Convex Function vs. Nonconvex Function: A Little Bit Theory

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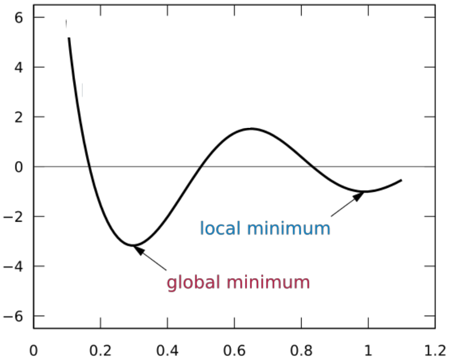
Global Extremum vs. Local Extremum



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

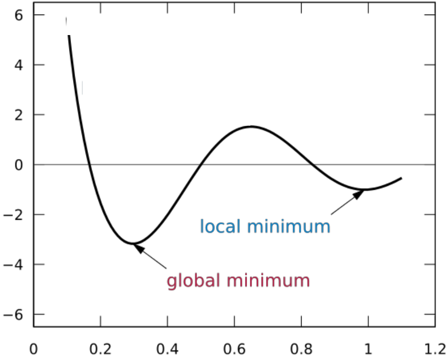
If $f(\mathbf{w}^\star) \leq f(\mathbf{w})$ for all $\mathbf{w}$ in a neighborhood of $\mathbf{w}^\star$, then $\mathbf{w}^\star$ is a **local minimum** of f.

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

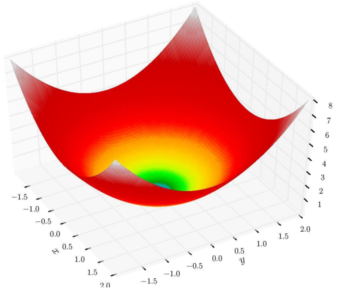


Assume f is defined on $\mathbb{R}^d$.

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



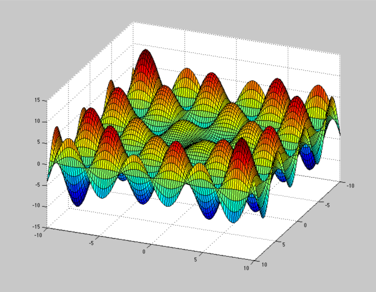
Graph of a convex function

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

Nonconvex Function

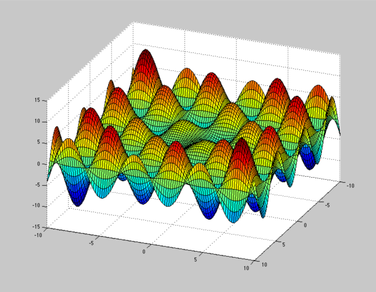


Graph of a nonconvex function

Properties:

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

Global Minimum is Unlikely to Reach

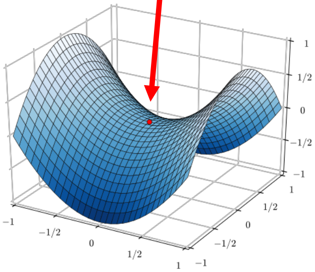


Graph of a nonconvex function

- Number of local minima ≫ number of global minima.
- The final solution depends on the initialization.
- Reaching one of the global minima is very unlikely.

Saddle Point

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



Graph of a nonconvex function

Definition of saddle point:

1. The gradient of f at a saddle point is all-zeros: $\nabla f(\mathbf{w}_{\text{sad}}) = \mathbf{0}$.
2. The Hessian matrix $\nabla^2 f(\mathbf{w}_{\text{sad}})$ 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

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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.

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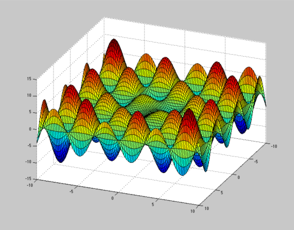

- In 2D, numbers of saddle points and local minimum are comparable.
- It is not true in high-dim.

Saddle Point vs. Local Minimum

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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.
  - The Hessian has d eigenvalues, each of which can be positive or negative.
  - ➡ 2^d combinations.
  - 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 $\mathbf{w}_{\text{sad}}$	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.

- 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.
- Heuristics:
  - 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.

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!

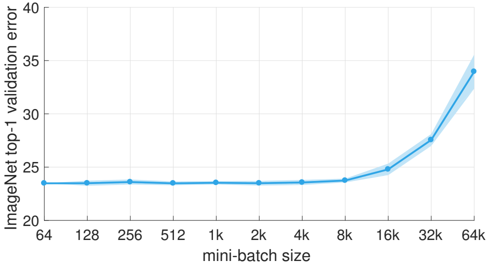
Be careful about the optimization algorithm!

Be careful about the batch size!

- Small batch size does not make full use of GPUs.
- 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

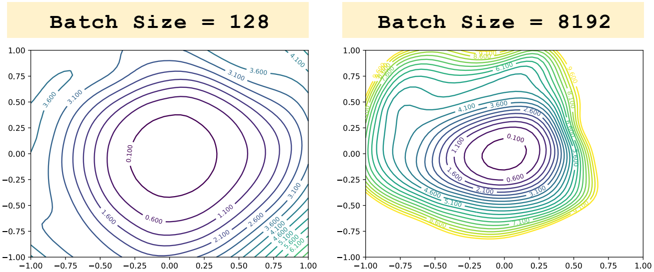
- Batch size larger than $8K$ results in poor generalization.
- Large batch size is good for computation.
- Lots of tricks are required in *large batch training*.



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).



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 $m = 4$.

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Training with large minibatches is bad for your health.
More importantly, it's bad for your test error.
Friends dont let friends use minibatches larger than 32. arxiv.org/abs/1804.07612

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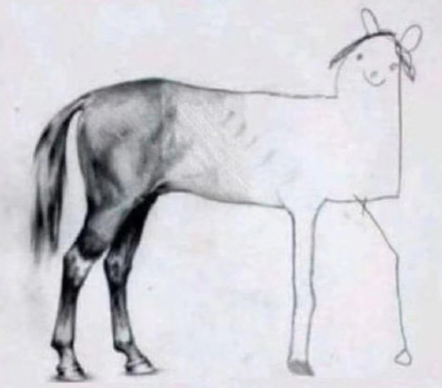
Do Not Believe Deep Learning Theories Blindly

Empirical study



Explanations