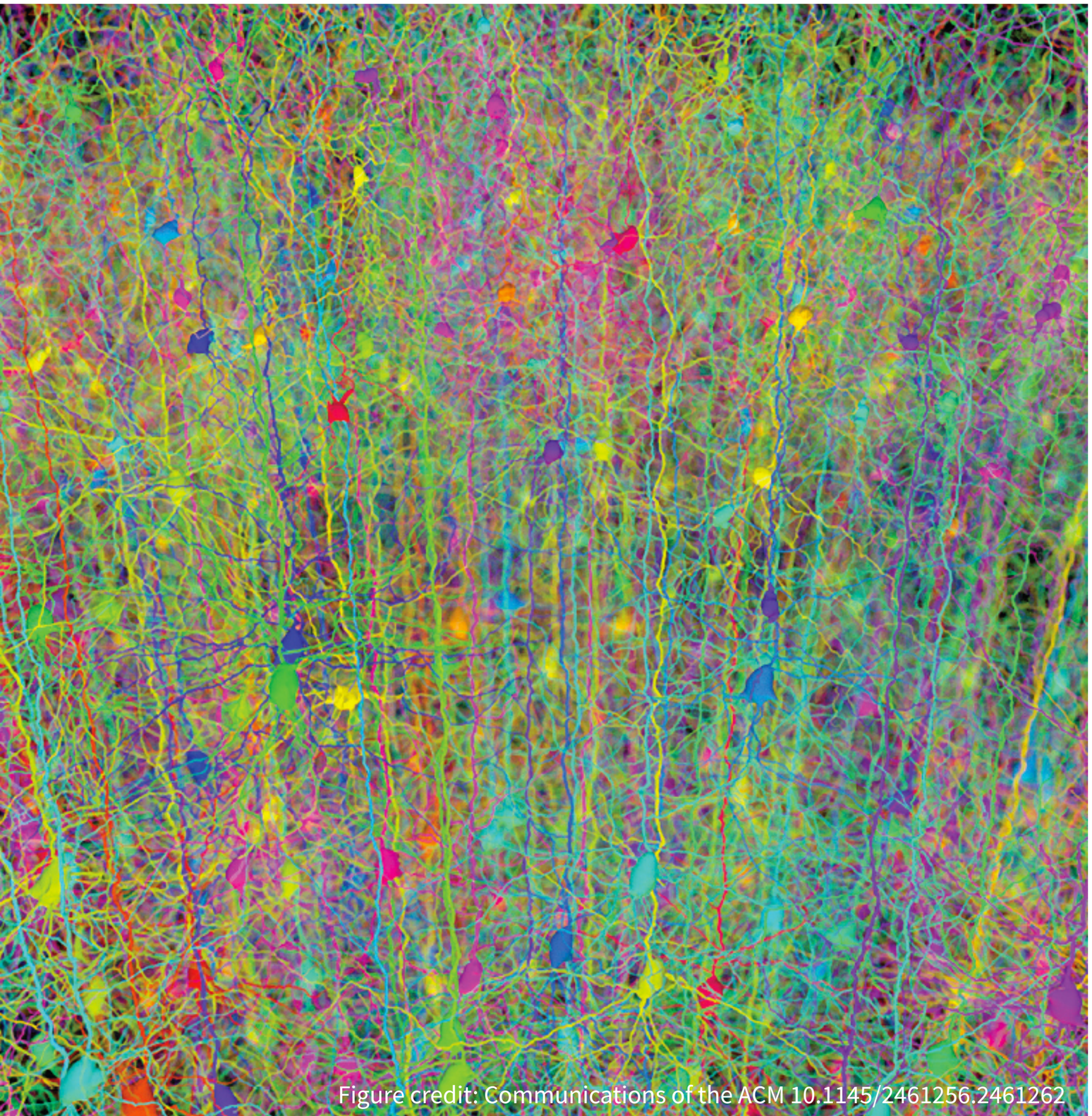
Optimization



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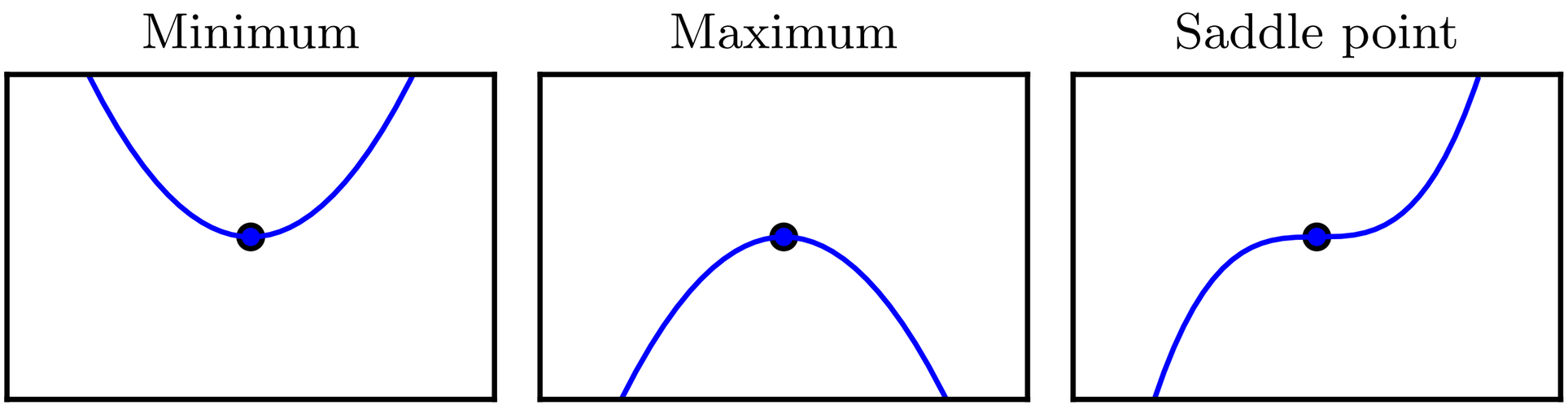
Optimization in Deep Learning

- There isn't a single global optimum (non-convex optimization)
- Non-identifiability:
  - We can permute the hidden units (with their connections) and get the same function
