How Infinitely Wide Neural Networks Can Benefit from Multi-task Learning
– an Exact Macroscopic Characterization

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Abstract
In practice, multi-task learning (through learning features shared among tasks) is an essential property of deep neural networks (NNs). While infinite-width limits of NNs can provide good intuition for their generalization behavior, the well-known infinite-width limits of NNs in the literature (e.g., neural tangent kernels) assume specific settings in which wide ReLU-NNs behave like shallow Gaussian Processes with a fixed kernel. Consequently, in such settings, these NNs lose their ability to benefit from multi-task learning in the infinite-width limit. In contrast, we prove that optimizing wide ReLU neural networks with at least one hidden layer using $\ell^2$-regularization on the parameters promotes multi-task learning due to representation-learning – also in the limiting regime where the network width tends to infinity. We present an exact quantitative characterization of this infinite width limit in an appropriate function space that neatly describes multi-task learning.

Keywords: Multi-task learning, Deep Learning, Neural Network Theory, Regularization, Bayesian Neural Networks, Overparametrized Neural Networks, infinite width limit

1. Introduction

One key difference of deep learning models, such as deep neural networks (NNs), in contrast to shallow learning models, such as Gaussian Processes (GPs)\(^1\), is that deep learning methods are capable of benefiting from multi-task learning. Standard deep NNs with multi-dimensional output share the same weights in the hidden layers, and only the last layer contains different weights for different outputs (or tasks). This shared representation learned by the hidden layers (representation learning, feature learning or metric learning) can be seen as the source for multi-task learning and transfer learning (Caruana et al., 1997). In various applications, training with high-dimensional output has outperformed separate training of the individuals tasks (Caruana et al., 1997; Ruder, 2017; Fifty et al., 2021; Tran

\(^1\). Within this paper “GPs” always refer to shallow GPs where a prior GP has a fixed kernel that is not learned from the data.
et al., 2021; Aribandi et al., 2021). Especially if the available data for some tasks is limited, these tasks greatly benefit from the other tasks in terms of improved generalization.

Due to the success of deep NNs, there is high interest in studying their generalization behavior (macroscopically, i.e., the inductive bias in function space). In the case of infinite-width neural networks Jacot et al. (2018); Neal (1996); Lee et al. (2018) have shown that in specific settings, deep NNs are equivalent to shallow GPs. Those however cannot benefit from multi-task learning, since their outputs are completely independent. The authors are aware of this problem and Neal (1996) suggests to define a specific prior for the weights to circumvent it. Roberts et al. (2021); Yaida (2021) in contrast suggest to use infinite depth NNs, with a fixed ratio of width and depth to circumvent this problem.

In contrast, we prove that ReLU-neural networks perfectly optimized under $\ell^2$-regularization can already (also for infinite width and finite depth) benefit from multi-task learning due to representation learning. We deduce this ability by giving an exact quantitative macroscopic characterization of the (generalization) behavior of wide $\ell^2$-regularized NNs.

1.1 Related Work

In concurrent work, Yang and Hu (2021) show that in specific settings (different from those studied in Jacot et al. (2018)) gradient descent enables feature learning also in the infinite width limit. This strongly suggests that in these settings, NNs can benefit from multi-task learning. However, Yang and Hu (2021) do not provide an easy-to-interpret characterization of the inductive bias in function space for those settings where feature learning is possible (Yang and Hu, 2021, Remark 3.11).

Chizat and Bach (2020); Neyshabur et al. (2014); Ongie et al. (2019); Savarese et al. (2019) also provide infinite-width limits of NNs, that do not share the generalization behavior of Gaussian Processes. However, they do not discuss multi-task learning and they do not consider NNs with multiple hidden layers (with nonlinear activation function). Moreover, none of these papers provide a precise theorem showing that the set of finite width networks minimizing the $\ell^2$-regularized loss converge to the set of minimizers of the continuous optimization problem in a certain function space equipped with a certain topology in the limit width to infinity.

