Deep Learning in Apache MxNet Gluon

Imperative, Dynamic and Distributed

gluon.mxnet.io

Aran Khanna, Alex Smola

AWS Machine Learning

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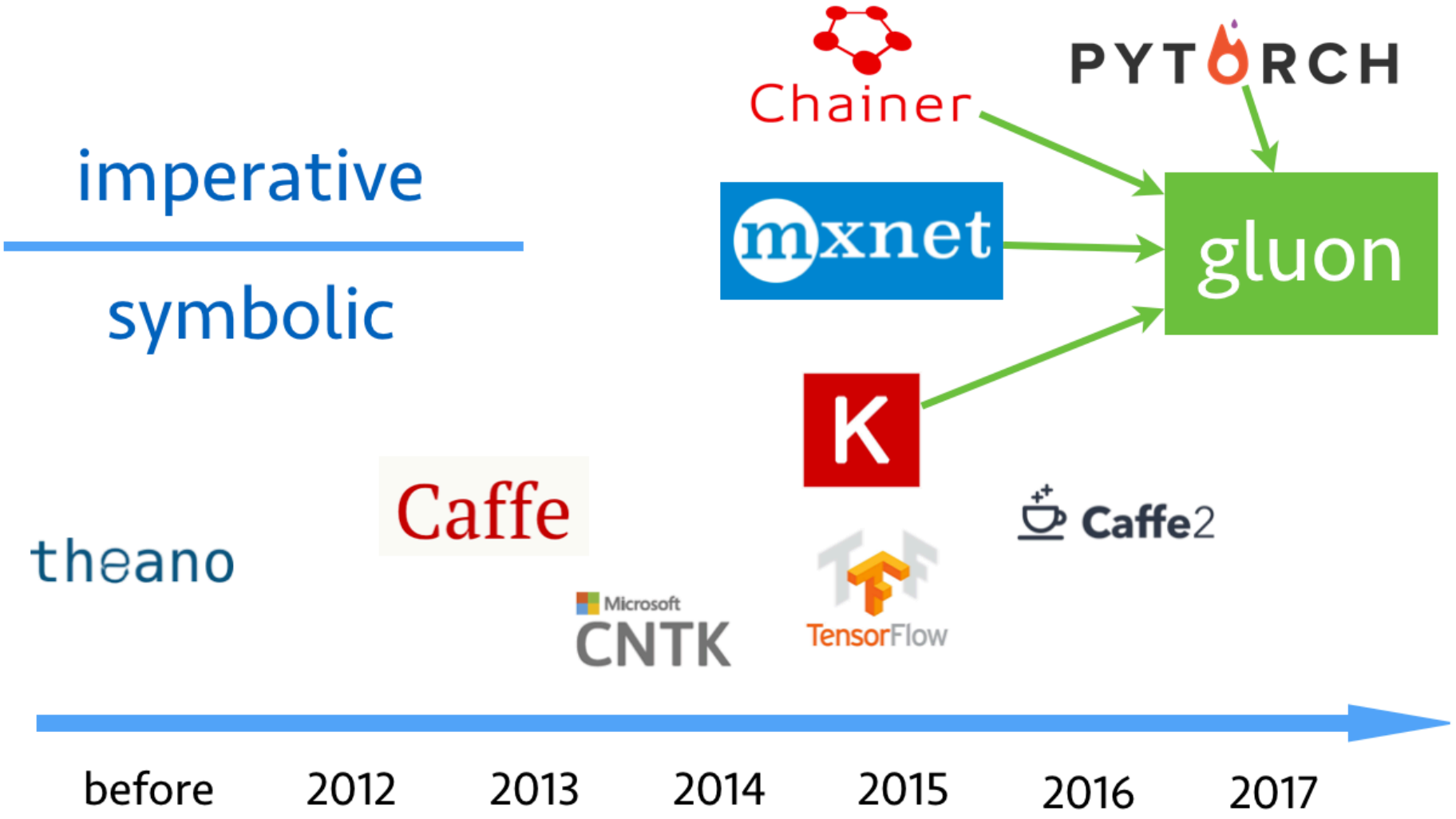
imperative
symbolic
Chainer
PYTORCH
mxnet
gluon
K
Caffe
theano
Caffe2
Microsoft
CNTK
TensorFlow
before
2012
2013
2014
2015
2016
2017

Outline

1. Deep Learning 101
2. NDArray
3. Multilayer Perceptrons
4. Convolutional Neural Networks
5. Generative Adversarial Networks
6. LSTMs
7. TreeLSTMs
8. Distributed Optimization
9. Parallel Training

1. Getting started with MxNet
2. Automatic Differentiation
3. Training from scratch/Gluon
4. Gluon layers
5. More than one gradient
6. Operator fusion
7. Dynamic graphs
8. Synchronous / asynchronous
9. (key, value) store

Installation

- **You need to update to the latest version of MxNet**
- **Build from source**

```
git clone git@github.com:apache/incubator-mxnet.git
git submodule update --init
mxnet.io/get_started/install.html
```

- **PIP install** (you should use Python 3)

```
pip install --upgrade pip
pip install --upgrade setuptools
pip install mxnet –pre
```

- **Deep Learning AMI**

```
bit.ly/deepami and bit.ly/deepubuntu
```

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Programming FizzBuzz

Code

```
var o='';
for (var i=1; i<=100; i++) {
    i%3 || (o+='Fizz ');
    i%5 || (o+='Buzz ');
    !(i%3 && i%5) || (o+=(i+' '));
}
console.log(o);
```

Programming with Data

- **Generate training data**
  (9,'Fizz'),(10,'Buzz'),(2,'2'),
  (15,'Fizz Buzz') …
- **Extract input features**
  x -> (x%3, x%5, x%15)
- **Train a classifier**
  mapping input x to output y
  using training data

Inspired by joelgrus.com

Programming FizzBuzz

Code

```
var o='';
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console.log(o);
```

That was silly.
Why would you do this?

Inspired by joelgrus.com

Programming with Data

- **Generate training data**
  (9,'Fizz'),(10,'Buzz'),(2,'2'),
  (15,'Fizz Buzz') …
- **Extract input features**
  x -> (x%3, x%5, x%15)
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  mapping input x to output y
  using training data

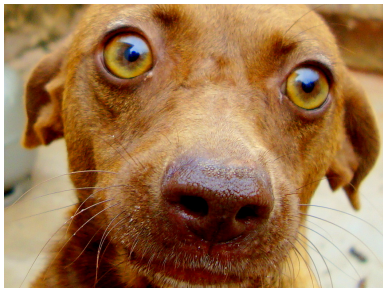
Programming with Data

- Given some input x we want to estimate output y
  - If it's a simple deterministic rule, probably don't bother
  - **Often quite complicated, vague but lots of examples**
  - **Impossible to write code but can train estimator**

cat

cat

dog

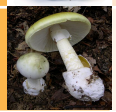


dog

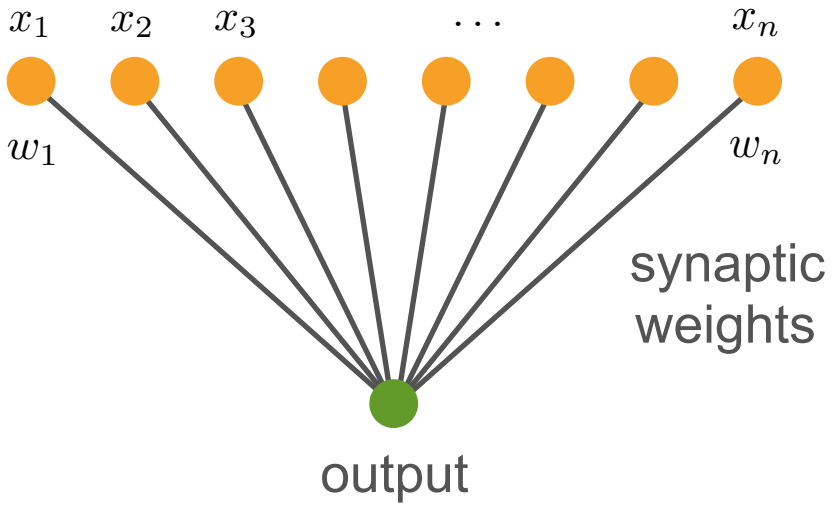
image credit - wikipedia

Programming with Data

- **Data** (patterns, labels)
  - Images (pictures / cat, dog, dinosaur, chicken, human)
  - Text (email / spam, ham)
  - Sound (recording / recognized speech)
  - Video (sequence / break-in, OK)
  - Images (X-ray image / size of cancer)
- **Goal** Learn mapping data to outputs
- **Loss function**
  measure how well we're doing

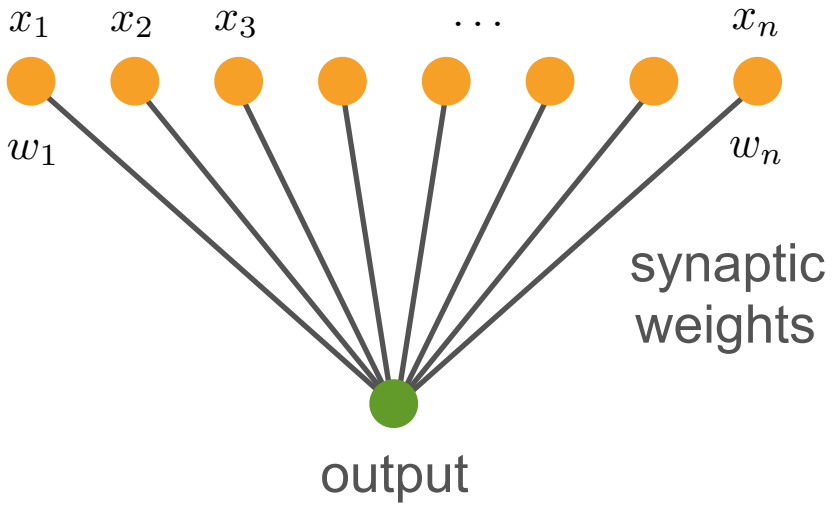
	Edible	Poison
Truffle 	0	10
Death cap 	1,000,000	0

Neural Networks



- **Input**
  Data vector x
- **Output**
  Linear function of inputs
- **Nonlinearity**
  Transform output into desired range of values, e.g. probabilities [0, 1]
- **Training**
  Learn the weights w and bias b

Neural Networks



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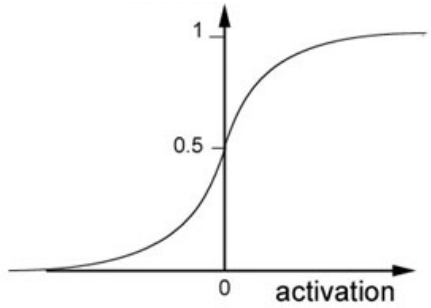
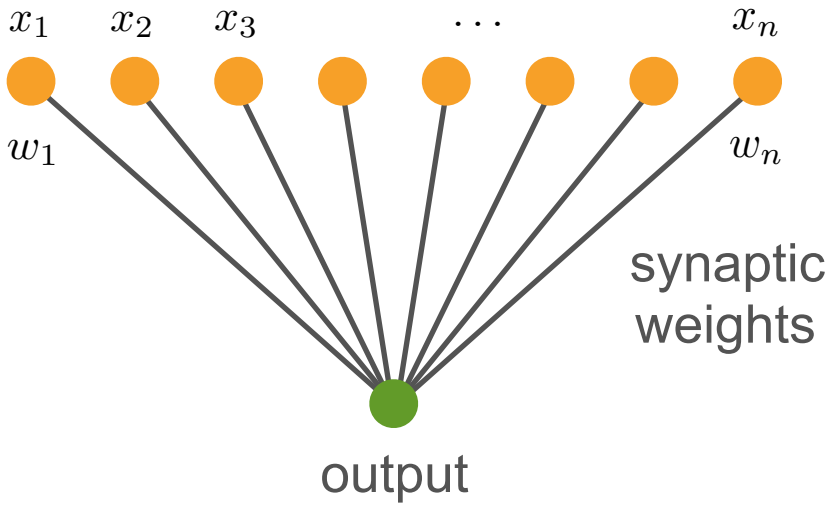


Neural Networks



- **Input**
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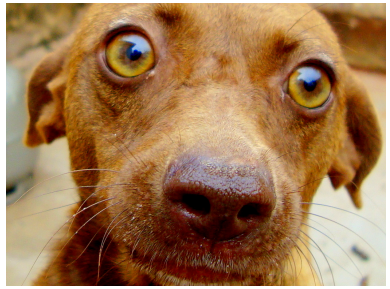
- **Training**
  Learn the weights w and bias b

$$f(x) = \sigma\left(\sum_{i=1}^{n} w_i x_i + b\right)$$

Artificial Neuron



$$f(x) = \sigma\left(\sum_{i=1}^{n} w_i x_i + b\right)$$

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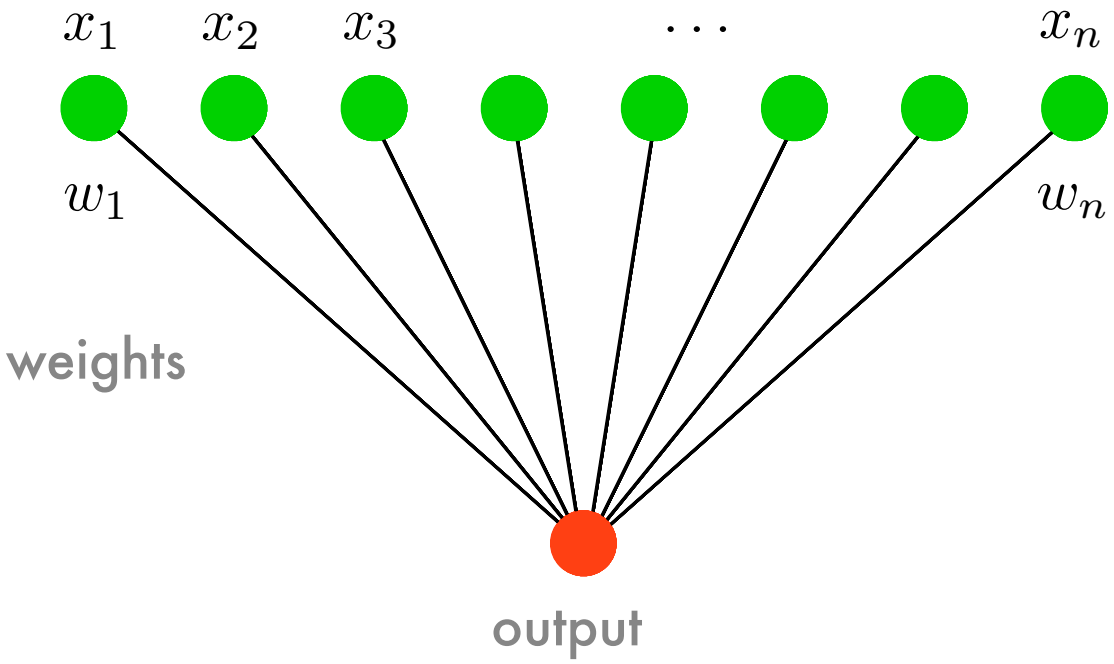
MxNet Code

```
import mxnet as mx
from mxnet import gluon

net = gluon.nn.Sequential()
net.add(gluon.nn.Dense(1))
loss = gluon.loss.SoftmaxCrossEntropyLoss()

+ iterator over data (and loader)
+ training loop
```

