# Strojové učení II

## Deep Feedforward Networks

Institute of Information Theory and Automation of the AS CR

# Cost Function

- Training data: $(x, y) \sim \hat{p}(x, y)$
- NN represents a function $f(x; \theta)$
- NN outputs $f(x; \theta)$ are not direct predictions of y
- You define $q(y|x; \theta)$
- ML principle give us the cost function as $-\log q(y|x; \theta)$
- NN provides parameters (e.g. mean) of $q(y|x; \theta)$

# Conditional Log-likelihood

- Empirical distribution of training data $(x, y) \sim \hat{p}(x, y)$

$$(\mathbb{X}, \mathbb{Y}) = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$$

$$\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} q(\mathbb{Y}|\mathbb{X}, \boldsymbol{\theta})$$

$$= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{m} \log q(y^{(i)}|x^{(i)}, \boldsymbol{\theta})$$

$$\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} \mathbb{E}_{(x,y)\sim\hat{p}(x,y)} \log q(y|x, \boldsymbol{\theta})$$

# Example – Gaussian Model

- Training data distribution: $p(x, y) = p(y|x)p(x)$
- Estimator of y: $f(x; \theta)$
- Model distribution: $q(y|x) \equiv N(y|f(x; \theta), \sigma^2)$

$$\hat{\theta} = \arg\min_{\theta} \mathbb{E}_{p(x,y)}[-\log q(y|f(x; \theta))]$$

$$L(\theta) = \int \left[ \int (y - f(x; \theta))^2 p(y|x) dy \right] p(x) dx + c$$

$$\frac{\partial L}{\partial \theta} \propto \mathbb{E}_{p(x)} \left[ \left( \mathbb{E}_{p(y|x)}[y] - f(x; \theta) \right) \times \frac{\partial f}{\partial \theta} \right] = 0$$

$$f(x; \hat{\theta}) = \mathbb{E}_{p(y|x)}[y]$$

# Linear Regression

- Training data: $p(x,y) \rightarrow \{(x^{(1)}, y^{(1)}), \ldots, (x^{(N)}, y^{(N)})\}$
- Linear estimator of y: $f(x) = wx + b \qquad \theta = \{w, b\}$
- Model distribution: $q(y|x) \equiv N(y|f(x;\theta), \sigma^2)$

$$\hat{\theta} = \arg\min_{\theta} \mathbb{E}_{p(x,y)}[-\log q(y|f(x;\theta))]$$

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{2\sigma^2} \sum_i (y^{(i)} - f(x^{(i)};\theta))^2 + \mathrm{c}$$

$$\arg\min_{w,b} \frac{1}{2\sigma^2} \sum_i (y^{(i)} - wx^{(i)} - b)^2 + \mathrm{c}$$

- Closed-form solution

# Example – Laplace Model

- Training data distribution: $p(x, y) = p(y|x)p(x)$
- Estimator of y: $f(x; \theta)$
- Model distribution: $q(y|x) \equiv \mathrm{Laplace}(y|f(x;\theta), \gamma)$

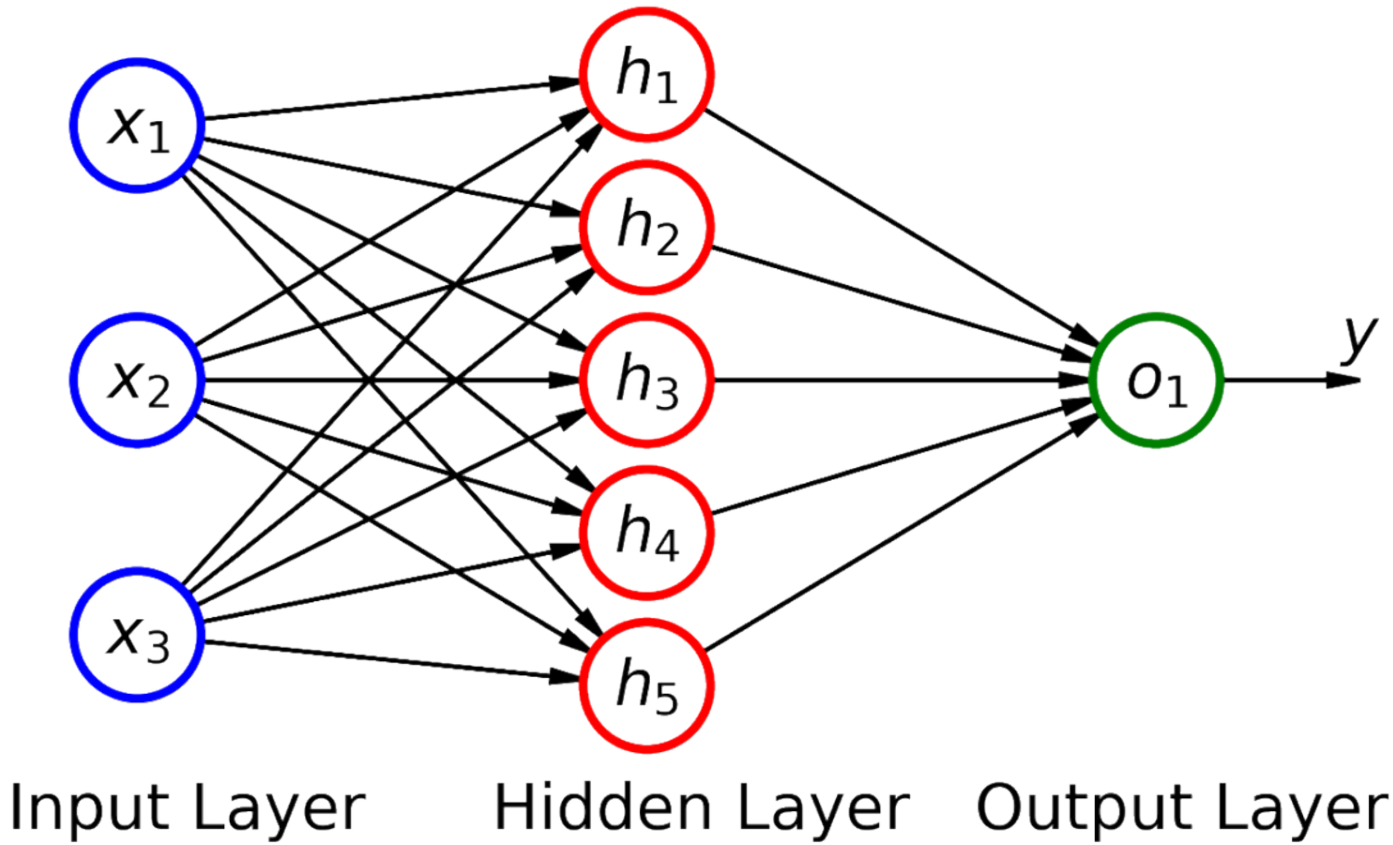
$$\hat{\theta} = \arg\min_{\theta} \mathbb{E}_{p(x,y)}[-\log q(y|f(x;\theta))]$$

$$L(\theta) = \int \left[ \int |y - f(x;\theta)|\, p(y|x) dy \right] p(x) dx + c$$

$$\frac{\partial L}{\partial \theta} \propto \mathbb{E}_{p(x)} \left[ \int \mathrm{sign}(y - f(x;\theta)) p(y|x) dy \times \frac{\partial f}{\partial \theta} \right] = 0$$

$f(x;\hat{\theta}) = m$ … median: $P(y \leq m|x) = P(y \geq m|x)$

# Feedforward Network



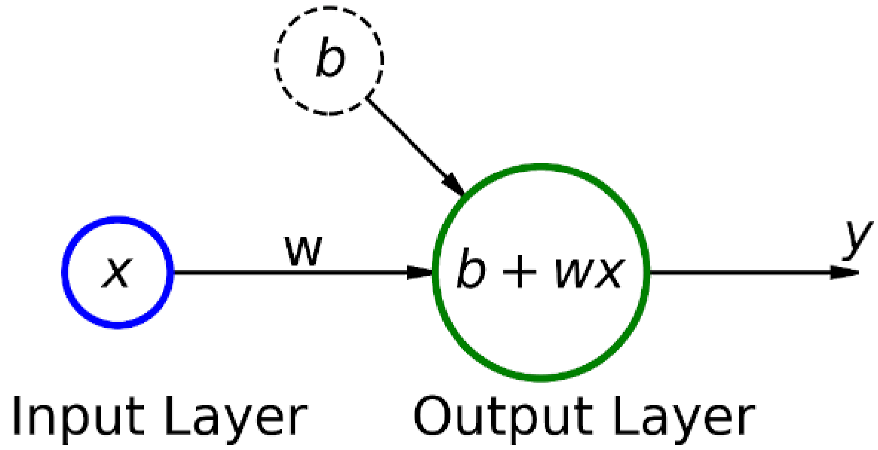
# Output Units

- Linear
- Sigmoid
- Softmax
- Softplus

# Linear Unit

- Affine transformation with no nonlinearity

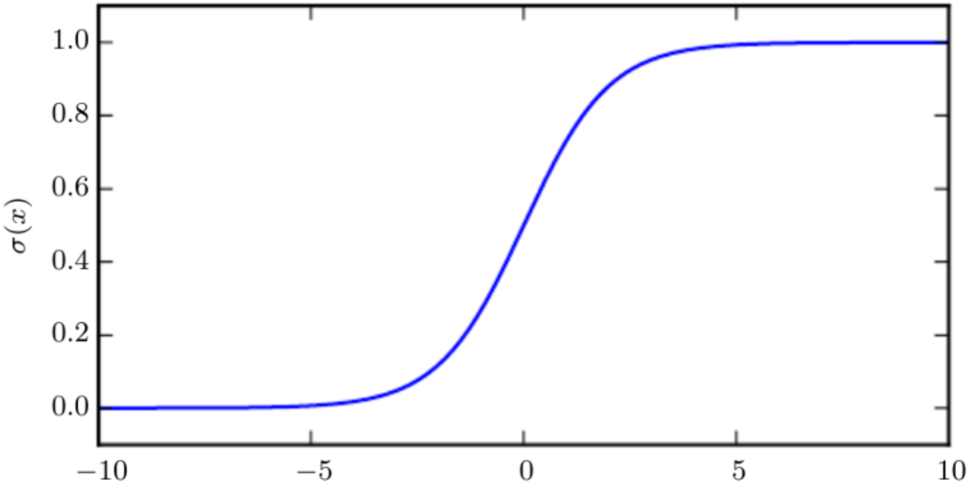
$$y = Wx + b$$




- e.g. predict mean of a Gaussian distribution

# Sigmoid

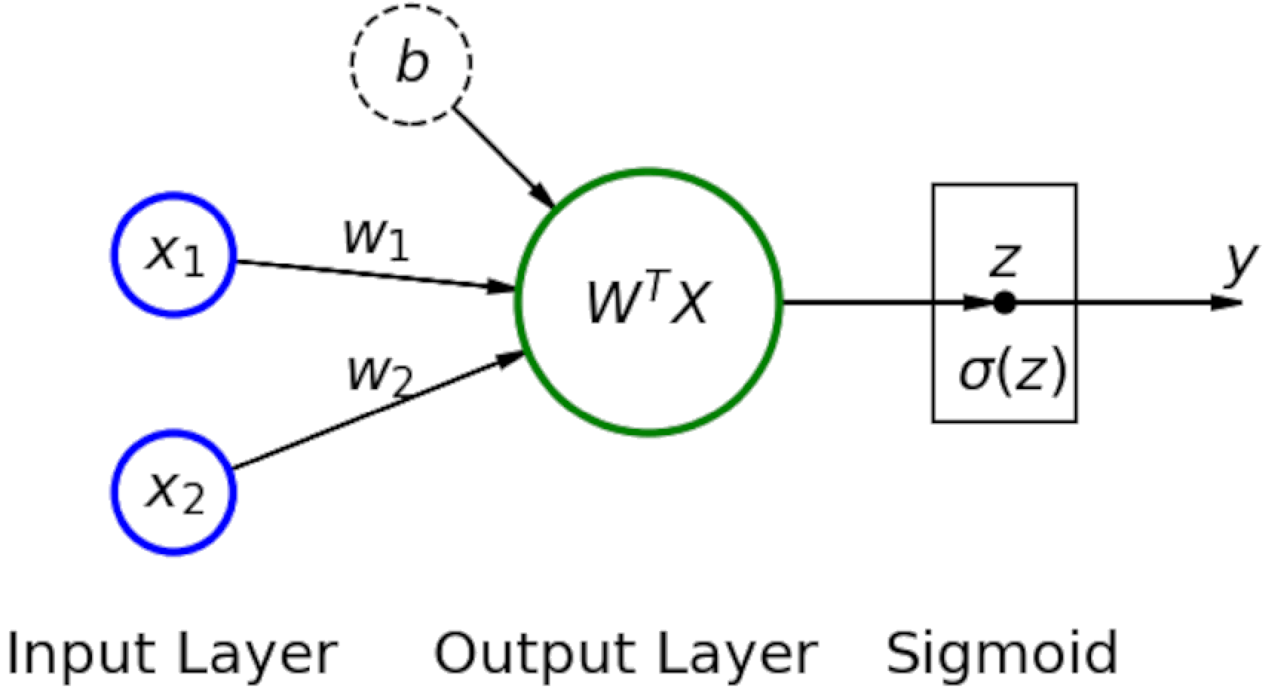
- Values in range (0,1)




$$\sigma(x) = \frac{1}{1+e^{-x}}$$

# Sigmoid output unit

- Predicting probability
- Ideal for Bernoulli output distributions



# Softmax

- Generalization of sigmoid
- Multi-class classification

$$z = Wx + b$$

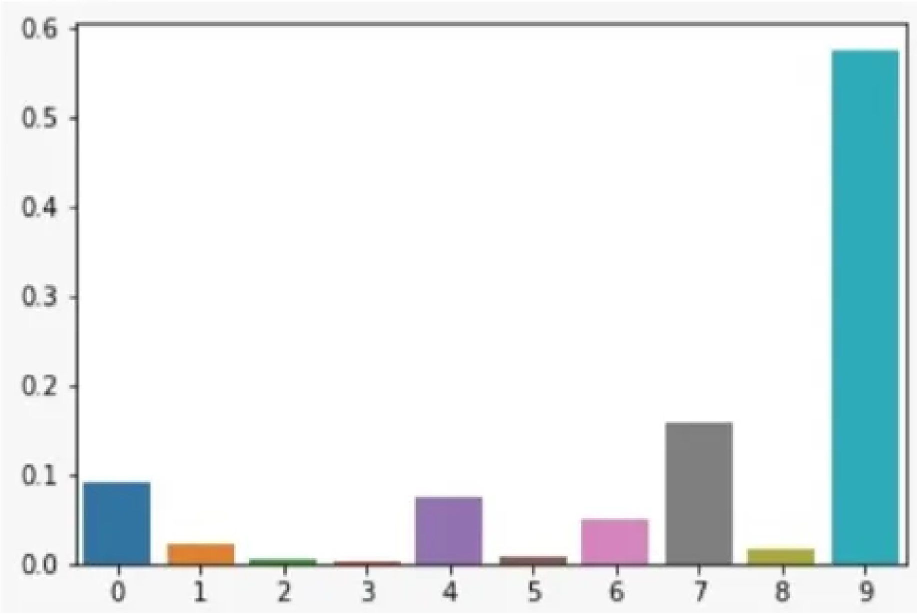
$$\mathrm{softmax}(\mathbf{z})_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

$$0 < \mathrm{softmax}(\mathbf{z})_i < 1 \qquad \sum_i \mathrm{softmat}(\mathbf{z})_i = 1$$

# Softmax

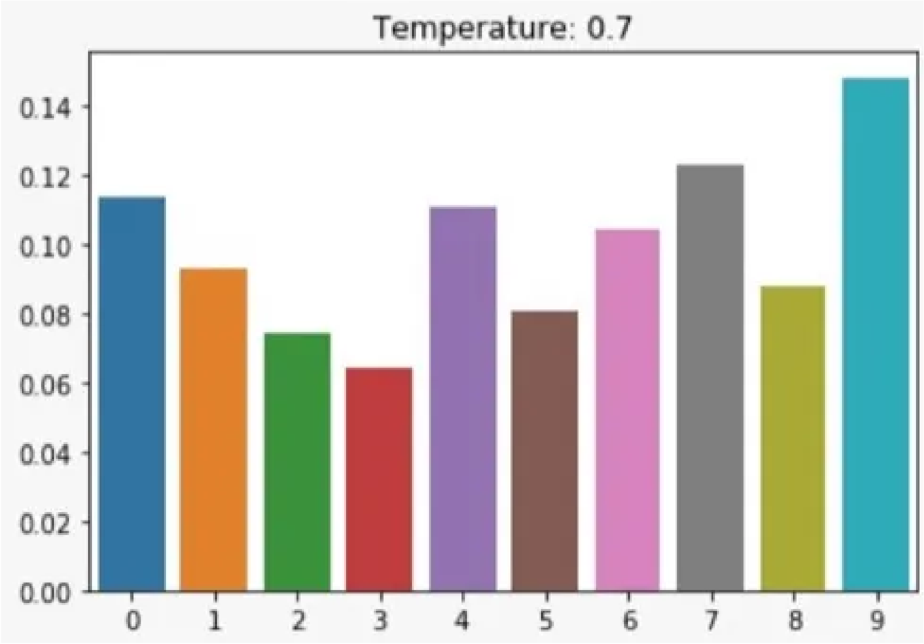
Softmax without temperature (T=1)

$$\frac{\exp(z_i)}{\sum_j \exp(z_j)}$$




Softmax with temperature

$$\frac{\exp(z_i/T)}{\sum_j \exp(z_j/T)}$$




Low entropy

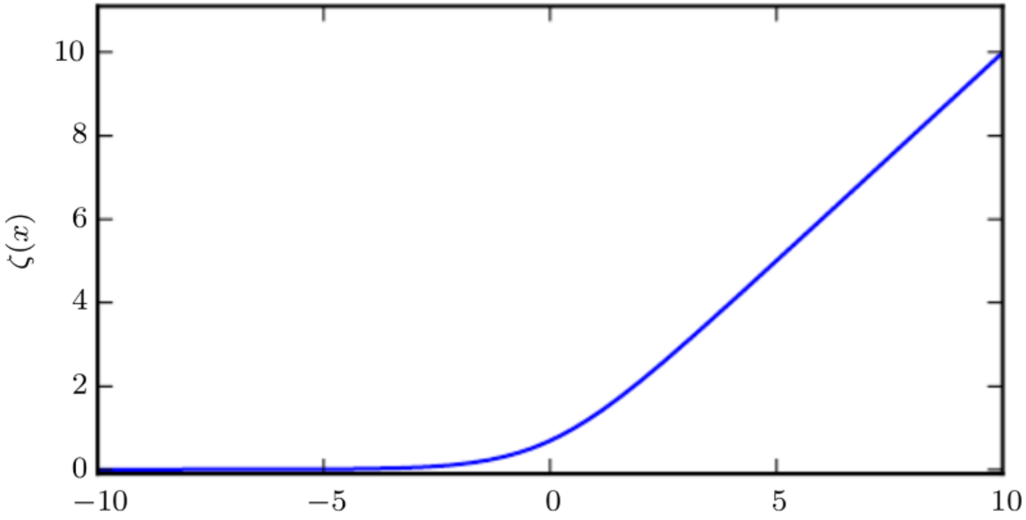
Increase in entropy

with increase in T

High entropy

# Softplus

- Non-negative values




$$\zeta(x) = \int_{-\infty}^{x} \sigma(y)dy$$

# Hidden Units

- Linear units with non-linear activation functions
- Activation functions:
  - Logistic Sigmoid
  - Hyperbolic Tangent

  old days

  - Rectification

  current

# Linear Layers

- Multiple linear layers <=> single linear layer

$$y_1 = W_1 x + b_1$$

$$y_2 = W_2 y_1 + b_2$$

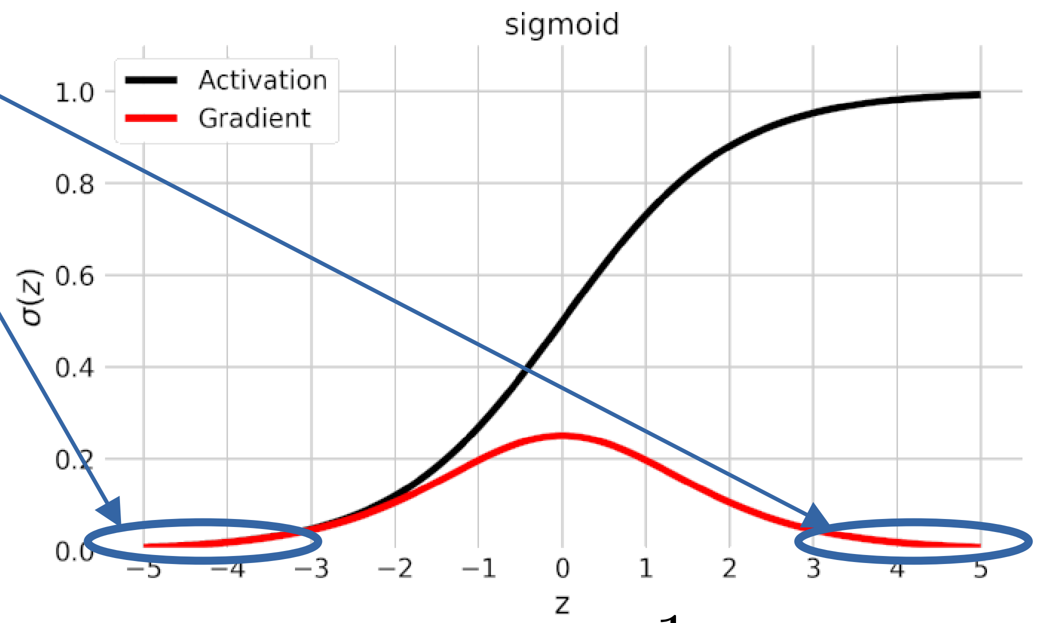
$$y_N = W_N y_{N-1} + b_N = W_N(W_{N-1}(\ldots) + b_{N-1}) + b_N$$

$$y_N = Wx + b$$

- We need a non-linear step in hidden units to go beyond!

