

MIT 9.520/6.860, Fall 2018

Class 11: Neural networks – tips, tricks & software

Andrzej Banburski

Last time - Convolutional neural networks

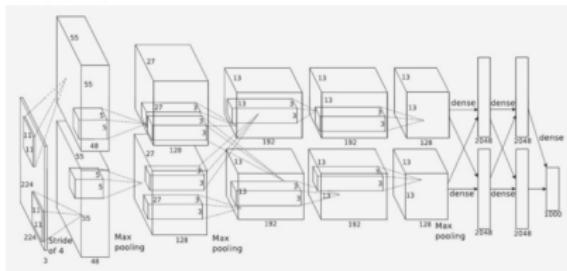
source: github.com/vdumoulin/conv_arithmetic

Large-scale Datasets



AlexNet
Krizhevsky
et al (2012)

General Purpose GPUs



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 :

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

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- ▶ If we go deeper however...
- ▶ 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 $x = (x_1, \dots, x_{n_{in}})$. 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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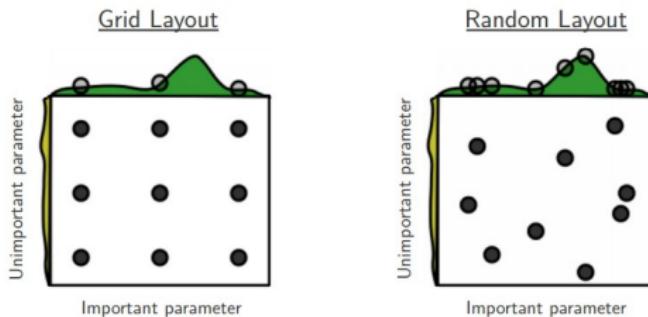
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Decaying learning rate

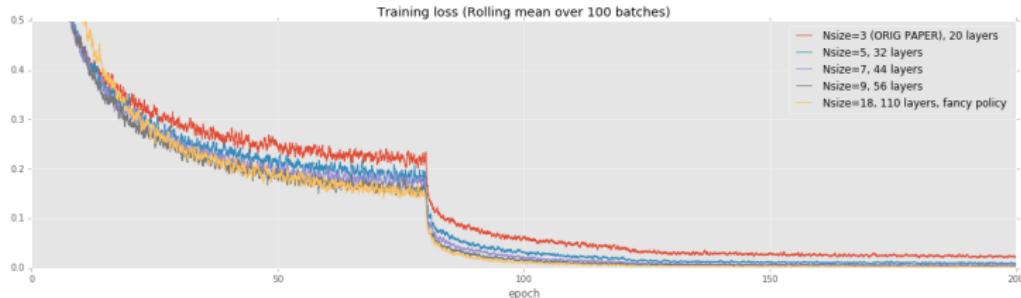
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- ▶ Typically we use a scheduler – decrease η after some fixed number of epochs.
- ▶ This allows the training loss to keep improving after it has plateaued



Batch-size & learning rate

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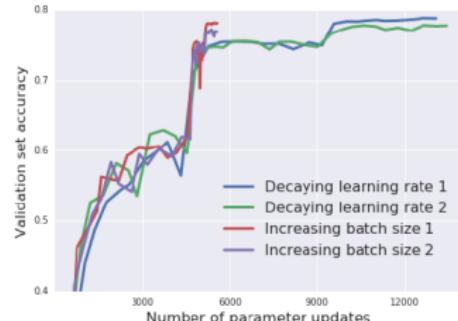
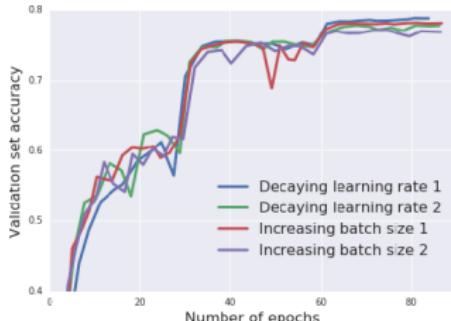
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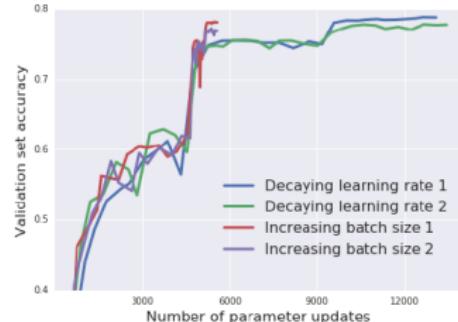
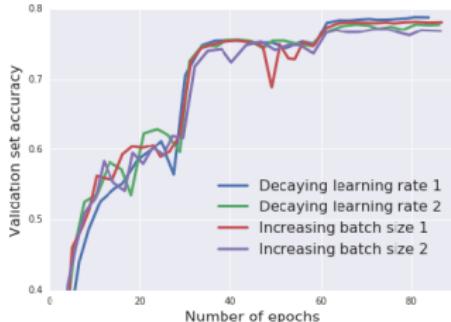