fully connected layer, 1 output

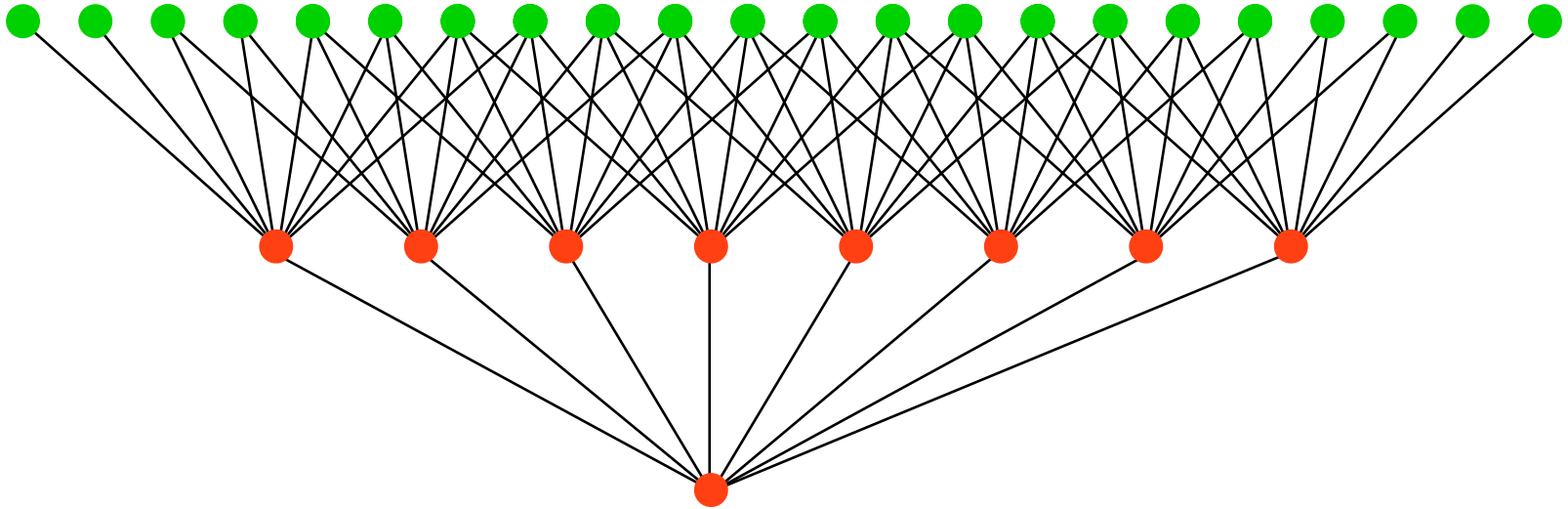
Multilayer Perceptron and Backprop

Perceptron



$$y(x) = \sigma(\langle w, x \rangle)$$

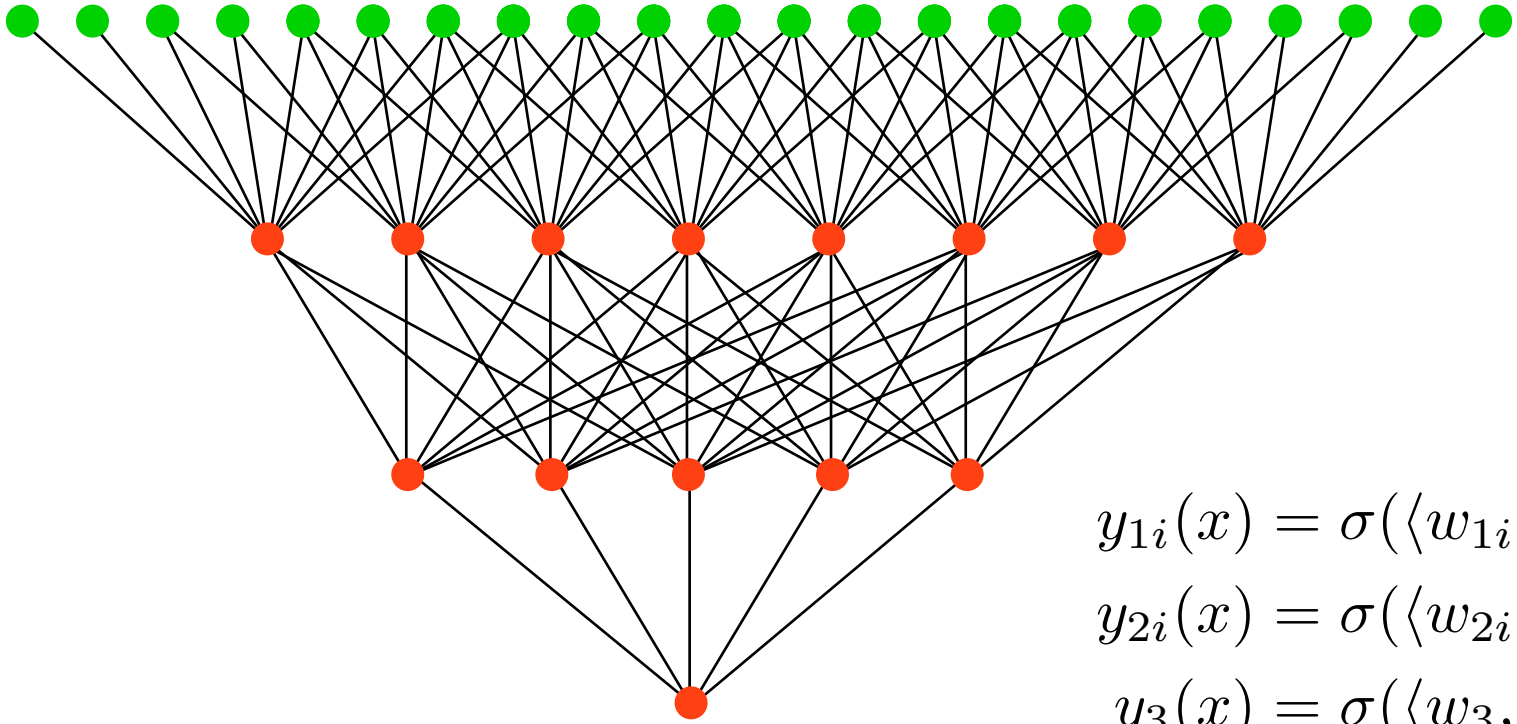
Multilayer Perceptron



$$y_{1i}(x) = \sigma(\langle w_{1i}, x \rangle)$$

$$y_2(x) = \sigma(\langle w_2, y_1 \rangle)$$

Multilayer Perceptron



$$y_{1i}(x) = \sigma(\langle w_{1i}, x \rangle)$$
$$y_{2i}(x) = \sigma(\langle w_{2i}, y_1 \rangle)$$
$$y_3(x) = \sigma(\langle w_3, y_2 \rangle)$$

Multilayer Perceptron Training

Layer Representation

$$y_i = W_i x_i$$

$$x_{i+1} = \sigma(y_i)$$

Gradient descent

$$W_i \leftarrow W_i - \eta \partial_{W_i} l(y, y_n)$$

- **Stochastic gradient descent** (use only one sample)
- **Minibatch** (small subset)

Multilayer Perceptron Training

Layer Representation

$$y_i = W_i x_i$$

$$x_{i+1} = \sigma(y_i)$$

Change in Objective

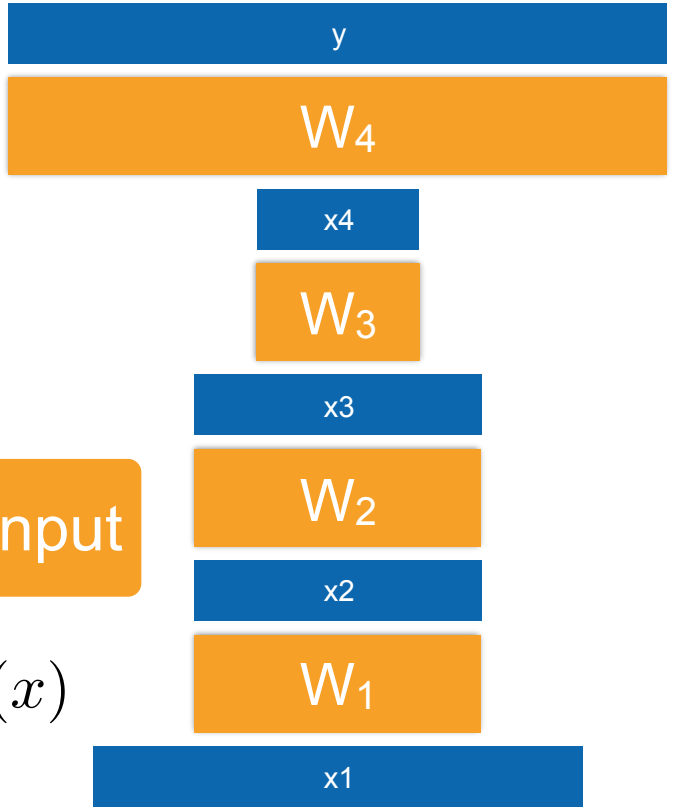
$$g_j = \partial_{W_j} l(y, y_i)$$

Chain Rule

$$\partial_x [f_2 \circ f_1](x) = [\partial_{f_1} f_2 \circ f_1](x) [\partial_x f_1](x)$$

effect of input

second layer



Multilayer Perceptron Training

Layer Representation

$$y_i = W_i x_i$$

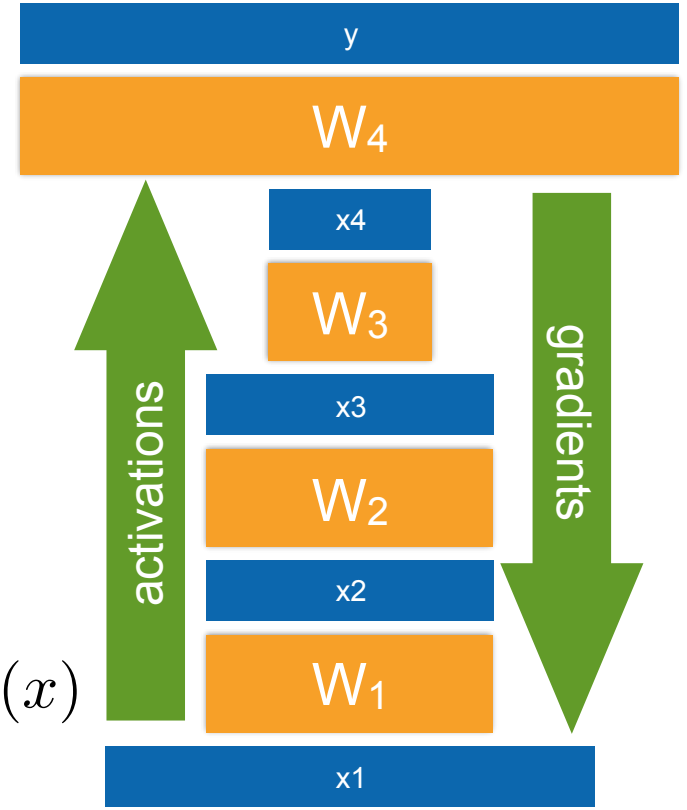
$$x_{i+1} = \sigma(y_i)$$

Change in Objective

$$g_j = \partial_{W_j} l(y, y_i)$$

Chain Rule

$$\partial_x [f_2 \circ f_1](x) = [\partial_{f_1} f_2 \circ f_1](x) [\partial_x f_1](x)$$



MxNet computes this automatically

That was complicated!
MXNet takes care of this for you …

```
import mxnet as mx
from mxnet import gluon

net = gluon.nn.Sequential()
with net.name_scope():
    net.add(gluon.Dense(128, activation='relu'))
    net.add(gluon.Dropout(dropout=0.5)
    net.add(gluon.Dense(64, activation='relu'))
    net.add(gluon.Dropout(dropout=0.5)
    net.add(gluon.Dense(1))

loss = gluon.loss.SoftmaxCrossEntropyLoss()
```

nonlinearity

regularization

second layer

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Matrices and Vectors

- **A Simple ML algorithm**

```
initialize function f(x,w)
for (x,y) in data:
      l = loss(y, f(x,w))
      g = gradient(l)
      w = w - eta * g
```

- Need vectors to deal with w
- Need matrices to deal with chain rule for loss gradient
- Need high performance linear algebra

NDArray (Linear Algebra on GPUs in Python)

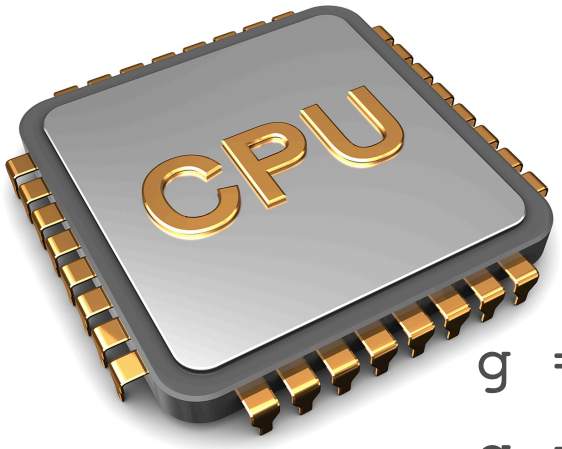
- **NumPy**
  - Limited to CPUs
  - No automatic differentiation
  - **Blocking (returns only once computation is performed)**
- **NDArray**
  - Multiple CPUs / GPUs via device context
  - Distributed systems in the cloud
  - **Nonblocking Python frontend (no GIL) & lazy evaluation**

http://mxnet.io/tutorials/basic/ndarray.html

NDArray Device Contexts

```
context = mx.cpu()
```

```
context = mx.gpu(0)
context = mx.gpu(1)
```

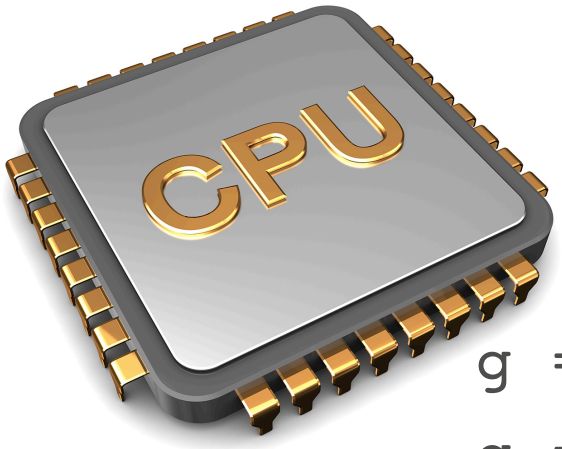


```
g = copyto(c)
g = c.as_in_context(mx.gpu(0))
```

NDArray Device Contexts

```
context = mx.cpu()
```

```
context = mx.gpu(0)
context = mx.gpu(1)
```



Caution!
NDArrays are
immutable on GPUs

```
g = copyto(c)
g = c.as_in_context(mx.gpu(0))
```

Automatic Differentiation

```
b = a * 2
while (nd.norm(b) < 1000).asscalar():
    b = b * 2
if (mx.nd.sum(b) > 0).asscalar():
    c = b
else :
    c = 100 * b
```

Compute dc/da?

Links & Notebooks

gluon.mxnet.io
github.com/zackchase/mxnet-the-straight-dope
mxnet.io/api/python/gluon.html

http://gluon.mxnet.io/P01-C03-linear-algebra.html
http://gluon.mxnet.io/P01-C05-autograd.html

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Linear Regression

- Model

$$f(x) = \langle w, x \rangle + b$$

- Loss

$$l(y, f(x)) = \frac{1}{2}(y - f(x))^2$$

- Optimization algorithm - SGD
  - Initialize w, b at random (or at zero)
  - Iterate over data

$$(w, b) \leftarrow (w, b) - \eta \partial_{(w,b)} l(y, f(x))$$

Logistic Regression (Multiclass)

- Model (single layer)

$$f(x) = Wx + b$$

- Multilayer Perceptron

$$x_1 = x_{\text{input}} \text{ and } x_{l+1} = \sigma\left(W_l x_l + b_l\right)$$

- Loss (exponential family)

$$-\log p(y|x) = \log \sum_{y'} \exp\left(f(x)_{y'}\right) - f(x)_y$$

Links & Notebooks

http://gluon.mxnet.io/P02-C01-linear-regression-scratch.html
http://gluon.mxnet.io/P02-C02-linear-regression-gluon.html
http://gluon.mxnet.io/P02-C04-softmax-regression-gluon.html
http://gluon.mxnet.io/P03-C02-mlp-gluon.html

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Where is Waldo?