# Sigmoid

Region of saturation



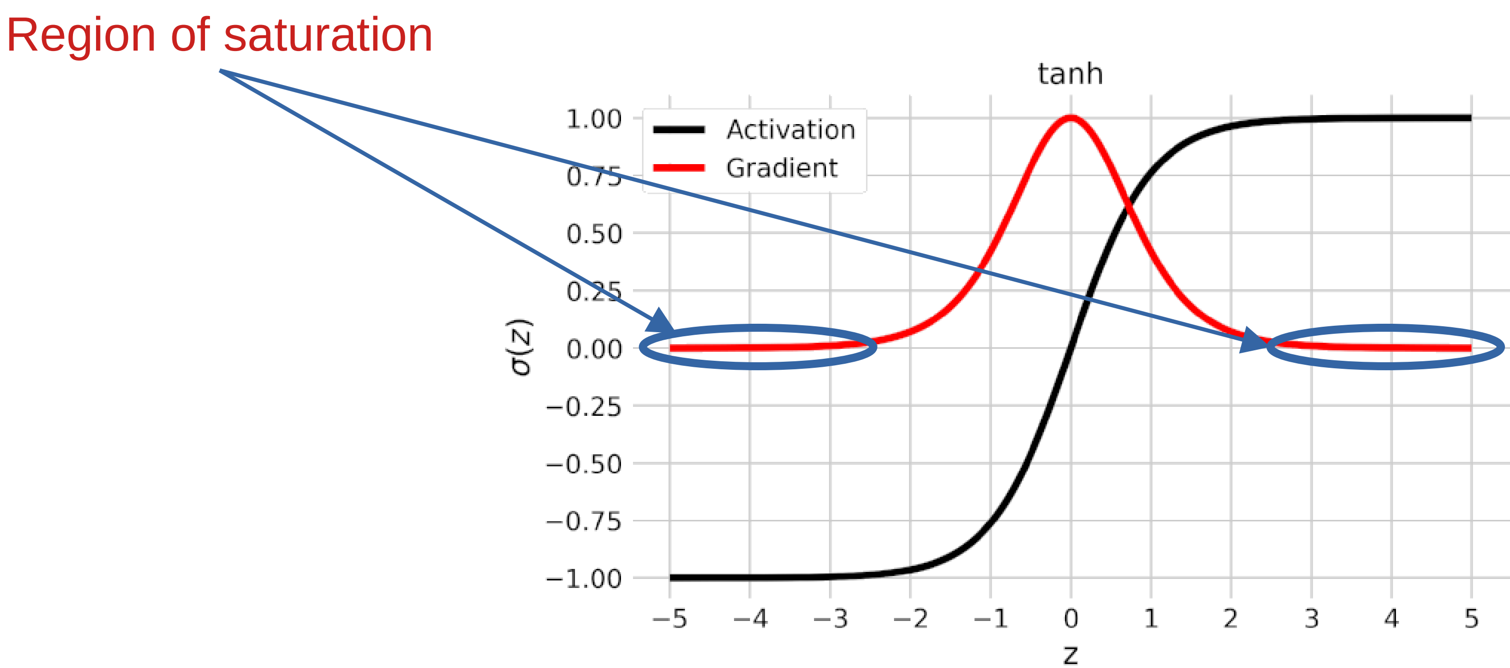

$$\sigma(z) = \frac{1}{1+e^{-z}}$$

- Cons: $\sigma(0) \neq 0$ shifted

  $\sigma'(0) = 0.25 < 1$

  vanishing gradient for small and large inputs

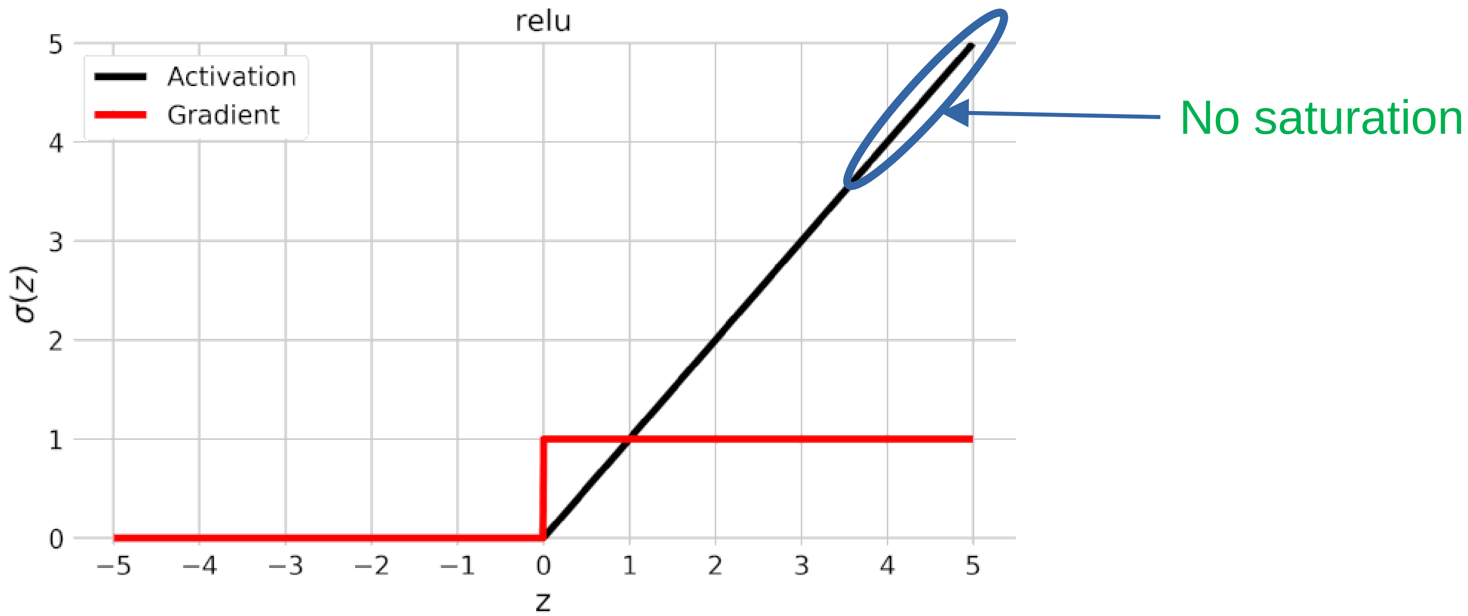
# Hyperbolic Tangent




$$\sigma(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

- Pros: $\sigma(0) = 0$ symmetric
  $\sigma'(0) = 1$
- Cons: vanishing gradient for small and large inputs

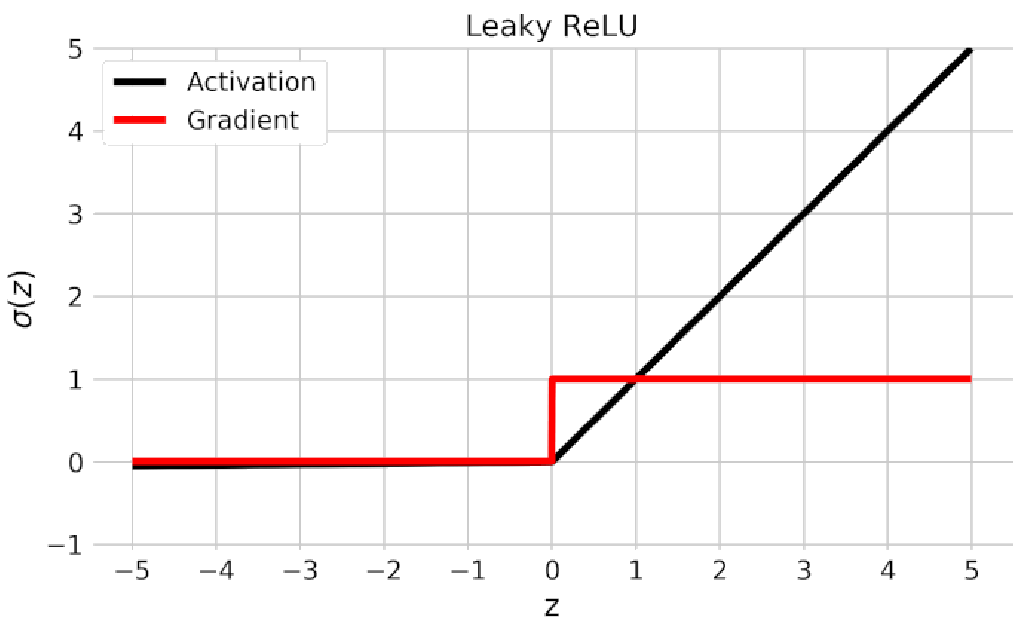
# ReLU




$$\sigma(z) = \max\{0, z\}$$

- Pros: derivatives in the positive domain are all 1
- Cons: output is not symmetric (internal covariate shift)
  “dead neuron” problem

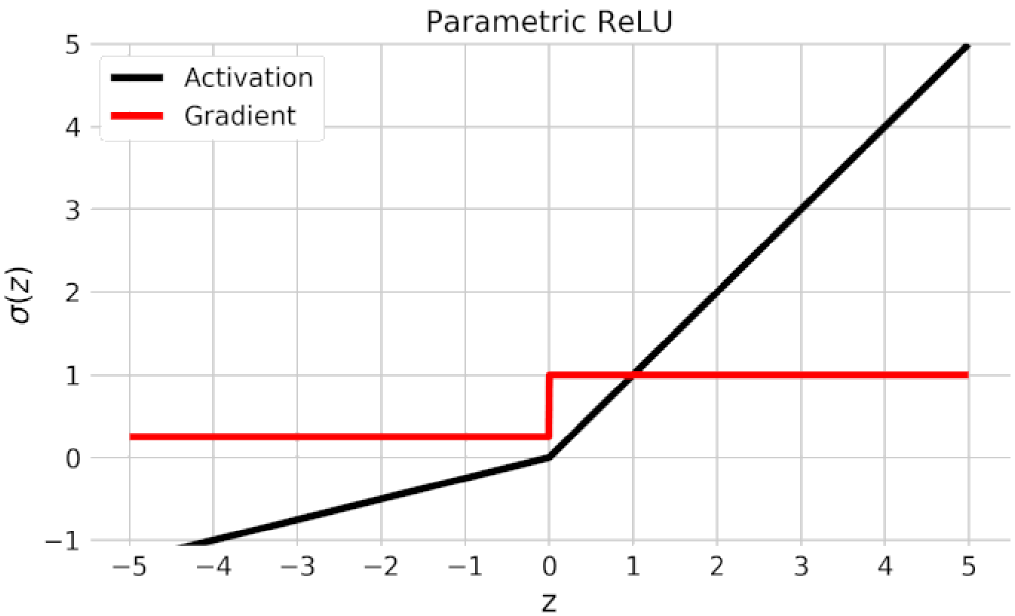
# Leaky ReLU




$$\sigma(z) = \max\{0, z\} + 0.01 \min\{0, z\}$$

- Pros: same as ReLU but solves "dead neuron" problem

# Parametric ReLU

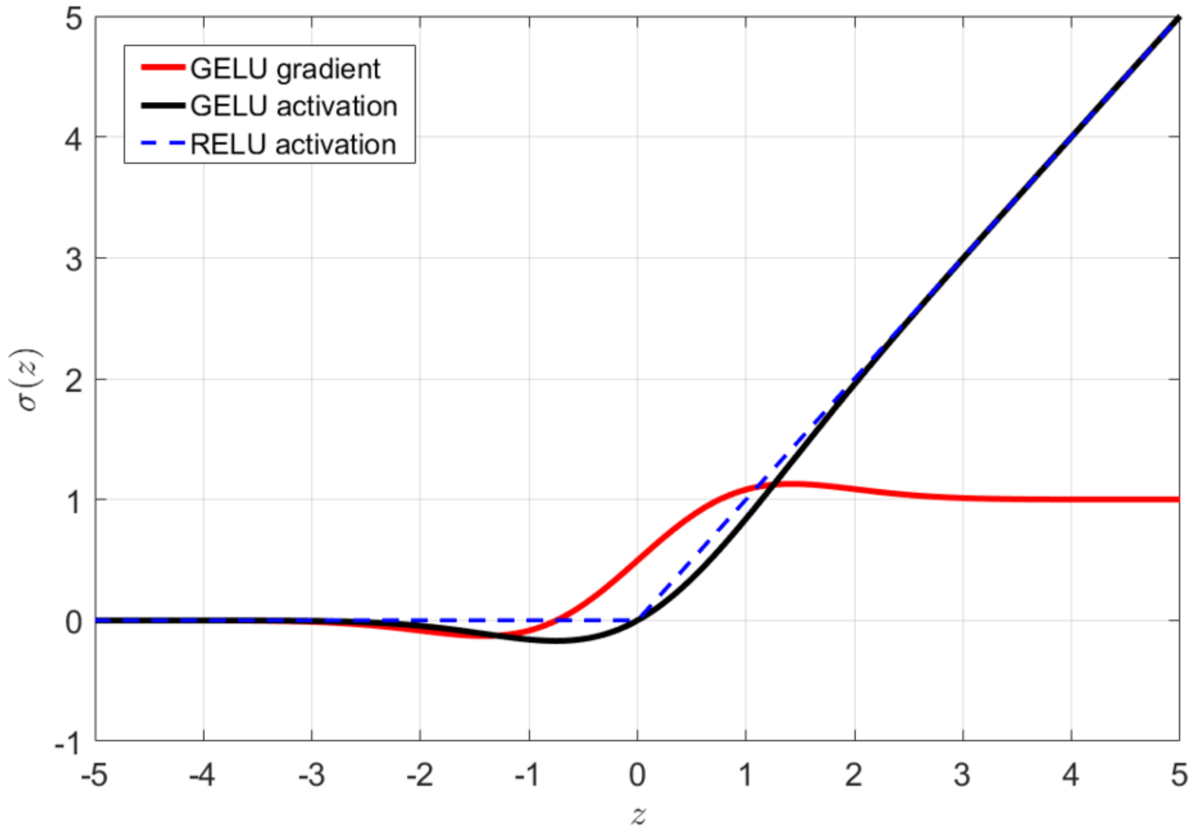



$$\sigma(z) = \max\{0, z\} + a \min\{0, z\}$$

- Pros: same as Leaky ReLU but parameterizes the leakage

# GELU

- Gaussian Error Linear Units



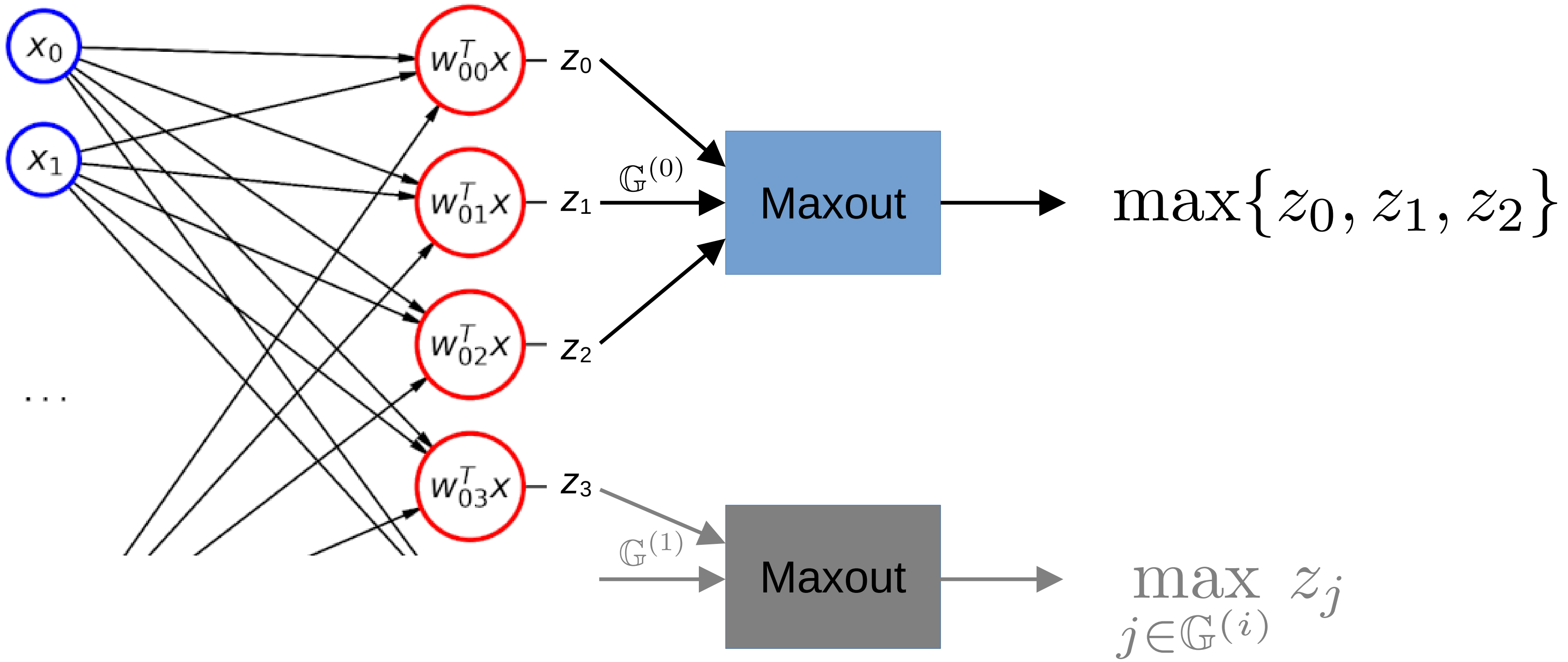

$$\sigma(z) = z\mathrm{P}(Z \leq z) \qquad Z \sim \mathcal{N}(0,1)$$

- Used in Transformers
- Similar: Swish, Mish

Hedrycks, Gimpel: GAUSSIAN ERROR LINEAR UNITS

# Maxout Units

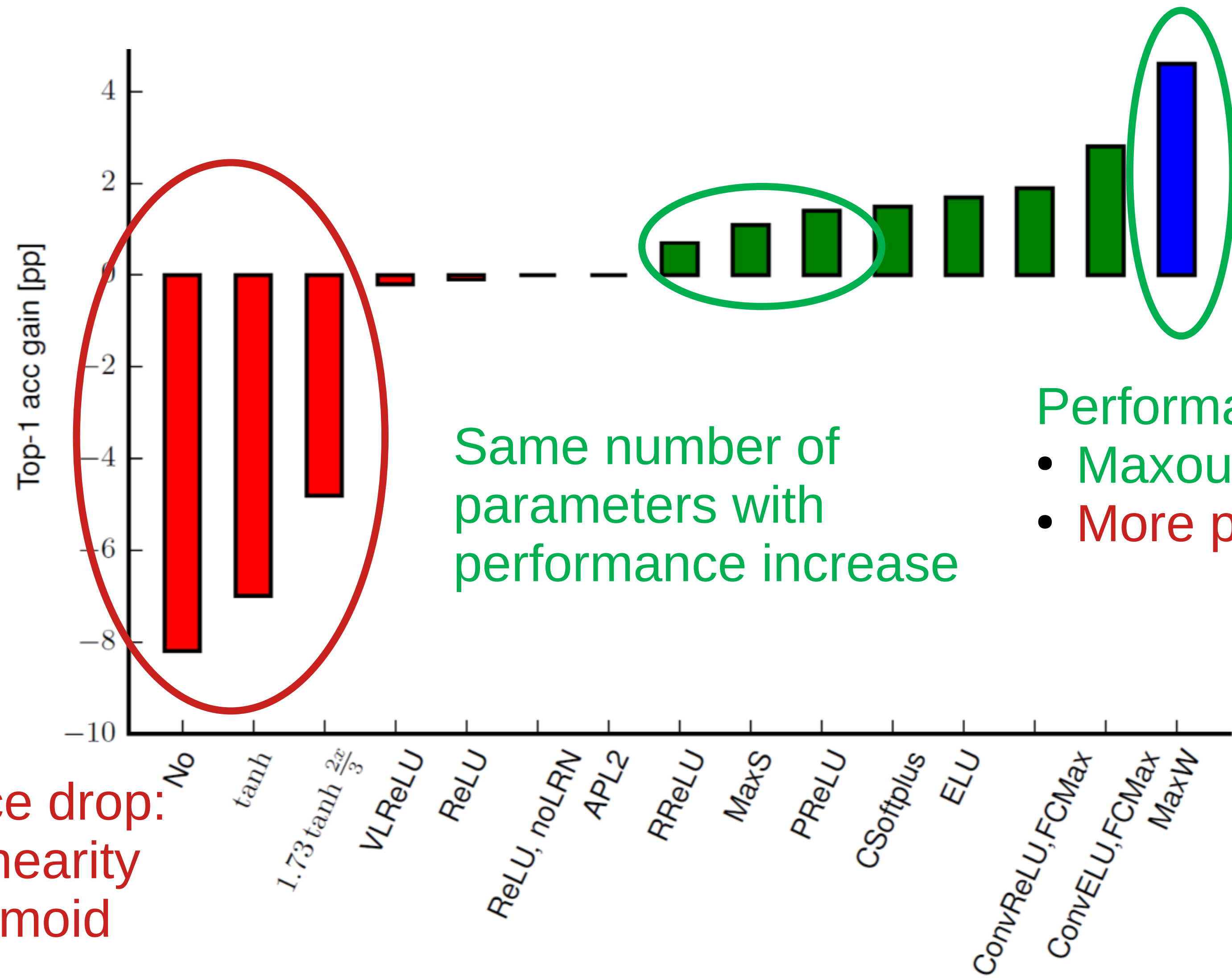
- Generalization of rectified linear units




- Can learn piecewise linear convex functions

# Quantitative Evaluation

- Classification performance vs. baseline with ReLU




Same number of parameters with performance increase

Performance increase
- Maxout
- More parameters

Performance drop:
- No non-linearity
- Tanh / sigmoid

Mishkin et.al., Systematic evaluation of CNN advances on the ImageNet, CoRR 2016

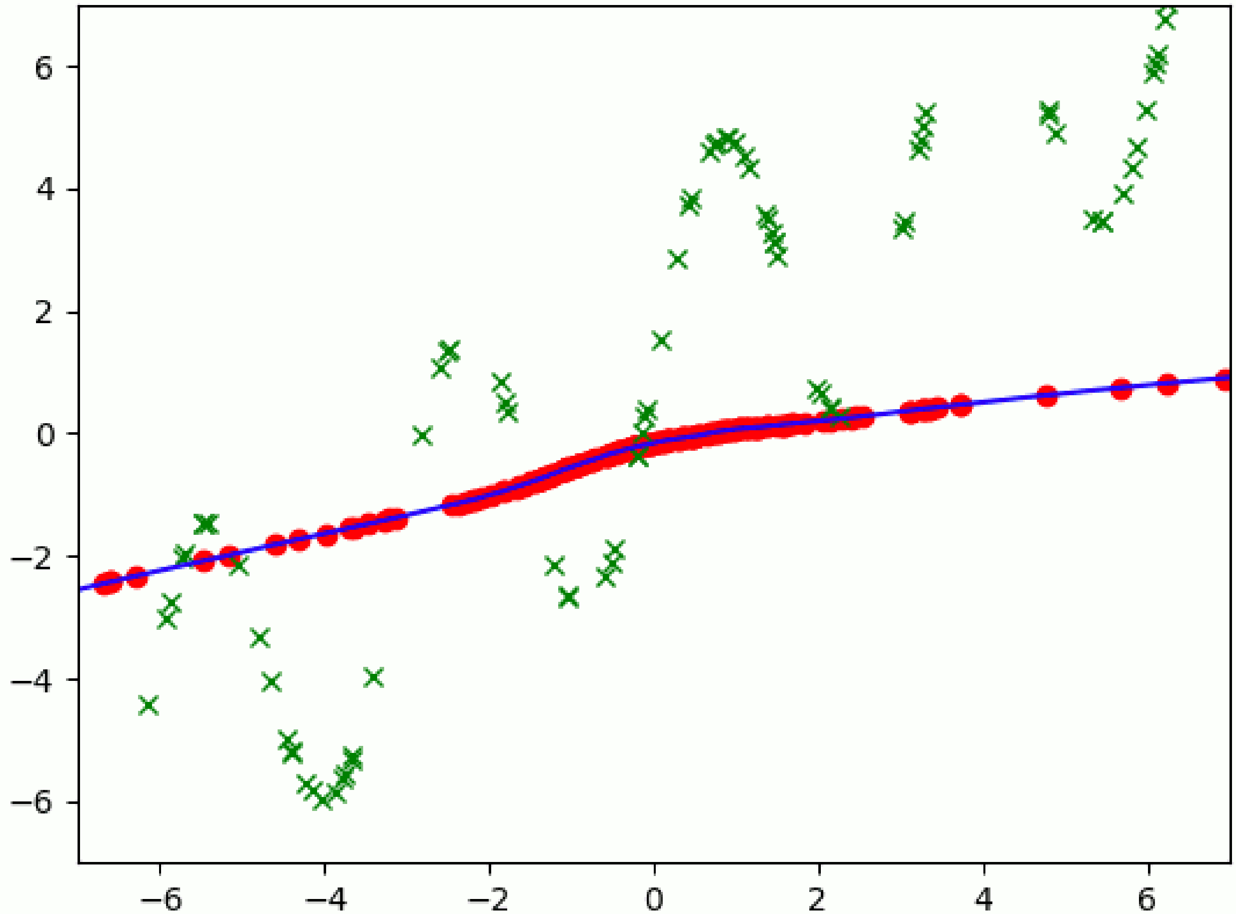
# Non-linearity conclusion

- Saturating non-linearities should be avoided
- ReLU is a standard choice for deep architectures
- Limited gains can be achieved with different types of non-linearities

# Universal Approximator

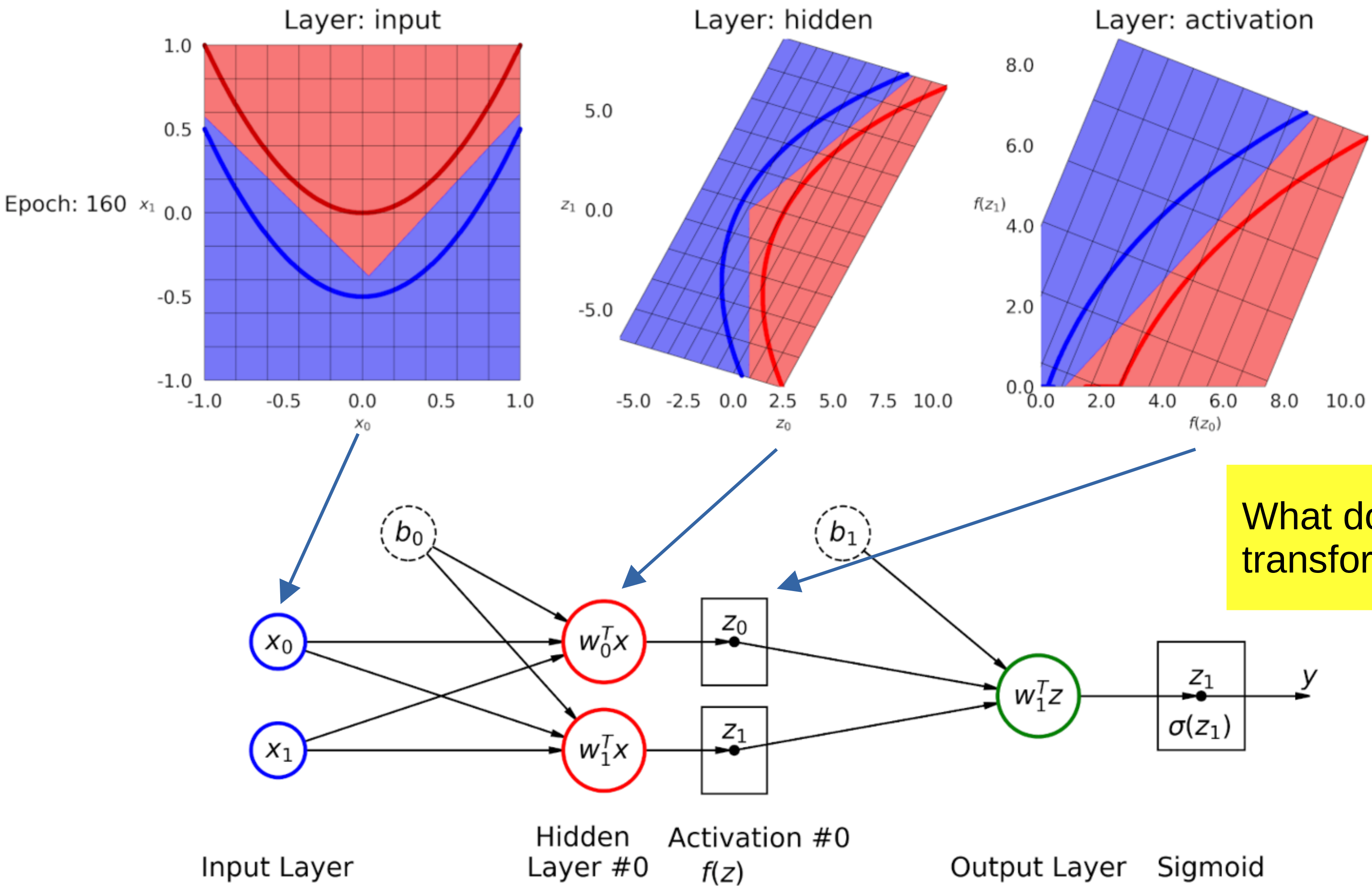
- Hornik [1989], Cybenko [1989]

