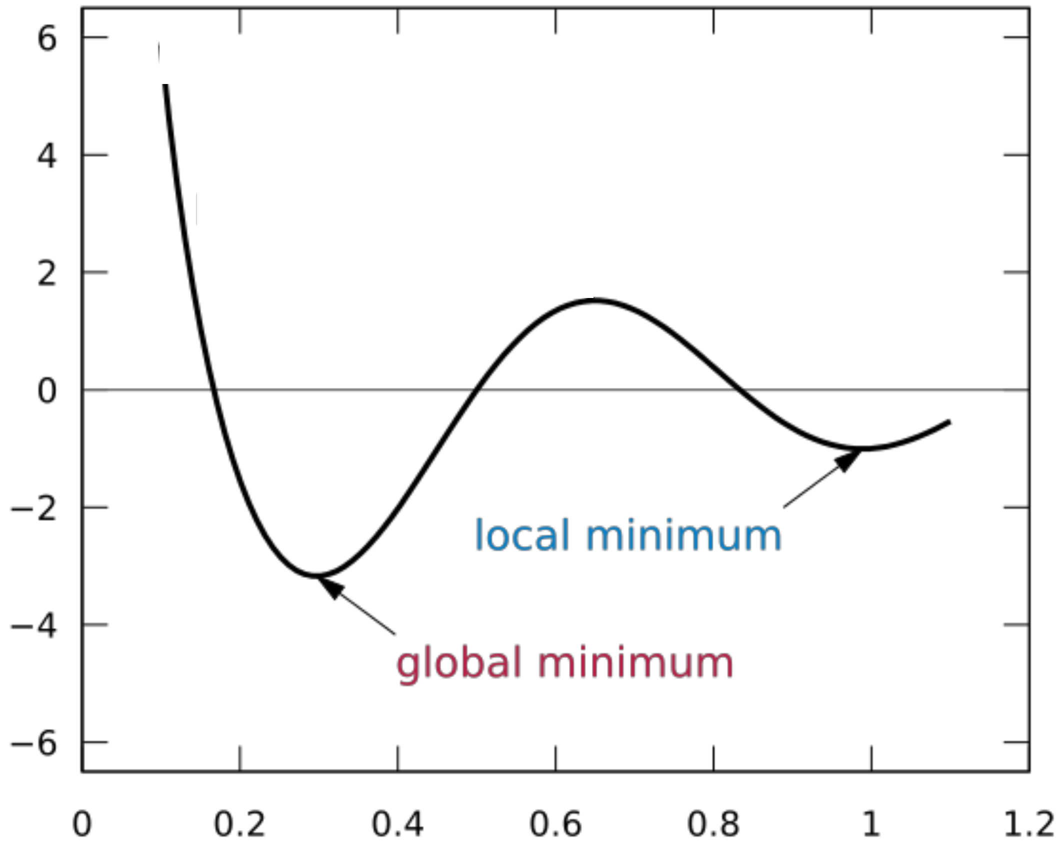
译者：此文数学内容偏多，不做翻译，仅作概要。
概要：
非凸优化中存在大量鞍点和局部极小值，找到全局极小值非常困难。训练的目标是至少逃过鞍点，找到一个较好的局部极小值。为此，需要：

慎重选择下降算法：SGD或Adam优于全梯度下降，能逃离鞍点。
慎重选择批量大小：小批量（32或更小）有助于逃离鞍点并提高泛化能力。
慎重选择初始化：好的初始化（如Xavier或预训练）可以避免陷入坏的区域。