Neal (1996); Jacot et al. (2018); Heiss et al. (2019); Williams et al. (2019); Lee et al. (2018) study settings in which NNs converge to GPs in the infinite width limit. Thus, in these settings the infinitely wide NNs cannot benefit from multi-task learning.

Agrawal et al. (2020) show that wide Bayesian Neural Networks (BNNs) with narrow bottleneck layers are deep Gaussian Processes. However, these deep GPs only deviate from shallow GPs due to narrow bottleneck layers, while our $\ell_2$-regularized wide NNs do not need any finite bottleneck layer in order to deviate from shallow GPs or in order to benefit from multi-task learning (see Proposition 10).

Independently and concurrently, Parhi and Nowak (2022) study the macroscopic behavior of deep neural networks with regularization similar to $\ell^2$-regularization. In contrast to their work, we derive an exact characterization of the infinite width-limit of $\ell_2$-regularized NNs (with and without regularization of the biases). For their choice of regularization on parameter space, they obtain in (Parhi and Nowak, 2022, Therorem 3.2 and Corollary 4.3) a similar regularization functional on function space as we do in Theorem 5. However, their
slightly different regularization prevents their model from benefiting from multi-task learning in the case of one hidden layer (as could be proven analogously to Proposition 19). We think that multi-task learning is one of the most exciting properties of our inductive bias, especially compared to infinite wide Gaussian BNNs. This is a main focus of our paper, which is not treated in Parhi and Nowak (2022). Moreover, we employ different proving techniques and provide different perspectives on the function space characterization: while their infinite width limit contains fractional derivatives and Radon transforms, our formulation of the infinite width limit is formulated as a natural extension of generalized additive models as we explain on page 8.

1.2 Contribution

- We give an exact characterization of the (out-of-sample) behavior of wide \( \ell^2 \)-regularized deep ReLU-NNs in function space with arbitrary input and output dimensions. This result also holds for NNs with more than one hidden layer. (Section 3)

- We show that wide \( \ell^2 \)-regularized NNs can benefit from multi-task learning. (Section 4)

- We explain a paradoxical contrast between infinitely wide \( \ell^2 \)-regularized NNs and infinitely wide Gaussian Bayesian Neural Networks (BNNs): While for finite width, the optimal \( \ell^2 \)-regularized NN is exactly the max a posteriori (MAP) on the parameter space of a Gaussian BNN, this does not hold anymore in the infinite width limit on function space (Section 5).

2. Setting and Notation

We denote fully connected, shallow NNs (i.e., NNs with one hidden layer) with ReLU activation as a “stack”. A fully connected, deep, stacked neural network \( \mathcal{NN}_\theta \) is then given as concatenation of stacks and an element-wise activation function \( \tilde{\sigma} \) (not necessarily ReLU as for the hidden layers of a stack),

\[
\mathcal{NN}_\theta := \ell^{-1} \circ \mathcal{NN}^{(#\text{stacks})} \circ \tilde{\sigma} \circ \mathcal{NN}^{(#\text{stacks}-1)} \circ \cdots \circ \tilde{\sigma} \circ \mathcal{NN}^{(1)},
\]

where \( \ell^{-1} \) is a Lipschitz continuous function (e.g. identity or soft-max which corresponds to the inverse of a link function in classical statistics) and \( \tilde{\sigma} \) is any Lipschitz continuous activation function. Throughout the paper, we focus on stacks as in Definition 1; see Appendix A for results on different stacks.