  - We can re-scale the inputs to a ReLU unit as long as we appropriately re-scale the outputs
- We have to deal with local minima, saddle points, and plateaus



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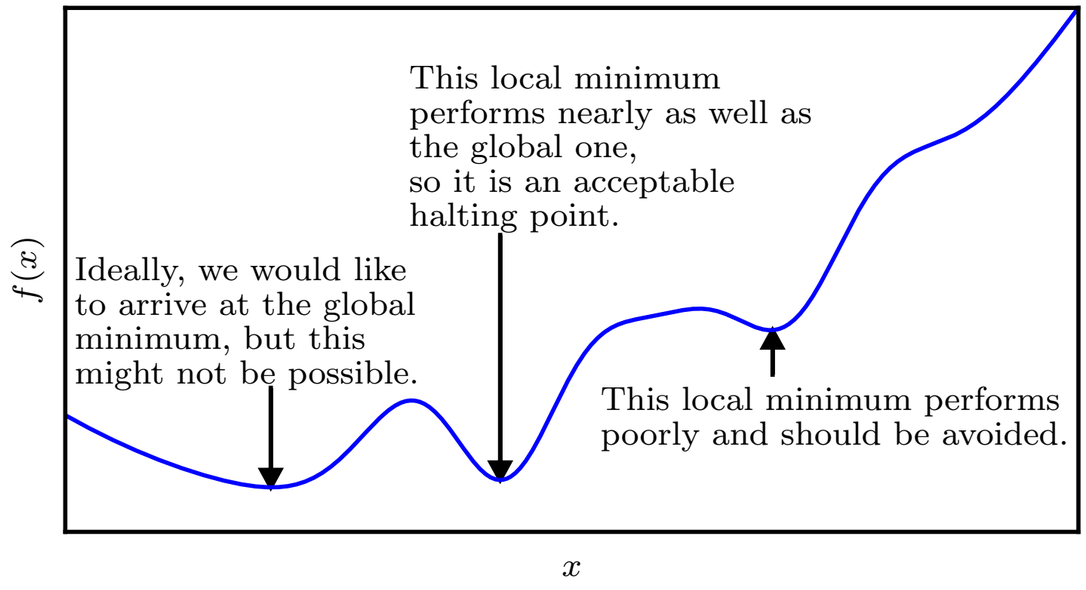
Historical vs. Modern Thinking

