. mean/std of pixel values, position, time, Δ of values (e.g. positions)

Example: XOR (1)

- XOR (Exclusive Or) of two inputs x_0 and x_1:

$$xor(x_0, x_1) = \begin{cases} 1, & \text{if } (x_0 \text{ or } x_1) \text{ and not } (x_0 \text{ and } x_1) \\ 0, & \text{otherwise} \end{cases}$$

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- Task: Learn XOR with NN with activation function a_{relu}:

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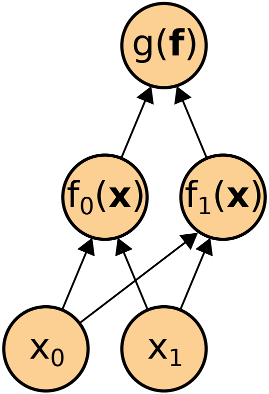
Example: XOR (2)

- Theoretically, this NN is enough for a solution:



Example: XOR (3)

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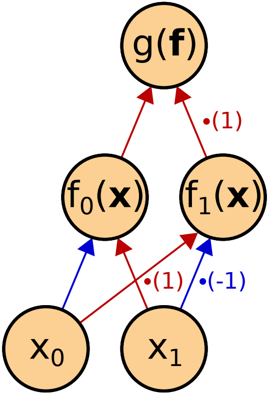

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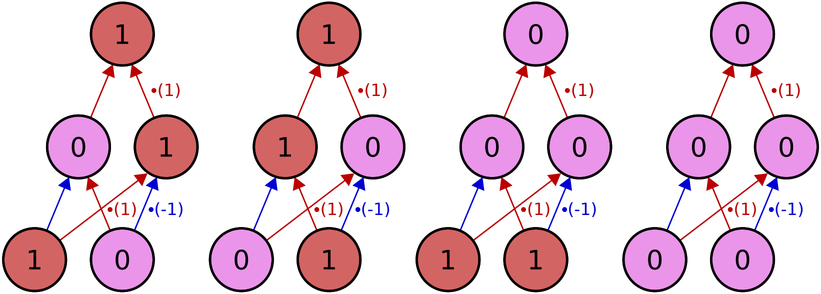


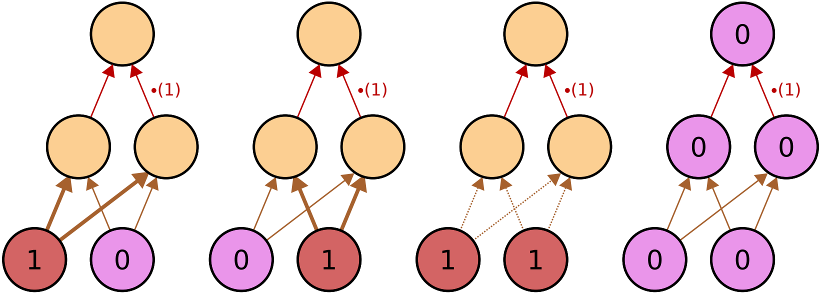
Example: XOR (5)

- But being able to represent the solution is not enough, we need to find it too!

$\rightarrow$ Can we find the solution via gradient descent starting from random weights?

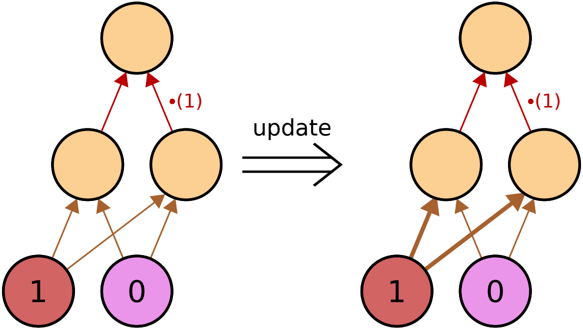
Example: XOR (6)

- This would be the updates for the weights for different inputs (bold: increase weight, dotted: decrease weight):



Example: XOR (7)

- Let's perform some consecutive update steps, given some samples:



Example: XOR (8)

