

CS639 Deep Learning for NLP

Deep Learning Basic

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Slides adapted from Graham

<https://junjiehu.github.io/cs639-spring26/>

Goals for Today

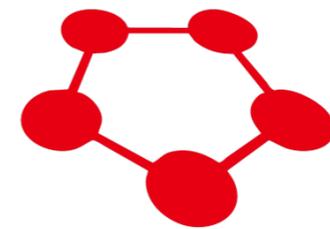
- Tensors and numerical computation
- **Model**: Define a **neural network architecture**
- **Forward**: computing predictions & Loss
- **Backpropagation**: computing gradients
- **Optimization**: parameter update
- Training Tricks

Neural Network Frameworks

theano

dy/net

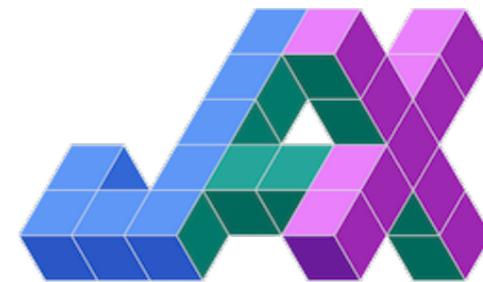
Caffe



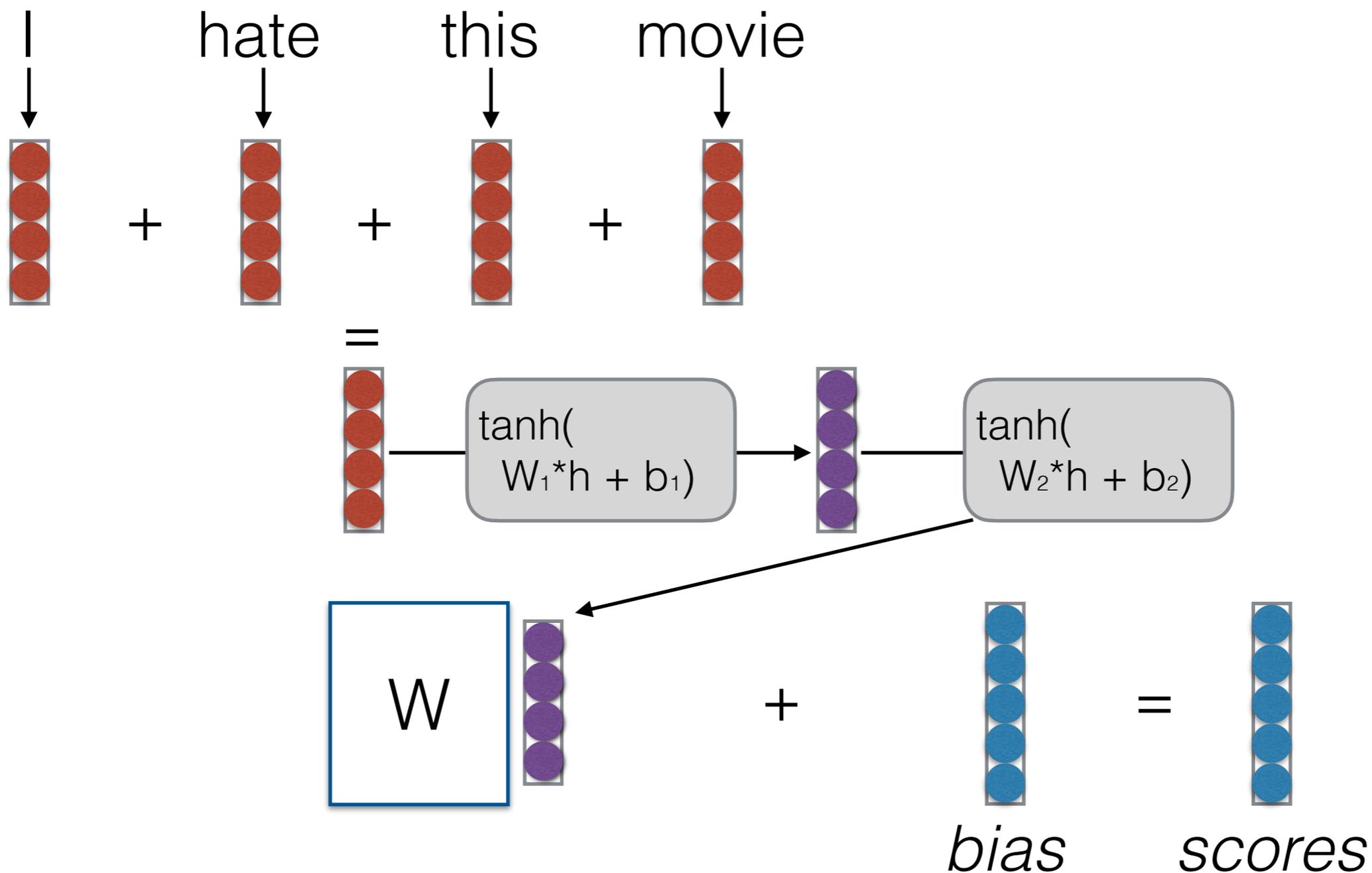
Chainer



PYTORCH



Example (HW1): Deep CBOW Model



NN App Algorithm Sketch

- Create a model and define a loss (i.e., **construct a computation graph**)
- For each example
 - **Forward: calculate the result** (prediction & loss) of that computation
 - if training
 - perform **back propagation**
 - **update** parameters

Tensors and Numerical Computation

Numerical Computation Backend

- Most neural network libraries use a backend for numerical computation
- **PyTorch/Tensorflow:** MKL, CUDNN, CUDA, OpenMP, custom-written kernels
- Support many numerical functions on **tensors**

```
import torch
import torch.nn as nn
print(*torch.__config__.show().split("\n"), sep="\n")
```

PyTorch built with:

- GCC 7.3
- C++ Version: 201402
- Intel(R) Math Kernel Library Version 2020.0.0 Product Build 20191114
- Intel(R) MKL-DNN v2.2.3 (Git Hash 7336ca9f055cf1b247e479d7e07226794c13931)
- OpenMP 201511 (a.k.a. OpenMP 4.5)
- LAPACK is enabled (usually provided by MKL)
- NNPACK is enabled
- CPU capability usage: AVX2
- CUDA Runtime 11.1
- NVCC architecture flags: -gencode;arch=compute_37
- CuDNN 8.0.5
- Magma 2.5.2
- Build settings: BLAS_INFO=mkl, BUILD_TYPE=Release

Tensors

- An n-dimensional array

Scalar



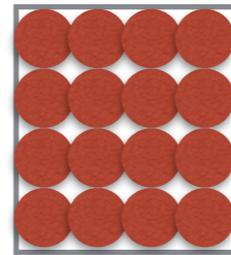
$$x \in \mathbb{R}$$

Vector



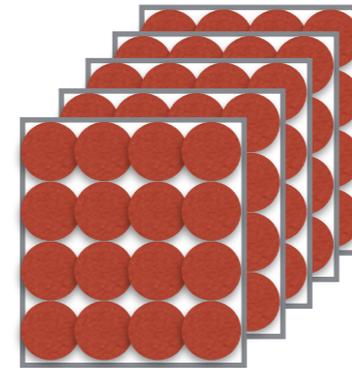
$$\mathbf{x} \in \mathbb{R}^4$$

Matrix



$$\mathbf{X} \in \mathbb{R}^{4 \times 4}$$

3-dim Tensor



$$\mathbf{X} \in \mathbb{R}^{4 \times 4 \times 5}$$

...

- Widely used in neural networks
- Parameters in NNs consist of different shape of tensors, which store both their **values** and **gradients**

Tensor Operations

- **PyTorch/Tensorflow:** Support many different matrix operations: matrix-multiply

```
import numpy as np
x = torch.Tensor([[2, 3], [1, 2]])
x = torch.Tensor(np.array([[ -1, 1], [2, 4]]))
x = torch.zeros([2, 3], dtype=torch.int32)
```

create tensors from list, numpy.array

```
▶ import torch
import torch.nn as nn
```

```
x = torch.randn((4, 2))
W = torch.randn((3, 4))
print(x)
print(W)
```

```
↳ tensor([[ -1.5372,  0.0845],
          [ 0.5752,  0.7634],
          [ 0.4265, -0.1287],
          [-1.8629, -0.8520]])
tensor([[ -1.1272, -1.1810,  0.0867,  0.0676],
        [-0.1070,  3.2586,  0.7446, -1.2094],
        [-1.7670,  0.2900, -1.0881, -1.5555]])
```

```
[10] torch.matmul(W, x) # results in a [3,2] matrix
```

```
tensor([[ 0.9646, -1.0656],
        [ 4.6092,  3.4132],
        [ 5.3167,  1.5373]])
```

matrix multiply

```
▶ x = torch.randn((4,2))
z = torch.randn((4,2))
print(x)
print(z)
```

```
↳ tensor([[ 0.0762,  1.5145],
          [-0.4747, -0.9141],
          [ 0.7106,  0.4888],
          [ 0.6959, -0.5305]])
tensor([[ -0.1766,  0.6187],
        [ 0.9254, -0.5931],
        [-0.9162,  0.3209],
        [ 0.0216, -0.7116]])
```

```
[13] x * z # results in a [4,2] matrix
```

```
tensor([[ -0.0135,  0.9371],
        [-0.4392,  0.5421],
        [-0.6510,  0.1569],
        [ 0.0151,  0.3775]])
```