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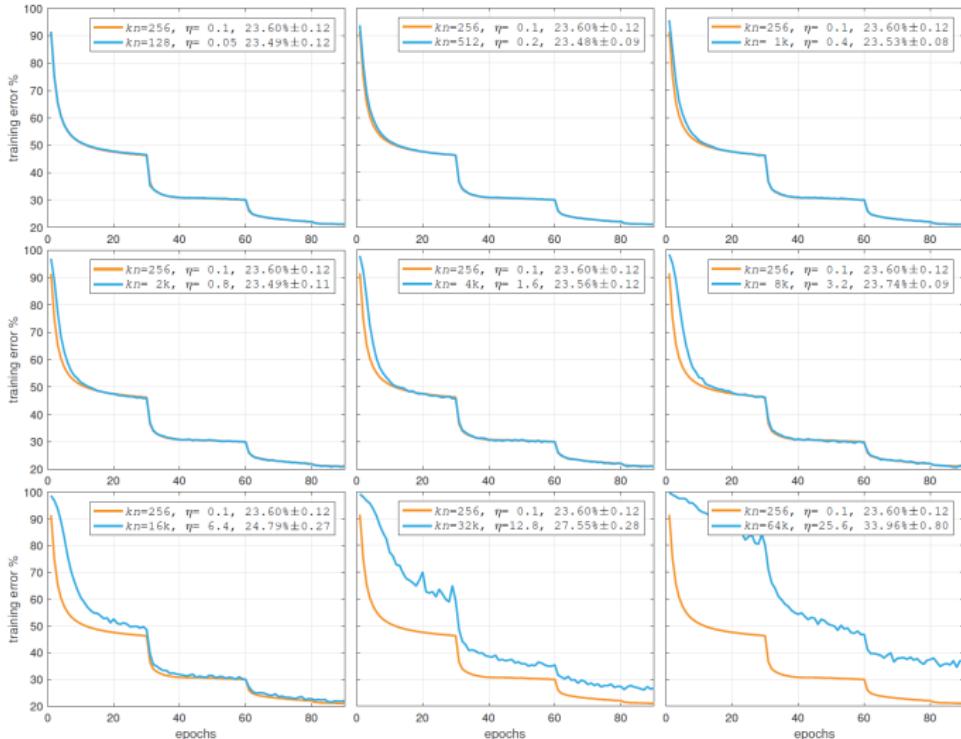
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- ▶ As b approaches N the dynamics become more and more deterministic and we would expect this relationship to vanish.

Batch-size & learning rate



source: [Goyal et al., 2017]

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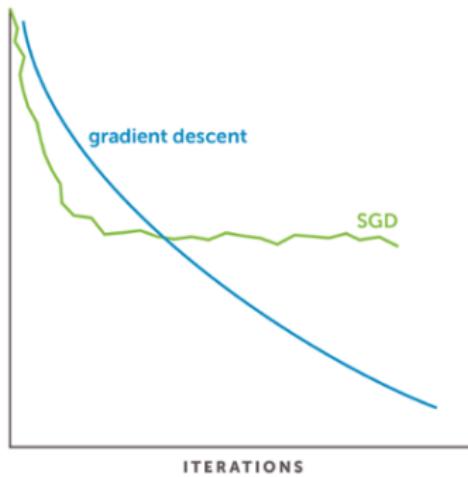
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SGD is kinda slow...