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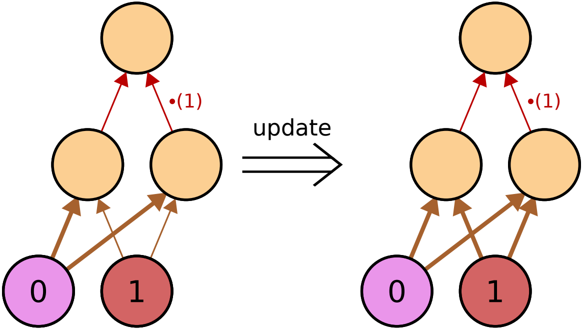

Example: XOR (9)

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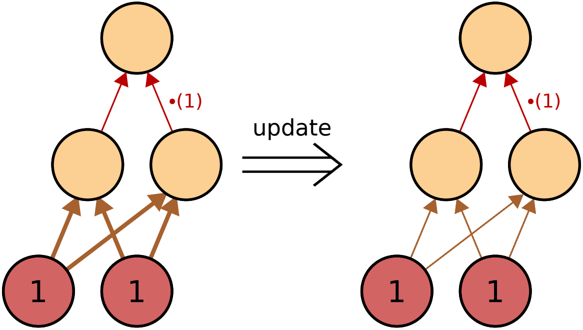
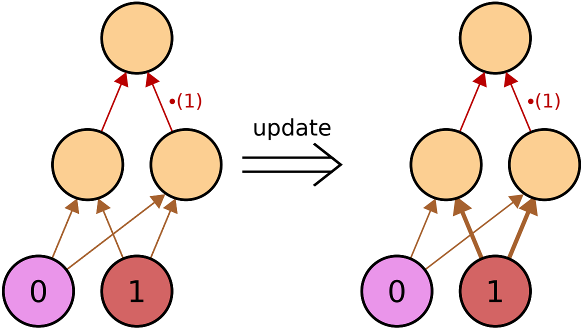


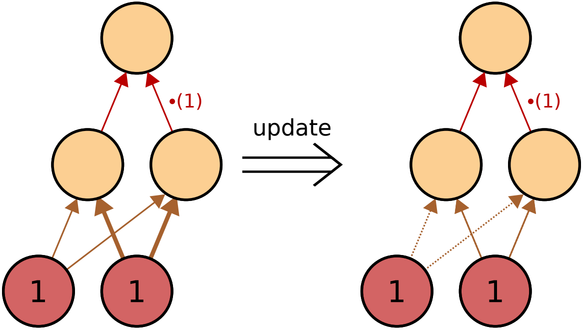
Example: XOR (10)

- Let's perform some consecutive update steps, given some samples:



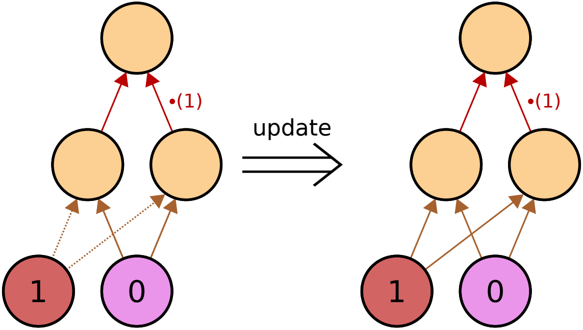
Example: XOR (11)

- Let's perform some consecutive update steps, given some samples:



Example: XOR (12)

- Let’s perform some consecutive update steps, given some samples:



Example: XOR (13)

- We are not reaching our solution :(

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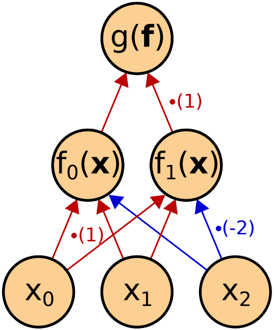
- We could add more units to our NN and hope to have a close-to-solution weight combination in the initialized weights or apply other fancy techniques…

Example: XOR (13)