Element-wise matrix multiply

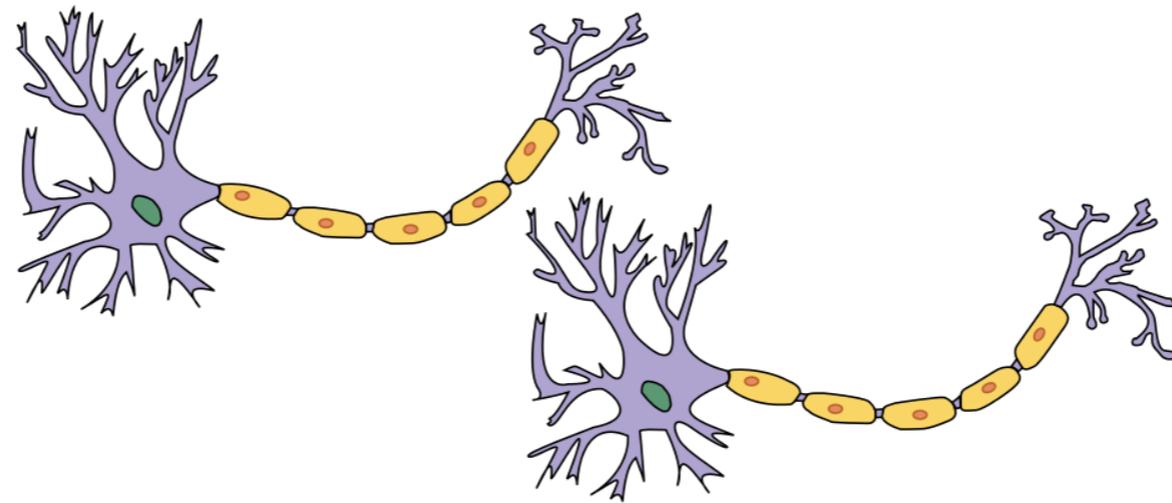
Model and Parameter Definition

NN App Algorithm Sketch

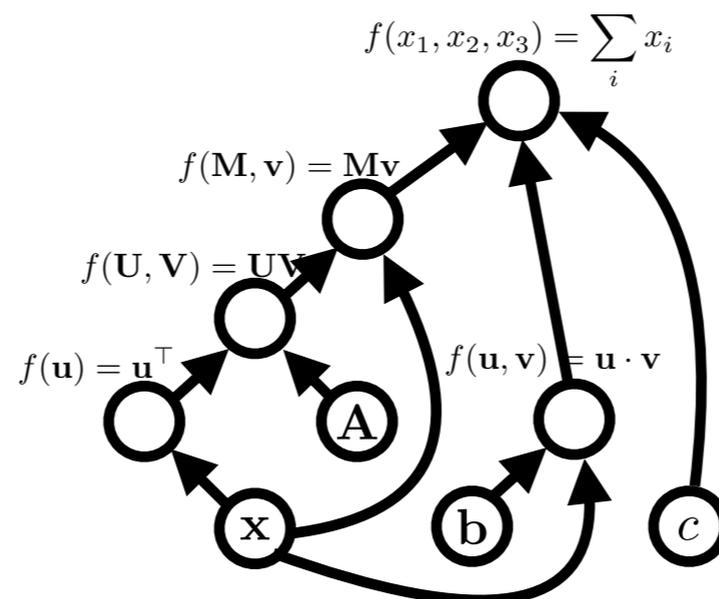
- Create a model and define a loss (i.e., **construct a computation graph**)
- For each example
 - **Forward: calculate the result** (prediction & loss) of that computation
 - if training
 - perform **back propagation**
 - **update** parameters

“Neural” Nets

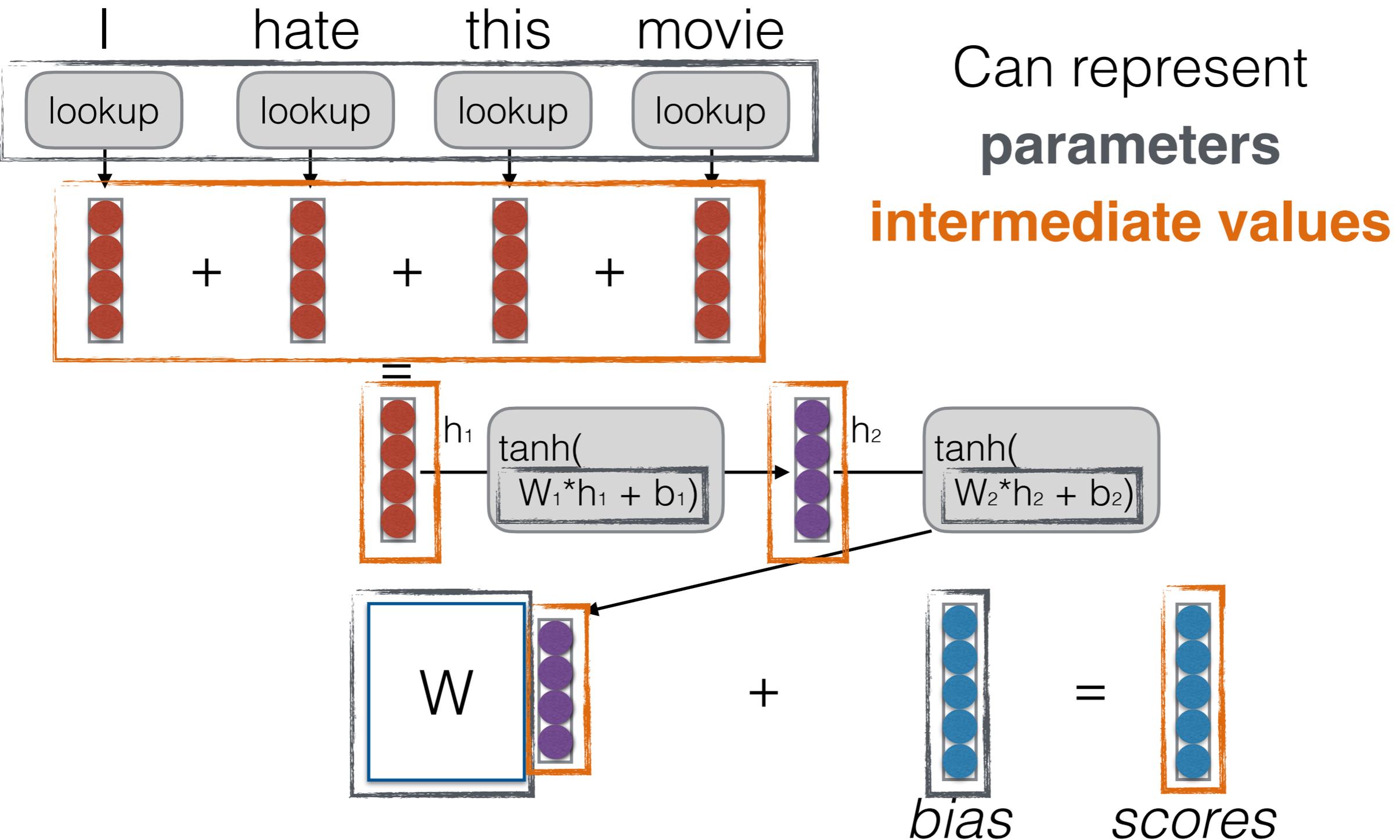
Original Motivation: Neurons in the Brain



Current Conception: Computation Graphs



Tensors in Neural Networks



Example Model Creation

- Define model's parameters:
 - Weight matrix W_0 for the input embedding layer
 - Weight matrix W_1 , W_2 and bias b_1 , b_2 for feedforward layers
 - Any other layers ...

```
class DanModel(BaseModel):
    def __init__(self, args, vocab, tag_size):
        super(DanModel, self).__init__(args, vocab, tag_size)
        self.define_model_parameters()
        self.init_model_parameters()

        # Use pre-trained word embeddings if emb_file exists
        if args.emb_file is not None:
            self.copy_embedding_from_numpy()
```

```
def define_model_parameters():
    """
    Define the model's parameters, e.g., embedding layer,
    """
    raise NotImplementedError()
```