image credit - wikipedia

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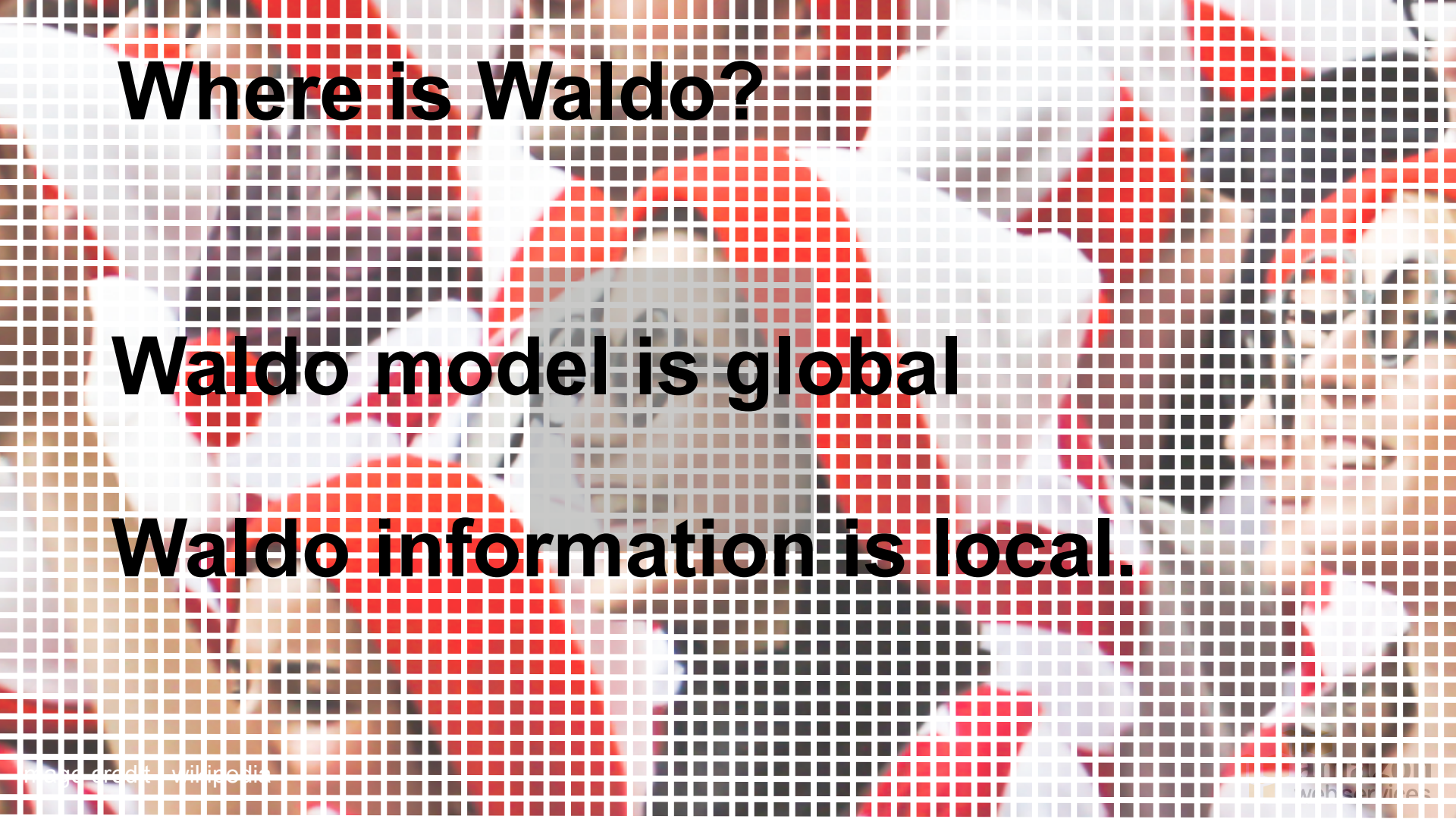
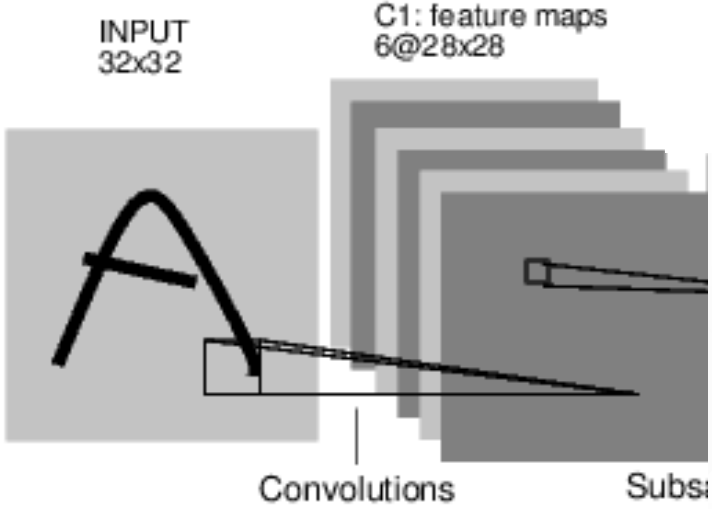

Where is Waldo?
Waldo model is global
Waldo information is local.

Convolutional Layers

- Images have shift invariance
- Low level mostly edge and feature detectors
- **Key Idea**
  Replace matrix multiplication with local computation

$$y_{ij} = \sum_{a=-\Delta}^{\Delta} \sum_{b=-\Delta}^{\Delta} W_{ab} x_{i+a,j+b}$$

- Backprop automatic in MXNet



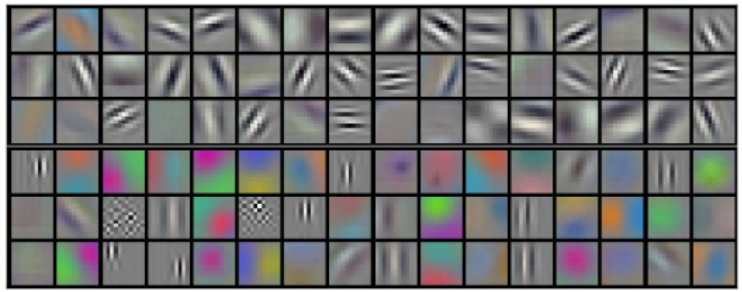
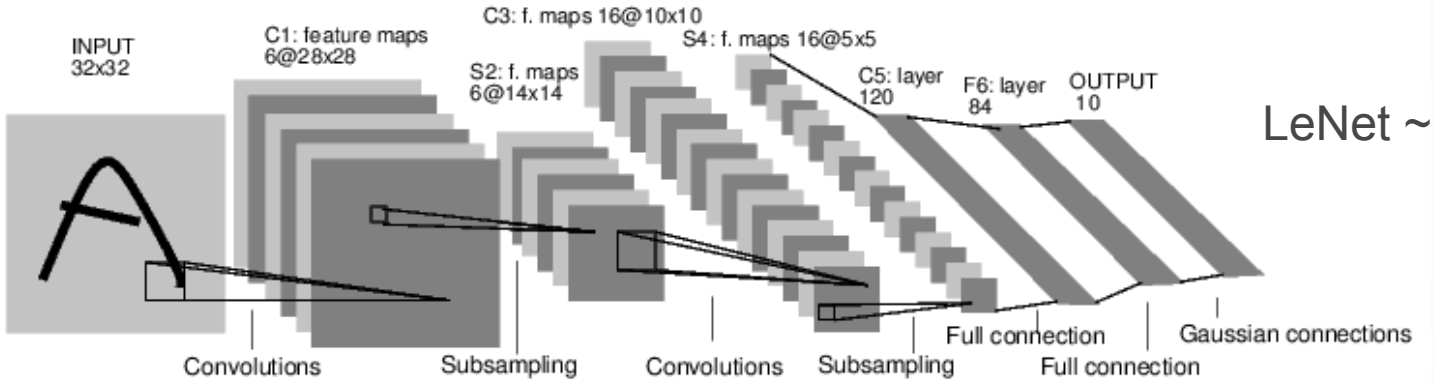


image credit - Le Cun et al, 1998, Olshausen and Field, 1998

Subsampling & MaxPooling

- Multiple convolutions blow up dimensionality



LeNet ~1995

- Subsampling - average over patches (works OK)
- MaxPooling - pick the maximum over patches (much better)

image credit - Le Cun et al, 1998

LeNet in MXNet

```
net = gluon.nn.Sequential()
with net.name_scope():
    net.add(gluon.nn.Conv2D(channels=20, kernel_size=5, activation='tanh'))
    net.add(gluon.nn.AvgPool2D(pool_size=2))
    net.add(gluon.nn.Conv2D(channels=50, kernel_size=5, activation='tanh'))
    net.add(gluon.nn.AvgPool2D(pool_size=2))
    net.add(gluon.nn.Flatten())
    net.add(gluon.nn.Dense(500, activation='tanh'))
    net.add(gluon.nn.Dense(10))

loss = gluon.loss.SoftmaxCrossEntropyLoss()

(size and shape inference is automatic)
```

More Layers

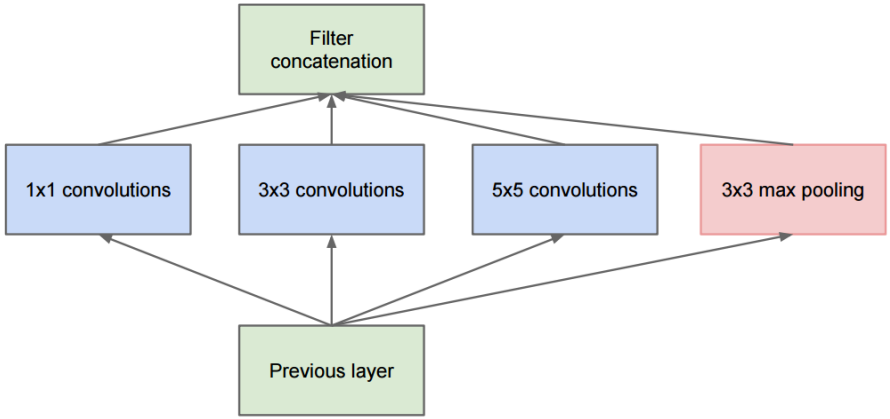
- **The usual suspects**
  - gluon.nn.Dense(units=50, …)
  - gluon.nn.Activation(activation='relu')
  - gluon.nn.Dropout(rate=0.3)
  - gluon.nn.BatchNorm(…)
  - gluon.nn.Embedding(…) for text
- **Convolutions**
  - gluon.nn.Conv1D, 2D, 3D
  - gluon.nn.Conv1DTranspose, 2D, 3D for Deconvolution
- **Pooling Layers**
  - gluon.nn.MaxPool1D, 2D, 3D, gluon.nn.AvgPool1D, 2D, 3D

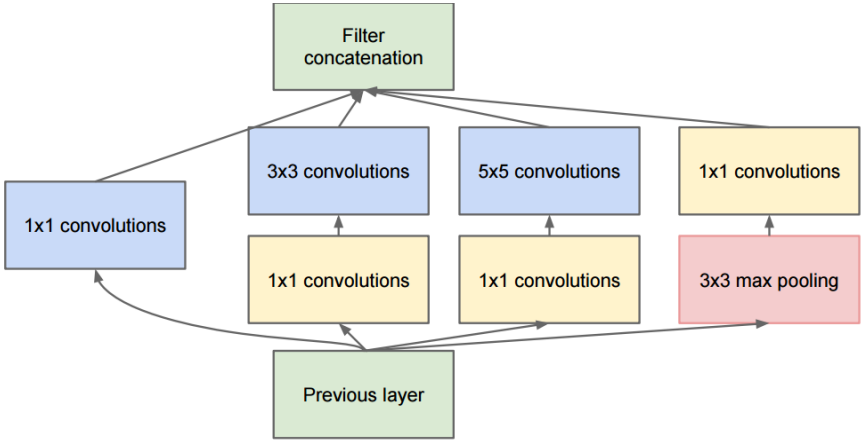
Links & Notebooks

http://gluon.mxnet.io/P04-C02-cnn-gluon.html
http://gluon.mxnet.io/P14-C05-hybridize.html

Fancy structures

- Compute different filters
- Compose one big vector from all of them
- Layer them iteratively





Szegedy et al. arxiv.org/pdf/1409.4842v1.pdf

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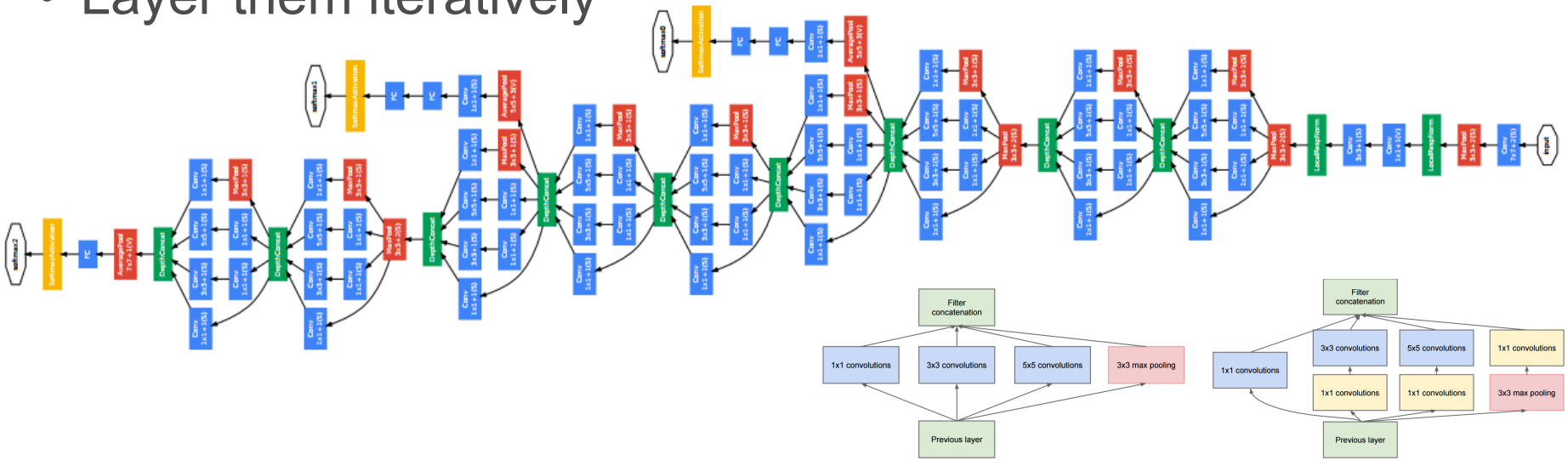

Szegedy et al. arxiv.org/pdf/1409.4842v1.pdf

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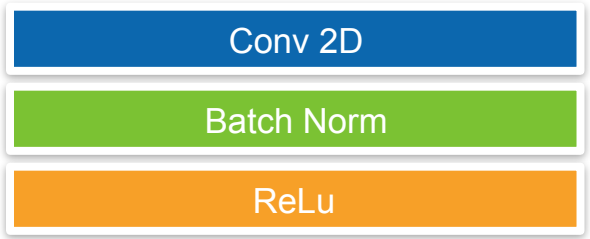
Networks of networks - Sequential Composition

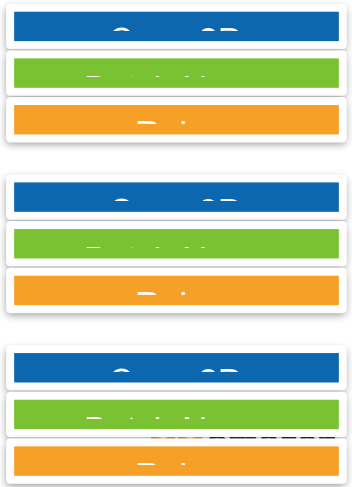
- **Define Single Block**

```
def _make_basic_conv(**kwargs):
  out = nn.HybridSequential(prefix='')
  out.add(nn.Conv2D(use_bias=False, **kwargs))
  out.add(nn.BatchNorm(epsilon=0.001))
  out.add(nn.Activation('relu'))
  return out
```



- **Compose Multiple Blocks into Branch**

```
def _make_branch(*conv_settings):
  out = nn.HybridSequential(prefix='')
  out.add(nn.MaxPool2D(pool_size=3, strides=2))
  setting_names = ['channels', 'kernel_size', 'strides', 'padding']
  for setting in conv_settings:
      kwargs = {}
      for i, value in enumerate(setting):
          if value is not None:
              kwargs[setting_names[i]] = value
      out.add(_make_basic_conv(**kwargs))
  return out
```



Networks of networks - Parallel Composition

- **Parallel composition of branches**

```
def def _make_A(pool_features, prefix):
    out = HybridConcurrent(concat_dim=1, prefix=prefix)
    with out.name_scope():
        out.add(_make_branch(None, (64, 1, None, None)))
        out.add(_make_branch(None, (48, 1, None, None),
                                   (64, 5, None, 2)))
        out.add(_make_branch(None, (64, 1, None, None),
                                   (96, 3, None, 1),
                                   (96, 3, None, 1)))
        out.add(_make_branch('avg',(pool_features, 1, None, None)))
    return out
```

