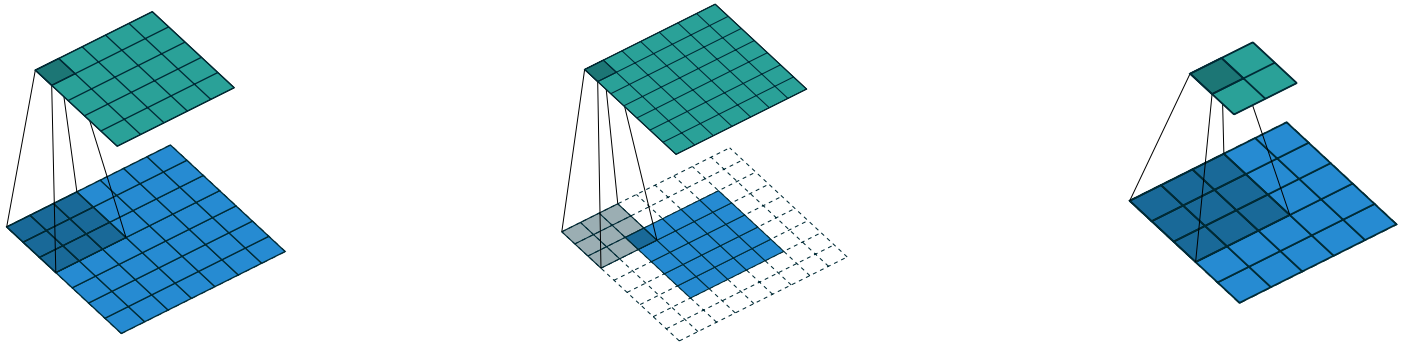
MIT 9.520/6.860, Fall 2018

Class 11: Neural networks – tips, tricks & software

Andrzej Banburski

Last time - Convolutional neural networks

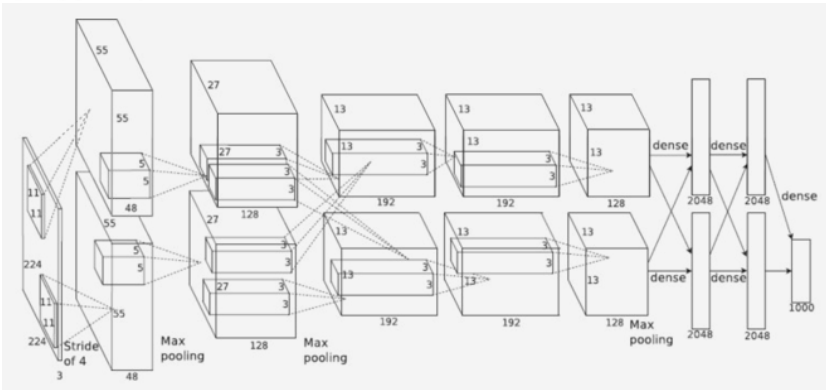


source: github.com/vdumoulin/conv_arithmetic

Large-scale Datasets

General Purpose GPUs

AlexNet
Krizhevsky
et al (2012)



Overview

Initialization & hyper-parameter tuning

Optimization algorithms

Batchnorm & Dropout

Finite dataset woes

Software

Initialization & hyper-parameter tuning

Consider the problem of training a neural network $f_\theta(x)$ by minimizing a loss

$$L(\theta, x) = \sum_{i=1}^{N} l_i(y_i, f_\theta(x_i)) + \lambda|\theta|^2$$

with SGD and mini-batch size b:

$$\theta_{t+1} = \theta_t - \eta \frac{1}{b} \sum_{i \in \mathcal{B}} \nabla_\theta L(\theta_t, x_i) \tag{1}$$

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- Super slow update of earlier layers 10^{-2L} for sigmoid or tanh activations – vanishing gradients. ReLU activations do not suffer so much from this.

Xavier & He initializations

- For tanh and sigmoid activations, near origin we deal with a nearly linear function $y = Wx$, with $x = (x_1, \ldots, x_{n_{in}})$. To stop vanishing and exploding gradients we need

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- Heuristically, ReLU is half of the linear function, so we can take

$$\text{Var}(w_i) = \frac{4}{n_{in} + n_{out}} \tag{3}$$

An analysis in [He et al., 2015] confirms this.

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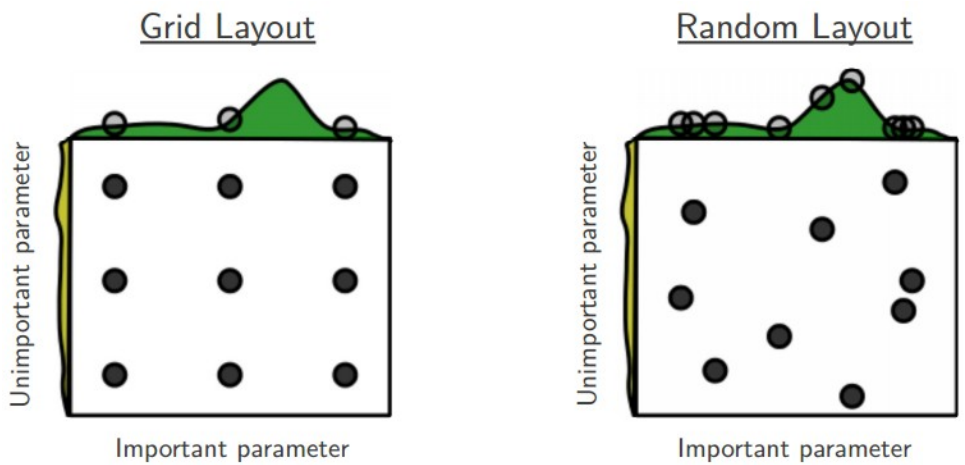

source: [Bergstra and Bengio, 2012]

Decaying learning rate

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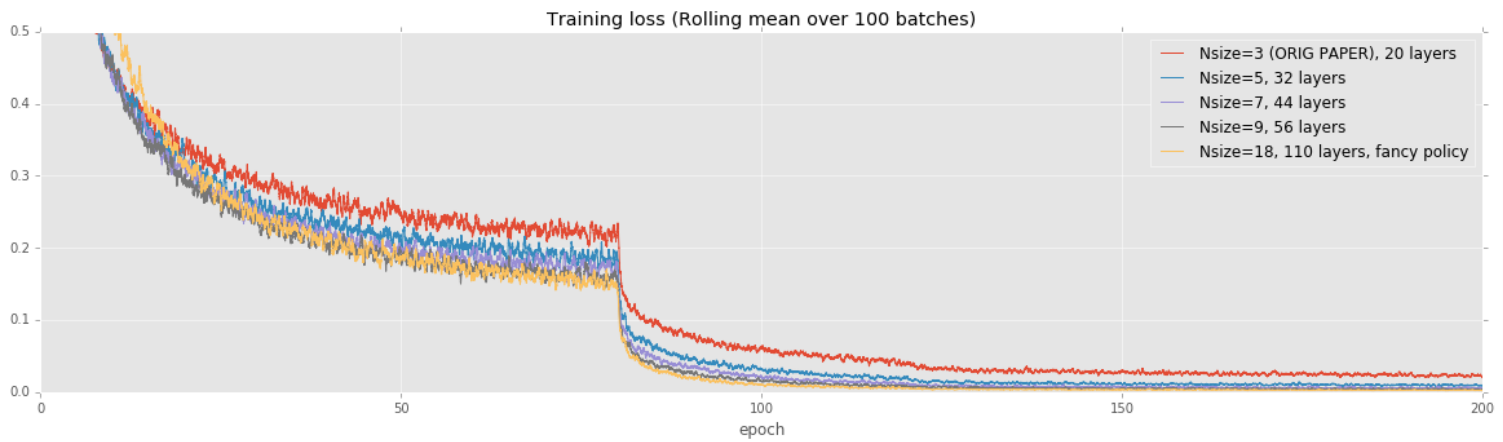
- This allows the training loss to keep improving after it has plateaued



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- As b approaches N the dynamics become more and more deterministic and we would expect this relationship to vanish.