+Proves existence
- Does not say how to learn
- No bounds for the capacity



# Effect of Activation Functions

- ReLU

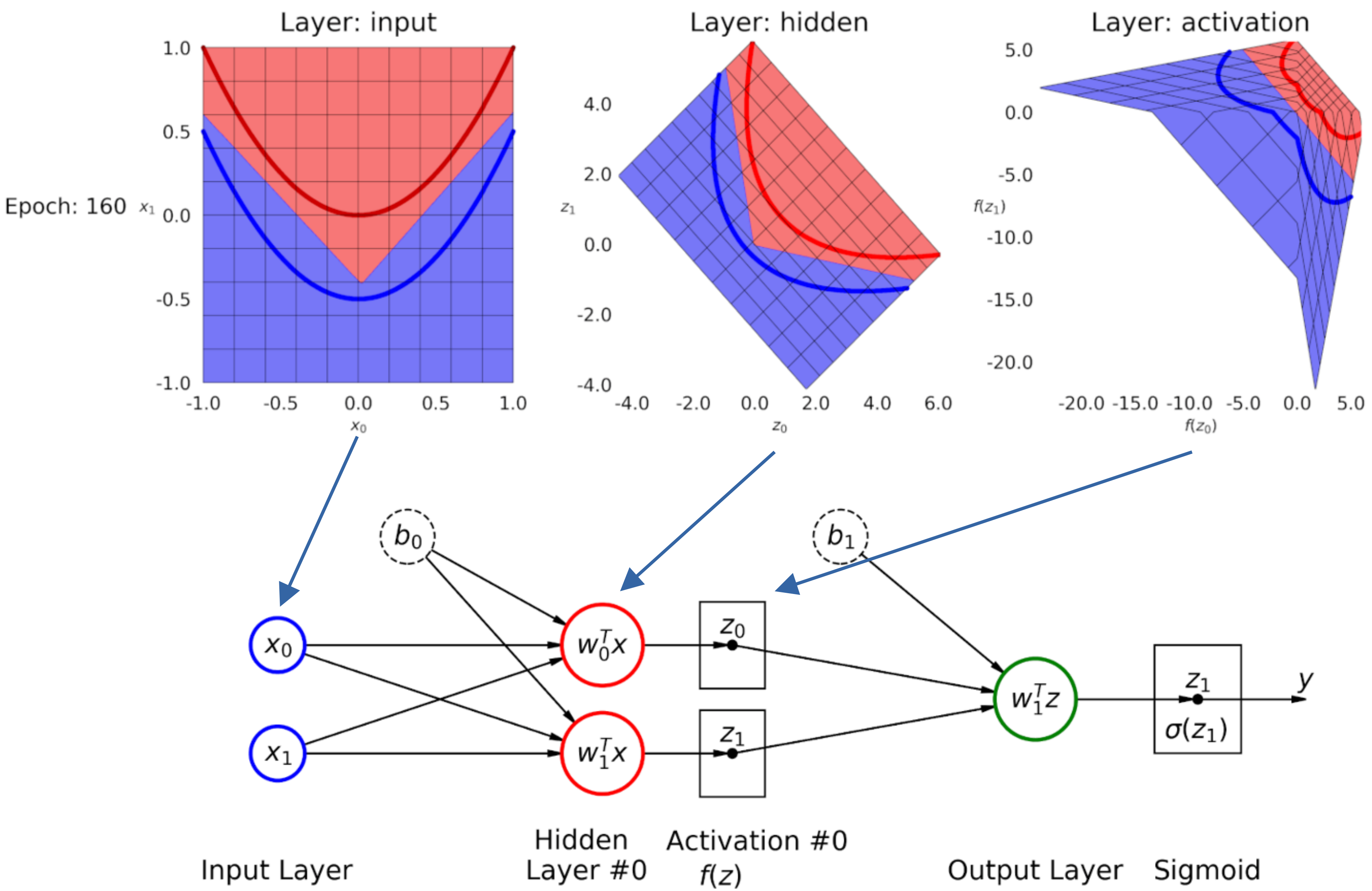



What does an affine transform preserve?

Godoy, Deep Learning with Pytorch, 2021

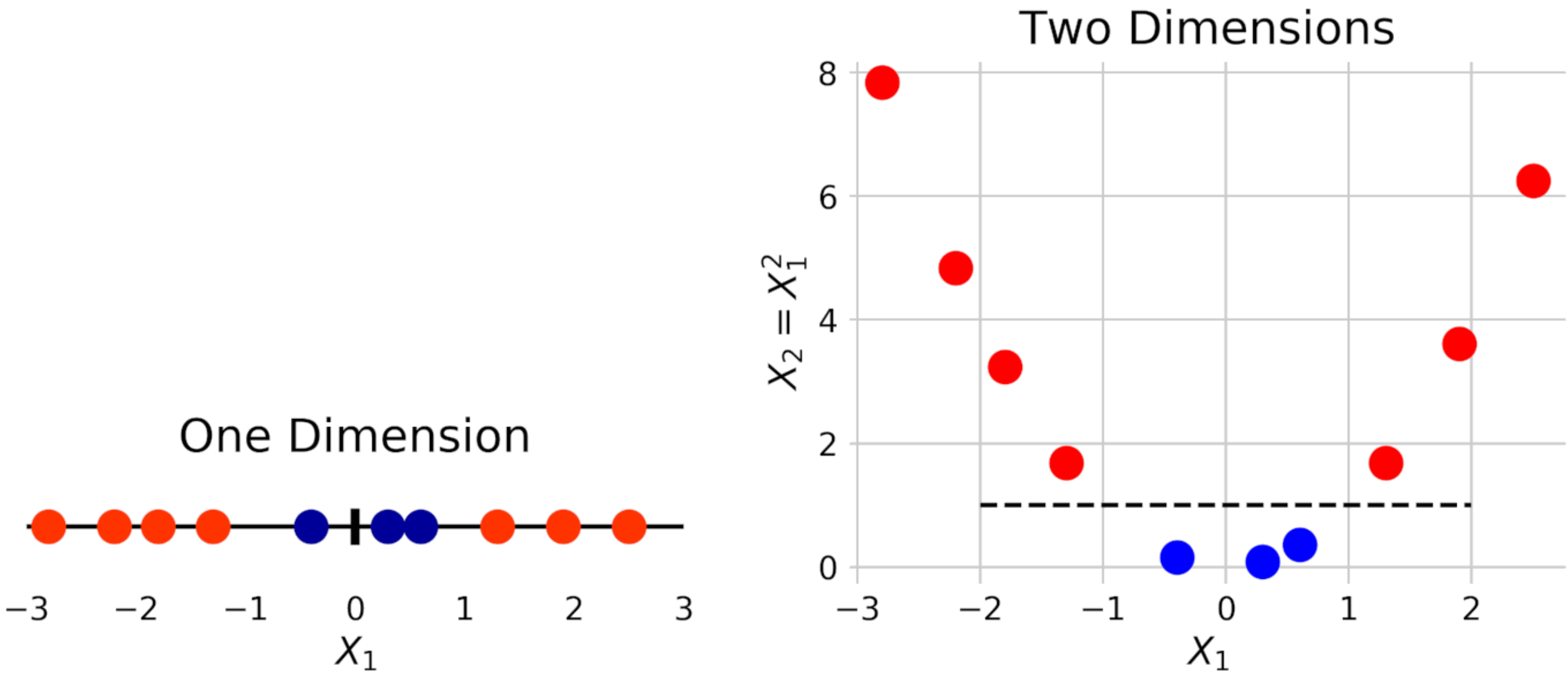
# Effect of Activation Functions

- PReLU




Godoy, Deep Learning with Pytorch, 2021

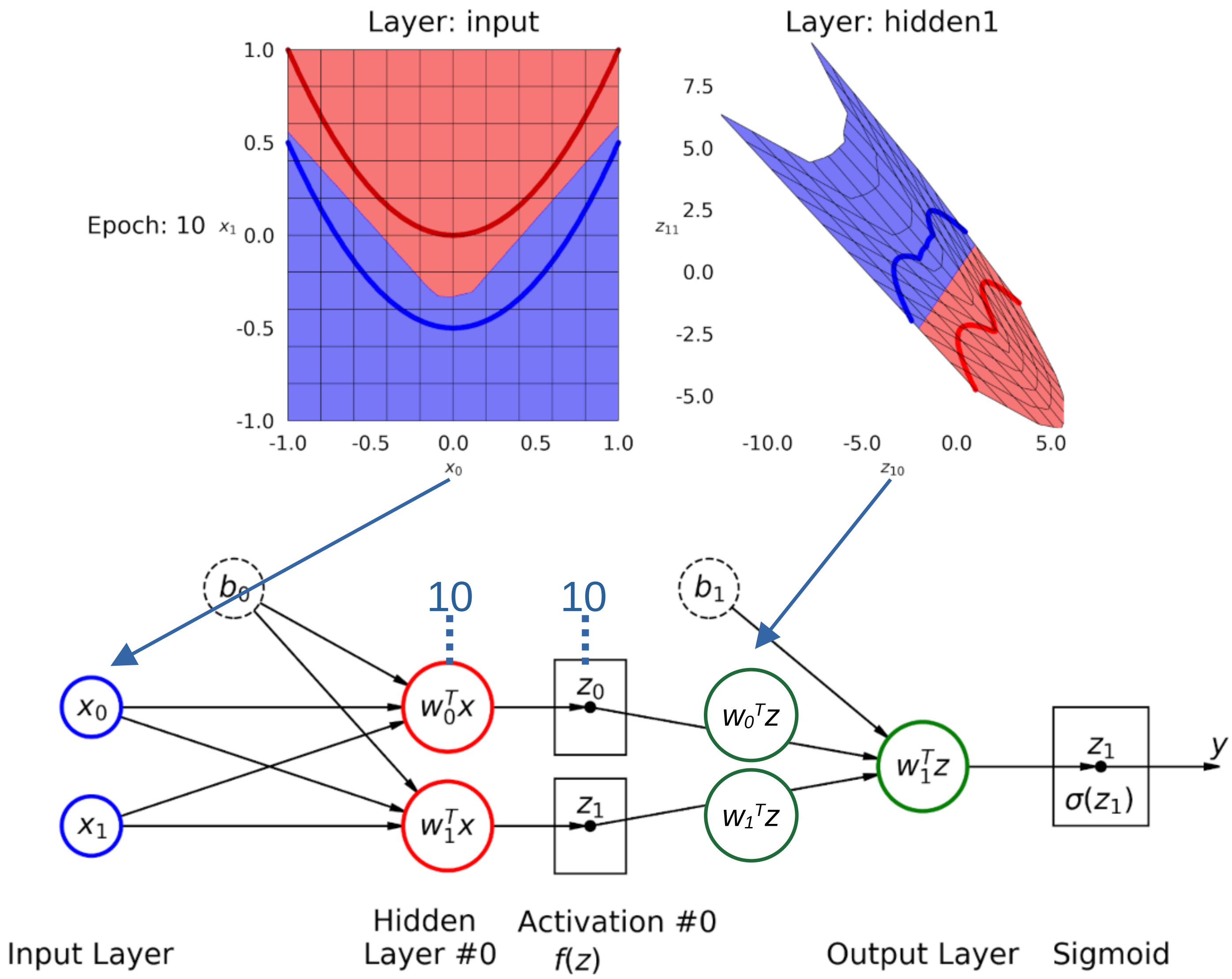
# Adding Dimensions




Godoy, Deep Learning with Pytorch, 2021

# Effect of Activation Functions

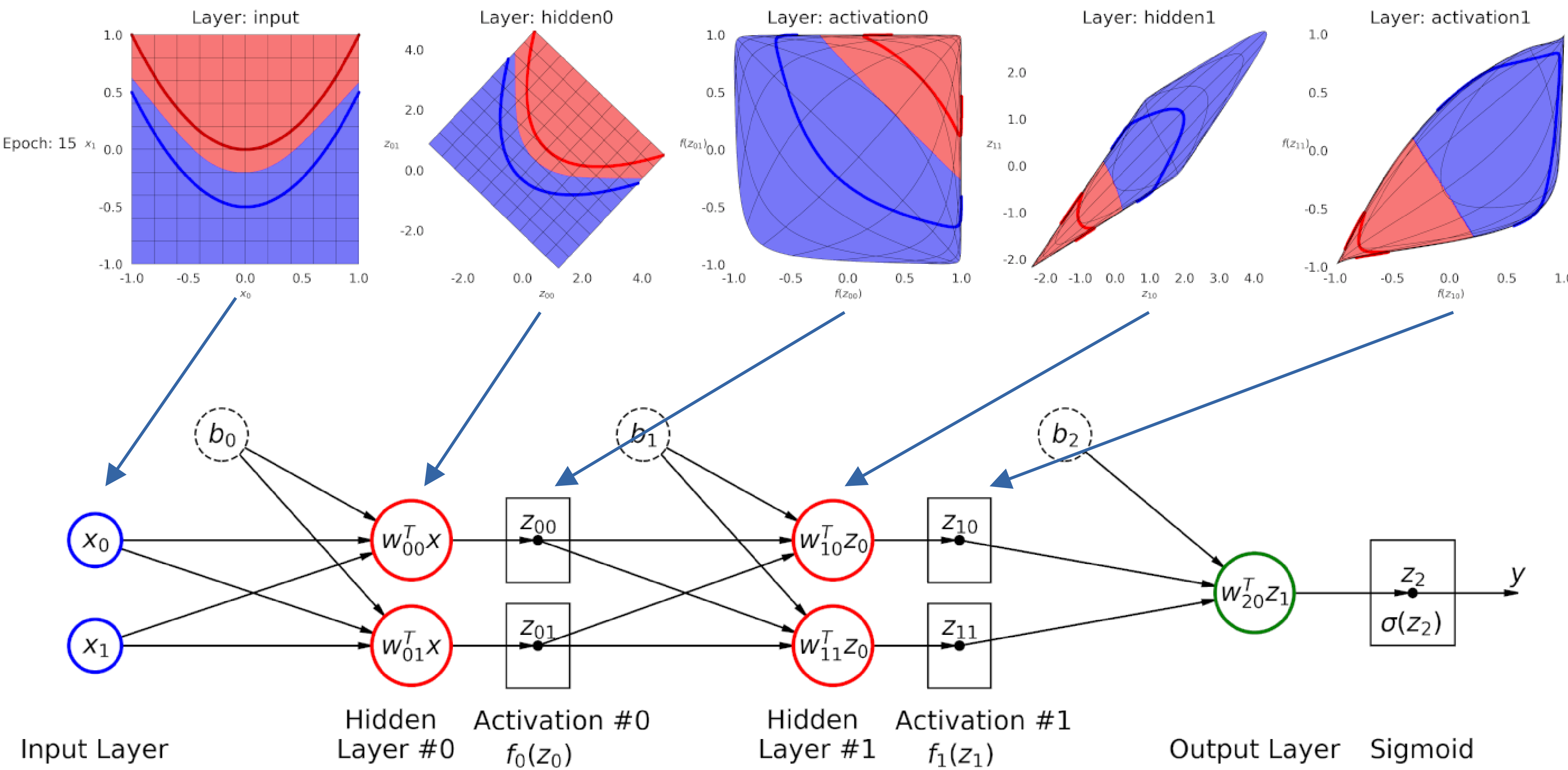
- More hidden units – only 10 epochs to learn




Godoy, Deep Learning with Pytorch, 2021

# Effect of Activation Functions

- More layers – only 15 epochs to learn




Godoy, Deep Learning with Pytorch, 2021

# Training Networks

- Find network parameters $\hat{\theta}$ (unit weights, biases, …) such that $\hat{\theta} = \arg\min_{\theta} J(\theta)$

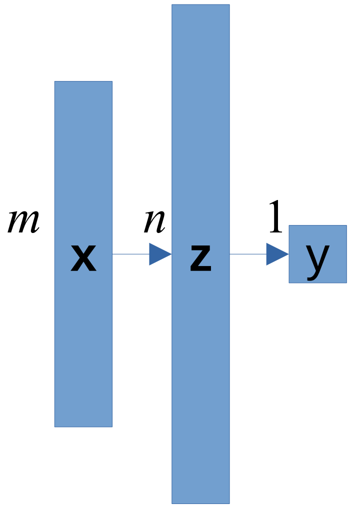
$$J(\theta) = \sum_{(x,y)\sim\hat{p}(x,y)} -\log q(y|f(x;\theta))$$

- Gradient descent is practically the only used minimization strategy
- Fast way to find gradients ==> back-propagation

# Chain Rule N-D

- N-D function composition: $y = g(f(\mathbf{x}))$

$$y = g(\mathbf{z}) : \mathbb{R}^n \to \mathbb{R}$$
$$\mathbf{z} = f(\mathbf{x}) : \mathbb{R}^m \to \mathbb{R}^n$$




- Jacobian:

$$\nabla_{\mathbf{x}} f = \begin{bmatrix} \frac{dz_1}{dx_1} & \frac{dz_1}{dx_2} & \cdots & \frac{dz_1}{dx_m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{dz_n}{dx_1} & \frac{dz_n}{dx_2} & \cdots & \frac{dz_n}{dx_m} \end{bmatrix}$$

$$\nabla_{\mathbf{z}} g = \begin{bmatrix} \frac{dy}{dz_1} & \frac{dy}{dz_2} & \cdots & \frac{dy}{dz_n} \end{bmatrix}$$

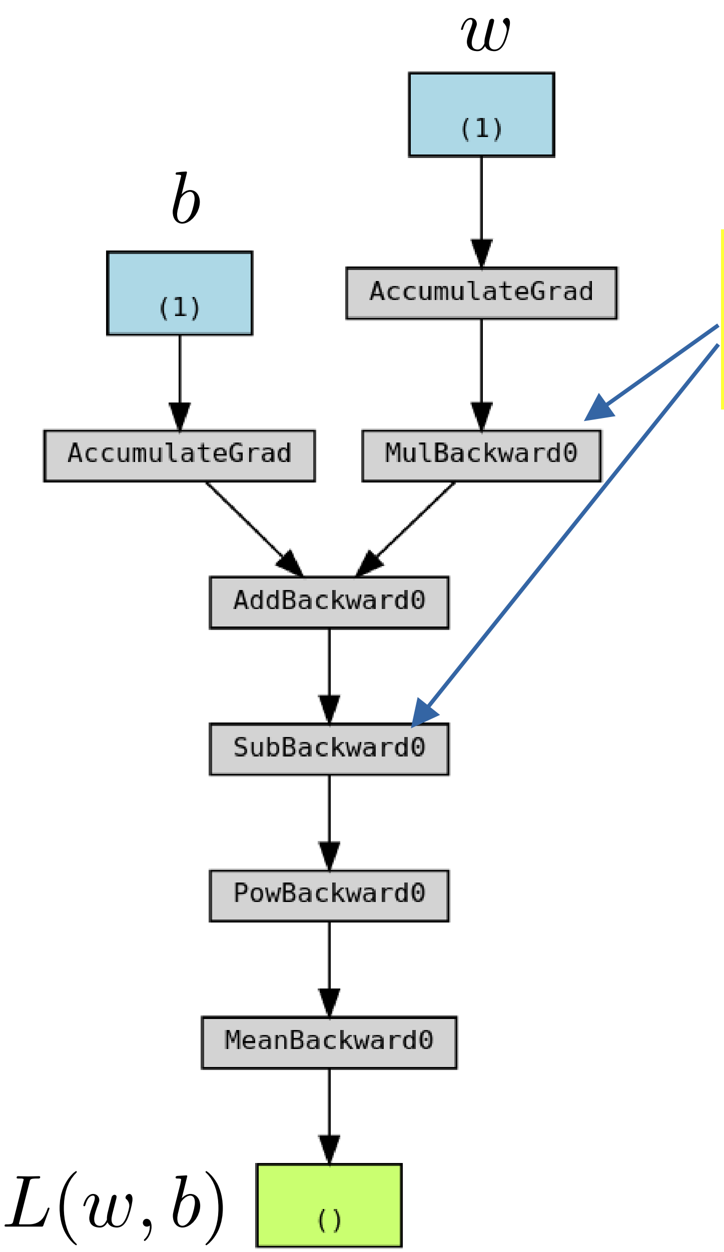
$$\frac{dy}{d\mathbf{x}} = \nabla_{\mathbf{z}} g . \nabla_{\mathbf{x}} f$$

# General Chain Rule

$$z^{(P)}(\dots z^{(p)}(z^{(1)}(z^{(0)}))\dots)$$

$$\frac{dz^{(P)}}{dz^{(0)}} = \prod_{p=0}^{P-1} \nabla_{z^{(P-p-1)}} z^{(P-p)}$$

# Computational Graph




Why are **x**, **y** missing in the graph?

$$L(w, b) = ||(w\mathbf{x} + b) - \mathbf{y})||^2$$

$$\mathbf{z}^{(0)} = w\mathbf{x}$$

$$\mathbf{z}^{(1)} = \mathbf{z}^{(0)} + b$$

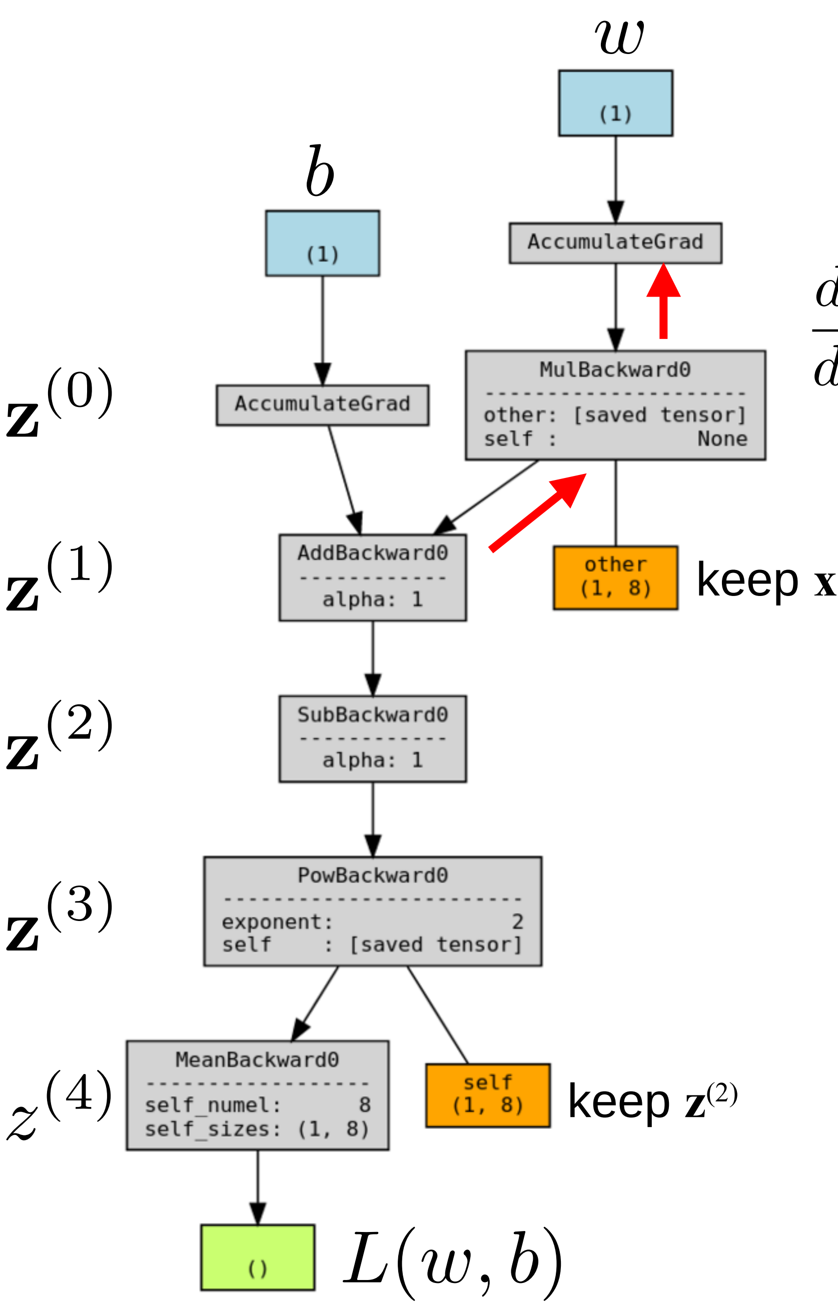
$$\mathbf{z}^{(2)} = \mathbf{z}^{(1)} - \mathbf{y}$$