- We are not reaching our solution :(
- We could add more units to our NN and hope to have a close-to-solution weight combination in the initialized weights or apply other fancy techniques...
- ...or we could just use better feature design!
  - Add more input features as combinations of x_0 and x_1
  - E.g.: Add $x_2 = (x_0 \wedge x_1)$

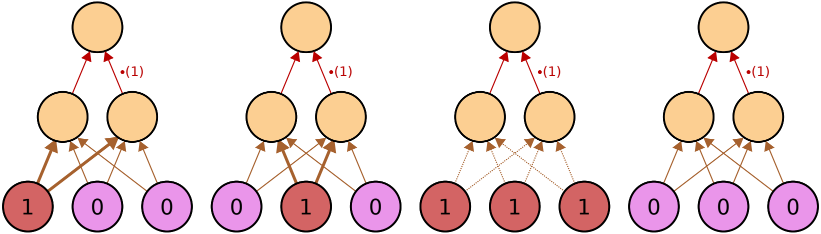
Example: XOR (14)

- With $x_2 = (x_0 \wedge x_1)$, a solution would be:



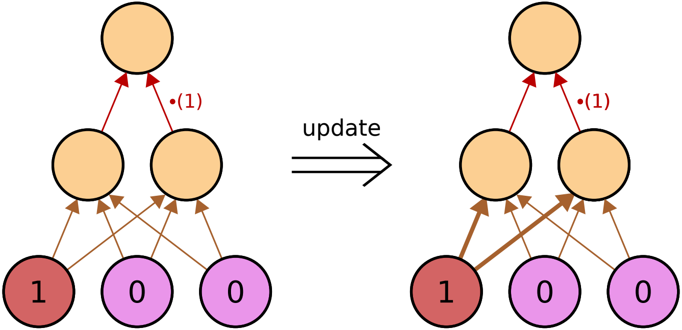
Example: XOR (15)

- Possible update steps for our network:



Example: XOR (16)

- Let's perform some consecutive update steps, given some samples:



Example: XOR (17)

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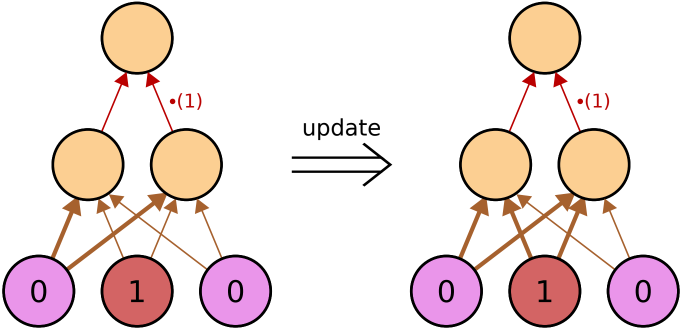
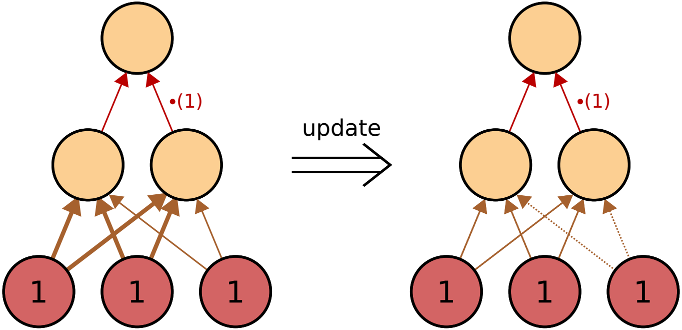


Example: XOR (18)

- Let's perform some consecutive update steps, given some samples:

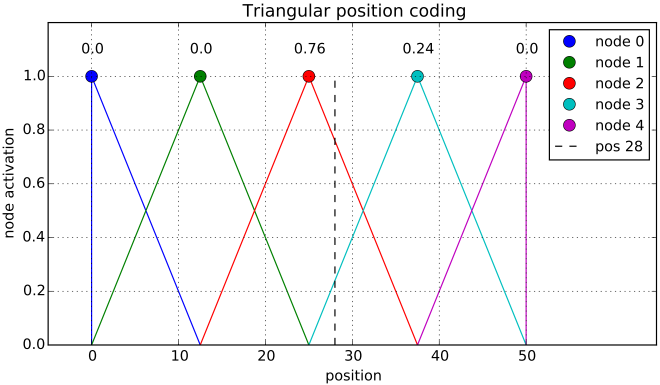


Example: XOR (19)

- We have found a solution easily just by adding 1 more input feature!