- ▶ 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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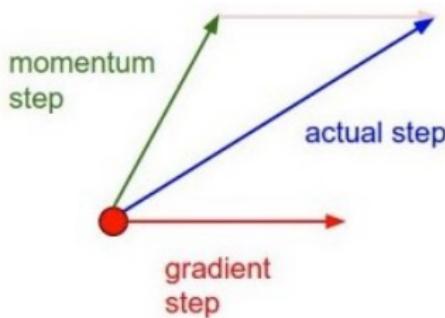
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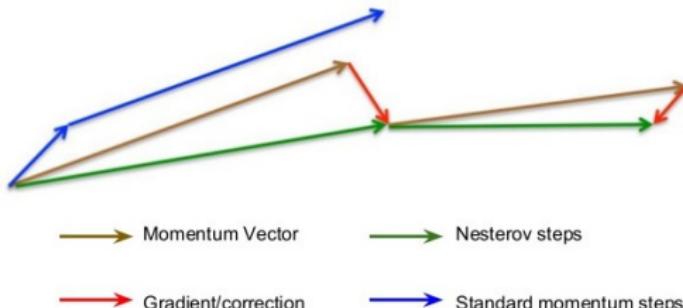
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source: Geoff Hinton's lecture

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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 $\{x^{(1)}, \dots, x^{(m)}\}$.

 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:
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Require: Initial parameters θ

Initialize 1st and 2nd moment variables $s = 0, r = 0$

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 Compute gradient: $g \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(x^{(i)}; \theta), y^{(i)})$

$t \leftarrow t + 1$

 Update biased first moment estimate: $s \leftarrow \rho_1 s + (1 - \rho_1)g$

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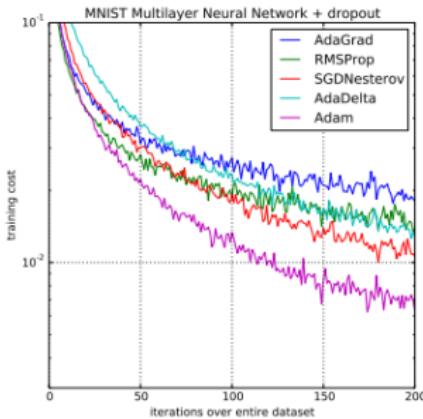
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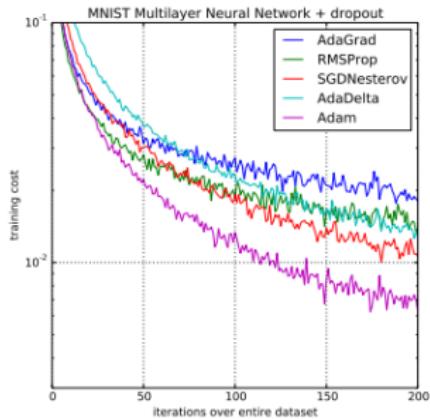
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[Kingma and Ba, 2014]

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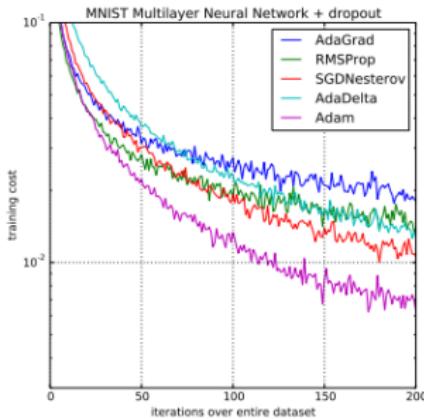
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[Kingma and Ba, 2014]

- ▶ 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).