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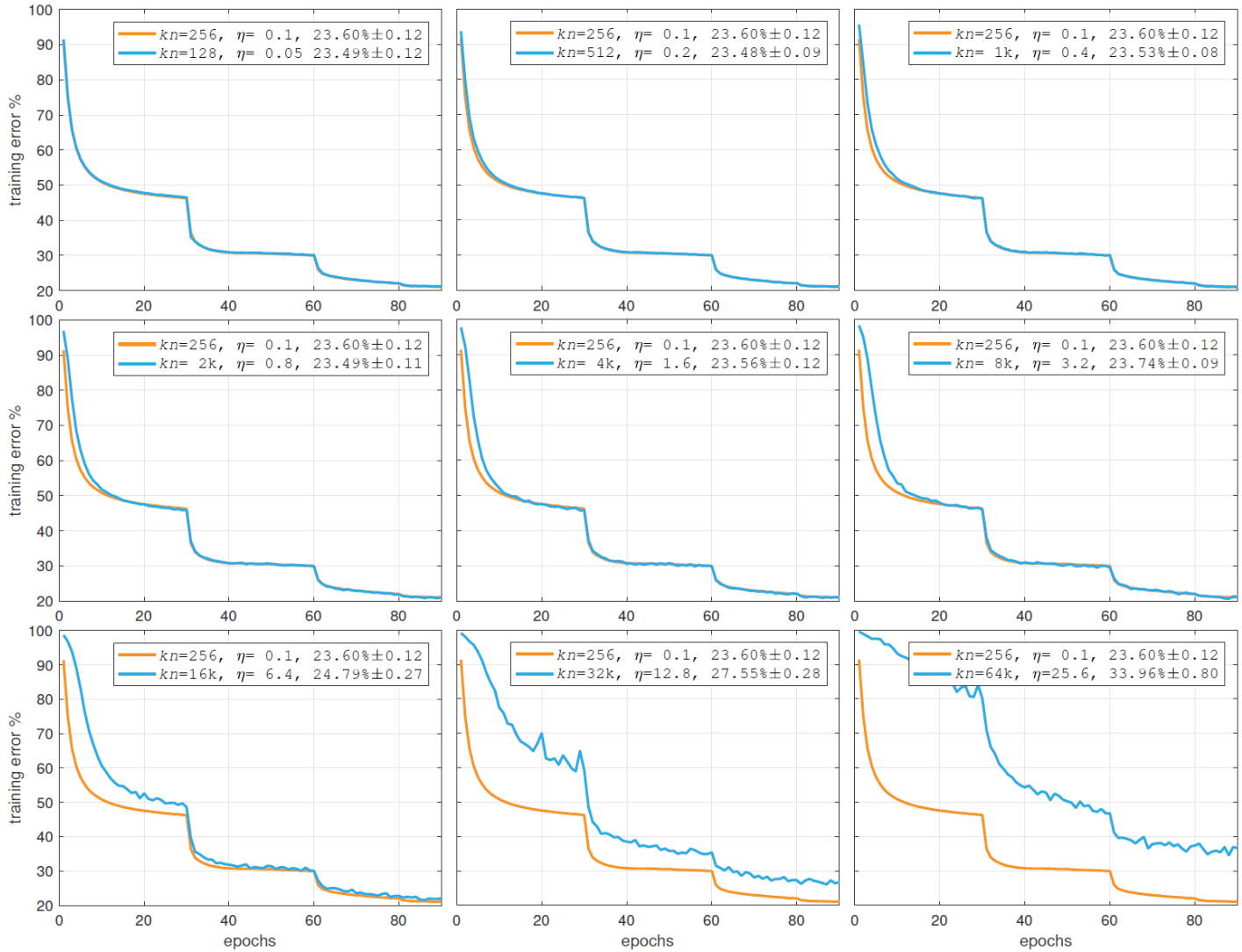

source: [Goyal et al., 2017]

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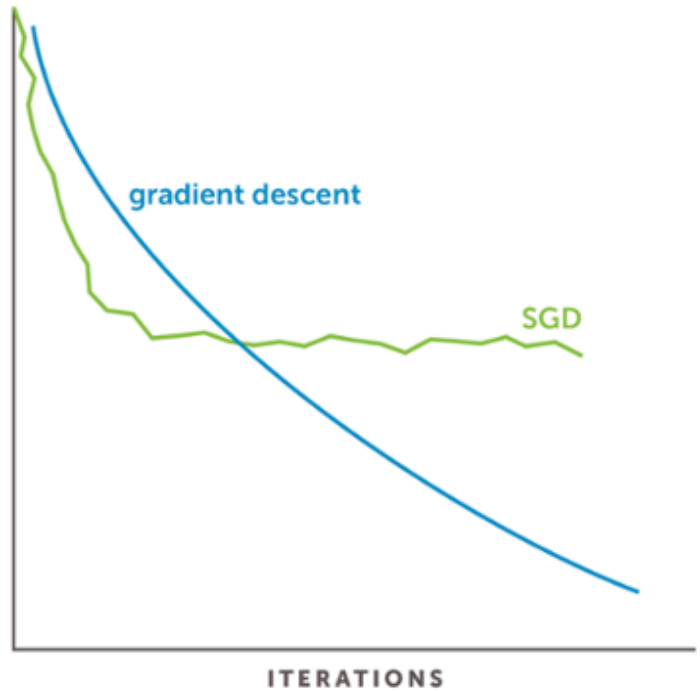
SGD is kinda slow...



- GD – use all points each iteration to compute gradient
- SGD – use one point each iteration to compute gradient
- **Faster:** Mini-Batch – use a *mini-batch* of points each iteration to compute gradient

Alternatives to SGD

Are there reasonable alternatives outside of Newton method?

Accelerations

- **Momentum**
- Nesterov's method
- Adagrad
- RMSprop
- Adam
- ...

SGD with Momentum

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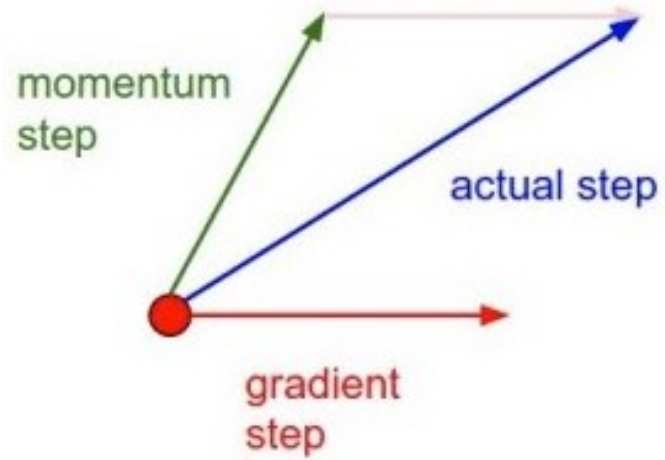

source: cs213n.github.io

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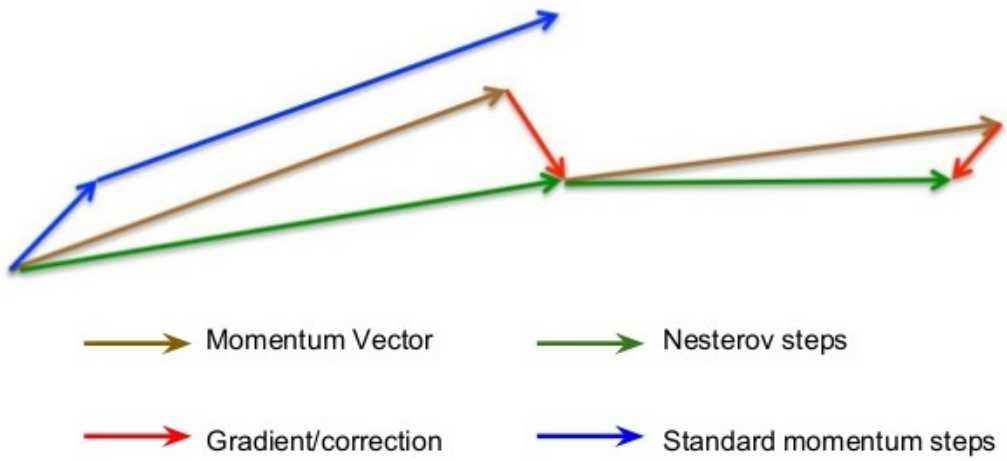

source: Geoff Hinton's lecture

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Algorithm 4 AdaGrad

Require: Global learning rate η

Require: Initial parameter θ

Initialize gradient accumulation variable $r = 0$

while Stopping criterion not met **do**

Sample a minibatch of m examples from the training set $\{x^{(1)}, \ldots, x^{(m)}\}$.