**Definition 1 (Deep Stacked Neural Network).** A deep stacked neural network is defined as in (1) with stacks \( \mathcal{NN}_{\theta(j)}^{(j)} : \mathbb{R}^{d_{j-1}} \to \mathbb{R}^{d_j} \) s.t.

\[
\forall x \in \mathbb{R}^{d_{j-1}} : \quad \mathcal{NN}_{\theta(j)}^{(j)}(x) = \sum_{k=1}^{n_j} w_k^{(j)} \max \left( 0, t_k^{(j)} + \langle v_k^{(j)}, x \rangle \right) + c^{(j)},
\]

with
• number of hidden neurons \( n_j \in \mathbb{N} \) in the \( j \)-th stack, not necessarily equal dimensions \( d_n = d_0, \ldots, d_j, \ldots, d_{\# \text{stacks}} = d_{\text{out}} \in \mathbb{N} \) that we call bottleneck dimensions and ReLU activation function (we collect these numbers in \( n = (n_j)_{j \in \{1, \ldots, \# \text{stacks}\}} \) and \( d = (d_j)_{j \in \{0, \ldots, \# \text{stacks}\}} \))

- weights \( v_k^{(j)} \in \mathbb{R}^{d_{j-1}}, w_k^{(j)} \in \mathbb{R}^{d_j}, k = 1, \ldots, n_j \) and
- biases \( c^{(j)} \in \mathbb{R}^{d_j}, b_k^{(j)} \in \mathbb{R}, k = 1, \ldots, n_j \).

Weights and biases are collected in \( \theta = (\theta^{(j)})_{j \in \{1, \ldots, \# \text{stacks}\}} \) with
\[
\theta^{(j)} := (v^{(j)}, b^{(j)}, w^{(j)}, c^{(j)}) \in \Theta^{(j)} := \mathbb{R}^{n_{j} \times d_{j-1}} \times \mathbb{R}^{n_{j}} \times \mathbb{R}^{d_{j}} \times \mathbb{R}^{n_{j}} \times \mathbb{R}^{d_{j}}.
\]

- All network parameters are then collected in
\[
\Theta := \Theta_{(n, d)} := \Theta^{(1)} \times \cdots \times \Theta^{(\# \text{stacks})}.
\]

![Figure 1: Schematic representation of a Deep Stacked NN from Definition 1 with \#stacks = 3 stacks, where we show the activation functions and the dimensions of the layers of this feed forward NN.](image)

Within this paper, for simplicity, we assume that NNs are trained to perform \( d_{\text{out}} \) one-dimensional regression tasks with quadratic training loss, where the \( k \)-th task learns from a subset of training data with indices \( I_k \subset \{1, \ldots, N\} = I_1 \cup \cdots \cup I_{d_{\text{out}}}, \) i.e.,

\[
L\left(\hat{f}\right) := \sum_{k=1}^{d_{\text{out}}} L_k(\hat{f}),
\]

\[
L_k(\hat{f}) := \sum_{i \in I_k} (\hat{f}_k(x_i^{\text{train}}) - y_i^{\text{train}})^2.
\]
Remark 2. Our main Theorem 5 also holds true for other losses of the form $L(\hat{f}) = \sum_{i=1}^{N} l_i \left( \hat{f}(x_{i}^{\text{train}}), y_{i}^{\text{train}} \right)$, with continuous loss-functions $l_i : \ell^{-1}(\mathbb{R}^{d_{\text{out}}}) \times \ell^{-1}(\mathbb{R}^{d_{\text{out}}}) \to \mathbb{R}$ (e.g. classification). While in (3b), it is $y_{i}^{\text{train}} \in \mathbb{R}$, within this remark, we have $y_{i}^{\text{train}} \in \ell^{-1}(\mathbb{R}^{d_{\text{out}}})$. Moreover, $l_i$ can ignore different dimensions for different indices $i$, depending on which output-labels are available for certain tasks at certain input points $x_{i}^{\text{train}}$.

2.1 Definition of Multi-task Learning

The idea of multi-task learning (Caruana et al., 1997) is that when training a model to perform multiple tasks simultaneously, the joint training induces a transfer of knowledge among the model’s outputs to improve each others generalization.