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Batchnorm & Dropout

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Data pre-processing

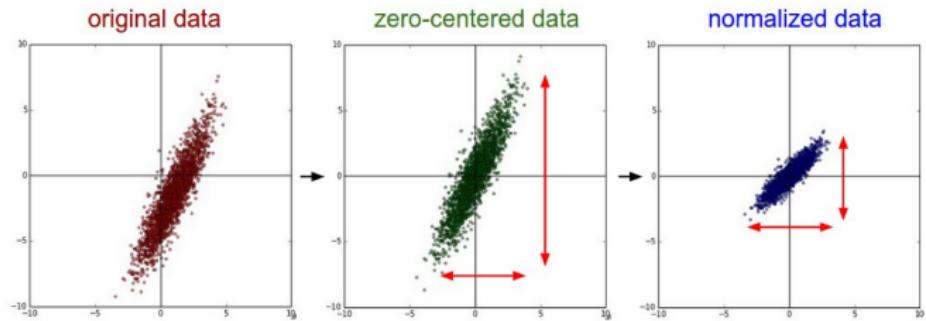
Since our non-linearities change their behavior around the origin, it makes sense to pre-process to zero-mean and unit variance.

$$\hat{x}_i = \frac{x_i - \mathbb{E}[x_i]}{\sqrt{\text{Var}[x_i]}} \quad (6)$$

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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: $\mathcal{B} = \{x_1 \dots m\}$;

Parameters to be learned: γ, β

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

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

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

$$\hat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \quad // \text{normalize}$$

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

[Ioffe and Szegedy, 2015]

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



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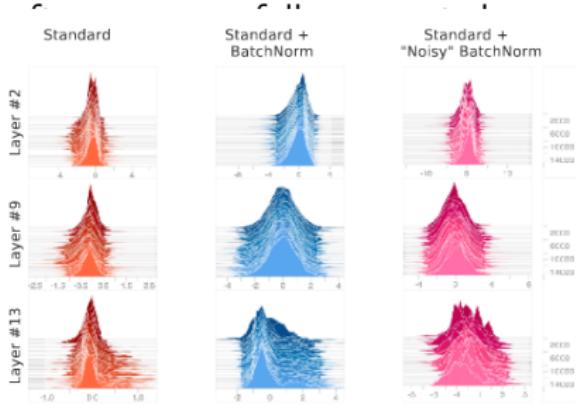
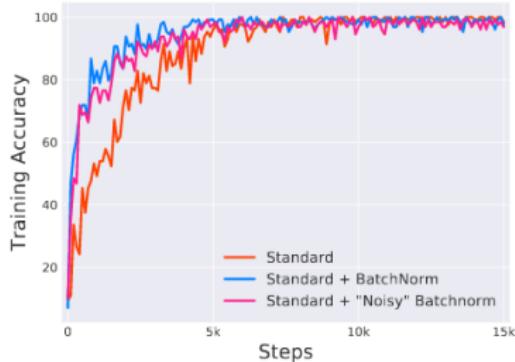
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[Santurkar, Tsipras, Ilyas, Madry, 2018]

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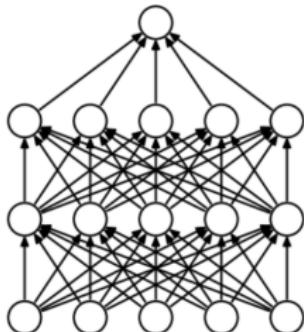
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- ▶ More obviously, this reduces 2nd-order correlations between layers. Recently shown that it actually doesn't change covariate shift! Instead it smooths out the landscape.
- ▶ In practice this reduces dependence on initialization and seems to stabilize the flow of gradient descent.
- ▶ Using BN usually nets you a gain of few % increase in test accuracy.

Dropout

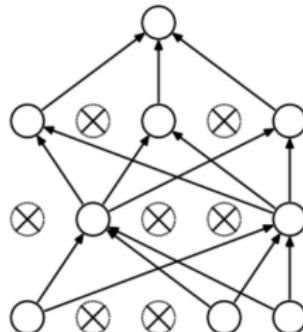
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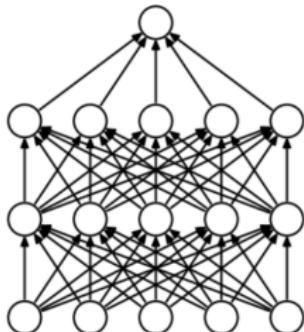
(a) Standard Neural Net