Apply interim update: $\theta \leftarrow \theta + \rho v$

Set $g = 0$

for $i = 1$ to m **do**

Compute gradient:

$$g \leftarrow g + \nabla_\theta L(f(x^{(i)}; \theta)), y^{(i)}; \theta).$$

end for

Accumulate gradient: $r \leftarrow r + g^2$ (square is applied element-wise)

Compute update: $\Delta\theta \leftarrow -\frac{\eta}{\sqrt{r}} g$ ($\frac{1}{\sqrt{r}}$ is applied element-wise)

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- AdaGrad accelerates in flat directions of optimization landscape and slows down in step ones.

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Algorithm 5 RMSprop

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Adam

Adaptive Moment – a combination of the previous approaches.

Algorithm 8.7 The Adam algorithm

Require: Step size ϵ (Suggested default: 0.001)
Require: Exponential decay rates for moment estimates, ρ_1 and ρ_2 in $[0, 1)$. (Suggested defaults: 0.9 and 0.999 respectively)
Require: Small constant δ used for numerical stabilization. (Suggested default: 10^{-8})
Require: Initial parameters $\boldsymbol{\theta}$
  Initialize 1st and 2nd moment variables $\boldsymbol{s} = \boldsymbol{0}, \boldsymbol{r} = \boldsymbol{0}$
  Initialize time step $t = 0$
  while stopping criterion not met **do**
    Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    $t \leftarrow t + 1$
    Update biased first moment estimate: $\boldsymbol{s} \leftarrow \rho_1 \boldsymbol{s} + (1 - \rho_1)\boldsymbol{g}$
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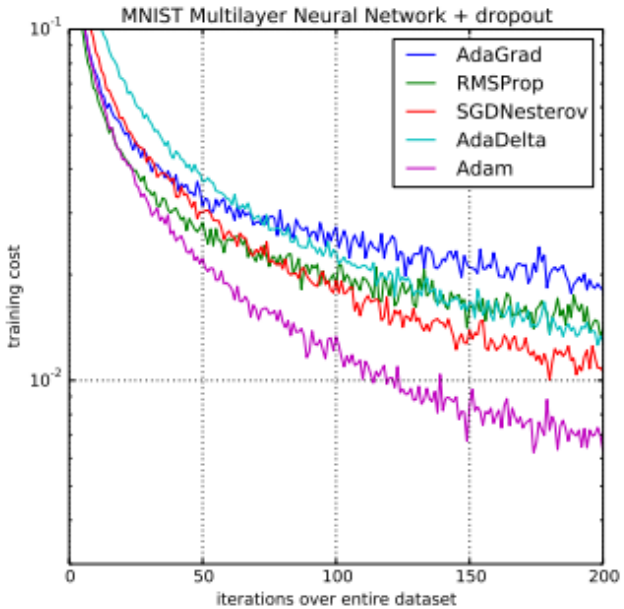

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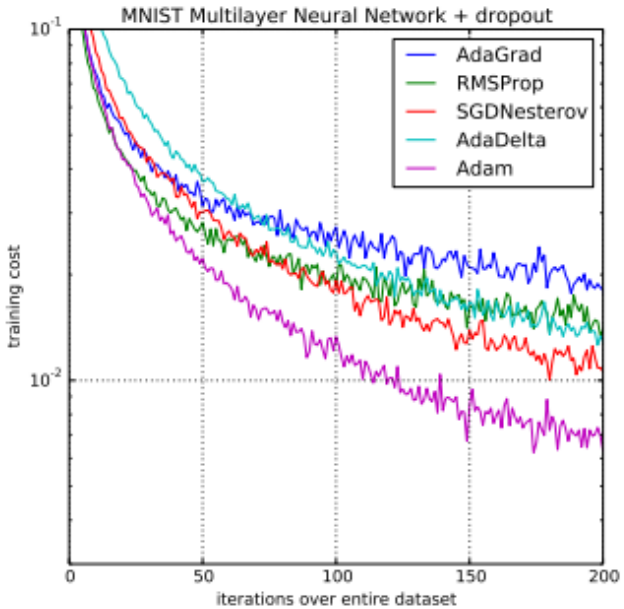

[Kingma and Ba, 2014]

- Ridiculously popular – more than 13K citations!

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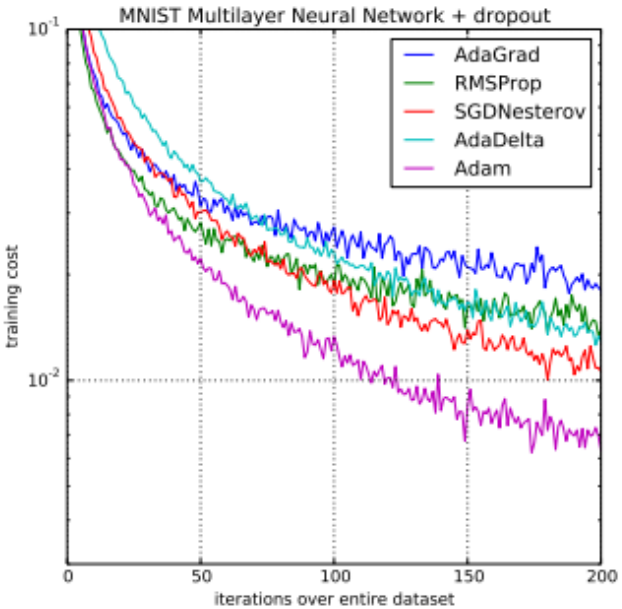
    Correct bias in first moment: $\hat{\boldsymbol{s}} \leftarrow \frac{\boldsymbol{s}}{1 - \rho_1^t}$
    Correct bias in second moment: $\hat{\boldsymbol{r}} \leftarrow \frac{\boldsymbol{r}}{1 - \rho_2^t}$
    Compute update: $\Delta\boldsymbol{\theta} = -\epsilon \frac{\hat{\boldsymbol{s}}}{\sqrt{\hat{\boldsymbol{r}}} + \delta}$ (operations applied element-wise)
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta\boldsymbol{\theta}$
  end while



[Kingma and Ba, 2014]

- Ridiculously popular – more than 13K citations!
- Probably because it comes with recommended parameters and came with a proof of convergence (which was shown to be wrong).

So what should I use in practice?

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Since our non-linearities change their behavior around the origin, it makes sense to pre-process to zero-mean and unit variance.

$$\hat{x}_i = \frac{x_i - \mathbb{E}[x_i]}{\sqrt{\mathsf{Var}[x_i]}} \tag{6}$$

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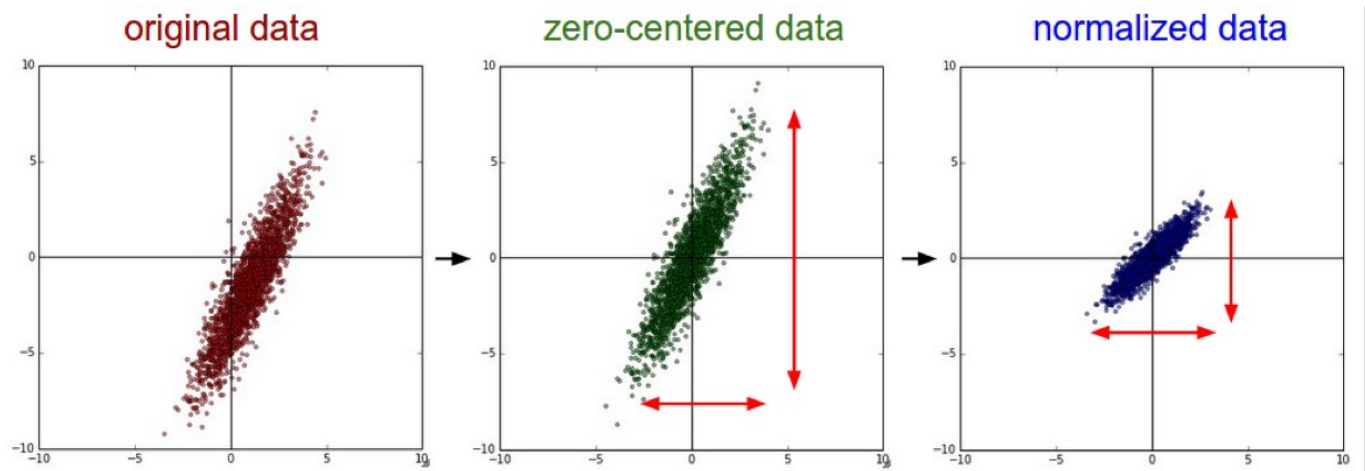

source: cs213n.github.io

Batch Normalization

A common technique is to repeat this throughout the deep network in a differentiable way:

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Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma^2_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

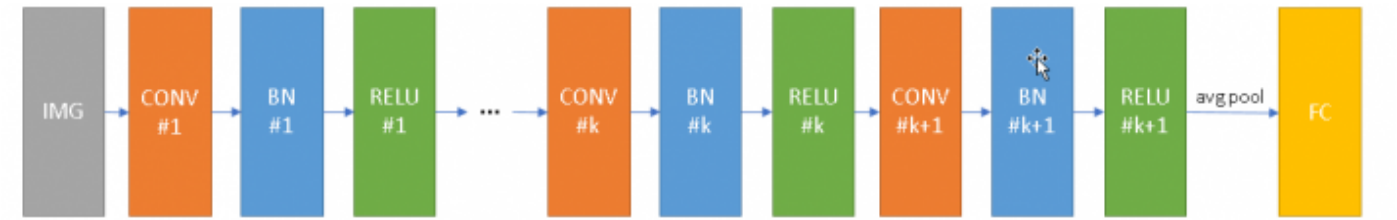
$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma^2_{\mathcal{B}} + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma\widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

[Ioffe and Szegedy, 2015]

Batch Normalization

In practice, a batchnorm layer is added after a conv or fully-connected layer, but before activations.



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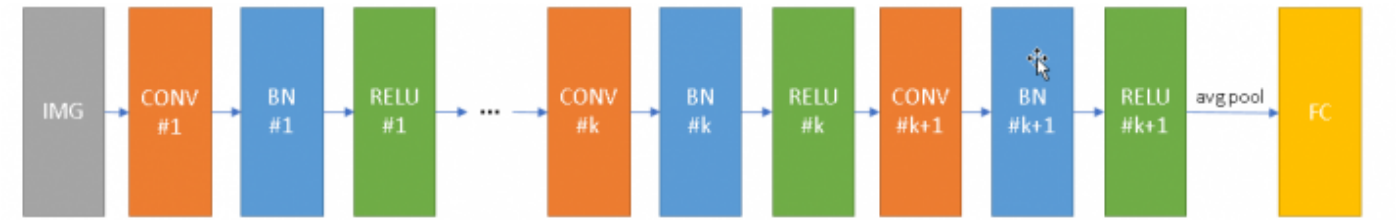

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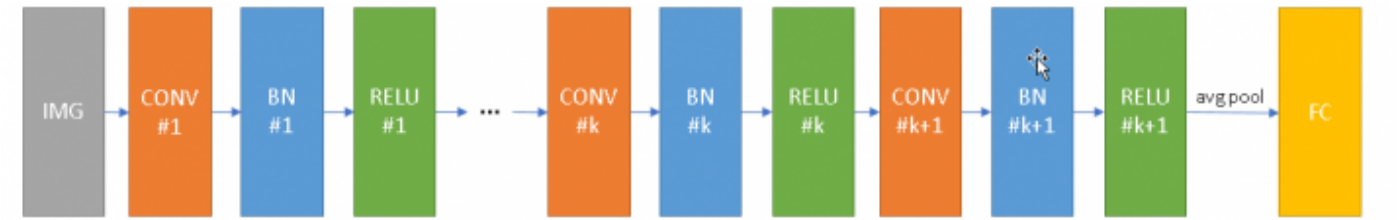

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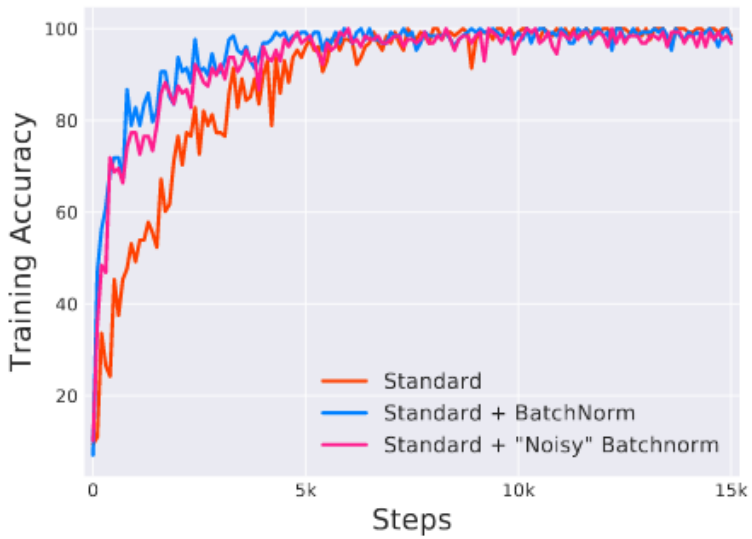

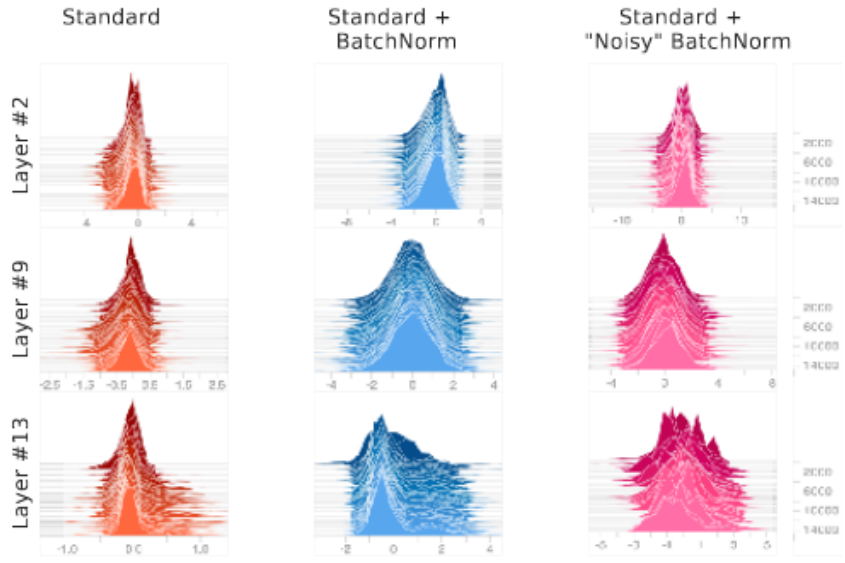

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[Santurkar, Tsipras, Ilyas, Madry, 2018]

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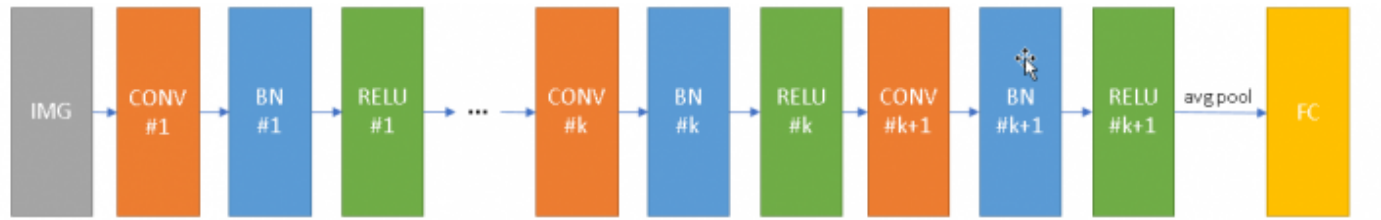

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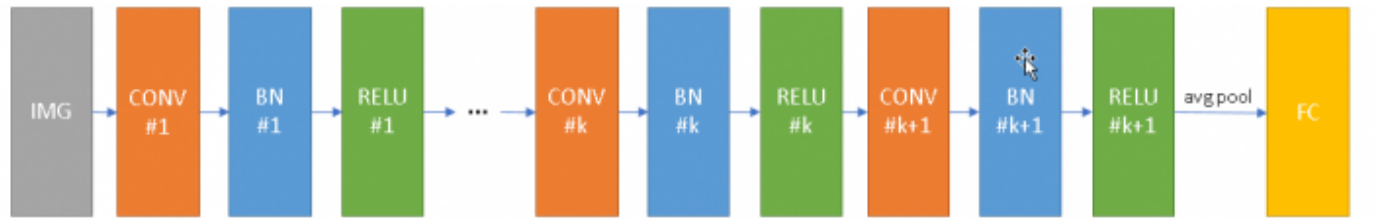

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- Using BN usually nets you a gain of few % increase in test accuracy.