Convex Function vs. Nonconvex Function: A Little Bit Theory

Shusen Wang

Global Extremum vs. Local Extremum



Local Minimum of a function $f(\mathbf{w})$

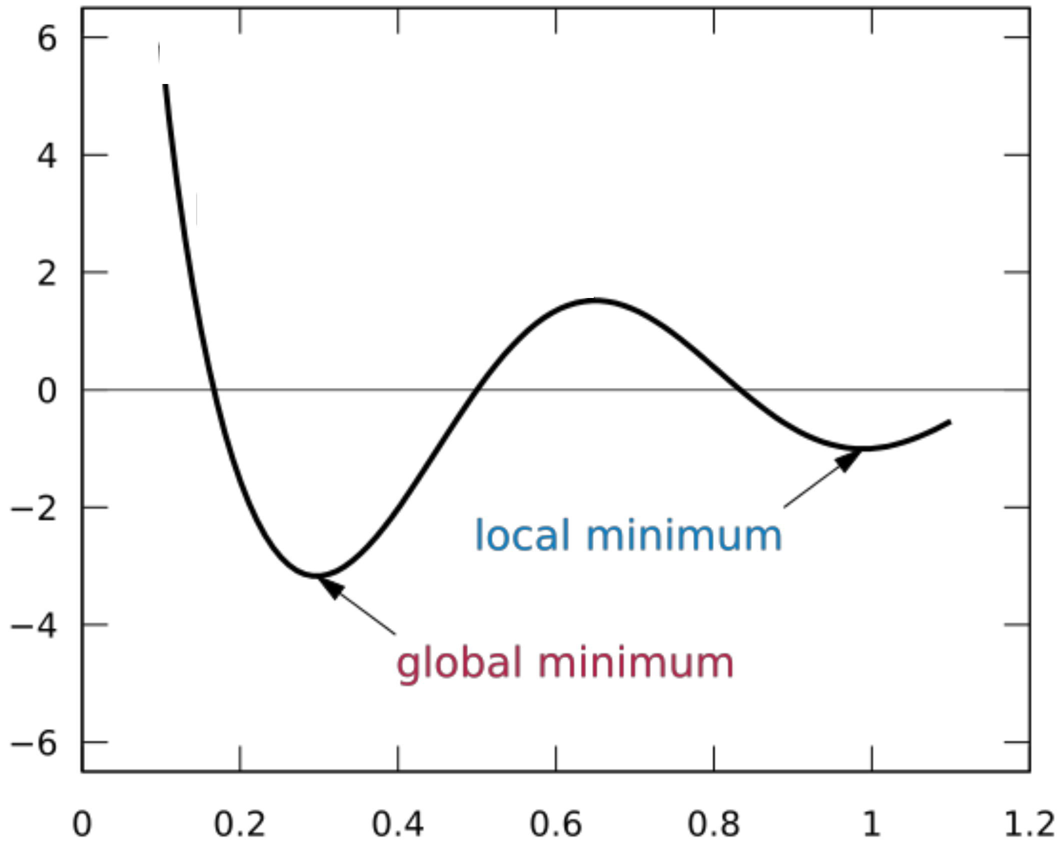
If $f(\mathbf{w}^\star) \leq f(\mathbf{w})$ for all $\mathbf{w}$ in a neighborhood of $\mathbf{w}^\star$, then $\mathbf{w}^\star$ is a **local minimum** of f.

Global Minimum of a function $f(\mathbf{w})$

If $f(\mathbf{w}^\star) \leq f(\mathbf{w})$ for all $\mathbf{w}$ in the domain of f, then $\mathbf{w}^\star$ is a **global minimum** of f.

- A global minimum is a local minimum.
- Global minimum may not be unique.

Properties of Local Minimum

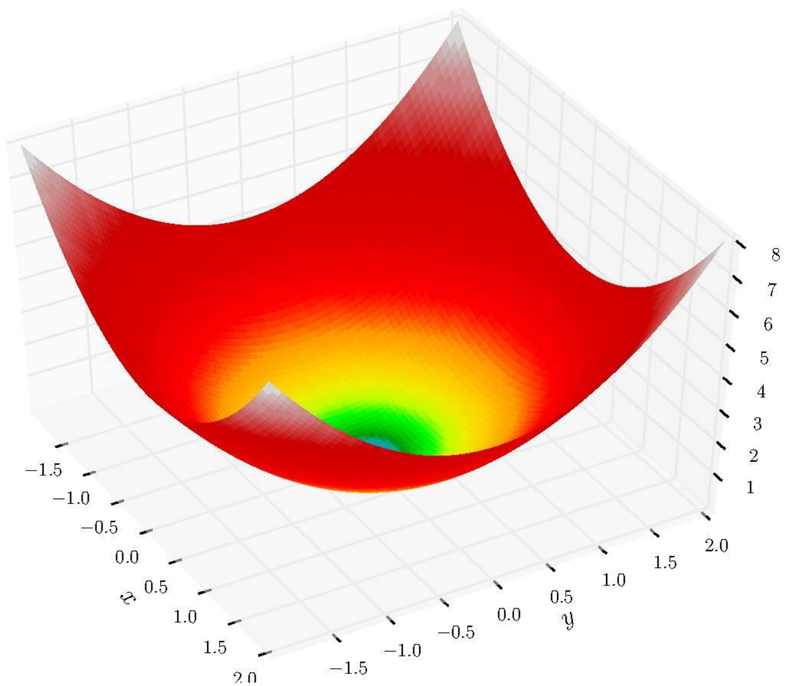


Assume f is defined on $\mathbb{R}^d$.