$$z_i^{(3)} = [z_i^{(2)}]^2$$

$$z^{(4)} = \sum_i z_i^{(3)}$$

# Back-Propagation

$$\mathbf{z}^{(0)} = w\mathbf{x}$$
$$\mathbf{z}^{(1)} = \mathbf{z}^{(0)} + b$$
$$\mathbf{z}^{(2)} = \mathbf{z}^{(1)} - \mathbf{y}$$
$$z_i^{(3)} = [z_i^{(2)}]^2$$
$$z^{(4)} = \sum_i z_i^{(3)}$$




$$\frac{dL}{dw} = \nabla_{\mathbf{z}^{(3)}} z^{(4)} . \nabla_{\mathbf{z}^{(2)}} \mathbf{z}^{(3)} . \nabla_{\mathbf{z}^{(1)}} \mathbf{z}^{(2)} . \nabla_{\mathbf{z}^{(0)}} \mathbf{z}^{(1)} . \nabla_{w} \mathbf{z}^{(0)}$$

$$\nabla_w \mathbf{z}^{(0)} = \mathbf{x}$$

$$\nabla_{\mathbf{z}^{(0)}} \mathbf{z}^{(1)} = \mathbf{I}$$

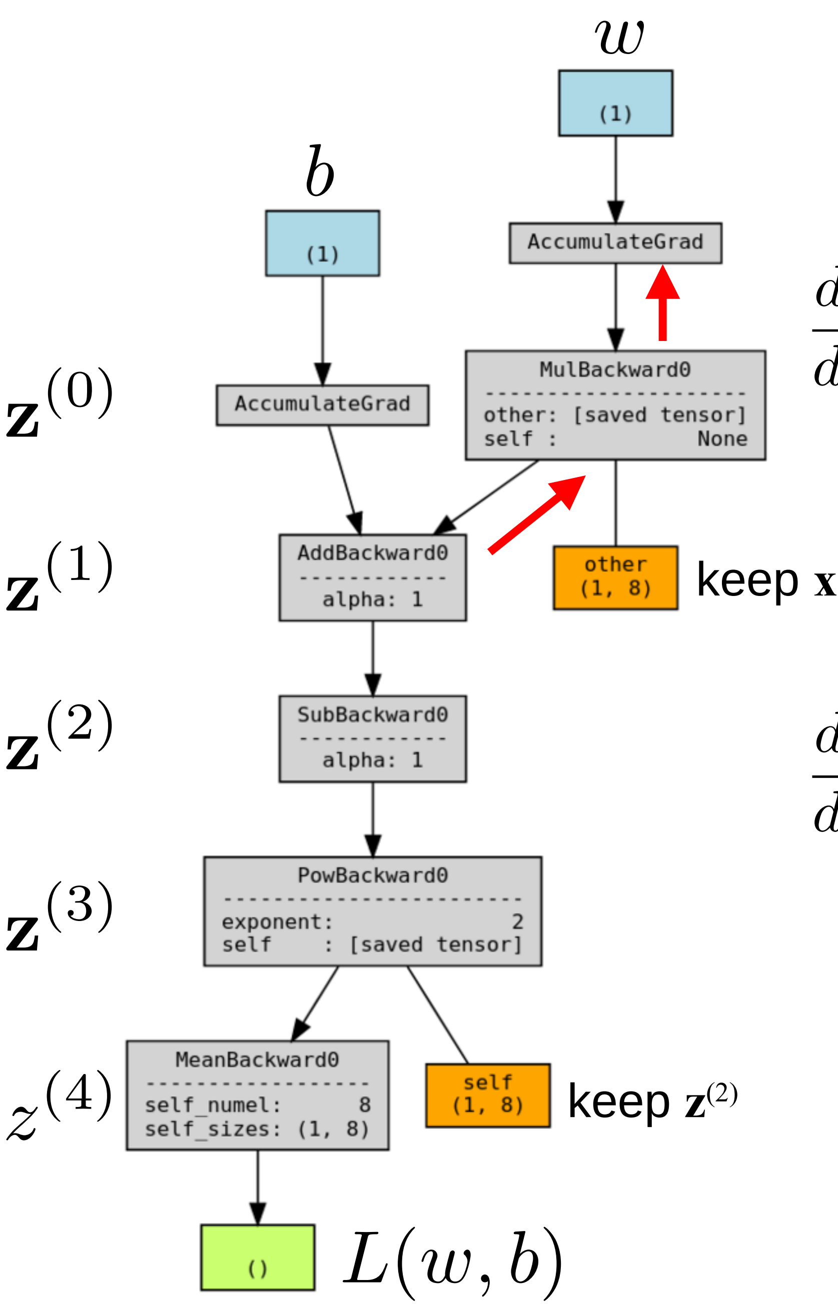
$$\nabla_{\mathbf{z}^{(1)}} \mathbf{z}^{(2)} = \begin{bmatrix} 1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 1 \end{bmatrix} = \mathbf{I}$$

$$\nabla_{\mathbf{z}^{(2)}} \mathbf{z}^{(3)} = \begin{bmatrix} 2z_1^{(2)} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 2z_n^{(2)} \end{bmatrix} = \mathrm{diag}(2\mathbf{z}^{(2)})$$

$$\nabla_{\mathbf{z}^{(3)}} z^{(4)} = [1, 1, \dots, 1] = \mathbf{1}^T$$

# Back-Propagation

$$
\begin{aligned}
\mathbf{z}^{(0)} &= w\mathbf{x} \\
\mathbf{z}^{(1)} &= \mathbf{z}^{(0)} + b \\
\mathbf{z}^{(2)} &= \mathbf{z}^{(1)} - \mathbf{y} \\
z_i^{(3)} &= [z_i^{(2)}]^2 \\
z^{(4)} &= \sum_i z_i^{(3)}
\end{aligned}
$$

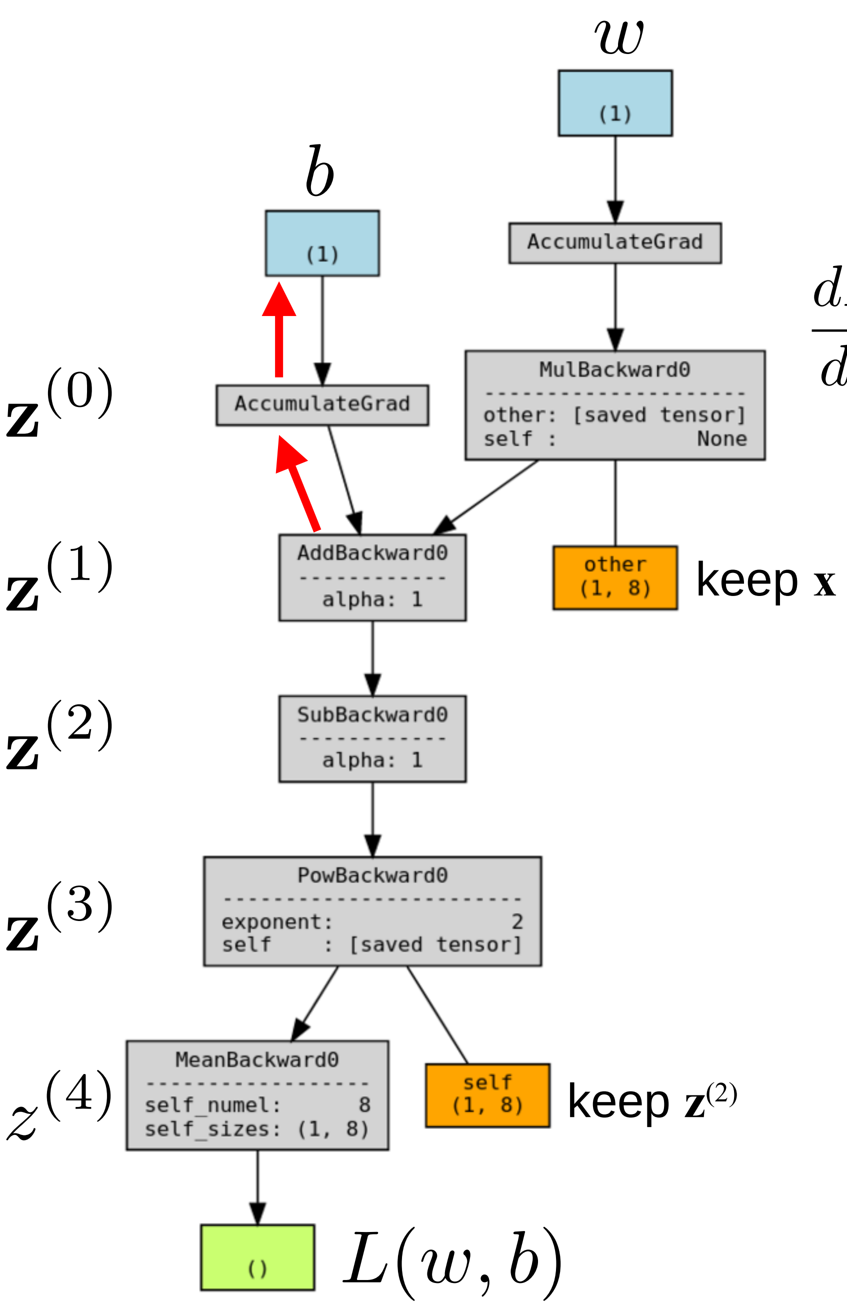



$$\frac{dL}{dw} = \nabla_{\mathbf{z}^{(3)}} z^{(4)} . \nabla_{\mathbf{z}^{(2)}} \mathbf{z}^{(3)} . \nabla_{\mathbf{z}^{(1)}} \mathbf{z}^{(2)} . \nabla_{\mathbf{z}^{(0)}} \mathbf{z}^{(1)} . \nabla_w \mathbf{z}^{(0)}$$

$$\frac{dL}{dw} = \sum_i 2 z_i^{(2)} x_i$$

# Back-Propagation

$$\mathbf{z}^{(0)} = w\mathbf{x}$$
$$\mathbf{z}^{(1)} = \mathbf{z}^{(0)} + b$$
$$\mathbf{z}^{(2)} = \mathbf{z}^{(1)} - \mathbf{y}$$
$$z_i^{(3)} = [z_i^{(2)}]^2$$
$$z^{(4)} = \sum_i z_i^{(3)}$$




$$\frac{dL}{db} = \nabla_{\mathbf{z}^{(3)}} z^{(4)} . \nabla_{\mathbf{z}^{(2)}} \mathbf{z}^{(3)} . \nabla_{\mathbf{z}^{(1)}} \mathbf{z}^{(2)} . \nabla_b \mathbf{z}^{(1)}$$

$$\nabla_b \mathbf{z}^{(1)} = \mathbf{1}$$

$$\nabla_{\mathbf{z}^{(1)}} \mathbf{z}^{(2)} = \begin{bmatrix} 1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 1 \end{bmatrix} = \mathbf{I}$$

$$\nabla_{\mathbf{z}^{(2)}} \mathbf{z}^{(3)} = \begin{bmatrix} 2z_1^{(2)} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 2z_n^{(2)} \end{bmatrix} = \mathrm{diag}(2\mathbf{z}^{(2)})$$

$$\nabla_{\mathbf{z}^{(3)}} z^{(4)} = [1, 1, \dots, 1] = \mathbf{1}^T$$

# Back-Propagation

$$\mathbf{z}^{(0)} = w\mathbf{x}$$
$$\mathbf{z}^{(1)} = \mathbf{z}^{(0)} + b$$
$$\mathbf{z}^{(2)} = \mathbf{z}^{(1)} - \mathbf{y}$$
$$z_i^{(3)} = [z_i^{(2)}]^2$$
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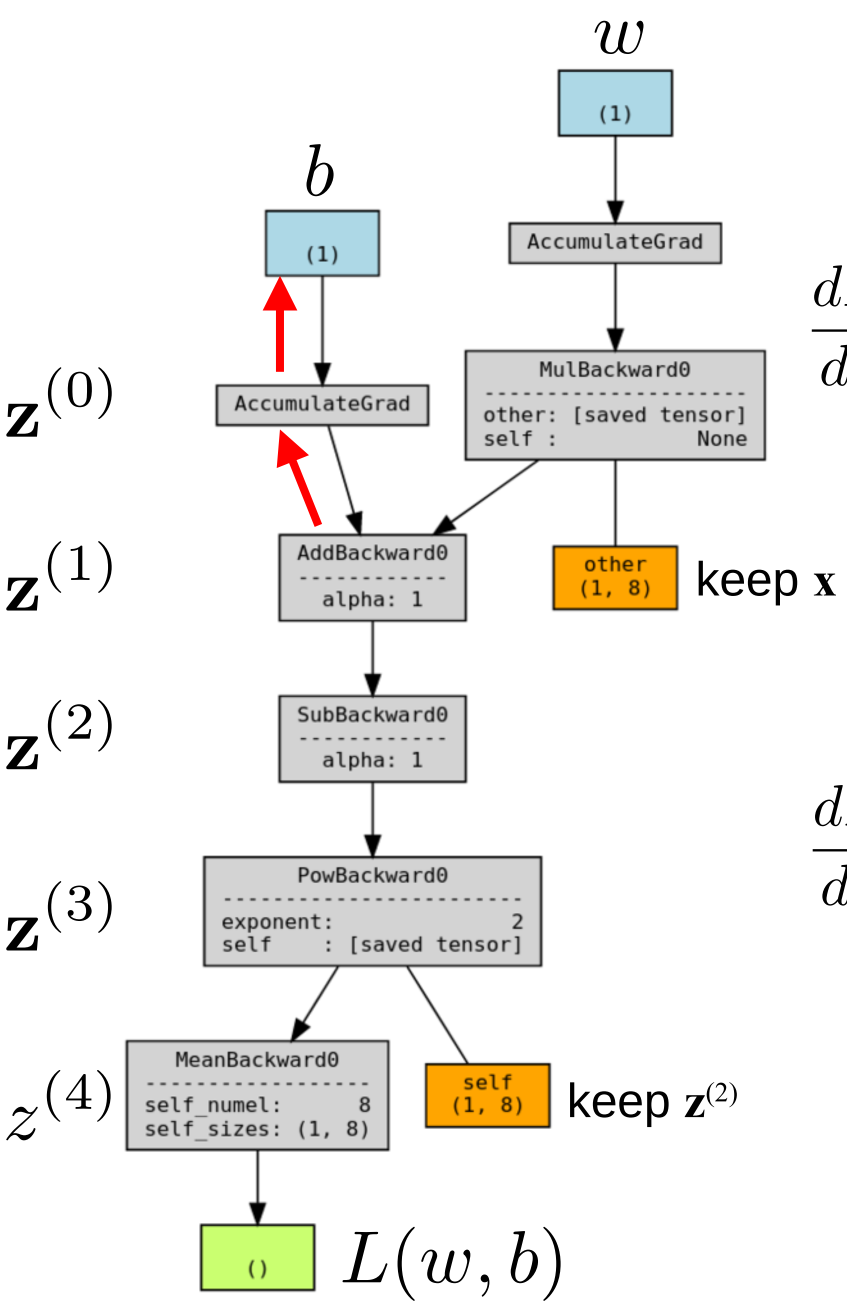
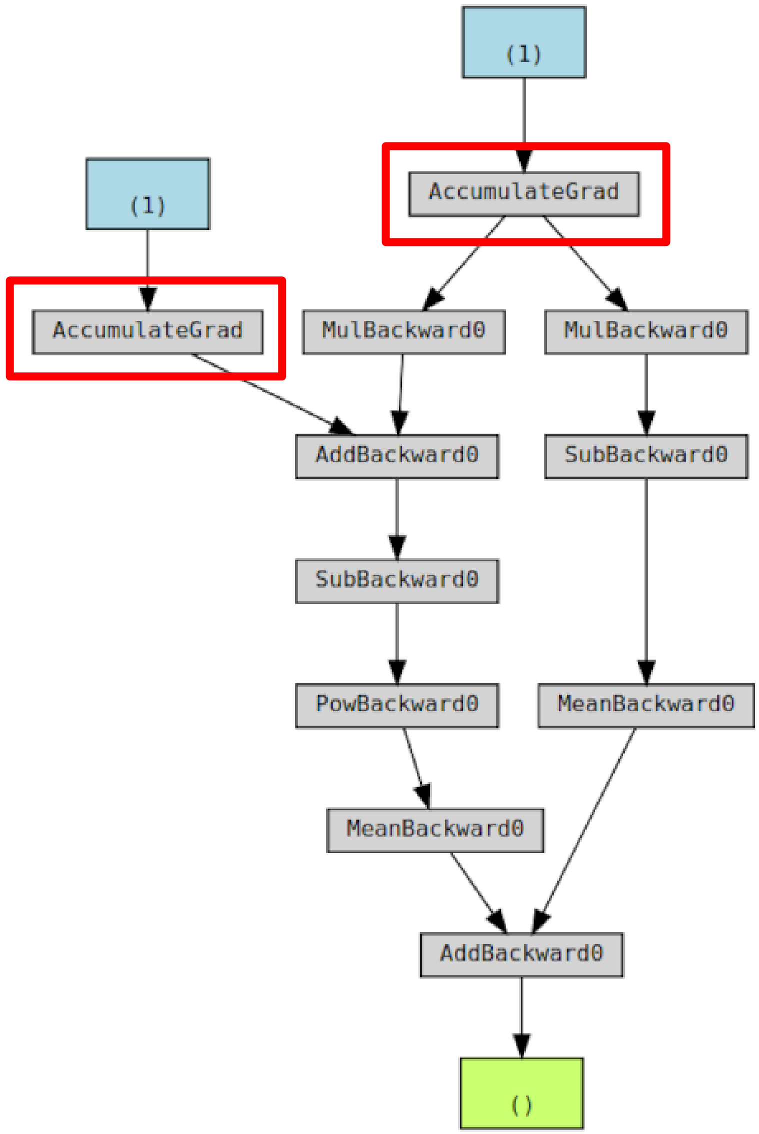



$$\frac{dL}{db} = \nabla_{\mathbf{z}^{(3)}} z^{(4)} . \nabla_{\mathbf{z}^{(2)}} \mathbf{z}^{(3)} . \nabla_{\mathbf{z}^{(1)}} \mathbf{z}^{(2)} . \nabla_b \mathbf{z}^{(1)}$$

$$\frac{dL}{db} = \sum_i 2 z_i^{(2)}$$

# Complex Computational Graphs




PytorchViz

# Learning vs Optimization

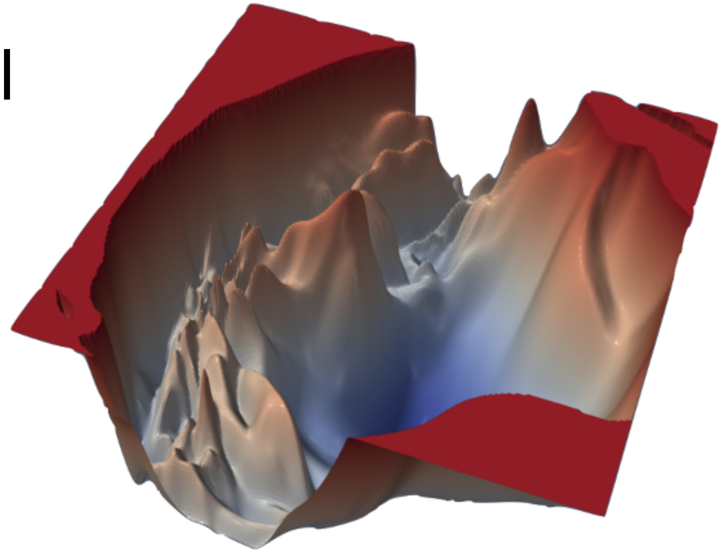
- Maximizing Performance $\neq$ Minimizing cost function
- Cost function

$$J(\theta) = \mathbb{E}_{(x,y)\sim p_{\text{data}}} L(f(x,\theta), y)$$

- Instead, Empirical risk

$$J^*(\theta) = \sum_i L(f(x^{(i)},\theta), y^{(i)})$$

- Many minima, which one is better?
- Reaching a minimum is often not a goal



# Batch vs Minibatch Gradient Methods

- Infeasible to calculate the derivative over the whole dataset

$$\{(x^{(i)}, y^{(i)})\}_{i \in \mathbb{D}} \qquad \nabla_\theta J^*(\theta) = \sum_{i \in \mathbb{D}} \nabla_\theta L(f(x^{(i)}, \theta), y^{(i)})$$

- Instead, derivatives over random data subsets (minibatches)

$$\mathbb{B} = \{\text{random set from } \mathbb{D}\}$$

$$\nabla_\theta J^*(\theta) \approx \sum_{i \in \mathbb{B}} \nabla_\theta L(f(x^{(i)}, \theta), y^{(i)})$$

  - Parallel implementation on GPUs
  - Small minibatches → good generalization properties

# Stochastic Gradient Descent

1. Initialization: parameters $\theta^{(0)}$, learning rate $\epsilon_t$

2. Sample a minibatch $\mathbb{B} \subset \mathbb{D}$

3. Compute gradient $g = \frac{1}{|\mathbb{B}|} \sum_{i \in \mathbb{B}} \nabla_\theta L(f(x^{(i)}, \theta^{(t)}), y^{(i)})$

4. Apply update $\theta^{(t+1)} = \theta^{(t)} - \epsilon_t g$

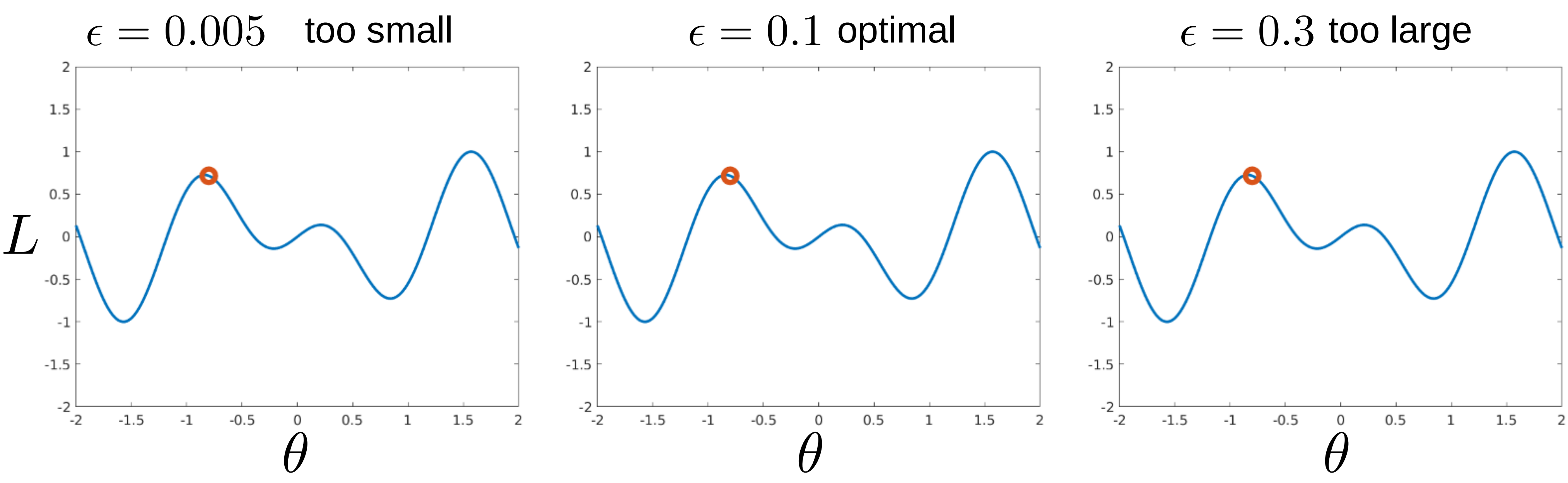
5. Repeat 2-4 until stopping criterion is met

# SGD

- Sufficient condition to guarantee convergence of SGD

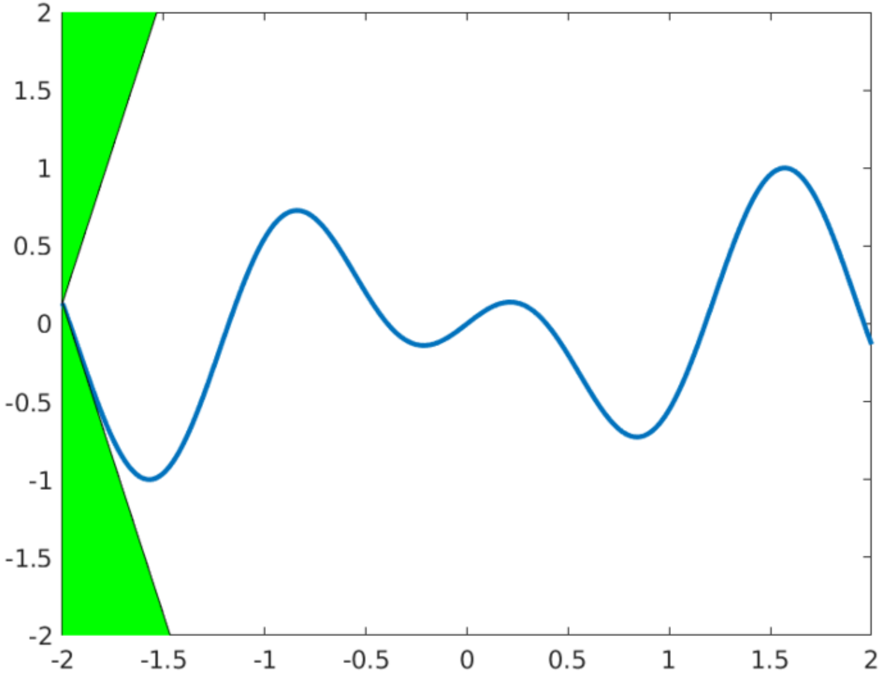
$$\sum_{t=1}^{\infty} \epsilon_t = \infty \qquad \sum_{t=1}^{\infty} \epsilon_t^2 < \infty$$

