

Loss Landscape Characterization of Neural Networks without Over-Parametrization

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Problem Formulation

We want to solve the finite-sum optimization problem

$$\min_{x \in \mathbb{R}^d} \left\{ f(x) \stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^n f_i(x) \right\} \quad (1)$$

Annotations:
 $f^* = \min_x f(x)$ (green box)
 non-convex (orange box)
 # of data points (orange box)
 # model parameters (orange box)
 Empirical risk/loss (orange box)
 Loss associated with one data point (orange box)
 $f_i^* = \min_x f_i(x)$ (green box)
 \mathcal{S} is the set of global minimizers (green box)

Limitations of Existing Conditions

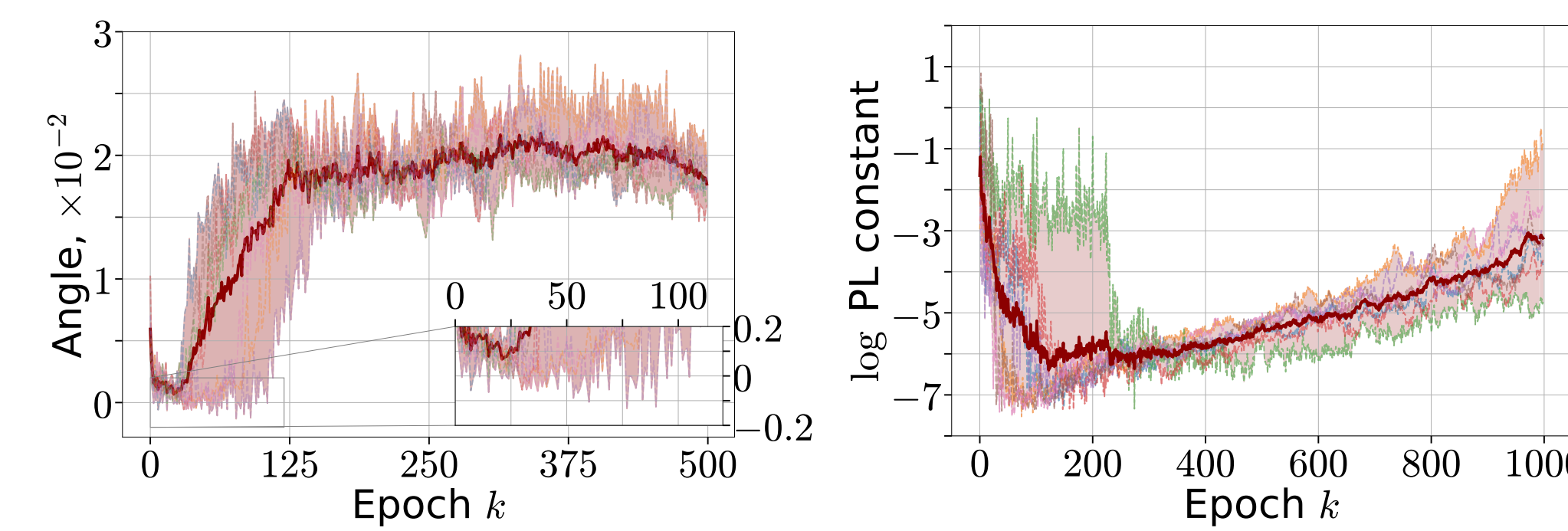


Figure 1: Training of 3 layer LSTM model that shows Aiming condition does not always hold since the angle $\angle(\nabla f(x^k), x^k - x^K)$ can be negative. The right figure demonstrates that the possible constant μ in PL condition should be small.

- **Necessity of Over-parameterization.** The theoretical justification of conditions such as Aiming [2] and PL [3] require a significant amount of overparameterization.
- **Necessity of Invexity.** The conditions imply that any stationary point is a global minimum (i.e., exclusion of saddle points and local minima).
- **Lack of Theory.** Several works have studied the empirical properties of the loss landscape of neural networks but fall short of providing theoretical explanations for this observed phenomenon.
- **Lack of Empirical Evidence.** Several theoretical works prove results on the loss landscape without supporting their claims using experimental validation on deep learning benchmarks.

