NONCONVEX PENALIZATION FOR SPARSE NEURAL NETWORKS

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Abstract. Training methods for artificial neural networks often rely on over-parameterization and random initialization in order to avoid spurious local minima of the loss function that fail to fit the data properly. To sidestep this, one can employ convex neural networks, which combine a convex interpretation of the loss term, sparsity promoting penalization of the outer weights, and greedy neuron insertion. However, the canonical $\ell_1$ penalty does not achieve a sufficient reduction in the number of nodes in a shallow network in the presence of large amounts of data, as observed in practice and supported by our theory. As a remedy, we propose a nonconvex penalization method for the outer weights that maintains the advantages of the convex approach. We investigate the analytic aspects of the method in the context of neural network integral representations and prove attainability of minimizers, together with a finite support property and approximation guarantees. Additionally, we describe how to numerically solve the minimization problem with an adaptive algorithm combining local gradient based training, and adaptive node insertion and extraction.

1. Introduction

The method we develop here builds upon the work on convex neural networks as outlined in, e.g., [4, 1]. In this approach the network architecture is adapted during training by gradually adding new neurons, while the outer weights are penalized by a convex sparsity promoting functional. The latter has the potential to set redundant network connections to zero during the training, which can be subsequently removed from the network. However, we will show that convex sparsity promoting penalties such as the $\ell_1$ norm do not always effectively eliminate redundancy, and the associated training procedures may still be affected by over-parametrization. As a remedy, we will develop a corresponding framework that incorporates nonconvex penalties but keeps most of the aforementioned advantages of convex neural networks. In order to do that, we focus on shallow networks with one hidden layer, which are of fundamental importance and, compared to deep networks, are relatively well understood theoretically. Moreover, we focus attention on the activation function given as the popular ReLU function $\sigma(x) = \max\{x, 0\}$; however most of our theory applies to a much larger class of activation functions and also other kernel based methods.

We define a shallow neural network with $N$ neurons to be a function $N : \mathbb{R}^d \rightarrow \mathbb{R}$ of the form

$$N_{\omega,c}(x) = \sum_{n=1}^{N} c_n \sigma(a_n \cdot x + b_n),$$

where $\sigma(a_n \cdot x + b_n)$ are the single neurons and $N$ is also called the width of the network. Additionally, by $\omega_n = (a_n, b_n) \in \mathbb{R}^{d+1}$ we denote the nodes consisting of inner weights $a_n \in \mathbb{R}^d$ and $b_n \in \mathbb{R}$. The numbers $c_n \in \mathbb{R}$ are called the outer weights. Let $f$ be a target function defined on some domain $D \subseteq \mathbb{R}^d$ (it can be an image, solution to a PDE, a specific parameter associated with a model, etc.). The aim is to find a neural network $N$ with as few as possible neurons $N$ such that $N$ fits the training points $\{(x_k, y_k)\}_{k=1,...,K}$. Here, $x_k \in D$ are the input data and $y_k$ the output data, which

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we assume to be given as \( y_k = f(x_k) + \varepsilon_k \). Additionally, \( \varepsilon_k \) represents error, which could be random in nature (e.g., measurement error) or have a deterministic origin (e.g., modeling or computational truncation error).

The network training considered here will be based on the following minimization problem:

\[
(2) \quad \min_{N \in \mathbb{N}, \{a_n,b_n,c_n\}_{n=1}^N, \|a_n\|^2 + |b_n|^2 \leq 1} l(N_{\omega,c}; y) + \alpha \sum_{n=1}^N \phi(|c_n|).
\]

For simplicity, we focus our attention on the least squares loss function

\[
(3) \quad l(N_{\omega,c}; y) = l_K(N_{\omega,c}; y) = \frac{1}{2K} \sum_{k=1}^K |N_{\omega,c}(x_k) - y_k|^2,
\]

although most of our results can be transferred to a much more general class of data fidelity terms. We emphasize that in problem (2) we do not fix the width \( N \) of the network, which will be chosen together with the corresponding coefficients to minimize the objective. To achieve a compromise between a good fit and a simple network (representing a hopefully regular function with few neurons \( N \)) we employ a sparsity promoting sublinear cost term involving the scalar penalty function \( \phi \) for the outer weights with hyperparameter \( \alpha > 0 \). Note that \( N_{\omega,c} \) is linear in \( c \) and that neurons with \( c_n = 0 \) can be dropped from the network. For the inner weights, we impose bound constraints. This does not limit the set of functions that can be written as (1), owing to the positive homogeneity of the ReLU activation function, but prevents the inner weights from growing arbitrarily large. Concerning the penalty \( \phi: \mathbb{R}_+ \to \mathbb{R}_+ \), we always impose the following assumption:

\((A1_\phi)\) The function \( \phi \) is a concave and nondecreasing with \( \phi(0) = 0 \), \( \phi'(0) = 1 \), and \( \phi(z) \to +\infty \) for \( z \to +\infty \); Moreover, \( \phi \) is \( \gamma \)-convex, i.e., there exists a \( \gamma \geq 0 \) such that the derivative \( \phi' \) fulfills

\[
0 \leq \phi'(z_1) - \phi'(z_2) \leq \gamma(z_2 - z_1) \quad \text{for all } 0 \leq z_1 \leq z_2.
\]

These assumptions imply that \( \phi \) fulfills \( \phi(z) \leq z \) for all \( z \geq 0 \) and that \( \phi \) is \textit{subadditive}, i.e. \( \phi(z_1 + z_2) \leq \phi(z_1) + \phi(z_2) \). This property enhances the sparsity of the solution, and in the case that the inequality is strict (referred to as \textit{strongly subadditive}), it actively promotes it. We will discuss this in more detail below. Moreover, positive homogeneity of the ReLU activation function and the monotonicity of \( \phi \) also imply that \( \| (a_n, b_n) \| = 1 \) will always be fulfilled for an optimal solution of the problem (2). Consequently, (2) is equivalent to the following problem

\[(P_\phi) \quad \min_{N \in \mathbb{N}, \{c_n\} \in \mathbb{R}^N, \{\omega_n=(a_n,b_n)\} \in (\mathbb{S}^d)^N} l(N_{\omega,c}; y) + \alpha \sum_{n=1}^N \phi(|c_n|),\]

where \( \mathbb{S}^d = \{(a,b) \in \mathbb{R}^{d+1} : \| (a,b) \|^2 = 1 \} \) is the unit sphere in \( \mathbb{R}^{d+1} \).

Note that the convex \( \ell_1 \) sparsity promoting penalty (i.e. \( \phi(z) = z \)) is still included in the above assumptions. It is known that the problem for \( \phi(z) = z \) can be understood as a convex problem on the space of measures, and always admits a global solution with \( N \leq K \). Moreover, this solution can be efficiently approximated with (generalized) conditional gradient methods (see, e.g., [1, 8, 7, 34]). While the \( \ell_1 \) problem with \( \phi(z) = z \) has many favorable theoretical properties, it does not completely solve the issue of over-parameterization, especially in the case where \( K \) is large. In Figure 1, we visualize this with a simple one-dimensional example, where we can interpret \( N_{\omega,c} \) as a piecewise linear spline with knot points \( x_n = -b_n/a_n \). We see that a nonconvex penalty term is able to substantially reduce the number of nodes without affecting the quality of the approximation.

To shed more light on this effect, we consider the limit of \( l_K \) where the number of data points grows infinitely large. If we interpret the data points \( x_k \) to be random samples from a probability distribution \( \nu \) on the domain \( D \), the loss function \( l_K \) can be understood as the empirical estimation
Figure 1. Comparison of solutions of \((P_\phi)\) in one dimension for \(f(x) = \cos(10(10^{-3} + x^2)^{1/8})\) with different convex and noncovex \(\phi\): We choose \(\alpha = 10^{-4}\), \(x_k\) by 5000 uniformly distributed points on the interval \([-1, 1]\), \(y_k = f(x_k) + \varepsilon_k\) perturbed by white noise with std. dev. \(\sigma = 0.05\). Top: outer weights \(c_n\) over the knot points \(x_n = -b_n/a_n\). Bottom: Noisy data \(y_k = f(x_k) + \varepsilon_k\) (blue), optimal network \(N_{\omega,c}\) (black), and knot points of the corresponding linear spline (orange).

of the loss
\[
l_\nu(N_{\omega,c}; y) = \frac{1}{2} \int_D (N_{\omega,c}(x) - y(x))^2 \, d\nu(x) = \frac{1}{2} \|N_{\omega,c} - y\|_{L^2(D, \nu)}^2,
\]
where \(y(x) = f(x) + \varepsilon(x)\), and \(\varepsilon(x)\) is an error term. Consequently, we consider the problem (2) with \(l = l_\nu\), which can be seen as approximating the function in the whole domain \(D\) instead of a finite number of points.

Remark 1. To make this precise from a statistical perspective, we consider a pair of random variables \((X, Y) \in \mathbb{R}^d \times \mathbb{R}\) where \(\nu\) is the (marginal) law of \(X\) and \(Y = f(X) + E\) with noise \(E\). We define its conditional expectation as \(\varepsilon(x) = \mathbb{E}[E|X = x]\). Now, if we consider \((x_k, y_k)\) to be independent draws from \((X, Y)\) we obtain
\[
\mathbb{E}[l_K(N_{\omega,c}; Y)] = \frac{1}{2} \mathbb{E}[(N_{\omega,c}(X) - Y)^2] = \frac{1}{2} \mathbb{E}[(N_{\omega,c}(X) - y(X))^2] + \frac{1}{2} \mathbb{E}[E^2 - \varepsilon(X)^2] = l_\nu(N_{\omega,c}; y) + \frac{1}{2} \mathbb{E}[\text{Var}(E|X)].
\]

Since the second term is independent of \(N_{\omega,c}\), minimizing the expectation of \(l_K\) corresponds to minimizing \(l_\nu\). In the case that the noise is unbiased, \(\mathbb{E}[E|X = x] = 0\), we simply have \(y = f\).

Since \(N\) is maintained as a free optimization variable in \((P_\phi)\), one may expect that in this case the problem may not have minimizers (local or global): a network with larger and larger number of nodes could decrease the value of the functional. That is indeed the case for the \(\ell_1\) penalization problem as our numerical experiments (performed for large \(K\)) indicate. The solutions of problem \((P_\phi)\) with the \(\ell_1\)-penalty \((\phi(z) = z)\) tend to form clusters of nodes \((a_n, b_n)\) with very small coefficients \(c_n\) (this effect is more severe for a larger number of training data \(K\)). The main disadvantage of the \(\ell_1\) cost functional is that it is not encouraging nodes \((a_n, b_n)\) that are very close to merge into one. This is related to the additivity of the absolute value on the positive real axis: if we replace
a node \((a, b)\) with coefficient \(c\) by two nodes \((a_1, b_1)\) and \((a_2, b_2)\) very closely placed to \((a, b)\), with corresponding coefficients \(c_1\) and \(c_2\) (of the same sign as \(c\)) with \(c = c_1 + c_2\) we obtain a network with the same \(\ell_1\)-norm, while potentially decreasing the fidelity term that measures \(\mathcal{N}(x_k) \approx y_k\). However, switching to a nonconvex, strongly subadditive penalty this effect is remedied; as illustrated in Figure 1b.

The above discussion highlights why the \(\ell_1\) norm penalized problem, which in our setting is given by

\[
(P_{\ell_1}) \quad \min_{\{c_n\} \in \mathbb{R}^N, \{\omega_n = (a_n, b_n)\} \in (\mathbb{S}^d)^N} l(\mathcal{N}_{\omega, c}; y) + \alpha \sum_{n=1}^{N} |c_n|
\]

is not the best choice for sparsity promoting regularization of neural networks. Certainly, this also affects formulations where we replace the penalty term in \((P_{\ell_1})\) with a constraint \(\|c\|_{\ell_1} \leq M\), or the fidelity term with a constraint \(\|\mathcal{N}_{\omega, c} - f\| \leq \delta\), since they essentially lead to the same solution manifolds (parameterized by different hyperparameters \(\alpha\), \(M\), and \(\delta\)). Moreover, we point out that the global solutions of the problem \((P_{\ell_1})\) are also global solutions of the popular formulation below, employing \(\ell^2\) regularization:

\[
(P_{\ell_2, \ell_2}) \quad \min_{\{(a_n, b_n, c_n)\} \in (\mathbb{R}^d \times \mathbb{R} \times \mathbb{R})^N} l(\mathcal{N}_{\omega, c}; y) + \frac{\alpha}{2} \sum_{n=1}^{N} \left[\|(a_n, b_n)\|^2 + |c_n|^2\right].
\]

This equivalence relies on the positive homogeneity of the ReLU activation function; see, e.g., [30]. Thus, \((P_{\ell_2, \ell_2})\) is surprisingly already equivalent to a sparsity regularized problem in this setting, and is also affected by the same issues as \((P_{\ell_1})\).