- Choice of the LR is critical! $\theta^{(t+1)} = \theta^{(t)} - \epsilon_t g$



# Lipschitz Constant

- $$|f(x_1) - f(x_2)| \leq K\|x_1 - x_2\| \quad \forall x_1, x_2$$




$$f(x) = \sin(x)\cos(4x)$$

$$\sup_{\mathbb{R}} f' = 4$$

$$K = 4$$

- Learning rate: $0 < \epsilon < 2/K$

# SGD with Momentum

- Adds momentum to the gradient

$$g = \frac{1}{|\mathbb{B}|} \sum_{i \in \mathbb{B}} \nabla_\theta L(f(x^{(i)}, \theta^{(t)}), y^{(i)})$$

Momentum factor

$$v^{(t+1)} = \alpha v^{(t)} + g$$

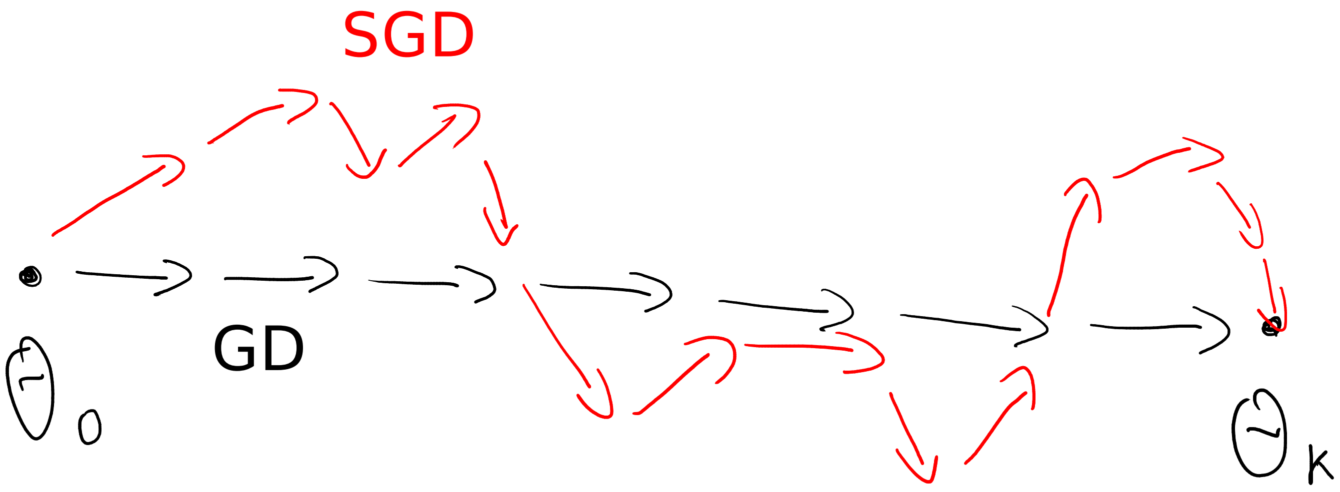
Velocity (momentum of unit mass)

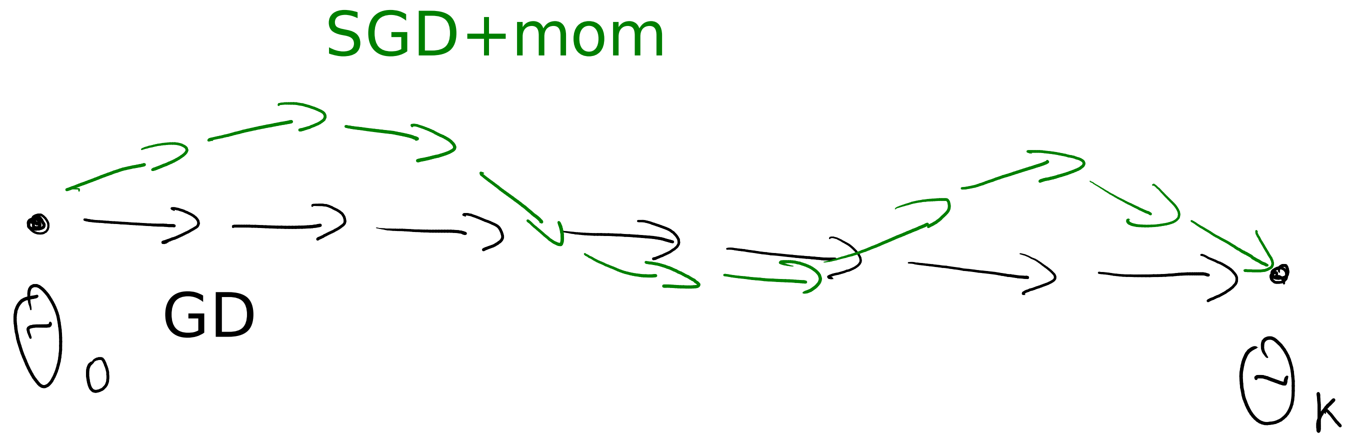
$$\theta^{(t+1)} = \theta^{(t)} - \epsilon v^{(t+1)}$$

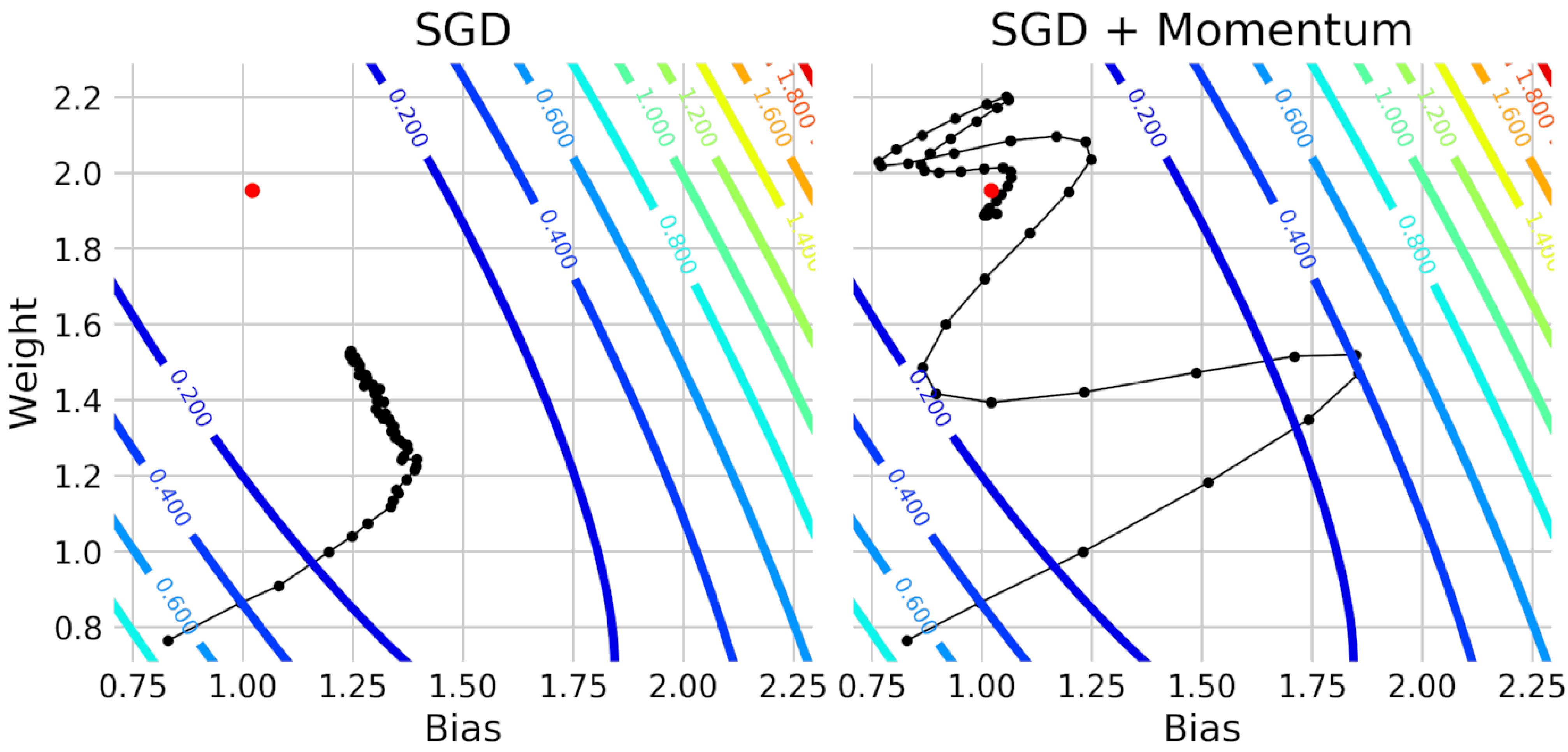
Learning rate

- For a constant gradient

$$\lim_{t \to \infty} v^{(t)} = \frac{g}{1 - \alpha}$$


SGD
GD


SGD+mom
GD


SGD
SGD + Momentum
Weight
Bias
Bias
0.200
0.400
0.600
0.800
1.000
1.200
1.400
1.600
1.800
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.75
1.00
1.25
1.50
1.75
2.00
2.25

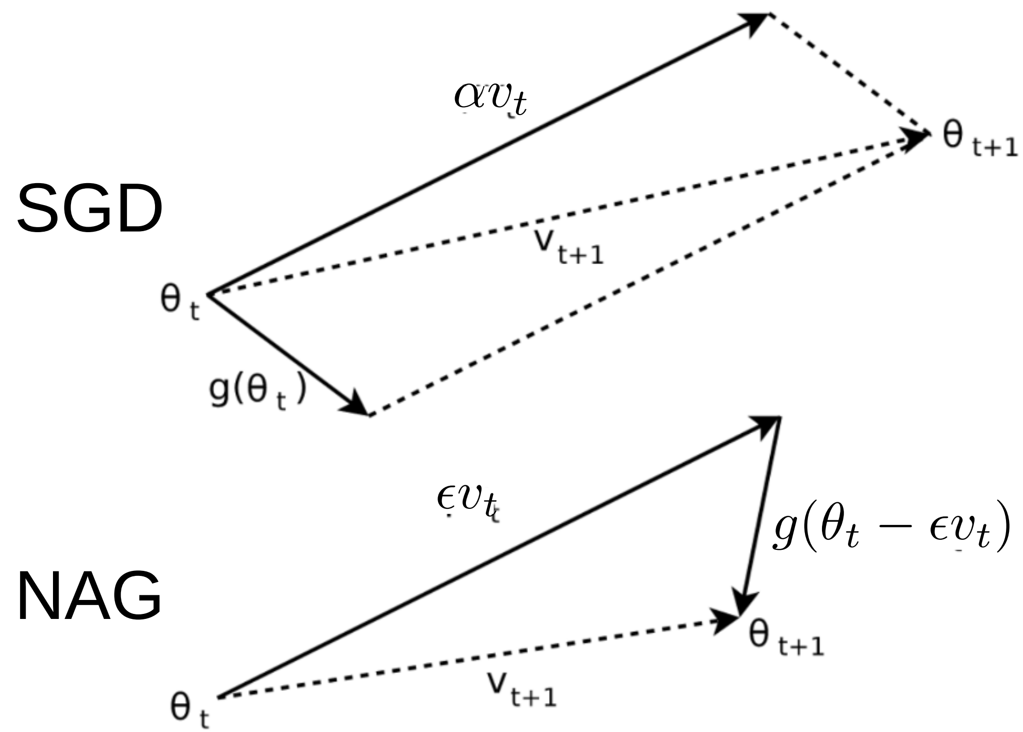
# SGD with Nesterov Momentum (NAG)

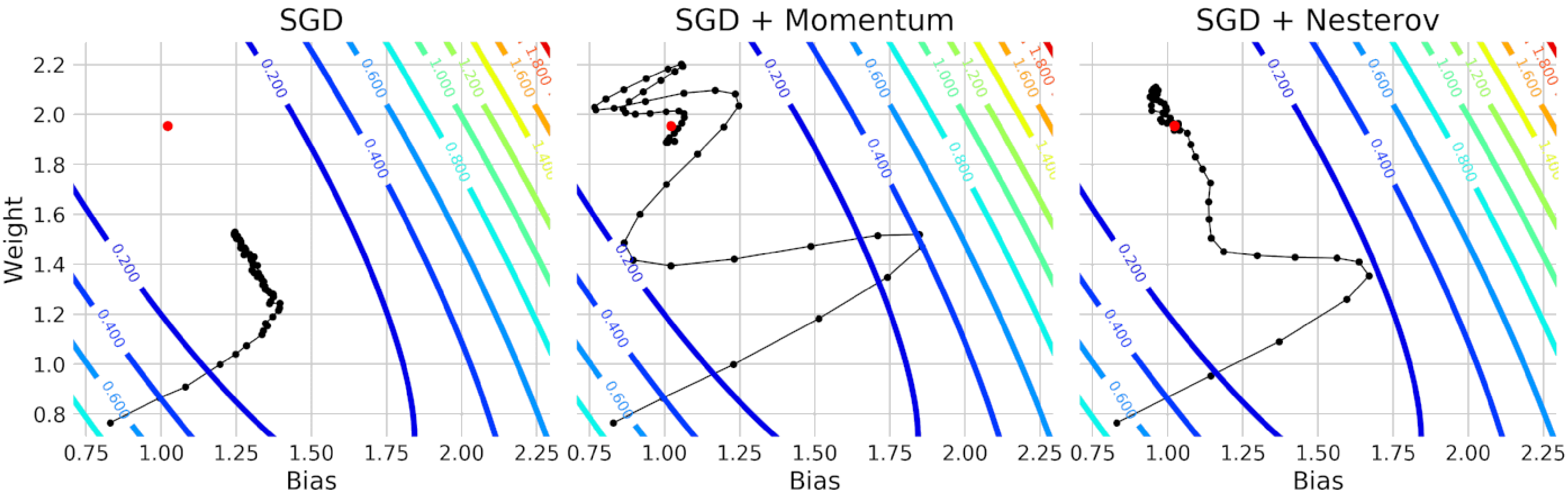
- Calculate gradient in the predicted future position

$$g = \frac{1}{|\mathbb{B}|} \sum_{i \in \mathbb{B}} \nabla_\theta L(f(x^{(i)}, \theta^{(t)} - \epsilon v^{(t)}), y^{(i)})$$

$$v^{(t+1)} = \alpha v^{(t)} + g$$

$$\theta^{(t+1)} = \theta^{(t)} - \epsilon v^{(t+1)}$$





SGD
SGD + Momentum
SGD + Nesterov
Weight
Bias
Bias
Bias
0.200
0.400
0.600
0.800
1.000
1.200
1.400
1.600
1.800

# Adaptive Learning Rate

- Slow progress in gently sloped directions, because

$$\theta^{(t+1)} = \theta^{(t)} - \epsilon_t g$$

- How to adapt LR, so the progress in all directions is approximately the same?

- AdaGrad
- AdaDelta
- RMSProp
- Adam

# RMSProp

$$g = \frac{1}{|\mathbb{B}|} \sum_{i \in \mathbb{B}} \nabla_\theta L(f(x^{(i)}, \theta^{(t)}), y^{(i)})$$

$$r^{(t+1)} = \beta r^{(t)} + (1 - \beta) g^2$$

Exponentially weighted moving average of $g^2$

$$v^{(t+1)} = \alpha v^{(t)} + \frac{1}{\delta + \sqrt{r^{(t+1)}}} g$$

Element-wise operations

$$\theta^{(t+1)} = \theta^{(t)} - \epsilon v^{(t+1)}$$

# Adam

$$g = \frac{1}{|\mathbb{B}|} \sum_{i \in \mathbb{B}} \nabla_\theta L(f(x^{(i)}, \theta^{(t)}), y^{(i)})$$

$$s^{(t+1)} = \beta_1 s^{(t)} + (1 - \beta_1) g$$

$$r^{(t+1)} = \beta_2 r^{(t)} + (1 - \beta_2) g^2$$

Exponentially weighted moving average of g and $g^2$

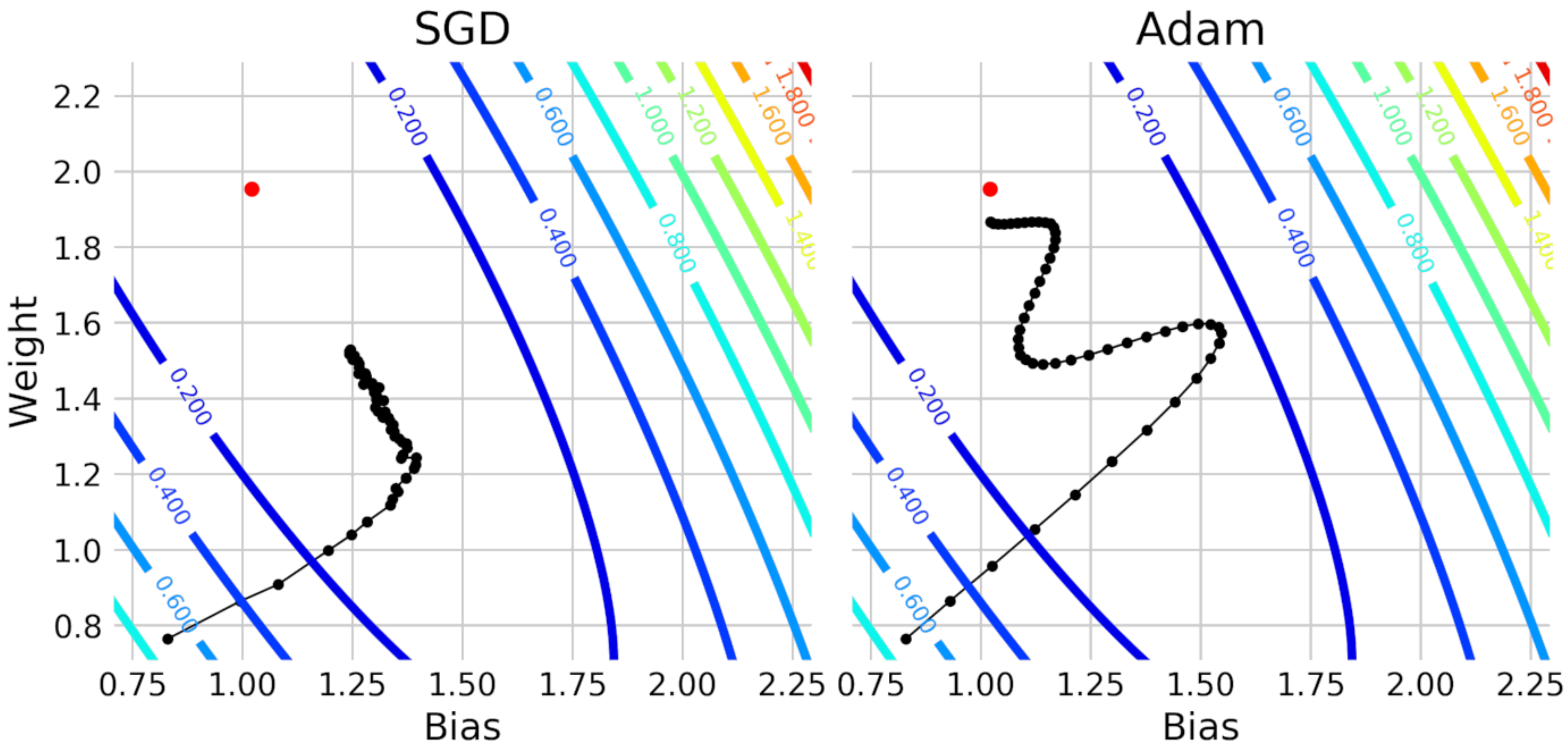
$$\hat{s} = \frac{s}{1 - \beta_1^{t+1}} \qquad \hat{r} = \frac{r}{1 - \beta_2^{t+1}}$$

Bias correction for correct initialization

$\hat{s}^{(1)} = g \quad \hat{r}^{(1)} = g^2$

$$\theta^{(t+1)} = \theta^{(t)} - \epsilon \frac{\hat{s}}{\delta + \sqrt{\hat{r}}}$$

Default values: $\beta_1 = 0.9,\ \beta_2 = 0.999,\ \delta = 10^{-8}$


SGD
Adam
Weight
Bias
Bias
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.75 1.00 1.25 1.50 1.75 2.00 2.25
0.75 1.00 1.25 1.50 1.75 2.00 2.25
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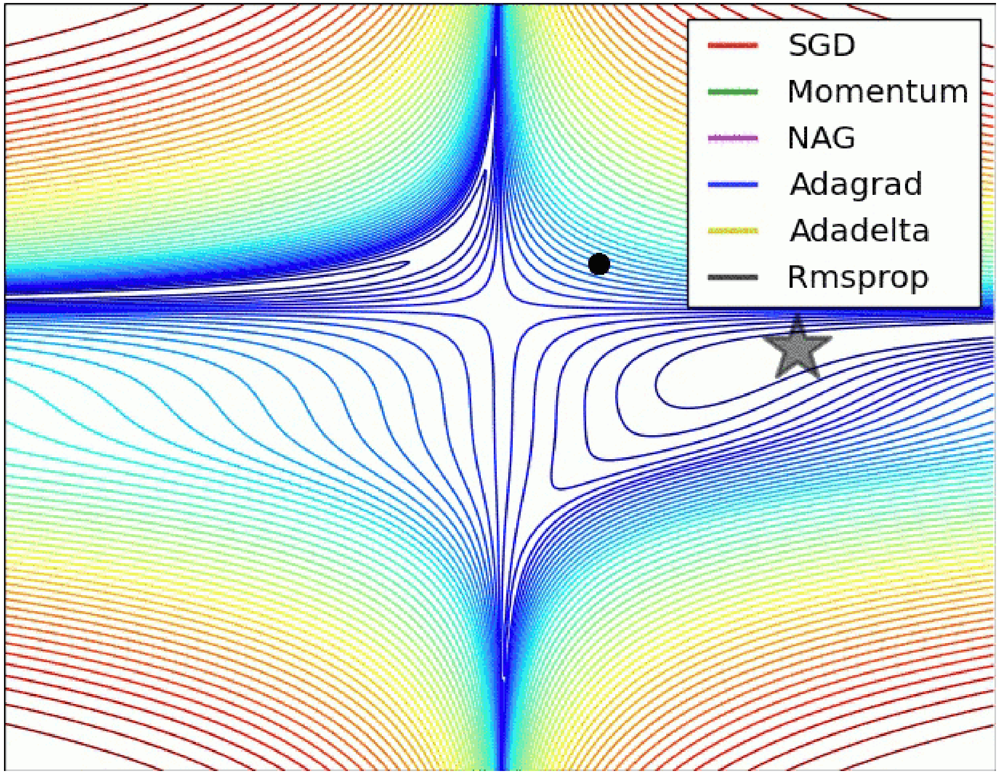
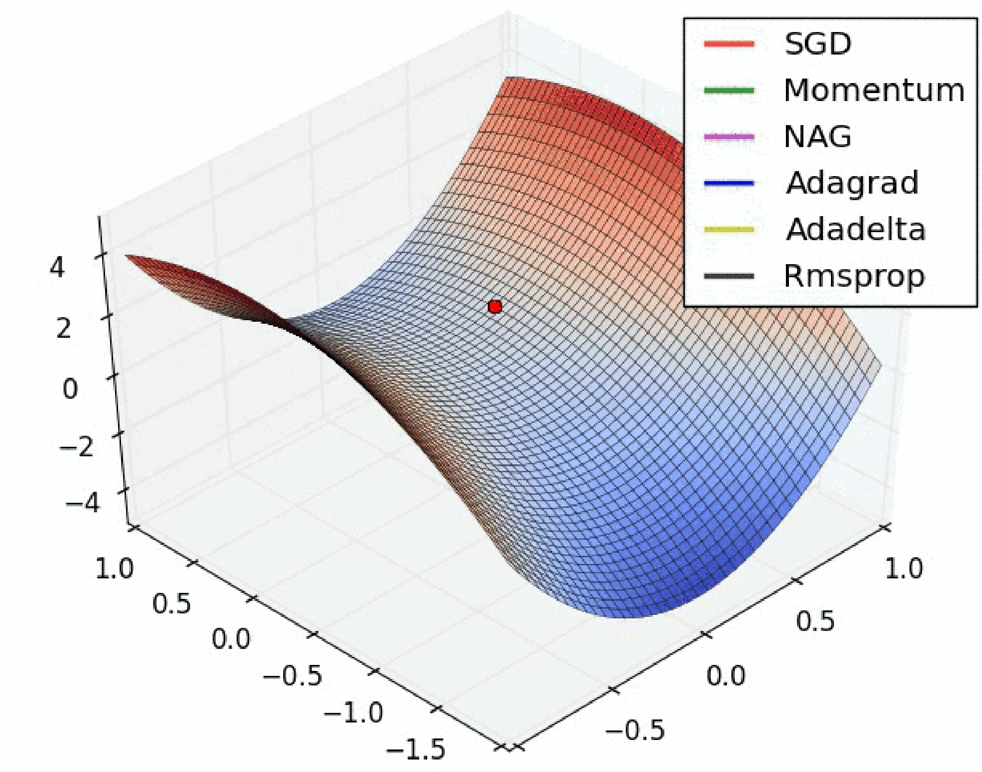
1.400
1.600
1.800

