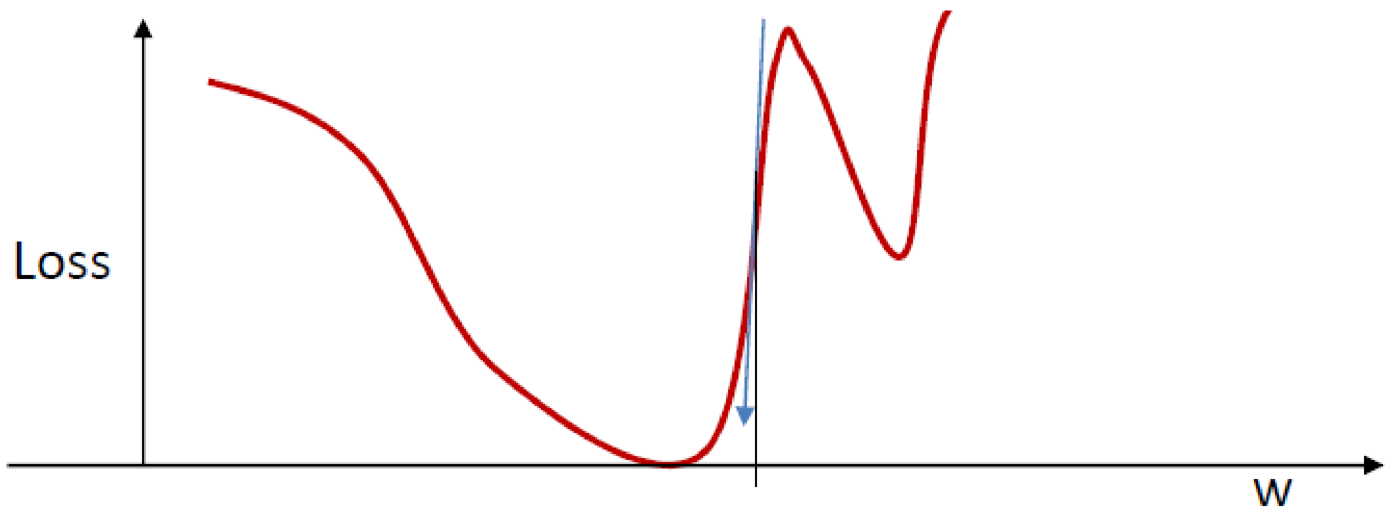
Important Techniques in Neural Network Training

Gradient Clipping

- The loss can occasionally lead to a steep descent
- This result in immediate instability
- If gradient norm bigger than a threshold, set the gradient to the threshold.