Properties of local minimum $\mathbf{w}^\star$:

1. The gradient at $\mathbf{w}^\star$, $\nabla f(\mathbf{w}^\star) \in \mathbb{R}^d$, is all-zeros.
2. The Hessian matrix at $\mathbf{w}^\star$, $\nabla^2 f(\mathbf{w}^\star) \in \mathbb{R}^{d\times d}$, is positive semidefinite (i.e., all of its d eigenvalues are nonnegative.)

Convex Function



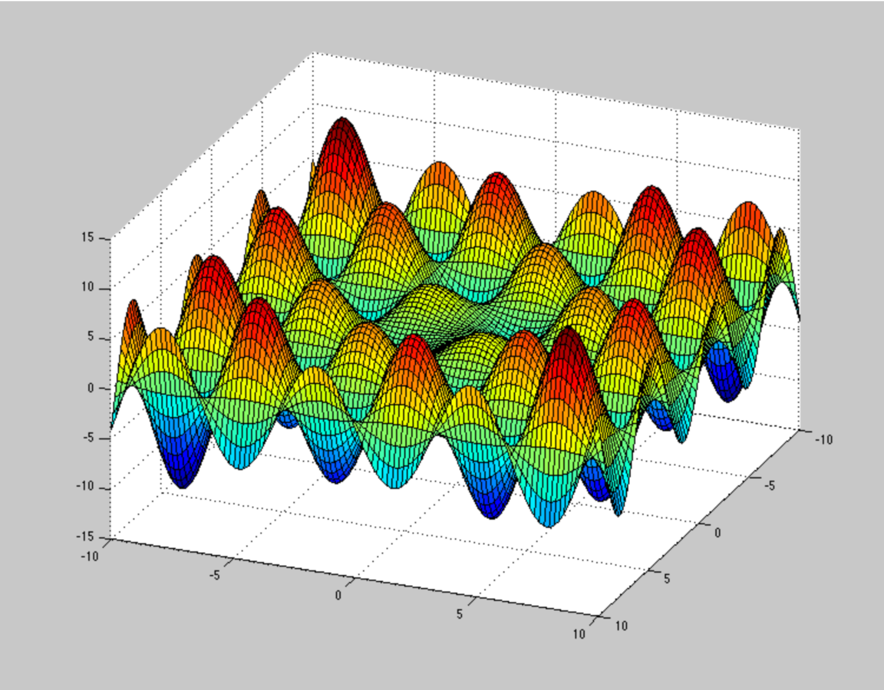
Graph of a convex function

- **Convex function**: The line segment between any two points on the graph of the function lies above or on the graph

Properties of a convex function f:

1. Local minimum = global minimum.
2. The Hessian matrix $\nabla^2 f(\mathbf{w})$ is positive semi-definite everywhere.
3. $\nabla f(\mathbf{w}^\star) = \mathbf{0} \Longleftrightarrow \mathbf{w}^\star$ is a global minimum.