Definition 3. We define a model $\mathcal{M}$ as a map that gets as input a loss functional $L$ in the form of (3) (including training data) and gives as output a set of functions $\mathcal{M}(L)$. (E.g. $\mathcal{M}(L) := \arg\min_{f} (L(f) + \lambda P(f))$ for some regularization functional $P$).

Definition 4. We say a model $\mathcal{M}$ cannot benefit from multi-task learning if for every $k$ and for every loss $L$ in the form of (3),

$$(\mathcal{M}(L))_k = (\mathcal{M}(L_k))_k,$$

where for any set $A$, we define $(A)_k := \{ a_k : a \in A \}$.

In simple words, Definition 4 says that a model cannot benefit from multi-task learning, if removing all the data for other tasks than task $k$ from the training set does not influence the behavior of the model on the task $k$.

3. Characterizing the Learned Function

In this paper we focus on understanding deep stacked ReLU-NNs (Definition 1) optimized with $\ell^2$-regularization (weight decay), i.e.,

$$\mathcal{N}\mathcal{N}_{\theta^*,\lambda} \text{ with } \theta^*,\lambda \in \arg\min_{\theta} \left( L(\mathcal{N}\mathcal{N}_{\theta}) + \lambda \|\theta\|_2^2 \right),$$

(4)

for the case of large numbers of $n_j$ for $j = 1, \ldots, \#\text{stacks}$. First, we formulate a characterization in function space for networks where the width of every second layer stays finite (i.e., $d_j \in \mathbb{N}$ stay fixed) and only the width of the other layers goes to infinity (i.e., $n \to \infty$). We use $\lim_{n \to \infty}$ as a shorthand notation for $\lim_{(n_1, \ldots, n_{\#\text{stacks}}) \to (\infty, \ldots, \infty)}$. Then, we proceed to derive the theory for the case where the width of every hidden layer goes to infinity (i.e., $n_j, d_j \to \infty$).

The goal of this section is to formulate $\lim_{n \to \infty} \mathcal{N}\mathcal{N}_{\theta^*,\lambda}$ as the solution of an optimization problem of the form

$$f^*,\lambda \in \arg\min_{f \in \mathcal{F}} \left( L(f) + \lambda P(f) \right)$$

(5)

for an appropriate function space $\mathcal{F}$ and regularization functional $P : \mathcal{F} \to \mathbb{R}_{\geq 0}$ to better understand how the solution of (4) behaves in function space in the case of many hidden neurons.

2. More discussion on the benefits of multi-task learning can be found in Appendix E.
The form of the regularization functional $P$ depends on the architecture of the network. As we will prove in Theorem 5, for a wide deep stacked NN as in Definition 1 the corresponding functional is given as

$$P(f) = \min_{(h_1, \ldots, h_{\#\text{stacks}}), \text{s.t. } f = e^{-1} o_{\#\text{stacks}} o_{\cdots} o_{\#\text{stacks}}} (P_1(h_1) + P_2(h_2) + \cdots + P_{\#\text{stacks}}(h_{\#\text{stacks}})),$$

where $P_j$ (and $T_j$) are given with slight abuse of notation (treating distributions as if they were functions)\(^3\) as

$$P_j(h_j) := \min_{\varphi \in T_j, c \in \mathbb{R}^{d_j}} \left( 2 \int_{S^{d_j-1}} \int_{\mathbb{R}} \left\| \frac{\partial^2}{\partial r^2} \varphi_s(r) \right\|_2^2 dr ds + 2\rho(\|c\|_2) \right),$$

where

$$T_j := \left\{ \varphi = (\varphi_s)_{s \in S^{d_j-1}} \mid \forall s \in S^{d_j-1}, \varphi_s : \mathbb{R} \to \mathbb{R}^{d_j}, \lim_{r \to -\infty} \varphi_s(r) = 0 = \lim_{r \to +\infty} \frac{\partial}{\partial r} \varphi_s(r) \right\}$$

handles a boundary condition, $S^{d-1}$ denotes the $(d - 1)$-dimensional unit sphere, $g(r) = \frac{1}{\sqrt{r^2 + 1}}$ denotes a weight function, and where $\rho(r) = \begin{cases} \frac{r^2}{2}, & \text{if } |r| \leq 1 \\ |r| - 1/2, & \text{else} \end{cases}$ is the Huber-loss.