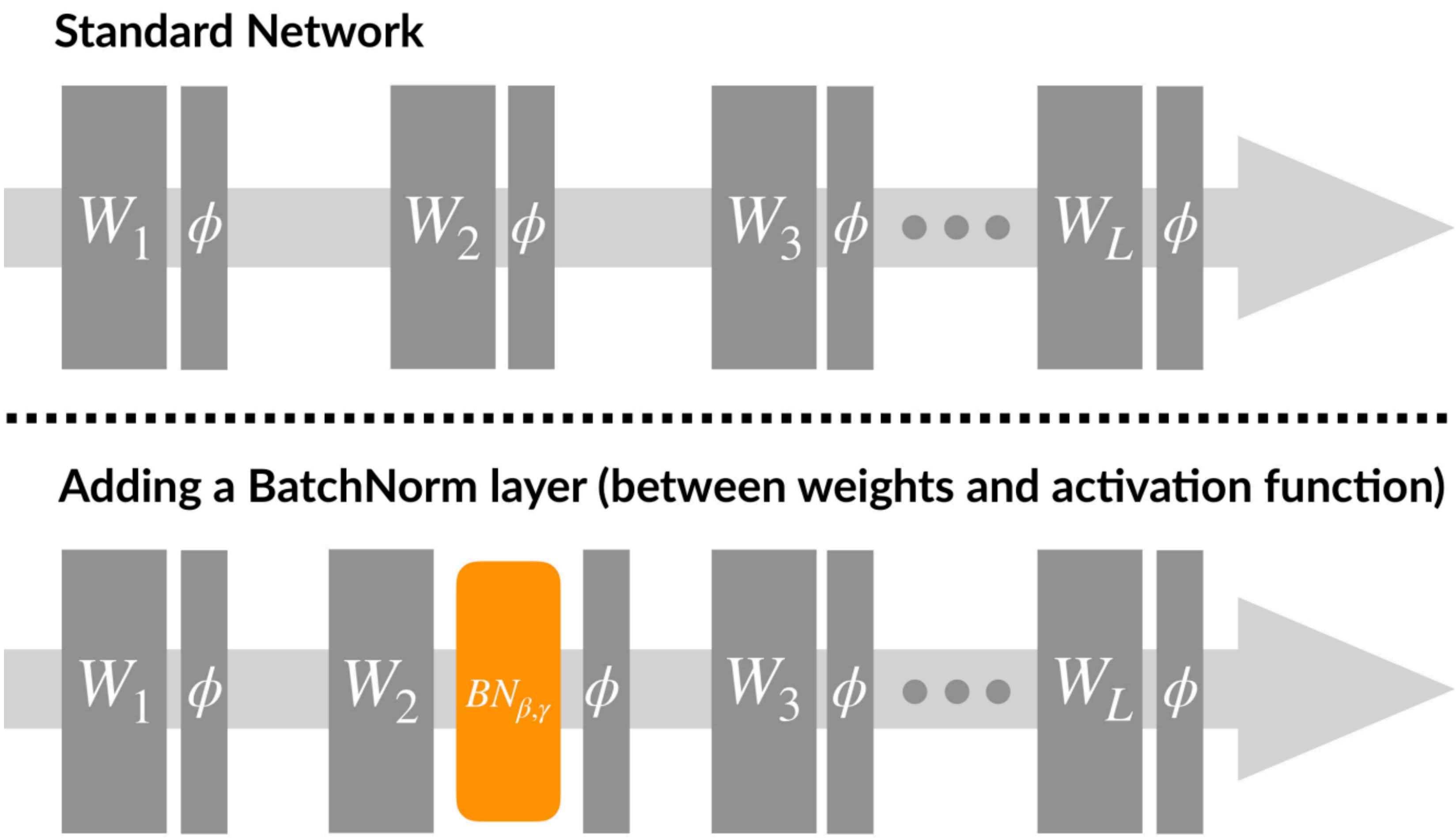


Batch Normalization (Ioffe & Szegedy, ’14)

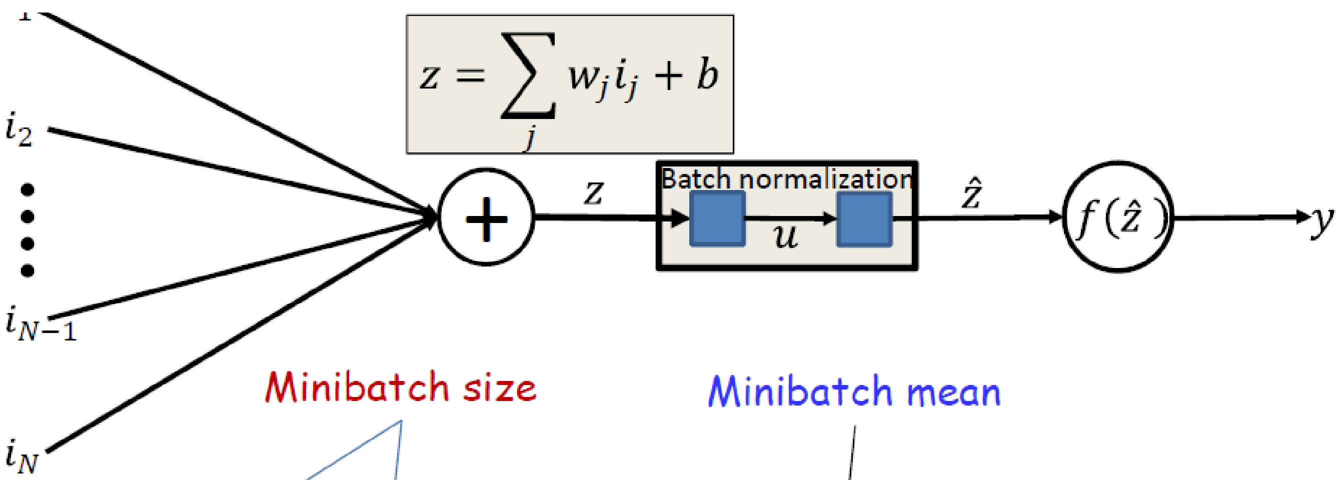
- Normalizing/whitening (mean = 0, variance = 1) the inputs is generally useful in machine learning.
  - Could normalization be useful at the level of hidden layers?
  - **Internal covariate shift**: the calculations of the neural networks change the distribution in hidden layers even if the inputs are normalized

- **Batch normalization** is an attempt to do that：
  - Each unit’s **pre-activation** is normalized (mean subtraction, std division)
  - During training, mean and std is computed for each minibatch (can be backproped!