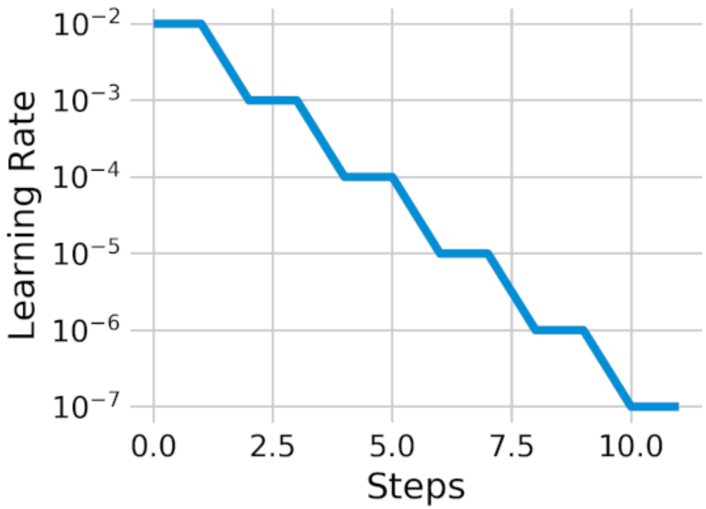


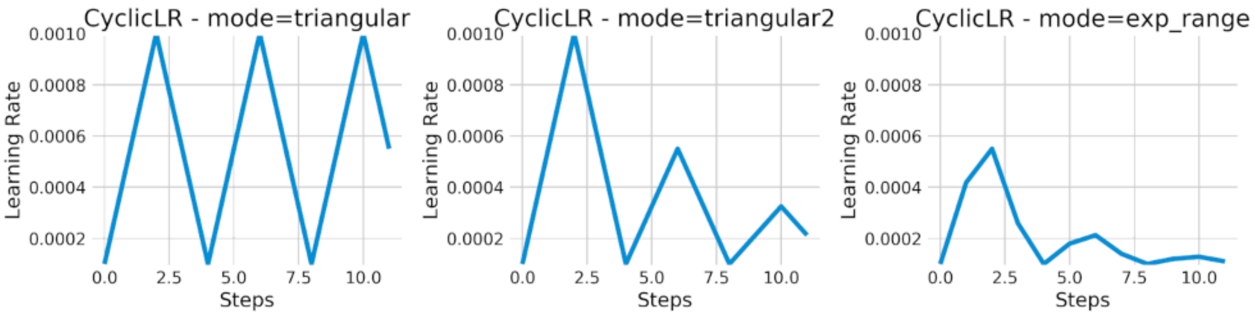




https://imgur.com/a/Hqolp

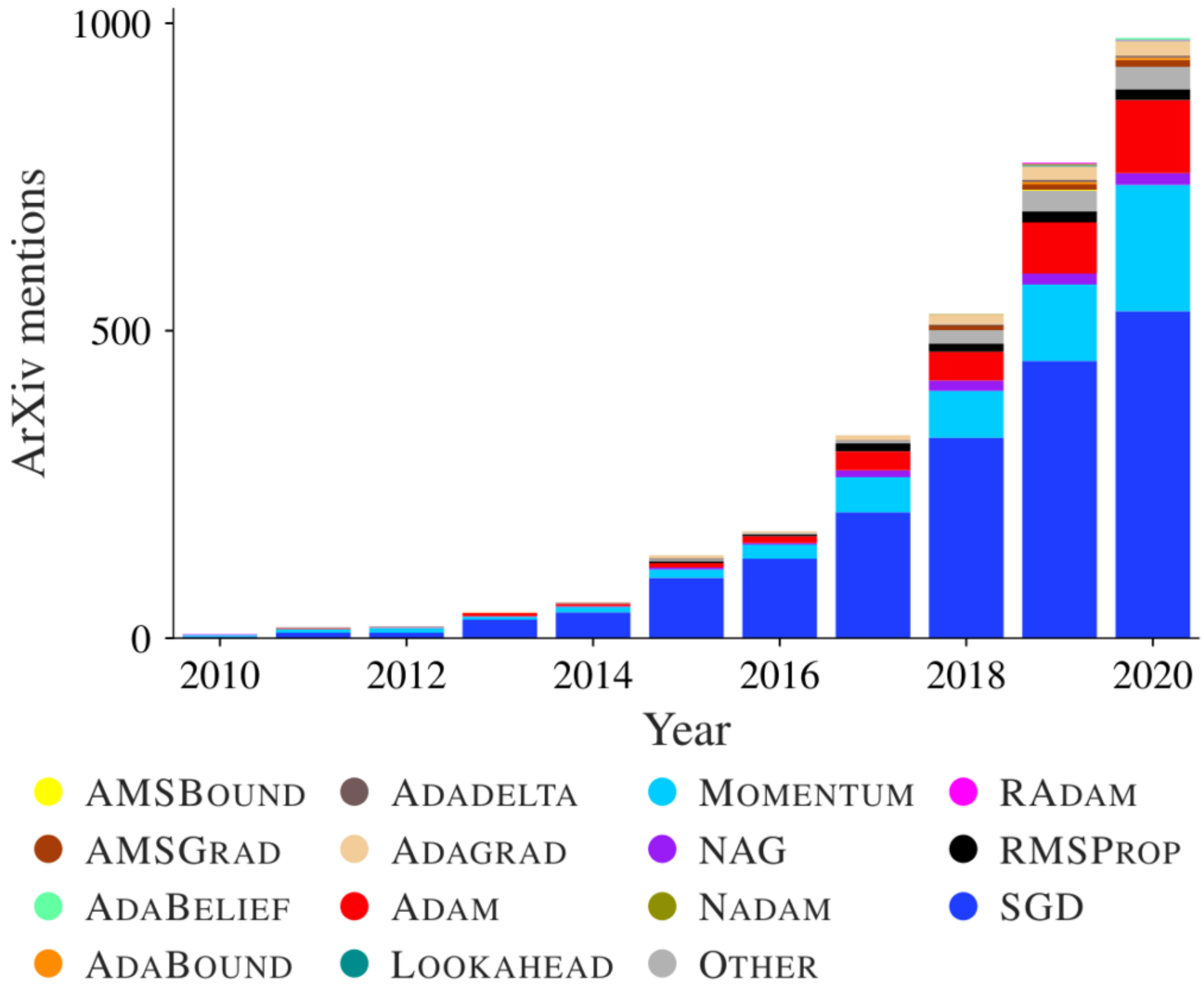
# Learning Rate Scheduler

- Linear decay
- Reduce on Plateau
- Cyclic LR
- ...



# Solver Popularity




Schmidt et al.,"Benchmarking Deep Learning Optimizers", ICML 2021.

# Solver takeaway

- No clear winner
- Adam (RMSprop, NAG) remains a viable choice for many problems

- Instead of trying a new solver, re-tuning and re-running your favorite one seems to be the best choice.

Schmidt et al.,"Benchmarking Deep Learning Optimizers", ICML 2021.

# Vanishing&Exploding Gradients

- Common in very deep nets

$$J(\theta) = z^{(P)}(\ldots z^{(p)}(z^{(2)}(z^{(1)}(x)))\ldots)$$

$$z^{(p)}(x) = Wx \quad p = 1, \ldots, P$$

$$J(\theta) = WW\ldots Wx = W^P x = V\Lambda^P V^{-1} x$$

$$\lim_{p\to\infty} \lambda_i^p$$

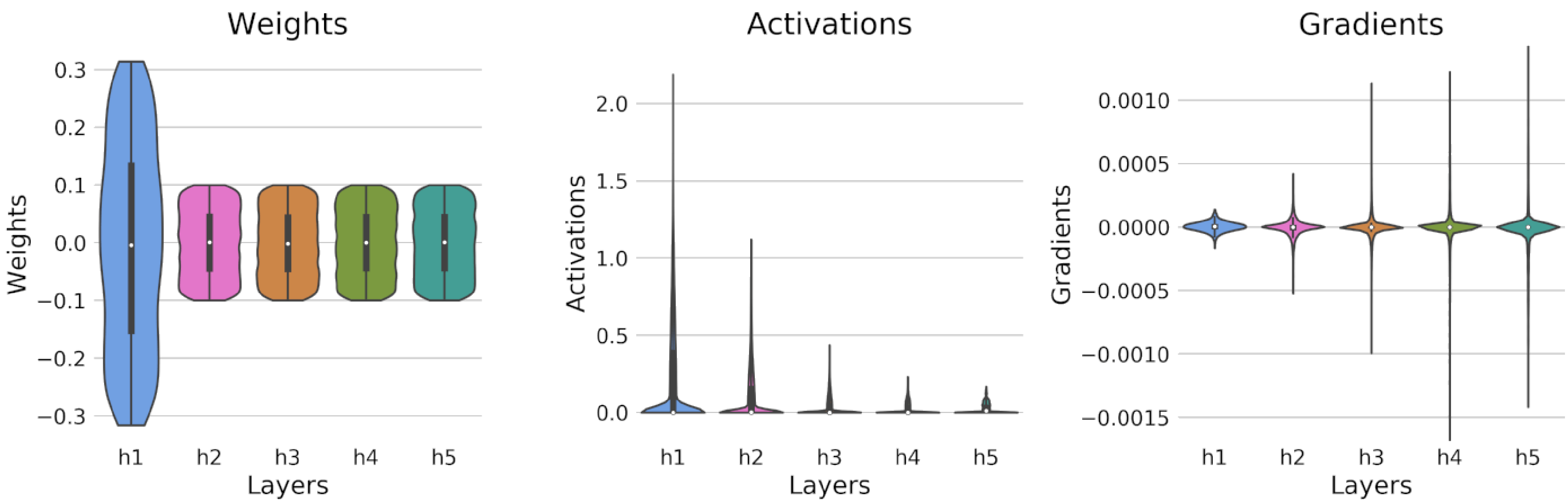
Eigenvalues<1 go to zero

Eigenvalues>1 go to infinity

- Proper initialization of weights
- Gradient clipping
- Batch normalization

# Initialization

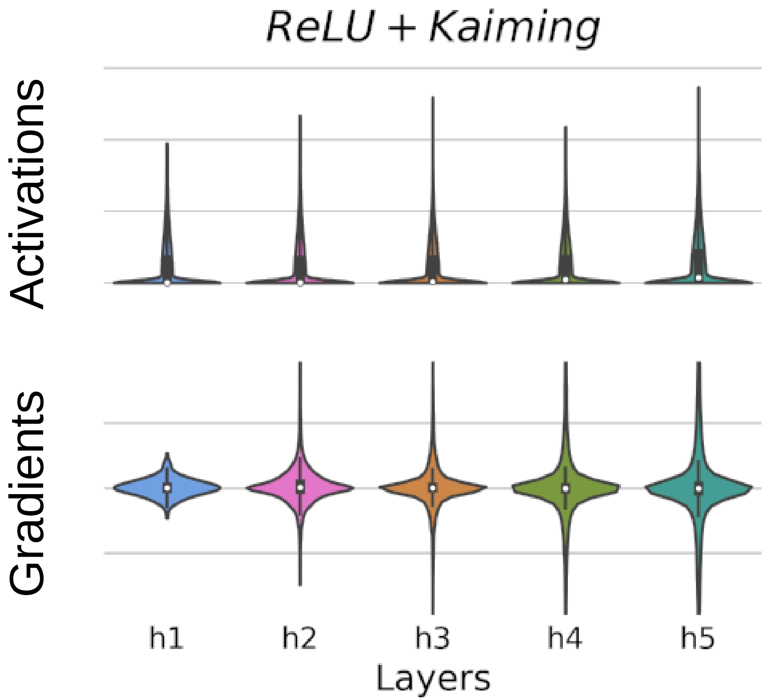
- Main principle: “break symmetry” - - > random initialization




- But we should also adapt the variance of random initialization

# Initialization

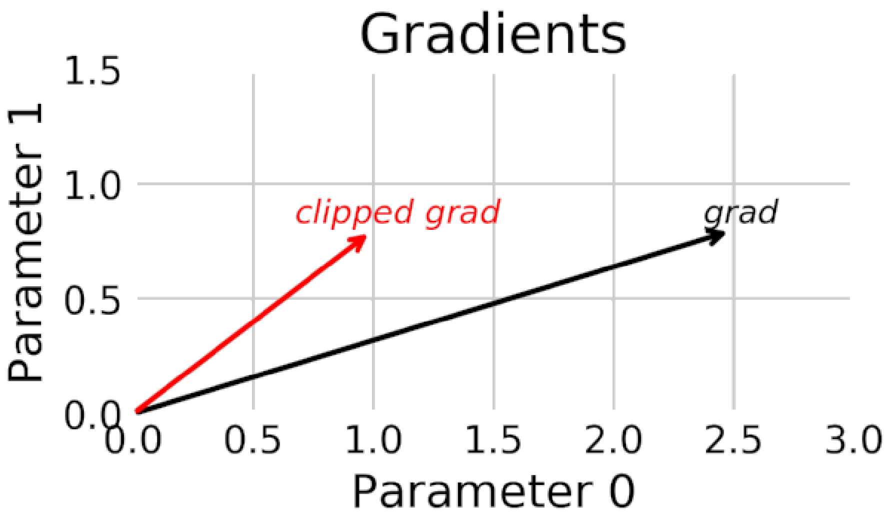
- *Kaiming* initilization for layers with ReLU activation



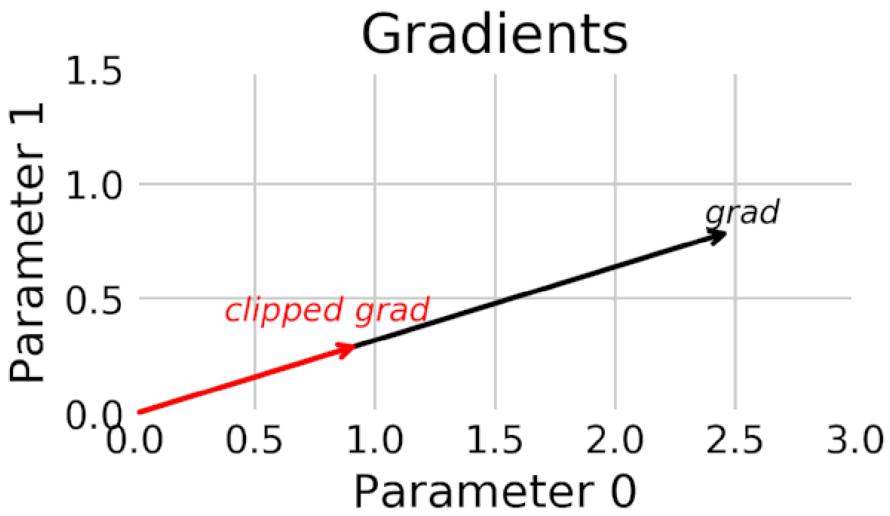

- *Glorot initialization* for layers with tanh activation

# Gradient Clipping

- Good for exploding gradients

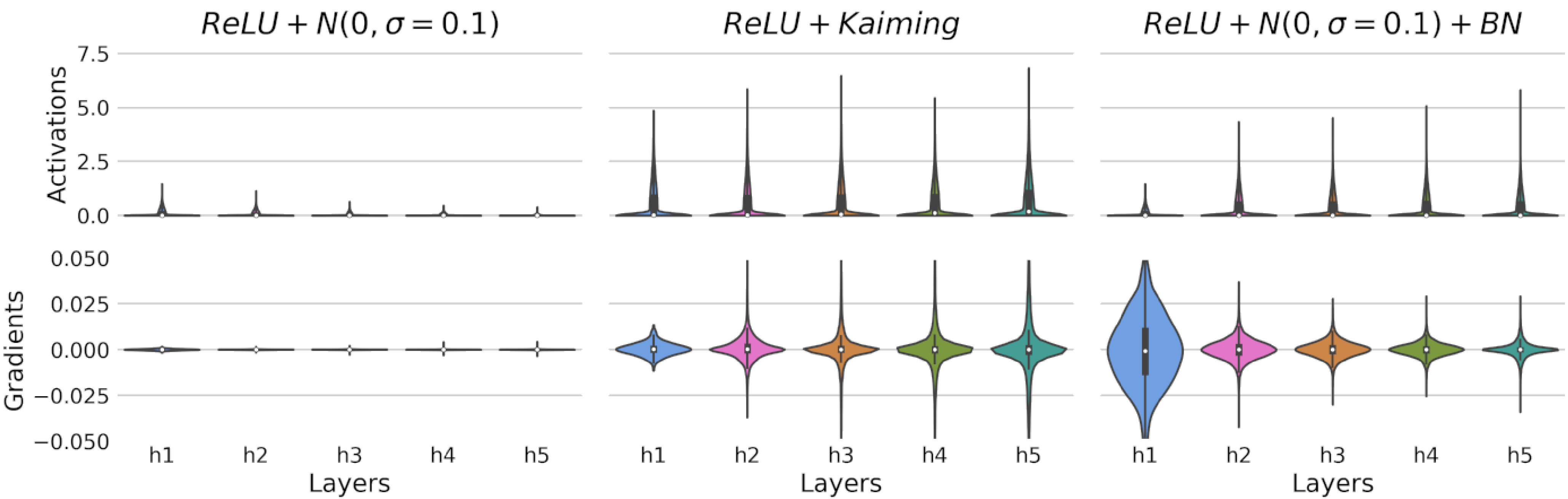



Value clipping




Norm clipping

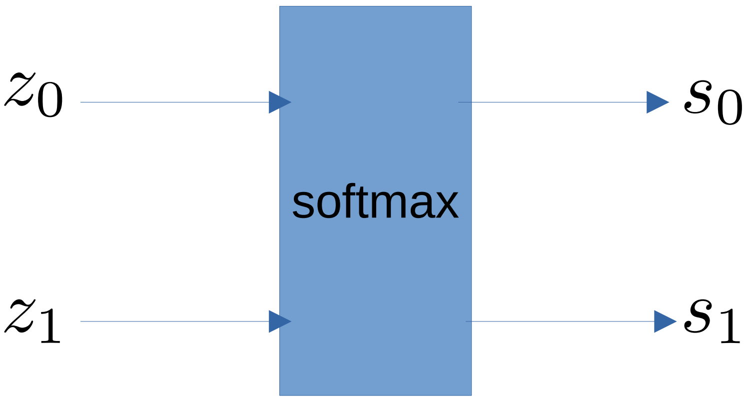
# Batch Normalization



- Extra Slides….

# Derivation of softmax

- Consider two-class problem
- z_0, z_1: network output (not probabilities)




$$s_0 + s_1 = 1$$

- S_0 ... probability of class 0
- S_1 ... probability of class 1

- GT labels: $\{t^i\}_{i=1}^{N} \quad \text{e.g.} \quad = \{0, 1, 1, \ldots\}$

$$(z_0^i, z_1^i) \quad i = 1, \ldots, N$$

# Derivation of softmax

- Maximize entropy $$s_0^i \log s_0^i + s_1^i \log s_1^i$$
- Subject to:

$$s_0^i, s_1^i \geq 0$$

$$s_0^i + s_1^i = 1$$

$$\sum_i s_0^i z_0^i = \sum_{\{i|t^i=0\}} z_0^i \equiv N\mu_0$$

$$\sum_i s_1^i z_1^i = \sum_{\{i|t^i=1\}} z_1^i \equiv N\mu_1$$

$$L = \sum_i s_0^i \log s_0^i + s_1^i \log s_1^i +$$
$$\lambda_0(\mu_0 - s_0^i z_0^i) + \lambda_1(\mu_1 - s_1^i z_1^i) +$$
$$\lambda(s_0^i + s_1^i - 1)$$

# Derivation of softmax

$$L = \sum_i s_0^i \log s_0^i + s_1^i \log s_1^i +$$
$$\lambda_0(\mu_0 - s_0^i z_0^i) + \lambda_1(\mu_1 - s_1^i z_1^i) +$$
$$\lambda(s_0^i + s_1^i - 1)$$

$$\frac{\partial L}{\partial s_0} = \log s_0 + 1 - \lambda_0 z_0 + \lambda = 0$$

$$\frac{\partial L}{\partial s_1} = \log s_1 + 1 - \lambda_1 z_1 + \lambda = 0$$

$$s_0 = e^{\lambda_0 z_0 - \lambda - 1}$$

$$s_1 = e^{\lambda_1 z_1 - \lambda - 1}$$

# Derivation of softmax

$$s_0 = e^{\lambda_0 z_0 - \lambda - 1}$$

$$s_1 = e^{\lambda_1 z_1 - \lambda - 1}$$

$$s_0 + s_1 = 1$$

$$e^{-\lambda - 1} = \frac{1}{e^{\lambda_0 z_0} + e^{\lambda_1 z_1}}$$

$$s_0 = \frac{e^{\lambda_0 z_0}}{e^{\lambda_0 z_0} + e^{\lambda_1 z_1}}$$

$$s_1 = \frac{e^{\lambda_1 z_1}}{e^{\lambda_0 z_0} + e^{\lambda_1 z_1}}$$

$$s_i = \mathrm{softmax}(\mathbf{z})_i$$

# Derivation of sigmoid

- One-class problem: Bernoulli distribution

$$z_1 = 0$$

$$s_0 = \frac{e^{\lambda_0 z_0}}{e^{\lambda_0 z_0} + 1} = \frac{1}{1 + e^{-\lambda_0 z_0}} = \sigma(z_0)$$

# Example – Gaussian Model

- Training data distribution: $p(x,y) = p(y|x)p(x)$
- Estimator of y: $f(x|\theta)$
- Model distribution: $q(y|x) \equiv N(y|f(x;\theta), \sigma^2)$

$$\hat{f}(x) = \arg\min_{f(x)} \mathbb{E}_{p(x,y)}[-\log q(y|f(x))]$$

$$L = \int \left[ \int (y - f(x))^2 p(y|x) dy \right] p(x) dx + c$$

$$\frac{\partial L}{\partial f} \propto \int (y - f(x)) p(y|x) dy = 0$$

$$\hat{f}(x) = \int y p(y|x) dy = \mathbb{E}_{p(y|x)}[y]$$

# Linear Regression

- Training data: $p(x,y) \to \{(x^{(1)}, y^{(1)}), \ldots, (x^{(N)}, y^{(N)})\}$
- Linear estimator of y: $f(x) = wx + b \qquad \theta = \{w, b\}$
- Model distribution: $q(y|x) \equiv N(y|f(x), \sigma^2)$

$$\hat{f}(x) = \arg\min_{f(x)} \mathbb{E}_{p(x,y)}[-\log q(y|f(x))]$$

$$\hat{f}(x) = \arg\min_{f} \frac{1}{2\sigma^2} \sum_i (y^{(i)} - f(x^{(i)}))^2 + \mathrm{c}$$

$$\arg\min_{w,b} \frac{1}{2\sigma^2} \sum_i (y^{(i)} - wx^{(i)} - b)^2 + \mathrm{c}$$

- Closed-form solution

# Example – Laplace Model

- Training data distribution: $p(x,y) = p(y|x)p(x)$
- Estimator of y: f(x)
- Model distribution: $q(y|x) \equiv \mathrm{Laplace}(y|f(x), \gamma)$

$$\hat{f}(x) = \arg\min_{f(x)} \mathbb{E}_{p(x,y)}[-\log q(y|f(x))]$$

$$L = \int \left[ \int |y - f(x)|\, p(y|x) dy \right] p(x) dx + c$$

$$\frac{\partial L}{\partial f} \propto \int \mathrm{sign}(y - f(x)) p(y|x) dy = 0$$

