Tractable Landscapes for Nonconvex Optimization

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Overview

Background

- Deep learning relies on optimizing a nonconvex loss.
- Even simple algorithms such as gradient descent often optimize the objective value to zero or near-zero.
- **Goal**: How to optimizate the nonconvex landscapes efficiently and identify their properties (for machine learning models)?
- Only apply to simpler nonconvex problems than deep learning.
- How to analyze deep learning with such landscape analysis is still open.

Global and Local Minimum

Definition 1 (Global/Local minimum)

1. For an objective function $f(w) : \mathbb{R}^d \to \mathbb{R}$, a point w^* is a global minimum if for every w we have $f\left(w^*\right) \leqslant f(w)$.
2. A point w is a local minimum/maximum if there exists a radius $\epsilon > 0$ such that for every $\|w' - w\|_2 \leqslant \epsilon$, we have $f(w) \leqslant f\left(w'\right)$ $\left(f(w) \geqslant f\left(w'\right)\right.$ for local maximum$\left.\right)$.
3. A point w with $\nabla f(w) = 0$ is called a critical point, and for smooth functions all local minimum/maximum are critical points.

- Here we work with functions whose global minimum exists, and use $f(w^*)$ to denote its optimal value.

Spurious Local Minimum

Definition 2 (Spurious local minimum)

For an objective function $f(w) : \mathbb{R}^d \to \mathbb{R}$, a point w is a spurious local minimum if it is a local minimum, but $f(w) > f\left(w^*\right)$.

- Many optimization algorithms are based on the idea of local search, thus cannot escape from a spurious local minimum.
- Many noncovex objectives do not have spurious local minima.

Saddle Points

Definition 3 (Saddle point)

For an objective function $f(w) : \mathbb{R}^d \to \mathbb{R}$, a point w is a saddle point if $\nabla f(w) = 0$, and for every radius $\epsilon > 0$, there exists w^+, w^- within distance ϵ of w such that $f(w^-) < f(w) < f(w^+)$.

- This definition covers all cases but makes it very hard to verify whether a point is a saddle point.
- In most cases, it is possible to tell whether a point is a saddle point, local minimum or local maximum based on its Hessian.

Second Order Sufficient Condition

Theorem 4

For an objective function $f(w) : \mathbb{R}^d \to \mathbb{R}$ and a critical point w ($\nabla f(w) = 0$), we know:
- If $\nabla^2 f(w) \succ 0$, w is a local minimum.
- If $\nabla^2 f(w) \prec 0$, w is a local maximum.
- If $\nabla^2 f(w)$ has both a positive and a negative eigenvalue, w is a saddle point.

- **Proof Hint**: looking at the second-order Taylor expansion.
- The three cases do not cover all the possible Hessian matrices.

Flat Regions

- **Challenge**: Even if a function does not have any spurious local minima or saddle point, it can still be hard to optimize.
- **Difficulty**: even if the norm $\|\nabla f(w)\|_2$ is small, unlike convex functions, one cannot conclude that $f(w)$ is close to $f(w^*)$.

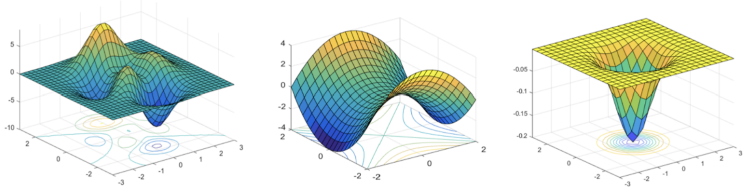

Figure: Obstacles for nonconvex optimization. From left to right: local minimum, saddle point and flat region.

Overview

Cases With a Unique Global Minimum

We first consider the case that is similar to convex objectives.

- The objective functions we look at have no spurious local minima or saddle points.
- **Obstacle**: points with small gradients may not be near-optimal.
- **Main Idea**: identify properties of the objective function, such that it keeps decreasing during the optimization process.

Cases With a Unique Global Minimum

Definition 5

Let $f(w)$ be an objective function with a unique global minimum w^*, then:

Polyak-Lojasiewicz: f satisfies Polyak-Lojasiewicz if there exists a value $\mu > 0$ such that for every w, $\|\nabla f(w)\|_2^2 \geqslant \mu \left(f(w) - f\left(w^*\right)\right)$

Weakly-quasi-convex: f is weakly-quasi-convex if there exists a value $\mu > 0$ such that for every w,
$\langle \nabla f(w), w - w^* \rangle \geqslant \mu \left(f(w) - f\left(w^*\right)\right)$

Restricted Secant Inequality (RSI): f satisfies RSI if there exists a value μ such that for every w, $\langle \nabla f(w), w - w^* \rangle \geqslant \mu \|w - w^*\|_2^2$

Cases With a Unique Global Minimum

Any one of these three properties can imply fast convergence together with some smoothness of f.

