

**10707**

# **Deep Learning: Spring 2021**

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Lecture 6: Advanced  
optimization

# Supervised learning

Empirical risk minimization approach:  
minimize a **training** loss  $l$  over a class of **predictors**  $\mathcal{F}$ :

$$\hat{f} = \operatorname{argmin}_{f \in \mathcal{F}} \sum_{(x,y): \text{training samples}} l(f(x), y)$$

Three pillars:

- (1) How expressive is the class  $\mathcal{F}$ ? (**Representational power**)
- (2) How do we minimize the training loss efficiently? (**Optimization**)
- (3) How does  $\hat{f}$  perform on unseen samples? (**Generalization**)

# Recap:continuous optimization

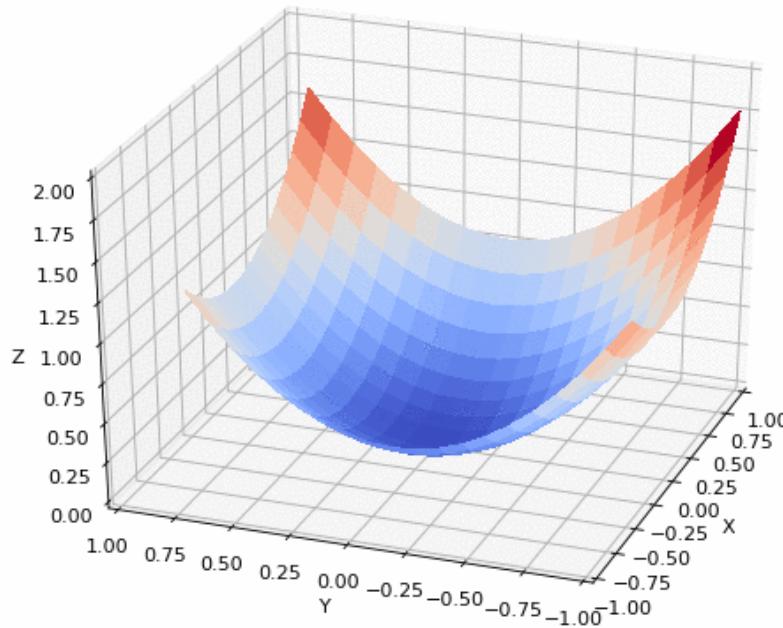
The typical training task in ML can be cast as:  $\min_{x \in \mathbb{R}^d} f(x)$

Most algorithms we will look at are iterative: they progressively pick points  $x_1, x_2, \dots$  that are supposed to bring “improvement”.

$$x_{t+1} = x_t - \eta \nabla f(x_t)$$

**Gradient descent**

# Recap:continuous optimization

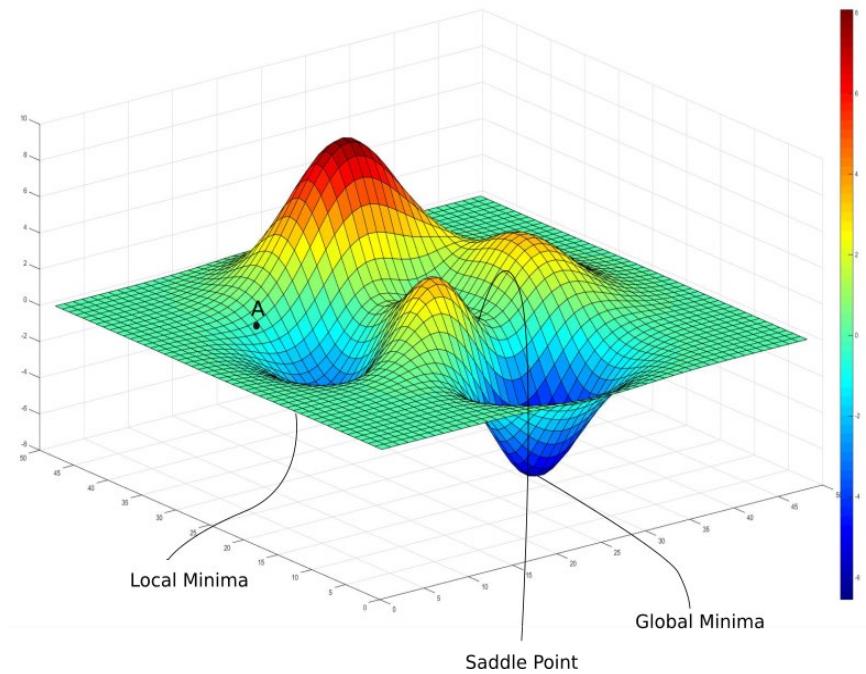


What can we hope for, in the case that  $\eta \rightarrow 0$ ?

We stop moving when  $\nabla f(x_t) \approx 0$ : these care called **stationary points**.

**What kinds of stationary points are there?**

# Recap:continuous optimization



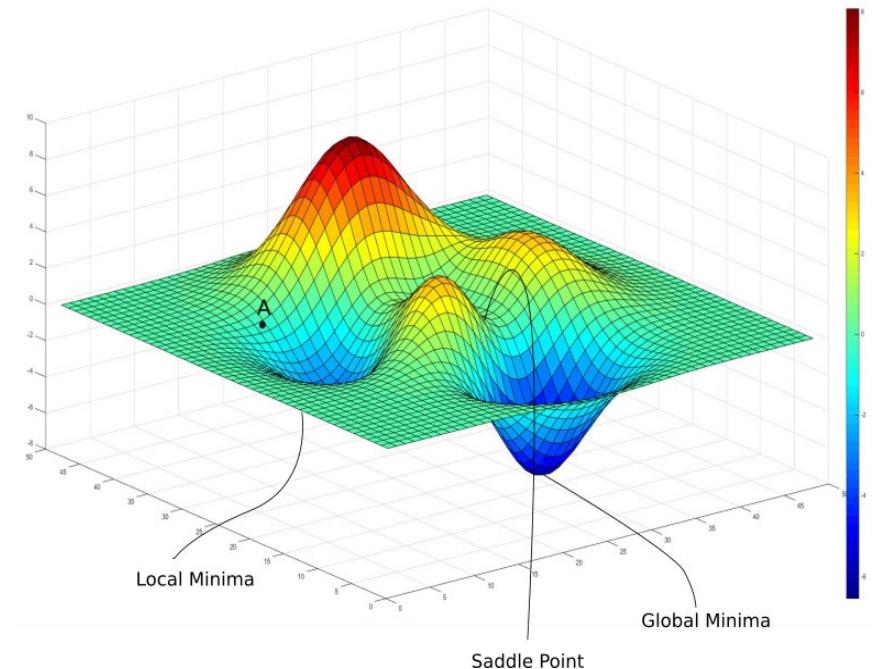
**Global minimum:** actual minimizer, namely  $f(\hat{x}) \leq f(x), \forall x \in \mathbb{R}^d$