More generally, if we replace the cost term in \((P_{\ell_2, \ell_2})\) with \(\mathcal{R}(a, b, c) = (1/p) \sum_n \|(a_n, b_n)\|^p + |c_n|^p\), we obtain the problem formulation \((P_{\phi})\) with \(\phi(z) = (2/p) z^{p/2}\) (see Appendix E). For \(0 < p < 2\), the choice of \(\phi(z) = (2/p) z^{p/2}\) is concave, monotonous, and subadditive, and would be appropriate for some parts of this paper. However, it does not fulfill the other requirements \((A1_\phi)\) imposed above, since it has an unbounded derivative at zero and can not be normalized to fulfill \(\phi'(0) = 1\). Since this assumption is crucial for this paper, we instead consider a strongly subadditive function \(\phi: \mathbb{R}_+ \to \mathbb{R}_+\) fulfilling \((A1_\phi)\) and the following additional assumption:

\[(A2_\phi)\] There exists a \(\tilde{\gamma} > 0\) and \(\bar{z} > 0\) such that

\[\tilde{\gamma}(z_2 - z_1) \leq \phi'(z_1) - \phi'(z_2) \quad \text{for all } 0 \leq z_1 \leq z_2 \leq \bar{z}.
\]

It can be observed that any \(\phi\) possessing the properties \((A1_\phi)\) and \((A2_\phi)\) also satisfies the inequalities \(z - (\gamma/2)z^2 \leq \phi(z) \leq z - (\tilde{\gamma}/2)z^2\) for \(z \in [0, \bar{z}]\). The function

\[
\phi_{\log, \gamma}(z) = \frac{1}{\gamma} \log(1 + \gamma z); \quad \gamma > 0,
\]

which is a scaled version of the log-penalty function (considered in, e.g., [28]) and its convex combination with the \(\ell_1\) norm, will be the main function of choice for us in the numerical examples. Another option is the MCP function [39],

\[
\text{MCP}_\gamma(z) = \begin{cases} 
  z - (\gamma/2)z^2 & \text{for } z < 1/\gamma, \\
  1/(2\gamma) & \text{else},
\end{cases}
\]

which however lacks the property \(\phi(z) \to +\infty\) for \(z \to +\infty\). However, a proper convex combination of MCP with \(\ell_1\), e.g. \(\phi(z) = (1/2)(z + \text{MCP}_{2\gamma}(z))\), fulfills both \((A1_\phi)\) and \((A2_\phi)\). We refer to Figure 2 for a visualization of different penalty functions.
1.1. Contribution. For $\phi$ satisfying the conditions \((A1_\phi)\) and \((A2_\phi)\) we show that the problem \((P_\phi)\) has global and local minimizers (with finite $N$) for finite and infinite data (see Theorem 3). Since the existence of finite minimizers of the convex problem relies on finite amount of data, and this is not the case for the nonconvex problem, this is a rather unexpected result.

Since the regularization term in \((P_\phi)\) is nonconvex, finding the global solution of the problem may not be feasible. In fact, for a nonconvex optimization problem of similar structure, finding global minima with very high precision is shown to be an NP-hard problem; see [11]. On the other hand, it is observed in practice and confirmed in theory (see, e.g., [25]) that local minima (or stationary points, in general) of nonconvex penalized problems tend to be well behaved. We will develop a similar theory for the problem \((P_\phi)\), where $N$ is a free optimization variable. First, we will define a concept of local minimality, which is based on the notion of locality in the space of shallow neural networks of the form \((1)\) defined in terms of the associated measure

\[
\mu = \sum_{n=1}^{N} c_n \delta(a_n,b_n),
\]

where $\delta(a_n,b_n)$ is the Dirac measure at $(a_n,b_n)$. This identification will be further explained in the context of integral neural networks discussed in Section 2. We only mention that a local solution in our setting will be any set of coefficients, where the $c_n$ are minimal in a suitable neighborhood, and where adding to $\mathcal{N}_{\omega,c}$ any additional node $(a,b) \in S^d$ (with suitably small outer weight $c$) will also increase the training objective; see Theorem 4.

For these local solutions of \((P_\phi)\) (which also include the global solutions), we show that:

- They are always finitely supported; see Theorem 3.
- In the case $K < \infty$ it holds $N \leq K$ for any local solution; see Theorem 6.
- The approximation error of the neural network can be estimated as follows:

\[
l(N_{\omega,c};f) \leq 2 C_f \alpha + l(y;f),
\]

where the constant $C_f$ depends only on the function $f$; see Theorem 5.

The last point quantitatively affirms the assertion that the hyperparameter $\alpha$ can be treated as a trade-off between the network sparsity and reconstruction accuracy. In particular, it shows that local solutions of \((P_\phi)\) can reduce the fitting term below the level of noise or bias in the data by an appropriate choice of $\alpha$. We remark that the property $\phi'(0) = 1$, which could be replaced by $\phi'(0) < +\infty$ with minor modifications, is required for the last result. For the $\phi(z) = (1/q) z^q$ with
$q < 1$ (and thus $\phi'(0) = +\infty$), the zero measure is always a local solution in the aforementioned sense, and thus no approximation guarantees can be given.

Finally, we propose a method to algorithmically approximate local solutions of $(P_0)$. This is based upon an extension of the methods developed for $\ell_1$ penalization [8, 7, 1, 34, 17] to the setting of nonconvex penalizers $\phi$. Here, we combine adaptive node insertion and deletion with local minimization of the outer weights (or, optionally, full gradient-based training of all the weights $(a, b, c)$). Again, we rely on the property $\phi'(0) = 1$ and the corresponding optimality conditions to guide the node insertion and deletion steps.

1.2. Related work. Sparsity has been widely employed with the dual purpose of removing non-informative connections from neural networks [15, 19] and also to guide adaptive architecture search [4, 1, 12]; in our case it is the adaptive choice of the network width.

Training procedures with nonconvex penalties have been employed in order to eliminate certain weights from the network. In [27] the authors imposed a nonconvex penalty with $\phi(z) = (\beta + 1)z / (\beta + z)$, combined with an additional $\ell_1(\ell_2)$ group sparsity penalty, and proposed a proximal gradient method. Note that the rescaled penalty $\phi(z) = \beta z / (\beta + z)$ fulfills all the requirements of our analysis. Unlike our case, they apply the penalty to all the weights in the network with a fixed architecture and do not consider $N$ to be variable. Similarly, in [38] a different nonconvex penalization strategy is adopted to sparsify a deep network architecture. The authors propose a penalty based on the ratio of $\ell_1$ and $\ell_2$ norms, which also can be considered as a nonconvex compromise between the $\ell_1$ norm and the counting measure. However, it does not have separable form as we consider in $(P_\phi)$.

Nonconvex penalties for sparse regularization have been considered in the statistics literature. The functions like SCAD, the MCP and capped $\ell_1$ are a popular choice [16, 40, 39, 37]. We remark that the MCP penalty fulfills most of the conditions of our analysis; cf. Figure 2. However, the setting we consider is different since the dictionary and the data set can be infinite in our work, and their results do not directly apply to the neural network model we consider here.

Nonconvex functionals on spaces of measures also appear in the study of minimization problems using gradient regularization, such as problems involving functions of bounded variation (BV-regularization, TV-norm of the gradient). In fact, such problems initially prompted the characterization of lower-semicontinuity of functionals of measures [5, 6]. In particular, a critical part of the proof in Theorem 1, follows from the lower-semicontinuity result in [5]. However, the gradient of a BV-function can only have atomic parts (Dirac delta functions) in one spatial dimension, and the picture in higher spatial dimensions is different. Therefore, nonconvex regularizers on the gradient of a function face additional challenges in a continuous setting [20], and are therefore often implemented after discretizing the problem. Due to this, these works do not consider the other important results we prove for local minimizers under the additional condition $(A_{2\phi})$; see Section 2.

Integral neural networks have been around for a while and there is a large volume of work in this direction. Some of the most related to this paper are those in [1] and [31]. Integral neural networks have, in particular, been used for demonstrating approximation capabilities of shallow neural networks [2, 24, 26]. Under the integral representation assumption, it is possible to prove certain convergence rates for greedy type algorithms. Other related work includes integral neural network representation results like those in [21, 23] and the ridgelet transform [10, 29, 35].

1.3. Organization. In section 2, we develop the main theoretical framework as outlined above. In subsection 2.1 we introduce integral neural networks, and extend problems $(P_{L1})$ and $(P_0)$ to this framework. In subsection 2.2 we state our main contributions concerning various properties of local solutions of $\phi$-penalized problem, their existence, necessary conditions, finiteness, and good fidelity. Section 3 is about the least total variational norm solution of the exact representation constrained problem. This problem is strongly connected to the fidelity estimate in Theorem 5.

In section 4 we propose a method for solving the problem $(P_0)$ which is an adaptation of the generalized conjugate gradient method to the nonconvex setting. We also provide detailed discussion
for the three main steps of the algorithm (network initialization, node insertion, and node extraction) in the proceeding subsections.

Finally, in section 5, we illustrate the developments of this paper with concrete examples. We conduct numerical experiments in one and two dimensions and compare the effect of $\gamma$ (which is the second derivative of $\phi$ at zero). Note that $\gamma$ is another hyperparameter along with $\alpha$ influencing the fidelity-sparsity trade-off in the approximating network.

The paper ends with an Appendix, where we provide proofs of the theorems from section 2.2.

## 2. General theory

Problem $(P_\phi)$ is a particular case of a more general framework that will be discussed in this section. We will make use of the concept of integral neural network which is a generalization of the neural network (1) where the sum in $\mathcal{N}_{\omega,c}(x)$ is replaced with an integral. We will introduce the extensions of problems $(P_\phi)$ and $(P_\delta)$ for integral neural networks, and obtain various analytic results concerning their local solutions. Most of the results here apply to a larger class of activation functions than just the ReLU so the theory will be developed in this setting.

### 2.1. Integral neural networks.

Let $\Omega$ be a compact subset of $\mathbb{R}^d$. Denote by $M(\Omega)$ the space of Borel measures on $\Omega$ of bounded total variation, and by $\|\mu\|_{M(\Omega)}$ the total variation norm of the measure $\mu \in M(\Omega)$. Consider a function $\sigma \in C(D \times \Omega)$ such that for some $\Lambda > 0$:

$$
|\sigma(\omega_1,x) - \sigma(\omega_2,x)| \leq \Lambda \|x\|_\infty \|\omega_1 - \omega_2\|.
$$

Note that with the ReLU activation function, i.e. $\sigma(\omega,x) = \max\{a \cdot x + b,0\}$, this condition is satisfied for $\Lambda = 1$ on $\Omega = S^d$. An integral neural network is a function of the form

$$
[\mathcal{N}\mu](x) = \int_\Omega \sigma(\omega,x) \, d\mu(\omega)
$$

where $\mu \in M(\Omega)$. Finally, by

$$
\langle \varphi, \mu \rangle = \int_\Omega \varphi(\omega) \, d\mu(\omega),
$$

we denote the canonical duality pairing of $\varphi \in C(\Omega)$ and $\mu \in M(\Omega) = C(\Omega)^*$.

To see that the above integral network is an extension of the network in (1), let $\Omega = S^d$, $\sigma(\omega,x) = \max\{a \cdot x + b,0\}$ for $\omega = (a,b) \in S^d$, and define the discrete measure

$$
\mu = \sum_{n=1}^N c_n \delta_{\omega_n} \in M(\Omega).
$$

Then it can be observed that

$$
[\mathcal{N}\mu](x) = \sum_{n=1}^N c_n \sigma(a_n \cdot x + b_n) = \mathcal{N}_{\omega,c}(x).
$$

Additionally, it holds that

$$
\|\mu\|_{M(\Omega)} = \sum_{n=1}^N |c_n| = \|c\|_{\ell_1}, \quad \langle \varphi, \mu \rangle = \sum_{n=1}^N \varphi(\omega_n) c_n = (\varphi(\omega),c)_{\mathbb{R}^N},
$$

which relates the total variation norm of $\mu$ to the $\ell_1$ norm of $c$ and the duality pairing to an Euclidean inner product of the vector $(\varphi(\omega_n))_n \in \mathbb{R}^N$ with $c$.

Now, we turn to the loss function. Let $\nu$ be a probability measure supported on the set $D \subseteq \mathbb{R}^d$ with finite first and second moments; i.e. $\int_D |x|^2 \, d\nu(x) = \|x\|^2_{L^2(D,\nu)} < \infty$. Associated to this, we
define the Hilbert space $L^2(D, \nu)$ of square integrable functions with respect to $\nu$. The last property, together with (6), ensures that $\mathcal{N}$ is bounded as an operator from $M(\Omega)$ to $L^2(D, \nu)$ and let

$$\|\mathcal{N}\| = \max_{\omega \in \Omega} \|\sigma(\omega, \cdot)\|_{L^2(D, \nu)} < \infty$$

be its operator norm. Moreover, let $f \in L^2(D, \nu)$ be the target function we aim to approximate with integral neural networks. From the observation above, the canonical extension of the $\ell_1$-penalized problem $(P_{\ell_1})$ can be easily deduced as

$$(P_{L_1}) \quad \min_{\mu \in M(\Omega)} L(\mu) + \alpha \|\mu\|_{M(\Omega)}$$

where

$$L(\mu) = l(\mathcal{N}\mu; y) = \frac{1}{2} \|[\mathcal{N}\mu](x) - y(x)\|_{L^2(D, \nu)}^2.$$  

Here, $y(x) = f(x) + \varepsilon(x) \in L^2(D, \nu)$ is a potentially biased or noisy version of function $f$ to be approximated. We remark that the empirical functional $l_K$ from (3) is still included in this formulation by the choice $\nu = \nu_K = (1/K) \sum_K \delta_{x_k}$ and identifying $y \in L^2(D, \nu_K)$ with the vector $y_k = y(x_k) = f(x_k) + \varepsilon(x_k) = f(x_k) + \varepsilon_k$.