Main Contributions

- We introduce the α - β -condition and theoretically demonstrate its applicability to a wide range of complex functions, notably those that include local saddle points and local minima.
- We empirically validate that the α - β -condition is a meaningful assumption that captures a wide range of practical functions, including matrix factorization and neural networks (ResNet, LSTM, GNN, Transformer, and other architectures).
- We analyze the theoretical convergence of several optimizers under α - β -condition, including vanilla SGD, SPS_{max}, and NGN.
- We provide empirical and theoretical counter-examples where the weakest assumptions, such as the PL and Aiming conditions, do not hold, but the α - β -condition does.

Table 1: Summary of existing assumptions on the optimization problem and their limitations. Here \mathcal{S} denotes the set of minimizers of f and $f_i^* := \arg\min_x f_i(x)$.

Condition	Definition	Comments
QCvx [1]	$\langle \nabla f(x), x - x^* \rangle \geq \theta(f(x) - f(x^*))$ for some fixed $x^* \in \mathcal{S}$	- excludes saddle points
Aiming [2]	$\langle \nabla f(x), x - \text{Proj}(x, \mathcal{S}) \rangle \geq \theta f(x)$	- excludes saddle points - in theory requires over-parameterization [2] - does not always hold in practice [Fig. 1 a-b]
PL [3]	$\ \nabla f(x)\ ^2 \geq 2\mu(f(x) - f^*)$	- excludes saddle points - in theory requires over-parameterization [4] - does not always hold in practice [Fig. 1 c-d]
α - β -condition [This work]	$\langle \nabla f_i(x), x - \text{Proj}(x, \mathcal{S}) \rangle \geq \alpha(f_i(x) - f_i(\text{Proj}(x, \mathcal{S}))) - \beta(f_i(x) - f_i^*)$	- might have saddles and local minima [Fig. 1 (b-c)] - in practice does not require over-parameterization [2 layer NN ex.]

The Proposed Condition and Examples

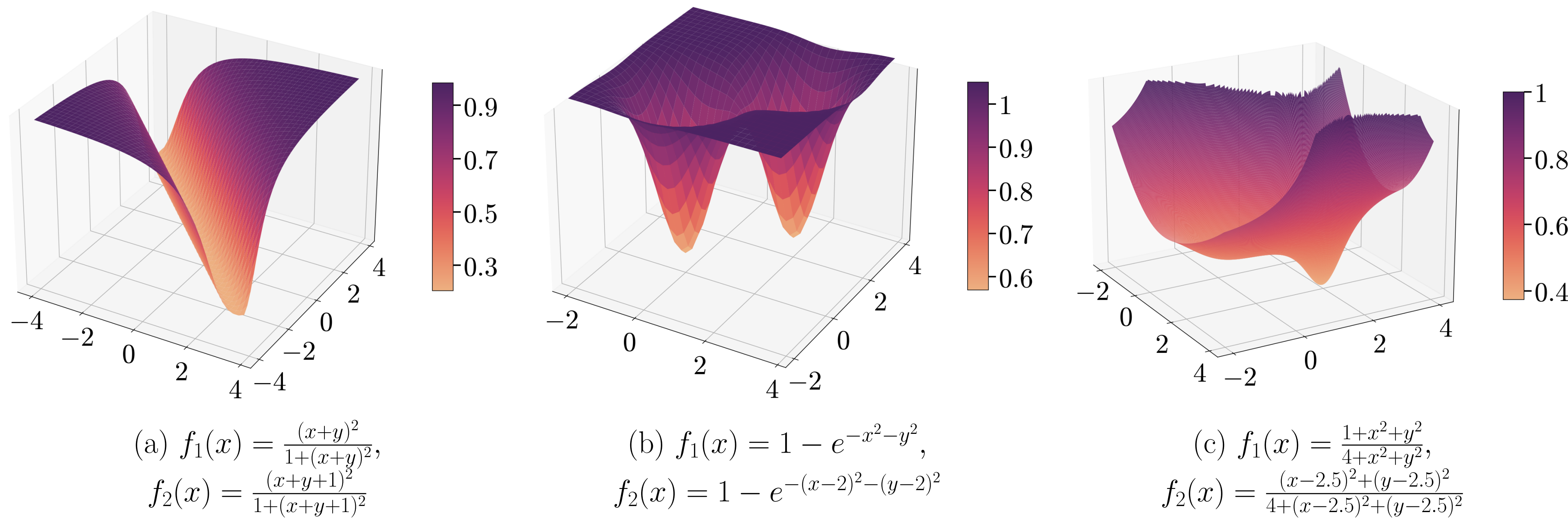


Figure 2: Loss landscape of f that satisfy α - β -condition. These examples demonstrate that the problem (1) that satisfies α - β -condition might have an unbounded set of minimizers \mathcal{S} (left), a saddle point (center), and local minima (right) in contrast to the PL and Aiming conditions.