**Local minimum:**  $f(\hat{x}) \leq f(x), \forall x$  s.t.  $\|x - \hat{x}\| \leq \epsilon$  for some  $\epsilon > 0$

**Local maximum:**  $f(\hat{x}) \geq f(x), \forall x$  s.t.  $\|x - \hat{x}\| \leq \epsilon$  for some  $\epsilon > 0$

**Saddle points:** stationary point that is \*not\* a local min/max.

# Recap:continuous optimization



**Global minimum:** finding these in general is very hard (both in theory – NP-hard, as well as in practice)

**Local minimum:** seem to work quite well often. Some theoretical understanding of why in very restricted cases.

**Saddle points:** typically bad, arise from invariances in input.  
Want to avoid these. (Stay tuned.)

# Why are local minima good?

**In short:** we don't know.

**Some results:**

*(Kawaguchi '16):* **Linear** neural networks (that is, neural networks with linear activation functions): **all local minima are also global minima.**

*(Hardt-Ma '18):* **Linear** residual networks (that is, ResNets with linear activation functions): **all stationary points are also global minima.**

**Evidence for the other side:**

*(Safran-Shamir '18, Yun-Sra-Jadbabie '19):* **Non-linear** nets with:

- Virtually any non-linearity.
- **Even** Gaussian inputs (about as simple as it gets)
- Labels **generated** by a neural net of the same architecture we are training can have **many** bad local minima.

**Overparametrization** (training larger net) breaks these examples.

# Why are local minima good?

**In short:** we don't know.

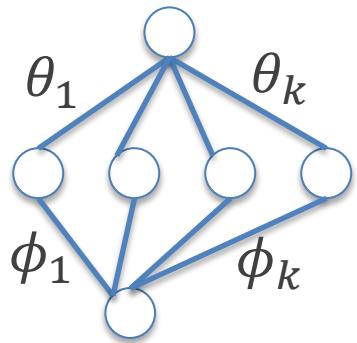
**Gradient descent w/ overparametrization:**

*(Allen-Zhu et al '18, Du et al '18):* **Sufficiently overparametrized** neural networks (that is neural nets with # parameters >> # of training samples, training from **random initialization**, converge to small **training error** solutions.

Interaction with **generalization** is still evolving/unclear.

# Intuition: saddle points arise due to symmetry

**Warning:** intuition only, not formal in any way!



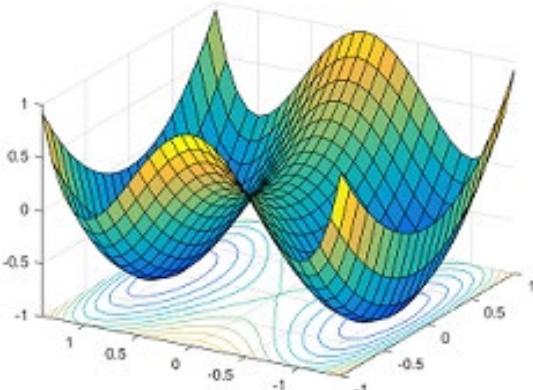
Permutation symmetry: loss function is  
 $f(\theta_1, \theta_2, \dots, \theta_k, \phi_1, \dots, \phi_k).$

Clearly same loss if we permute neurons, e.g.

$$f(\theta_3, \theta_1, \theta_2, \dots, \theta_k, \phi_3, \phi_1, \phi_2, \dots, \phi_k)$$

However, averaging likely will give different (larger) loss

$$f\left(\frac{\theta_1+\theta_3}{2}, \frac{\theta_2+\theta_1}{2}, \frac{\theta_3+\theta_2}{2}, \dots, \theta_k, \frac{\phi_1+\phi_3}{2}, \frac{\phi_2+\phi_1}{2}, \frac{\phi_3+\phi_2}{2}, \dots, \phi_k\right).$$



Isolated minima corresponding to permutations, connected via a “flat” region inbetween. (We’ll see later this intuition may be deficient in some ways.)

# First order methods on the cheap: stochastic gradient descent

In the supervised learning setup, function we are optimizing has the form of a sum:

$$\min_{\theta} \sum_{(x,y): \text{training samples}} l(f_{\theta}(x), y)$$

## Stochastic gradient descent

- **Initialize:**  $\theta_0 := \{W^{(1)}, b^{(1)}, \dots, W^{(L+1)}, b^{(L+1)}\}$
- For  $t=1$  to  $T$ 
  - Pick a uniformly random training example  $(x, y)$ :
  - Set  $\theta_{t+1} = \theta_t - \eta \nabla_{\theta} l(f_{\theta}(x), y))$



*Random variable w/ expectation true  
gradient*

# First order methods on the cheap: stochastic gradient descent

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$$\min_{\theta} \sum_{(x,y): \text{training samples}} l(f_{\theta}(x), y)$$

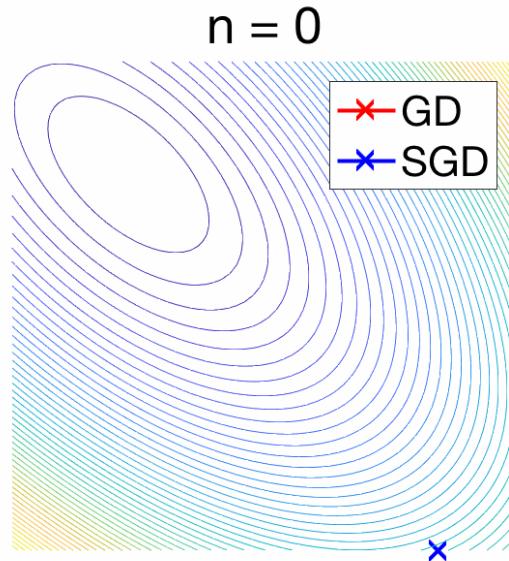
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*Actually, typically, one takes a **mini-batch** of  $B$  samples, and calculates gradient over those samples*

# First order methods on the cheap: stochastic gradient descent

Due to randomness, more jittery than gradient descent:



*Bug?* Longer convergence time

*Feature?* Regularization effect / better generalization.

*Feature?* Can help escape saddles.

# Recap: local minima

**Second order checks:** Hessian approximates a function to second order

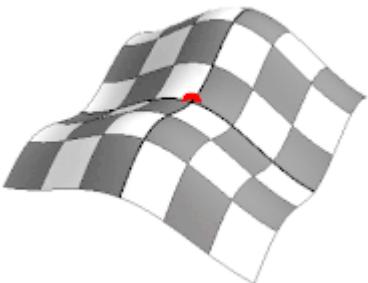
$$\begin{aligned}\textbf{Taylor's thm: } f(x + \Delta) &\approx f(x) + \Delta^T \nabla f(x) + \frac{1}{2} \Delta^T \nabla^2 f(x) \Delta + O(||\Delta||^3) \\ &\approx f(x) + \frac{1}{2} \Delta^T \nabla^2 f(x) \Delta + O(||\Delta||^3)\end{aligned}$$



If  $\nabla^2 f(x) > 0$ : for any direction  $\Delta$ , and small enough  $||\Delta||$

$$\Delta^T \nabla^2 f(x) \Delta + O(||\Delta||^3) \geq 0, \text{ so } f(x + \Delta) > f(x)$$

**Local minimum!** (Flipped for local maximum)



If  $\nabla^2 f(x)$  has both positive and negative eigenvalues:

**Saddle point** (not a local minimum/maximun)

**If neither of these attains, test is inconclusive!**

# First order methods on the cheap: stochastic gradient descent

**Feature:** can help escape (second-order) saddle points

- 🌀 Consider  $f(x) = \frac{1}{2}x^\top Ax$ , A is *strict saddle*: has **negative eval**
- 🌀 Gradient descent updates:  $x_{t+1} = x_t - \eta \nabla f(x_t) = (I - \eta A)x_t$
- 🌀 Write  $x_t = \sum_i \mu_i^t v_i$ , for the **eigenbasis**  $\{(v_i, \lambda_i)\}_i$  of A.
- 🌀 Then,  $x_{t+1} = \sum_i (1 - \eta \lambda_i) \mu_i^t v_i$
- 🌀 In other words,  $x_T = \sum_i (1 - \eta \lambda_i)^T \mu_i^0 v_i$

**In other words:** component in direction of negative eigenvalue grows  
– we don't get stuck!

Stochastic noise helps no component to get too small.