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Another common technique: during forward pass, set some of the weights to 0 randomly with probability p. Typical choice is $p = 50\%$.

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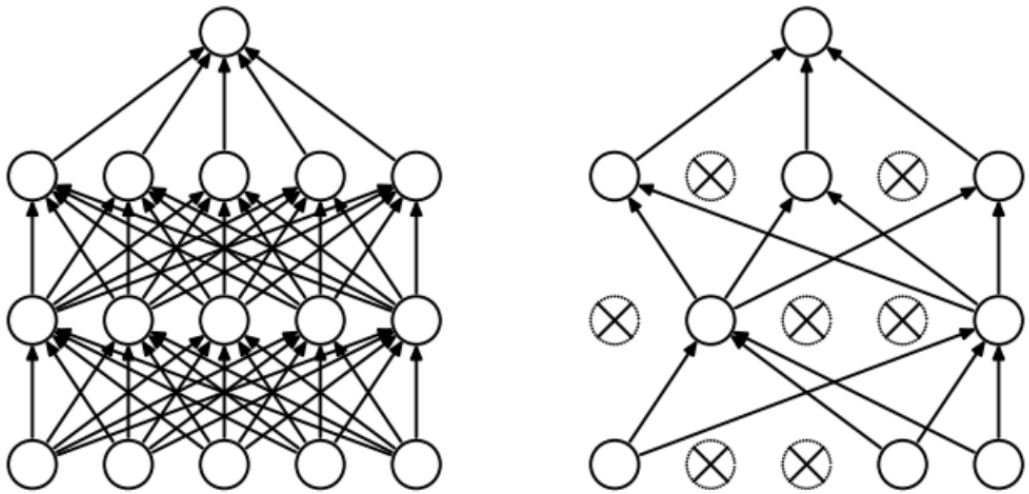

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(b) After applying dropout.

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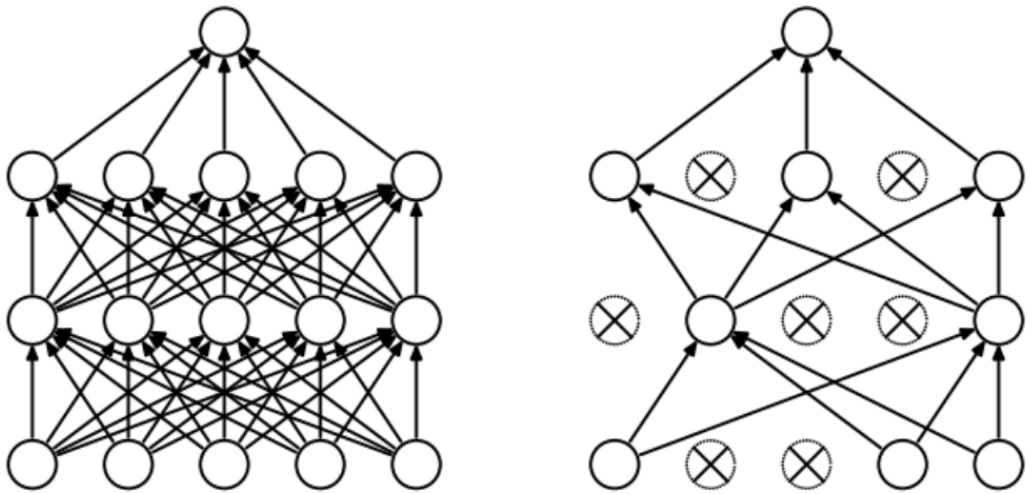

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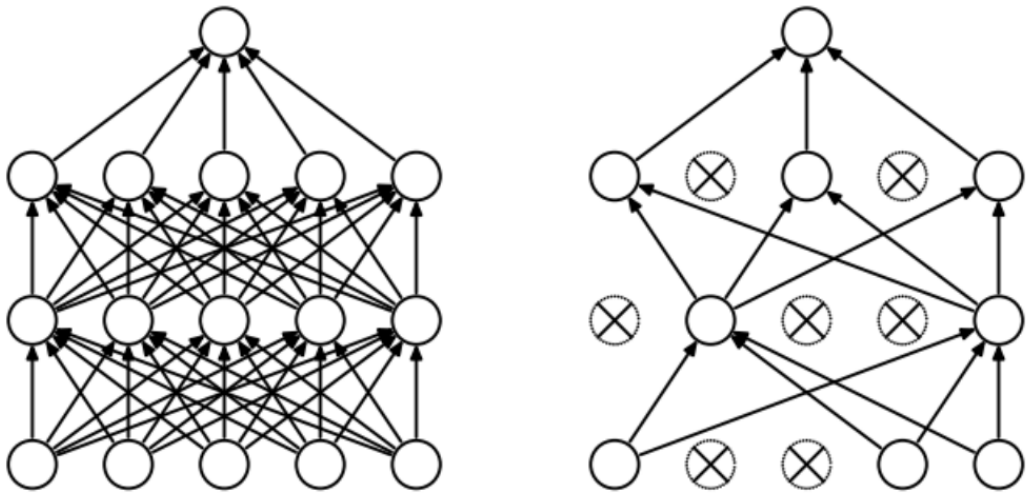

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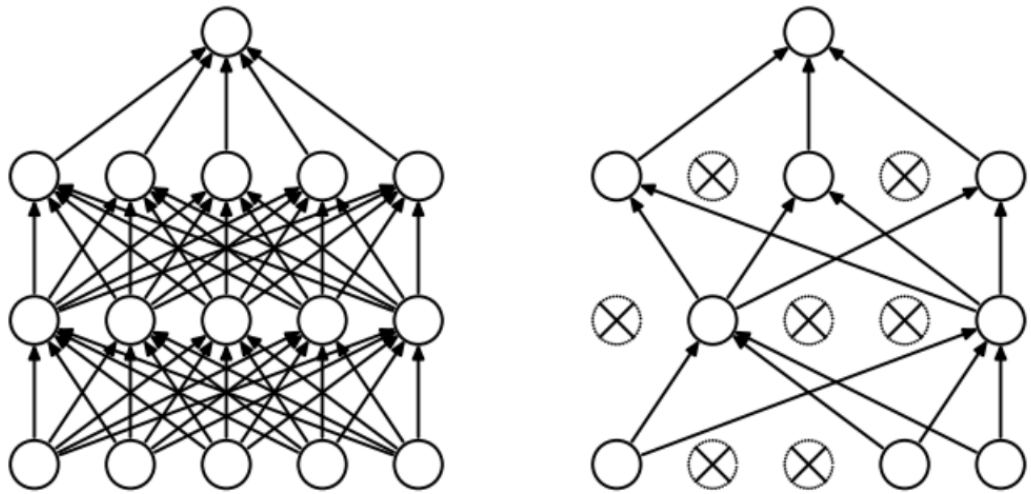

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- Dropout is more commonly applied for fully-connected layers, though its use is waning.