To extend the problem $(P_\phi)$ for integral neural networks, we need to define the analog of the cost term in $(P_\phi)$ for arbitrary measures $\mu \in M(\Omega)$. To do this, we first recall that any finite measure $\mu$ can be uniquely decomposed into an atomic part, which is a (potentially infinite) sum of Dirac-delta measures, and the remaining continuous part. Denote by $\text{atom}(\mu) = \{\omega_n\}$ the atoms of $\mu \in M(\Omega)$, of which there are either a finite number or countably infinitely many. Then, $\mu = \mu_{\text{atom}} + \mu_{\text{cont}}$, where $\mu_{\text{atom}} = \sum_n \epsilon_n \delta_{\omega_n}$ with $\epsilon_n = \mu(\{\omega_n\})$ and $\mu_{\text{cont}} = \mu|_{\Omega \setminus \text{atom}(\mu)}$, and define

$$\Phi(\mu) = |\mu| (\Omega \setminus \text{atom}(\mu)) + \sum_n \phi(|\mu|(\{\omega_n\}))$$

where $|\mu|$ is the total variation measure of $\mu$. We note that this functional is weakly lower semicontinuous with respect to weak-* convergence (see [5]), which will be important in the following. Moreover, it is the only possible extension of $\Phi(\mu_{\text{atom}}) = \sum_n \phi(|\mu_{\text{atom}}|(\{\omega_n\}))$ for a purely atomic measure $\mu_{\text{atom}}$ to arbitrary measures with this property; see [6]. We remark that, for a continuous measure with no atoms, we obtain $\Phi(\mu_{\text{cont}}) = \int_{\Omega} \phi(0) \, d|\mu_{\text{cont}}| = \|\mu_{\text{cont}}\|_{M(\Omega)}$. As the canonical generalization of the problem $(P_\phi)$, we then consider the following problem

$$(P_\phi) \quad \min_{\mu \in M(\Omega)} L(\mu) + \alpha \Phi(\mu).$$

One advantage we gain from expanding the definition of finite width neural networks to infinite width neural networks is that measures come equipped with the total variation norm topology that allows us to define a concept of locality in a straightforward way.

### 2.2. Local solutions of the $\phi$-penalized problem.
Finding the global solution of the nonconvex problem $(P_\phi)$ may not be realistic, so instead, we will investigate its local minima, and show that they possess desirable properties. The first result is to show that minima of the functional

$$J(\mu) = L(\mu) + \alpha \Phi(\mu)$$

in fact, exist. To this purpose, we introduce an appropriate notion of a local minimum.

**Definition 1.** $\bar{\mu} \in M(\Omega)$ is a local minimum if there exists an $\epsilon > 0$, such that

$$J(\mu) \leq J(\bar{\mu}) \quad \text{for all } \mu \in M(\Omega) \text{ with } \|\mu - \bar{\mu}\|_{M(\Omega)} \leq \epsilon.$$

The next theorem establishes the existence of minimizers under the minimal assumptions $(A1_\phi)$, which also cover the $\ell_1$-penalty function.

**Theorem 1.** If $\phi$ satisfies conditions $(A1_\phi)$, then (10) admits at least one global minimizer.
Note, that the global minimum is also a local minimum; however, the optimization algorithm that we employ in practice can only approximate a local minimum. Moreover, the local and global solutions of \((P_\phi)\) only correspond to solutions of \((P_\phi)\) in a generalized sense, since, thus far, there is no guarantee that the solutions are discrete, i.e. have a representation as in (7). To analyze this, we first derive first-order conditions for the local solutions.

To characterize local solutions of \((P_\phi)\) with a first-order necessary condition, we require some additional notation. Denote by \(\nabla L(\mu)\) the gradient (Fréchet derivative) of the loss function \(L\), which is defined as

\[
\langle \nabla L(\mu), u \rangle = \lim_{\tau \to 0} \left( \frac{1}{\tau} [L(\mu + \tau u) - L(\mu)] \right), \quad \forall u \in M(\Omega).
\]

It holds that \(\nabla L(\mu) = N^*\nabla l(N\mu; y) = N^*(N\mu - y) \in C(\Omega)\), where

\[
N^*: L^2(D, \nu) \to C(\Omega), \quad [N^* g](\omega) = \int_D \sigma(x; \omega) g(x) d\nu(x) \quad \forall g \in L^2(D, \nu)
\]
is the (pre-)adjoint of \(N\). The gradient \(p = N^*(N\mu - y) \in C(\Omega)\) will be called the dual variable in the following. We note that the dual variable gives the inner product of the residual \(N\mu - y\) with \(\sigma(\cdot; \omega)\), i.e.

\[
\bar{p}(\omega) = \int_D \sigma(x; \omega) [N\mu - y](x) d\nu(x) = (\sigma(\cdot; \omega), N\mu - y)_{L^2(D, \nu)}.
\]

It serves to characterize the local solutions of \((P_\phi)\) as follows.

**Theorem 2.** Let \(\phi\) fulfill the conditions \((A_{1\phi})\). If \(\bar{\mu}\) is a local minimum of functional \(J\), then the optimal dual variable \(\bar{p} = \nabla L(\bar{\mu}) = N^*(N\bar{\mu} - y) \in C(\Omega)\) has the following properties:

\[
|\bar{p}(\omega)| \leq \alpha \quad \text{ for } \omega \in \Omega,
\]

\[
\bar{p}(\omega) = -\alpha \phi'(|\bar{\mu}(\{\omega\})|) \text{ sign}(\bar{\mu})(\omega) \quad \text{ for } \omega \in \text{supp } \bar{\mu}.
\]

Here, \(\text{sign}(\bar{\mu})\): \(\text{supp } \bar{\mu} \to \{-1, 1\}\) denotes the signum of \(\mu\), defined \(\bar{\mu}\)-a.e. uniquely for \(\omega \in \text{supp } \bar{\mu}\) (by the Hahn decomposition).

We refer to Appendix B for the proof of this result. We note that this only gives a necessary condition for optimality, and that the interpretation of the second condition requires abstract tools from measure theory.

In the previous results, we still include the case \(\phi(z) = z\) corresponding to \((P_{L1})\). In this situation, we can not guarantee that a solution of the form (7) exists (which is also evidenced by our numerical experiments in Section 5). However, if \((A_{2\phi})\) holds, we derive that the local solutions to \((P_\phi)\) are finitely supported and thus of the form (7).

**Theorem 3.** Suppose function \(\phi\) satisfies conditions \((A_{1\phi})\) and \((A_{2\phi})\). If \(\bar{\mu}\) is a local solution of \((P_\phi)\), then there exists \(N < \infty, \bar{\omega}_n\) and corresponding coefficients \(\bar{c}_n \neq 0, n = 1, \ldots, N\), with \(\bar{\mu} = \sum_n \bar{c}_n \delta_{\bar{\omega}_n}\).

In the case of an atomic local minimum, the necessary optimality conditions from Theorem 2 can be simplified.

**Remark 2.** Let \(\phi\) fulfill the conditions \((A_{1\phi})\). Let \(\bar{\mu}\) be a finite local minimum of \(J\) (as in Theorem 3) with \(\bar{c}_n \neq 0\). Then, the second condition of Theorem 2 reads as

\[
(11) \quad \bar{p}(\bar{\omega}_n) = -\alpha \phi'(|\bar{c}_n|) \text{ sign } \bar{c}_n, \quad n = 1, \ldots, N,
\]

where the dual variable is \(\bar{p} = N^*(N_{\bar{\omega}, \bar{c}} - y)\). Define also the functional

\[
J_{\omega}(c) = l(N_{\bar{\omega}, \bar{c}}; y) + \alpha \sum_{n=1}^{N} \phi(|c_n|),
\]

It can be seen that condition (11) is the necessary optimality condition of local optimality of \(\bar{c}\) being a local minimizer of \(J_{\omega}\).
We note that with (A2φ), due to \( \phi'(z) \leq z - (\gamma/2)z^2 \), these conditions imply that \( |\bar{p}(\tilde{\omega}_n)| < \alpha \) for all \( n = 1, \ldots, N \), in addition to \( |\bar{p}| \leq \alpha \), which holds uniformly on \( \Omega \). However, for a nonconvex problem, the necessary conditions above are not sufficient for optimality. The next theorem provides a slightly stronger condition that turns out to be sufficient for local optimality.

**Theorem 4.** Let \( \phi \) fulfill the conditions (A1φ) and (A2φ). Let \( \bar{\mu} = \sum_{n=1}^{N} \bar{c}_n \delta_{\tilde{\omega}_n} \) be a finite measure such that:

i) \( \tilde{c} \in \mathbb{R}^N \) is a local minimum of \( J_\omega \).

ii) For all \( \omega \in \Omega \setminus \{\tilde{\omega}_n\}_{n=1,\ldots,N} \) it holds \( |\bar{p}(\omega)| < \alpha \), where \( \bar{p} = N^*(N_{\omega,\tilde{c}} - y) \) is the associated dual variable.

Then, \( \bar{\mu} \) is a local minimum of \( J \) (i.e., a local solution of \( (P_\phi) \)).

**Proof.** First, since \( \tilde{c} \in \mathbb{R}^N \) is a local minimum of \( J_\omega \), there exists an \( \epsilon > 0 \), such that \( J_\omega(c) \geq J_\omega(\tilde{c}) \) for all \( c \in \mathbb{R}^N \) with \( \|c - \tilde{c}\|_{\ell_1} \leq \epsilon \). Due to Remark 2, \( |\bar{p}(\tilde{\omega}_n)| = \alpha \phi'(\tilde{c}_n) < \alpha \phi'(0) = \alpha \), and thus there exists a \( \delta > 0 \), such that \( \sup_{\omega \in \Omega} |\bar{p}(\omega)| \leq (1 - \delta) \alpha \). Without restriction, assume in the following that \( \epsilon \leq \alpha \delta/(\|N\|^2 + \alpha \gamma/2) \), where \( \gamma \) is from (A1φ). To verify local optimality of \( \bar{\mu} \), let \( \mu \in M(\Omega) \) be arbitrary with \( \|\mu - \bar{\mu}\|_{M(\Omega)} \leq \epsilon \). By the Lebesgue decomposition theorem, we can write

\[
\mu = \mu_0 + \bar{\mu}, \quad \text{with} \quad \mu_0 = \sum_{n=1}^{N} c_n \delta_{\omega_n} \quad \text{and} \quad \bar{\mu} = \sum_{n} \bar{c}_n \delta_{\tilde{\omega}_n} + \mu_{\text{cont}},
\]

where \( \{\tilde{\omega}_n\} \subset \Omega \setminus \text{atom} \bar{\mu} \) are the atoms of \( \bar{\mu} \), \( c_n = \mu(\{\omega_n\}) \), \( \bar{c}_n = \bar{\mu}(\{\tilde{\omega}_n\}) \), and \( \mu_{\text{cont}} \) is the continuous part of \( \mu \). Therefore, it follows \( N_{\bar{\mu}} = N_{\mu_0} + N_{\bar{\mu}} \). Moreover, \( \|c - \tilde{c}\|_{\ell_1} + \|\bar{c}\|_{\ell_1} + \|\mu_{\text{cont}}\|_{M(\Omega)} = \|\mu - \bar{\mu}\|_{M(\Omega)} \leq \epsilon \). By the quadratic form of the loss, we obtain

\[
\frac{1}{2}\|N_{\mu} - y\|^2_{L^2(D,y)} = \frac{1}{2}\|N_{\mu_0} - y\|^2_{L^2(D,y)} + (N_{\mu_0} - y,N_{\bar{\mu}})_{L^2(D,y)} + \frac{1}{2}\|N_{\bar{\mu}}\|^2_{L^2(D,y)}
\]

\[
\geq \frac{1}{2}\|N_{\omega,c} - y\|^2_{L^2(D,y)} + (N_{[\mu_0 - \bar{\mu}]} + N_{[\bar{\mu} - \mu_0]} = (N_{\bar{\mu}} - y,N_{\bar{\mu}})_{L^2(D,y)}
\]

\[
\geq \frac{1}{2}\|N_{\omega,c} - y\|^2_{L^2(D,y)} - \|N\|^2 \epsilon^2 + (\bar{p},\bar{\mu}),
\]

using that

\[
|N_{[\mu_0 - \bar{\mu}]}| = \|N\|^2 \epsilon - \|\mu_{\text{cont}}\|_{M(\Omega)} \leq \|N\|^2 \epsilon^2.
\]