Nonconvex Function

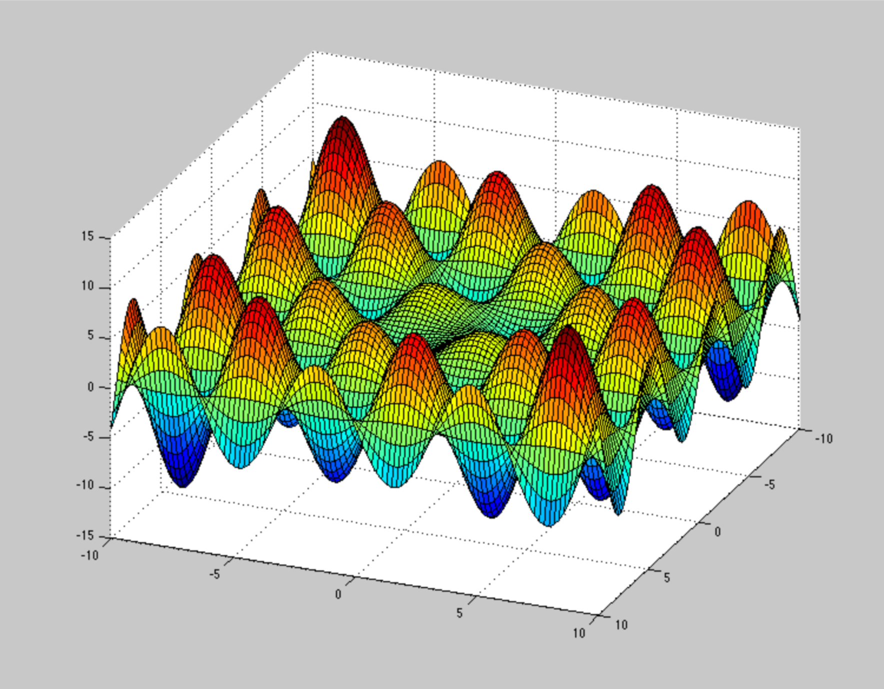


Graph of a nonconvex function

Properties:

1. Local minimum $\cancel{=}$ global minimum.
2. The Hessian ~~matrix $\nabla^2 f(\mathbf{w})$ is positive semi-definite everywhere~~.
3. $\nabla f(\mathbf{w}^\star) = \mathbf{0} \; \cancel{\Longleftarrow} \; \mathbf{w}^\star$ is a global minimum.

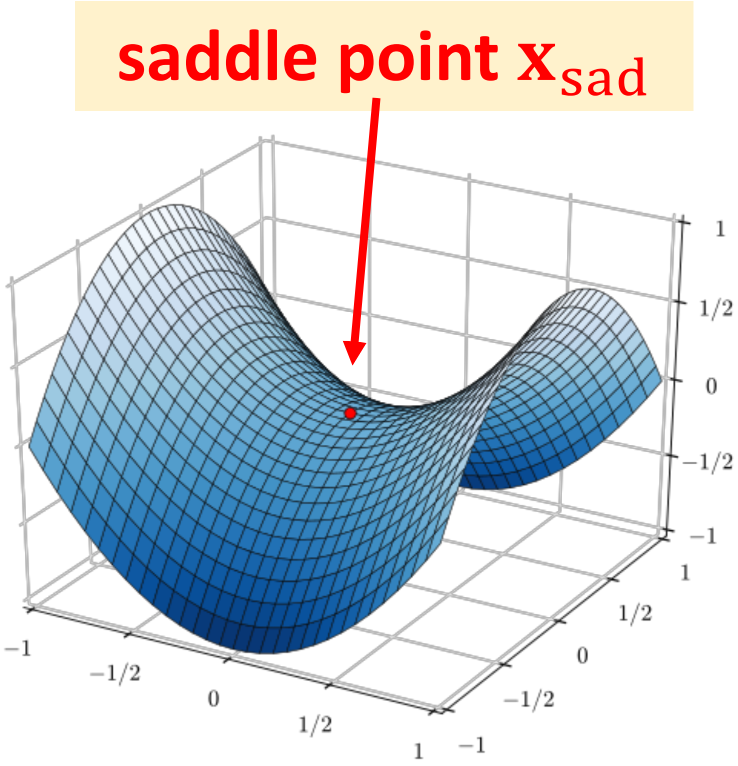
Global Minimum is Unlikely to Reach



Graph of a nonconvex function

- #local minima $\gg$ #global minima.
- The final solution depends on the initialization.
- Reaching one of the global minima is very unlikely.

Saddle Point



Graph of a nonconvex function

Definition of saddle point:

1. The gradient of f at a saddle point is all-zeros: $\nabla f(\mathbf{w}_{\mathrm{sad}}) = \mathbf{0}$.
2. The Hessian matrix $\nabla^2 f(\mathbf{w}_{\mathrm{sad}})$ has **both positive** and **negative eigenvalues**..

Saddle Point vs. Local Minimum

saddle point $\mathbf{w}_{\text{sad}}$	local minimum $\mathbf{w}^\star$
• Gradient: $\nabla f(\mathbf{w}_{\text{sad}}) = \mathbf{0}$. • Hessian: $\nabla^2 f(\mathbf{w}_{\text{sad}})$ has **both positive** and **negative eigenvalues**.	• Gradient: $\nabla f(\mathbf{w}^\star) = \mathbf{0}$. • Hessian: $\nabla^2 f(\mathbf{w}^\star)$ does **not** have **negative eigenvalues**.