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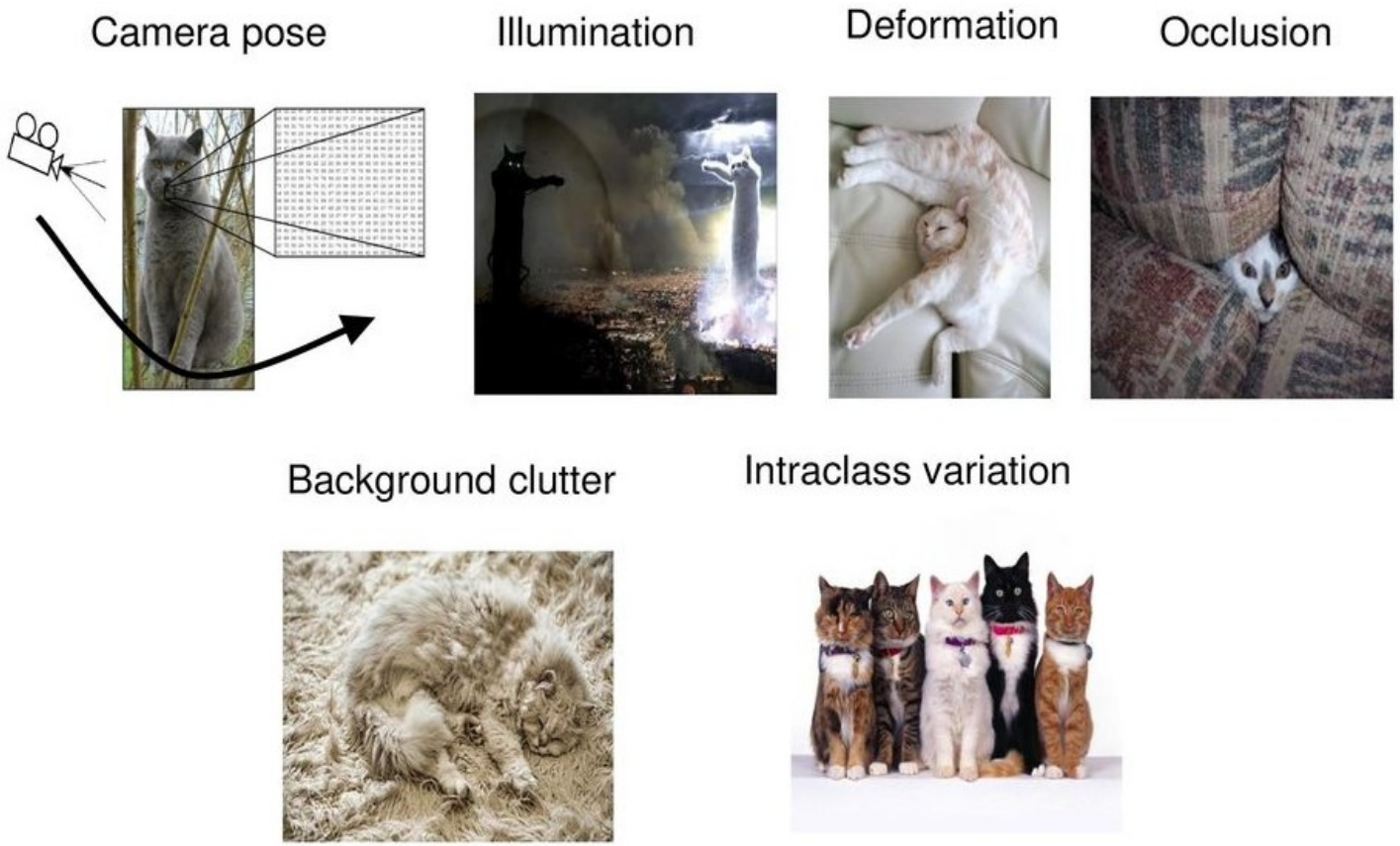
- What if collecting more data is slow/difficult?
- Can we squeeze out more from what we already have?

Invariance problem

An often-repeated claim about CNNs is that they are invariant to small translations. Independently of whether this is true, they are not invariant to most other types of transformations:



source: cs213n.github.io

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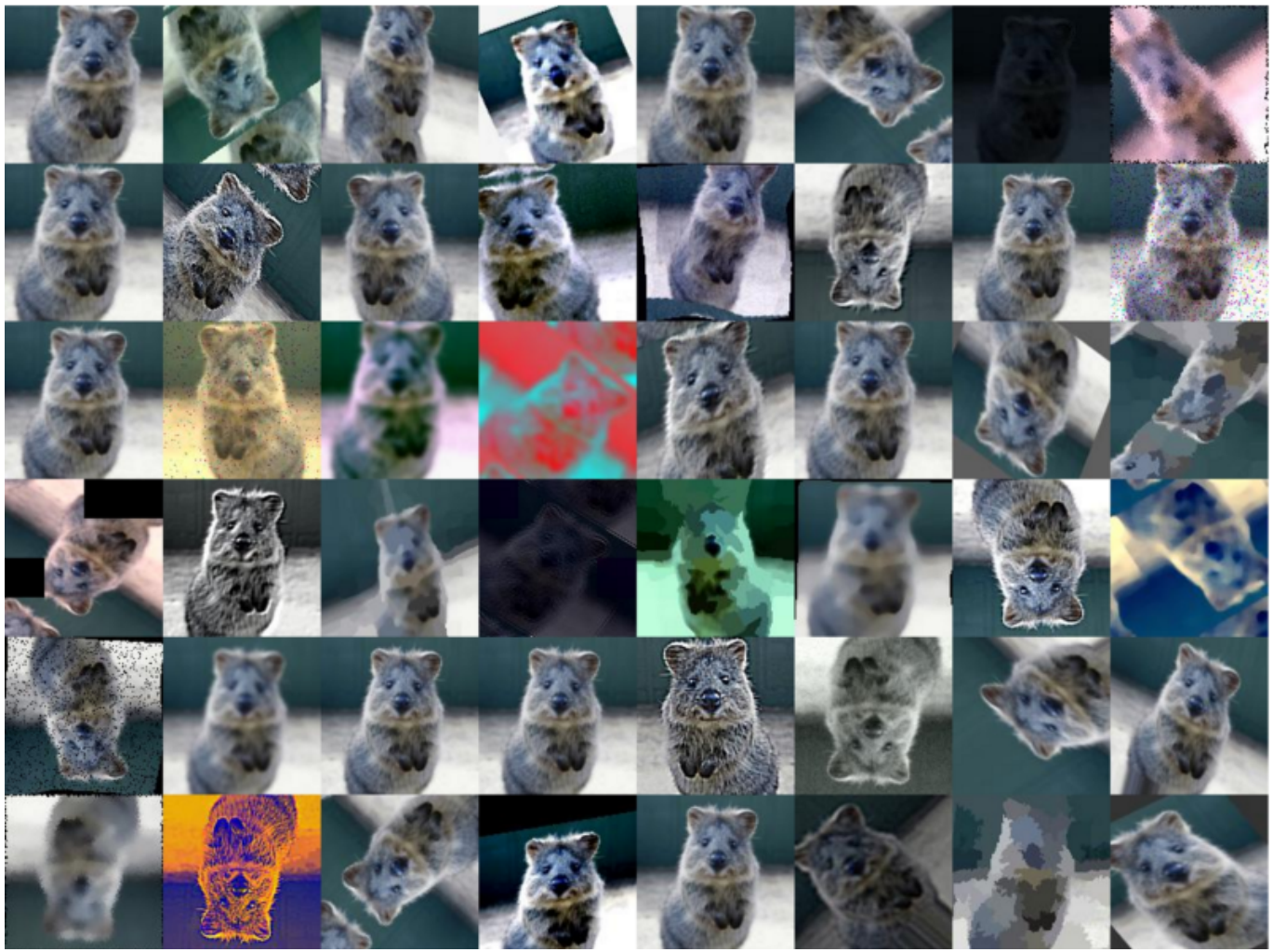
- Crucial for achieving state-of-the-art performance!
- For example, ResNet improves from 11.66% to 6.41% error on CIFAR-10 dataset and from 44.74% to 27.22% on CIFAR-100.