[Can be formalized for fresh noise, *Jin, Ge, Netrapalli, Jordan, Kakade '17*]

# Recap:continuous optimization

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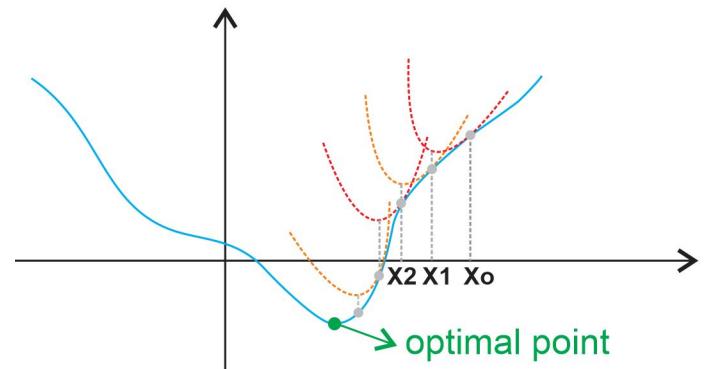
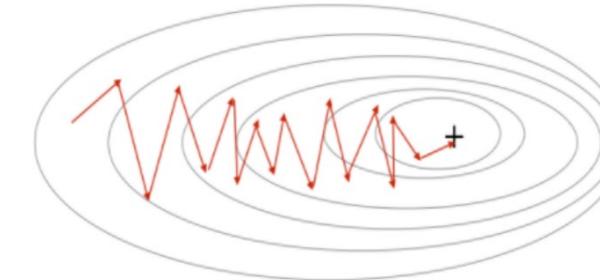
Most algorithms we will look at are iterative: they progressively pick points  $x_1, x_2, \dots$  that are supposed to bring “improvement”.

$$x_{t+1} = x_t - \eta \nabla f(x_t)$$

**Gradient descent**

$$\text{Set } x_{t+1} = x_t - \eta (\nabla^2 f(x_t))^{-1} \nabla f(x_t)$$

**Newton's method.**



# Second order methods on the cheap: AdaGrad

Recall the problem with Newton: inverting large matrices

$$\text{Set } x_{t+1} = x_t - \eta (\nabla^2 f(x_t))^{-1} \nabla f(x_t)$$

**Newton's method.**

**AdaGrad (simplified):** have a separate learning rate for every parameter

$$(G_t)_{ii} = \sqrt{\sum_{j=1}^{t-1} (\nabla f(x_t)_{ji})^2}, \quad \text{else 0}$$

$$\text{Set } x_{t+1} = x_t - \eta G_t^{-1} \nabla f(x_t),$$

$$(G_t)^{-1}_{ii} = \frac{1}{\sqrt{\sum_{j=1}^{t-1} (\nabla f(x_t)_{ji})^2}}, \quad \text{else 0}$$

# Second order methods on the cheap: RMSProp

AdaGrad (simplified): have a separate learning rate for every parameter

$$\text{Set } x_{t+1} = x_t - \eta G_t^{-1} \nabla f(x_t), \quad (G_t)_{ii} = \sqrt{\sum_{j=1}^{t-1} (\nabla f(x_t)_{ji})^2}, \quad \text{else 0}$$

**RMSProp**: since we keep summing the norms of the gradient, the learning rate could keep getting smaller. [NOTE: For convex functions, this is standard and in fact works.] Instead, keep a weighted exponential avg.

$$(g_{t+1})_i = \beta(g_t)_i + (1 - \beta)(\nabla f(x_t)_{ii})^2$$

$$(x_{t+1})_i = (x_t)_i - \frac{\eta \nabla f(x_t)_i}{\sqrt{(g_{t+1})_i}}$$

# Recap:continuous optimization

The typical training task in ML can be cast as:  $\min_{x \in \mathbb{R}^d} f(x)$

Most algorithms we will look at are iterative: they progressively pick points  $x_1, x_2, \dots$  that are supposed to bring “improvement”.

$$x_{t+1} = x_t - \eta \nabla f(x_t)$$

**Gradient descent**

*Linear combination of  
prior gradients + current one*

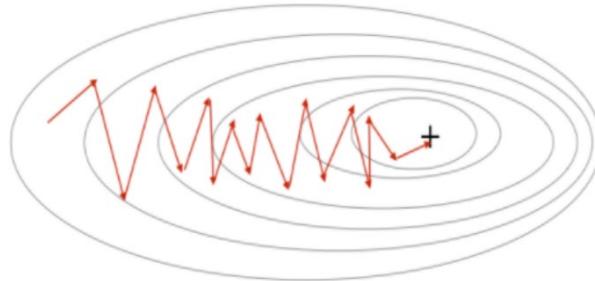
$$v_{t+1} = -\nabla f(x_t) + \beta v_t$$