Theorem 6

If an objective function f satisfies one of Polyak-Lojasiewicz, weakly-quasi-convex or RSI, and f is smooth, then gradient descent converges to global minimum with a geometric rate.

- Polyak-Lojasiewicz and RSI requires standard smoothness, weakly-quasi-convex requires a special smoothness property detailed in [Hardt et al., 2016].
- We will use generalized linear model (GLM) as an example to show how some of these properties can be used.

Generalized Linear Model

In GLM ([Kalai and Sastry, 2009], [Kakade et al., 2011]), the input consists of samples $\left\{x^{(i)}, y^{(i)}\right\}$ that are drawn from a distribution $\mathcal{D}$, where $(x, y) \sim \mathcal{D}$ satisfies

$$y = \sigma\left({w_*}^\top x\right) + \epsilon$$

Generalized Linear Model

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$$y = \sigma\left({w_*}^\top x\right) + \epsilon$$

- $\sigma : \mathbb{R} \to \mathbb{R}$ is a known monotone function, ϵ is a noise that satisfies $\mathbb{E}[\epsilon \mid x] = 0$.
- Consider Expected loss: $L(w) = \frac{1}{2} \underset{(x,y)\sim\mathcal{D}}{\mathbb{E}} \left[\left(y - \sigma\left(w^\top x\right)\right)^2\right]$.

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- GLM: learn a single neuron where σ is its nonlinearity.

Generalized Linear Model

How to prove prop. (e.g., weakly-quasi-convex or RSI) for GLM?

The objective is rewritten as:

$$\begin{aligned} L(w) &= \frac{1}{2} \mathop{\mathbb{E}}_{(x,y)\sim\mathcal{D}} \left[\left(y - \sigma\left(w^\top x \right) \right)^2 \right] \\ &= \frac{1}{2} \mathop{\mathbb{E}}_{(x,\epsilon)} \left[\left(\epsilon + \sigma\left(w_*^\top x \right) - \sigma\left(w^\top x \right) \right)^2 \right] \\ &= \frac{1}{2} \mathop{\mathbb{E}}_{\epsilon} \left[\epsilon^2 \right] + \frac{1}{2} \mathop{\mathbb{E}}_{x} \left[\left(\sigma\left(w_*^\top x \right) - \sigma\left(w^\top x \right) \right)^2 \right]. \end{aligned} \tag{1}$$

- This decomposition is helpful as $\frac{1}{2}\mathop{\mathbb{E}}_{\epsilon}\left[\epsilon^2\right]$ is just a constant.

Generalized Linear Model

Consider the derivative of the objective:

$$\nabla L(w) = \mathop{\mathbb{E}}_{x}\left[\left(\sigma\left(w^\top x\right) - \sigma\left(w_*^\top x\right)\right)\sigma'\left(w^\top x\right)x\right]. \tag{2}$$

Then we have:

$$\begin{aligned} &\langle \nabla L(w), w - w^* \rangle \\ =&\mathop{\mathbb{E}}_{x}\left[\left(\sigma\left(w^\top x\right) - \sigma\left(w_*^\top x\right)\right)\sigma'\left(w^\top x\right)\left(w^\top x - w_*^\top x\right)\right] \\ =&\mathop{\mathbb{E}}_{x}\left[\sigma'(\xi)\sigma'\left(w^\top x\right)\left(w^\top x - w_*^\top x\right)^2\right]. \end{aligned} \tag{3}$$

By making more assumptions on σ and the distribution of x, it is possible to lowerbound $\langle \nabla L(w), w - w^* \rangle$ in the form required by either weakly-quasi-convex or RSI.

Overview

Permutation Symmetry for Neural Networks

Consider a two-layer neural network $h_\theta(x) : \mathbb{R}^d \to \mathbb{R}$. The parameters θ is $(w_1, w_2, \cdots, w_k)$.