Data augmentation



source: github.com/aleju/imgaug

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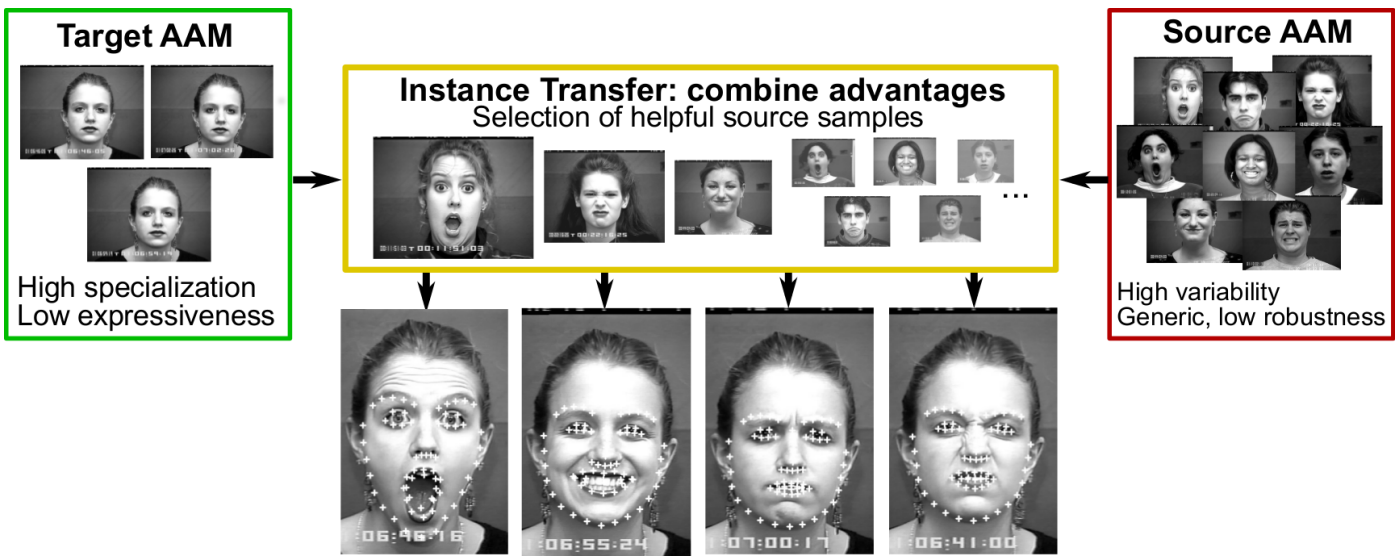

source: [Haase et al., 2014]

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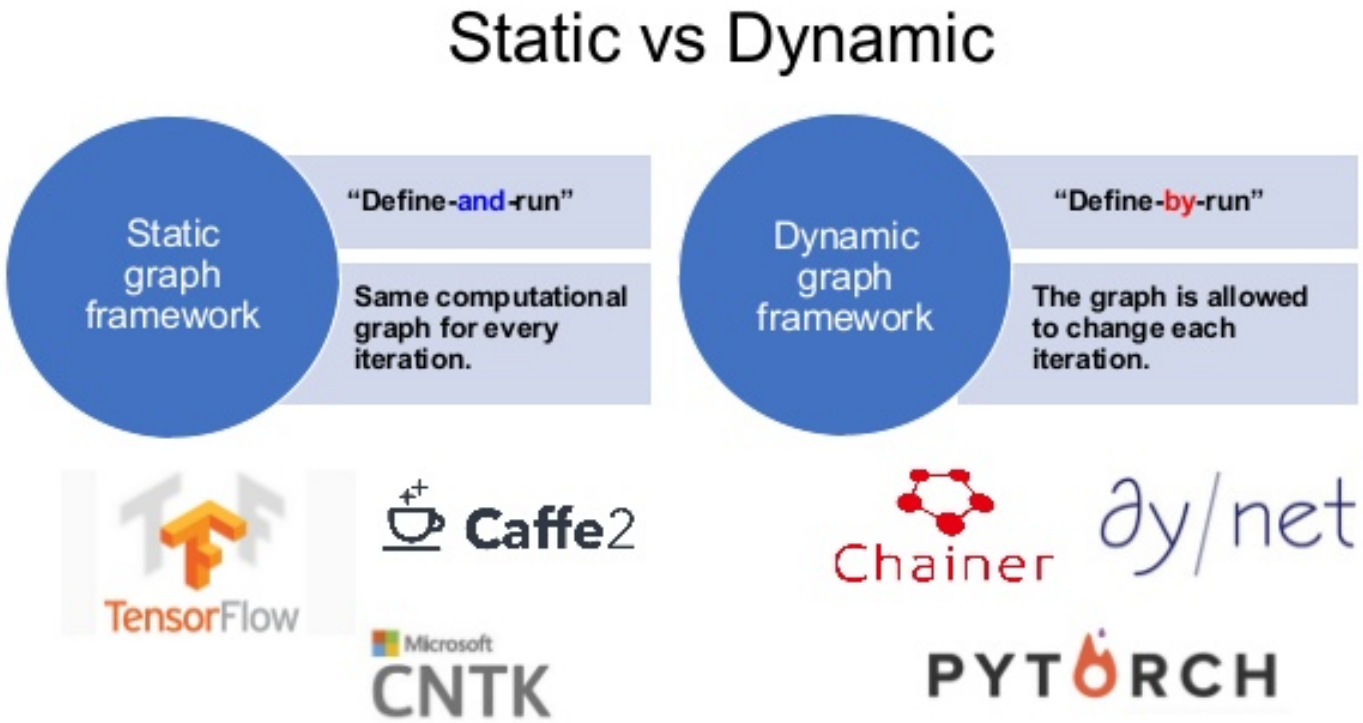
- You don't have to implement everything yourself.
- Many inbuilt modules allow quick iteration of ideas – building a neural network becomes putting simple blocks together and computing backprop is a breeze.
- Someone else already wrote CUDA code to efficiently run training on GPUs (or TPUs).

Main design difference



source: Introduction to Chainer

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- Autograd: package for automatic computation of backprop and construction of computational graphs.
- Module: neural network layer storing weights
- Dataloader: class for simplifying efficient data loading

```
import torch
from torchvision import transforms, datasets

data_transform = transforms.Compose([
        transforms.RandomSizedCrop(224),
        transforms.RandomHorizontalFlip(),
        transforms.ToTensor(),
        transforms.Normalize(mean=[0.485, 0.456, 0.406],
                             std=[0.229, 0.224, 0.225])
    ])
hymenoptera_dataset = datasets.ImageFolder(root='hymenoptera_data/train',
                                           transform=data_transform)
dataset_loader = torch.utils.data.DataLoader(hymenoptera_dataset,
                                             batch_size=4, shuffle=True,
                                             num_workers=4)
```

PyTorch - optimization

```
import torch

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)

model = torch.nn.Sequential(
          torch.nn.Linear(D_in, H),
          torch.nn.ReLU(),
          torch.nn.Linear(H, D_out))

learning_rate = 1e-4
optimizer = torch.optim.Adam(model.parameters(),
                             lr=learning_rate)
for t in range(500):
    y_pred = model(x)
    loss = torch.nn.functional.mse_loss(y_pred, y)

    loss.backward()

    optimizer.step()
    optimizer.zero_grad()
```

PyTorch - ResNet in one page

```
class BnLayer(nn.Module):
    def __init__(self, ni, nf, stride=2):
        super().__init__()
        self.conv = nn.Conv2d(ni, nf, kernel_size=3, stride=stride, bias=False, padding=1)
        self.a = nn.Parameter(torch.zeros(nf,1,1))
        self.m = nn.Parameter(torch.ones(nf,1,1))

    def forward(self, x):
        x = F.relu(self.conv(x))
        x_chan = x.transpose(0,1).contiguous().view(x.size(1), -1)
        if self.training:
            self.means = x_chan.mean(1)[:,None,None]
            self.stds  = x_chan.std (1)[:,None,None]
        x = x - self.means
        x = x / self.stds
        return x*self.m+self.a
```

```
class ResnetLayer(BnLayer):
    def forward(self, x): return x + super().forward(x)
```

```
class Resnet(nn.Module):
    def __init__(self, layers, c):
        super().__init__()
        self.layers = nn.ModuleList([BnLayer(layers[i], layers[i+1])
            for i in range(len(layers) - 1)])
        self.layers2 = nn.ModuleList([ResnetLayer(layers[i+1], layers[i + 1], 1)
            for i in range(len(layers) - 1)])
        self.layers3 = nn.ModuleList([ResnetLayer(layers[i+1], layers[i + 1], 1)
            for i in range(len(layers) - 1)])
        self.out = nn.Linear(layers[-1], c)

    def forward(self, x):
        for l,l2,l3 in zip(self.layers, self.layers2, self.layers3):
            x = l3(l2(l(x)))
        x = F.adaptive_max_pool2d(x, 1)
        x = x.view(x.size(0), -1)
        return F.log_softmax(self.out(x), dim=-1)
```