Batch Normalization (Ioffe & Szegedy, ’14)



Batch Normalization (Ioffe & Szegedy, ’14)



$$z = \sum_j w_j i_j + b$$

Minibatch size

Minibatch mean

Minibatch standard deviation

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

$$\sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B}(z_i - \mu_B)^2$$

$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

$$\hat{z}_i = \gamma u_i + \beta$$

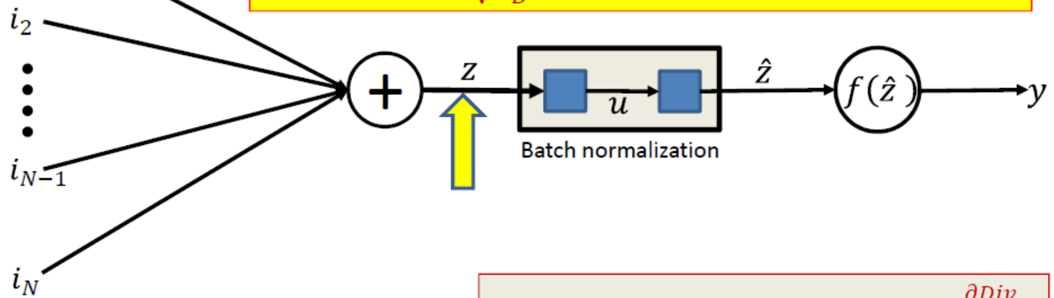
Batch Normalization (Ioffe & Szegedy, ’14)

- BatchNorm at training time
  - Standard backprop performed for each single training data
  - Now backprop is performed over entire batch.

$$\frac{\partial Div}{\partial \sigma_B^2} = \frac{-1}{2}(\sigma_B^2 + \epsilon)^{-3/2} \sum_{i=1}^{B} \frac{\partial Div}{\partial u_i}$$

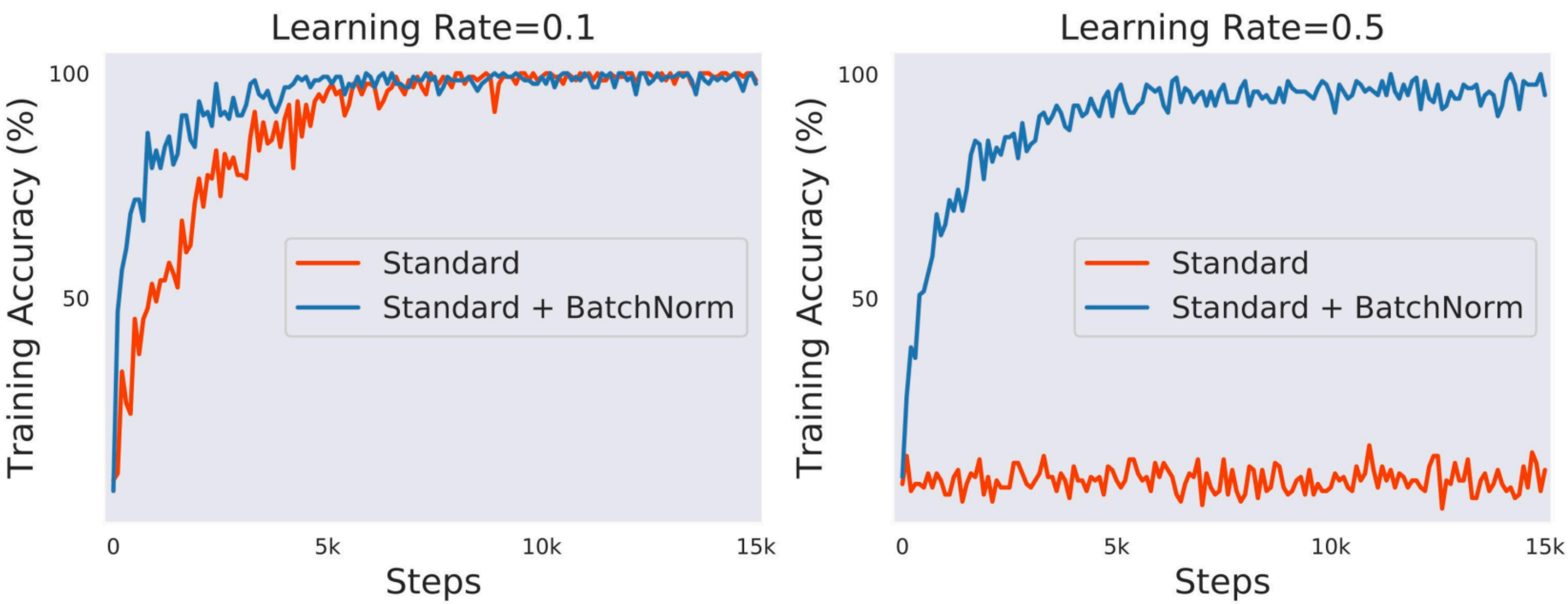
$$\frac{\partial Div}{\partial \mu_B} = \frac{-1}{\sqrt{\sigma_B^2 + \epsilon}} \sum_{i=1}^{B} \frac{\partial Div}{\partial u_i}$$