$$x_{t+1} = x_t + \eta v_{t+1}$$

**Momentum  
(Polyak and Nesterov)**

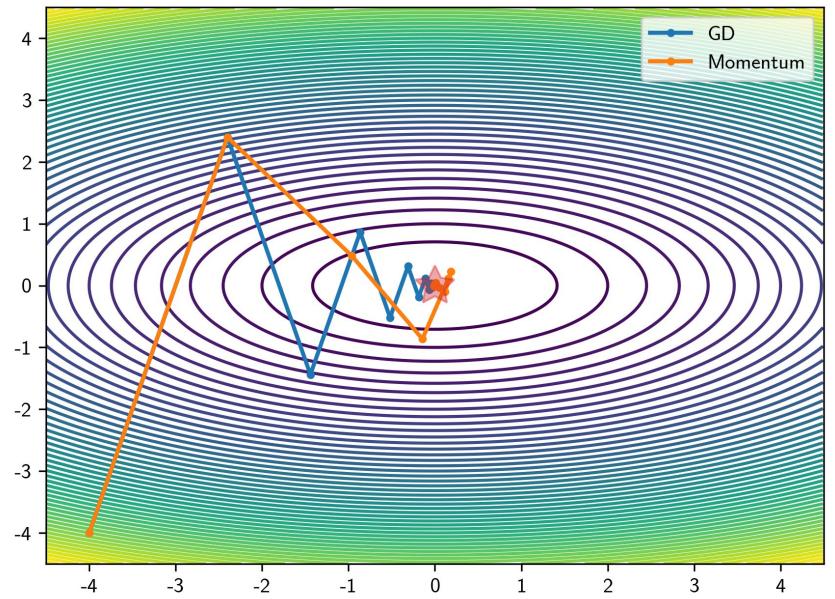
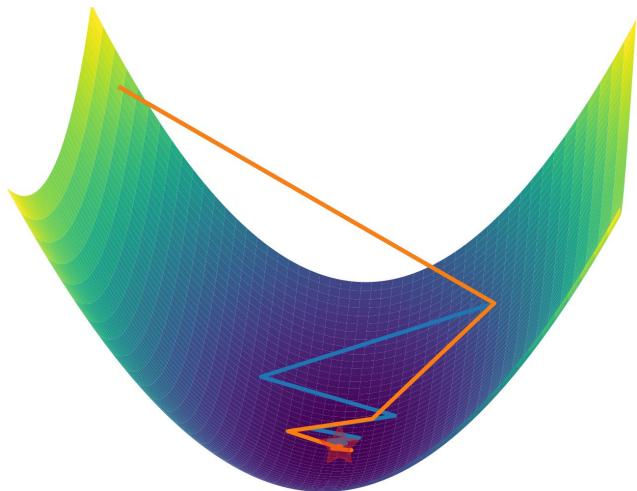
$$v_{t+1} = -\nabla f(x_t + \beta v_t) + \beta v_t$$

$$x_{t+1} = x_t + \eta v_{t+1}$$



*Evaluate gradient at a  
“lookahead” point*

# Recap:continuous optimization



**Momentum vs grad. descent**

<https://tangbinh.github.io/01/04/Optimizers.html>

# Momentum + AdaGrad = Adam

**Adam:** Frankenstein momentum and AdaGrad together:

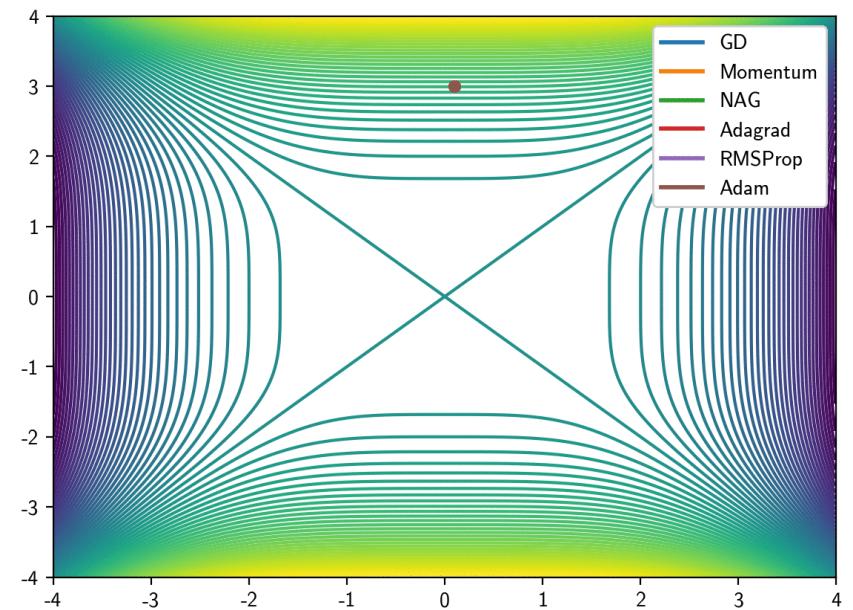
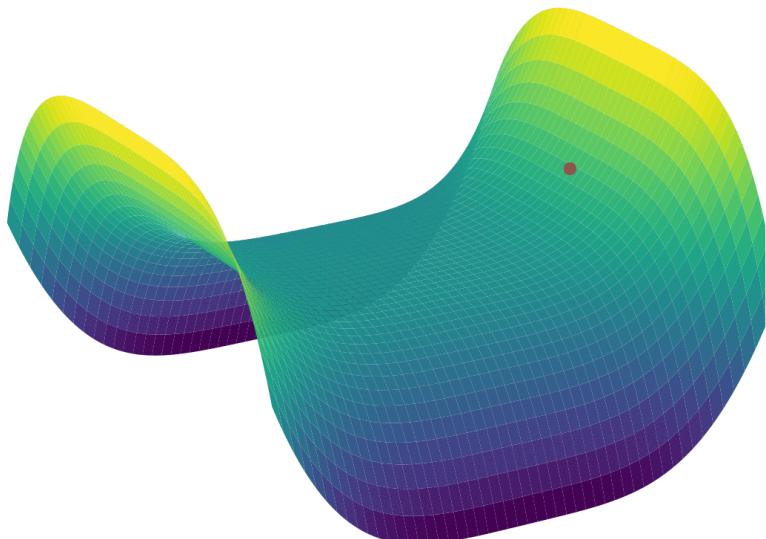
The diagram illustrates the Adam update rule as a combination of two components: Momentum and AdaGrad. It features three equations within a light blue rounded rectangle. The first equation,  $v_{t+1} = \beta_1 v_t + (1 - \beta_1) \nabla f(x_t)$ , is labeled 'Momentum' with a blue arrow pointing to it. The second equation,  $(g_{t+1})_i = \beta_2 (g_t)_i + (1 - \beta_2) (\nabla f(x_t))_{ii}^2$ , is labeled 'AdaGrad' with a blue arrow pointing to it. The third equation,  $(x_{t+1})_i = (x_t)_i - \frac{\eta v_{t+1}}{\sqrt{(g_{t+1})_i}}$ , is labeled 'Combine the two' with a blue arrow pointing to it.

$$v_{t+1} = \beta_1 v_t + (1 - \beta_1) \nabla f(x_t)$$
$$(g_{t+1})_i = \beta_2 (g_t)_i + (1 - \beta_2) (\nabla f(x_t))_{ii}^2$$
$$(x_{t+1})_i = (x_t)_i - \frac{\eta v_{t+1}}{\sqrt{(g_{t+1})_i}}$$

Default choice nowadays.