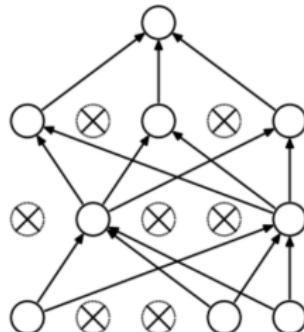
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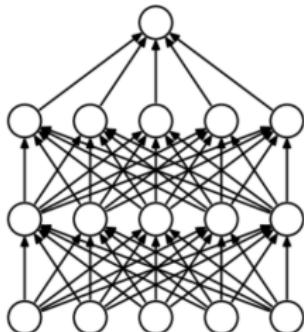


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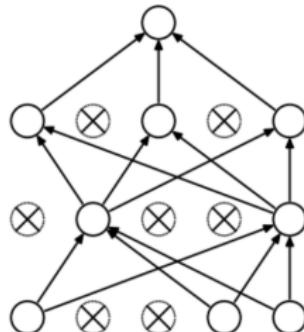
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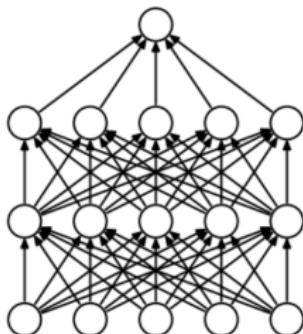


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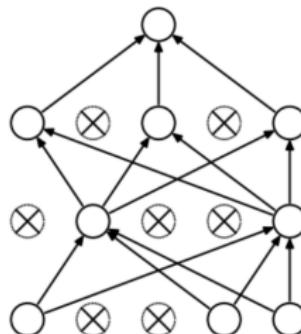
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- ▶ Dropout is more commonly applied for fully-connected layers, though its use is waning.

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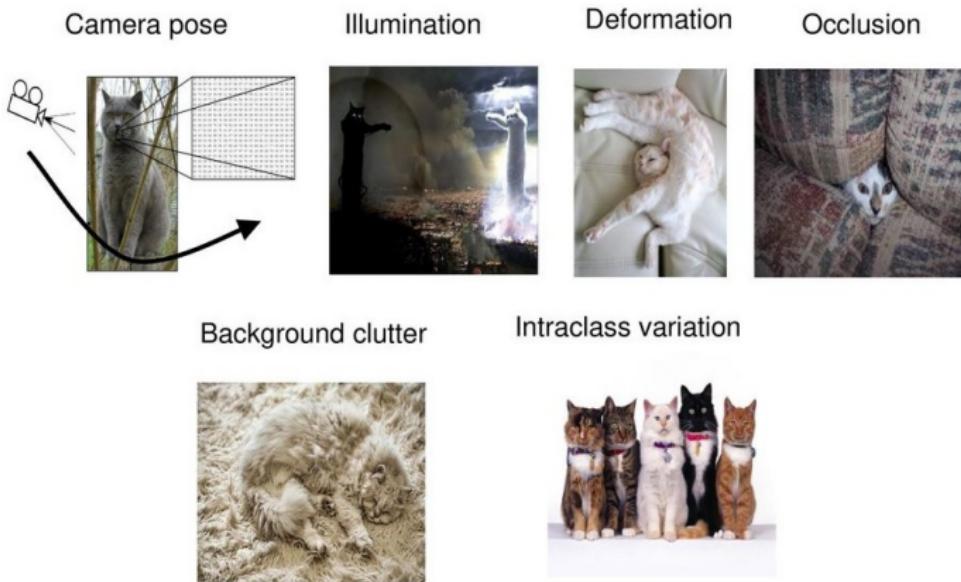
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- ▶ Can we squeeze out more from what we already have?