Parameter Initialization

- Neural nets must have weights that are not identical to learn non-identical features
- **Uniform Initialization:** Initialize weights in some range, such as $[-v, v]$, $v = 0.01$ for example
 - *Problem!* Depending on the size of the net, inputs to downstream nodes may be very large
- **Glorot (Xavier) Initialization, He Initialization:** Initialize based on the size of the matrix

$$\text{Glorot Init: } v = \sqrt{\frac{6}{d_{\text{in}} + d_{\text{out}}}}$$

15

Example Model Initialization

- Initialize model's parameters using **Glorot** or others:
- Create initial random values within $[-v, v]$ for tensors such as W_0, W_1, W_2, b_1, b_2 , and any others before training.

```
def init_model_parameters(self):  
    """  
    Initialize the model's parameters by uniform sampling from a range  $[-v, v]$   
    """  
    raise NotImplementedError()
```

Loss Function

- Given a labeled example (x, y^*) , we use a NN $f(x)$ to estimate the condition probability and predict the label as $y = \arg \max P_{\theta}(y|x)$. Then we compute how close our predict w.r.t. the true label by a loss function.

$$P_{\theta}(y|x) = \text{Softmax}(f(x))$$

- **Classification:** Cross-Entropy

$$\mathcal{L}(x, y^*) = -\log P_{\theta}(y = y^* | x)$$

- **Regression:** L1 loss, L2 loss (a.k.a. Mean Square Error)

$$\mathcal{L}(x, y^*) = \|f(x) - y^*\|_1$$

$$\mathcal{L}(x, y^*) = \|f(x) - y^*\|_2$$

Forward Propagation: Computing Predictions & Loss

NN App Algorithm Sketch

- Create a model and define a loss (i.e., **construct a computation graph**)
- For each example
 - **Forward: calculate the result** (prediction & loss) of that computation
 - if training
 - perform **back propagation**
 - **update** parameters

expression:

x

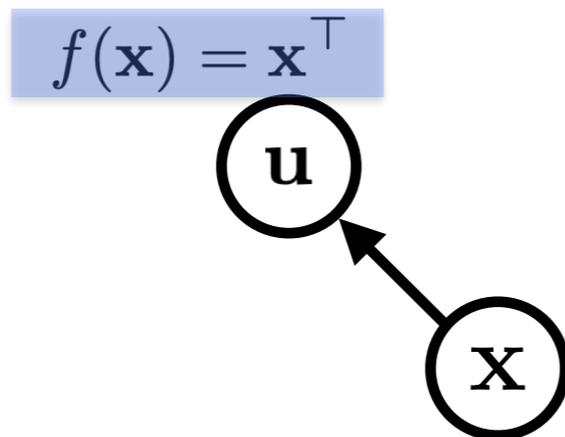
graph:

A **node** is a {tensor, matrix, vector, scalar} value

x

An **edge** represents a function argument (and also a data dependency). They are just pointers to nodes.

A **node** with an incoming **edge** is a **function** of that edge's tail node.

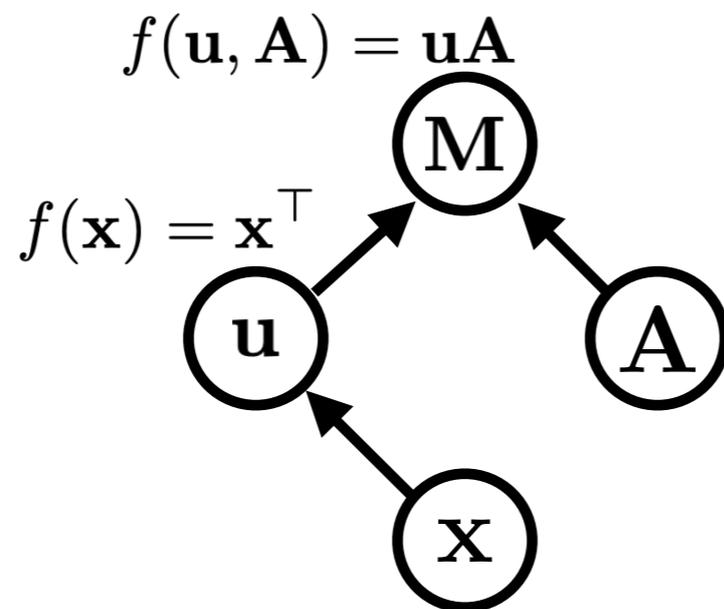


expression:

$$\mathbf{x}^\top \mathbf{A}$$

graph:

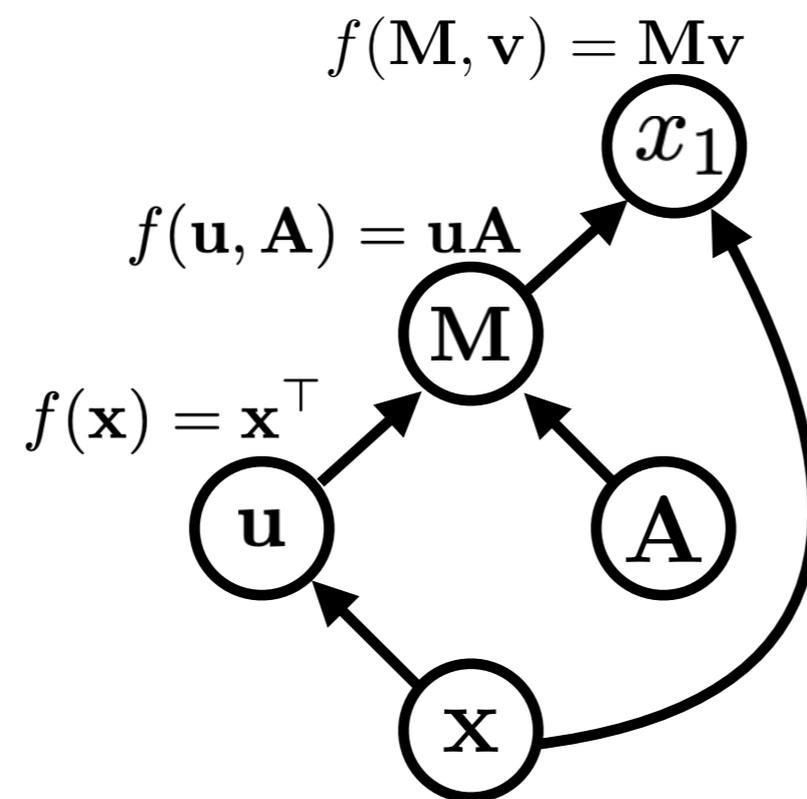
Functions can be unary, binary, ... n -ary (no. of inputs).
Often they are unary or binary.



expression:

$$\mathbf{x}^\top \mathbf{A} \mathbf{x}$$

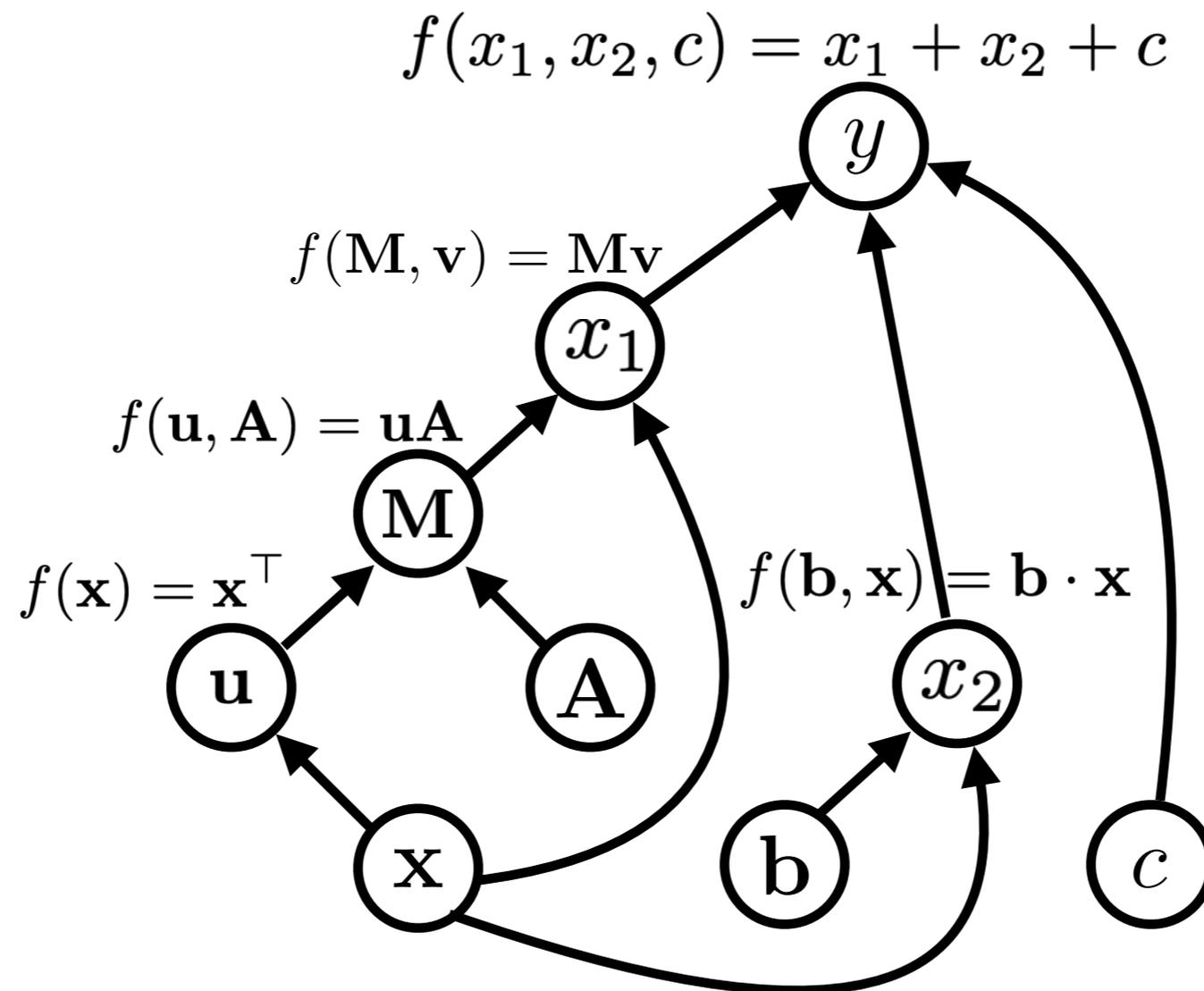
graph:



expression:

$$\mathbf{x}^\top \mathbf{A} \mathbf{x} + \mathbf{b} \cdot \mathbf{x} + c$$

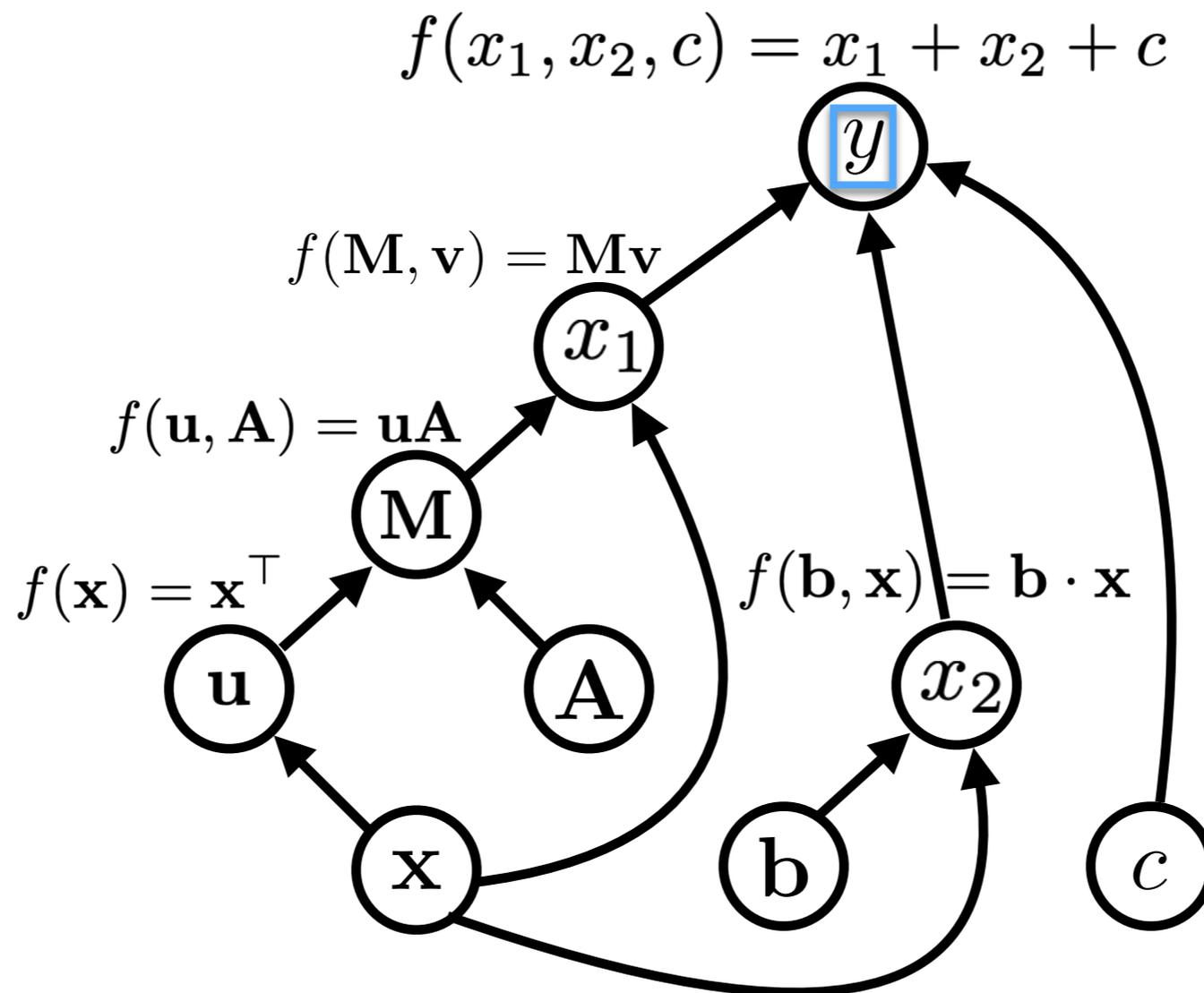
graph:



expression:

$$y = \mathbf{x}^\top \mathbf{A} \mathbf{x} + \mathbf{b} \cdot \mathbf{x} + c$$

graph:

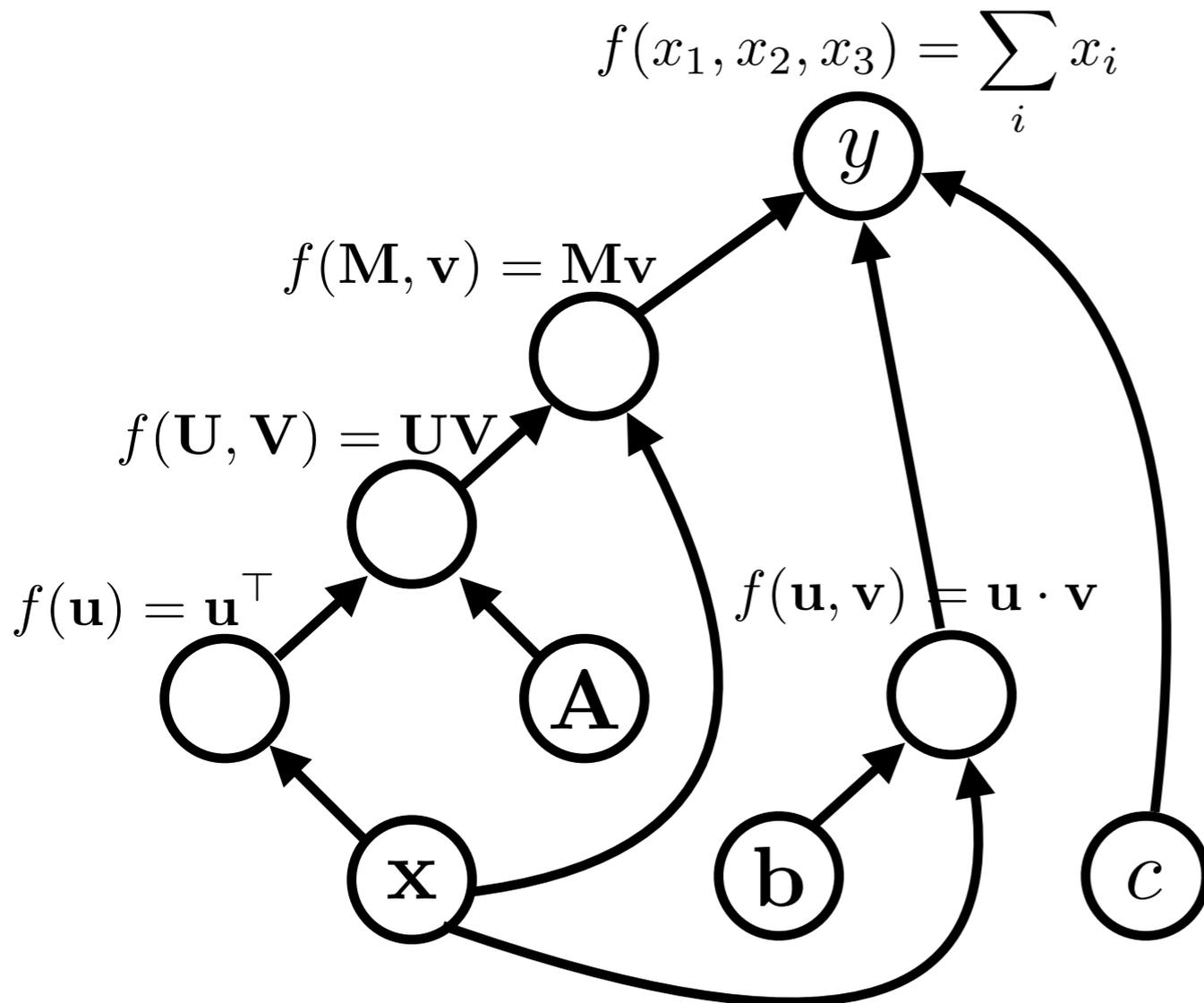


Computation graphs are generally directed and acyclic

expression:

$$y = \mathbf{x}^\top \mathbf{A} \mathbf{x} + \mathbf{b} \cdot \mathbf{x} + c$$

graph:



```
# x: 5-dimensional vector  
# Model's parameters contain:  
#   A: 5x5 matrix  
#   b: 5-dimensional vector  
#   c: scalar
```

```
class SimpleModel(nn.Module):  
    def __init__(self):  
        super(SimpleModel, self).__init__()  
        self.define_model_parameters()
```

```
def define_model_parameters(self):  
    self.A = nn.Parameter(torch.randn((5,5)))  
    self.b = nn.Parameter(torch.randn(5))  
    self.c = nn.Parameter(torch.randn(1))
```