It actually does **not** converge, even on convex instances without some modification of updates. (*Reddi, Kale, Kumar, Best paper at ICLR '18*)

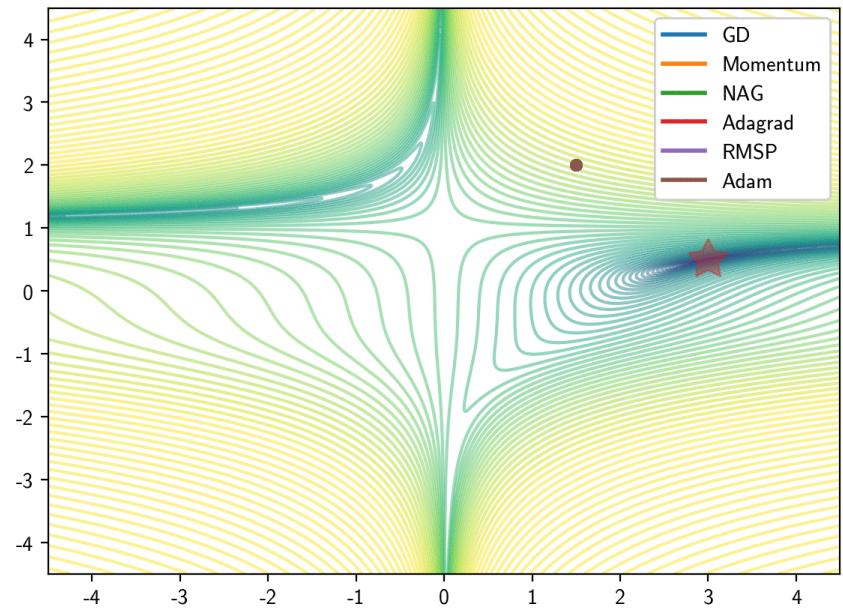
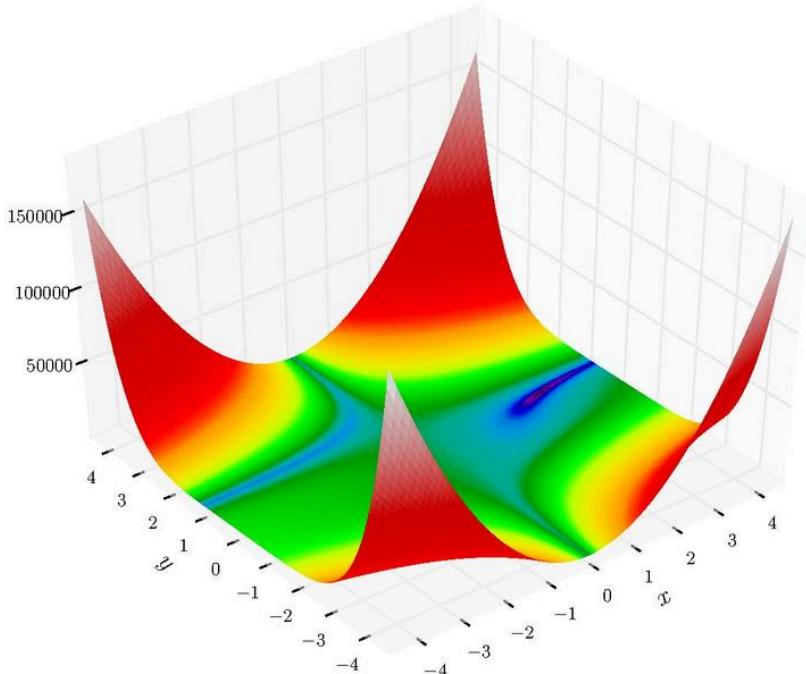
# Moving around saddles with various methods



<https://tangbinh.github.io/01/04/Optimizers.html>

Loss function  $f(x, y) = y^4 - x^4$ , saddle point at  $(0,0)$ , minimized at  $x=\infty$ .

# Beale's function using various methods

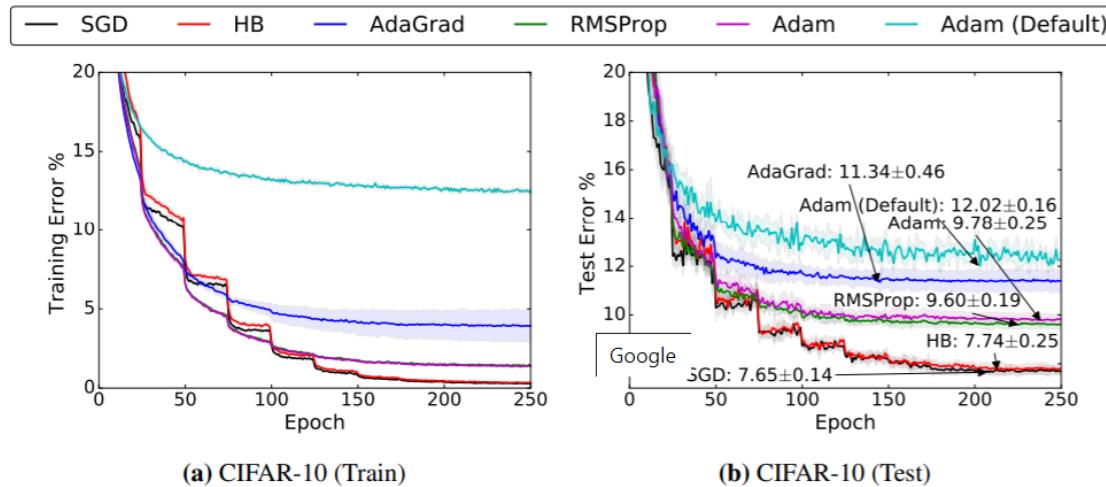


<https://tangbinh.github.io/01/04/Optimizers.html>

Beale's function minimized at (3,0).

# Are these actually helpful?

Remember, what we are trying to do is minimize \*test error\*. There's still the question of whether the solution generalizes well.



**Figure 1:** Training (left) and top-1 test error (right) on CIFAR-10. The annotations indicate where the best performance is attained for each method. The shading represents  $\pm$  one standard deviation computed across five runs from random initial starting points. In all cases, adaptive methods are performing worse on both train and test than non-adaptive methods.

*(Wilson, Roelofs, Stern, Srebro, Recht '18)*

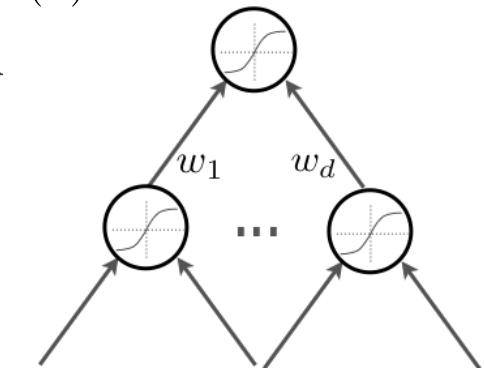
# Batch Normalization

Normalizing/whitening (mean = 0, variance = 1) the inputs speeds up training (*Lecun et al. 1998*)

- Could normalization be useful at the level of the hidden layers?