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

challenge

A. Banburski

Data augmentation

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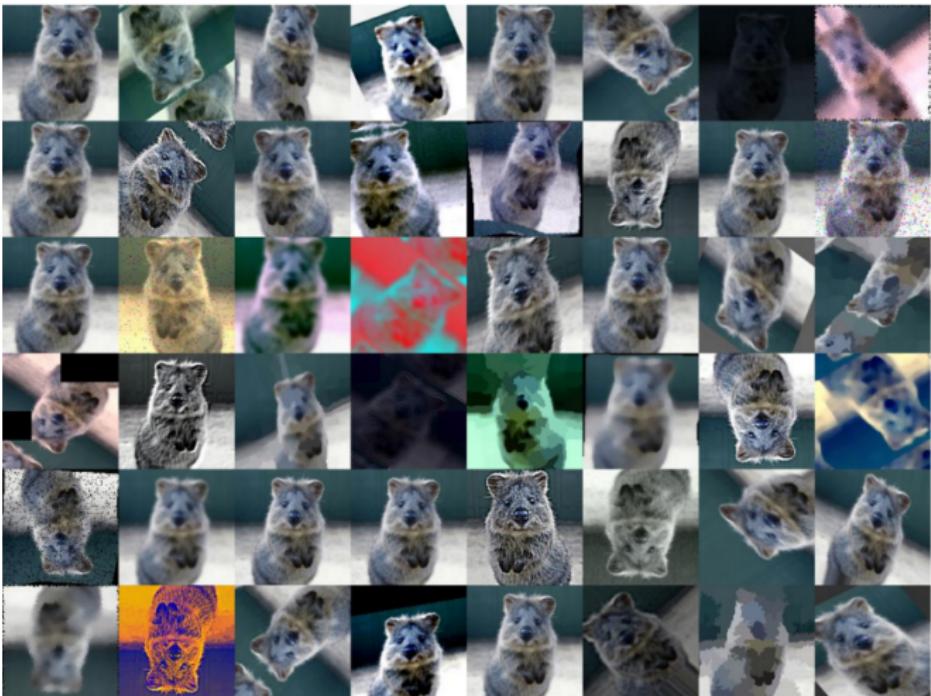
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- ▶ For example, ResNet improves from 11.66% to 6.41% accuracy on CIFAR-10 dataset and from 44.74% to 27.22% on CIFAR-100.

Data augmentation



source: github.com/aleju/imgaug

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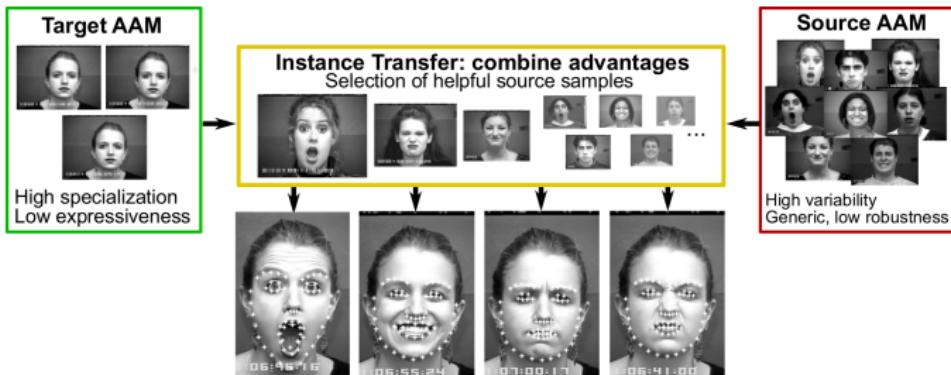
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source: [Haase et al., 2014]

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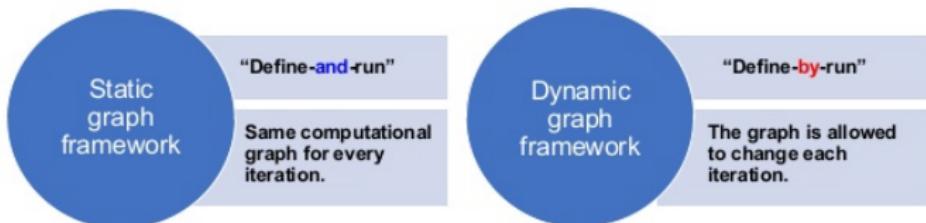
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- ▶ You don't have to implement everything yourself.
- ▶ Many inbuilt modules allow quick iteration of ideas – building a neural network becomes putting simple blocks together and computing backprop is a breeze.
- ▶ Someone else already wrote CUDA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