Saddle Point vs. Local Minimum

saddle point $\mathbf{w}_{\text{sad}}$	local minimum $\mathbf{w}^\star$
• Gradient: $\nabla f(\mathbf{w}_{\text{sad}}) = \mathbf{0}$. • Hessian: $\nabla^2 f(\mathbf{w}_{\text{sad}})$ has **both positive** and **negative eigenvalues**.	• Gradient: $\nabla f(\mathbf{w}^\star) = \mathbf{0}$. • Hessian: $\nabla^2 f(\mathbf{w}^\star)$ does **not** have **negative eigenvalues**.

- Full gradient descent stops at either a saddle point or a local minimum.

Saddle Point vs. Local Minimum

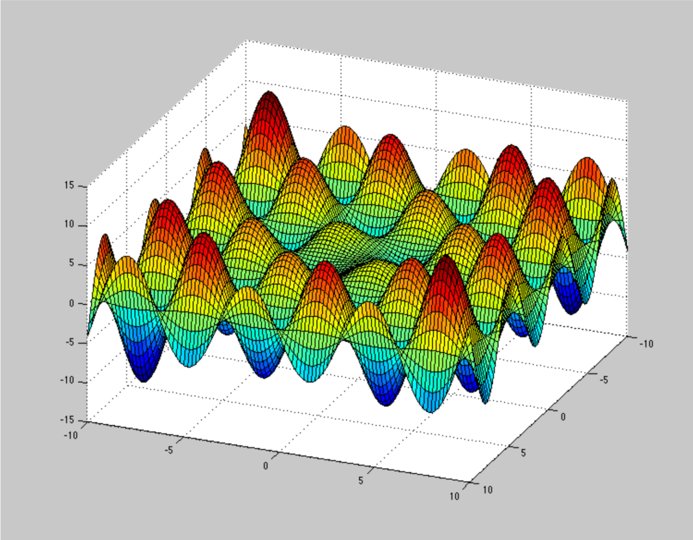
saddle point $\mathbf{w}_{\text{sad}}$

- Gradient: $\nabla f(\mathbf{w}_{\text{sad}}) = \mathbf{0}$.
- Hessian: $\nabla^2 f(\mathbf{w}_{\text{sad}})$ has **both positive** and **negative eigenvalues**.

local minimum $\mathbf{w}^\star$

- Gradient: $\nabla f(\mathbf{w}^\star) = \mathbf{0}$.
- Hessian: $\nabla^2 f(\mathbf{w}^\star)$ does **not** have **negative eigenvalues**.

- Full gradient descent stops at either a saddle point or a local minimum.



- In 2D, #saddle points and #local minimum are comparable.
- It is not true in high-dim.

Saddle Point vs. Local Minimum

saddle point $\mathbf{w}_{\text{sad}}$

- Gradient: $\nabla f(\mathbf{w}_{\text{sad}}) = \mathbf{0}$.
- Hessian: $\nabla^2 f(\mathbf{w}_{\text{sad}})$ has **both positive** and **negative eigenvalues**.

local minimum $\mathbf{w}^\star$

- Gradient: $\nabla f(\mathbf{w}^\star) = \mathbf{0}$.
- Hessian: $\nabla^2 f(\mathbf{w}^\star)$ does **not** have **negative eigenvalues**.

- Full gradient descent stops at either a saddle point or a local minimum.

- In high dim, #saddle points is much greater than #local minima.
  - The Hessian has d eigenvalues, each of which can be positive or negative.
  - ➡ 2^d combinations of positive and negative eigenvalues.
  - One out of the 2^d combinations corresponds to local minima.
  - $2^d - 2$ combinations corresponds to saddle points.

Saddle Point vs. Local Minimum

saddle point $\mathbf{w}_{\text{sad}}$

- Gradient: $\nabla f(\mathbf{w}_{\text{sad}}) = \mathbf{0}$.
- Hessian: $\nabla^2 f(\mathbf{w}_{\text{sad}})$ has **both positive** and **negative eigenvalues**.

local minimum $\mathbf{w}^\star$

- Gradient: $\nabla f(\mathbf{w}^\star) = \mathbf{0}$.
- Hessian: $\nabla^2 f(\mathbf{w}^\star)$ does **not** have **negative eigenvalues**.

