Optimal Sets and Solution Paths of ReLU Networks

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Introduction

Main Contribution: characterize all optimal two-layer ReLU nets.

- **Critical Points**: we extend our expression to all Clarke stationary points.
- **Uniqueness**: we give conditions for optima to be permutation-unique.
- **Pruning**: we show how to compute the "narrowest" optimal ReLU networks.

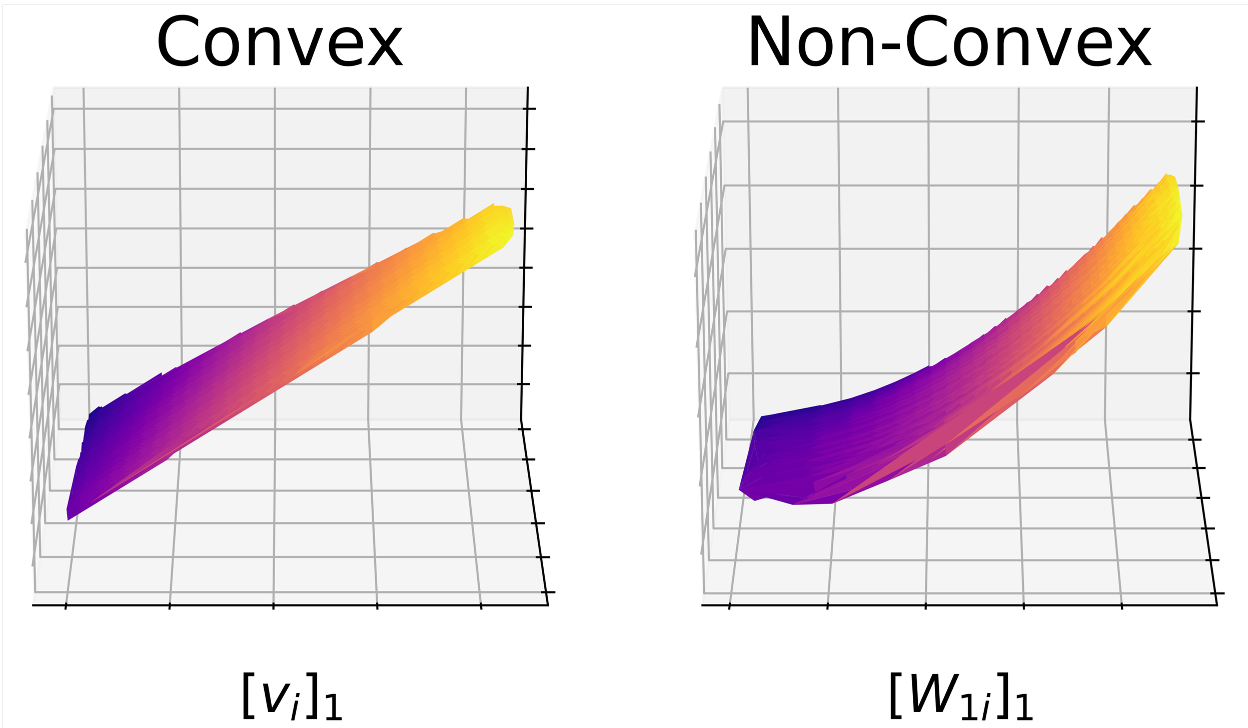


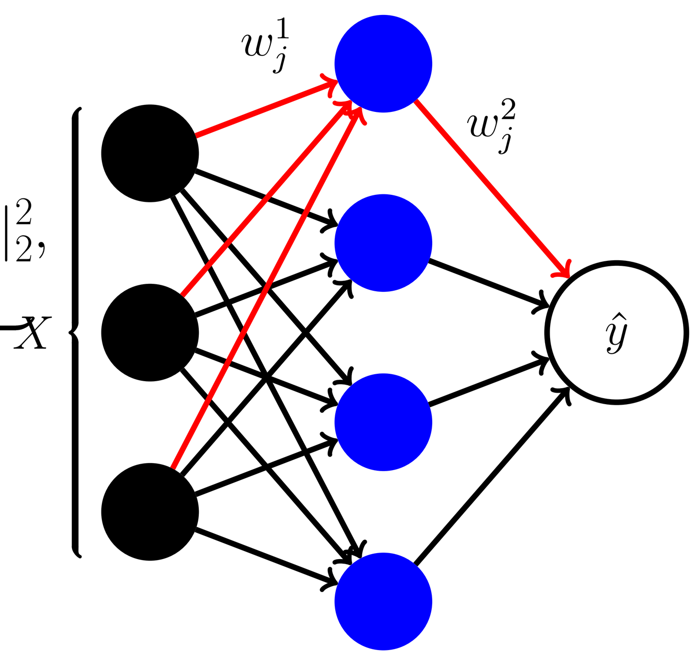
Figure 1. **Optimal set** for the first features of three different neurons.