Main design difference

Static vs Dynamic



source: Introduction to Chainer

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- ▶ 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 l1,l2,l3 in zip(self.layers, self.layers2, self.layers3):
            x = l3(l2(l1(x)))
        x = F.adaptive_max_pool2d(x, 1)
        x = x.view(x.size(0), -1)
        return F.log_softmax(self.out(x), dim=-1)
```

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
```

Keras wrapper - closer to PyTorch

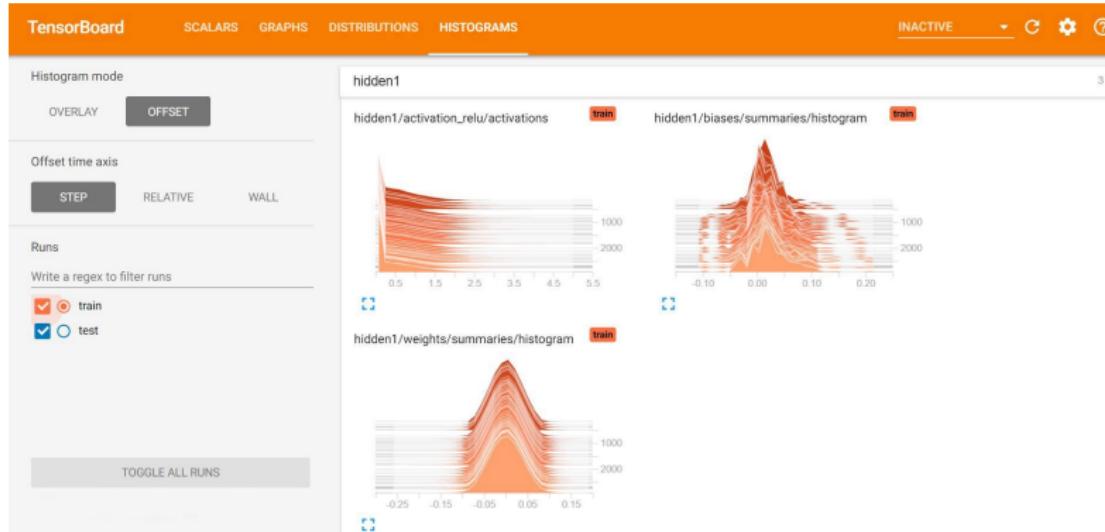
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N, D, H = 64, 1000, 100
x = tf.placeholder(tf.float32, shape=(N, D))
y = tf.placeholder(tf.float32, shape=(N, D))

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(1e-0)
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)
```

Tensorboard - very useful tool for visualization



Tensorflow overview

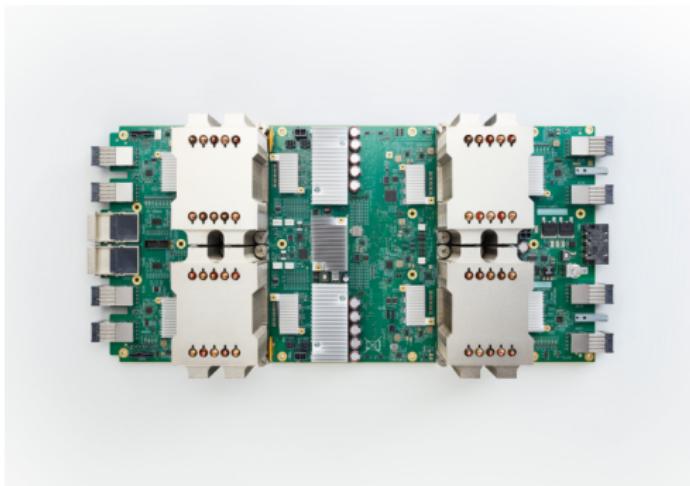
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- ▶ With Keras wrapper code is more similar to PyTorch however.
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- ▶ PyTorch is merging with Caffe2, which will provide static graphs too!
- ▶ Which one to choose then?
 - **PyTorch** is more popular 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.