Moreover, for the penalty it holds

\[
\Phi(\mu) = \Phi(\mu_0) + \Phi(\bar{\mu}) = \sum_{n=1}^{N} \phi(|c_n|) + \sum_{n} \phi(|\bar{c}_n|) + \int_{\Omega} d\mu_{\text{cont}}
\]

Combining this, we obtain

\[
J(\mu) \geq J_\omega(c) = J_\omega(c) - \|N\|^2 \epsilon^2 + \int_{\Omega} [\alpha - |\bar{p}|] d\mu_{\text{cont}} + \sum_n [\alpha \phi(\bar{c}_n)] - |\bar{p}(\tilde{\omega}_n)||\bar{c}_n|
\]

By the optimality of \( \tilde{c} \), it follows that \( J_\omega(c) \geq J_\omega(\tilde{c}) = J(\bar{\mu}) \). For the remaining two terms, we use that

\[
\int_{\Omega} [\alpha - |\bar{p}|] d\mu_{\text{cont}} \geq \delta \alpha \epsilon,
\]

also, from \( \phi(|\bar{c}_n|) \geq |\bar{c}_n| - (\gamma/2)|\bar{c}_n|^2 \geq |\bar{c}_n|(1 - (\gamma/2)\epsilon) \),

\[
\sum_n [\alpha \phi(\bar{c}_n) - |\bar{p}(\tilde{\omega}_n)||\bar{c}_n|] \geq -(\gamma/2)\alpha \epsilon \sum_n |\bar{c}_n| \geq -(\gamma/2)\alpha \epsilon^2.
\]

Consequently,

\[
J(\mu) \geq J(\bar{\mu}) + \epsilon(\delta \alpha - (\gamma/2)\alpha \epsilon - \|N\|^2 \epsilon) \geq J(\bar{\mu}).
\]

\( \square \)
We can interpret the conditions from the previous result in terms of the original problem \((P_\phi)\). Condition \(i)\) simply requires the outer weights \(c\) in \((P_\phi)\) to be chosen as a local minimum. Condition \(ii)\) can be read as follows: Adding any number of additional nodes \(\omega\) with small outer weights to \(N\) will increase the training objective of \((P_\phi)\).

The next theorem proves that any local minimizer is not only sparse, guaranteed by Theorem 3, but also fits the data properly. To state the theorem we need to introduce the following notation; cf. \([1, 31]\). Let \(W(D)\) be the space of functions \(f\) on \(D\) that satisfy \(f(x) = [N\mu](x)\) for every \(x \in D\) and some \(\mu \in M(\Omega)\). It can be easily seen that any such \(f\) is Lipschitz continuous on \(D\). For \(f \in W(D)\), denote

\[
\|f\|_{W(D)} = \min_{\mu \in M(\Omega)} \|\mu\|_{M(\Omega)} \quad \text{subject to } f(x) = [N\mu](x) \quad \text{for every } x \in D.
\]

Note that, for any \(f \in W(D)\), there exists a minimizer \(\mu_f\) with \(f = N\mu_f\) such that \(\|f\|_{W(D)} = \|\mu_f\|_{M(\Omega)}\). The existence of the optimal measure in (12) follows from the direct method of variational calculus.

**Theorem 5.** If \(\phi\) satisfies conditions \((A1_\phi)\), and \(f \in W(D)\) then, for any local solution of \((P_\phi)\),

\[
\|N\bar{\mu} - f\|_{L^2(D,\nu)}^2 \leq 2\alpha \|f\|_{W(D)}^2 + \|y - f\|_{L^2(D,\nu)}^2.
\]

**Proof.** Let \(\mu_f\) be such that \(f(x) = [N\mu_f](x)\) for all \(x \in D\) and \(\|\mu_f\|_{M(\Omega)} = \|f\|_{W(D)}\). Then, for any local minimizer \(\bar{\mu}\) of \((P_\phi)\), we have

\[
\|N\bar{\mu} - f\|_{L^2(D,\nu)}^2 = (N\bar{\mu} - y, N(\bar{\mu} - \mu_f))_{L^2(D,\nu)} + (y - f, N\bar{\mu} - f)_{L^2(D,\nu)}
\]

\[
\leq \langle N^*(N\bar{\mu} - y), \bar{\mu} - \mu_f \rangle + \frac{1}{2} \|y - f\|_{L^2(D,\nu)}^2 + \frac{1}{2} \|N\bar{\mu} - f\|_{L^2(D,\nu)}^2,
\]

using Young’s inequality. With \(\bar{p} = N^*(N\bar{\mu} - y)\) and bringing the last term to the left-hand side, we arrive at

\[
\frac{1}{2} \|N\bar{\mu} - f\|_{L^2(D,\nu)}^2 \leq \langle \bar{p}, \bar{\mu} \rangle - \langle \bar{p}, \mu_f \rangle + \frac{1}{2} \|y - f\|_{L^2(D,\nu)}^2.
\]

Now, we can estimate the first term by zero, due to

\[
\langle \bar{p}, \bar{\mu} \rangle = -\alpha \int_{\Omega} \phi'(|\bar{\mu}(\omega)|) \text{sign}(\bar{\mu})(\omega) \, d\bar{\mu}(\omega) = -\alpha \int_{\Omega} \phi'(|\bar{\mu}(\omega)|) \, d|\bar{\mu}|(\omega) \leq 0,
\]

using the optimality conditions for \(\bar{\mu}\) from Theorem 2. Finally, the second term is estimated as

\[-\langle \bar{p}, \mu_f \rangle \leq \alpha \|\mu_f\|_{M(\Omega)}\] using \(\|\bar{p}\|_{C(\Omega)} \leq \alpha\), resulting in the desired estimate. \(\square\)

The condition \(f \in W(D)\) may appear restrictive, but it turns out that a large class of functions is included. In particular, when \(\sigma\) is given by the ReLU function, all sufficiently smooth functions are contained in \(W(D)\). Moreover, if additionally \(D = \mathbb{R}^d\), the quantity \(\|f\|_{W(\mathbb{R}^d)}\) can be explicitly computed. We will discuss this topic further in Section 3.

Finally, we give an additional upper bound in the case of finite data. The representer theorem for the \(\ell_1\) minimization (see, e.g., \([1, \text{Sec. 2.2}]\)) claims that the problem \((P_{\ell_1})\) has a global solution with at most \(K\) nodes. A similar but stronger version of the representer theorem holds for the problem \((P_\phi)\).

**Theorem 6.** If \(\phi\) satisfies conditions \((A1_\phi)\) and \((A2_\phi)\), and \(\text{supp}(\nu) = \{ x_k \}_{k=1,...,K}\) is a finite set with \(K\) points (finite data case) then any local solution of \((P_\phi)\) has at most \(K\) nodes.
3. Exact representation with integral neural networks

We return to the space $\mathcal{W}(D)$, more specifically to the case when the activation function is the ReLU function, $\Omega = S^d$. First, we set $D = \mathbb{R}^d$. First, we characterize the kernel of $\mathcal{N}$, which is given by $M_-(S^d)$, the set of all odd measures $\mu$, i.e. $d\mu(-a, -b) = -d\mu(a, b)$, that satisfy the conditions

$$\int_{S^d} a \, d\mu(a, b) = 0 \quad \text{and} \quad \int_{S^d} b \, d\mu(a, b) = 0.$$ 

It can be seen that $\mathcal{N}_{\mu} \equiv 0$, if and only if $\mu \in M_-(S^d)$. Next, we derive an explicit formula for the measure $\mu_f$ that represents exactly a given smooth function $f$.

**Theorem 7.** For a compactly supported function $f \in C^{d+1}(\mathbb{R}^d)$, we define the coefficient function

$$c_f(a, b) = \begin{cases} 
\frac{(-1)^{(d+1)/2}}{2(2\pi)^{d-1}} \frac{1}{|a|^{d+2}} \frac{\partial^{d+1}}{\partial y^{d+1}} \mathcal{R}[f](a, b) & \text{if } d \text{ is odd}; \\
\frac{1}{2(2\pi)^{d-1}} \frac{1}{|a|^{d+2}} \frac{\partial^{d+1}}{\partial y^{d+1}} \mathcal{H}[\mathcal{R}[f](a, b)](b) & \text{if } d \text{ is even}.
\end{cases}$$

Then $f(x) = [\mathcal{N}_{\mu_f}](x)$ where $d\mu_f(a, b) = c_f(a, b) \, d(a, b)$ is the measure with density $c_f(a, b)$ with respect to the Lebesgue measure $d(a, b)$ on $\mathbb{S}^d$. Moreover, $f(x) = [\mathcal{N}_{\mu}](x)$ for $\mu \in M(\mathbb{R}^d)$ if and only if $\mu = \mu_f + \mu_-$, where $\mu_- \in M_-(\mathbb{S}^d)$.

The proof of Theorem 7 follows by combining results from [13, 31]. Here, $\mathcal{R}[f]$ is the Radon transform of $f$, given by the formula

$$\mathcal{R}[f](a, b) = \int_{a \cdot x + b = 0} f(x) \, dx,$$

where integration is with respect to $(d - 1)$-dimensional Lebesgue measure on the hyperplane \{x $\in \mathbb{R}^d$: a $\cdot$ x + b = 0\} and $\mathcal{H}[g]$ is the Hilbert transform of a function $g: \mathbb{R} \rightarrow \mathbb{R}$ is defined as

$$\mathcal{H}[g](b) = \frac{1}{\pi} \text{p.v.} \int_{-\infty}^{\infty} \frac{g(z)}{b - z} \, dz.$$ 

Observe that the value of $\|f\|_{\mathcal{W}(\mathbb{R}^d)}$ in (12) is attained at $\mu_f$. It is not necessarily the only global minimizer but it is the unique minimizer among even measures [31].

**Corollary 1.** $C_c^{d+1}(\mathbb{R}^d) \subset \mathcal{W}(\mathbb{R}^d)$ and, for any $f \in C_c^{d+1}(\mathbb{R}^d)$, $\|f\|_{\mathcal{W}(\mathbb{R}^d)} = \|\mu_f\|_{M(S^d)}$.

When $D$ is a compact subset of $\mathbb{R}^d$, for $f \in C^{d+1}(D)$, we will still have $C^{d+1}(D) \subset \mathcal{W}(D)$, but Theorem 7 only provides an upper bound for $\|f\|_{\mathcal{W}(\mathbb{R}^d)}$. Here we say that $f \in C^{d+1}(D)$ if there exists an extension $F \in C_c^{d+1}(\mathbb{R}^d)$ such that $F|_D = f$.

**Corollary 2.** Let $f \in C^{d+1}(D)$, where $D$ is a compact subset of $\mathbb{R}^d$. Then $f \in \mathcal{W}(D)$, and for any extension $F \in C_c(\mathbb{R}^d)$ with $F|_D = f$, we have

$$\|f\|_{\mathcal{W}(D)} \leq \|F\|_{\mathcal{W}(\mathbb{R}^d)} = \|\mu_F\|_{M(S^d)}.$$ 

**Proof.** It easily follows from the observation that

$$\{\mu \in M(S^d): f(x) = [\mathcal{N}_{\mu}](x), \forall x \in D\} \subseteq \{\mu \in M(S^d): F(x) = [\mathcal{N}_{\mu}](x), \forall x \in \mathbb{R}^d\}.$$ 

Additionally, in the setting where $D$ is bounded, we point out that the $\mathcal{W}$ norm can be estimated by what is know as the Barron constant in the literature (going back to [2] and [9]). In particular, it can be shown that, for any continuous function $f: \mathbb{R}^d \rightarrow \mathbb{R}$ with Fourier transform $\hat{f}$ and

$$C_f = \int_{\mathbb{R}^d} \|\omega\|^2 |\hat{f}(\omega)| \, d\omega < \infty,$$
the restriction of $f$ to the bounded set $D$ is in $\mathcal{W}(D)$ with norm bounded by a constant factor of $C_f$. We refer to the introduction of [22] (cf. also [26]), where we note that the variation of the function $f$ introduced there is equivalent to the definition (12) given above due to density of Dirac-delta functions in the space of measures and the equivalence in $\mathbb{R}^{d+1}$ of the 1-norm to the Euclidean norm. This implies that the class of functions in $\mathcal{W}(D)$ is larger than $C^{d+1}$.

Finally, we comment on the form of the reconstruction formula derived in Theorem 7, which shows that a smooth function will be represented by a smooth density $d\mu_f = c(a, b) \, d(a, b)$. Moreover, the optimization problem in $(P_\phi)$ can also be seen as an unconstrained and approximate version of the problem (12). As such, when $f$ is smooth, we can expect that the solution of $(P_\phi)$ will try to approximate the non-atomic measure $\mu_f$, indirectly pointing towards the numerical observation that the $\ell_1$ penalization does not promote sufficiently sparse networks.