Model Zoo

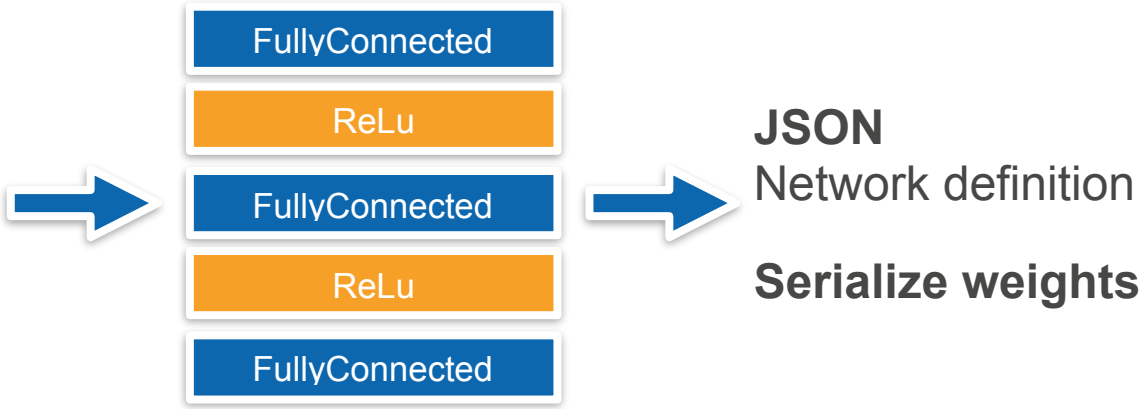
- Lots more networks at mxnet.gluon.model_zoo.vision (with all the model parameters you want)
  - AlexNet (because, why not)
  - SqueezeNet
  - Inception
  - VGG
  - DenseNet
  - ResNet

… import from PyTorch is trivial …

Hybridization (a JIT compiler for Networks)

- Loops and control flow are easy to understand
- Runtime engine needs to parse them each time (slow)
- Use JIT compiler to convert into compute graph (no need to parse the code more than once)

```
x = F.relu(self.fc1(x))
x = F.relu(self.fc2(x))
return self.fc3(x)
```



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Generative Adversarial Networks Primer

- **Traditional Statistics**
  Given data X, try to find some distribution p that would have generated X.
- **Why?**
  - Assess how well some observation x’ fits with the data, by evaluating p(x’).
  - Draw new fake data x' that looks like it came from X
  - Summarize X concisely (sufficient statistics)

Generative Adversarial Networks Primer

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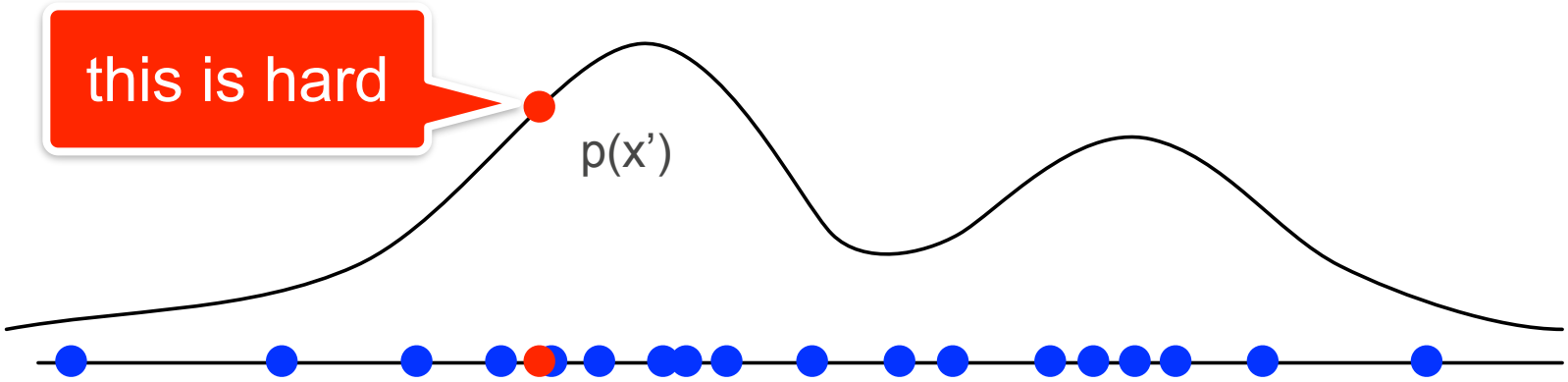

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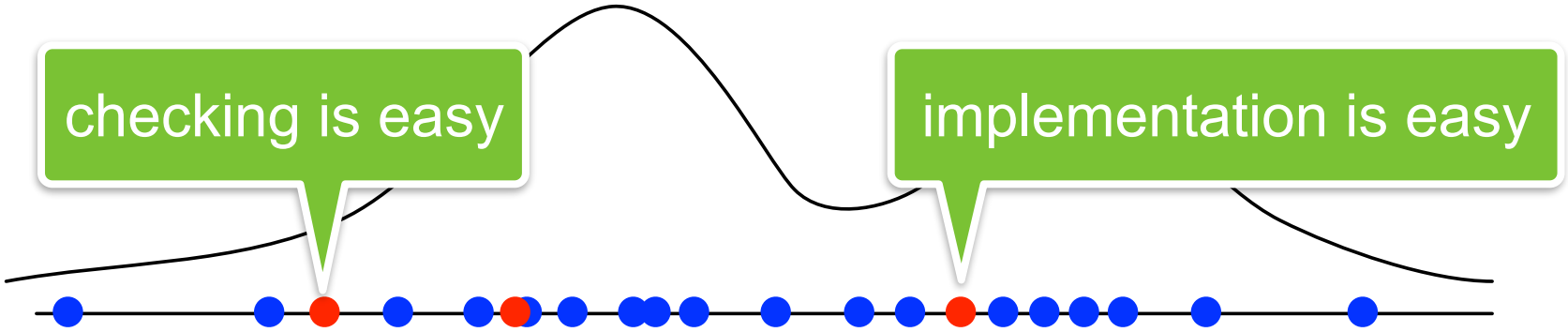

Generative Adversarial Networks Primer

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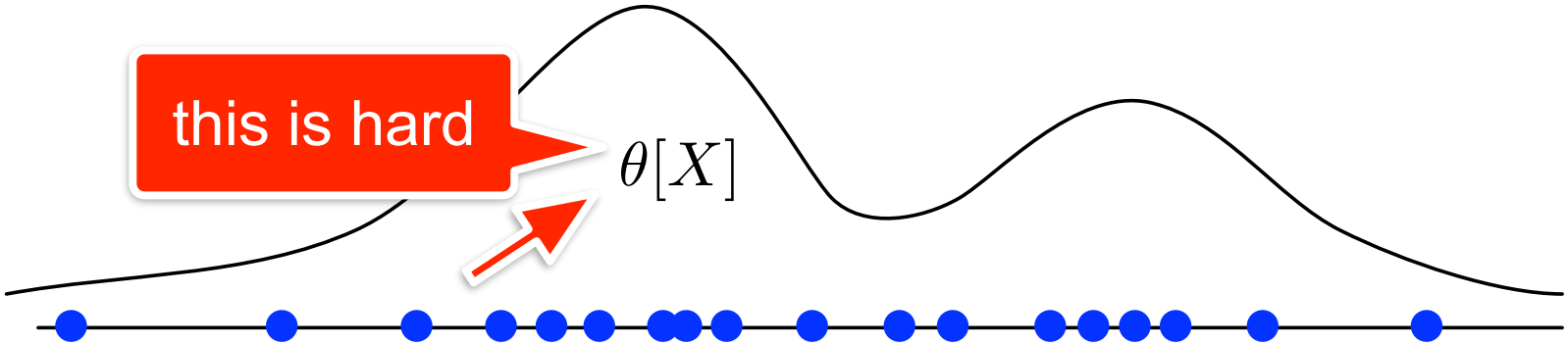
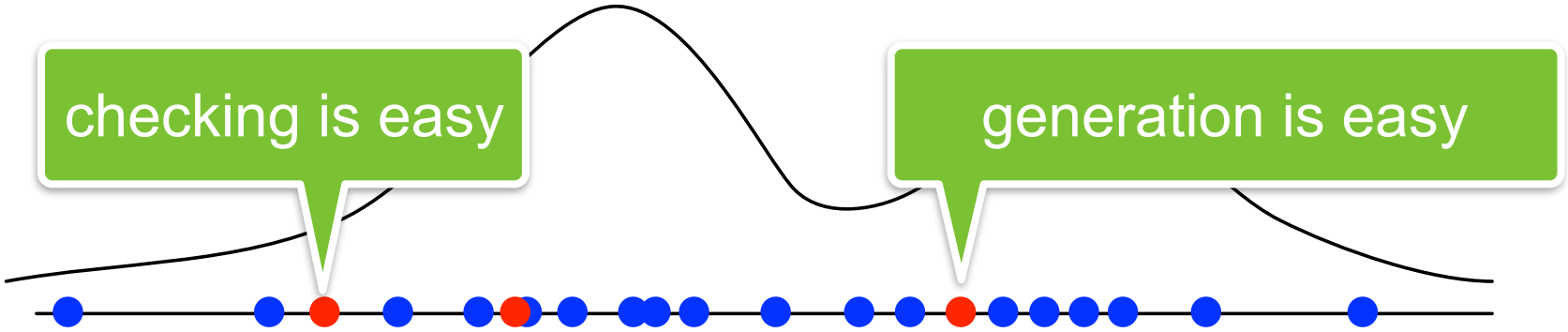


Key Idea - Focus on generating data

- **Generator network** x' = g(z) that produces 'fake' data
  - Start with some random z
  - Transform it via neural network
- **Discriminator network** d(x) distinguishing x from fake x'



Objective Functions

- Discriminator Network uses logistic regression (binary classification between real and fake data)

$$\frac{1}{n}\sum_{i=1}^{n}\log(1+\exp(d(x_i))+\mathbf{E}_{x'\sim q(x')}\left[\log(1+\exp(-d(x'))\right]$$

real data

fake data

- Generative Network tries to fool data (maximize acceptance or minimize rejection)

$$\mathbf{E}_u\left[\log(1+\exp(d(g(z))\right]$$

Multiple Gradients

- ‘Normal’ SGD loop
  - Iterate over data and compute loss
  - Update parameters w.r.t. loss gradient
- GAN loop
  - Iterate over data and sample from generator
    - Compute loss and gradient on real & fake data
    - Update parameters for discriminator
  - Sample from generator
    - Compute loss and gradient on real data
    - Update parameters for generator

Links & Notebooks

http://gluon.mxnet.io/P10-C01-gan-intro.html

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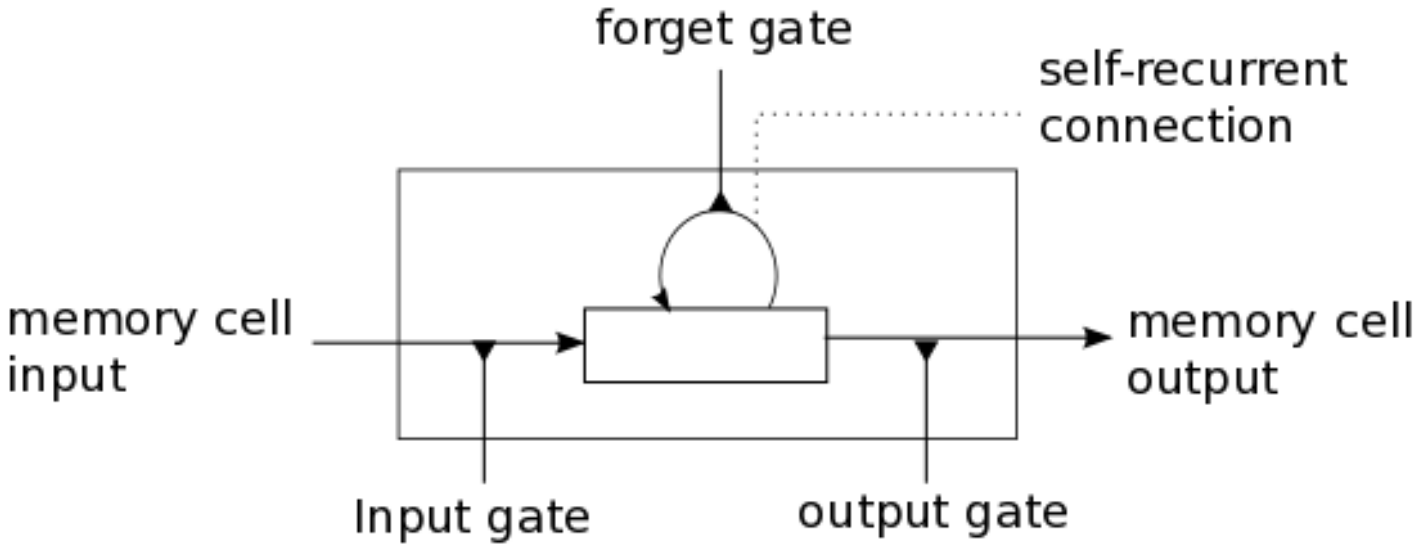
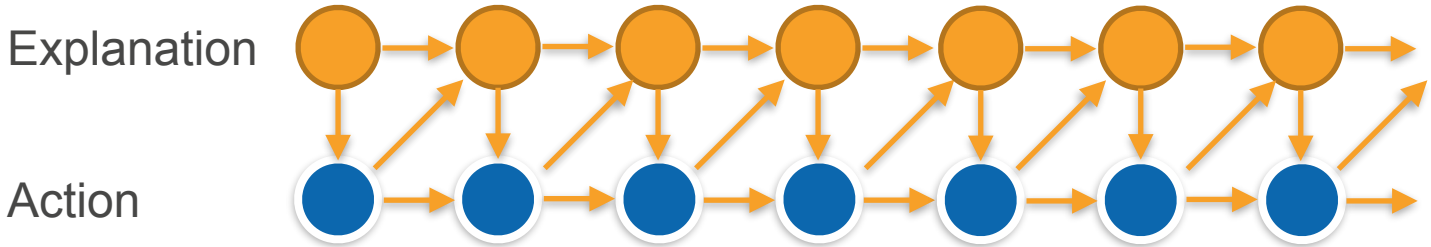
Sequence Models



Hochreiter & Schmidhuber, 1997

Latent Variable Models

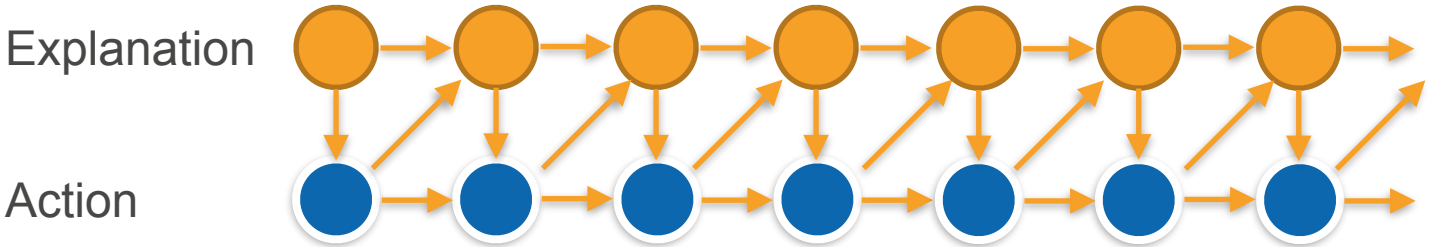
- **Temporal sequence of observations**
  Purchases, likes, app use, e-mails, ad clicks, queries, ratings
- **Latent state to explain behavior**
  - Clusters (navigational, informational queries in search)
  - Topics (interest distributions for users over time)
  - Kalman Filter (trajectory and location modeling)



Latent Variable Models

- **Temporal sequence of observations**
  Purchases, likes, app use, e-mails, ad clicks, queries, ratings
- **Latent state to explain behavior**

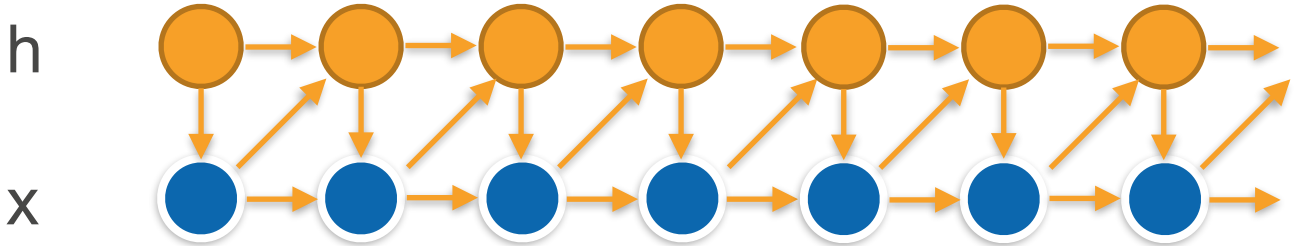
Are the parametric models really true?