Example: Position encoding

- Note how the encoded ranges overlap by $1/2$
  - No cut-offs between positions
  - All positions have accumulated activation 1 $\rightarrow$less initial bias



PYTHON II PROJECT

Types of data – Python II Project

- We are dealing with measurements of light (continuous),
- which have been quantized to `uint8` pixel values (discrete)
- We do not need high precision (do not need to single out precise brightness values)

→ Encoding a discrete pixel value as a `float` value is sufficient

- Could we include features that make prediction of the unknown image parts easier? (Assignment 2)

Further reading

- Courses and lecture materials in AI-study
- ML-, statistics-, image-/signal-processing courses at JKU
- *Pattern Recognition and Machine Learning* (C. Bishop)
- *Statistics For Dummies*: `https://www.dummies.com/education/math/statistics/types-of-statistical-data-numerical-categorical-and-ordinal/`
- *Dive into Deep Learning* (A. Zhang, Z. Lipton, M. Li, A. Smola): `https://d2l.ai/`

LOADING DATA: BOTTLENECKS

Bottlenecks: Bandwith (1)

- General
  - Transfer as little data as possible
  - Prefer smaller data types
  - Make use of sparseness of data (compression and optimized computations)
- Network $\Longrightarrow$ disk
  - Copy dataset to storage with fast connection to training device
- Disk $\Longrightarrow$ RAM
  - Store dataset in RAM if possible
- RAM $\Longrightarrow$ GPU memory
  - Only copy what you really need (input and output)
  - Prefer large coherent array vs. many small arrays

Bottlenecks: Bandwith (2)

- Example: One-hot feature vectors
- Setting:
  - We want to transfer many one-hot feature vectors to our GPU
  - Or mini-batch consists of 20 one-hot feature vectors of length 50

Bottlenecks: Bandwith (2)

- Example: One-hot feature vectors
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  - We want to transfer many one-hot feature vectors to our GPU
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- Possible solutions:
  - Stack our feature vectors to one array before transfer
  - Only transfer indices of 1-elements and create full feature vector on GPU
    - $\rightarrow$ Reduced from $20 \cdot 50 = 1,000$ to $20 \cdot 1 = 20$ bits!

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  - (We only need 50 indices, we can use `uint8` to store indices)

Bottlenecks: Bandwith (3)

- Important:
  - Introduces possibility for bugs, always check if final sample on GPU equals sample on CPU
  - Check where the actual bottleneck is in you code (timeit module*)
  - Check if your approach is really faster
  - Performance-optimization is a trade-off $\rightarrow$how far do you need to go?

*) `https://docs.python.org/3/library/timeit.html`

Bottlenecks: Computation (1)

- Loading data often involves on-the-fly preprocessing and data augmentation
- Large datasets are typically stored with high compression and need to be decompressed
- For each NN update we need to load multiple samples (mini-batch learning)

$\rightarrow$ Considerable computational effort for loading data

Bottlenecks: Computation (2)

- Solution:
  Data loading is performed by multiple processes the background
- Background processes can prepare new mini-batch during weight update
- Typicially done on CPUs
  - Access to large RAM with dataset
  - “Cheap” mass of CPUs
  - Exceptions: Embedding/preprocessing/data augmentation that require GPUs
- Multiprocessing often removes deterministic sample order
  - Less/no reproducibility

LOADING DATA: PYTORCH

PyTorch for loading dada

- PyTorch offers various tools for data loading*
- General: `torch.utils.data`**
  - Dataset classes, templates, unified interfaces
  - Loading data with support for background workers
- Relevant for vision-based tasks: `torchvision`***
  - Pre-processing and data augmentation pipe-lines
  - Pre-trained models
  - Standard public datasets