Definition of α - β -condition

Let $\mathcal{X} \subseteq \mathbb{R}^d$ be a set and consider a function $f: \mathcal{X} \rightarrow \mathbb{R}$ as defined in (1). Then f satisfies the α - β -condition with positive parameters α and β such that $\alpha > \beta$ if for any $x \in \mathcal{X}$ there exists $x_p \in \text{Proj}(x, \mathcal{S})$ such that for all $i \in [n]$

$$\langle \nabla f_i(x), x - x_p \rangle \geq \alpha(f_i(x) - f_i(x_p)) - \beta(f_i(x) - f_i^*).$$

Matrix Factorization. Let f, f_{ij} be such that

$$f(W, S) = \frac{1}{2nm} \|X - W^\top S\|_F^2 = \frac{1}{2nm} \sum_{i,j} (X_{ij} - w_i^\top s_j)^2,$$

$$f_{ij}(W, S) = \frac{1}{2} (X_{ij} - w_i^\top s_j)^2,$$

where $X \in \mathbb{R}^{n \times m}$, $W = (w_i)_{i=1}^n \in \mathbb{R}^{k \times n}$, $S = (s_j)_{j=1}^m \in \mathbb{R}^{k \times m}$, and $\text{rank}(X) = r \geq k$. We assume that X is generated using matrices W^* and S^* with non-zero additive noise that minimize empirical loss, namely, $X = (W^*)^\top S^* + (\varepsilon_{ij})_{i \in [n], j \in [m]}$ where $W^*, S^* = \arg\min_{W, S} f(W, S)$. Let \mathcal{X} be any bounded set that contains \mathcal{S} . Then α - β -condition is satisfied with $\alpha = \beta + 1$ and some $\beta > 0$.

Two Layer Neural Network. Consider training a two-layer neural network with a logistic loss

$$f(W, v) = \frac{1}{n} \sum_{i=1}^n f_i(W, v), \quad f_i(W, v) = \phi(y_i \cdot v^\top \sigma(W x_i))$$

for a classification problem where $\phi(t) := \log(1 + \exp(-t))$, $W \in \mathbb{R}^{k \times d}$, $v \in \mathbb{R}^k$, σ is a ReLU function applied coordinate-wise, $y_i \in \{-1, +1\}$ is a label and $x_i \in \mathbb{R}^d$ is a feature vector. Let \mathcal{X} be any bounded set that contains \mathcal{S} . Then the α - β -condition holds in \mathcal{X} for some $\alpha \geq 1$ and $\beta = \alpha - 1$.

Convergence under α - β -condition

Theorem. Assume that each f_i is L -smooth and the interpolation error $\sigma_{\text{int}}^2 := \mathbb{E}[f^* - f_i^*]$ is bounded. Then the iterates of SGD with stepsize $\gamma \leq \frac{\alpha - \beta}{2L}$ satisfy

$$\min_{0 \leq k < K} \mathbb{E}[f(x^k) - f^*] \leq \frac{\mathbb{E}[\text{dist}(x^0, \mathcal{S})^2]}{K} \frac{1}{\gamma(\alpha - \beta)} + \frac{2L\gamma}{\alpha - \beta} \sigma_{\text{int}}^2 + \frac{2\beta}{\alpha - \beta} \sigma_{\text{int}}^2.$$

Empirical Verification

Model's width \nearrow	Model's depth \nearrow	Batch size \nearrow
Change in $\beta \sigma_{\text{int}}^2$ \searrow		

Table 2: Summary of how the non-vanishing term $\beta \sigma_{\text{int}}^2$ changes as a function of specific quantities of interest.