Neither the solutions $\mathcal{N} \mathcal{N}_{\gamma^{*}, \lambda}$ to eq. (4) nor the solutions $f^{*, \lambda}$ to eq. (5) have to be unique. But even in cases where they are not unique, the set of solutions to eq. (4) converges to the set of solutions to eq. (5) as $n \to \infty$.

**Theorem 5.** Using the definitions from Sections 2 and 3, it holds that for a sufficiently large\(^4,5\) number of neurons $n$ every solution $\mathcal{N} \mathcal{N}_{\gamma^{*}, \lambda}$ to eq. (4) is a solution to eq. (5) too, i.e.,

$$\mathcal{N} \mathcal{N}_{\gamma^{*}, \lambda} \in \arg \min_{f \in \mathcal{F}} (L(f) + \lambda P(f)).$$

Furthermore, it holds that for every compact $K \subset \mathbb{R}^{d_{\text{in}}}, \forall \epsilon \in \mathbb{R}_{>0}$:

$$\forall f^{*, \lambda} \in \arg \min_{f \in \mathcal{F}} (L(f) + \lambda P(f)) : \exists \bar{n} \in \mathbb{N}^{\#\text{stacks}} : \forall n \geq \bar{n} :$$

$$\exists \theta^{*, \lambda} \in \arg \min_{\theta \in \Theta(n, d)} \left( L(\mathcal{N} \mathcal{N}_{\theta}) + \lambda \|\theta\|_2^2 \right) : \sup_{x \in K} \|f^{*, \lambda}(x) - \mathcal{N} \mathcal{N}_{\gamma^{*}, \lambda}(x)\|_\infty < \epsilon.$$  

---

3. To be mathematically precise, the “function” $\varphi : s \mapsto \varphi_s$ does not have to be a classical function, but can also be a distribution. First derivatives are understood in a weak sense and second derivatives are distributional. See Appendix B for different formulations of $P_j$ in precise mathematical notation.
4. In Appendix C we discuss explicit bounds on how many neurons are sufficient for the result to hold.
5. Note that $\mathcal{N} \mathcal{N}_{\gamma}$ depends on $n$ since it refers to a network with $n_j$ neurons in the corresponding layers. Moreover, $n \geq \bar{n}$ is always understood component-wise. By “sufficiently large $n$”, we mean that every $n_j$ has to be sufficiently large.
Proof We prove the theorem in Appendix F.3, while proving all necessary lemmas in Appendix F. Some basic intuition for the proof can be obtained from Lemma 31 for finite-width networks, from Lemma 32 for (8), and from Lemma 33 for (9).

Moreover, we can describe the limiting regime $d_j \to \infty$ for $j \in \{1, \ldots, \#\text{stacks} - 1\}$, i.e., the regime of letting the width of all hidden layers go to infinity.

Corollary 6. Let $\tilde{\sigma}$ be ReLU or linear. For every number of training data points $N$, there exist $n^* \in \mathbb{N}^{\#\text{stacks}}$ and $d^* \in \mathbb{N}^{\#\text{stacks} - 1}$ such that in the limit where all layers tend to infinity, all solutions are characterized as

$$ S := \lim_{(n,d) \to \infty} \left\{ \mathcal{N} \mathcal{N}_{\theta^*,\lambda} : \theta^*,\lambda \in \arg\min_{\theta \in \Theta_{(n,d)}} \left( L(\mathcal{N} \mathcal{N}_{\theta}) + \lambda \|\theta\|_2^2 \right) \right\} $$