**Batch normalization** is an attempt to do that (*Ioffe and Szegedy, 2014*)

- each unit's pre-activation is normalized (mean subtraction, stddev division)
- during training, mean and stddev is computed for each minibatch
- backpropagation takes into account the normalization
- at test time, the global mean / stddev is used



# Batch Normalization

**Input:** Values of  $x$  over a mini-batch:  $\mathcal{B} = \{x_{1\dots m}\}$ ;

Parameters to be learned:  $\gamma, \beta$

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

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

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

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

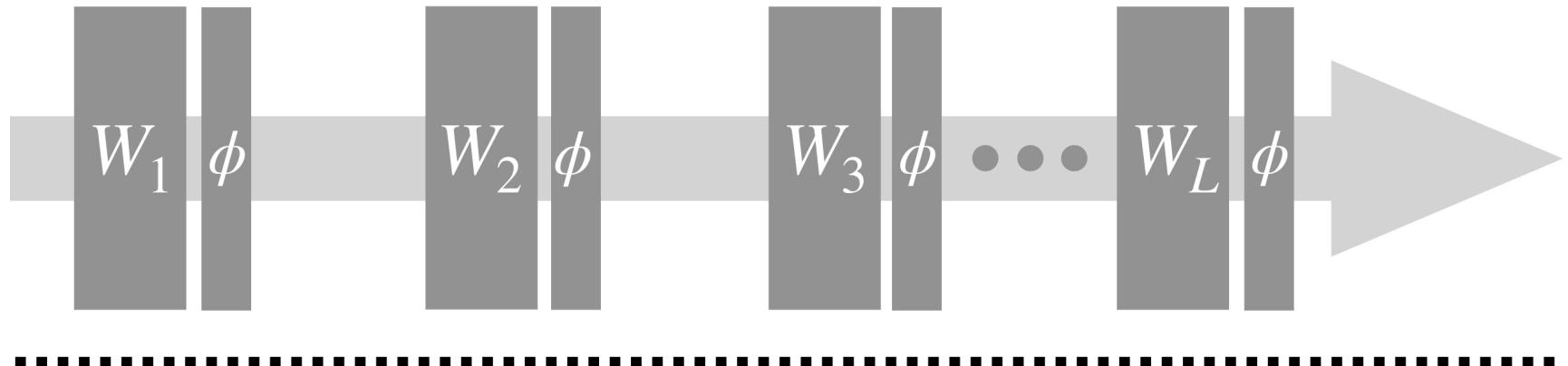
$$y_i \leftarrow \gamma \hat{x}_i + \beta \equiv \text{BN}_{\gamma, \beta}(x_i) \quad // \text{scale and shift}$$



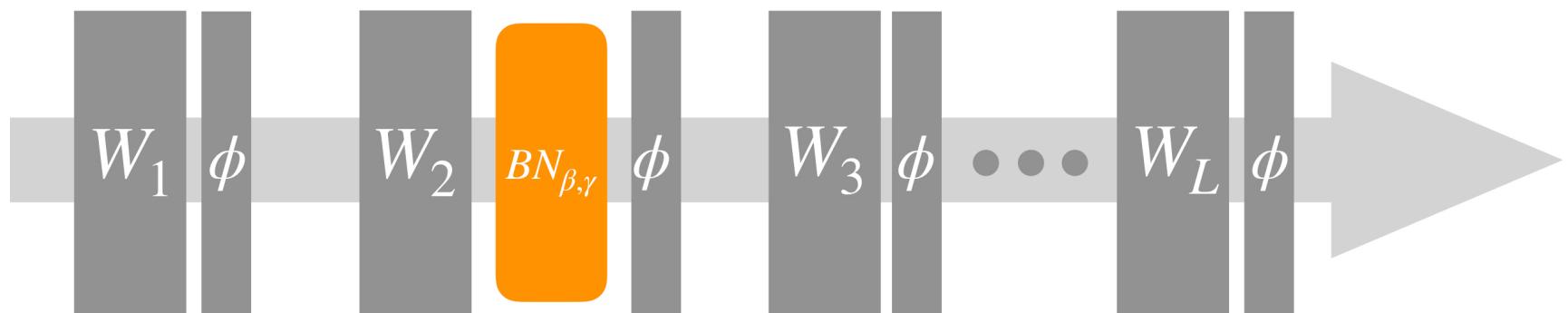
Learned linear transformation to adapt to non-linear activation function ( $\gamma$  and  $\beta$  are trained)

# Batch Normalization

## Standard Network

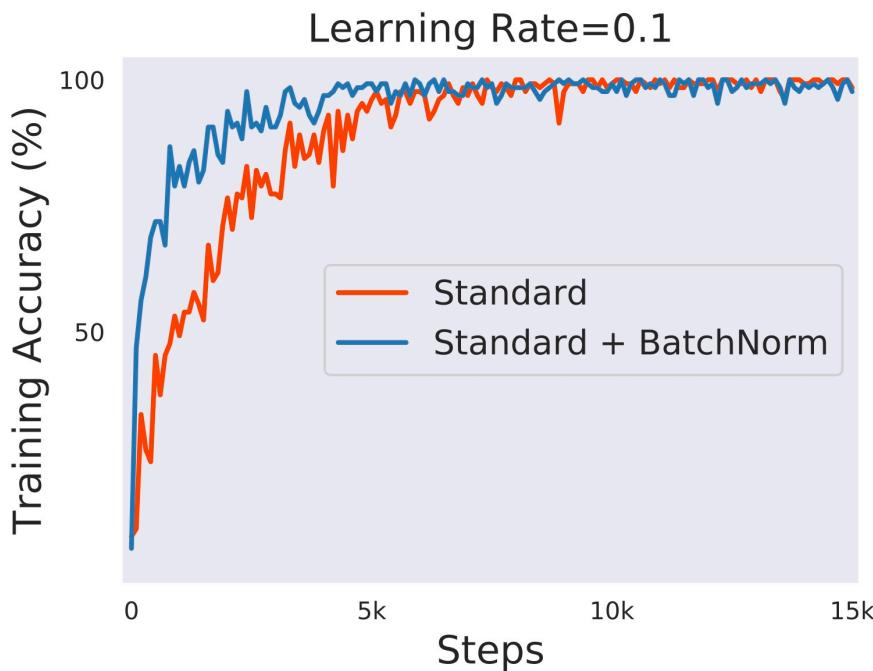


**Adding a BatchNorm layer (between weights and activation function)**



<http://gradientscience.org/batchnorm/>

# Batch Normalization



<http://gradientscience.org/batchnorm/>

# Batch Normalization

Why normalize the pre-activation?

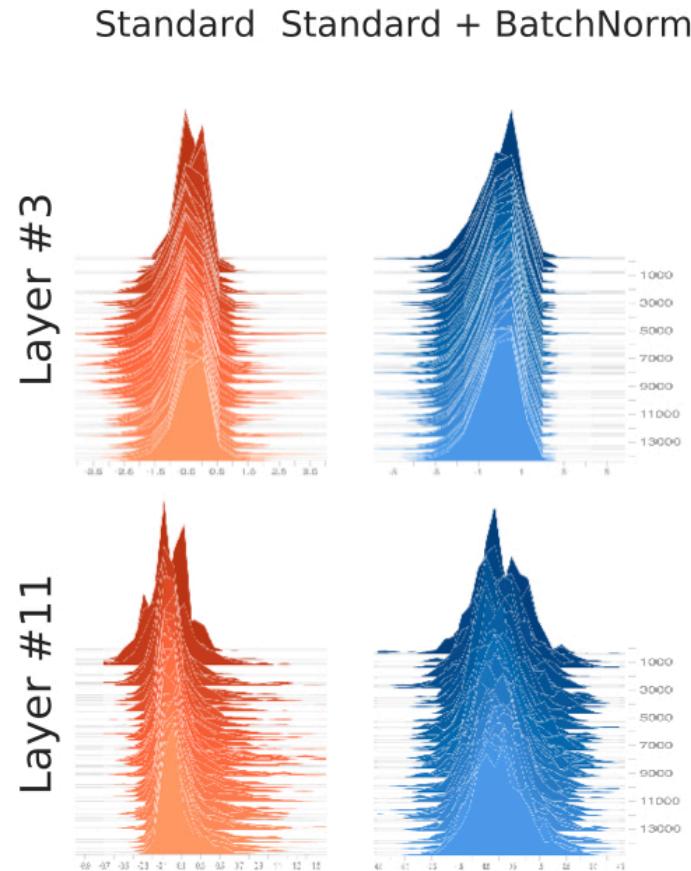
- Can help keep the pre-activation in a non-saturating regime
- Could condition Hessian better (in linear 1-layer nets, *Lecun et al. 1998*)

Why use minibatches?