@jeremyphoward

A. Banburski

Tensorflow static graphs

```
N, D, H = 64, 1000, 100
x = tf.placeholder(tf.float32, shape=(N, D))
y = tf.placeholder(tf.float32, shape=(N, D))
w1 = tf.placeholder(tf.float32, shape=(D, H))
w2 = tf.placeholder(tf.float32, shape=(H, D))

h = tf.maximum(tf.matmul(x, w1), 0)
y_pred = tf.matmul(h, w2)
diff = y_pred - y
loss = tf.reduce_mean(tf.reduce_sum(diff ** 2, axis=1))

grad_w1, grad_w2 = tf.gradients(loss, [w1, w2])

with tf.Session() as sess:
    values = {x: np.random.randn(N, D),
              w1: np.random.randn(D, H),
              w2: np.random.randn(H, D),
              y: np.random.randn(N, D),}
    out = sess.run([loss, grad_w1, grad_w2],
                   feed_dict=values)
    loss_val, grad_w1_val, grad_w2_val = out
```

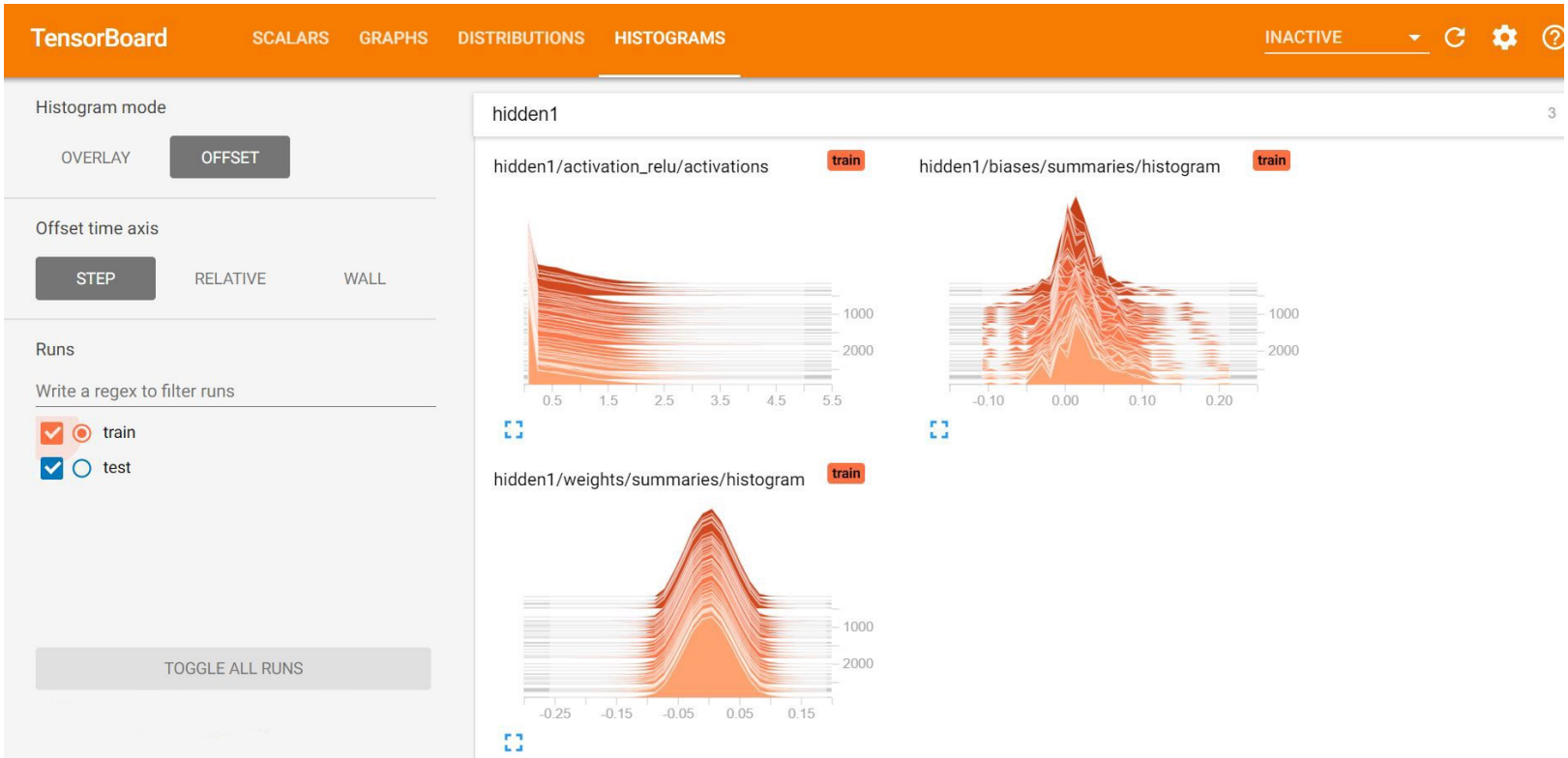
source: cs213n.github.io

Keras wrapper - closer to PyTorch

```
N, D, H = 64, 1000, 100
x = tf.placeholder(tf.float32, shape=(N, D))
y = tf.placeholder(tf.float32, shape=(N, D))

model = tf.keras.Sequential()
model.add(tf.keras.layers.Dense(H, input_shape=(D,),
                                activation=tf.nn.relu))
model.add(tf.keras.layers.Dense(D))
y_pred = model(x)
loss = tf.losses.mean_squared_error(y_pred, y)

optimizer = tf.train.GradientDescentOptimizer(1e0)
updates = optimizer.minimize(loss)

with tf.Session() as sess:
    sess.run(tf.global_variables_initializer())
    values = {x: np.random.randn(N, D),
              y: np.random.randn(N, D)}
    for t in range(50):
        loss_val, _ = sess.run([loss, updates],
                               feed_dict=values)
```

source: cs213n.github.io

Tensorboard - very useful tool for visualization



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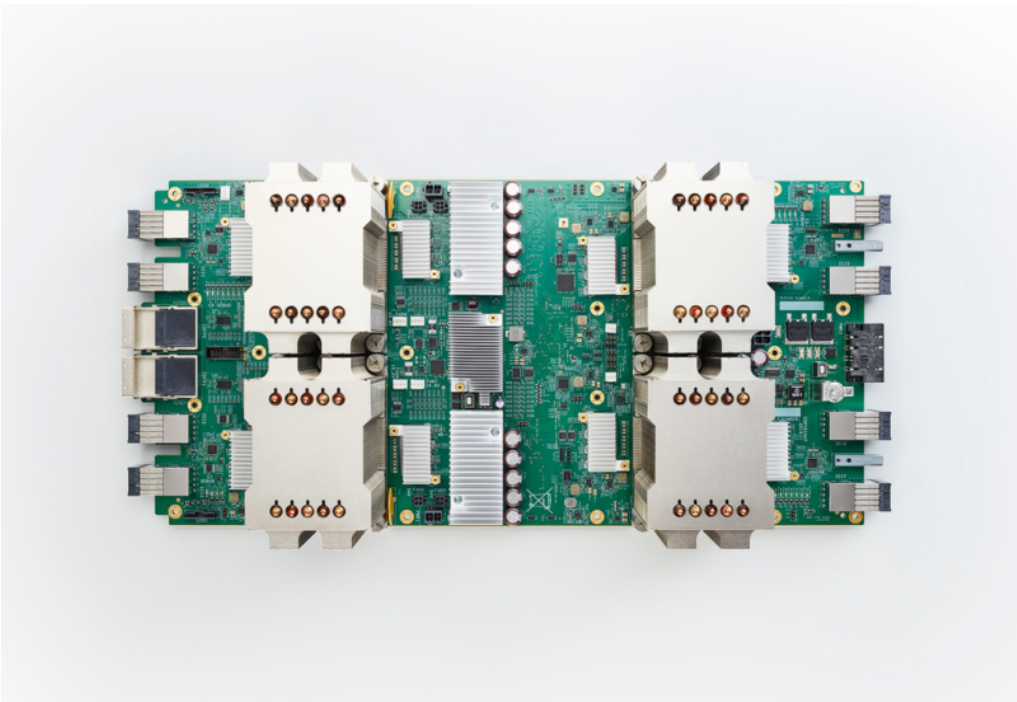
- Can use TPUs



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- Which one to choose then?
  - **PyTorch** is more popular in the research community for easy development and debugging.
  - In the past a better choice for production was **Tensorflow**. Still the only choice if you want to use TPUs.