Convex Reformulations: ReLU Networks

Non-Convex Problem:

$$\min_{w^1,w^2} \underbrace{\Big\| \sum_{j=1}^m (Xw_j^1)_+ w_j^2 - y\Big\|_2^2}_{\text{Squared Error}} + \underbrace{\lambda \sum_{j=1}^m \|w_j^1\|_2^2 + \|w_j^2\|_2^2}_{\text{Weight Decay}},$$

where $(x)_+ = \max\{x, 0\}$ is the ReLU activation.

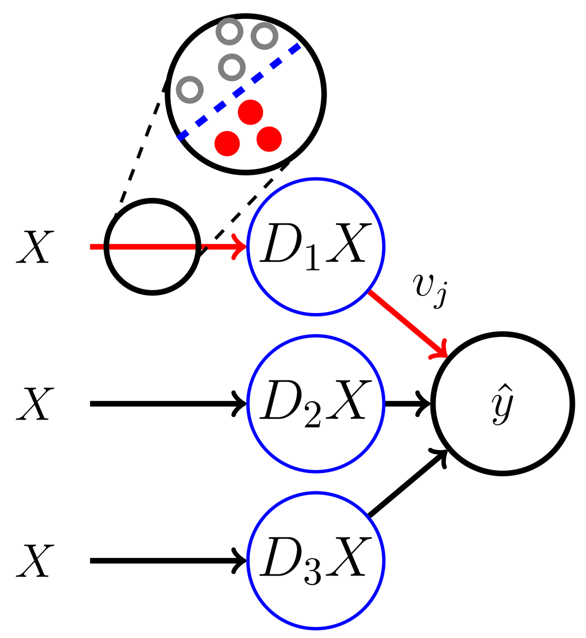


Convex Reformulation: (Pilanci & Ergen, 2020)

$$\min_{v,h} \Big\| \sum_{j=1}^p D_j X(v_j - h_j) - y\Big\|_2^2 + \lambda \sum_{j=1}^p \|v_j\|_2 + \|h_j\|_2$$

s.t. $v_j, h_j \in \mathcal{K}_j := \{w : (2D_j - I)Xw \geq 0\}$,

where $D_j = \text{diag}[\mathbb{1}(Xg_j \geq 0)]$.



Equivalence:

- If $m \geq m^*$, where $m^* \leq n$, then both programs have the same optimal value.
- The convex and non-convex solutions are related by a **solution mapping**.

Proof Strategy

Approach: We use convex reformulations as an analytical tool!

1. Re-write convex reformulation as a **constrained group lasso** (CGL) problem,

$$p^*(\lambda) = \min_w \frac{1}{2}\|Zw - y\|_2^2 + \lambda \sum_{b_i \in \mathcal{B}} \|w_{b_i}\|_2$$

s.t. $K_{b_i}^\top w_{b_i} \leq 0$ for all $b_i \in \mathcal{B}$.

2. Derive optimal set for CGL using the **KKT conditions**: if $w_{b_i} \neq 0$,

$$\underbrace{Z_{b_i}^\top (y - Zw) - K_{b_i}\rho_{b_i}}_{v_{b_i}} = \lambda \frac{w_{b_i}}{\|w_{b_i}\|_2}$$

3. Obtain ReLU optimal set using the **solution mapping**: for $s_i \in \{+1, -1\}$,

$$W_{1i} = w_{b_i}^* / \sqrt{\|w_{b_i}^*\|}, \quad w_{2i} = s_i \cdot \sqrt{\|w_{b_i}^*\|}$$

The ReLU Optimal Set

Define the set of blocks supported by *a solution* to the convex reformulation:

$$\mathcal{S}_\lambda = \{b_i \in \mathcal{B} : \exists w \in \mathcal{W}^*(\lambda), w_{b_i} \neq 0\},$$

and let $Zw^* = \hat{y}$ be the (unique) optimal model fit.

Corollary 4.1 (informal): Suppose $m \geq m^*$ and $\lambda > 0$. Then the set of optimal two-layer ReLU MLPs is,

$$\mathcal{O}_\lambda = \Big\{(W_1, w_2) : f_{W_1,w_2}(Z) = \hat{y}, \; W_{1i} = \left(\frac{\alpha_i}{\lambda}\right)^{\frac{1}{2}} v_i, w_{2i} = (\alpha_i \lambda)^{\frac{1}{2}}, \; \alpha_i \geq 0, \; i \in [2p] \setminus \mathcal{S}_\lambda \Rightarrow \alpha_i = 0\Big\},$$

Interpretation: optimal neurons are scalings of the correlation vector v_{b_i} on the manifold of optimal predictors.

Conditions for Uniqueness

Q: When are optimal networks unique up to permutations/splits?

A: When the convex reformulation has a unique solution!