- since hidden units depend on parameters, can't compute mean/stddev once and for all
- adds stochasticity to training, which might regularize

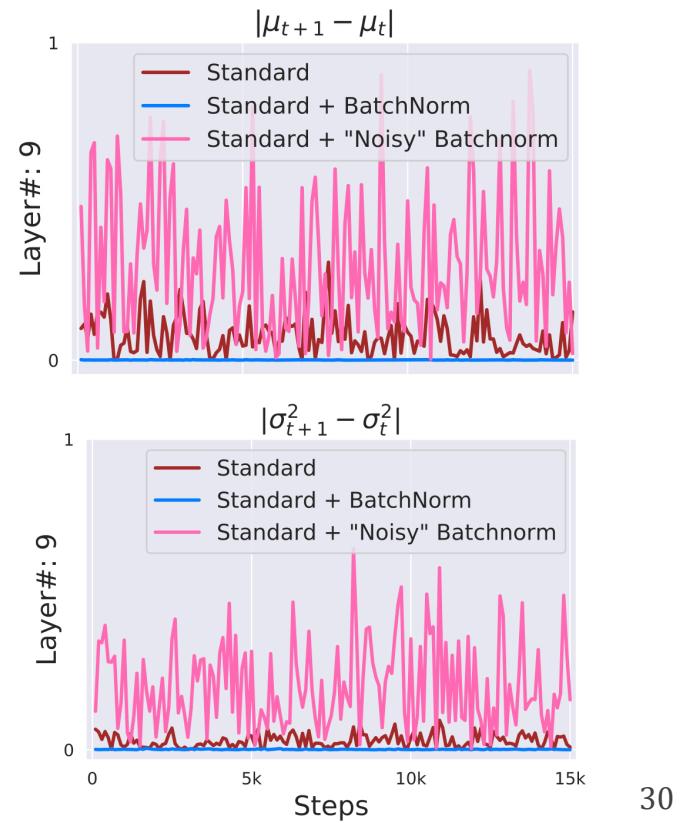
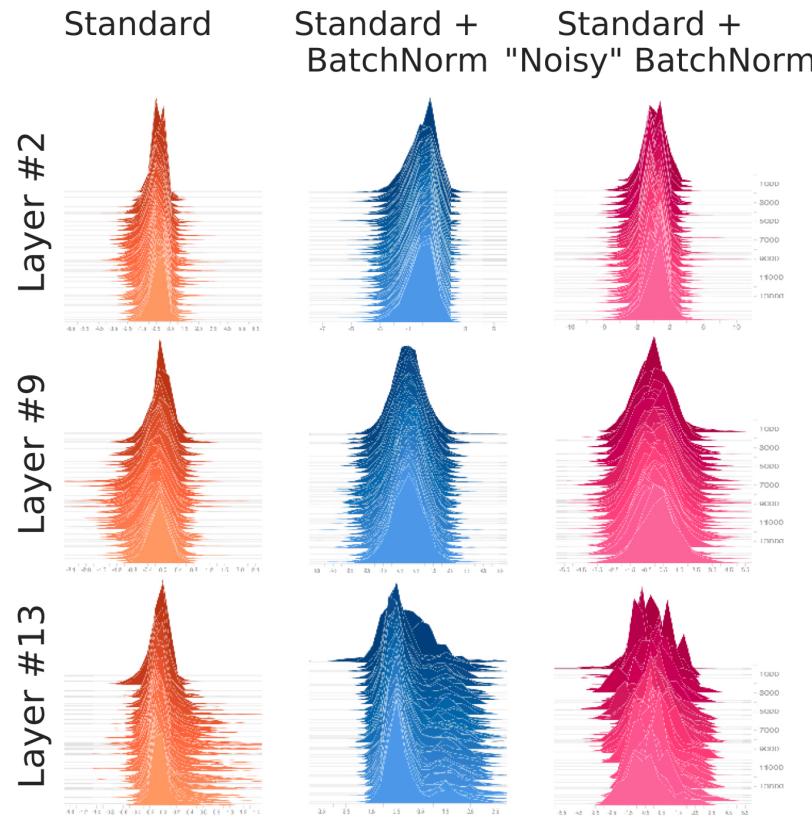
# Batch Normalization

Recent observations cast some doubts on distribution shift explanation  
(*Santurka, Tspiras, Ilyas, Madry '18*)



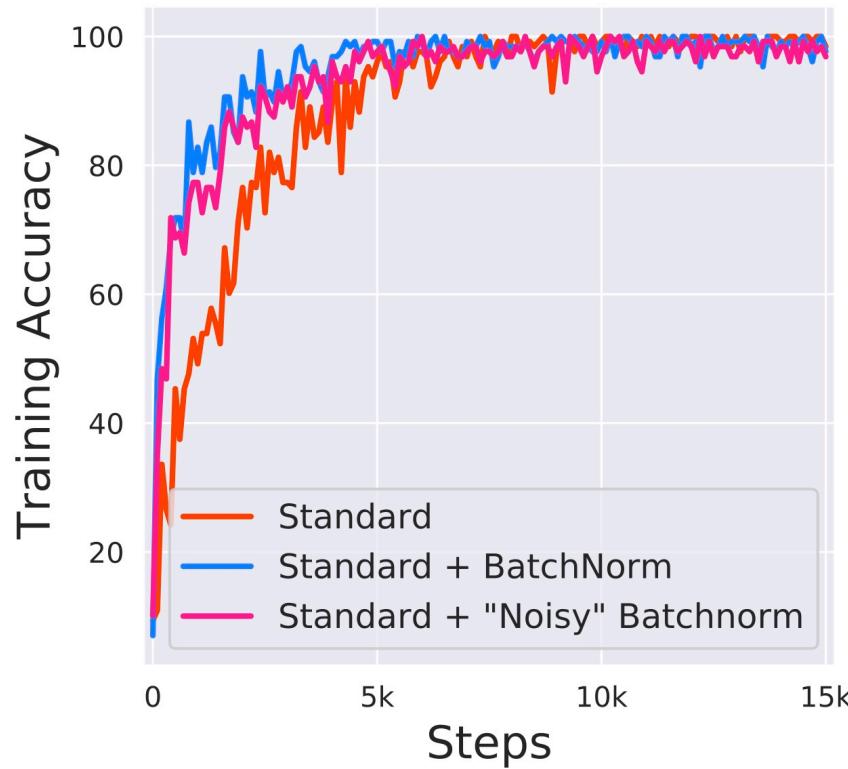
# Batch Normalization

Simple experiment: inject non-stationary Gaussian noise after BN layer.  
This removes the alleged whitening effect of BN layers.