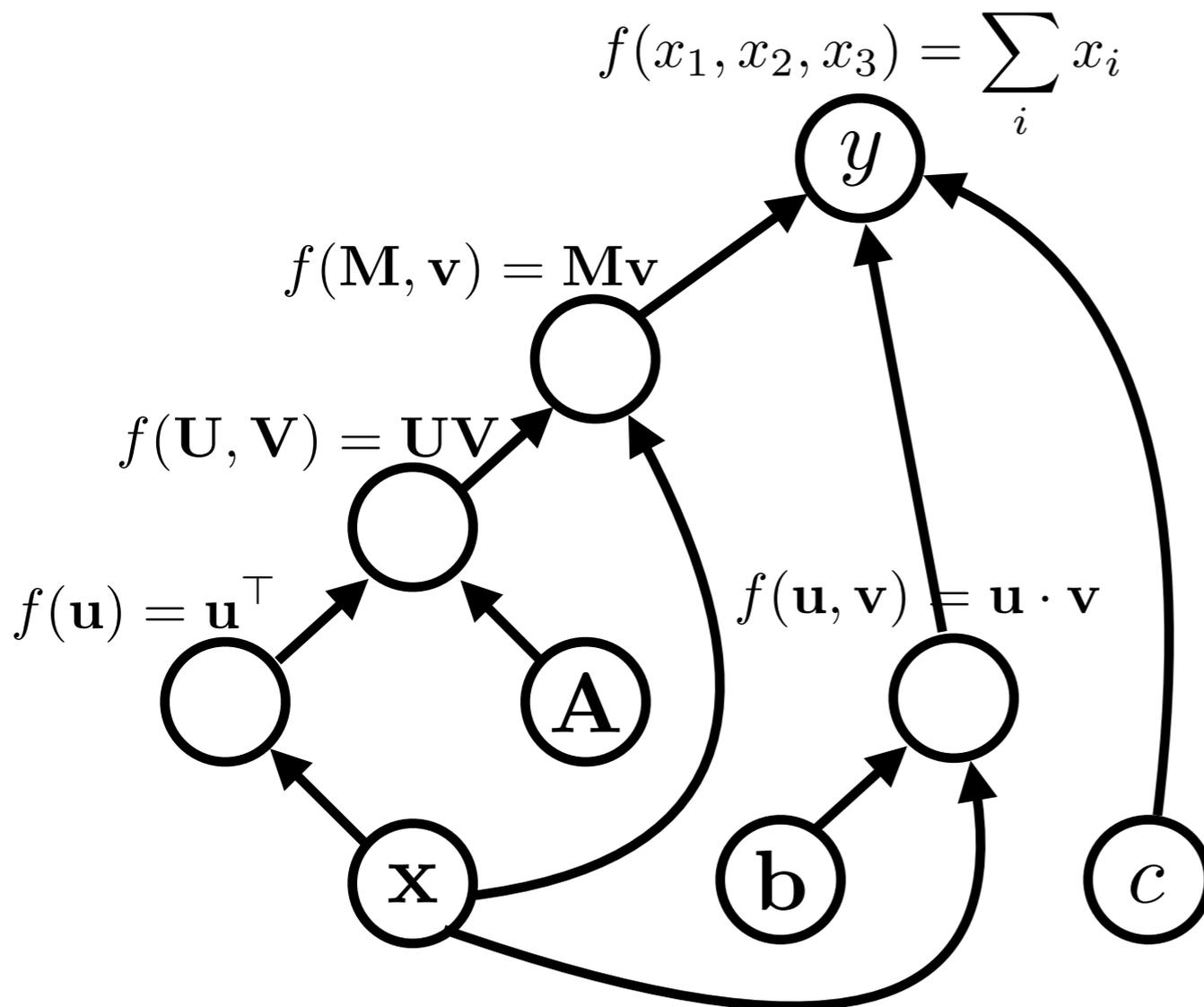
```
def forward(self, x):  
    U = x.T  
    print('U', U)  
    M = torch.matmul(U, self.A)  
    print('M', M)  
    Mv = torch.matmul(M, x)  
    print('Mv', Mv)  
    bx = torch.dot(self.b, x)  
    print('bx', bx)  
    y = Mv + bx + self.c  
    return y
```

```
x = torch.randn(5)  
model = SimpleModel()  
y = model(x)  
print(y)
```

expression:

$$y = \mathbf{x}^\top \mathbf{A} \mathbf{x} + \mathbf{b} \cdot \mathbf{x} + c$$

graph:



```
# x: 5-dimensional vector
# Model's parameters contain:
#   A: 5x5 matrix
#   b: 5-dimensional vector
#   c: scalar
```

```
class SimpleModel(nn.Module):
    def __init__(self):
        super(SimpleModel, self).__init__()
        self.define_model_parameters()

    def define_model_parameters(self):
        self.A = nn.Parameter(torch.randn((5,5)))
        self.b = nn.Parameter(torch.randn((5)))
        self.c = nn.Parameter(torch.randn((1)))
```

```
def forward(self, x):
    U = x.T
    print('U', U)
    M = torch.matmul(U, self.A)
    print('M', M)
    Mv = torch.matmul(M, x)
    print('Mv', Mv)
    bx = torch.dot(self.b, x)
    print('bx', bx)
    y = Mv + bx + self.c
    return y
```

```
x = torch.randn((5))
model = SimpleModel()
y = model(x)
print(y)
```

Operations

- Operations must know:
- **Forward:** Calculate their predictions/loss given input
 - Prediction: $y = f(\mathbf{x}) = \mathbf{x}^\top \mathbf{A} \mathbf{x} + \mathbf{b} \cdot \mathbf{x} + c$
 - Loss: $\mathcal{L} = (y - y^*)^2$
- **Backward:** Calculate the derivative of model parameters w.r.t. the loss

$$\frac{\partial \mathcal{L}}{\partial \mathbf{A}}, \quad \frac{\partial \mathcal{L}}{\partial \mathbf{b}}, \quad \frac{\partial \mathcal{L}}{\partial c}$$

Back Propagation

NN App Algorithm Sketch

- Create a model and define a loss (i.e., **construct a computation graph**)
- For each example
 - **Forward: calculate the result** (prediction & loss) of that computation
 - if training
 - perform **back propagation**
 - **update** parameters

Back Propagation

- Mean-square error: $\mathcal{L} = (y - y^*)^2$

graph:

$$y = f(x_1, x_2, c) = x_1 + x_2 + c$$

$$\frac{\partial \mathcal{L}}{\partial y} = 2(y - y^*)$$

$$\frac{\partial \mathcal{L}}{\partial x_1} = \frac{\partial \mathcal{L}}{\partial y} \cdot \frac{\partial y}{\partial x_1} = 2(y - y^*) \quad f(\mathbf{M}, \mathbf{x}) = \mathbf{M}\mathbf{x}$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{M}} = \frac{\partial \mathcal{L}}{\partial x_1} \cdot \frac{\partial x_1}{\partial \mathbf{M}} = 2(y - y^*)\mathbf{x}$$