- The function can be evaluated as $h_\theta(x) = \sum_{i=1}^{k} \sigma(\langle w_i, x \rangle)$.
- Given a dataset $\left(x^{(1)}, y^{(1)}\right), \ldots, \left(x^{(n)}, y^{(n)}\right) \overset{\text{i.i.d.}}{\sim} \mathcal{D}$.
- The objective $f(\theta) = L(h_\theta) = \mathbb{E}_{(x,y)\sim\mathcal{D}}\left[\ell\left((x, y), h_\theta\right)\right]$ has permutation symmetry.
- That is, for any permutation $\pi(\theta)$ that permutes the weights of the neurons, $f(\theta) = f(\pi(\theta))$.

Permutation Symmetry for Neural Networks

The permutation symmetry has many implications:

- If the global minimum θ^* is a point where not all neurons have the same weight, then there must be equivalent global minimum $f(\pi(\theta^*))$ for every permutation π.
- An objective with this symmetry must also be nonconvex, because if it were convex, the point $\bar{\theta} = \frac{1}{k!}\sum_{\pi} \pi(\theta^*)$ must be a global minimum.
- However, for $\bar{\theta}$ the weight vectors of the neurons are all equal to $\frac{1}{k}\sum_{i=1}^{k} w_i$, so $h_{\bar{\theta}}(x) = k\sigma\left(\left\langle \frac{1}{k}\sum_{i=1}^{k} w_i, x\right\rangle\right)$ is equivalent to a neural network with a single neuron.

Permutation Symmetry for Neural Networks

The permutation symmetry has many implications:

- f must be nonconvex.
- It is also possible to show that functions with symmetry must have saddle points.

- To optimize f, the algorithm needs to be able to either avoid or escape from saddle points.
- More concretely, one would like to find a second order stationary point.

Second order stationary point (SOSP)

Definition 7 (Second order stationary point (SOSP))

For an objective function $f(w) : \mathbb{R}^d \to \mathbb{R}$, a point w is a second order stationary point if $\nabla f(w) = 0$ and $\nabla^2 f(w) \succeq 0$

- The conditions for SOSP are known as the second order necessary conditions for a local minimum.
- The optimization algorithms can be used to find an approximate second order stationary point.

Definition 8 (Approximate second order stationary point)

For an objective function $f(w) : \mathbb{R}^d \to \mathbb{R}$, a point w is a (ϵ, γ)-second order stationary point ((ϵ, γ)-SOSP) if $\|\nabla f(w)\|_2 \leqslant \epsilon$ and $\lambda_{\min}\left(\nabla^2 f(w)\right) \geqslant -\gamma$

Locally Optimizable

Define a class of functions that can be optimized efficiently and allow symmetry and saddle points.

Definition 9 (Locally optimizable functions)

An objective function $f(w)$ is locally optimizable, if for every $\tau > 0$, there exists $\epsilon, \gamma = \text{poly}(\tau)$ such that every $(\epsilon, \gamma) - \text{SOSP}$ w of f satisfies $f(w) \leqslant f(w_*) + \tau$.

- Roughly speaking, an objective function is locally optimizable if every local minimum of the function is also a global minimum, and the Hessian of every saddle point has a negative eigenvalue.

Locally Optimizable Functions

Locally optimizable objective functions:

- Matrix sensing [Hardt et al., 2016]
- Matrix completion [Ge et al., 2016]
- Dictionary learning [Sun et al., 2016]
- Tensor decomposition [Ge et al., 2015]
- Certain objective for two-layer neural network [Ge et al., 2017]

Overview

Top Eigenvector of a Matrix

Here we look at a simple example of a locally optimizable function.

- Given a symmetric PSD matrix $M \in \mathbb{R}^{d \times d}$, the goal is to find its top eigenvector.
- More precisely, using SVD we can write M as

$$M = \sum_{i=1}^{d} \lambda_i v_i v_i^\top$$

  Here v_i's are orthonormal vectors that are eigenvectors of M, and λ_i's are the eigenvalues.
- For simplicity, we assume $\lambda_1 > \lambda_2 \geqslant \lambda_3 \geqslant \cdots \geqslant \lambda_d > 0$

Top Eigenvector of a Matrix

There are many objective functions whose global optima give the top eigenvector.

- For PSD matrix M, the global optima of

$$\max_{\|x\|_2=1} x^\top M x$$

  is the top eigenvector of M. However, this formulation requires a constraint.