- Full gradient descent stops at either a saddle point or a local minimum.

- In high dim, the number of saddle points is much larger than local minima.

- If a neural net is optimized by the full gradient descent, it will converge to a saddle point.

Be Careful When Optimizing a Nonconvex Function

Be careful about the initialization!

- Bad initialization results in convergence to bad regions.
  - Because of the nonconvexity, global minimum cannot be attained.

Be Careful When Optimizing a Nonconvex Function

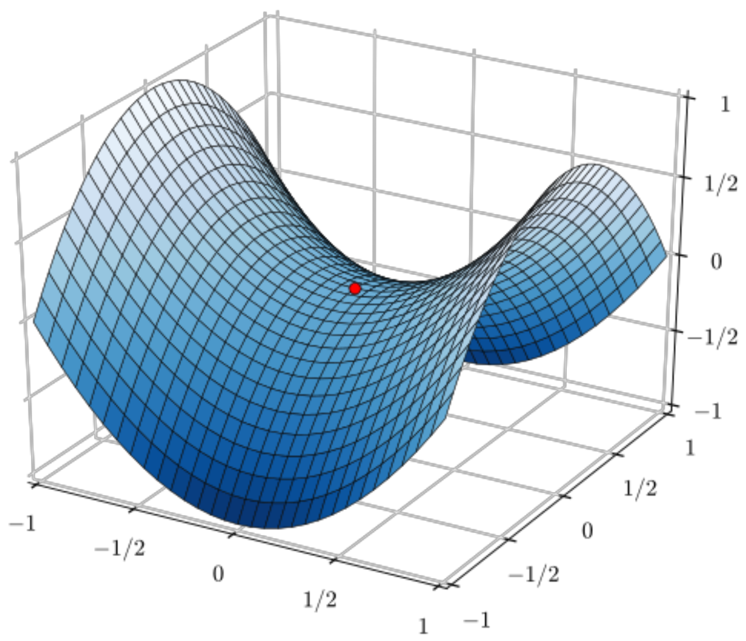
Be careful about the initialization!

- Bad initialization results in convergence to bad regions.
  - Because of the nonconvexity, global minimum cannot be attained.
- Rule of thumb :
  - The trainable parameters (e.g., the filters of ConvNet) are randomly initialized with proper scaling.
  - Bad scaling leads to terrible results.
  - All-zero and all-one initializations are bad ideas.
  - Pretrained parameters can be very good initialization.

Be Careful When Optimizing a Nonconvex Function

Be careful about the initialization!

Be careful about the optimization algorithm!



- Full gradient descent will be stuck in a saddle point.
  - Because the gradient is near zero when approaching the saddle point.
- Stochastic gradient descent (SGD) can escape the saddle points.
  - Because it is random and noisy.

Be Careful When Optimizing a Nonconvex Function

Be careful about the initialization!

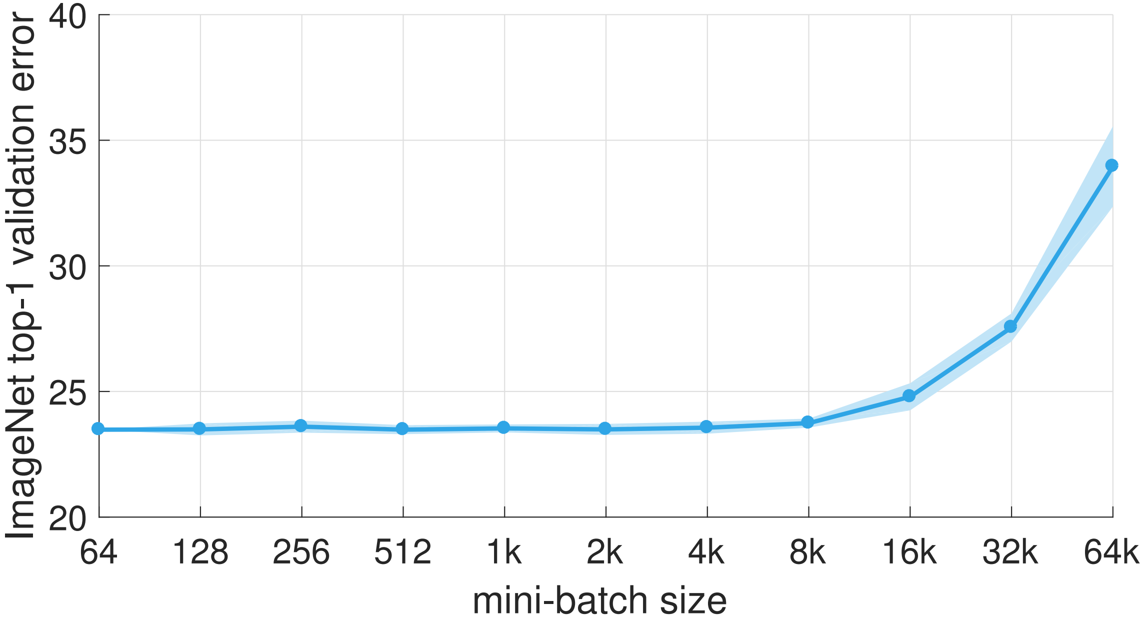
Be careful about the optimization algorithm!