*) https://pytorch.org/tutorials/beginner/data_loading_tutorial.html
**) https://pytorch.org/docs/stable/data.html
***) https://pytorch.org/docs/stable/torchvision/index.html

Standardized Interfaces and Overloading

- PyTorch makes heavy use of standardized interfaces between objects and overloading
- We will now go through the first part of code file for Unit 05

PyTorch Dataset

- `torch.utils.data.Dataset`
- Dataset represented as class with standardized interface
- Derive your dataset class from `Dataset`
- Add your own method for reading a sample via `__getitem__()`
  - Should return 1 sample
  - Can include pre-processing and data augmentation
  - E.g. returns tuple of image as numpy array, label as `int`, and ID as `int`
- Provide number of samples in `__len__()`
- Can be wrapped by other classes, e.g. `torch.utils.data.Subset`

MINI-BATCH LEARNING

Mini-batch learning

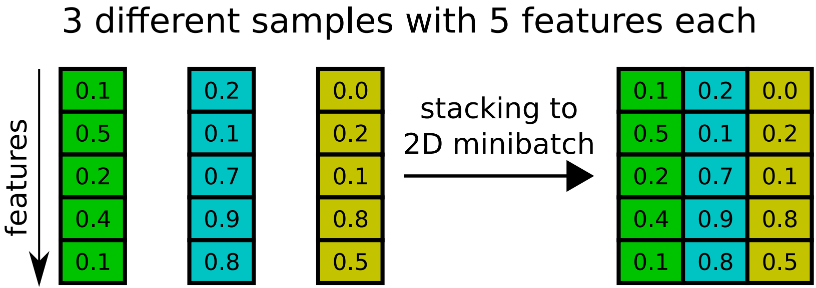
- 3 types of utilizing samples to train NN:
  - Full-batch learning
    - All training samples used for 1 NN update
    - Gradients are averaged over samples
    - Smooth but weak gradients $\rightarrow$slow learning, overfitting
  - Online learning
    - 1 sample per weight update (shuffled samples)
    - Strong but not smooth gradients $\rightarrow$gradients might be contradicting
  - Mini-batch learning
    - b samples per weight update (shuffled samples)
    - Smooth gradients but strong enough to train fast with less overfitting
    - b is a hyperparameter that we need to optimize

Mini-batch implementation: stacking

- Typically, we would create a mini-batch by stacking the feature arrays
  - Introduce new dimension for samples in mini-batch
  - Stack feature arrays along this dimension (each feature array is 1 element in mini-batch dimension)
- Benefits:
  - Sending data/allocating memory on e.g. GPU ist faster for consecutive memory
    - 1 large array performs better than many small arrays
  - Computations can be broadcasted along mini-batch dimensions
    - Large speed up on CPU and especially GPU (matrix operations)

Mini-batch implementation: 1D

- If our input data are 1D feature vectors, we can stack them to 2D mini-batches
  - Assumes that all feature vectors have same length (e.g. same number of measurements)

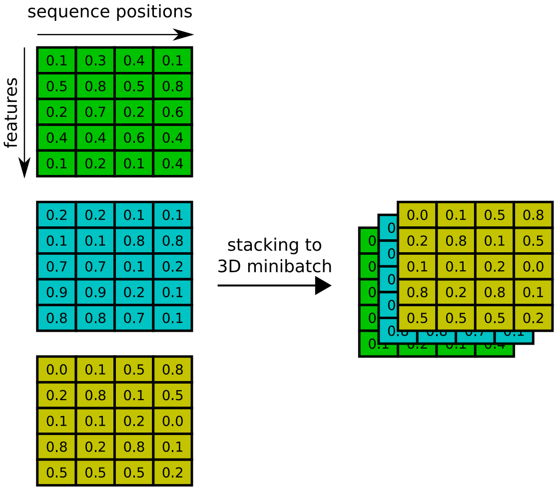


Mini-batch implementation: 2D

- If our input data are 2D feature arrays, we can stack them to 3D mini-batches
  - E.g. gray-scale images or sequences (multiple features per sequence position)
  - Assumes that all arrays have same shape (e.g. same number of pixels or sequence positions)