$$\frac{\partial Div}{\partial z_i} = \frac{\partial Div}{\partial u_i} \cdot \frac{1}{\sqrt{\sigma_B^2 + \epsilon}} + \frac{\partial Div}{\partial \sigma_B^2} \cdot \frac{2(z_i - \mu_B)}{B} + \frac{\partial Div}{\partial \mu_B} \cdot \frac{1}{B}$$



The rest of backprop continues from $\frac{\partial Div}{\partial z_i}$

Batch Normalization (Ioffe & Szegedy, '14)



What is BatchNorm actually doing?

- May not due to covariate shift (Santurkar et al. ‘18):
  - Inject non-zero mean, non-standard covariance Gaussian noise after BN layer: removes the whitening effect
  - Still performs well.

- Only training β, γ with random convolution kernels gives non-trivial performance (Frankle et al. ’20)

- BN can use exponentially increasing learning rate! (Li & Arora ’19)

More normalizations

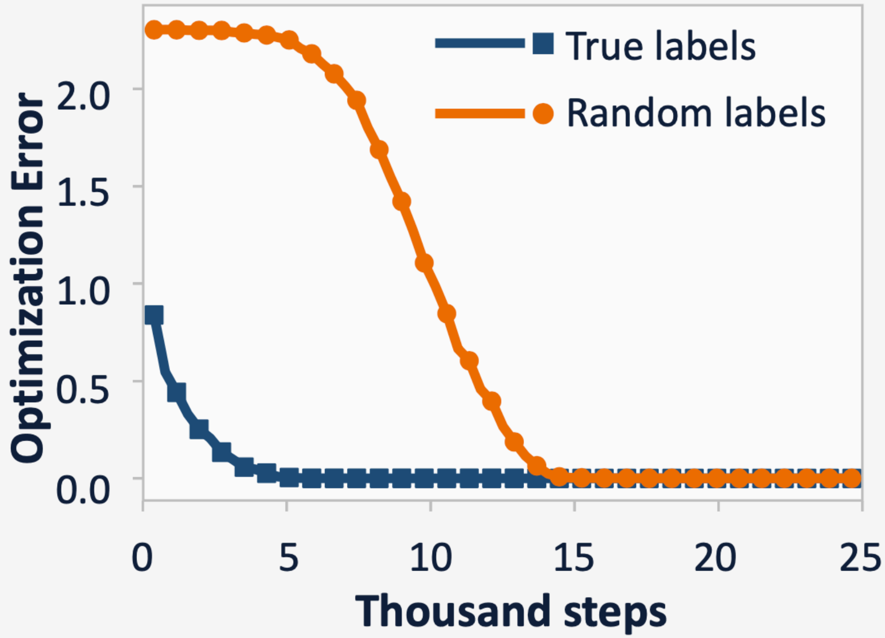
- Layer normalization (Ba, Kiros, Hinton, ’16)
  - Batch-independent
  - Suitable for RNN, MLP
- Weight normalization (Salimans, Kingma, ’16)
  - Suitable for meta-learning (higher order gradients are needed)
- Instant normalization (Ulyanov, Vedaldi, Lempitsky, ’16)
  - Batch-independent, suitable for generation tasks
- Group normalization (Wu & He, ‘18)
  - Batch-independent, improve BatchNorm for small batch size