$$f(\mathbf{u}, \mathbf{A}) = \mathbf{u}\mathbf{A}$$

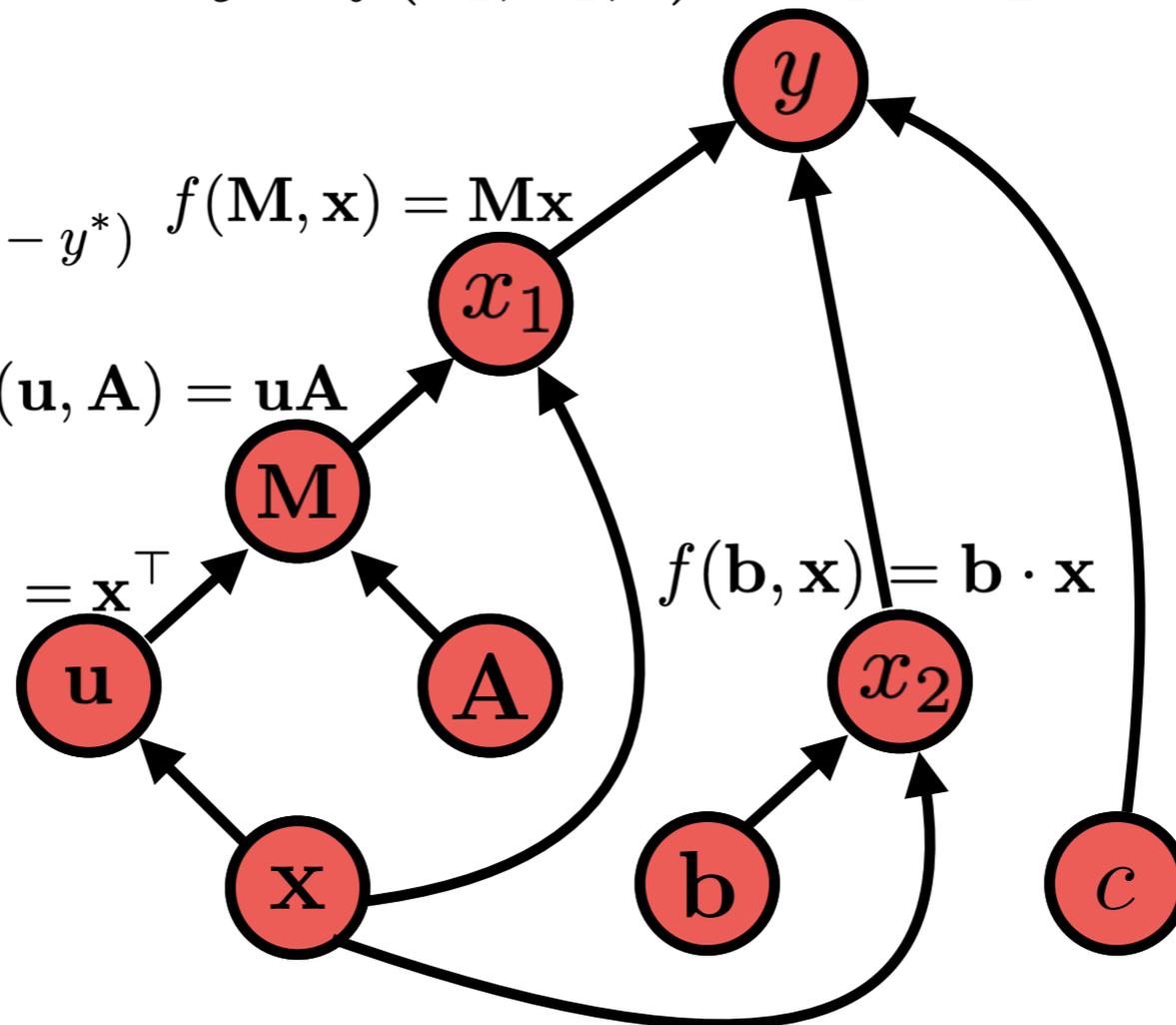
$$f(\mathbf{x}) = \mathbf{x}^\top$$

$$f(\mathbf{b}, \mathbf{x}) = \mathbf{b} \cdot \mathbf{x}$$

$$\frac{\partial \mathcal{L}}{\partial x_2} = \frac{\partial \mathcal{L}}{\partial y} \cdot \frac{\partial y}{\partial x_2} = 2(y - y^*)$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{A}} = \frac{\partial \mathcal{L}}{\partial \mathbf{M}} \cdot \frac{\partial \mathbf{M}}{\partial \mathbf{A}} = 2(y - y^*)\mathbf{x}\mathbf{x}^\top$$

$$\frac{\partial \mathcal{L}}{\partial c} = \frac{\partial \mathcal{L}}{\partial y} \cdot \frac{\partial y}{\partial c} = 2(y - y^*)$$



Model parameters: \mathbf{A} , \mathbf{b} , c

$$\frac{\partial \mathcal{L}}{\partial \mathbf{b}} = \frac{\partial \mathcal{L}}{\partial x_2} \cdot \frac{\partial x_2}{\partial \mathbf{b}} = 2(y - y^*)\mathbf{x}$$

Back Propagation

graph:

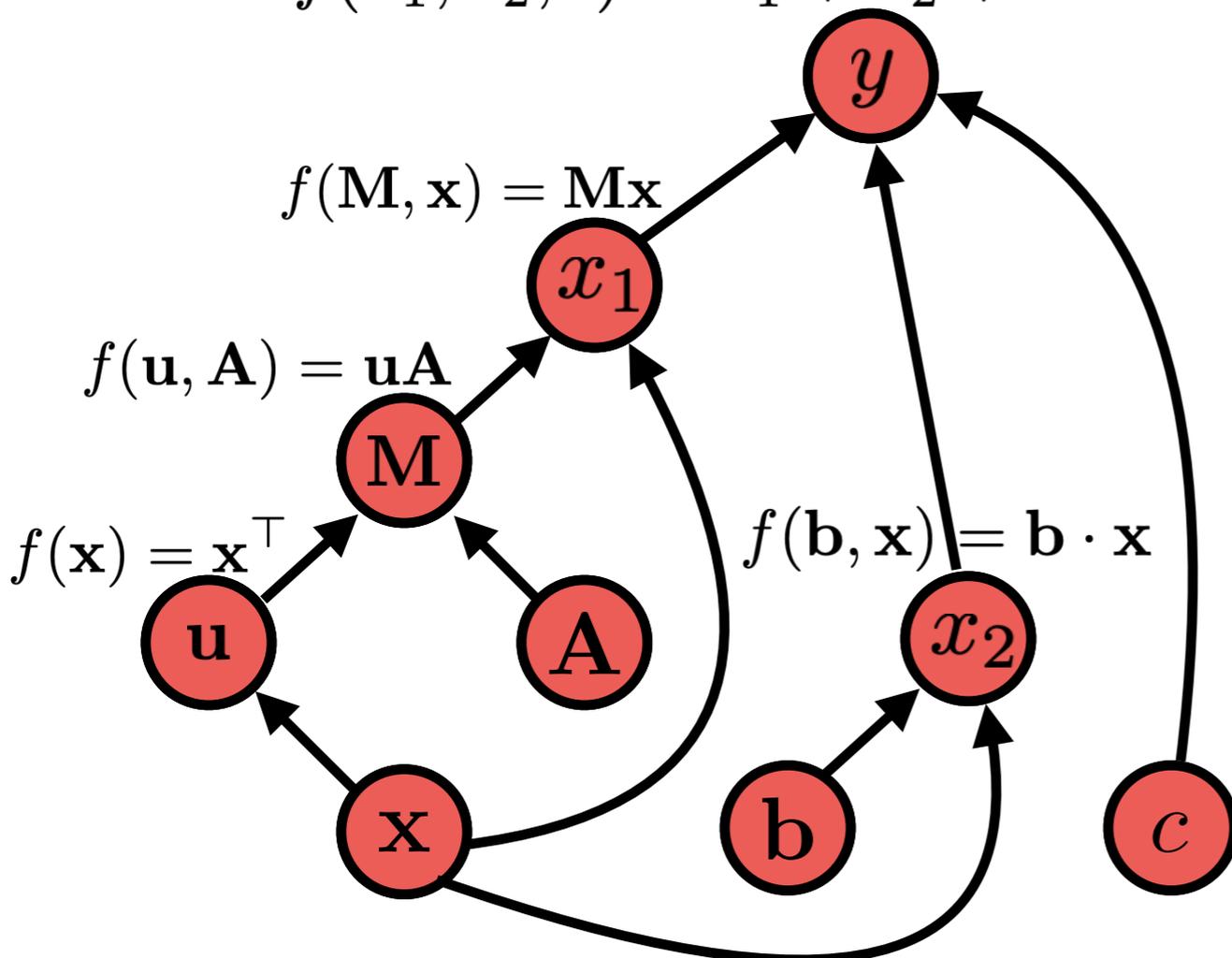
$$f(x_1, x_2, c) = x_1 + x_2 + c$$

$$f(\mathbf{M}, \mathbf{x}) = \mathbf{M}\mathbf{x}$$

$$f(\mathbf{u}, \mathbf{A}) = \mathbf{u}\mathbf{A}$$

$$f(\mathbf{x}) = \mathbf{x}^\top$$

$$f(\mathbf{b}, \mathbf{x}) = \mathbf{b} \cdot \mathbf{x}$$



- Mean-square error: $\mathcal{L} = (y - y^*)^2$

```
optimizer = torch.optim.Adagrad(model.parameters(), lr=0.01)
loss_func = nn.MSELoss()

y_true = torch.FloatTensor([1.0]) # ground true
loss = loss_func(y, y_true)
print(loss)
```

tensor(34.0528, grad_fn=<MseLossBackward0>)

- Compute gradients automatically by most tools: $\frac{\partial \mathcal{L}}{\partial A}$, $\frac{\partial \mathcal{L}}{\partial b}$, $\frac{\partial \mathcal{L}}{\partial c}$

```
optimizer.zero_grad()
loss.backward(retain_graph=True)
for name, param in model.named_parameters():
    print(name, param.grad)
```