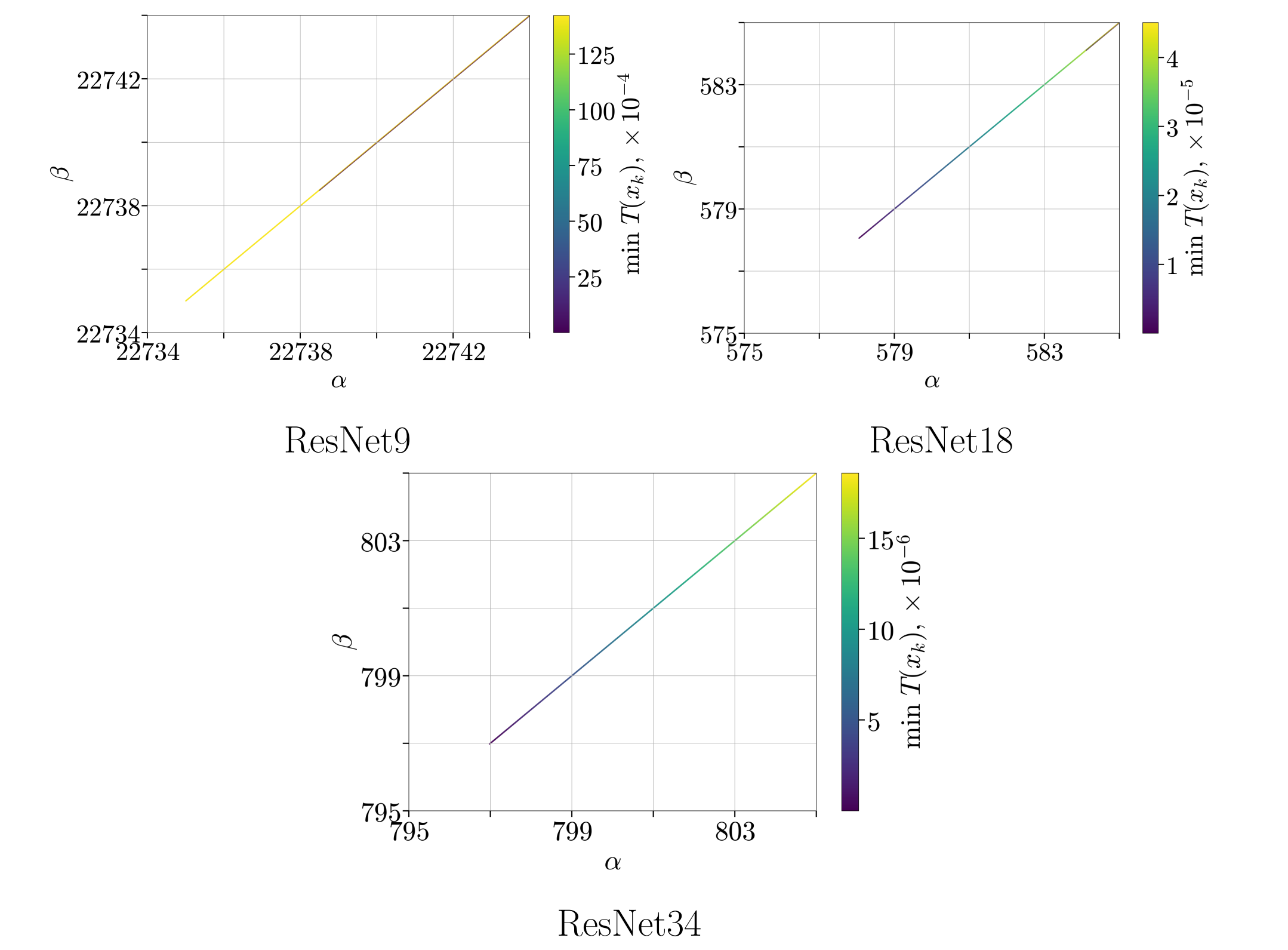


Figure 3: Training of ResNet models on CIFAR100 dataset. Here $T(x_k) = \langle \nabla f_{i_k}(x^k), x^k - x^K \rangle - \alpha(f_{i_k}(x^k) - f_{i_k}(x^K)) - \beta f_{i_k}(x^k)$ assuming that $f_i^* = 0$. Minimum is taken across all runs and iterations for a given pair of (α, β) .