4. The optimization algorithm

To numerically solve the problem $(P_\phi)$, we deploy the following algorithm which consists of three phases that are executed consecutively. The first phase is a greedy node insertion step requiring a global search over $\Omega$. The second phase involves a standard local gradient-based training of the outer weights. Optionally, in phase two the inner weights can be optimized together with the outer weights. And finally, in the third phase, we remove the nodes whose outer weights had been set to zero by the sparse penalty method in phase two. The major advantage of this method is that it is dynamic: we can start with any network as initialization, and both extract and insert new nodes at every step of the algorithm. This way we maintain a sparse network and gradually improve its predictive performance. The proposed method can be considered an accelerated version of the conditional gradient method [1, 34]. The differences are that the problem is nonconvex, and we allow simultaneously several node insertions, thus potentially accelerating the approximation rate after each iteration. It also resembles the gradient boosting [18] in that it fits the current residual with a new network in a greedy fashion on each iteration.

In the following, we give more details on the concrete implementation of the above-mentioned steps summarized in Algorithm 1. Let $\omega^{(t)} = [\omega_1^{(t)}, \ldots, \omega_{N(t)}^{(t)}]$, $c^{(t)} = [c_1^{(t)}, \ldots, c_{N(t)}^{(t)}]$ be the lists of network inner and outer weights on the $t$-th iteration of the algorithm and $N(t)$ is the number of nodes in the network. In addition, denote by $\mathcal{N}_{\omega^{(t)}, c^{(t)}}(x)$ the corresponding neural network. Network initialization is arbitrary. One can start from any network, including the empty network, then add and extract nodes to derive an optimal network.

Algorithm 1: Iterative node insertion and optimization

1: Initial network $\omega^{(0)}, c^{(0)}$ of width $N(0)$
2: while $t < T$ do
3: Sample $N_{\text{trial}}$ random nodes $\omega \in \Omega$
4: Optimize (in parallel) the function (13) starting from the initial nodes.
5: Select distinct nodes with $|p_t(\omega)| > \alpha$ and add them to the network (of width $N(t + 1/2)$).
6: Perform local training based on (14).
7: Remove nodes with weight zero (resulting in width $N(t + 1)$).
8: $t = t + 1$.
9: end while

To determine new points to insert, in the greedy insertion step, we compute the nodes $\omega \in \Omega$ for which the correlation of $\sigma(\omega, x)$ with the residual $g_t(x) = \mathcal{N}_{\omega^{(t)}, c^{(t)}}(x) - y(x)$ is largest. Thus, we maximize the absolute value of

$$p_t(\omega) = \int_D \sigma(\omega, x) g_t(x) \, d\nu(x) = \frac{1}{K} \sum_{k=1}^{K} \sigma(\omega, x_k) g_k^{(t)}$$

where $\mathcal{N}_{\omega^{(t)}, c^{(t)}}(x)$ is the corresponding neural network.
where we assume that $K$ is finite and $g_k^{(t)} = g_t(x_k)$. Note that $p_t(\omega)$ is exactly the dual variable as defined in Subsection 2.2. Finding a global maximum in a high dimensional space is a challenging problem which requires expensive computations, and its reliable determination up to a guaranteed tolerance for the specific problem here is subject of ongoing research; cf. [1]. As an ersatz, we use the following heuristic which is commonly employed in practice: we test all local maxima of

$$\Omega \ni \omega \mapsto |p_t(\omega)|,$$

which are found by a gradient maximization, initialized at $N_{\text{trial}}$ random points on $\Omega$. This corresponds to solving $N_{\text{trial}}$ simple unconstrained optimization problems (in parallel); cf., e.g., [7]. Of these points, we insert all that violate the constraint $|p_t(\omega)| \leq \alpha$ (after removing possible duplicates). Here, we rely on the random initialization of the $N_{\text{trial}}$ problems in order to have a chance to identify the global maximum with some probability. Moreover, more than one identified local maximum can be added to the network in each iteration to identify a potentially wide network faster. According to Theorem 4, at any node $\omega \in \Omega$ where $|p_t(\omega)| < \alpha$, it is not possible to decrease the objective by inserting the corresponding node with small non-zero weight. Conversely, the nodes $\omega \in \Omega$ where $|p_t(\omega)| > \alpha$, represent locations where local decrease can still be achieved. All the corresponding outer weights at the trial nodes are initialized to zero, and are going to be optimized in the next phase of the algorithm.

Before we address the next phase, we point out that in the case when we consider $\Omega$ to be the sphere and $\sigma$ be the ReLU activation function, we opt to parametrize $\omega$ by its stereographic projection $\omega = (a, b) = (2x, 1 - ||z||^2)/(1 + ||z||^2)$, where $z \in \mathbb{R}^d$. This is done to avoid dealing with the algebraic constraint $||\omega|| = 1$. Here, we use the southern pole as the projection point, which corresponds to $(a, b) = (0, -1)$. The corresponding neuron represents the zero function and removing it from $\Omega$ does not affect the approximation capability of the network.

Let $N(t + 1/2) \leq N(t) + N_{\text{trial}}$ denote the number of nodes in the resulting network. Next, we compute an approximate local solution to the following problem

$$(\Omega \times \mathbb{R})^{N(t+1/2)} \ni (a, b, c) \mapsto l(N_{\omega,c}; y) + \alpha \sum_{n=1}^{N(t+1/2)} \phi(|c_n|)$$

in terms of all weights, using the old values as initialization for the weights from the previous iteration. The resulting nonsmooth optimization problem can be solved by standard training methods based on (proximal) gradient descent. In particular, we can eliminate the constraint for the inner weights by stereographic projection and use gradient descent, and treat the outer weights with proximal gradient descent (see, e.g., [32]). We note that the proximal map for the cost term $\phi$ can still determined uniquely for small stepsize due to $\gamma$-convexity. For instance, for the function $\phi_\gamma(z) = \log(1 + \gamma z)/\gamma$ from the introduction (4), it is given as

$$\text{Prox}_\lambda \phi_\gamma(q) = \arg\min_{c \in \mathbb{R}^N} \frac{1}{2} ||c - q||^2 + \lambda \phi_\gamma(c)$$

$$= \begin{cases} 
\text{sign } q \left( (\gamma |q| - 1) + \sqrt{(\gamma |q| - 1)^2 + 4 \gamma (|q| - \lambda)} \right), & \text{for } |q| > \lambda, \\
0, & \text{else.}
\end{cases}$$

In the case that $\lambda < 1/\gamma$, this proximal mapping is uniquely determined. We note that this has the potential to set a number of outer weights to zero because of the proximal descent step. In phase three of the method, once (14) is solved to a desired accuracy, we drop the nodes with outer weight equal to zero from the network.

We do not specify the details here (in particular, the optimal choices of the stopping criteria for the different nonlinear and nonsmooth optimization routines that we employ), and leave a detailed analysis to future work.
4.1. **Second-order methods for outer weights.** The aforementioned gradient-based methods in phase two of Algorithm 1 are efficient in that they only require derivatives of the objective function in terms of inner and outer weights, which are readily available in modern computational toolboxes via automatic differentiation. However, these methods suffer from slow convergence once we are close to the minimum, and can be slow to eliminate redundant nodes \( \omega \) (as already observed in the context of a convex sparse problem with measures; cf. [34]). In order to provide accurate results (that are not influenced by the choice of the solver), in our numerical experiments we employ a second order semi-smooth Newton method for the outer weights. In an additional step after step 6. of Algorithm 1 this solves the problem in terms of outer weights up to machine precision for the fixed inner weights \( \omega^{(t+1/2)} \), which in particular serves to reliably eliminate redundant nodes.

We first rewrite

\[
\begin{align*}
& l \left( N_{\omega^{(t+1/2)},c}; y \right) + \alpha \sum_{n=1}^{N(t+1/2)} \phi(|c_n|) = F(c) + \|c\|_1 \\
& F(c) = l \left( N_{\omega^{(t+1/2)},c}; y \right) + \alpha \sum_{i=1}^{N(t+1/2)} \left[ \phi(|c_i|) - |c_n| \right]
\end{align*}
\]

is a two times continuously differentiable function of \( c = [c_1, \ldots, c_{N(t+1/2)}] \) due to conditions (A1_\( \phi \)) we imposed on \( \phi \). Note that if \( c \) is a local minimizer of (15) then

\[
- \nabla F(c) \in \alpha \partial \|c\|_1
\]

where \( \partial \|c\|_1 \) is the subdifferential of the \( \ell_1 \) norm. For \( \lambda > 0 \) and \( q = [q_1, \ldots, q_{N(t+1/2)}] \), let \( \text{Prox}_\lambda(q) \) be the proximal operator of the \( \ell_1 \) norm (also known as the soft-thresholding operator) which modifies each entry of \( q \) according to the formula

\[
\text{Prox}_\lambda(q)_n = \text{sign} \ q_n \ \max \{ \lambda - q_n, 0 \}.
\]

Using a reformulation of the condition optimality condition in terms of Robinson's normal map, \( c \) satisfies (16) if and only if \( c = \text{Prox}_\lambda(q) \) for some \( q \) and

\[
\nabla F(\text{Prox}_\lambda(q)) + \frac{\alpha}{\lambda} \ (q - \text{Prox}_\lambda(q)) = 0;
\]

see, e.g., [33, Prop. 3.5]. The first advantage of this reformulation is that the inclusion condition (16) is replaced with an equation. This nonsmooth equation can then be solved using a semi-smooth Newton method (see, e.g., [36]), which exhibits locally superlinear convergence. In particular, once the optimal sparsity pattern is identified, it converges at the quadratic rate of the classical Newton method. The second important advantage is that at each iteration, the soft-thresholding operator outputs a sparse \( c \): we use this feature to drop the zero entries and reduce the number of nodes in the network.

5. **Numerical examples**

In this section, we supply numerical examples of function approximation in one and two dimensions using \((P_\phi)\) and compare it against the \((P_{\ell_1})\). We perform experiments to demonstrate the effect of the \( \gamma \) parameter on the number of nodes in the network. Here, the penalizing function is taken to be

\[
\phi_\gamma(z) = \frac{1}{2} \ (z + \phi_{\text{log,2}\gamma}(z))
\]

for various values of \( \gamma \), which fulfills \((A1_\phi)\) and \((A2_\phi)\) with \( \tilde{\gamma} = \gamma/2 \) and \( \tilde{z} = 1/\gamma \), where \( \phi_{\text{log,2}\gamma}(z) \) is defined in (4).
5.1. One dimensional example. In Figure 3, we consider the function

\[ f(x) = \exp \left( -\frac{x^2}{2} \right) \left| \sin \left( 7\sqrt{1 + x^2} \right) \right| \]

on the interval \( D = [-1, 1] \). The dataset consists of 1000 uniformly arranged points and corresponding values of the function at these points. We apply the algorithm from Section 4 for both \((P_{\ell_1})\) and \((P_\phi)\) problems. In this example the hyperparameter \( \gamma \) is set to the value \( \gamma = 1 \) and the hyperparameter \( \alpha \) is set to the value \( \alpha = 1 \cdot 10^{-5} \). The number of iterations is \( M = 15 \). During each iteration, up to \( N_{\text{trial}} = 50 \) nodes can be added to the network. For \((P_{\ell_1})\) problem in the numerical example, the primal-dual gap is \( 2 \cdot 10^{-9} \) which means the method was able to find a good approximation to the global minimum of the problem. In Figure 3, we report the \( \ell_2 \) error on the training data and the number of resulting nodes to demonstrate that the \( \phi \) minimization achieves better trade-off between sparsity and reconstruction accuracy.

\begin{figure}[h]
\centering
\begin{subfigure}{0.45\textwidth}
\centering
\includegraphics[width=\textwidth]{figure_a.png}
\caption{Global \( \ell_1 \)-solution: \( N = 200 \) nodes and \( \|N_{\omega,c} - f\| = 4.45 \cdot 10^{-3} \).}
\end{subfigure}\hspace{0.5cm}
\begin{subfigure}{0.45\textwidth}
\centering
\includegraphics[width=\textwidth]{figure_b.png}
\caption{Local \( \phi_\gamma \)-penalized solution for \( \gamma = 1 \): \( N = 15 \) nodes and \( \|N_{\omega,c} - f\| = 4.15 \cdot 10^{-3} \).}
\end{subfigure}
\caption{Comparison between solutions of \((P_{\ell_1})\) and \((P_\phi)\), for \( \phi_\gamma(z) \) in (18) in one dimension. Top: Location and values of nodes in angular coordinates. Bottom: True function (black) and reconstructed function values (blue).}
\end{figure}

In the next experiment, results of which are reported in Table 1, we compare the number of nodes for different values of \( \gamma \). We use the network for smaller \( \gamma \) as initialization for the next larger value, and observe a reduction of the number of nodes from one network to the next. For a smaller value of \( \gamma \), \( \phi_\gamma \) minimization performs similar to \( \ell_1 \). We also plot the nodes and corresponding dual variables for two values of \( \gamma \) in Figure 4. Again, we observe that dense clusters of nodes in the \( \ell_1 \) solution are replaced by fewer better separated nodes in the nonconvex penalized solution.

| \( \gamma \)   | Nodes | \( \|N_{\omega,c} - f\| \)     |
|--------------|------|----------------|
| \( 10^{-4} \) | 130  | \( 4.46 \cdot 10^{-3} \)       |
| \( 10^{-3} \) | 71   | \( 4.45 \cdot 10^{-3} \)       |
| \( 10^{-2} \) | 37   | \( 4.31 \cdot 10^{-3} \)       |
| \( 10^{-1} \) | 20   | \( 3.84 \cdot 10^{-3} \)       |
| \( 1 \)      | 18   | \( 3.51 \cdot 10^{-3} \)       |

Table 1. Number of nodes and fidelity for the solution of \((P_\phi)\) with \( \phi_\gamma(z) \) in (18), for different values of \( \gamma \).
5.2. Two-dimensional example. For the two dimensional experiment, we uniformly sample the function
\[ f(x_1, x_2) = \exp\left(-\frac{x_1^2 + x_2^2}{2}\right) \cos(10x_1x_2). \]
on a $51 \times 51$ grid in $[-1, 1]^2$ and apply the $(P_{\ell_1})$ and $(P_{\phi})$ with $\phi_\gamma$ from (18) and hyperparameter values $\alpha = 10^{-5}$ and $\gamma = 5$. For both methods, the algorithm is iterated 10 times, with up to 50 nodes added at each iteration. The network nodes are plotted on the plane via the stereographic projection. We give the results in Figure 5. As before, we observe a reduction in the number of nodes for the nonconvex penalization with essentially the same approximation quality. In contrast to the convex penalized solution, the nonconvex penalization is not affected by the clustering of nodes in a small area of the sphere.