A tensor([[-0.0313, -0.0386, -0.8571, 0.7265, 0.9405],
 [-0.0386, -0.0476, -1.0572, 0.8961, 1.1601],
 [-0.8571, -1.0572, -23.4711, 19.8953, 25.7557],
 [0.7265, 0.8961, 19.8953, -16.8643, -21.8319],
 [0.9405, 1.1601, 25.7557, -21.8319, -28.2627]])
 b tensor([0.6044, 0.7455, 16.5508, -14.0294, -18.1619])
 c tensor([-11.6710])

Parameter Update

NN App Algorithm Sketch

- Create a model and define a loss (i.e., **construct a computation graph**)
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Optimizer Update

- Most deep learning toolkits implement the parameter updates by calling **optimizer.step()** function

```
[59] # Before gradient update
      for name, param in model.named_parameters():
          print(name, param)

A Parameter containing:
tensor([[ -0.2267,  0.6521, -0.8193,  0.7723, -0.6456],
        [ 1.2410, -2.4380, -0.5612, -0.1144, -0.2687],
        [ 0.4792,  0.4543, -1.3530,  1.2934, -0.9943],
        [ 0.7565,  0.9449,  0.2796,  0.4703,  0.2926],
        [ 0.4143,  0.5891,  0.4370,  0.6060,  0.0161]])
b Parameter containing:
tensor([ 0.3592,  0.3455, -0.2517, -0.5678, -0.6016], :
c Parameter containing:
tensor([-1.5490], requires_grad=True)
```

Before optimizer update

```
[61] # Gradient update:
      optimizer.step()
      # After gradient update
      for name, param in model.named_parameters():
          print(name, param)

A Parameter containing:
tensor([[ -0.2167,  0.6621, -0.8093,  0.7623, -0.6556],
        [ 1.2510, -2.4280, -0.5512, -0.1244, -0.2787],
        [ 0.4892,  0.4643, -1.3430,  1.2834, -1.0043],
        [ 0.7465,  0.9349,  0.2696,  0.4803,  0.3026],
        [ 0.4043,  0.5791,  0.4270,  0.6160,  0.0261]])
b Parameter containing:
tensor([ 0.3492,  0.3355, -0.2617, -0.5578, -0.5916], :
c Parameter containing:
tensor([-1.5390], requires_grad=True)
```

After optimizer update

Many Different Optimizers

- **Simple SGD:** update with only gradients
- **Momentum:** update w/ running average of gradient
- **Adagrad:** update downweighting high-variance values
- **Adam:** update w/ running average of gradient, downweighting by running average of variance

Standard SGD

- **Reminder:** Standard stochastic gradient descent does

$$g_t = \frac{\nabla_{\theta_{t-1}} \ell(\theta_{t-1})}{\text{Gradient of Loss}}$$

$$\theta_t = \theta_{t-1} - \frac{\eta g_t}{\text{Learning Rate}}$$

- There are many other optimization options! (see Ruder 2016 in references)

SGD With Momentum

- Remember gradients from past time steps

$$v_t = \gamma v_{t-1} + \eta g_t$$

Momentum

Previous Momentum

Momentum
Conservation
Parameter

$$\theta_t = \theta_{t-1} - v_t$$

- Intuition:** Prevent instability resulting from sudden changes

Adagrad

- Adaptively reduce learning rate based on accumulated variance of the gradients

$$G_t = G_{t-1} + \underline{g_t \odot g_t}$$

Squared Current Gradient

$$\theta_t = \theta_{t-1} - \frac{\eta}{\sqrt{G_t + \epsilon}} g_t$$

— Small Constant

- **Intuition:** frequently updated parameters (e.g. common word embeddings) should be updated less
- **Problem:** learning rate continuously decreases, and training can stall -- fixed by using rolling average in *AdaDelta* and *RMSProp*

Adam

- Most standard optimization option in NLP and beyond
- Considers rolling average of gradient, and momentum

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t \quad \text{Momentum}$$

$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t \odot g_t \quad \text{Rolling Average of Gradient}$$

- Correction of bias early in training, because $\mathbb{E}[v_t]$ is a biased estimation of variance: $\mathbb{E}[v_t] = \mathbb{E}[g_t^2] \cdot (1 - \beta_2^t)$

$$\hat{m}_t = \frac{m_t}{1 - (\beta_1)^t} \quad \hat{v}_t = \frac{v_t}{1 - (\beta_2)^t}$$

- Final update

$$\theta_t = \theta_{t-1} - \frac{\eta}{\sqrt{\hat{v}_t} + \epsilon} \hat{m}_t$$

Training Tricks

Shuffling the Training Data

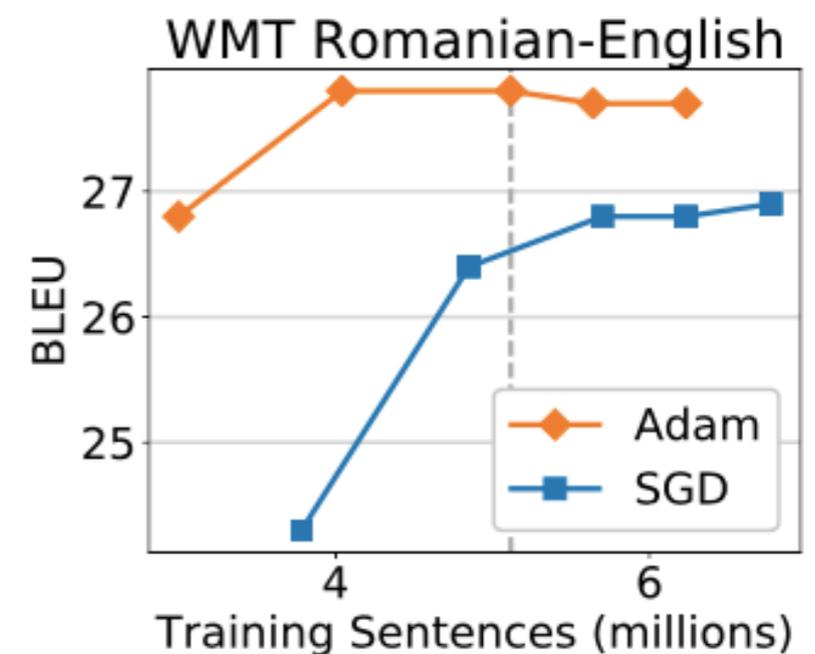
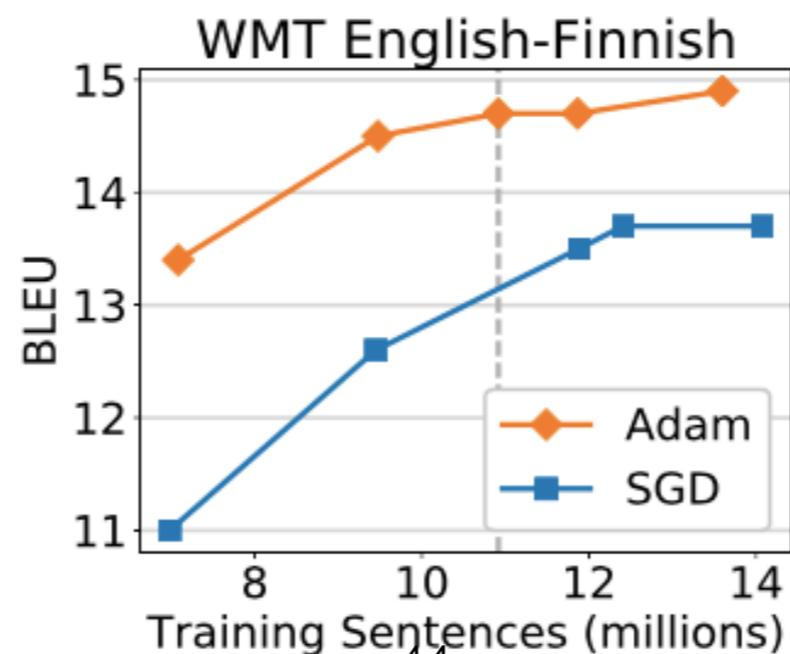
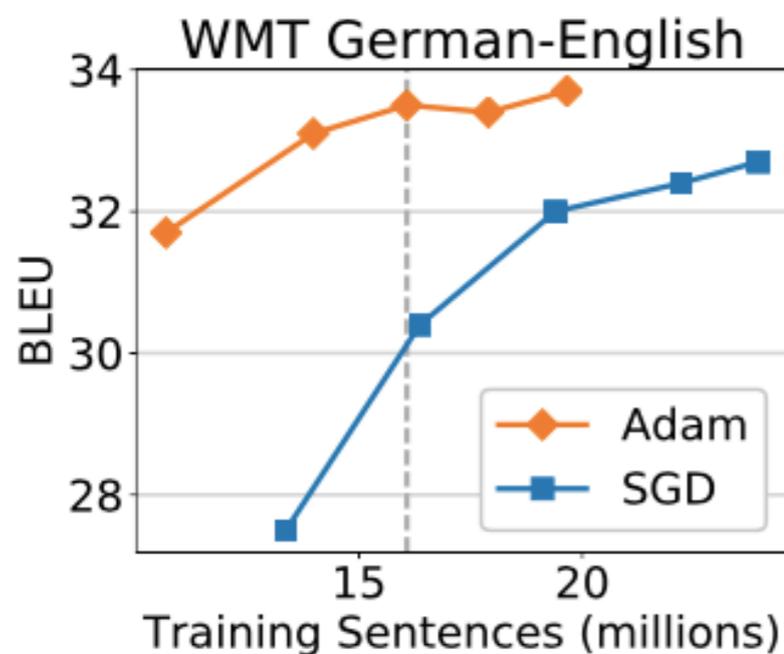
- Stochastic gradient methods update the parameters a little bit at a time
 - What if we have the sentence “I love this sentence so much!” at the end of the training data 50 times?
- To train correctly, we should randomly shuffle the order at each time step