Be careful about the batch size!

- For parallel computing with multiple GPUs, larger batch size ➔ lower per-epoch runtime.
- Large batch size, e.g., $10K$, may result in bad generalization.

… More about the Batch Size

- Batch size larger than $8K$ results in poor generalization.
- Large batch size is good for time-efficiency.
- Lots of tricks are required in *large batch training*.

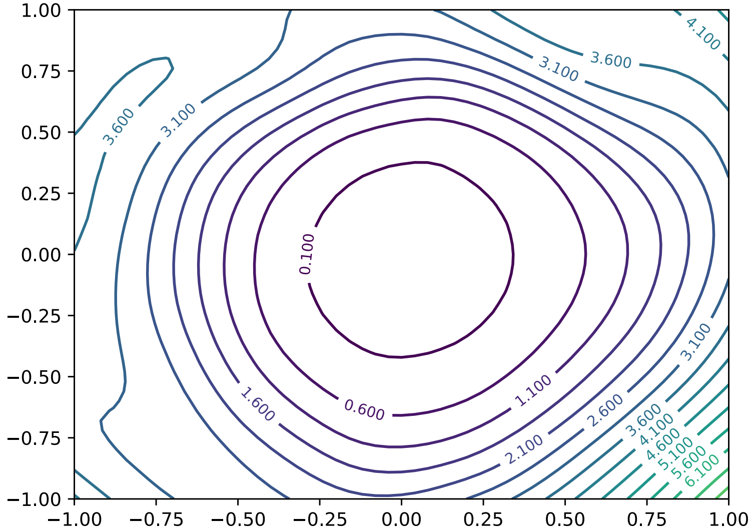


The figure is from the paper *"Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour"*

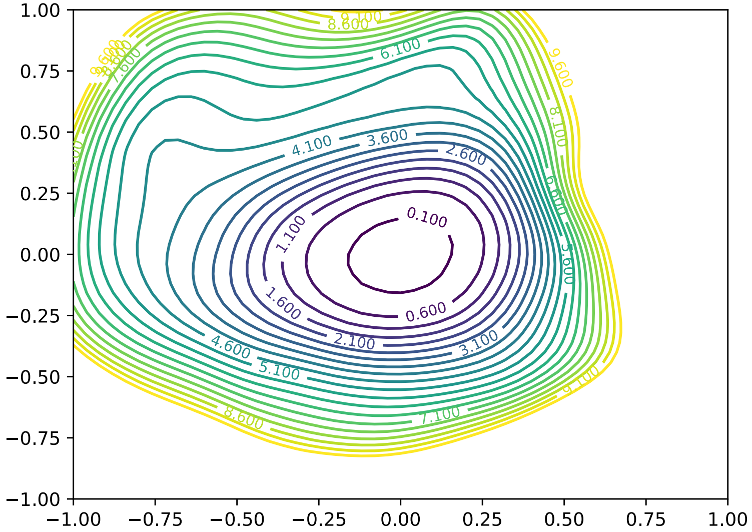
… More about the Batch Size

- Researchers’ conjecture:
  - Small batch size ➔ flat local minima; Big batch size ➔ shape local minima.
  - Flat local minima generalizes better (on the test set).