- Pre-2012: “The problem with neural nets is that they get stuck in local minima”
- Now: the local minima arising from nonidentifiability are equivalent to each other in cost function value
  - As a result, they’re not a problematic form of nonconvexity
- Open issue: Do cost surfaces have many local minima of high cost, and do optimization algorithms encounter them?



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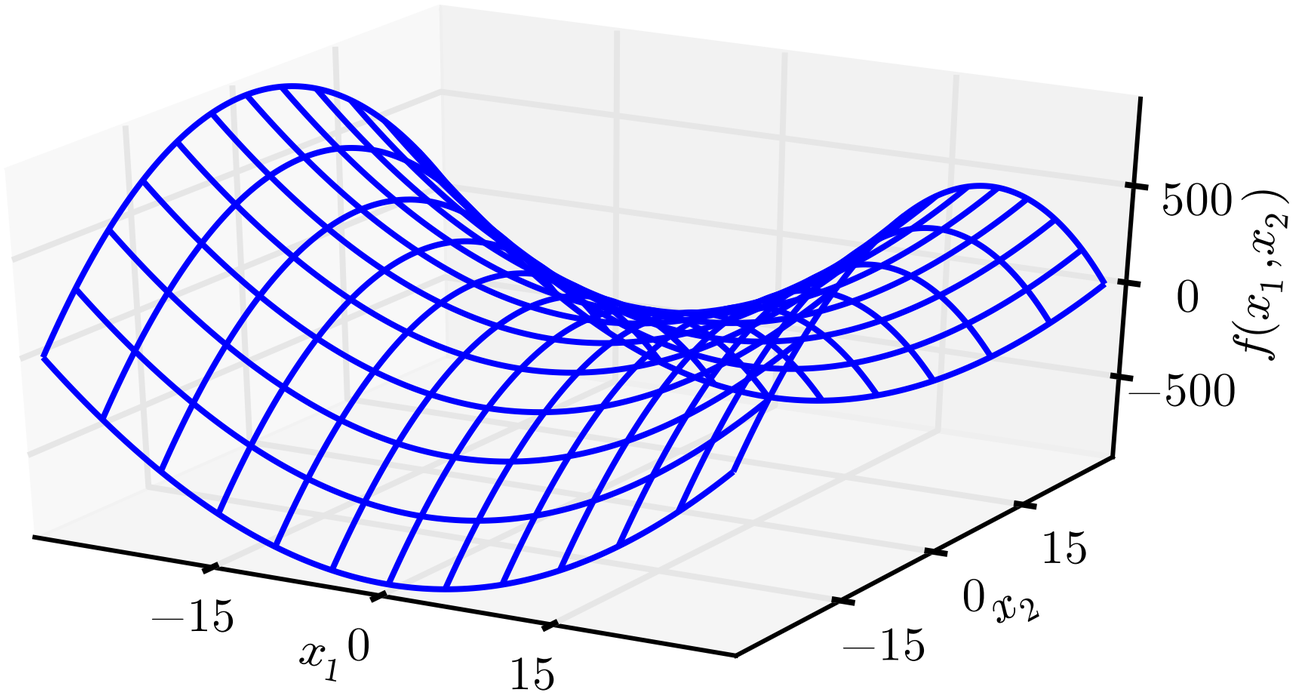
Saddle Points

- Many classes of random functions exhibit the following behaviour:
  - local minima are rare
  - saddle points are more common
- It has been shown experimentally that real neural networks also have loss functions that contain many high-cost saddle points
- What are the implications?
  - for first order methods, still unclear
  - but, second order methods seem to be attracted to saddle points