Again, we compare the effect of the hyperparameter $\gamma$ on the number of nodes in the network. This time we apply $M = 10$ iterations of the algorithm with the function
\[ f(x) = \|x - \hat{x}\|_\infty = \sqrt{(x_1 - \hat{x}_1)^2 + (x_2 - \hat{x}_2)^2}, \quad \text{where } \hat{x} = (0.1.0.1) \]
uniformly sampled on a $21 \times 21$ grid in $[-1, 1]^2$. The results are provided in Table 2.

| $\gamma$       | Nodes | $\|N_{\omega,c} - f\|$     |
|----------------|-------|----------------------------|
| $1.00 \cdot 10^{-3}$ | 75    | $1.91 \cdot 10^{-4}$       |
| $2.50 \cdot 10^{-2}$ | 60    | $1.89 \cdot 10^{-4}$       |
| $1.25 \cdot 10^{-1}$ | 43    | $2.05 \cdot 10^{-4}$       |
| $6.25 \cdot 10^{-1}$ | 27    | $3.58 \cdot 10^{-4}$       |
| $3.12$          | 18    | $6.38 \cdot 10^{-4}$       |

Table 2. Number of nodes and fidelity in the solution of the two dimensional $(P_{\phi})$ problem with $\phi_\gamma(z) = (1/\gamma) \log(1 + \gamma z)$, for different values of $\gamma$.

Concerning the number of nodes, we observe a steady reduction with increased $\gamma$ from 75 to 18, whereas in
Global $\ell_1$-solution: $N = 167$ nodes and $\|N_{\omega,c} - f\| = 9.76 \cdot 10^{-3}$.

Local $\phi_{\gamma}$-penalized solution for $\gamma = 5$: $N = 69$ nodes and $\|N_{\omega,c} - f\| = 9.13 \cdot 10^{-3}$.

Figure 5. Comparison between solutions of $(P_{\ell_1})$ and $(P_\phi)$, for $\phi_{\gamma}(z)$ in (18) in two dimensions. Top: Location and values of nodes under stereographic projection. Bottom: Original and reconstructed values of the function.

this example the approximation quality is slightly reduced. However, it is still consistently small following the estimate $\|N_{\omega,c} - f\| \leq \|f\|_{W(D)}^\alpha$ in Theorem 5.

For this example, we can give the integral representation exactly (cf. Theorem 7). Using the fact that $f$ is radial around the point $\hat{x}$, one can show that $f = N\mu_f$ for a measure $\mu_f$ supported on the great circle $S_{\hat{x}} = \{(a, b) \in S^2 \mid a \cdot \hat{x} = b\}$. In fact, we have

$$f(x) = \int_{S_{\hat{x}}} \max\{a \cdot x + b, 0\} \frac{1}{2\|a\|} dS(a, b) = \frac{1}{2} \left[\int_{S_0} \max\{a \cdot y, 0\} dS(a, b)\right]_{y = x - \hat{x}},$$

where $dS$ is the one-dimensional line integral on $S_{\hat{x}}$, resp. $S_0$. Therefore, $\mu_f$ is given by $d\mu_f = 1/(2\|a\|) dS(a, b)|_{S_{\hat{x}}}$. In Figure 6 we look a little bit more closely on the two solutions corresponding to the smallest and largest $\gamma$. We observe that the nodes of the solution for $\gamma = 10^{-3}$ (still close to the $\ell_1$ norm) densely clusters essentially everywhere on the great circle $S_{\hat{x}}$. Up to gaps due to the lack of enforcing the symmetry of the measure with respect to $(a, b) \sim (-a, -b)$ (cf. Theorem 7), the circle is densely filled by the 75 nodes. This is remarkable since here the support of the penalized solution – representing a compromise between a good fit of the data and a small regularization term – is essentially the same as the exact measure $\mu_f$, which achieves the perfect fit. In contrast, for large $\gamma$, the points are sparsely placed on the circle and spaced with almost perfect regularity (modulo symmetry $(a, b) \sim (-a, -b)$). By reducing the dual variable far enough below the bound $|\bar{p}| \leq \alpha$ in the existing nodes, no additional point with a small weight can be inserted without increasing the penalized objective.
6. Conclusions

In this work, we introduce a nonconvex penalization method for finding sparse neural networks. Even though it is challenging to solve the problem globally, we provide theoretical confirmation of local minimizers satisfying the desirable sparsity and approximation properties. We numerically solve the problem using an adaptive method that gradually adds and removes nodes from the network until a certain approximation accuracy is achieved.

We assumed that the target function outputs scalar values. However this restriction can be easily lifted by considering the outer weights $c_n$ to be vectors, and by replacing the penalty term $\phi(|c_n|)$ with $\phi(\|c_n\|)$ in the problem formulation. Then, the generalized problem with measures will be modified by switching from signed measures to vector-valued measures. We can expect all the results of this paper to hold true with small modifications.

Throughout the paper, we largely limited ourselves to the ReLU activation function, although the optimization problem is not specific to this choice and many activation functions that fulfill the Lipschitz continuity requirement could be employed instead. However, ReLU allowed us to restrict the inner weights from $\mathbb{R}^{d+1}$ to $S^d$. For other activation functions that are not positively homogeneous (in particular smoother ones), the restriction from the whole space to a bounded set can impose restrictions on the approximation properties of the resulting architecture. For various widely used activation functions this can be an interesting problem to explore. Additionally, in light
of the equivalence result in Appendix E, restricting to different subsets of \( \mathbb{R}^{d+1} \) may lead to optimal networks with different properties.

A more thorough investigation of the numerical optimization algorithm, algorithmic choices, and implementation details may warrant more attention. Additionally, we only consider nonconvex regularization and adaptive training for shallow neural networks. For the case of deep neural networks, a direct reformulation in terms of appropriate integral representations is a challenging problem. There are two currently existing approaches that can be potential candidates: one way is consider sub-blocks as atoms instead of single neurons (cf., e.g., [12]). A second way is the greedy layer-wise training method as in, e.g., [3] and the references therein.

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**Appendix A. Proof of Theorem 1**

We introduce some notation and auxiliary results that will be used in the proof. For a sequence of measures μ(k) ∈ M(Ω), k = 1, 2, . . . , and a measure μ ∈ M(Ω), denote μ(k) →* μ if μ(k) ∈ M(Ω) converges to μ in weak-* sense as functionals on C(Ω), i.e. for any g ∈ C(Ω),

\[
\lim_{n \to \infty} \langle \varphi, \mu^{(k)} \rangle = \langle \varphi, \mu \rangle.
\]

We require the following auxiliary results:

**Lemma 1** (e.g., Theorem 4.10 in [14]). If μ(k) ∈ M(Ω) are non-negative then μ(k) →* μ if and only if for any (relatively) open set O ⊆ Ω

\[
\liminf_k \mu^{(k)}(O) \geq \mu(O).
\]

**Lemma 2.** For any μ ∈ M(Ω),

\[
\Phi(\|\mu\|_{M(\Omega)}) \leq \Phi(\mu) \leq \|\mu\|_{M(\Omega)}.
\]
Proof. The second inequality follows directly from $\phi(|z|) \leq |z|$. Concerning the first, we let $\text{atom}(\mu) = \{\omega_n\}_n$ be the atoms of $\mu$ and estimate

$$\Phi(\mu) \geq \phi \left( |\mu| (\Omega \setminus \text{atom}(\mu)) \right) + \sum_n \phi \left( |\mu|(\{\omega_n\}) \right)$$

$$\geq \phi \left( |\mu| (\Omega \setminus \text{atom}(\mu)) + \sum_n |\mu|(\{\omega_n\}) \right) = \phi(\|\mu\|_{M(\Omega)}),$$

where we used first the subadditivity of $\phi$ and second the $\sigma$-additivity of $\mu$. \hfill \Box

The next lemma can also be derived from Theorem 3.3 in [5]. We provide independent proof for the sake of a self-contained exposition.

Lemma 3. $\Phi$ is weak-* lower semicontinuous on $M(\Omega)$: if $\mu^{(k)} \rightharpoonup^* \mu$ then

$$\liminf_{n \to \infty} \Phi(\mu^{(k)}) \geq \Phi(\mu). \tag{19}$$

Proof. First let us show that (19) holds when $\mu^{(k)} \rightharpoonup^* \mu$ and $\mu^{(k)}$ are non-negative measures. Let $\text{atom}(\mu) = \{\omega_n\}$ and $c_n = \mu(\{\omega_n\}) > 0$. If $\mu$ has countably infinite atoms, for a given $\varepsilon > 0$ select $N_\varepsilon \in \mathbb{N}$ such that $c_n \leq \varepsilon$ for all $n > N_\varepsilon$ (this exists since $c_n \to 0$). Let $\theta > 0$ be such that

$$B_\theta(\omega_n) \cap B_\delta(\omega_m) = \emptyset$$

for any $1 \leq n < m \leq N_\varepsilon$ where $B_\delta(\omega) \subset \Omega$ denotes the open ball in $\Omega$ around $\omega$ of the radius $\delta$. Abbreviate $A_\delta = \cup_{n=1}^{N_\varepsilon} B_\delta(\omega_n)$ and denote by $A_\delta^c = \Omega \setminus A_\delta$ its complement in $\Omega$. Using subadditivity of $\phi$ and Lemma 2, we have

$$\Phi \left( \mu^{(k)} \right) \geq \Phi \left( \mu^{(k)}_{|A_\delta^c} \right) + \Phi \left( \mu^{(k)}_{|A_\delta} \right) \geq \sum_{n=1}^{N_\varepsilon} \Phi \left( \mu^{(k)}_{|B_\delta(\omega_n)} \right) + \Phi \left( \mu^{(k)}_{|A_\delta^c} \right).$$

If $k$ is sufficiently large then, for any $\omega \in \Omega \setminus \cup_{n=1}^{N_\varepsilon} B_\delta(\omega_n)$, we have $\mu^{(k)}(\{\omega\}) \leq 3\varepsilon$. Indeed, let $g_\gamma$ be a smooth function on $\mathbb{R}^p$ with $\text{supp} \ g_\gamma \subset B_\delta(0)$, $0 \leq g_\gamma \leq 1$ and $g_\gamma(0) = 1$. Notice that the functions $L_k(\omega) = \langle g_\gamma(\cdot - \omega), \mu^{(k)} \rangle$ are uniformly bounded and equicontinuous due to compactness of $\Omega \setminus \cup_{n=1}^{N_\varepsilon} B_\delta(\omega_n)$ and uniform boundedness of $\|\mu^{(k)}\|_{M(\Omega)}$. Additionally,

$$L_k(\omega) \to \langle g_\gamma(\cdot - \omega), \mu \rangle \quad \text{for} \ k \to \infty$$

pointwise which combined with Arzelá–Ascoli theorem implies that in fact, $L_k(\omega)$ converges to $\langle g_\gamma(\cdot - \omega), \mu \rangle$ uniformly in $\Omega \setminus \cup_{n=1}^{N_\varepsilon} B_\delta(\omega_n)$. For every $\omega \in \Omega \setminus \cup_{n=1}^{N_\varepsilon} B_\delta(\omega_n)$, we have $\mu(\{\omega\}) \leq \varepsilon$. From dominated convergence theorem, by picking $\gamma$ small enough we can ensure that $\langle g_\gamma(\cdot - \omega), \mu \rangle \leq \varepsilon$. And then take $k$ large enough so that $3\varepsilon \geq L_k(\omega) \geq \mu^{(k)}(\{\omega\})$.