- We instead work with an unconstrained version whose correctness follows from Eckart-Young Theorem:

$$\min_{x\in\mathbb{R}^d} f(x) := \frac{1}{4}\left\|M - xx^\top\right\|_F^2$$

Top Eigenvector of a Matrix

Consider the following unconstrained optimization problem:

$$\min_{x \in \mathbb{R}^d} f(x) := \frac{1}{4} \left\| M - xx^\top \right\|_F^2$$

- This function does have a symmetry in the sense that $f(x) = f(-x)$.
- Under the assumptions, the only global minima of it are $x = \pm\sqrt{\lambda_1} v_1$. They are the only 2^{nd}-order stationary points.

- Two proof strategies:
    - Characterizing all critical points
    - Finding directions of improvements

Characterizing All Critical Points

The first idea is simple:

- Solve the Eq. $\nabla f(x) = 0$ to get the position of all critical points.

Characterizing All Critical Points

The first idea is simple:

- Solve the Eq. $\nabla f(x) = 0$ to get the position of all critical points.
- For the critical points that are not the desired global minimum, try to prove that they are local maximum or saddle points.

Computing Gradient and Hessian

Expand $f(x+\delta)$ as follows:

$$
\begin{aligned}
f(x+\delta) =& \frac{1}{4}\left\|M-(x+\delta)(x+\delta)^\top\right\|_F^2 \\
=& \frac{1}{4}\left\|M-xx^\top-\left(x\delta^\top+\delta x^\top\right)-\delta\delta^\top\right\|_F^2 \\
=& \frac{1}{4}\left\|M-xx^\top\right\|_F^2-\frac{1}{2}\left\langle M-xx^\top, x\delta+\delta x^\top\right\rangle \\
&+\left[\frac{1}{4}\left\|x\delta^\top+\delta x^\top\right\|_F^2-\frac{1}{2}\left\langle M-xx^\top, \delta\delta^\top\right\rangle\right]+o\left(\|\delta\|_2^2\right)
\end{aligned}
$$

Thus we have:

$$
\nabla f(x)=\left(xx^\top-M\right)x, \quad \nabla^2 f(x)=\|x\|_2^2 I+2xx^\top-M
$$

Characterizing Critical Points

Set $\nabla f(x) = 0$, we have:

$$Mx = xx^\top x = \|x\|_2^2 x$$

- The only solutions to $Mx = \lambda x$ are if λ is an eigenvalue and x is (a scaled version) of the corresponding eigenvector.
- $x = \pm\sqrt{\lambda_i} v_i$ or $x = 0$. And $x = \pm\sqrt{\lambda_1} v_1$ are intended solutions.

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- $x = \pm\sqrt{\lambda_i}v_i$ or $x = 0$. And $x = \pm\sqrt{\lambda_1}v_1$ are intended solutions.
- Next we need to show for every other critical point, its Hessian has a negative direction, i.e., there exists a δ such that $\delta^\top \left[\nabla^2 f(x)\right] \delta < 0$.
- Key: The main step of the proof involves guessing what is this direction δ. In this case we will choose $\delta = v_1$.

Characterizing Critical Points

When $x = \pm\sqrt{\lambda_i} v_i$, and $\delta = v_1$, we have:

$$\delta^\top \left[\nabla^2 f(x)\right] \delta = v_1^\top \left[\left\|\sqrt{\lambda_i} v_i\right\|_2^2 I + 2\lambda_i v_i v_i^\top - M\right] v_1 = \lambda_i - \lambda_1 < 0$$

The proof for $x = 0$ is very similar.
Combining all the steps above, we proved the theorem:

Theorem 10 (Properties of critical points)

The only critical points of $f(x)$ are of the form $x = \pm\sqrt{\lambda_i} v_i$ or $x = 0$. For all critical points except $x = \pm\sqrt{\lambda_1} v_1$, $\nabla^2 f(x)$ has a negative eigenvalue.

Characterizing Critical Points

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- The only 2^{nd}-order stationary points are $x = \pm\sqrt{\lambda_1} v_1$, so all 2^{nd}-order stationary points are also global minima.

Finding Directions of Improvements

It is often infeasible to enumerate all the solutions for $\nabla f(x) = 0$.
Key: For every point x that is not a global minimum, we define its direction of improvements as below:

Definition 11

— For an objective function f and a point x, we say δ is a direction of improvement (of f at x) if $|\langle \nabla f(x), \delta \rangle| > 0$ or $\delta^\top [\nabla^2 f(x)] \delta < 0$.
— We say δ is an (ϵ, γ)-direction of improvement $($of f at $x)$ if $|\langle \nabla f(x), \delta \rangle| > \epsilon \|\delta\|_2$ or $\delta^\top [\nabla^2 f(x)] \delta < -\gamma \|\delta\|_2^2$.