Simple Methods to Prevent Over-fitting

- Neural nets have tons of parameters: we want to prevent them from over-fitting
- **Early stopping:**
 - monitor performance on held-out development data and stop training when it starts to get worse
- **Learning rate decay:**
 - gradually reduce learning rate as training continues, or
 - reduce learning rate when dev performance plateaus
- **Patience:**
 - learning can be unstable, so sometimes avoid stopping or decay until the dev performance gets worse n times

Which One to Use?

- Adam is usually fast to converge and stable
- But simple SGD tends to do very well in terms of generalization (Wilson et al. 2017)
- You should use learning rate decay, (e.g. on Machine translation results by Denkowski & Neubig 2017)



Dropout

(Srivastava+ 14)

- Neural nets have lots of parameters, and are prone to overfitting
- Dropout: randomly zero-out nodes in the hidden layer with probability p at **training time only**



- Because the number of nodes at training/test is different, scaling is necessary:
 - **Standard dropout:** scale by $1-p$ at test time
 - **Inverted dropout:** scale by $1/(1-p)$ at training time
- An alternative: **DropConnect** (Wan+ 2013) instead zeros out weights in the NN

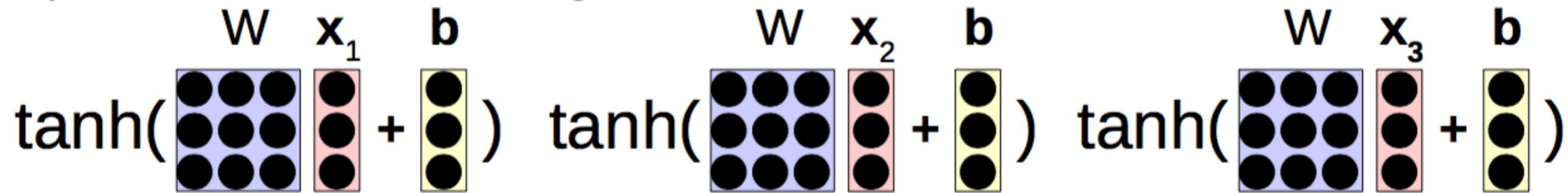
Efficiency Tricks: Operation Batching

Efficiency Tricks: Mini-batching

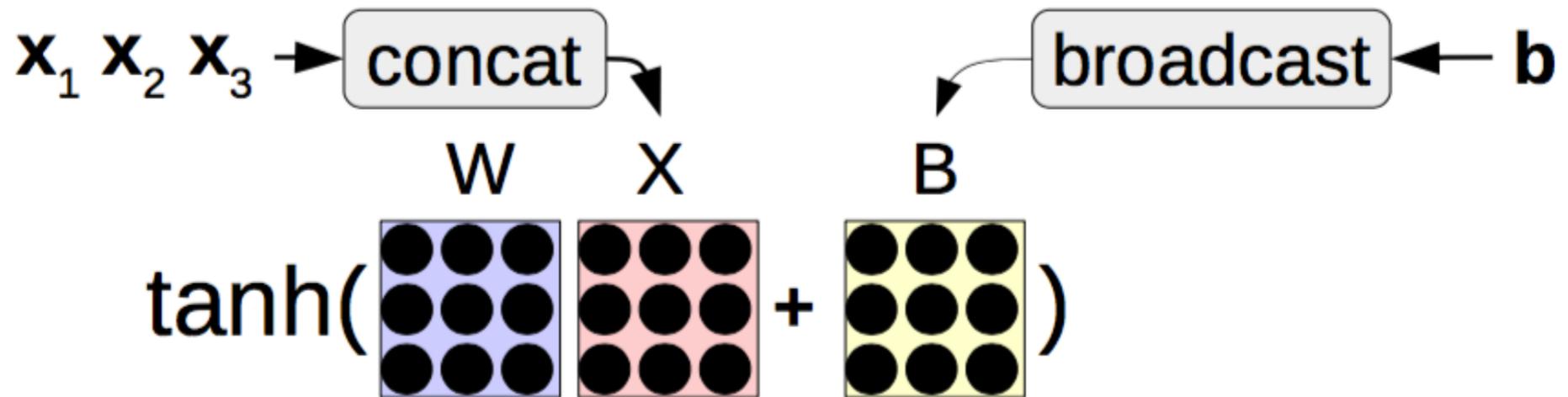
- On modern hardware 10 operations of size 1 is **much slower than** 1 operation of size 10
- Minibatching combines together smaller operations into one big one

Minibatching

Operations w/o Minibatching



Operations with Minibatching



Procedure of Minibatching

- **Group together similar operations** (e.g. loss calculations for a single word) and execute them all together
 - In the case of a feed-forward language model, each word prediction in a sentence can be batched
 - For recurrent neural nets, etc., more complicated
- How this works depends on toolkit
 - Most toolkits have require you to **add an extra dimension** representing the batch size
 - Some toolkits have **explicit tools** that help with batching

Assignment

Still Some Things Left!

- We've left off the details of some underlying parts.
- What about more operations?
- What about more optimizers?
- **Challenge:** can you make a more sophisticated model?

<https://github.com/JunjieHu/cs639-assignments/tree/main/hw1>

load_embedding

- Load a pretrained word embedding matrix from a text file (GloVe/ FastText)

```
def load_embedding(vocab, emb_file, emb_size):  
    """  
    Read embeddings for words in the vocabulary from the emb_file (e.g., GloVe, FastText).  
    Args:  
        vocab: (Vocab), a word vocabulary  
        emb_file: (string), the path to the embedding file for loading  
        emb_size: (int), the embedding size (e.g., 300, 100) depending on emb_file  
    Return:  
        emb: (np.array), embedding matrix of size (|vocab|, emb_size)  
    """  
    raise NotImplementedError()
```

- Copy the numpy embedding matrix to torch embeddings

```
class DanModel(BaseModel):  
    def copy_embedding_from_numpy(self):  
        """  
        Load pre-trained word embeddings from numpy.array to nn.embedding  
        Pass hyperparameters explicitly or use self.args to access the hyperparameters.  
        """  
        raise NotImplementedError()
```

DanModel

```
class DanModel(BaseModel):
    def __init__(self, args, vocab, tag_size):
        super(DanModel, self).__init__(args, vocab, tag_size)
        self.define_model_parameters()
        self.init_model_parameters()

        # Use pre-trained word embeddings if emb_file exists
        if args.emb_file is not None:
            self.copy_embedding_from_numpy()

    def define_model_parameters(self):
        """
        Define the model's parameters, e.g., embedding layer, feedforward layer.
        Pass hyperparameters explicitly or use self.args to access the hyperparameters.
        """
        raise NotImplementedError()

    def init_model_parameters(self):
        """
        Initialize the model's parameters by uniform sampling from a range [-v, v], e.g., v=0.08
        Pass hyperparameters explicitly or use self.args to access the hyperparameters.
        """
        raise NotImplementedError()

    def copy_embedding_from_numpy(self):
        """
        Load pre-trained word embeddings from numpy.array to nn.embedding
        Pass hyperparameters explicitly or use self.args to access the hyperparameters.
        """
        raise NotImplementedError()

    def forward(self, x):
        """
        Compute the unnormalized scores for P(Y|X) before the softmax function.
        E.g., feature: h = f(x)
            scores: scores = w * h + b
            P(Y|X) = softmax(scores)
        """
```

Mini-batch of varying length sequences

Add padding tokens to the end of the sentences to make sure that the minibatch has all sentences of the same length

Example: The maximum length is 5.

- $X_1 =$ “ I love this interesting movie” // 5 real-words
- $X_2 =$ “ great movie [pad] [pad] [pad]” // 2 real-words
- $X_3 =$ “This movie is bad [pad] ” // 4 real-words

When computing the average word embedding, we should (1) zero-out the padding tokens, (2) sum out the embeddings over words, and (3) divide the sum by the number of real-words

Questions?