Latent Variable Models

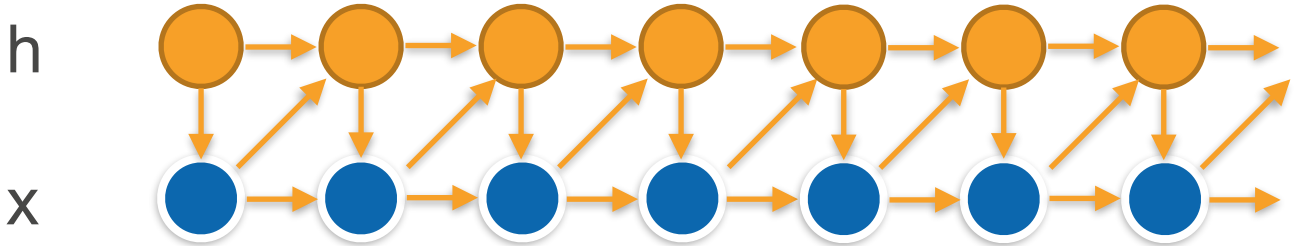
- **Temporal sequence of observations**
  Purchases, likes, app use, e-mails, ad clicks, queries, ratings
- **Latent state to explain behavior**
  - Nonparametric model / spectral
  - Use data to determine shape
  - Sidestep approximate inference

$$h_t = f(x_{t-1}, h_{t-1})$$
$$x_t = g(x_{t-1}, h_t)$$



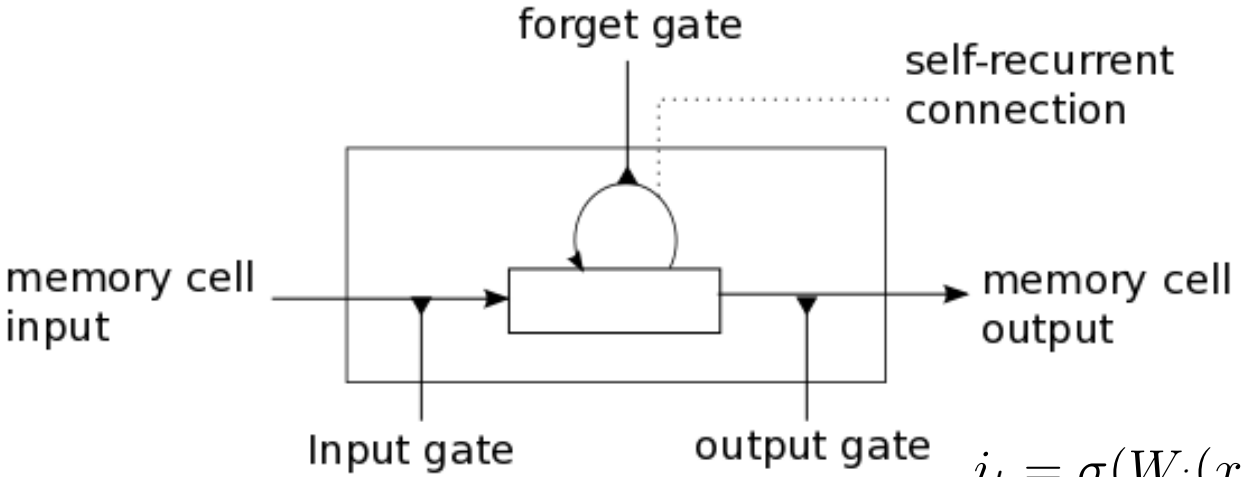
Latent Variable Models

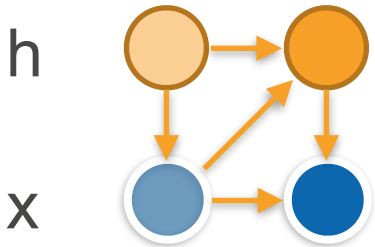
- **Temporal sequence of observations**
  Purchases, likes, app use, e-mails, ad clicks, queries, ratings
- **Latent state to explain behavior**
  - Plain deep network = RNN
  - Deep network with attention = LSTM / GRU …
    (learn when to update state, how to read out)



Long Short Term Memory

Hochreiter & Schmidhuber, 1997

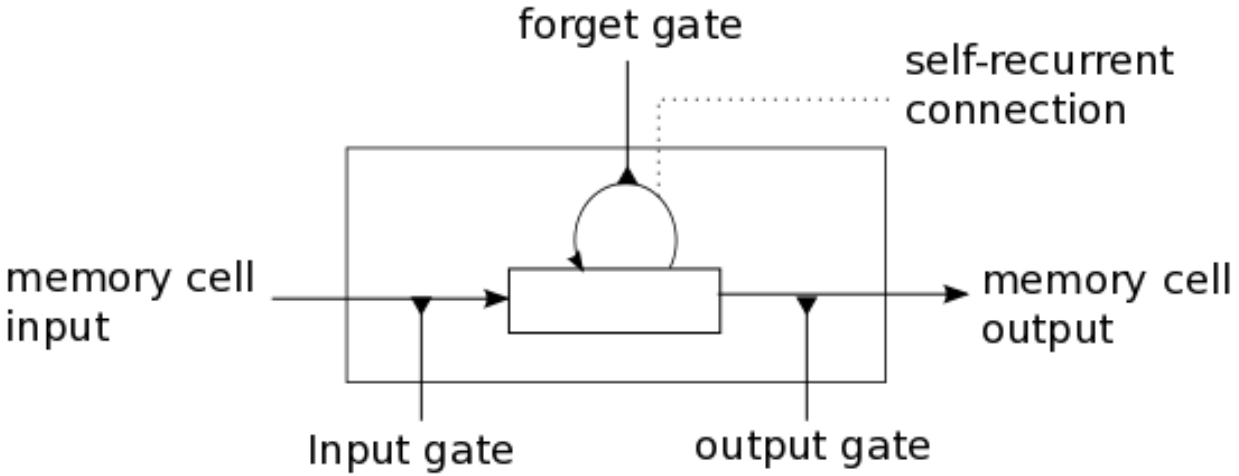


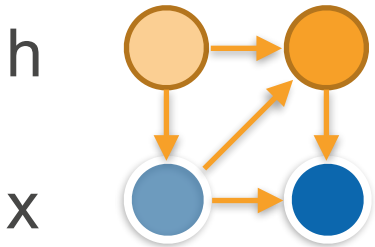


$$
\begin{aligned}
i_t &= \sigma(W_i(x_t, h_t) + b_i) \\
f_t &= \sigma(W_f(x_t, h_t) + b_f) \\
z_{t+1} &= f_t \cdot z_t + i_t \cdot \tanh(W_z(x_t, h_t) + b_z) \\
o_t &= \sigma(W_o(x_t, h_t, z_{t+1}) + b_o) \\
h_{t+1} &= o_t \cdot \tanh z_{t+1}
\end{aligned}
$$

Long Short Term Memory

Hochreiter & Schmidhuber, 1997





$$(z_{t+1}, h_{t+1}, o_t) = \mathrm{LSTM}(z_t, h_t, x_t)$$

```
rnn.LSTM(num_hidden, num_layers, dropout, input_size)
```

The anatomy of an RNN language model

- **Statistical Model**

$$p(x) = \prod_{i=0}^{n-1} p(x_{i+1}|x_i \dots x_1) = \prod_{i=0}^{n-1} p(x_{i+1}|\mathrm{LSTM}(x_i, h_i))$$

- **Truncated Backpropagation Through Time (BPTT)**
  - Sequence is often too long for exact computation
  - Truncate and predict smaller segments (approximation)

$$p(x) = \prod_{j=0}^{\lfloor n/L \rfloor} \prod_{i=0}^{L-1} p(x_{i+1+JL}|\mathrm{LSTM}(x_{i+JL}, h_{i+JL}))$$

The anatomy of an RNN language model

- **Data**
  - `Some sequence to predict the next …`
  - Break into batches
  - Tokenize words (or characters)
  - Truncate for limited Backprop through Time (BPTT)
- **Encoder**
  - Map token i into vector v_i
    (one-hot encoding followed by an MLP)

The anatomy of an RNN language model

- **RNN**
  - Initialize with some state s
  - Recurse through sequence to compute

$$(h_{i+1}, o_{i+1}) = \mathrm{LSTM}(h_i, x_i)$$

- **Decoder**
  - Softmax decoding for output, i.e

$$p(x_i|o_i) = \mathrm{softmax}(\mathrm{MLP}(o_i))$$

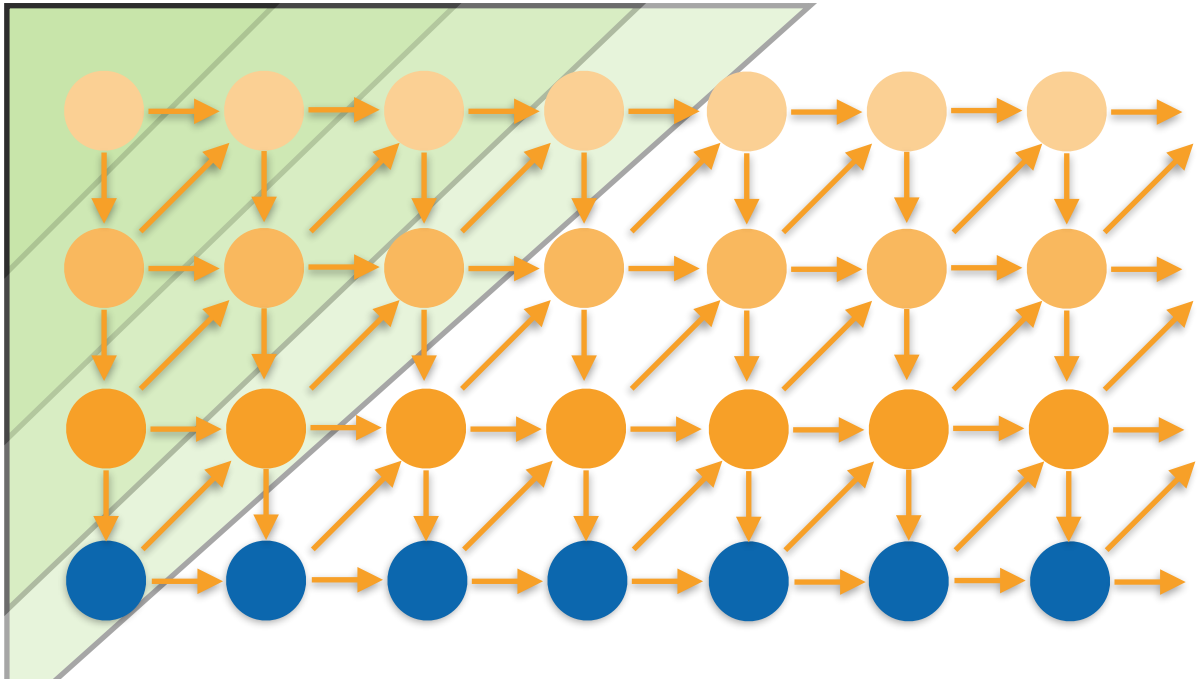
  - Better decoders possible (beam search, WFST …)

Links & Notebooks

gluon.mxnet.io/P05-C01-simple-rnn.html
gluon.mxnet.io/P05-C03-lstm-scratch.html
gluon.mxnet.io/P05-C04-rnns-gluon.html

Fusion for RNNs

- GPUs too fast to call a matrix-vector product every time
- Fuse CUDA kernels (automatic if you use Gluon RNNs)



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Tree LSTMs

- **LSTM**
  sequential dependence between states

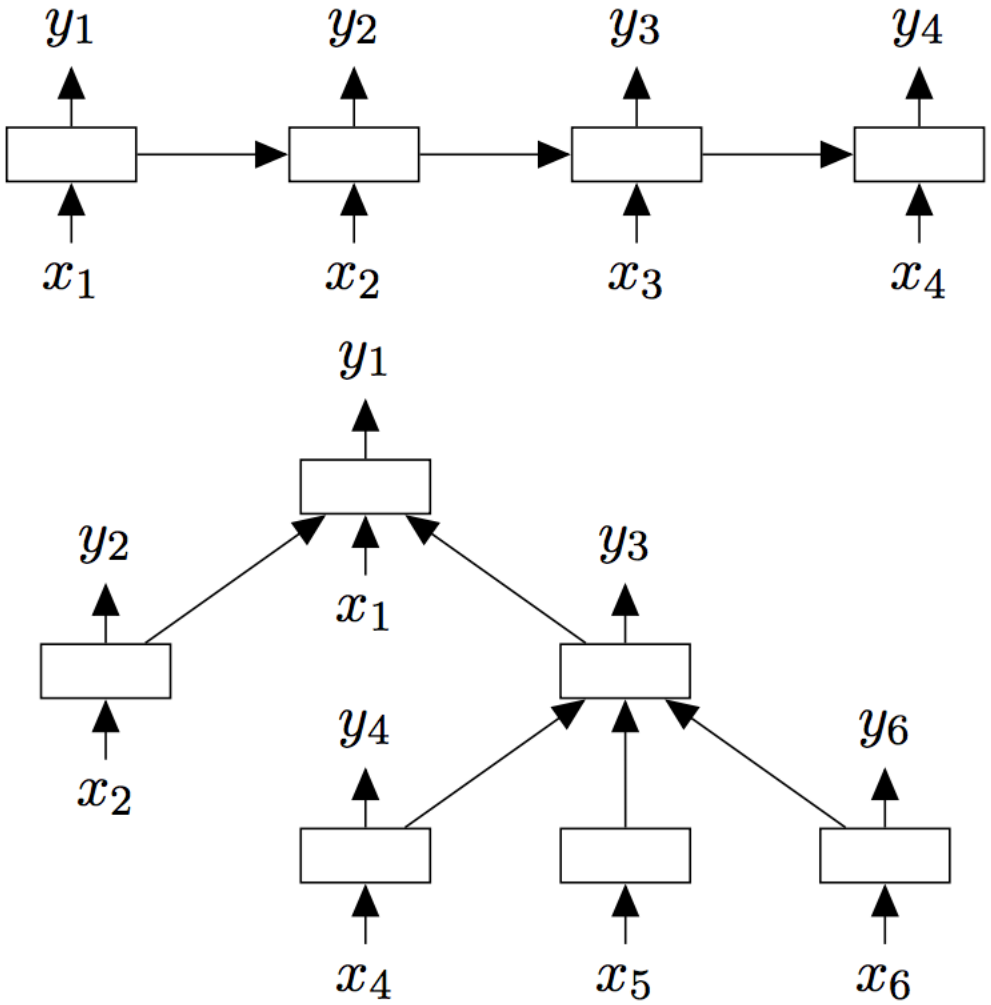
$$o_t = f(x_t, h_{t-1})$$

$$(c_t, h_t) = g(x_t, h_{t-1}, c_{t-1})$$

- **Tree LSTM**
  hierarchical dependence

$$o_t = f(x_t, H_{t-1})$$

$$(c_t, h_t) = g(x_t, H_{t-1}, C_{t-1})$$



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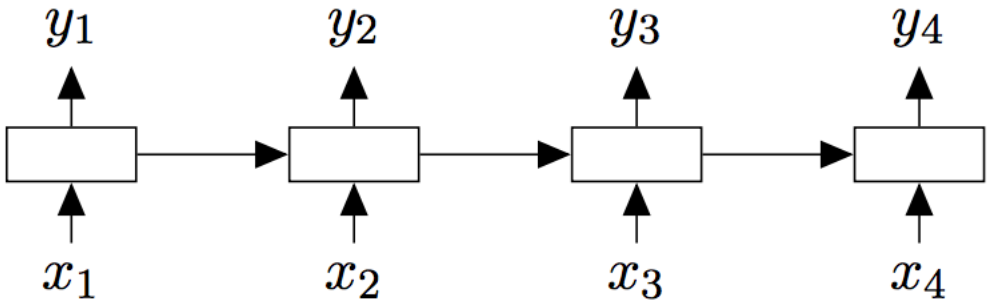
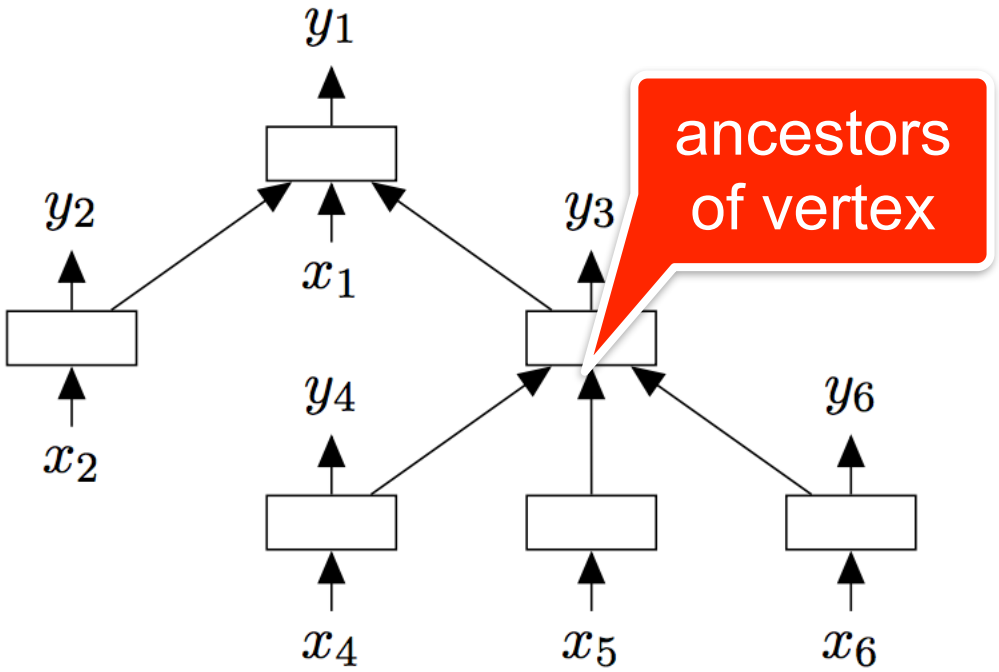