We use the fact that $z - \phi(z) \leq \gamma z^2$, so

$$\Phi \left( \mu^{(k)}_{|A_\delta^c} \right) = \sum_{\omega \in A_\delta^c} \left[ \phi \left( \mu^{(k)}(\{\omega\}) \right) - \mu^{(k)}(\{\omega\}) \right] + \mu^{(k)}(A_\delta^c) \geq -\gamma \sum_{\omega \in A_\delta^c} \mu^{(k)}(\{\omega\})^2 + \mu^{(k)}(A_\delta^c) \geq -3\varepsilon \sum_{\omega \in A_\delta^c} \mu^{(k)}(\{\omega\}) + \mu^{(k)}(A_\delta^c) \geq (1 - 3\varepsilon) \mu^{(k)}(A_\delta^c).$$
Furthermore, denote by $\hat{A}^C_\delta = \Omega \setminus \left( \bigcup_{n=1}^{N_\delta} \tilde{B}_\delta(\omega_n) \right)$ the relative interior of $A^C_\delta$. Combining the previous estimates, we have

$$
\Phi(\mu^{(k)}) \geq \sum_{n=1}^{N_\delta} \phi(\mu^{(k)}(B_\delta(\omega_n))) + (1 - 3\gamma \epsilon) \mu^{(k)}(\hat{A}^C_\delta).
$$

Thus, it follows that

$$
\liminf_k \Phi(\mu^{(k)}) \geq \liminf_k \sum_{n=1}^{N_\delta} \phi(\mu^{(k)}(B_\delta(\omega_n))) + (1 - 3C\epsilon) \liminf_k \mu^{(k)}(\hat{A}^C_\delta)
$$

$$
\geq \sum_{n=1}^{N_\delta} \phi(\mu(B_\delta(\omega_n))) + (1 - 3C\epsilon) \mu(\hat{A}^C_\delta)
$$

where we used Lemma 1 and the monotonicity of $\phi$ to obtain the last estimate. By letting $\delta \to 0$ and then $\epsilon \to 0$ in the last expression, we get

$$
\liminf_k \Phi(\mu^{(k)}) \geq \sum_{n=1}^{\infty} \phi(\mu(\{\omega_n\})) + \mu(\Omega \setminus \{\omega_n\}_{n=1}^{\infty} = \Phi(\mu)
$$

proving the lower semi-continuity for non-negative measures.

Now let $\mu^{(k)} \rightharpoonup^* \mu$ where $\mu^{(k)}$ are signed measures. Since every weak-* convergent sequence is bounded, we have $\|\mu^{(k)}\|_{M(\Omega)} \leq M$. Take a subsequence of $\mu^{(k)}$ (denoted for simplicity by the same symbol) that realizes $\liminf_k \Phi(\mu^{(k)})$. $|\mu^{(k)}|$ is bounded, so due to sequential compactness of closed balls in $M(\mathbb{R}^d)$, there exists a weak-* convergent subsequence. W.l.o.g. assume $|\mu^{(k)}| \rightharpoonup^* \hat{\mu} \in M^+(\Omega)$. Hence,

$$
\langle |\varphi|, \hat{\mu} \rangle = \lim_{k \to \infty} \langle |\varphi|, |\mu^{(k)}| \rangle \geq \lim_{k \to \infty} \langle \varphi, \mu^{(k)} \rangle = \langle \varphi, \mu \rangle
$$

for any continuous function $\varphi$. Thus,

$$
|\mu|(B) = \sup_{\varphi \in C^0(B), \|\varphi\|_C \leq 1} \langle |\varphi|, \mu \rangle \leq \sup_{\varphi \in C^0(B), \|\varphi\|_C \leq 1} \langle |\varphi|, \hat{\mu} \rangle \leq \hat{\mu}(B)
$$

for any relatively open set $B \subset \Omega$. Additionally, since $|\mu|$ and $\hat{\mu}$ are regular, for any Borel set $A \in \mathcal{B}(\Omega)$ it holds

$$
|\mu|(A) = \inf_{A \subseteq B, B \text{ open}} |\mu|(B) \leq \inf_{A \subseteq B, B \text{ open}} \hat{\mu}(B) = \hat{\mu}(A).
$$

Note that $\Phi(|\mu^{(k)}|) = \Phi(|\mu^{(k)}|)$. $|\mu^{(k)}|$ are positive measures, hence by assumption

$$
\liminf_{k \to \infty} \Phi(\mu^{(k)}) = \liminf_{k \to \infty} \Phi(|\mu^{(k)}|) \geq \Phi(\hat{\mu}).
$$

We finish the proof by observing that $\Phi(\hat{\mu}) \geq \Phi(\mu)$, taking into account the definition (9) and $|\mu| \leq \hat{\mu}$. \hfill \square

To finish the proof of Theorem 1, we employ the direct method of variational calculus. Since $J \geq 0$, we can select a minimizing sequence $\mu^{(n)} \in M(\Omega)$. Now, with

$$
\phi(\|\mu^{(n)}\|_{M(\Omega)}) \leq \Phi(\mu^{(n)}) \leq J(\mu^{(n)}) \to \inf_{\mu \in M(\Omega)} J(\mu)
$$

and the fact that $\phi(z) \to +\infty$ for $z \to \infty$, $\|\mu^{(n)}\|_{M(\Omega)}$ is bounded and we can select a subsequence that converges to $\hat{\mu} \in M(\Omega)$ in the weak-* sense. By weak-* lower semicontinuity of $\Phi$ and continuity of the loss function $L(\mu)$, we conclude that the minimum is attained at $\hat{\mu}$.
APPENDIX B. PROOF OF THEOREM 2

In the following, we let $\bar{\mu}$ be a local solution of $(P_\mu)$, i.e. a local minimum of $J$. To derive the conditions for the given local solution, we consider

$$J(\bar{\mu} + \tau u) - J(\bar{\mu}) = L(\bar{\mu} + \tau u) - L(\bar{\mu}) + \alpha \bar{\Phi}(\bar{\mu} + \tau u) - \alpha \bar{\Phi}(\bar{\mu}) \geq 0$$

with arbitrary $u \in M(\Omega)$ and $0 < \tau < \epsilon / \|u\|_{M(\Omega)}$ where $\epsilon$ is the radius from Definition 1. Dividing by $\tau > 0$ and letting $\tau \to 0$, from local optimality, it follows

$$\left\langle \nabla L(\bar{\mu}), u \right\rangle = -\langle \bar{\Phi}, u \rangle \leq \alpha \lim_{\tau \to 0^+} (1/\tau) [\bar{\Phi}(\bar{\mu} + \tau u) - \bar{\Phi}(\bar{\mu})],$$

as long as the limit on the right exists. We consider different values of $u$ in the following:

For $u = \pm \delta \omega$ for $\omega \notin \text{atom}(\mu)$, i.e. $\mu(\{\omega\}) = 0$, we obtain

$$\exists \bar{p}(\omega) = -\langle \bar{p}, u \rangle \leq \alpha \lim_{\tau \to 0^+} (1/\tau) \phi(\tau) = \alpha \lim_{\tau \to 0^+} (1/\tau) [\phi(\tau) - \phi(0)] = \alpha \phi'(0) = \alpha.$$

Hence, $|\bar{p}(\omega)| \leq \alpha$ for $\omega \notin \text{atom}(\mu)$.

Now, take $u = \pm \delta \omega$ for $\omega \in \text{atom}(\mu)$, i.e. $\bar{\mu}(\{\omega\}) = c \neq 0$. Here, we obtain

$$\exists \bar{p}(\omega) = \langle \bar{p}, u \rangle \leq \alpha \lim_{\tau \to 0^+} (1/\tau) [\phi(\pm \tau) - \phi(|c|)] = \pm \alpha \phi'(|c|) \text{ sign } c.$$

Hence, it follows

$$\bar{p}(\omega) = -\alpha \phi'(|c|) \text{ sign } c.$$

Using the fact that $\phi'(0) = 1$, $\phi$ is increasing and $\phi'$ is decreasing we have that $\phi'(\omega) \in [0, 1]$ for $\omega \geq 0$. Hence $|\bar{p}(\omega)| \leq \alpha$ for $\omega \in \text{atom}(\mu)$ also proving the first estimate in the lemma: $|\bar{p}(\omega)| \leq \alpha$ for all $\omega \in \Omega$.

Next, we take $u = \bar{\mu}_{\text{cont}} = \bar{\mu}|_{\Omega \setminus \text{atom}(\mu)}$ be the continuous part of $\bar{\mu}$ and deduce

$$\exists \langle \bar{p}, \bar{\mu}_{\text{cont}} \rangle \leq \alpha \lim_{\tau \to 0^+} (1/\tau) \|\bar{\mu}_{\text{cont}}\|_{M(\Omega)} = \pm \alpha \|\bar{\mu}_{\text{cont}}\|_{M(\Omega)}$$

and thus $-\langle \bar{p}, \bar{\mu}_{\text{cont}} \rangle = \alpha \|\bar{\mu}_{\text{cont}}\|_{M(\Omega)}$, which together with $|\bar{p}(\omega)| \leq \alpha$ for $\omega \in \Omega$ implies that $\bar{p} = -\alpha \text{ sign } \bar{\mu}_{\text{cont}}$ for $\bar{\mu}_{\text{cont}}$ almost all $\omega \in \Omega$. Combined with the atomic case above and the continuity of $\bar{p}$, we get the second part of the theorem.

APPENDIX C. PROOF OF THEOREM 3

First, let us show that $\bar{\mu}$ is atomic. Assume otherwise and let $\bar{\mu}_{\text{cont}} = \bar{\mu}|_{\Omega \setminus \text{atom}(\mu)} \neq 0$ be the continuous part of $\bar{\mu}$. Then there exist a point $\hat{\omega} \in \text{supp} \mu_{\text{cont}} \setminus \text{atom}(\mu)$, i.e., such that $\bar{\mu}(\hat{\omega}) = 0$ and for any $\delta > 0$, $|\bar{\mu}(B_\delta(\hat{\omega}))| > 0$ where $B_\delta(\hat{\omega})$ is the open ball of radius $\delta$ in $\Omega$ around $\hat{\omega}$. Without restriction, let $\hat{\omega} \in \text{supp} \mu_{\text{cont},+}$ where $\mu_{\text{cont},+}$ is the positive part of $\mu_{\text{cont}}$. Let $D_+ \subset \Omega \setminus \text{atom}(\mu)$ be a set with $\mu_{\text{cont},+} = \bar{\mu}|_{D_+}$ (given by the Hahn decomposition theorem) and $D_\delta = D_+ \cap B_\delta(\hat{\omega})$. Now, we define

$$\mu_\delta = \bar{\mu} - \bar{\mu}|_{D_\delta} + C_\delta \delta \omega, \quad \text{where } C_\delta = \bar{\mu}(D_\delta) > 0$$

which replaces $\bar{\mu}$ on $D_\delta$ for any $\delta > 0$ by a single Dirac measure of the same total variation norm. We note that by construction $C_\delta$ is positive and converges to zero for $\delta \to 0$. We will show that $\mu_\delta$, for $\delta$ small enough, improves the function value of $J$ in contradiction to optimality of $\bar{\mu}$.

Using the Lipschitz continuity assumption on $\sigma$, i.e. $|\sigma(\hat{\omega}; x) - \sigma(\omega; x)| \leq \delta \|x\|\|\bar{\mu}(\hat{\omega} - \omega)|$, one readily obtains that

$$|\mathcal{N}(\mu_\delta - \bar{\mu})(x)| = |\mathcal{N}(\bar{\mu}|_{D_\delta} - C_\delta \delta \omega)(x)| \leq \left| \int_{D_\delta} \sigma(\omega, x) \text{ d}\bar{\mu}(\omega) - C_\delta \sigma(\hat{\omega}, x) \right|$$