Proposition 4.3 (informal): Suppose $m \geq m^*$ and $\lambda > 0$. If there does not exist $\alpha \neq 0$ such that

$$\sum_{i \in \mathcal{S}_\lambda} \alpha_i (XW_{1i})_+ = 0,$$

then the non-convex solution is permutation unique (p-unique).

Continuity: p-uniqueness on a neighbourhood $\mathcal{N}$ implies continuity of the regularization path $\lambda \mapsto (W_1(\lambda), w_2(\lambda))$ on $\mathcal{N}$.

Optimal Pruning

Definition: a ReLU network is minimal if there does not exist an optimal network with strictly fewer non-zero neurons.

Proposition 3.6 (informal): Let $m \geq m^*$ and $\lambda > 0$. A model is minimal if and only if the non-zero activations $(XW_{1i})_+$ are linearly independent.

Algorithm 1 Optimal Pruning

Input: data matrix X, solution w^0.
while $\exists \beta \neq 0$ s.t. $\sum_{b_i \in \mathcal{A}_\lambda(w^k)} \beta_{b_i} X_{b_i} w_{b_i}^k = 0$ **do**
  $b_i^k \leftarrow \arg\max_{b_i} \{|\beta_{b_i}| : b_i \in \mathcal{A}_\lambda(w^k)\}$
  $t^k \leftarrow 1/|\beta_{b_i^k}|$
  $w^{k+1} \leftarrow w^k(1 - t^k \beta_{b_i})$
end while
Output: final weights w^k

Proposition (informal): Algorithm 1 computes an optimal and minimal ReLU network with $m^* \leq n$ non-zero neurons in $O(n^3 m + nd)$ time.

Direct Pruning: We give equivalent algorithm for non-convex params.

Experiments

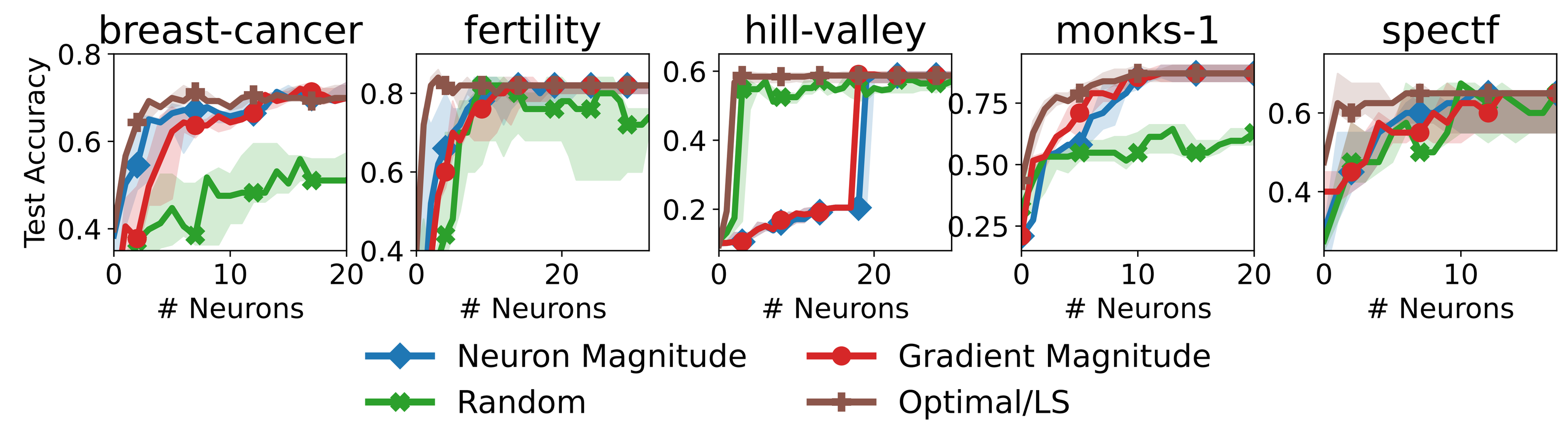


Figure 2. Test accuracy for theory-inspired pruning (Optimal/LS) and baseline methods.

- We consider pruning neurons on several UCI classification datasets.
- Our approach dominates every baseline considered.

Dataset	Min L_2	EP	V-MSE	T-MSE	Max Diff.
mammogr.	0.77	0.77	0.57	0.78	**0.21**
horse-colic	0.75	0.59	0.74	0.85	**0.26**
ilpd-indian	0.59	0.59	0.53	0.72	**0.19**
parkinsons	0.74	0.74	0.65	0.88	**0.23**
pima	0.68	0.68	0.68	0.87	**0.2**

- We tune ReLU networks by direct optimization over the optimal set.
- Same training performance, but test accuracy differs by over 20 points!

References

Pilanci, M. and Ergen, T. Neural networks are convex regularizers: Exact polynomial-time convex optimization formulations for two-layer networks. In *ICML 2020*, volume 119 of *Proceedings of Machine Learning Research*, pp. 7695–7705. PMLR, 2020.