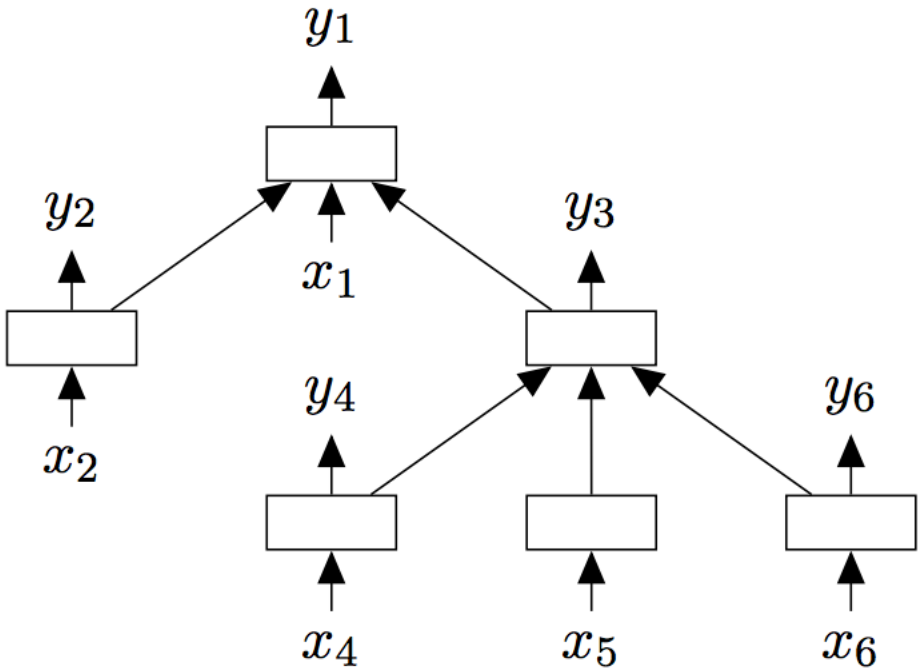


Tree LSTMs (Tsai et al, 2015)

- **Applications**
  - dependency parsing
  - sentiment
  - document similarity
- **Problems**
  - **Variable inputs H and C**
  - Specialization (left, right)
  - **Model has variable dependency structure**

$$o_t = f(x_t, H_{t-1})$$

$$(c_t, h_t) = g(x_t, H_{t-1}, C_{t-1})$$



LSTM

$$
\begin{aligned}
z &= Wx_t + Uh_{t-1} + b \\
[i_t, f_t, o_t, u_t] &= [\sigma(z_i), \sigma(z_f), \sigma(z_o), \tanh(z_u)] \\
c_t &= i_t \circ u_t + f_t \circ c_{t-1} \\
h_t &= o_t \circ \tanh(c_t)
\end{aligned}
$$

Tree LSTM

$$
\begin{aligned}
\tilde{h} &= \sum_{j \in C(t)} h_j \\
z &= Wx_t + U\tilde{h} + b \\
f_{tj} &= \sigma\left(W_f x_t + U_f h_j + b_f\right) \\
[i_t, o_t, u_t] &= [\sigma(z_i), \sigma(z_o), \tanh(z_u)] \\
c_t &= i_t \circ u_t + \sum_{j \in C(t)} f_{tj} \circ c_j \\
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\end{aligned}
$$

Tree LSTM

$$
\tilde{h} = \sum_{j \in C(t)} h_j
$$

aggregate hidden state

$$
\begin{aligned}
z &= W x_t + U \tilde{h} + b \\
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\end{aligned}
$$

Tree LSTM

$$\tilde{h} = \sum_{j \in C(t)} h_j$$

aggregate hidden state

individual forget weights

$$
\begin{aligned}
z &= W x_t + U \tilde{h} + b \\
f_{tj} &= \sigma\left(W_f x_t + U_f h_j + b_f\right) \\
[i_t, o_t, u_t] &= [\sigma(z_i), \sigma(z_o), \tanh(z_u)] \\
c_t &= i_t \circ u_t + \sum_{j \in C(t)} f_{tj} \circ c_j \\
h_t &= o_t \circ \tanh(c_t)
\end{aligned}
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LSTM

$$
\begin{aligned}
z &= W x_t + U h_{t-1} + b \\
[i_t, f_t, o_t, u_t] &= [\sigma(z_i), \sigma(z_f), \sigma(z_o), \tanh(z_u)] \\
c_t &= i_t \circ u_t + f_t \circ c_{t-1} \\
h_t &= o_t \circ \tanh(c_t)
\end{aligned}
$$

Tree LSTM (individual weights)

$$
\begin{aligned}
z &= W x_t + U \left[h_j, \ldots h_{j'}\right] + b \\
\left[i_t, o_t, \left[f_{tj} \ldots f_{tj'}\right], u_t\right] &= \left[\sigma(z_i), \sigma(z_o), \left[\sigma(z_{fj}) \ldots \sigma(z_{fj'})\right], \tanh(z_u)\right] \\
c_t &= i_t \circ u_t + \sum_{j \in C(t)} f_{tj} \circ c_{tj} \\
h_t &= o_t \circ \tanh(c_t)
\end{aligned}
$$

LSTM

$$z = Wx_t + Uh_{t-1} + b$$

$$[i_t, f_t, o_t, u_t] = [\sigma(z_i), \sigma(z_f), \sigma(z_o), \tanh(z_u)]$$

$$c_t = i_t \circ u_t + f_t \circ c_{t-1}$$

$$h_t = o_t \circ \tanh(c_t)$$

Tree LSTM (individual weights)

$$z = Wx_t + U\left[h_j, \ldots h_{j'}\right] + b$$

$$\left[i_t, o_t, \left[f_{tj} \ldots f_{tj'}\right], u_t\right] = \left[\sigma(z_i), \sigma(z_o), \left[\sigma(z_{fj}) \ldots \sigma(z_{fj'})\right], \tanh(z_u)\right]$$

$$c_t = i_t \circ u_t + \sum_{j \in C(t)} f_{tj} \circ c_{tj}$$

$$h_t = o_t \circ \tanh(c_t)$$

individual forget weight

LSTM

$$z = W x_t + U h_{t-1} + b$$

$$[i_t, f_t, o_t, u_t] = [\sigma(z_i), \sigma(z_f), \sigma(z_o), \tanh(z_u)]$$

$$c_t = i_t \circ u_t + f_t \circ c_{t-1}$$

$$h_t = o_t \circ \tanh(c_t)$$

Tree LSTM (individual weights)

individual weight

$$z = W x_t + U \left[h_j, \ldots h_{j'}\right] + b$$

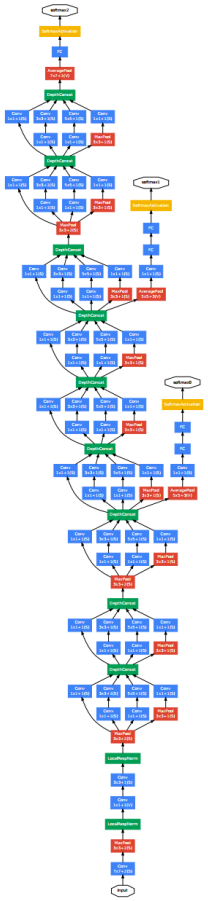
$$\left[i_t, o_t, \left[f_{tj} \ldots f_{tj'}\right], u_t\right] = \left[\sigma(z_i), \sigma(z_o), \left[\sigma(z_{fj}) \ldots \sigma(z_{fj'})\right], \tanh(z_u)\right]$$

$$c_t = i_t \circ u_t + \sum_{j \in C(t)} f_{tj} \circ c_{tj}$$

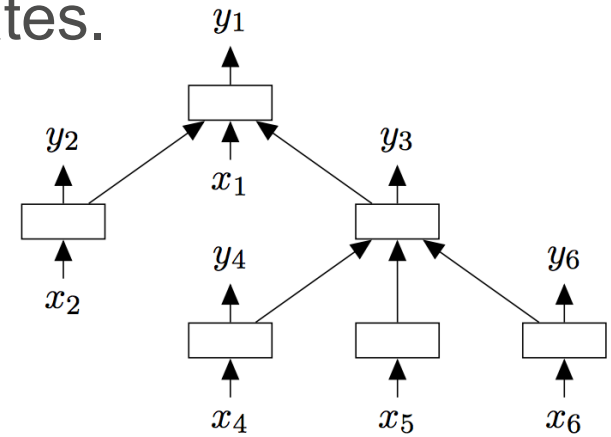
individual forget weight

$$h_t = o_t \circ \tanh(c_t)$$

Static and Dynamic Graphs



- **Static Graph**
  Predefined concatenation of layers. Easy to do with a symbolic framework.
- **Dynamic Graph**
  Implicitly defined via code in **imperative** framework. Automatic differentiation for updates.
  - Compute solution
  - Update parameters



Links & Notebooks

gluon.mxnet.io/P07-C08-tree-lstm.html
gluon.mxnet.io/P14-C05-hybridize.html

Hybridization - (JIT for Deep Networks)

- **Forward Definition**

```
def hybrid_forward(self, F, x):
        print('type(x): {}, F: {}'.format(type(x).__name__, F.__name__))
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        return self.fc3(x)
```

- **Without Hybridization**
  Executes the full program (including print)
- **With Hybridization**
  Executes only the compute graph that was **implicitly** defined. JIT for compute graphs (no need to parse repeatedly), as efficient as symbolic definition.

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8. **Distributed Optimization**
9. Parallel Training

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9. (key, value) store

Optimization Basics

- **Optimization Problem**

$$\underset{w}{\text{minimize}} \frac{1}{m} \sum_{i=1}^{m} l(y_i, f(x_i, w)) + \lambda \|w\|_2^2$$

- **Stochastic Gradient Approximation**
  - **Gradient on Minibatch**

$$g_B := \frac{1}{b} \sum_{i \in B} \partial_w l(y_i, f(x_i, w)) \text{ and } w \leftarrow \text{Optimizer}(w, g_B)$$

  - **Update w with advanced first order solver**
    (Adam, AdaGrad, Momentum, Eve, SGD, SGLD …)

Optimization Basics

- SGD
- DCASGD
- NAG
- Adam
- SGLD
- AdaGrad
- RMSProp
- AdaDelta
- Ftrl
- Adamax
- Nadam

- **Stochastic Gradient Descent (SGD)**

$$w \leftarrow (1 - 2\eta\lambda)w - \eta g_b$$

- **SGD with Momentum and Clipping**

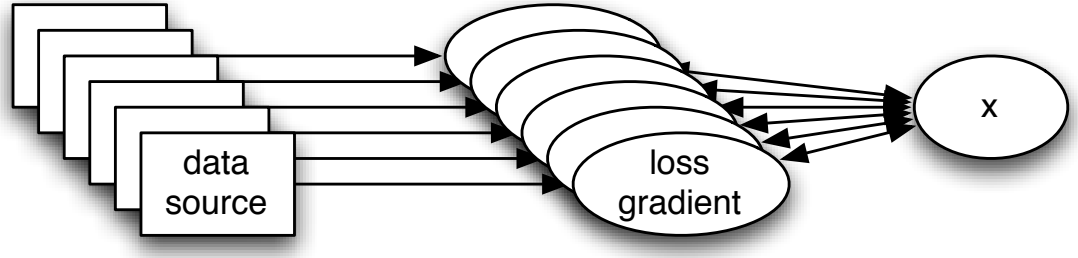
$$s \leftarrow \mu s + \eta \operatorname{clip}(g_b) + \eta\lambda w$$
$$w \leftarrow w - s$$

Quite often learning rate is piecewise constant (this yields better accuracy in practice, albeit convergence is slower)

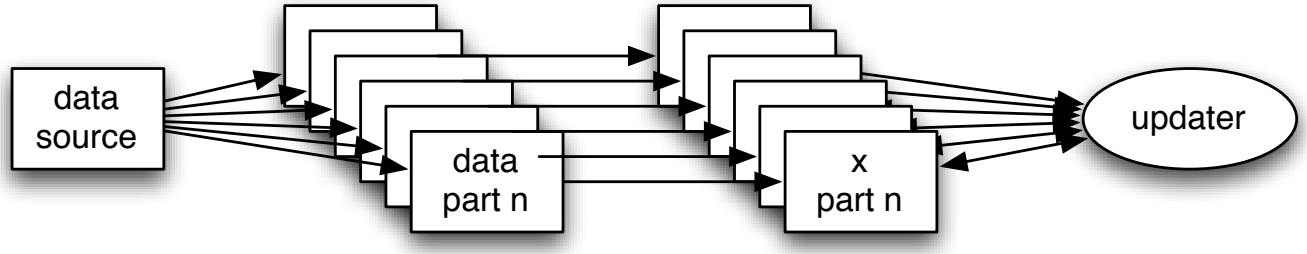
- **Improved conditioning, momentum, precision …**

Parallelization

- **Data Parallel (easier & more efficient)**
  Distribute data over multiple GPUs / CPUs / machines

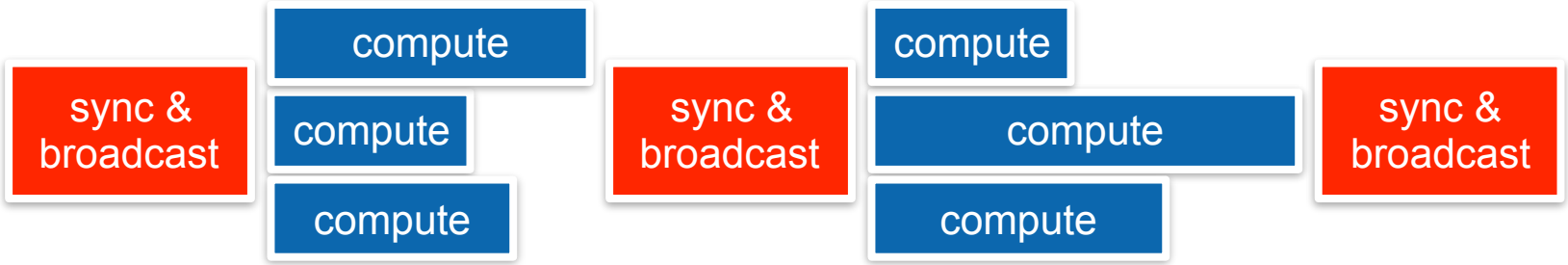


- **Model Parallel (only for huge models)**
  Distribute parts of the computation over multiple GPUs / CPUs

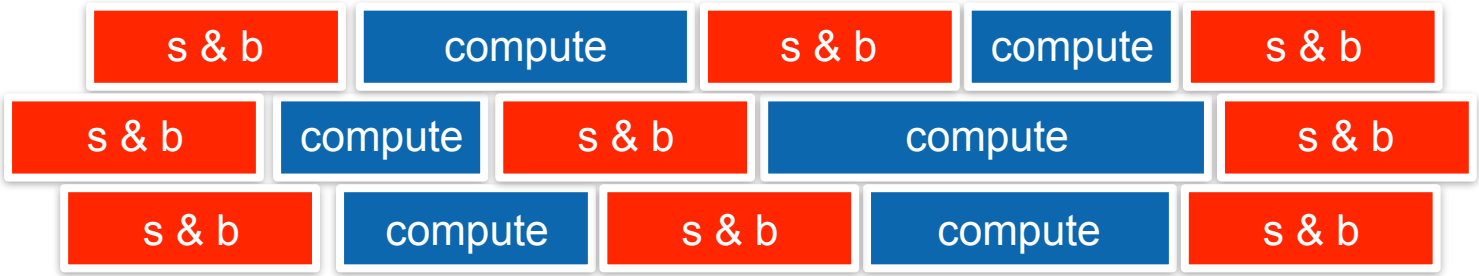


Parallelization

- Synchronous - easy for homogeneous jobs



- Asynchronous - efficient for high time dispersion



Parallelization - Pragmatic Strategy

- **Data Parallel & Synchronous**
  - Even for 512 GPUs you only need 32 P2.16xlarge (so the speed dispersion is negligible).
  - GPUs have plenty of RAM (only an inefficient framework needs model parallel)
- **Algorithm Template** (shard data over machines)
  - Compute gradient on mini batch on each GPU
  - Aggregate gradients into (key,value) store
  - Broadcast them back to GPUs