$\hat{f}(x) = m$ … median: $P(y \leq m|x) = P(y \geq m|x)$

# Example – Bernoulli Model

- Training data distribution: $p(x,y) = p(y|x)p(x)\,, \quad y \in \{0,1\}$
- Estimator of y: f(x)
- Model distribution: $q(y|x) \equiv \mathrm{Bernoulli}(y|f(x))$

$$\hat{f}(x) = \arg\min_{f(x)} \mathbb{E}_{p(x,y)} \boxed{[-\log q(y|f(x))]}$$

$$L = \int \sum_{y=0}^{1} \left( \boxed{[y \log f(x) + (1-y)\log(1-f(x))]}\, p(y|x) \right) p(x)\,dx$$

$$\frac{\partial L}{\partial f} = p(x) \sum_{y=0}^{1} \left( y \frac{1}{f(x)} - (1-y) \frac{1}{1-f(x)} \right) p(y|x)$$

$$= p(x) \left( p(y=1|x) \frac{1}{f(x)} - (1 - p(y=1|x)) \frac{1}{1-f(x)} \right)$$

$$= 0$$

# Example – Bernoulli Model

$$p(x)\left(p(y=1|x)\frac{1}{f(x)}-(1-p(y=1|x))\frac{1}{1-f(x)}\right)=0$$

$$\hat{f}(x)=p(y=1|x)=\mathbb{E}_{p(y|x)}[y]$$

$$\mathbb{E}_{p(x)}[\hat{f}(x)]=\int\hat{f}(x)p(x)dx$$

$$=\int p(y=1|x)p(x)dx=p(y=1)$$

… Bernoulli mean

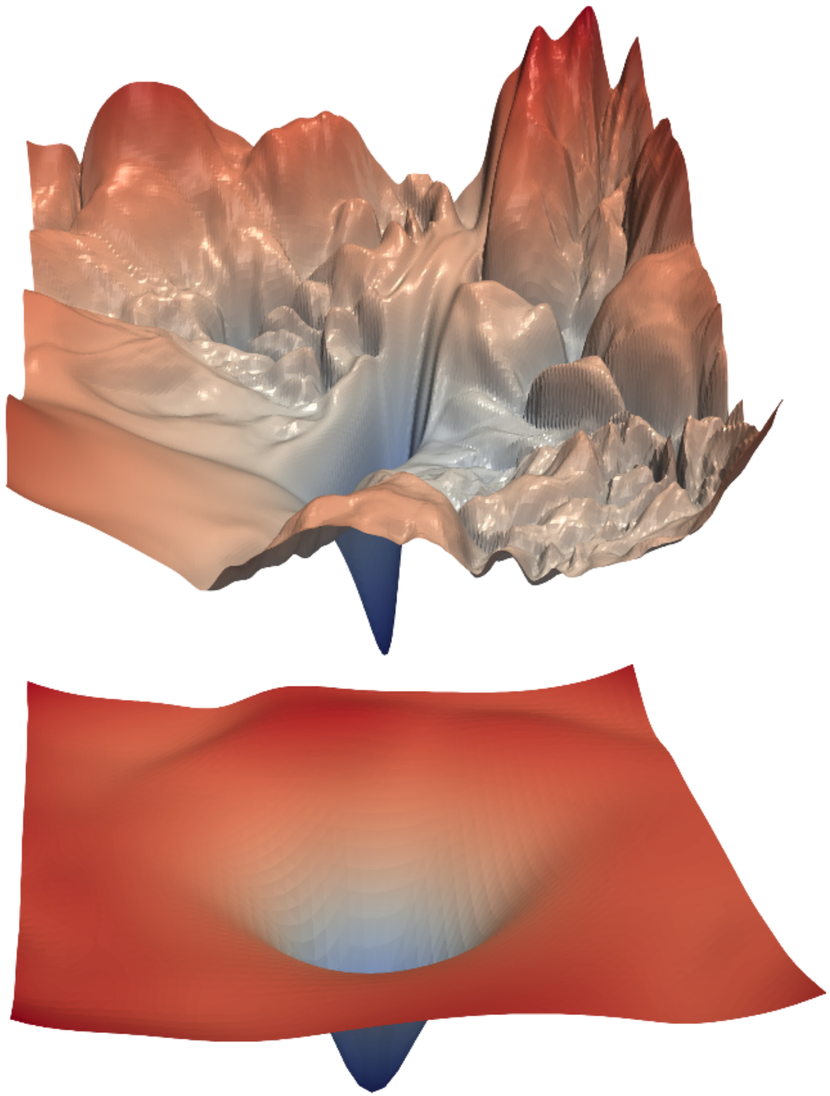
# Strojové učení II

## Regularization

Institute of Information Theory
and Automation of the AS CR

# Regularization

- Reduce overfitting, improve generalization
- Loss terms
  - Parameter Regularization
- Dataset
  - Augmentation
  - Label Smoothing
- Architecture
  - Parameter Tying
  - Bagging
  - Dropout
  - Batch Normalization
  - Residual Connections



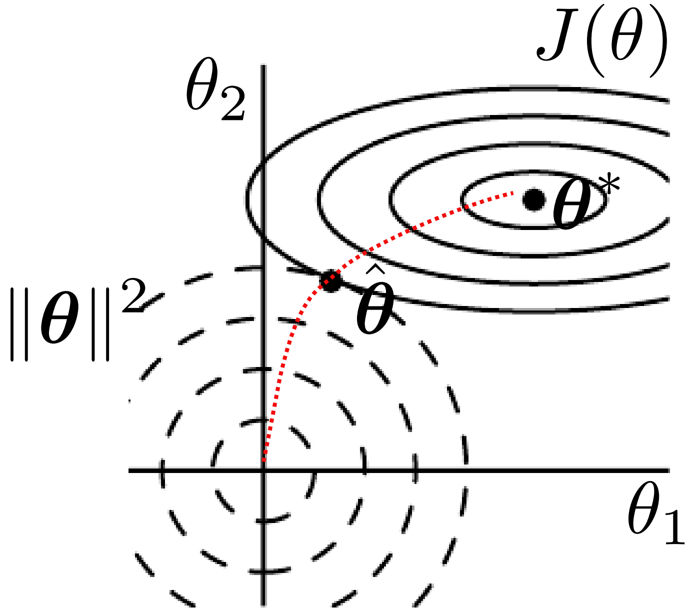
Li et al., NIPS 2018

# Parameter Regularization

- Original loss function $J(\theta)$

  with regularization $\tilde{J}(\theta) = J(\theta) + \lambda \|\theta\|^2$

- L2 norm of parameters is called "Weight Decay"



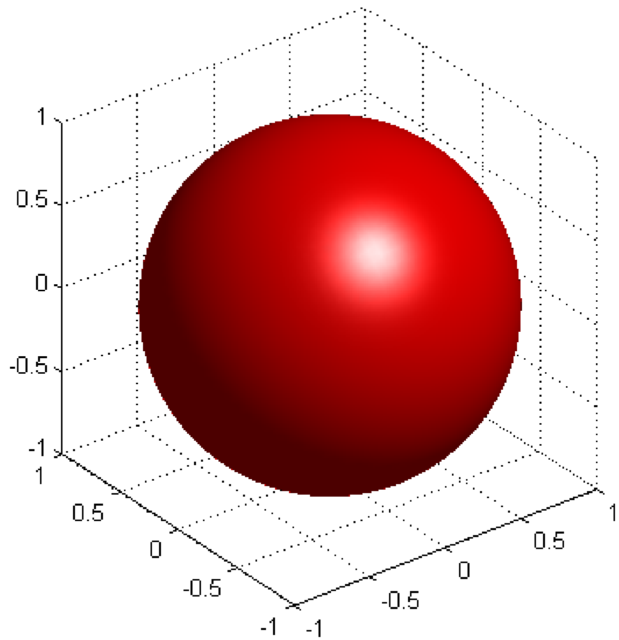

Position on the curve depends on λ

# Unit Ball

$$\tilde{J}(\theta) = J(\theta) + \lambda\|\theta\|_2^2$$

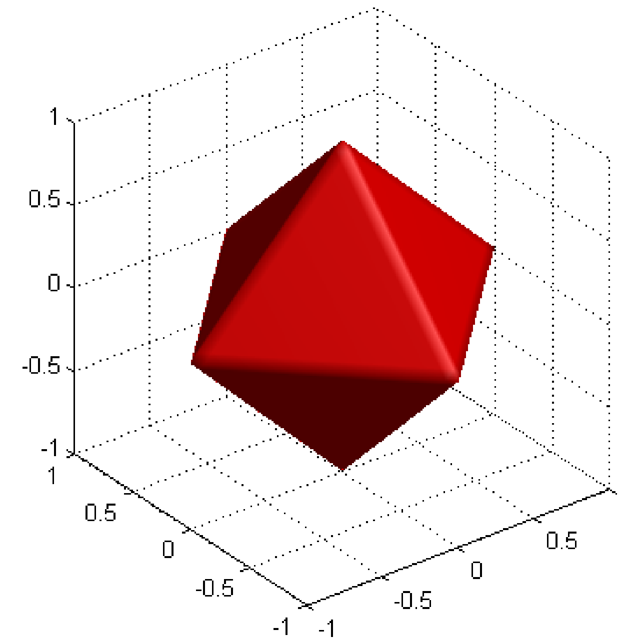
Sometimes is better to use explicit constraints

$$\min J(\theta) \quad \text{s.t.} \quad \|\theta\|_2^2 \leq \epsilon$$




$$\|\theta\|_2^2 = \sum_i |\theta_i|^2$$

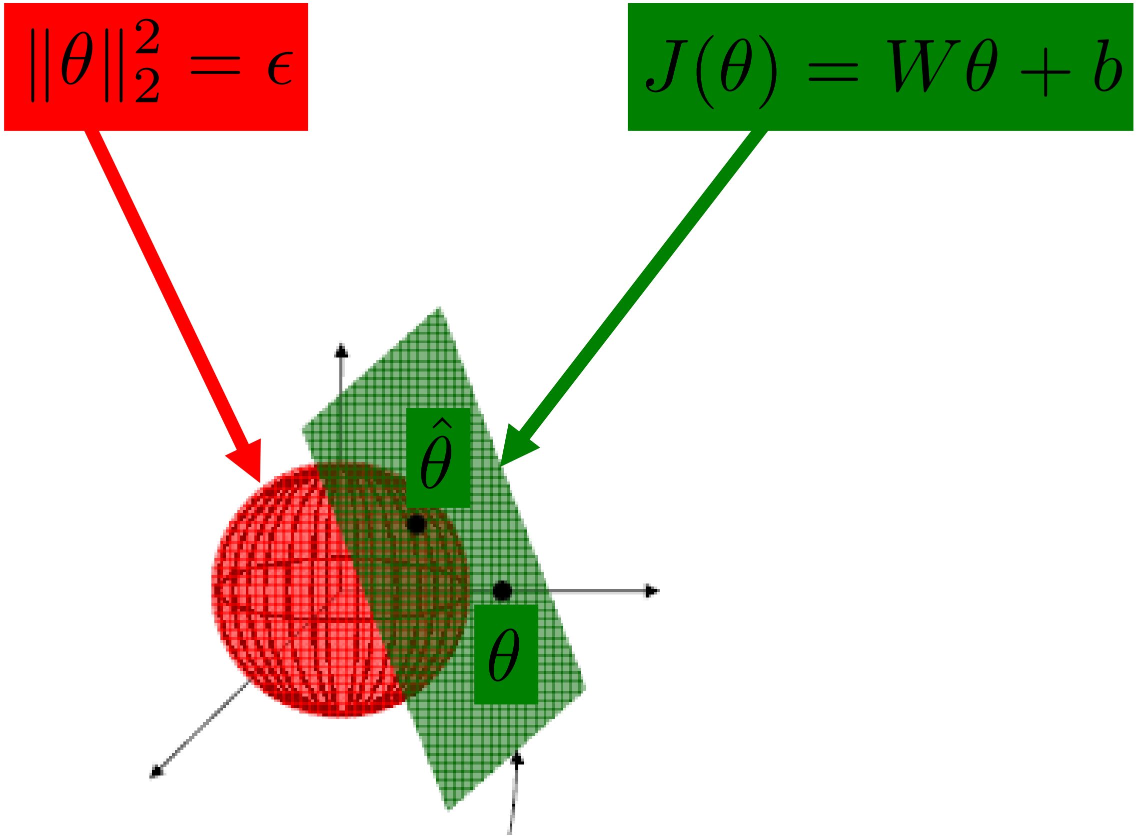
L$_2$ norm



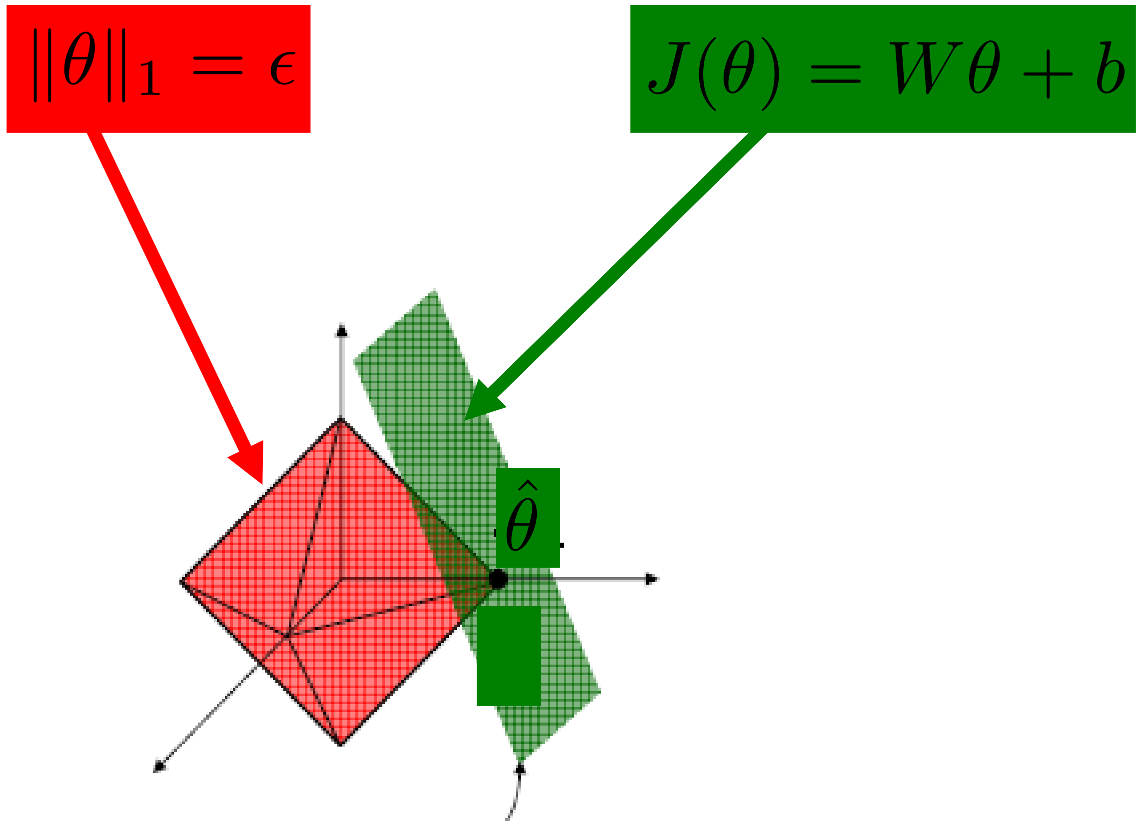

$$\|\theta\|_1 = \sum_i |\theta_i|$$

L$_1$ norm

# L$_2$-norm

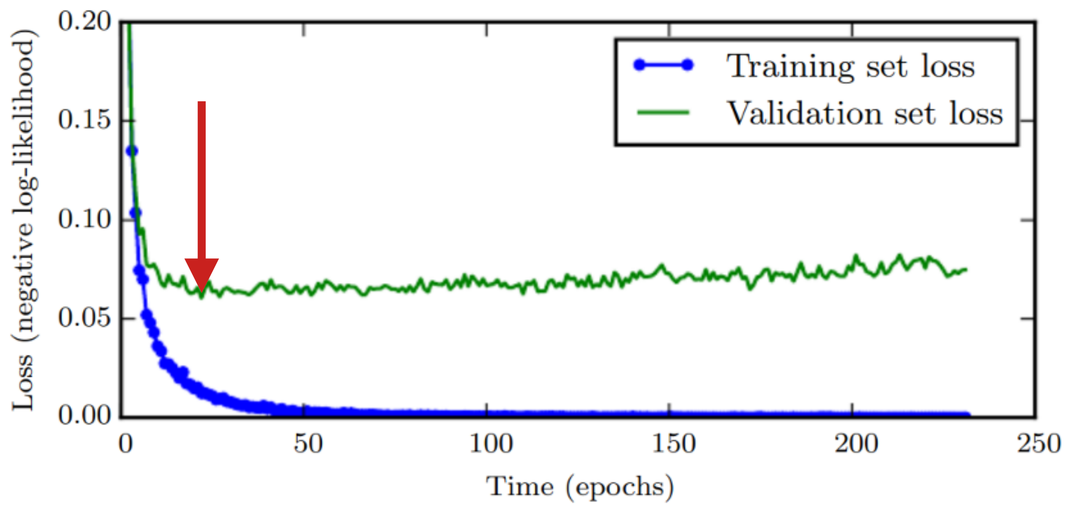


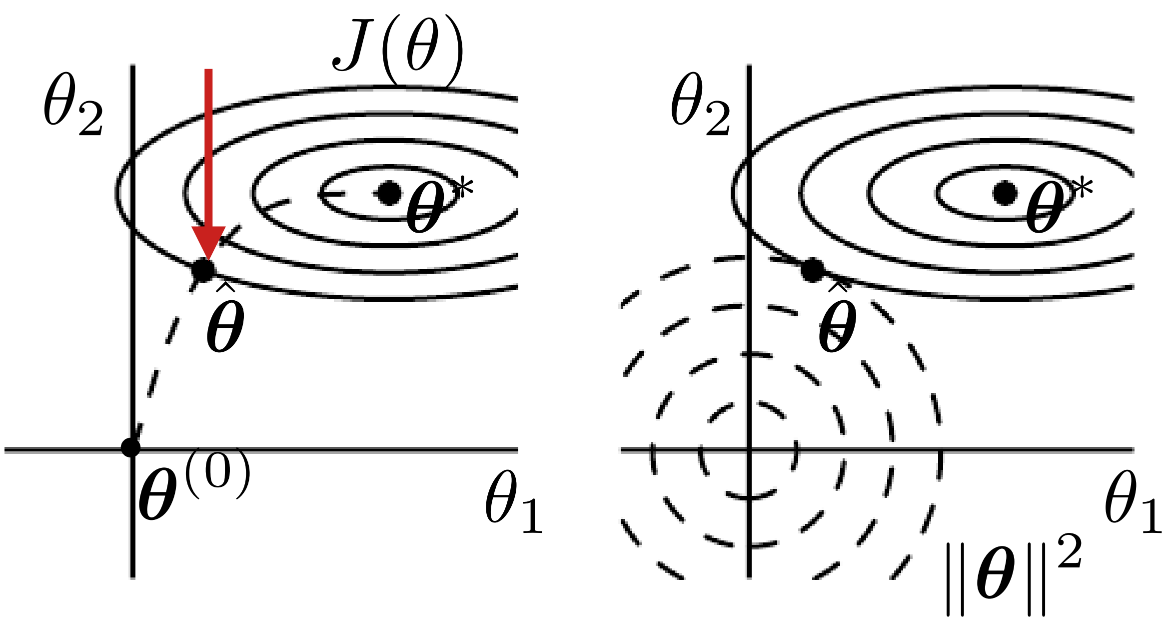
# $L_1$-norm




- Sparse solution

# Early Stopping




Early stopping

L2-norm regularization

# Dataset Augmentation

- Apply random transformation T to inputs
- T = {cropping, rotation, scaling,…}
- This way we learn a representation invariant to T
- Particularly effective for object recognition
- Other transformations: blur, noise, …

# Noise Robustness

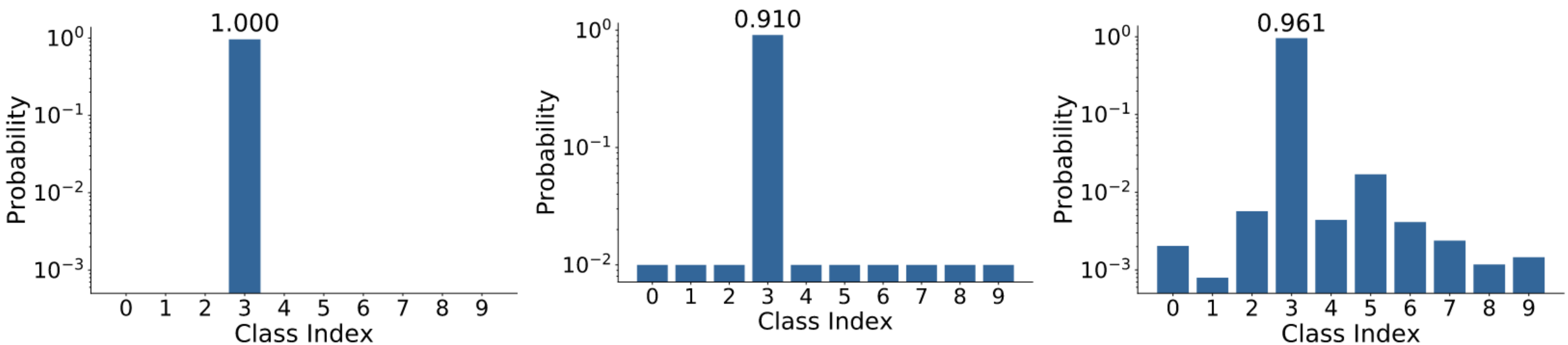
- Injecting noise in
  - Inputs
  - Outputs (labels)
  - Parameters

# Noise in Inputs

- Same principle as data augmentation
- Increases invariance (robustness) to noise

# Noise in Outputs

- Label smoothing




(a) Hard Label (b) LS (c) Ours

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 0 – *airplane* | 1 – *automobile* | 2 – *bird* | 3 – *cat* | 4 – *deer* | 5 – *dog* | 6 – *frog* | 7 – *horse* | 8 – *ship* | 9 – *truck* |

Zhang et al., Delving deep into label smoothing, TIP 2021

# Noise in Parameters

- Adding noise to weights during learning

  training data: $(x, y) \sim \hat{p}(x, y)$

  loss: $J(\theta) = \mathbb{E}_{p(x,y)}[f(x, \theta) - y]$

  with noise: $\tilde{J}(\theta) = \mathbb{E}_{p(x,y)}[f(x, \theta + n) - y] \quad n \sim N(0, \eta\mathbf{I})$

- Similar to a regularized problem:

$$\tilde{J}(\theta) \sim \mathbb{E}_{p(x,y)}[(f(x, \theta) - y) + \eta\|\nabla_\theta f(x, \theta)\|^2]$$

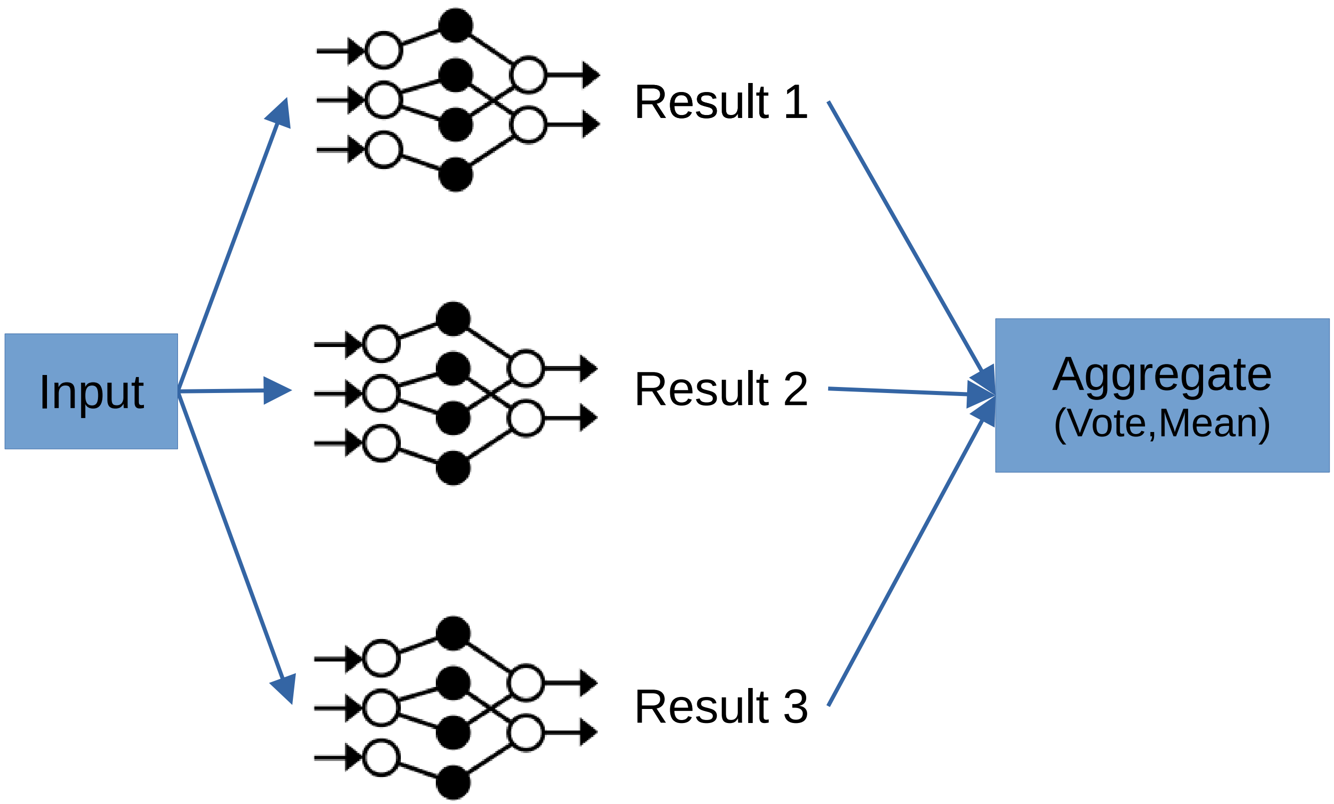
# Parameter Tying

- Decrease the number of parameters
  - Share parameters across layers
  - Share parameters across tasks
  - By assuming structured W in linear units (e.g. convolution)

$$y = Wx + b$$

# Bagging

- Bootstrap aggregation

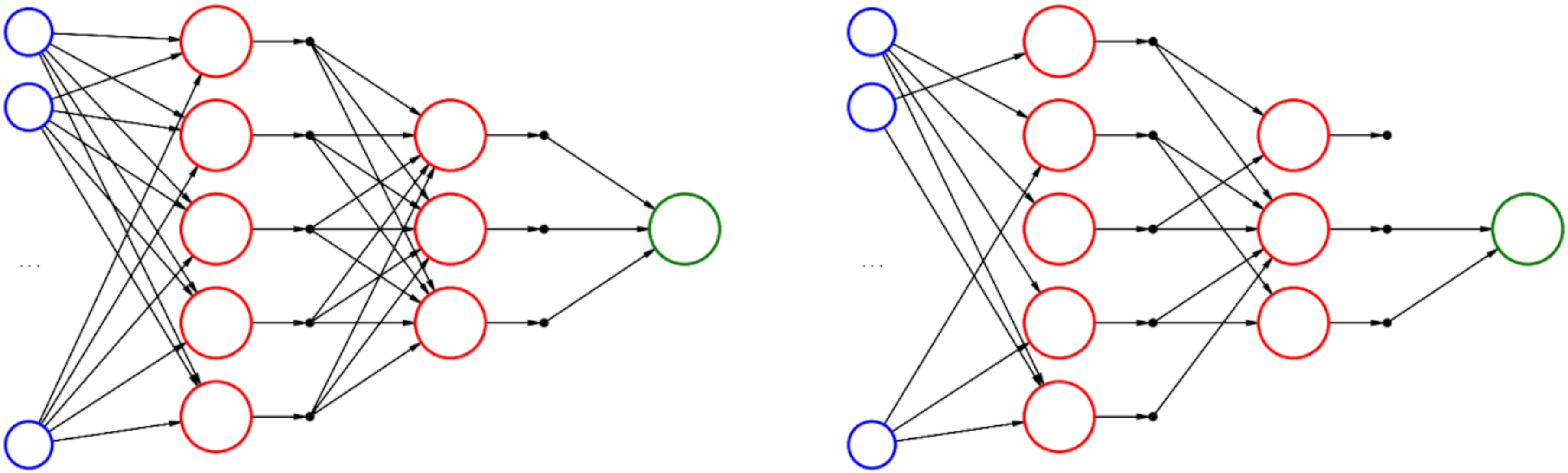



- Uncorrelated results: squared error decreases linearly

Can you prove it?