# Batch Normalization

Simple experiment: inject non-stationary Gaussian noise after BN layer.  
This removes the alleged whitening effect of BN layers.



Performance doesn't suffer...

# Batch Normalization

*Authors suggestions (can be formalized):*

**Lipschitz constant** of the loss improves.

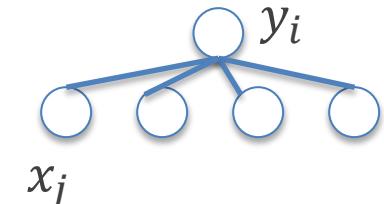
The **Hessian** evaluated in the direction of the gradient (i.e. second-order term in the Taylor expansion *decreases* in magnitude.  
[i.e. first-order term gets comparatively bigger]

# Initialization

**Warning:** lots of handwaving, intuitions

Typically, the goal of initialization is to make sure the non-linearities are in the “active” (linear) regime.

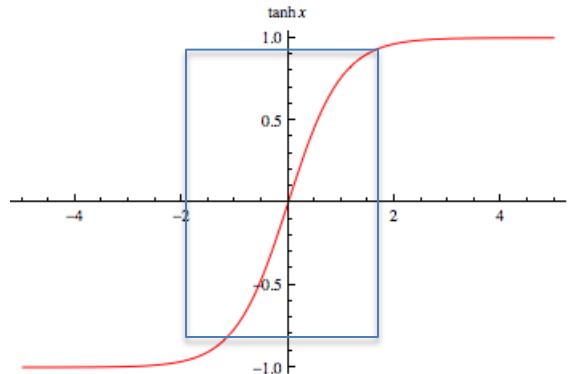
**LeCun initialization:**  $\mathbb{E}[w_{ij}] = 0, \text{Var}[w_{ij}] = \frac{1}{\text{fan-in}}$



If  $x_i$ 's are 0-mean, var-1, and  $y_i = \sum_j w_{ij}x_j, \mathbb{E}[y_i] = 0, Var(y_i) = \sqrt{w_{ij}^2}$

Gradient of tanh is around 1 in the linear regime.

So,  $\tanh(y_i)$  has variance 1.



# Initialization

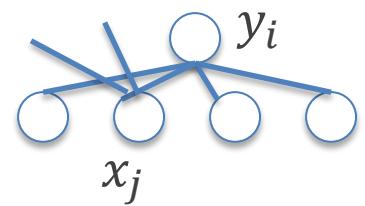
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Typically, the goal of initialization is to make sure the non-linearities are in the “active” (linear) regime.

**Xavier** initialization:  $\mathbb{E}[w_{ij}] = 0, \text{Var}[w_{ij}] = \frac{2}{\text{fan-in} + \text{fan-out}}$

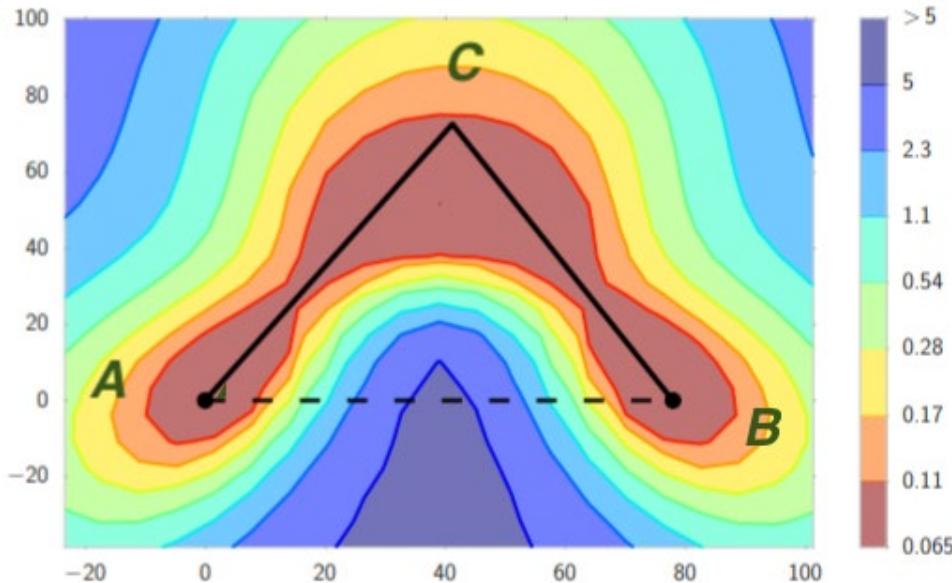
(e.g.:  $N\left(0, \frac{2}{\text{fan-in} + \text{fan-out}}\right)$ ,  $\text{unif}\left(\left[\frac{-\sqrt{6}}{\sqrt{\text{fan-in} + \text{fan-out}}}, \frac{\sqrt{6}}{\sqrt{\text{fan-in} + \text{fan-out}}}\right]\right)$ ,

Same argument as before, except when doing backprop,  
we take transposes of matrices. So, this keeps  
“backproped” activations also in the active regime.



# Surprises: mode connectivity

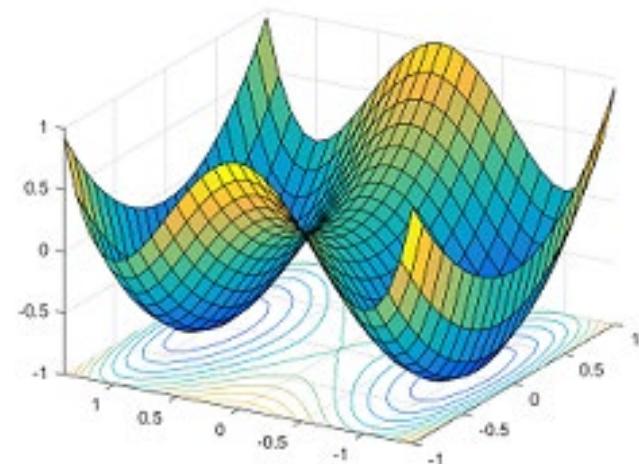
(*Freeman and Bruna, 2016, Garipov et al. 2018, Draxler et al. 2018*): Local minima can be connected by simple paths of near-same cost.



**Surprising!**

Remember our intuition,  
permutations should give  
rise to isolated solutions

Some explanations due to [*Kuditipudi et al '19*]: robustness of the network to “dropping out” some neurons can ensure this.



# Surprises: lottery hypothesis

(Frankle, Carbin ICLR '20, Best paper award): Typical neural nets have **much** smaller subnetworks that “could have been trained” in isolation to give comparable results.

More precisely, the following works reliably:

1. Initialize a network and train it.
2. “Prune” superfluous structure. (e.g. smallest weights)
3. Reset unpruned weights to values in 1.
4. Repeat 2+3.

B/w 15% and 1% of the original network!

The small network won the “**initialization lottery**” – it could’ve been trained to a good network w/o rest of weights.

We’re training networks that are way larger than in principle necessary!