Links & Notebooks

gluon.mxnet.io/P14-C02-multiple-gpus-scratch.html
gluon.mxnet.io/P14-C03-multiple-gpus-gluon.html

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Amazon Machine Image for Deep Learning

bit.ly/deepami bit.ly/deepubuntu

- Tool for data scientists and developers
- Setting up a DL system takes (install) time & skill
  - Keep packages up to date and compiled (MXNet, TensorFlow, Caffe, Torch, Theano, Keras)
  - Anaconda, Jupyter, Python 2 and 3
  - **NVIDIA** Drivers for G2 and P2 instances
  - **Intel MKL** Drivers for all other instances (C4, M4, …)

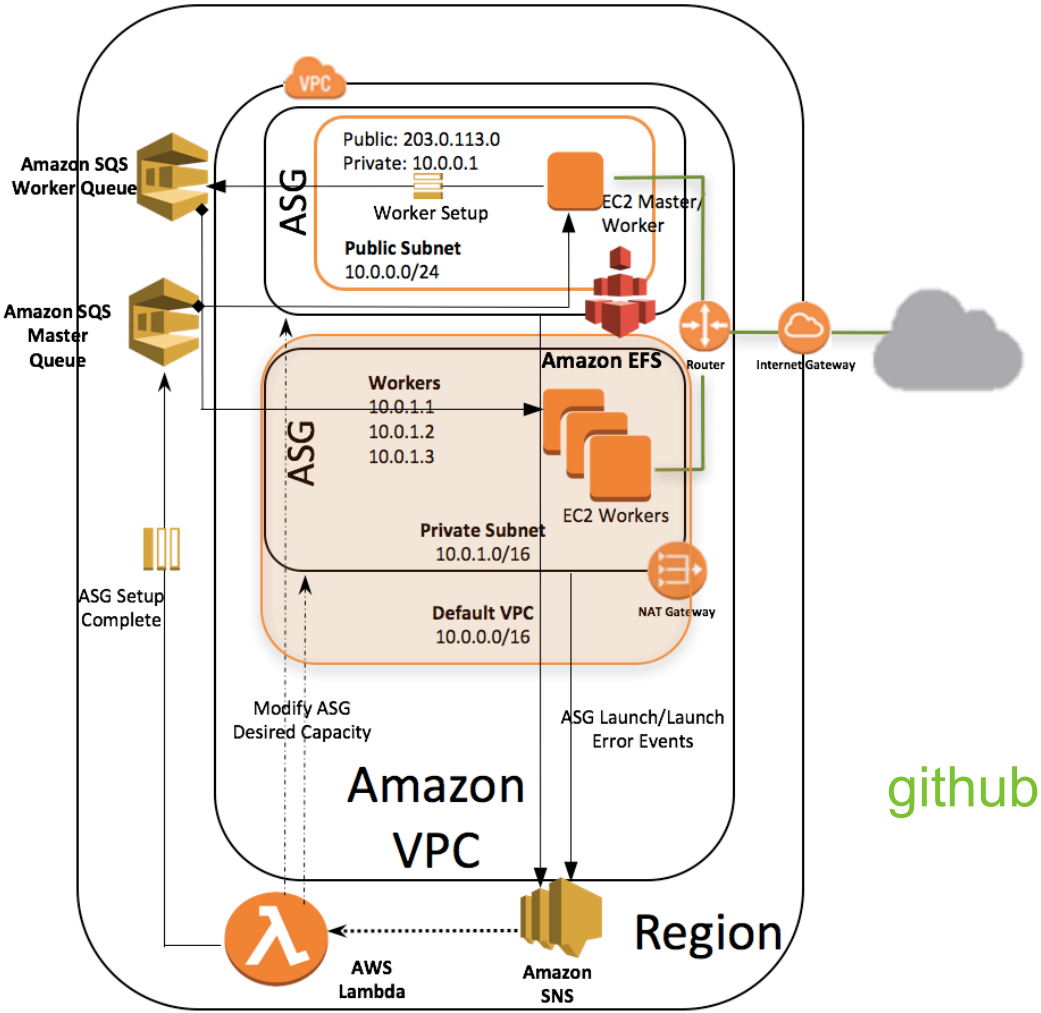
Getting started

```
acbc32cf4de3:image-classification smola$ ssh ec2-user@54.210.246.140
Last login: Fri Nov 11 05:58:58 2016 from 72-21-196-69.amazon.com
================================================================================
       __|  __|_  )
       _|  (     /   Deep Learning AMI for Amazon Linux
      ___|\___|___|

This is beta version of the Deep Learning AMI for Amazon Linux.

The README file for the AMI →→→→→→→→→→→→→→→→→→→  /home/ec2-user/src/README.md
Tests for deep learning frameworks →→→→→→→→→→→→   /home/ec2-user/src/bin
================================================================================

7 package(s) needed for security, out of 75 available
Run "sudo yum update" to apply all updates.
Amazon Linux version 2016.09 is available.
[ec2-user@ip-172-31-55-21 ~]$ cd src/
[ec2-user@ip-172-31-55-21 src]$ ls
anaconda2  bazel  caffe   cntk   keras  mxnet                 OpenBLAS  README.md   Theano
anaconda3  bin    caffe3  demos  logs   Nvidia_Cloud_EULA.pdf  opencv    tensorflow  torch
```



AWS CloudFormation Template for Deep Learning

github.com/awslabs/deeplearning-cfn

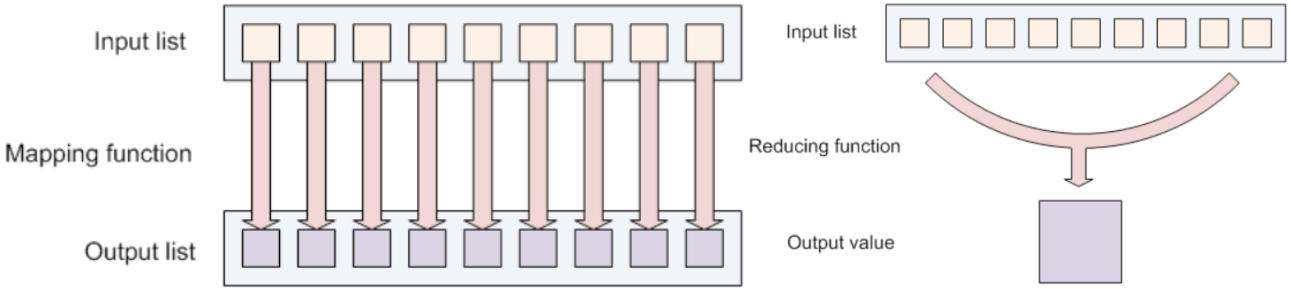
amazon web services

AWS CloudFormation Components

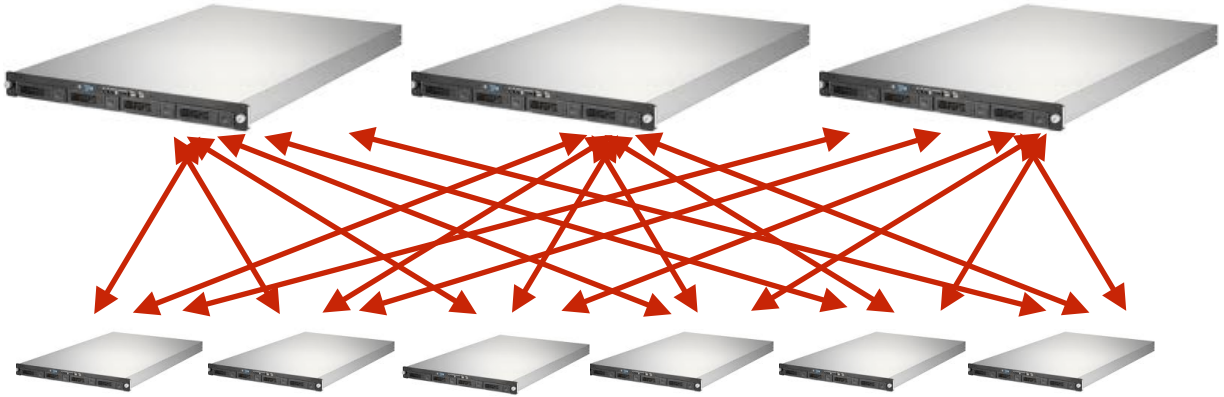
- **VPC** in the customer account.
- The requested number of **worker instances** in an Auto Scaling group within the VPC. Workers are launched in a **private subnet**.
- **Master instance** in a separate Auto Scaling group that acts as a proxy to enable connectivity to the cluster via **SSH**.
- Two security groups that open ports on the **private subnet** for communication between the master and workers.
- **IAM role** that allows users to access and query Auto Scaling groups and the private IP addresses of the EC2 instances.
- **NAT gateway** used by instances within the VPC to talk to the outside.

Why (not) MapReduce?

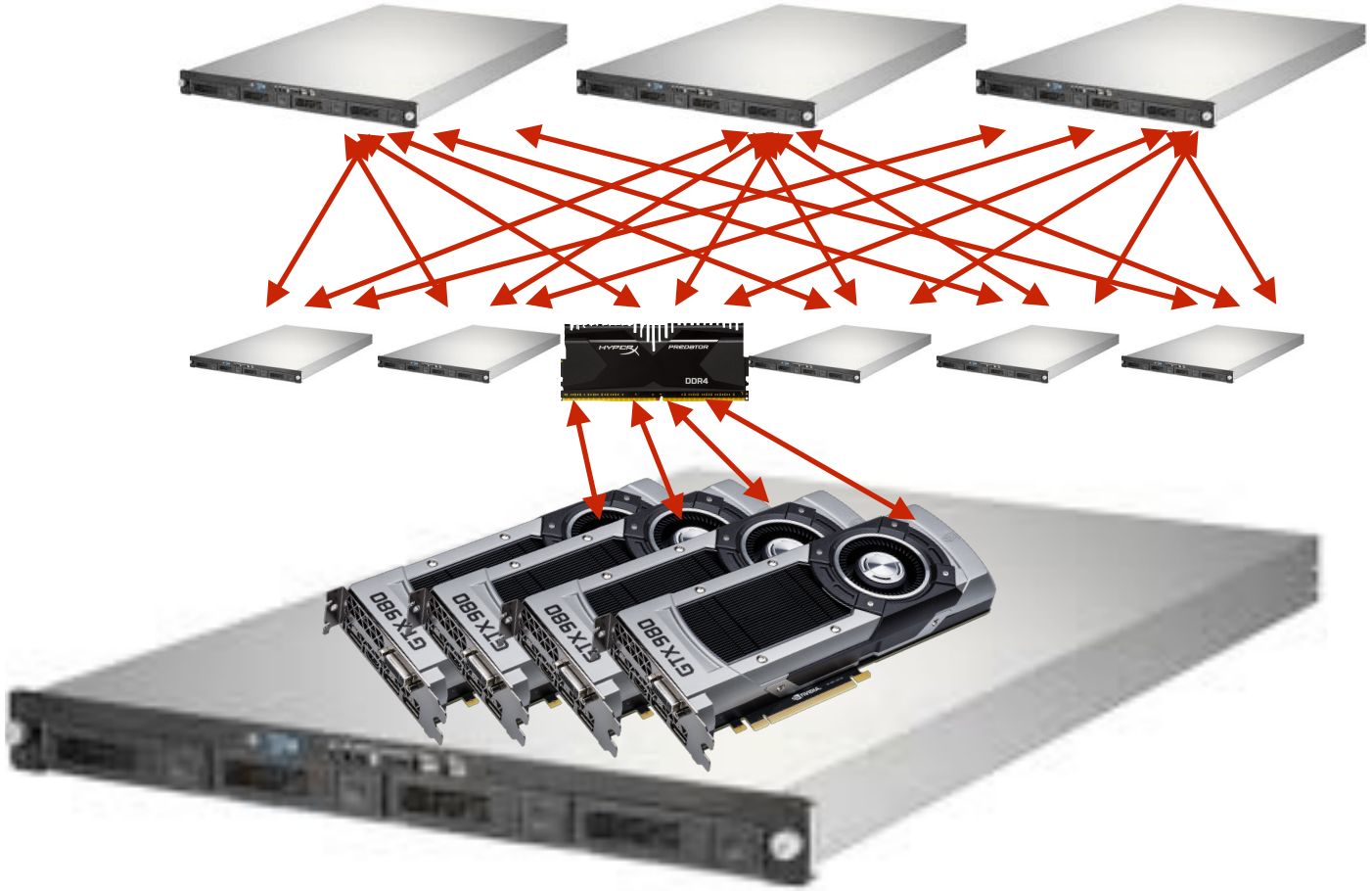
- **Map(key, value)**
  Process subset of the data (and emit gradients)
- **Reduce(key, value)**
  Aggregate gradients from machines and update parameters
- **Simple parameter exchange**
  - **Great if only small number of syncs needed (slow mixing)**
  - **Huge overhead per iteration**
  - **Fully synchronous (bad for large number of machines)**