# Dropout

- Training: randomly remove connections with the probability p and multiply layer outputs by 1/p
- Evaluation: keep all connections



Regular Connections                Applying Dropout

p = 0.5

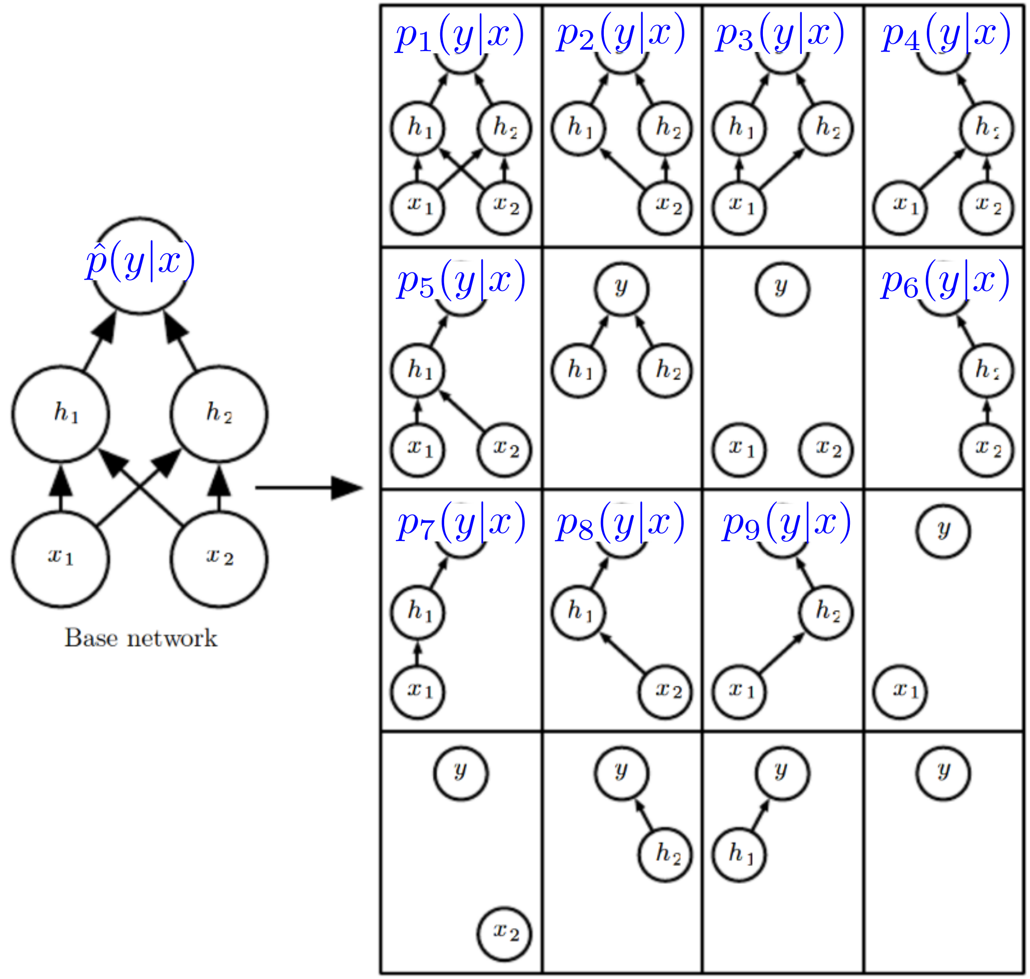
- In 2D (images) dropout removes channels and not pixels!

Why channels and not pixels?

# Dropout

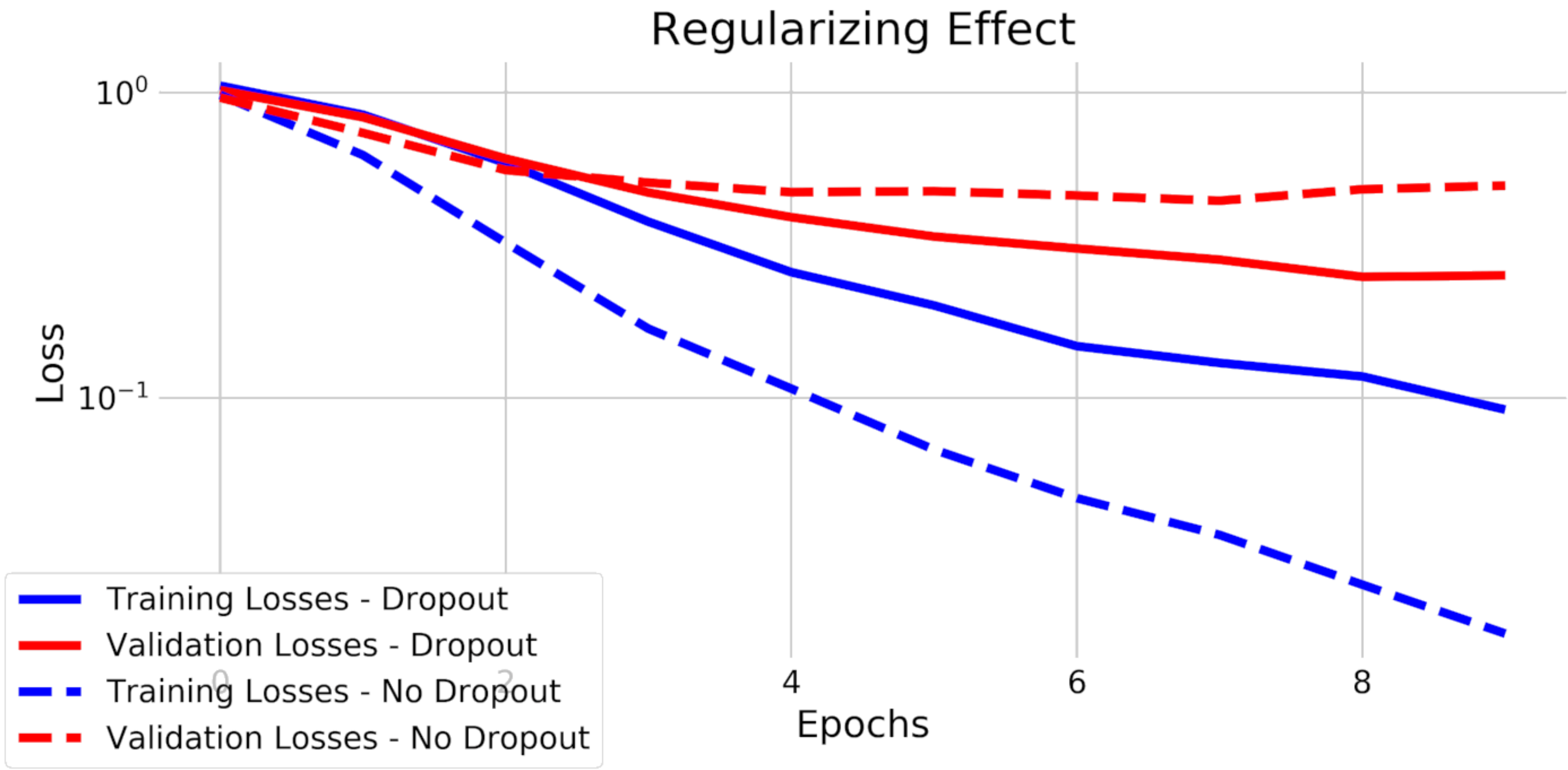
- Equivalent to bagging with an ensemble of subnets
- Inference on the full network is geometric mean

$$\hat{p}(y|x) \approx \sqrt[d]{\prod_{i=1}^{d} p_i(y|x)}$$



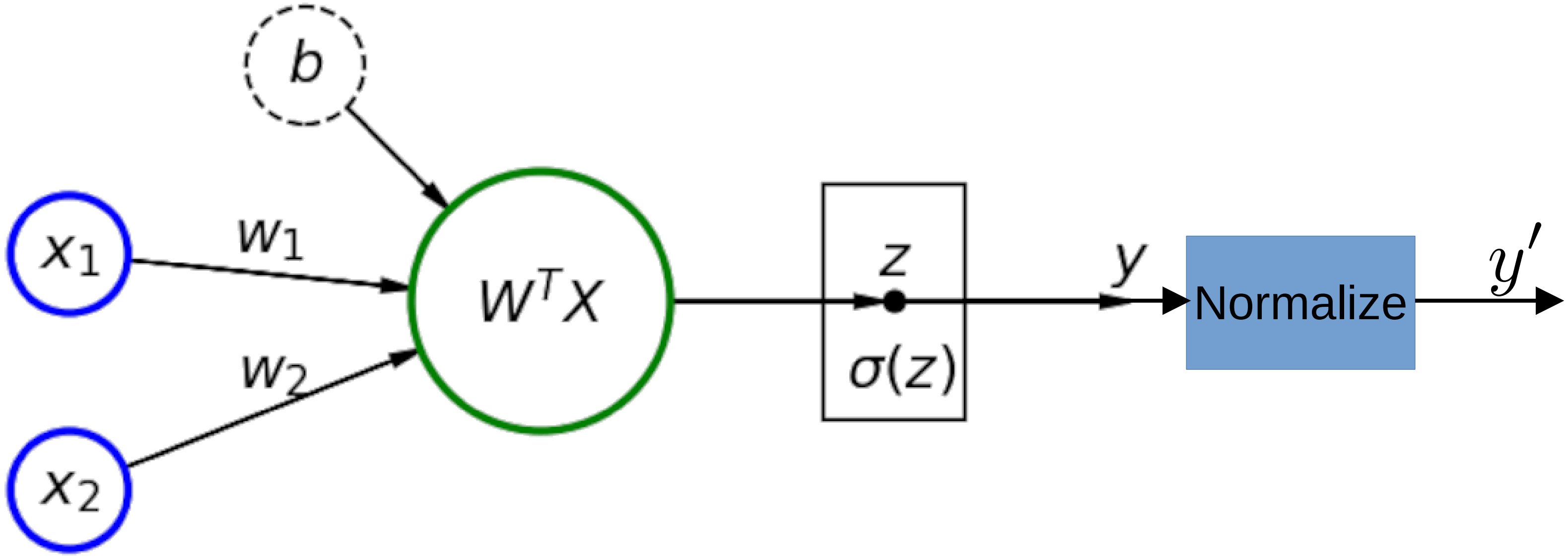

Ensemble of subnetworks

# Dropout Performance



# Batch Normalization

- Standard hidden unit: $y = \sigma(Wx + b)$




- Normalize output across the minibatch $y' = \dfrac{y - \bar{y}}{\sqrt{\mathrm{var}(y) + \epsilon}}$

$$\bar{y} = \frac{1}{|\mathbb{B}|} \sum_{i \in \mathbb{B}} y^{(i)} \qquad \mathrm{var}(y) = \frac{1}{|\mathbb{B}|} \sum_{i \in \mathbb{B}} (y^{(i)} - \bar{y})^2$$

# Batch Normalization

- Training: update $\bar{y}, \mathrm{var}(y)$ with every batch
- Evaluation: keep learned statistics $\bar{y}, \mathrm{var}(y)$ (EWMA) from the training phase
- Output of hidden layers have mean=0 and var=1

Exponential Weighted Moving Average

- Helps to solve Vanishing/Exploding gradients
- In reality BN makes the loss surface smoother!

- Implementation:
  - Extra affine transf. param. are learnable: $\gamma * y' + \beta$
  - Why? - > gradients w.r.t. param. are simpler
  - BN before or after the activation function?

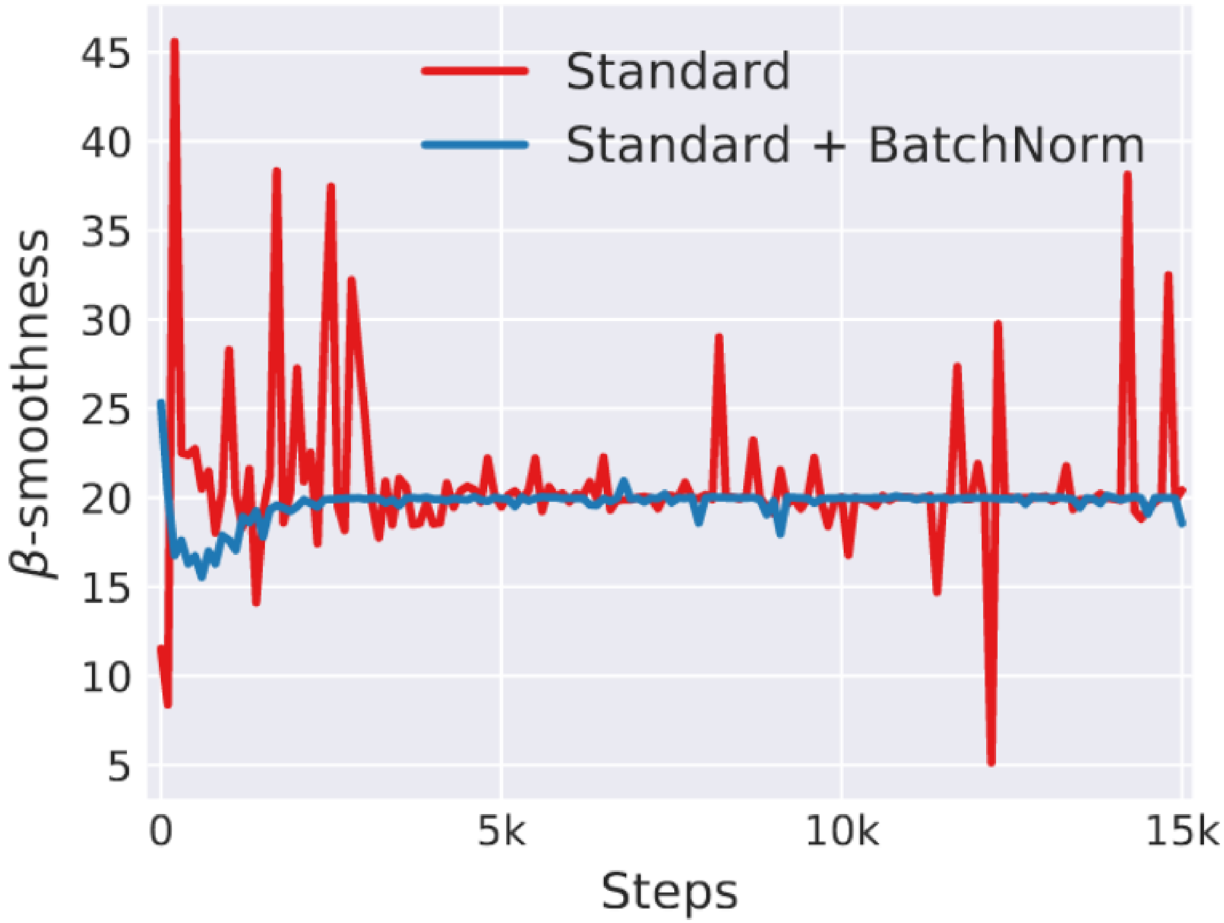
That is the question.

# BN and loss smoothness

- BN decreases Lipschitz constant of the loss

  making it more smooth

$$|f(x_1) - f(x_2)| \leq \beta \|x_1 - x_2\| \quad \forall x_1, x_2$$




Santurkar et al., CoRR 2018

# BN takeaway

- Use BN
  - Architectures with LARGE batches
  - Mean & variance stable across batches
  - Image classification
- Avoid BN
  - Architectures with SMALL batches
  - Unstable mean & variance
  - Object detection / Segmentation / Synthesis

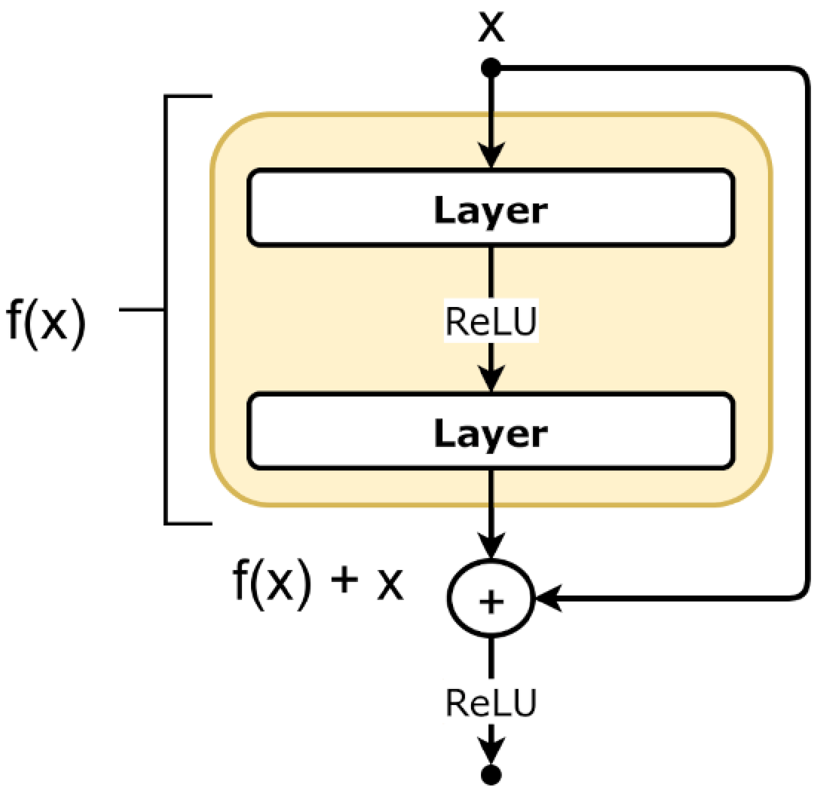
# Residual Connections

- Not trivial to learn "trivial" identity with nonlinearities.

  $y = f(x;\theta)$ learn $\theta$ such that $y = x$

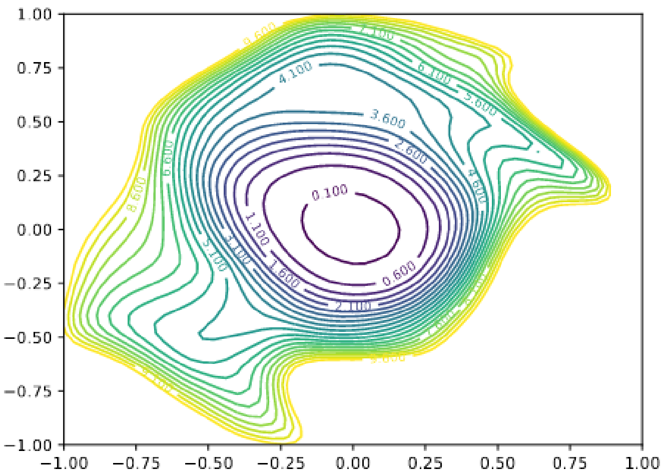
- Easy if

  $$y = f(x;\theta) + x$$

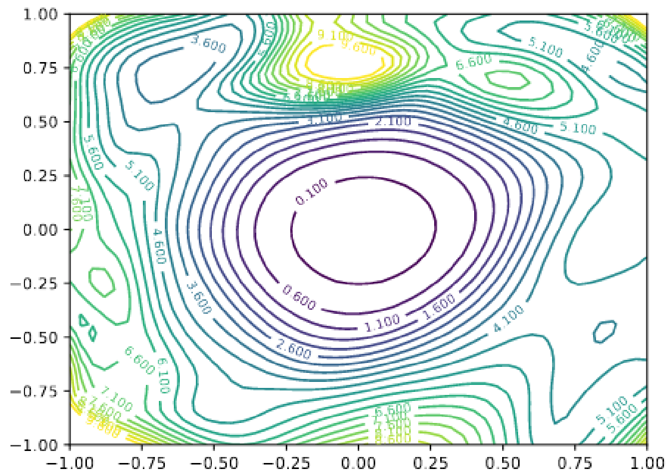


Residual Block

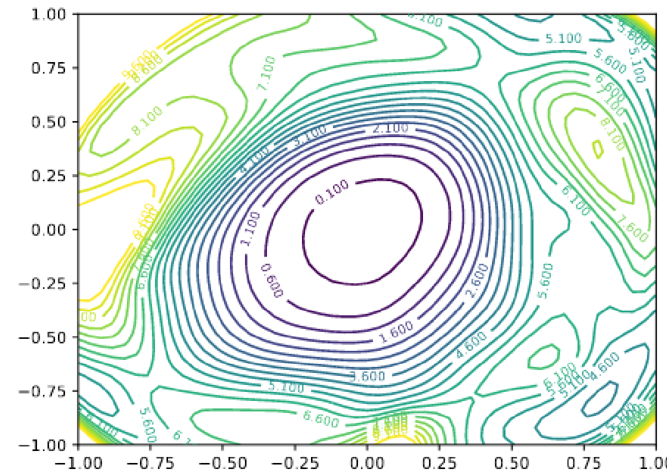
- RC makes the loss surface smoother



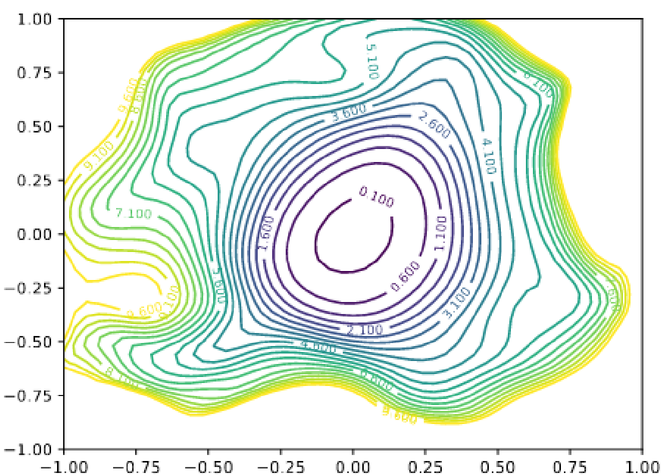
(a) ResNet-20, 7.37%



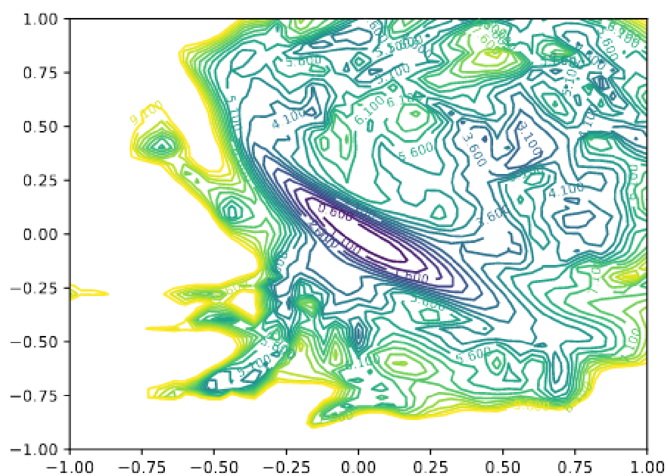
(b) ResNet-56, 5.89%



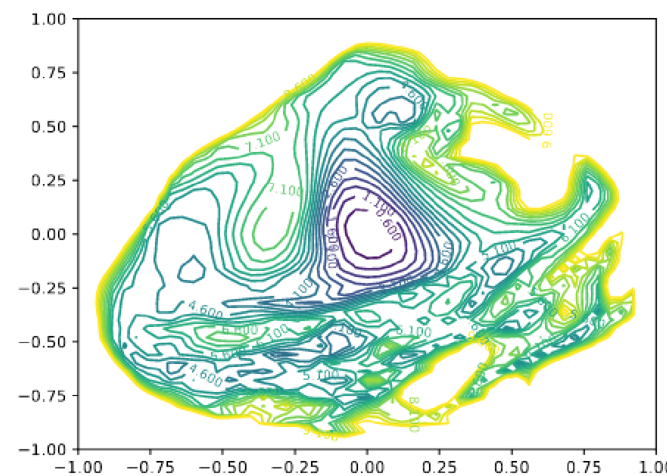
(c) ResNet-110, 5.79%



(d) ResNet-20-NS, 8.18%



(e) ResNet-56-NS, 13.31%



(f) ResNet-110-NS, 16.44%

Li et al., Visualizing the loss landscape, 2018