Mini-batch implementation: 2D

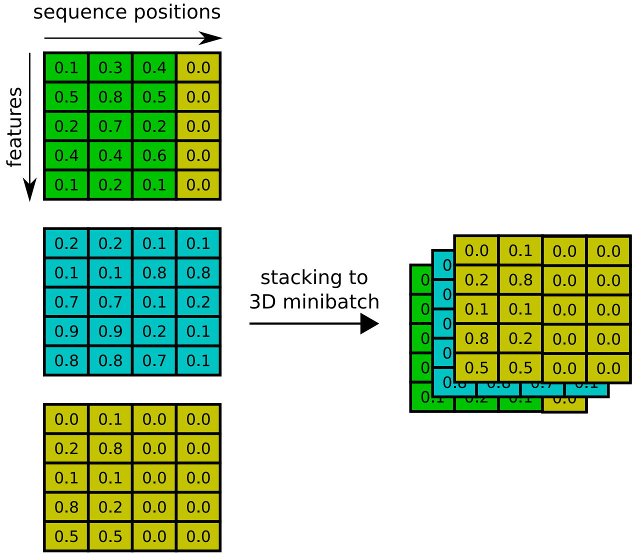
3 different samples with 4 sequence positions
and 5 features per sequence position



Mini-batch implementation: 2D with padding

- If arrays are not of same shape, they are often padded to same shape
  - Padding with zeros (zero-padding) or heuristics
  - Depending on method will influence predictions!
- Recurrent NNs (LSTMs, GRUs)
  - Pad end of sequences, store original lengths of sequences
  - Use model output at last original sequence position as final model output
- CNNs:
  - Zero-padding or heuristic (tries to extrapolate array without introducing too much new information)
- Good padding depends on data!

Mini-batch implementation: 2D with padding



Mini-batch implementation: 2D without padding

- In some cases it is be better to omit padding
  - Array shapes too different (e.g. very small and very long sequences)
    - Sending and allocating many unnecessary values
  - Padding hurts model performance or introduces undesired information
  - Memory consumption too high to process consecutive mini-batch array
- Alternative:
  - No stacking, keep feature arrays in a list
  - Send to GPU array-by-array
  - Compute outputs and gradients iteratively for arrays in list
  - Perform gradient step based on all arrays in list

PyTorch DataLoader

- `torch.utils.data.DataLoader`
- Extracts mini-batch of samples from `Dataset` instance
  - Supports shuffling and multiprocessing (not deterministic!)
  - Stacks samples to mini-batch automatically (=batching)
  - Custom batching via `collate_fn` argument
  - Looping over `DataLoader` instance will return all samples of `Dataset` instance, one mini-batch at a time

Classic usage

- Derive a class from `Dataset`: `MyDataset(Dataset)`
- Add `__getitem__()` (to read and return sample)
- Add `__len__()` (to return number of samples in dataset)
- Create dataset instance: `mydataset = MyDataset()`
- Create dataset splits via `torch.utils.data.Subset`:
  - `trainingset = torch.utils.data.Subset(mydataset, training_indices)`
- Create data loader (mini-batch size 16, using 4 background workers)

  ```
  training_loader = DataLoader(trainingset,
  batch_size=16, shuffle=True, num_workers=4)
  ```
- Loop over data loader to get mini-batches
  - `for mini-batch in training_loader: ...`

Hints

- Shuffling and multiprocessing is not deterministic (reproducability)
- Store indices of dataset splits in separate file and use `torch.utils.data.Subset` to create training, validation, and test set (reproducability)
- Disable shuffling in validationset/testset
- Warning: Avoid using DataLoaders in threads of `multiprocessing` (buggy), instead call Python scripts using `subprocess.call`/`subprocess.Popen`
- No need to use tensors in `Dataset`, you can stay in numpy
- Include sample ID in return from `__getitem__()` (debugging)