- If δ is a direction of improvement for f at x, then moving along one of δ or $-\delta$ for a small enough step can decrease the objective function.

Finding Directions of Improvements

For simplicity, consider an simpler version of the top eigenvector problem, where $M = zz^\top$ is a rank-1 matrix, and z is a unit vector. Then

$$\min_x f(x) = \frac{1}{4} \left\| zz^\top - xx^\top \right\|_F^2 \tag{4}$$

- Which direction should we move to decrease the objective?
- One only have the optimal direction z and the current direction x, so the natural guesses would be z, x or $z - x$.

Finding Directions of Improvements

Lemma 12

For objective function f, there exists a universal constant $c > 0$ such that for any $\tau < 1$, if neither x or z is an $(c\tau, 1/4)$-direction of improvement for the point x, then $f(x) \leqslant \tau$.

- The proof of this lemma involves some detailed calculation.
- To get some intuition, we first think about what happens if neither x or z is a direction of improvement.

Finding Directions of Improvements

Lemma 13

For objective function f, if neither x or z is a direction of improvement of f at x, then $f(x) = 0$.

Proof.

If x is not a direction of improvement, we must have:

$$\langle \nabla f(x), x \rangle = 0 \Longrightarrow \|x\|_2^4 = \langle x, z \rangle^2$$

If z is not a direction of improvement, we know $z^\top \left[\nabla^2 f(x)\right] z \geqslant 0$ which means

$$\|x\|^2 + 2\langle x, z \rangle^2 - 1 \geqslant 0 \Longrightarrow \|x\|^2 \geqslant 1/3$$

□

Finding Directions of Improvements

Proof.

Consider the fact that $\langle x, z\rangle^2 \leqslant \|x\|_2^2\|z\|_2^2 = \|x\|_2^2$, thus we have $\langle x, z\rangle^2 = \|x\|_2^4 \geqslant 1/9$.
Finally, since z is not a direction of improvement, we know $\langle \nabla f(x), z\rangle = 0$, which implies $\langle x, z\rangle \left(\|x\|_2^2 - 1\right) = 0$. We have already proved $\langle x, z\rangle^2 \geqslant 1/9 > 0$, thus $\|x\|_2^2 = 1$.
Again we know $\langle x, z\rangle^2 = \|x\|_2^4 = 1$. The only two vectors with $\langle x, z\rangle^2 = 1$ and $\|x\|_2^2 = 1$ are $x = \pm z$. $\square$

Finding Directions of Improvements

- The proof of Lemma 12 is very similar to Lemma 13, except we need to allow slacks in every equation and inequality we use.
- Lemma 12 and Lemma 13 both use directions x and z. It is also possible to use the direction $x - z$ when $\langle x, z\rangle \geqslant 0$ (and $x + z$ when $\langle x, z\rangle < 0$).
- Both ideas can be generalized to handle the case when $M = ZZ^\top$ where $Z \in \mathbb{R}^{d\times r}$, so M is a rank-r matrix.

Overview

Mode Connectivity

- Although the loss landscape of DNNs is nonconvex with many minima, there are some tractable structures.
- Mode connectivity: Different local minima can be connected by simple paths [Garipov et al., 2018, Draxler et al., 2018].

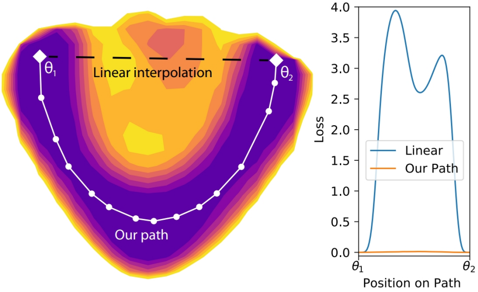

Figure: Two minima (found by SGD) are connected by a polygonal chain of low loss, but the loss along the linear path is high [Draxler et al., 2018].

Linear Mode Connectivity

- Mode connectivity suggests that different local minima are not isolated, but essentially form a connected manifold.
- Linear mode connectivity (LMC): Connected by a linear path.

Definition 14 (Linear mode connectivity)

Given dataset D and two modes θ_A, θ_B that $\mathrm{Err}_D(\theta_A) = \mathrm{Err}_D(\theta_B)$, two mode θ_A and θ_B satisfy the linear mode connectivity if

$$\forall \alpha \in [0, 1], \mathrm{Err}_D(\alpha\theta_A + (1-\alpha)\theta_B) \approx \mathrm{Err}_D(\theta_A)$$

- LMC implies that the minima are in the same basin.
- SGD converges to a basin $\rightarrow$ flat minima.
- When LMC happens?