Parameter Server aka (key,value) store

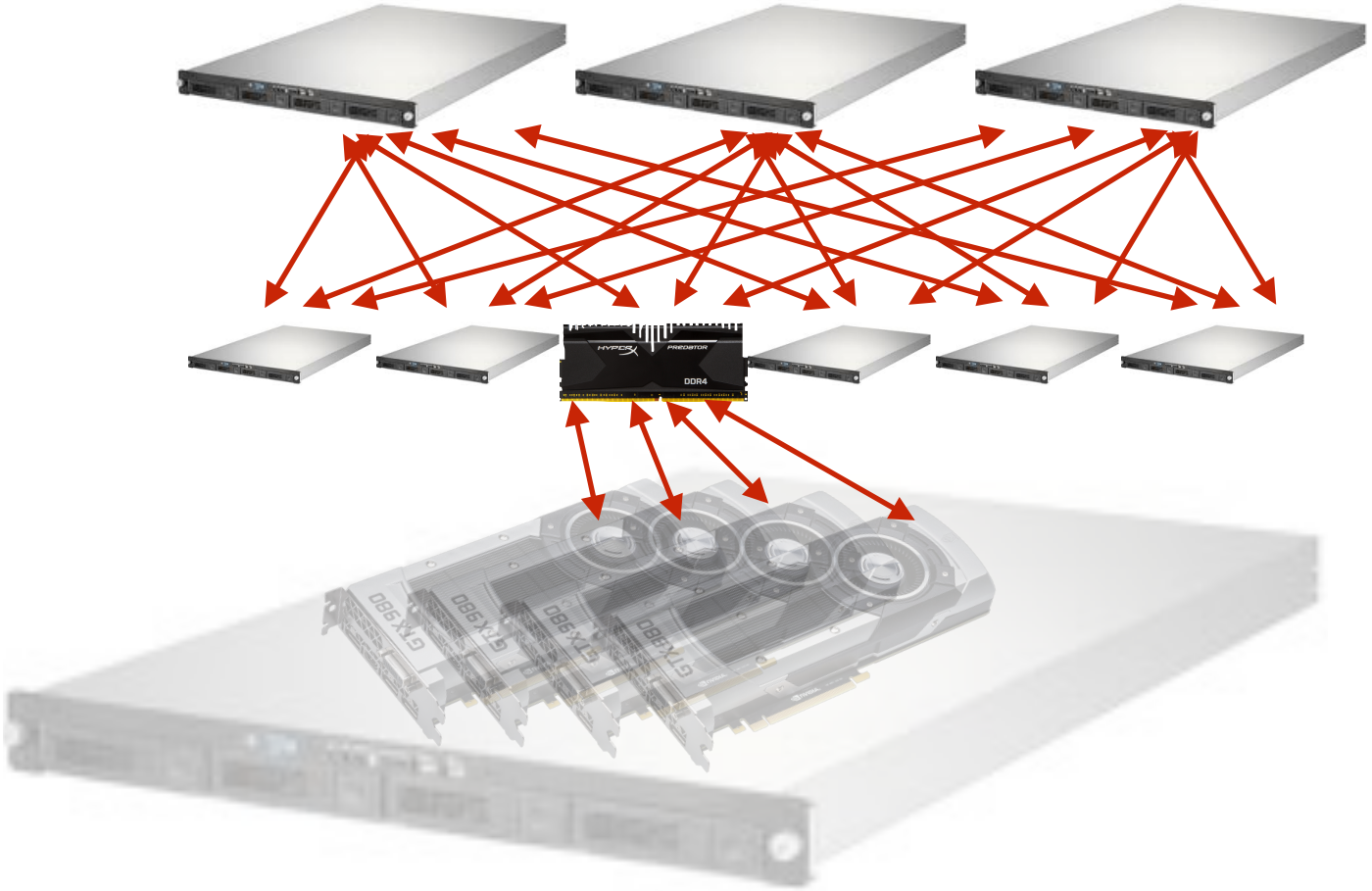


Parameter Server aka (key, value) store



amazon web services

Parameter Server aka (key, value) store



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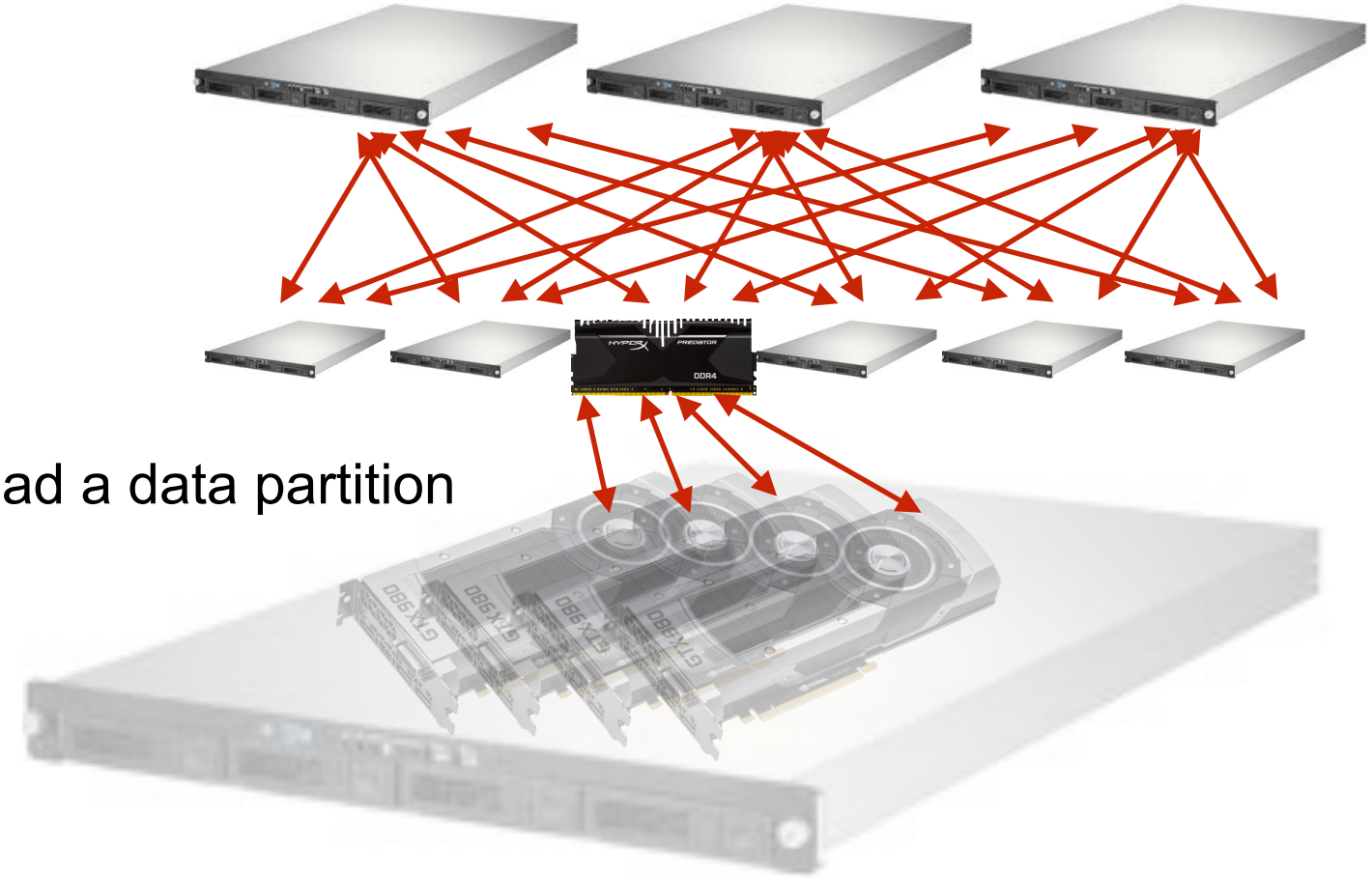
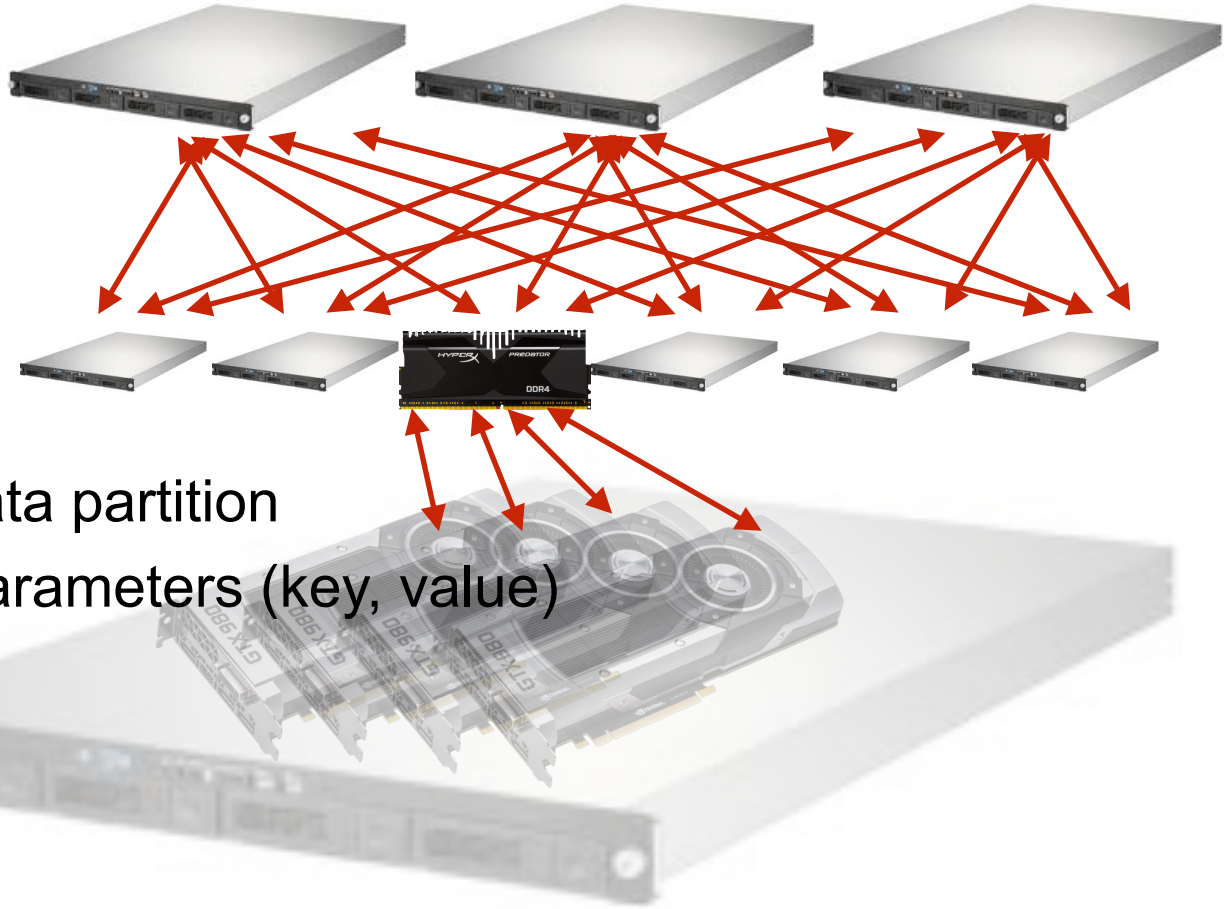
Parameter Server aka (key, value) store



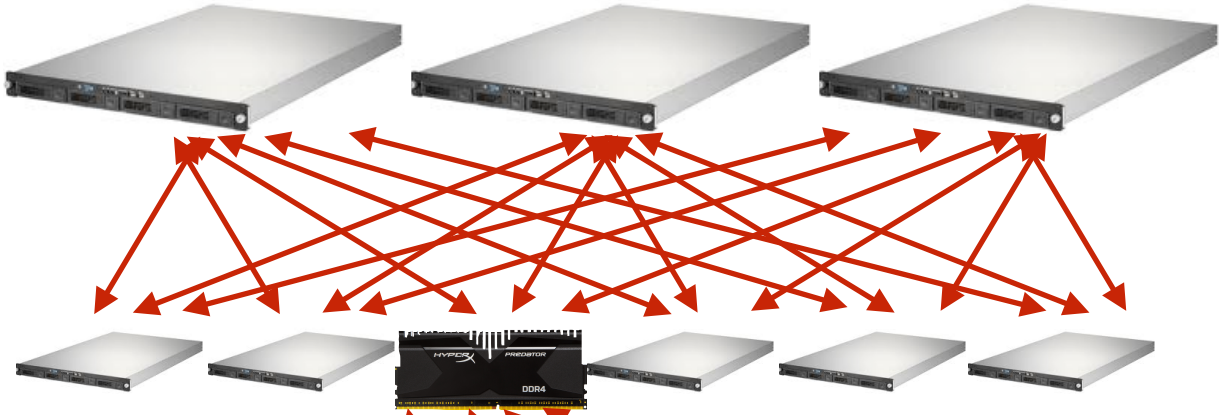
1. Read a data partition

Parameter Server aka (key, value) store



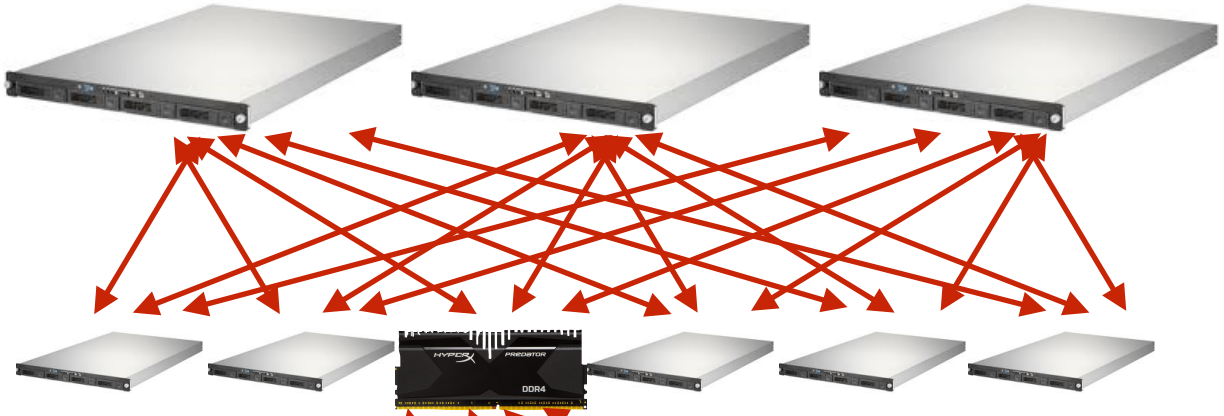
1. Read a data partition
2. Pull the parameters (key, value)

Parameter Server aka (key, value) store



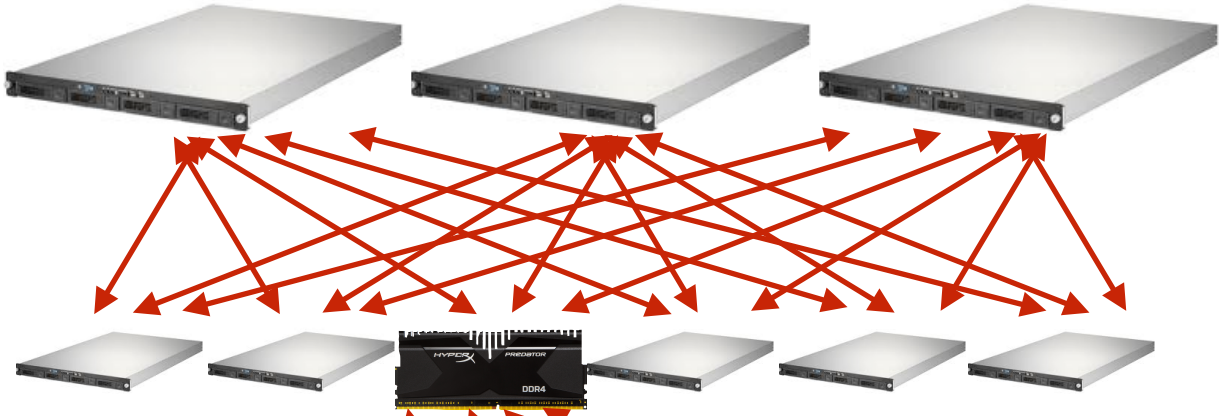
1. Read a data partition
2. Pull the parameters (key, value)
3. Compute the gradient

Parameter Server aka (key, value) store



1. Read a data partition
2. Pull the parameters (key, value)
3. Compute the gradient
4. Push the gradient (key, value)

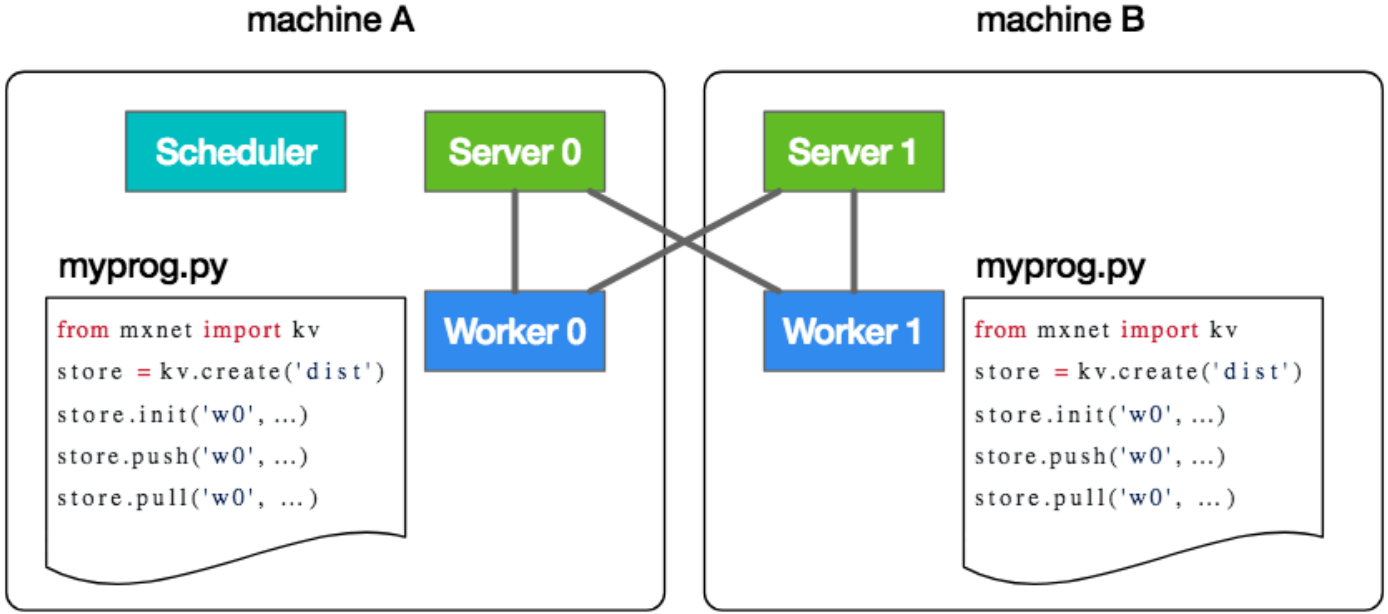
Parameter Server aka (key, value) store



1. Read a data partition
2. Pull the parameters (key, value)
3. Compute the gradient
4. Push the gradient (key, value)
5. Update the parameters (on server)

Multiple Machines (in practice)

- Each machine has server and worker job
- One machine has scheduler for task distribution



Links & Notebooks

gluon.mxnet.io/P14-C04-training-with-multi-machines.html
mxnet.io/api/python/kvstore.html

Notebooks github.com/zackchase/mxnet-the-straight-dope

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