$$= \left| \int_{D_\delta} \left| \sigma(\omega, x) - \sigma(\hat{\omega}, x) \right| \text{ d}\bar{\mu}(\omega) \right| \leq \delta \Lambda \|x\| \|\bar{\mu}(D_\delta)\| = \delta \Lambda \|x\| \|\bar{\mu}(D_\delta)\| = \delta \Lambda \|x\| C_\delta.$$
Therefore for any \( x \in \mathbb{R}^d \). Thus, it also follows
\[
\|N(\mu_\delta - \bar{\mu})\|_{L^2(D, \nu)} \leq \delta A L^2(D, \nu) \|N\|_{L^2(D, \nu)} C_\delta = \delta A_1 C_\delta.
\]
Here, we define \( \|x\|_{L^2(D, \nu)}^2 = \int_D \|x\|^2 \, d\nu(x) \) and \( A_1 = \|N\|_{L^2(D, \nu)} \). Consequently, by the quadratic form of \( L \) and, using the fact that \( \bar{\mu} = N^*(N\bar{\mu} - y) \), we have
\[
L(\mu_\delta) = L(\bar{\mu}) + \langle N\bar{\mu} - y, N(\mu_\delta - \bar{\mu}) \rangle_{L^2(D, \nu)} + \frac{1}{2} \|N(\mu_\delta - \bar{\mu})\|^2_{L^2(D, \nu)}
\]
\[
\leq L(\bar{\mu}) + \langle \bar{\mu}, \mu_\delta - \bar{\mu} \rangle + \frac{1}{2} \delta^2 A_1^2 C_\delta^2
\]
By the optimality condition, we have \( \bar{p}(\omega) = -\alpha \) for all \( \omega \in D_\delta \cap \text{supp } \bar{\mu} \subset \text{supp } \mu_{\text{cont,+}} \) (note that also \( \hat{\omega} \in D_\delta \)) and therefore the term \( \langle \bar{p}, \mu_\delta - \bar{\mu} \rangle = \langle \bar{p}, -\bar{\mu} \rangle_{D_\delta} + C_\delta \delta \hat{\omega} \) vanishes. Hence
\[
L(\mu_\delta) \leq L(\bar{\mu}) + \frac{1}{2} \delta^2 A_1^2 C_\delta^2
\]
Note that
\[
\Phi(\mu_\delta) = \Phi(\bar{\mu}) - \rho(D_\delta) + \phi(C_\delta) = \Phi(\bar{\mu}) + \phi(C_\delta) - C_\delta
\]
\[
= \Phi(\bar{\mu}) + \int_{C_\delta} (\phi'(\xi) - \phi'(0)) \, d\xi \leq \Phi(\bar{\mu}) + \hat{\gamma} \int_{C_\delta} (\xi - 1) \, d\xi = \Phi(\bar{\mu}) - \frac{1}{2} \hat{\gamma}^2 C_\delta^2,
\]
for \( \delta \) small enough, using \( \phi'(0) = 1 \), the definition of \( \Phi \) and \( (A2_\phi) \). Combining both estimates, we obtain
\[
J(\mu_\delta) = L(\mu_\delta) + \alpha \Phi(\mu_\delta) \leq J(\bar{\mu}) + \frac{1}{2} \delta^2 A_1^2 - \alpha \hat{\gamma}^2 \delta^2 \hat{\gamma} C_\delta^2.
\]
Therefore
\[
J(\mu_\delta) \leq J(\bar{\mu}) - \frac{1}{2} \left( \alpha \hat{\gamma}^2 - \delta^2 A_1^2 \right) C_\delta^2 < J(\bar{\mu}),
\]
for \( \delta < \sqrt{\alpha \hat{\gamma}} / A_1 \), contradicting the optimality of \( \bar{\mu} \).

Now let us show that the number of atoms in \( \bar{\mu} \) is finite. Assume otherwise, then there exists a subsequence of distinct atoms \( \omega_n \) converging to some \( \hat{\omega} \) due to compactness of \( \Omega \). Without restriction, assume that \( c_n = \bar{\mu}(\{\omega_n\}) > 0 \) for all \( n \). By optimality of \( \bar{\mu} \) and continuity of \( \bar{p} \), from Theorem 2, it holds
\[
\alpha \phi'(c_n) = -\bar{p}(\omega_n) \Rightarrow -\bar{p}(\hat{\omega}) \quad \text{for } n \to \infty.
\]
Since \( \phi'(c_n) \to 1 \) due to \( c_n \to 0 \), it follows that \( \bar{p}(\hat{\omega}) = -\alpha \). Hence, from Theorem 2, \( \hat{\omega} \) cannot be an atom of \( \bar{\mu} \). Define now
\[
\mu_N = \bar{\mu} - \sum_{n=N}^\infty c_n \delta_{\omega_n} + C_N \delta_{\hat{\omega}} \quad \text{where } C_N = \sum_{n=N}^\infty c_n > 0,
\]
replacing an infinite number of atoms by a single one. Set \( \delta_N = \max_{n \geq N} |\omega_n - \hat{\omega}| \). As before, we obtain
\[
L(\mu_N) \leq L(\bar{\mu}) + \langle \bar{p}, \mu_N - \bar{\mu} \rangle + \frac{1}{2} \delta_N^2 C_N A_1^2.
\]
Here, the second term is given as
\[
\langle \bar{p}, \mu_N - \bar{\mu} \rangle = C_N \bar{p}(\hat{\omega}) - \sum_{n=N}^\infty c_n \bar{p}(\omega_n) = -\alpha C_N + \alpha \sum_{n=N}^\infty c_n \phi'(c_n),
\]
using the optimality conditions. Concerning \( \Phi \), there holds
\[
\Phi(\mu_N) = \Phi(\bar{\mu}) - \sum_{n=N}^\infty \phi(c_n) + \phi(C_N).
\]
Combining these estimates, we obtain

\[ J(\mu_N) = L(\mu_N) + \alpha \Phi(\mu_N) \leq J(\tilde{\mu}) - \alpha \sum_{n=N}^{\infty} [\phi(c_n) - \phi'(c_n)c_n] - \alpha [C_N - \phi(C_N)] + \frac{1}{2} \delta_N^2 C_N^2 A_1^2. \]

Now, we use concavity of \( \phi \) for \( \phi(c_n) - \phi'(c_n)c_n \geq \phi(c_n - c_n) = \phi(0) = 0 \) and uniform concavity of \( \phi \) on \([0, \tilde{z}]\), using (A2\( \phi \)), for \( \phi(C_N) = \phi(0) + \phi'(0)C_N + \int_0^{C_N} [\phi'(\xi) - \phi'(0)] d\xi \leq C_N - (\hat{\gamma}/2)C_N^2 \) when \( N \) is large enough, to obtain

\[ J(\mu_N) \leq J(\tilde{\mu}) - \frac{1}{2} (\alpha \hat{\gamma} - \delta_N^2 A_1) C_N^2. \]

Similar to the previous case, we choose now \( N \) such that \( \delta_N < \sqrt{\alpha \hat{\gamma}}/A_1 \), which again results in a contradiction to the optimality of \( \tilde{\mu} \).

This, together with the optimality conditions obtained in Theorem 2, concludes the proof.

**Appendix D. Proof of Theorem 6**

For the total variation norm (i.e. \( \phi(z) = z \)), the Carathéodory lemma implies an upper bound on the number of atoms for some optimal solution \( \tilde{\mu} \) in some cases. In particular, we consider the special case of finitely supported \( \nu \), which is given by a sum of \( K \) Dirac delta measures. In this case, the space \( L^2(D, \nu) \) is finite dimensional, i.e. \( \dim L^2(D, \nu) = K \). To prove the Theorem 6 we need to show that any local solution of \((P_\phi)\) is atomic and its support consists of at most \( K \) points.

By the previous result we know that any locally optimal solution is representable as

\[ \tilde{\mu} = \sum_{n=1}^{N} \tilde{c}_n \delta_{\tilde{w}_n}, \quad |\tilde{c}_n| > 0, \quad \tilde{w}_n \in \Omega, \quad N \in \mathbb{N}. \]

Clearly,

\[ N \tilde{\mu} = \sum_{n=1}^{N} \tilde{c}_n N (\delta_{\tilde{w}_n}) = \sum_{n=1}^{N} \tilde{c}_n \sigma(\cdot, \tilde{w}_n). \]

Assume that \( N > K \). Then there exists a nontrivial vector \( \lambda \in \mathbb{R}^N \) such that

\[ \sum_{n=1}^{N} \lambda_n c_n \sigma(x_k, \tilde{w}_n) = 0 \quad \text{for all} \quad k = 1, \ldots, K \]

or, equivalently, \( \sum_{n=1}^{N} \lambda_n c_n \sigma(\cdot, \tilde{w}_n) = 0 \) in \( L^2(D, \nu) \). For any \( \tau \in \mathbb{R} \) we define

\[ \tilde{\mu}_\tau = \sum_{n=1}^{N} (1 + \tau \lambda_n) \tilde{c}_n \delta_{\tilde{w}_n}. \]

Note that \( N \tilde{\mu}_\tau = N \tilde{\mu} + \tau \sum_{n=1}^{K+1} \lambda_n c_n \sigma(\cdot, \tilde{w}_n) = N \tilde{\mu} \) in \( L^2(D, \nu) \) for any \( \tau \). Now, we assume also that \( \tau \) is small enough such that \( 1 + \lambda_n \tau \geq 0 \) for all \( n \) and turn our attention to the objective functional of \((P_\phi)\). Taking into account the previous argument, we have, for any \( \tau \neq 0 \), that

\[ J(\tilde{\mu}_\tau) - J(\tilde{\mu}) = \Phi(\tilde{\mu}_\tau) - \Phi(\tilde{\mu}) = \alpha \sum_{n=1}^{N} [\phi((1 + \tau \lambda_n) |\tilde{c}_n|) - \phi(|\tilde{c}_n|)] \]

\[ < \tau \alpha \sum_{n=1}^{N} \phi'(|\tilde{c}_n|) \lambda_n |\tilde{c}_n| = \tau \alpha \Phi'(\tilde{\mu}; \delta \mu). \]
where \( \delta \mu = \bar{\mu}_1 - \bar{\mu} \), taking into account that \( f(\bar{\mu}_r) = f(\bar{\mu}) \), the restrictions on \( \tau \) and the strict concavity of \( \phi \). Depending on the sign of \( \Phi'(\bar{\mu}; \delta \mu) \), we choose \( \tau > 0 \) or \( \tau < 0 \) sufficiently small such that

\[
J(\bar{\mu}_r) - J(\bar{\mu}) < 0,
\]

contradicting the local optimality of \( \bar{\mu} \).

\section*{Appendix E. Equivalences of outer- and all-weights penalizations}

Here, we consider networks with the ReLU activation function \( \sigma(\omega, x) = \max\{a \cdot x + b, 0\} \), and prove the equivalence of certain cost terms.

\textbf{Proposition 1.} Let \( p \geq 1 \) and \( q \geq 1 \) and \( r(\omega) \) be a 1-homogeneous functional:

\[
r(\tau \omega) = |\tau| r(\omega) \quad \text{for any } \omega = (a, b) \in \mathbb{R}^{d+1}.
\]

Then the problems

\begin{equation}
(20) \quad \min_{N \in \mathbb{N}, \{a_n, b_n, c_n\} \in \mathbb{R}^d \times \mathbb{R} \times \mathbb{R}} l(N_{\omega,c}; y) + \alpha \sum_{n=1}^{N} [(1/p)|c_n|^p + (1/q)r(\omega_n)^q],
\end{equation}

and

\[
\min_{\{c_n\} \in \mathbb{R}^N, \{\omega_n=(a_n,b_n): r(\omega_n) \leq (1/q)\}} l(N_{\omega,c}; y) + \frac{\alpha}{s} \sum_{n=1}^{N} |c_n|^{s/2},
\]

where \( s = 2pq/(q+p) = 2/(1/p + 1/q) \) is the harmonic mean of \( p \) and \( q \), are equivalent.

\textbf{Proof.} Note that due to positive homogeneity of the ReLU activation function \( \sigma \), we have

\[
N_{\omega,c} = N_{\omega_\tau,c_\tau} \quad \text{where } \omega_\tau = \tau \omega, c_\tau = c/\tau.
\]

It is easy to see that the problem (20) is equivalent to

\[
\min_{\{c_n\} \in \mathbb{R}^N, \{\omega_n=(a_n,b_n): r(\omega_n) \leq (1/q)\}, \tau_n \geq 0} l(N_{\omega,c}; y) + \alpha \sum_{n=1}^{N} [(1/p)|c_n|^p/\tau_n^p + (1/q)|\tau_n|^q].
\]

Moreover, since the first term does not depend on \( \tau \), we can compute \( \tau_n \) as the minimum of

\[
\tau \mapsto (1/p)|c_n|^p \tau^{-p} + (1/q)|\tau|^q.
\]

Differentiating with respect to \( \tau \), we obtain

\[
0 = -|c_n|^p \tau_n^{-p-1} + \tau_n^{-q-1} \leftrightarrow \tau_n^{q+p} = |c_n|^p \tau_n^{-q} \leftrightarrow \tau_n = |c_n|^{p/(q+p)}.
\]

Inserting the analytical solution for \( \tau_n \) into the cost term above, we obtain

\[
(1/p)|c_n|^{p-p^2/(q+p)} + (1/q)|c_n|^{qp/(q+p)} = (1/p + 1/q)|c_n|^{qp/(q+p)}
\]

which completes the proof. \(\square\)

As a corollary, by taking \( r(\omega) = \|\omega\|_p \) for \( \omega \in \mathbb{R}^{d+1} \), we get that solving the problem

\[
\min_{\{c_n\} \in \mathbb{R}^N, \{\omega_n=(a_n,b_n)\} \in (S^d_p)^N} l(N_{\omega,c}; y) + \alpha \sum_{n=1}^{N} |c_n|^{p/2},
\]

where \( S^d_p = \{(a, b) \in \mathbb{R}^{d+1} : \|a\|_p^p + \|b\|_p^p = 1\} \) is the unit \( p \)-sphere in \( \mathbb{R}^{d+1} \), is equivalent to solving the problem

\[
\min_{(a_n,b_n,c_n) \in \mathbb{R}^d \times \mathbb{R} \times \mathbb{R}} l(N_{\omega,c}; y) + \frac{\alpha}{p} \sum_{n=1}^{N} \left[ \|a_n\|_p^p + \|b_n\|_p^p + |c_n|^p \right].
\]