Non-convex Optimization Landscape

Gradient descent finds global minima

Practice: gradient descent

$$\theta(t+1) \leftarrow \theta(t) - \eta \frac{\partial L(\theta(t))}{\partial \theta(t)}$$



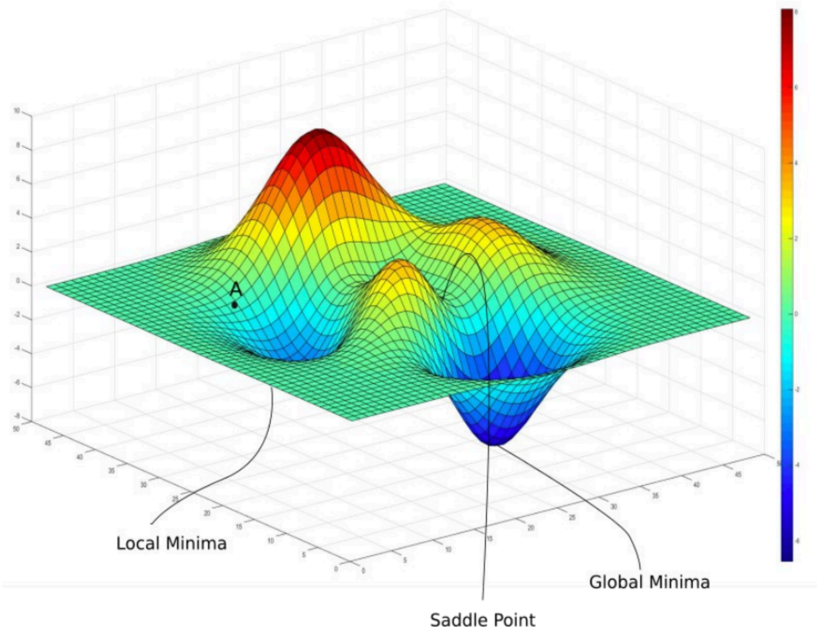
Optimization error **-> 0** for both ***true labels*** and ***random labels*** !

Zhang Bengio Hardt Recht Vinyals 2017

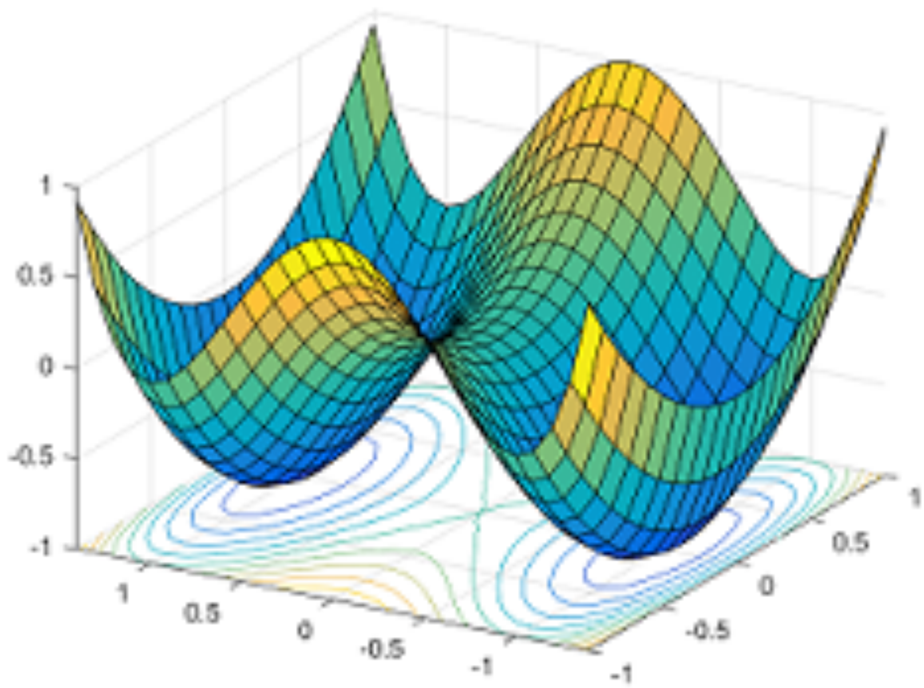
Understanding DL Requires Rethinking Generalization