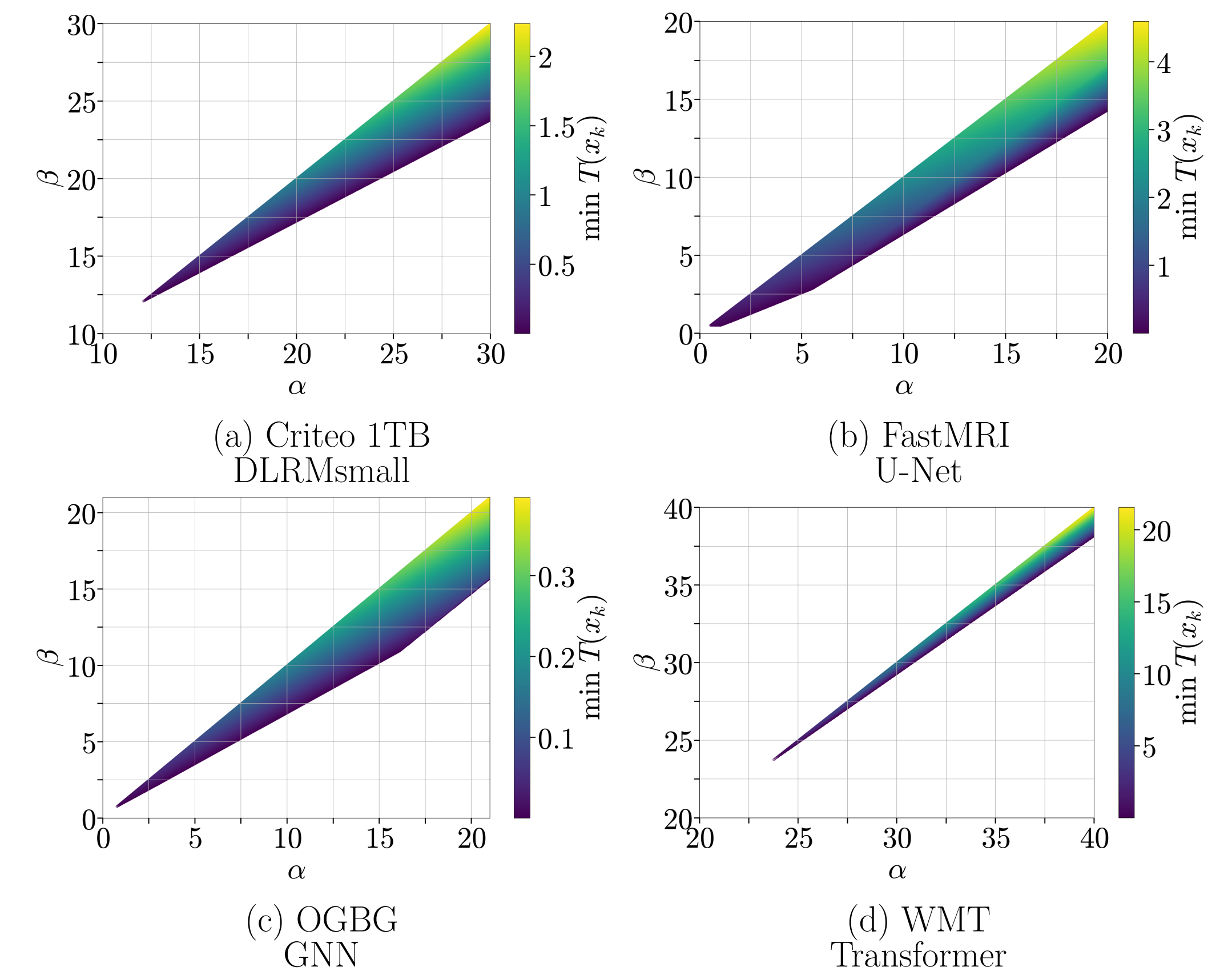


Figure 4: α - β -condition in the training of some large models from AlgoPerf. Here $T(x_k) = \langle \nabla f_{i_k}(x^k), x^k - x^K \rangle - \alpha(f_{i_k}(x^k) - f_{i_k}(x^K)) - \beta f_{i_k}(x^k)$ assuming that $f_i^* = 0$. Minimum is taken across all runs and iterations for a given pair of (α, β) .

References

- [1] Hardt et al., Gradient descent learns linear dynamical systems. JMLR, 2018.
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- [3] Polyak. Gradient methods for the minimisation of functionals. USSR Comp. Math. and Math. Phys., 1963.
- [4] Chaoyue Liu, Libin Zhu, and Mikhail Belkin. Loss landscapes and optimization in overparameterized non-linear systems and neural networks. Appl. and Comp. Harm. Analysis, 2022.