Batch Size = 128



Batch Size = 8192



The figure is from paper https://arxiv.org/abs/1712.09913

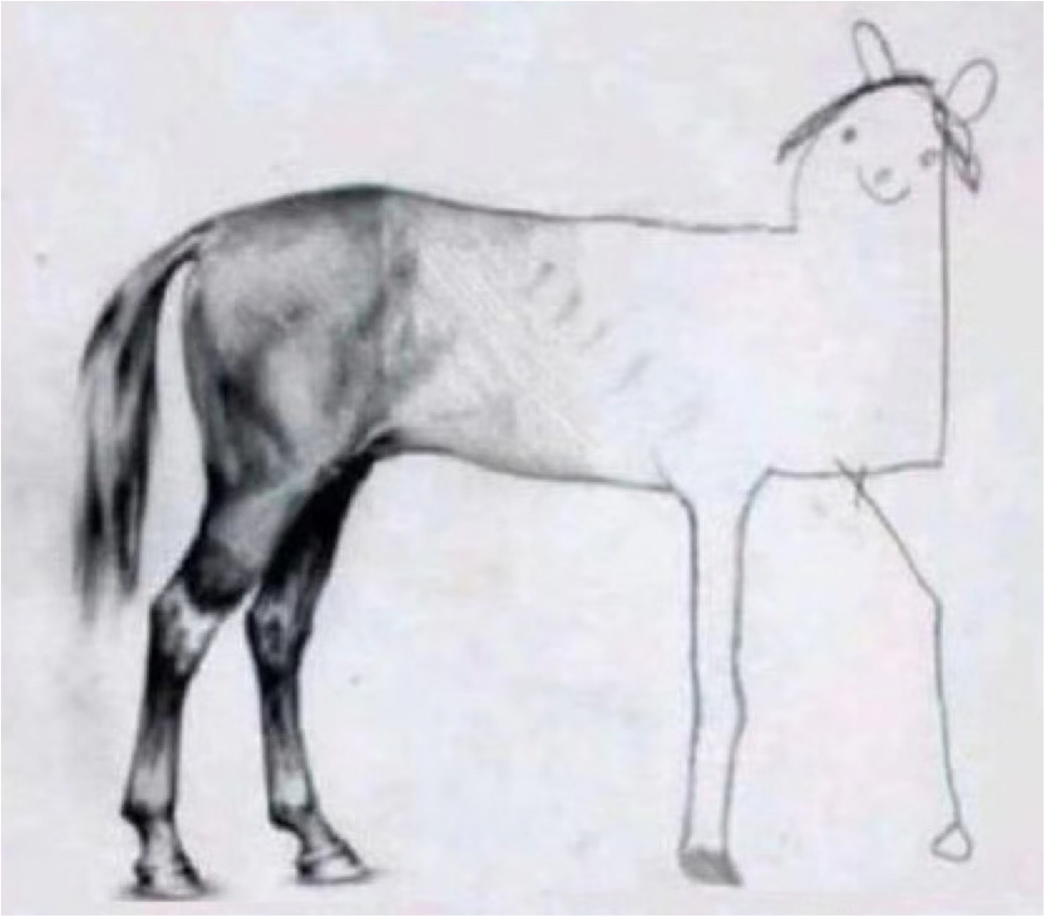
… More about the Batch Size

- There are papers supportive of small batch training, e.g., https://arxiv.org/pdf/1804.07612.pdf

The presented results confirm that using small batch sizes achieves the best training stability and generalization performance, for a given computational cost, across a wide range of experiments. In all cases the best results have been obtained with batch sizes $m = 32$ or smaller, often as small as $m = 2$ or $m = 4$.

Do Not Believe Deep Learning Theories Blindly

Empirical study



Explanations

Summary

- #global minima $\ll$ #local minima $\ll$ #saddle points.
- Full gradient descent converges to a saddle point.
- SGD converges to a local minimum.

Summary

- #global minima $\ll$ #local minima $\ll$ #saddle points.
- Full gradient descent converges to a saddle point.
- SGD converges to a local minimum.

- Initialization is crucial.
  - Proper scaling.
  - Pretrain.

Summary

- #global minima $\ll$ #local minima $\ll$ #saddle points.
- Full gradient descent converges to a saddle point.
- SGD converges to a local minimum.

- Initialization is crucial.
  - Proper scaling.
  - Pretrain.

- Batch size affects time efficiency and generalization.