Types of stationary points

- Stationary points: $x : \nabla f(x) = 0$
- Global minimum: $x : f(x) \leq f(x') \forall x' \in \mathbb{R}^d$
- Local minimum: $x : f(x) \leq f(x') \forall x' : \|x - x'\| \leq \epsilon$
- Local maximum: $x : f(x) \geq f(x') \forall x' : \|x - x'\| \leq \epsilon$
- Saddle points: stationary points that are not a local min/max

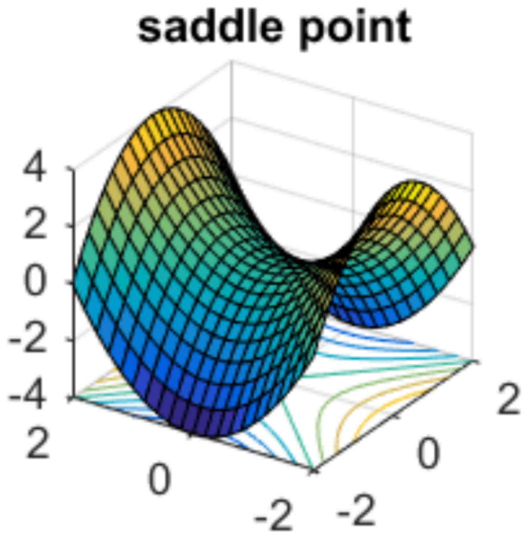


Landscape Analysis



- All local minima are global!
- Gradient descent can escape saddle points.

Strict Saddle Points (Ge et al. ’15, Sun et al. ’15)



- Strict saddle point: a saddle point and $\lambda_{\min}(\nabla^2 f(x)) < 0$

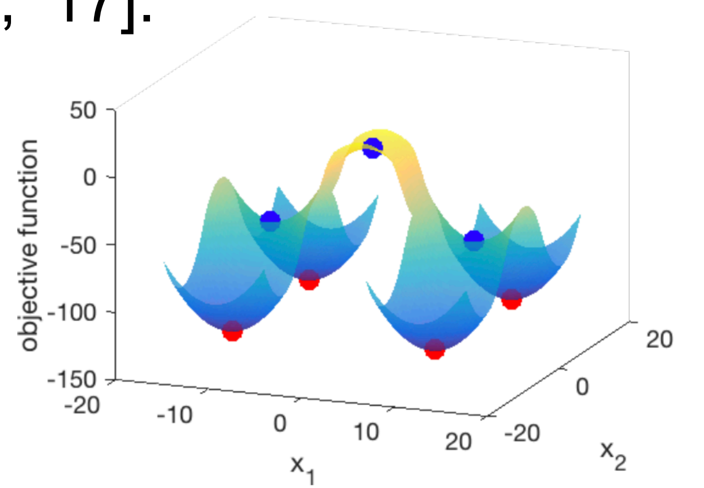
Escaping Strict Saddle Points

- Noise-injected gradient descent can escape strict saddle points in polynomial time [Ge et al., ’15, Jin et al., ’17].

- Randomly initialized gradient descent can escape all strict saddle points asymptotically [Lee et al., ’15].
  - Stable manifold theorem.

- Randomly initialized gradient descent can take exponential time to escape strict saddle points [Du et al., ’17].

If 1) all local minima are global, and 2) are saddle points are strict, then noise-injected (stochastic) gradient descent finds a global minimum in polynomial time



What problems satisfy these two conditions

- Matrix factorization
- Matrix sensing
- Matrix completion
- Tensor factorization
- Two-layer neural network with quadratic activation

What about neural networks?

- Linear networks (neural networks with linear activations functions): all local minima are global, but there exists saddle points that are not strict [Kawaguchi ’16].

- Non-linear neural networks with:
  - Virtually any non-linearity,
  - Even with Gaussian inputs,
  - Labels are generated by a neural network of the same architecture,

There are many bad local minima [Safran-Shamir ’18, Yun-Sra-Jadbaie ’19].

Trajectory-based Analysis for Non-convex optimization

Gradient Flow: a Kernel Point of View

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