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Convergence Conditions

- Stochastic gradient descent will converge if:

$$\sum_{k=1}^{\infty} \epsilon_k = \infty, \text{and}$$

$$\sum_{k=1}^{\infty} \epsilon_k^2 < \infty$$

- Several recipes for decreasing the learning rate:

$$\epsilon_k = \frac{\epsilon_0}{1 + \delta k}$$

$$\epsilon_k = \frac{\epsilon_0}{k^\delta} \quad 0.5 < \delta \leq 1$$

$$\epsilon_k = (1 - \alpha)\epsilon_0 + \alpha\epsilon_\tau \quad \alpha = \frac{k}{\tau}$$

Batch and Minibatch Algorithms

- Optimization algorithms that use the entire training set are called batch or deterministic gradient methods
  - process examples simultaneously in a large “batch”
  - a lot of computation to get one gradient update
- Optimization algorithms that use only a single example are called stochastic and sometimes online methods
  - noisy estimates of the true gradient
- Most algorithms used for deep learning fall in-between, using more than one, but fewer than all training examples
  - traditionally called minibatch, but commonly called stochastic methods

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Choosing Minibatch Sizes

- Larger batches provide a more accurate estimate of the gradient, but require more computation
- Multicore architectures are underutilized by extremely small batches
- When processing all examples in a batch in parallel, amount of memory scales with batch size
- Some kinds of hardware (e.g. GPUs) benefit with specific sizes of arrays; powers of 2 are common (typically 32 to 256)
- Small batches can offer some regularizing effect

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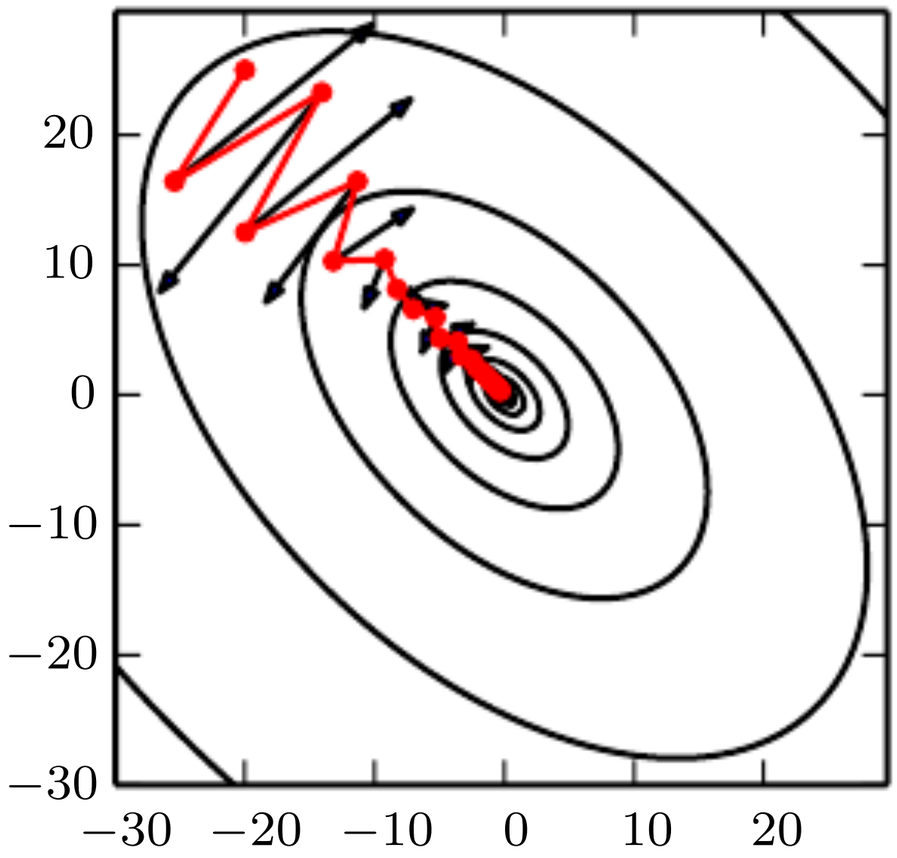
Momentum

- Use an exponential average of previous gradients:

$$\boldsymbol{v} \leftarrow \alpha \boldsymbol{v} - \epsilon \nabla_{\boldsymbol{\theta}} \left(\frac{1}{m} \sum_{i=1}^{m} L(f(\boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)}) \right)$$