Spawning Method [Frankle et al., 2020]

1. A network is randomly initialized, trained for some epochs.
2. Spawned into two copies which continue to be independently trained by different SGD randomnesses.

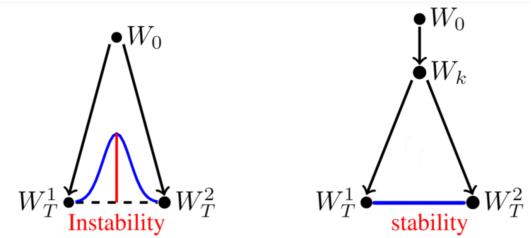

Figure: **Left:** MC; **Right:** LMC after spawning [Frankle et al., 2020].

- **Insight:** The result of optimization is determined in early stage.

Permutation Method [Entezari et al., 2021]

- Recall that DNNs satisfy permutation symmetry.
- **Conjecture:** SGD solutions are LMC after proper permutation.

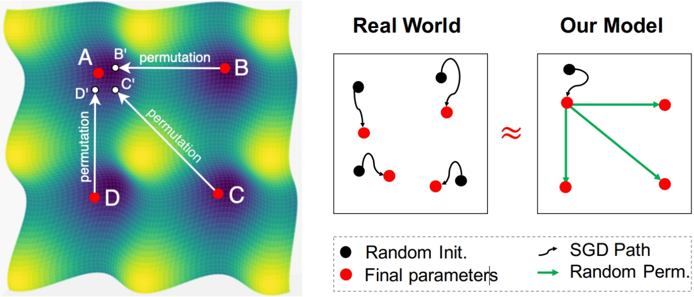

Figure: Permuting minima to the same basin [Entezari et al., 2021].

- **Insight:** Permutation symmetry leads to different basins, yet SGD can converge to minima with similar performance.

Ways to Find Proper Permutation

- Align the neurons of independently trained models via permutation [Ainsworth et al., 2022, Qu and Horvath, 2024].
  - **Weight matching:** $\min_\pi \sum_{\ell=1}^{L} \left\| \boldsymbol{W}_A^{(\ell)} - \boldsymbol{P}^{(\ell)} \boldsymbol{W}_B^{(\ell)} \boldsymbol{P}^{(\ell-1)^\top} \right\|_F^2$
  - **Activation matching:** $\min_\pi \sum_{\ell=1}^{L} \left\| \boldsymbol{H}_A^{(\ell)} - \boldsymbol{P}^{(\ell)} \boldsymbol{H}_B^{(\ell)} \right\|_F^2$
- LMC allows us to merge models by “teleporting” solutions into a single basin.

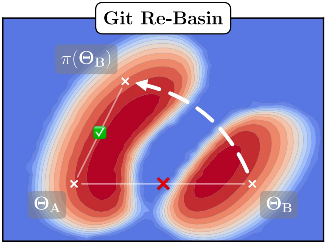

Figure: Git Re-Basin, a weight averaging method [Ainsworth et al., 2022].

LMC Leads to better Model Averaging

- **Goal:** Merge models trained on disjoint datasets.
  - Federated Learning
  - Distributed Training
- **Method:** Weight averaging in the same basin via permutation.

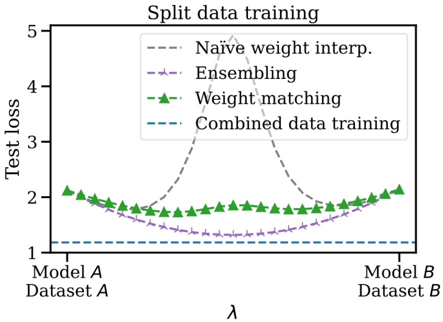

Figure: Merging ResNets on CIFAR100 outperforms both input models while using half compute required for ensembling [Ainsworth et al., 2022].

Overview

Summary

- **Cases with a unique global minimum:** identify properties of the objective function, such as PL, weakly-quasi-convex and RSI conditions.
- **The permutation symmetry has many implication:** nonconvex, saddle points and so on.
- **Two strategies for analyzing the landscape:**
  - Characterizing all critical points
  - Finding directions of improvements
- **(Linear) mode connectivity reveals the relationship between local minima in nonconvex landscape:** Connected by simple (linear) paths.

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