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$$

- Aims primarily to solve two problems:
  - poor conditioning of the Hessian
  - variance of the stochastic gradients



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Parameter Initialization

- Modern strategies are simple and heuristic
- Only property known with complete certainty is to "break symmetry"
- The goal of having each unit compute a different function motivates initialization with small random values

- Biases are typically set to heuristic chosen constants and only the weights are chosen randomly (almost always Gaussian or uniform)
- Common recipe (Glorot and Bengio 2010):

$$W_{i,j} \sim U\left(-\sqrt{\frac{6}{m+n}}, \sqrt{\frac{6}{m+n}}\right)$$

m - # of inputs ("fan-in")

n - # of outputs ("fan-out")

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Choosing the Right Optimization Algorithm

- Unfortunately, there is no consensus
- See Unit Tests for Stochastic Optimization (Schaul et al. 2014)
  - results suggest that the family of algorithms with adaptive learning rates performed fairly robustly
- Currently, the most popular optimization algorithms actively in use include:
  - SGD, SGD with momentum
  - RMSProp, RMSProp with momentum
  - AdaDelta and Adam

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Batch Normalization (Ioffe and Szegedy 2015)

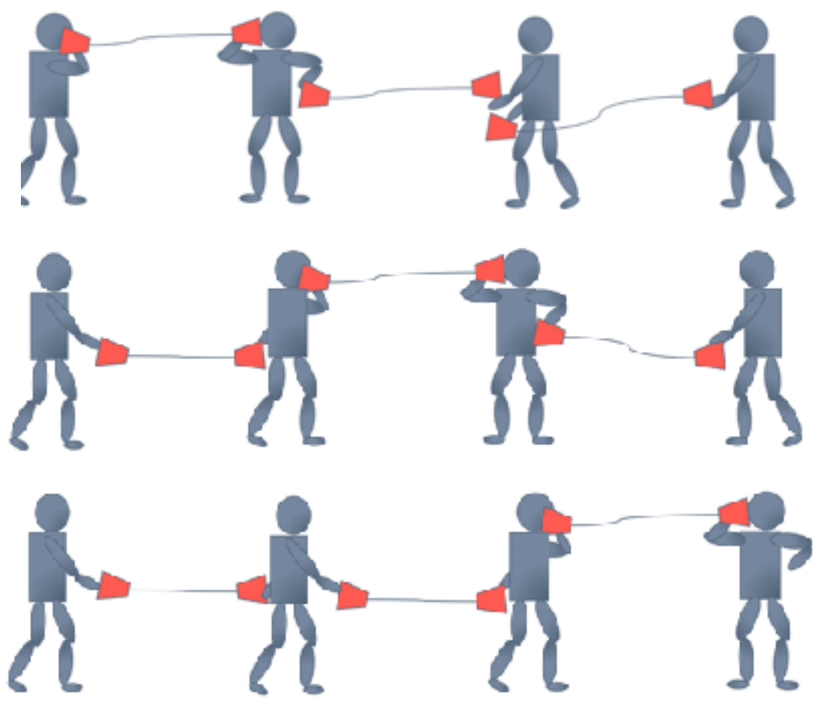
- A method of adaptive reparametrization, motivated by the difficulty of training very deep models
- Significantly reduces the problem of coordinating updates across many layers ("internal covariate shift")
- Reparametrize a minibatch of activations at any layer:

$$\boldsymbol{Z} = \boldsymbol{X}\boldsymbol{W}$$

$$\tilde{\boldsymbol{Z}} = \boldsymbol{Z} - \frac{1}{m}\sum_{i=1}^{m} \boldsymbol{Z}_{i,:}$$

$$\hat{\boldsymbol{Z}} = \frac{\tilde{\boldsymbol{Z}}}{\sqrt{\epsilon + \frac{1}{m}\sum_{i=1}^{m} \tilde{\boldsymbol{Z}}_{i,:}^2}}$$

$$\boldsymbol{H} = \max\{0, \boldsymbol{\gamma}\hat{\boldsymbol{Z}} + \boldsymbol{\beta}\}$$



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