$$ = \bigcup_{(n,d) \geq (n^*,d^*)} \left\{ \mathcal{N} \mathcal{N}_{\theta^*,\lambda} : \theta^*,\lambda \in \arg\min_{\theta \in \Theta_{(n,d)}} \left( L(\mathcal{N} \mathcal{N}_{\theta}) + \lambda \|\theta\|_2^2 \right) \right\} $$

$$ = \lim_{d \to \infty} \arg\min_{f \in \mathcal{F}} (L(f) + \lambda P(d)(f)) $$

$$ = \bigcup_{d \geq d^*} \arg\min_{f \in \mathcal{F}} (L(f) + \lambda P(d)(f)), $$

(10a, 10b, 10c, 10d)

where $P(d)$ denotes $P$ with bottleneck-dimensions $d_j$, and the closure $(\overline{\cdot})$ is understood with respect to the topology of locally uniform convergence in function space.)

Moreover, there exists a solution in $f^*,\lambda \in S$ that can be represented as a neural network $\mathcal{N} \mathcal{N}_{\theta^*,\lambda} = f^*,\lambda$ with dimensions $n^*$ and $d^*$. This network satisfies

$$ \theta^*,\lambda \in \arg\min_{\theta \in \Theta_{(n^*,d^*)}} \left( L(\mathcal{N} \mathcal{N}_{\theta}) + \lambda \|\theta\|_2^2 \right) $$

and

$$ \mathcal{N} \mathcal{N}_{\theta^*,\lambda} \in \arg\min_{f \in \mathcal{F}} (L(f) + \lambda P(d^*)(f)) . $$

Proof See Appendix F.4 for the proof and different points of view on Corollary 6.

Remark 7 (No regularization on biases). If one does not regularize the biases but only the weights, one obtains given the same abuse of notation as above (treating distributions as if they were functions)

$$ P_j(h_j) := \min_{\varphi \in \mathcal{T}_j, c \in \mathbb{R}^{d_j}} \left( 2 \int_{S^{d_{j-1}}} \int_{\mathbb{R}} \varphi_s(r)^2 dr ds \right), $$

(11)

6. Note that $\mathcal{N} \mathcal{N}_i$ depends on $d$ and $n$ since it refers to a network with $d_j$ and $n_j$ neurons in the corresponding layers. Moreover, $d \geq d^*$ is always understood component-wise, i.e., $\forall j \in \{1, \ldots, \#\text{stacks} - 1\}$: $d_j \geq d^*_j$, while $d_0 = d_{in}$ and $d_{\#\text{stacks}} = d_{out}$ are considered constant throughout the paper.

7. $P$ always depends on the bottleneck-dimensions $d$, but by writing $P(d)$ we make the dependency on $d$ more explicit at this point.
where $T_j$ simplifies to

$$T_j := \{ \varphi = (\varphi_s)_{s \in S^{d_j-1}} : \forall s \in S^{d_j-1} : \varphi_s : \mathbb{R} \rightarrow \mathbb{R}^{d_j}, \lim_{r \rightarrow -\infty} \frac{\partial}{\partial r} \varphi_s(r) = 0 \}. $$

In this case, and if $d_j = 1$, Savarese et al. (2019) provides a simpler reformulation of $P_j$ from eq. (11), i.e., given the same abuse of notation as above (treating distributions as if they were functions)

$$P_j(h_j) := \min_{\varphi = (\varphi_s)_{s \in S^{d_j-1}}, c \in \mathbb{R}^{d_j}} \left( 2 \int_{S^{d_j-1}} \max \left( \int_{\mathbb{R}} \| \varphi_s(r)'' \|_2^2 \, dr, \lim_{r \rightarrow -\infty} \varphi_s(r)' + \lim_{r \rightarrow +\infty} \varphi_s(r)' \right) \, ds \right). \quad (12)$$

Equation (12) can be particularly intuitively interpreted as a generalized additive model (GAM), where

1. instead of only using the coordinate directions $(e_1, \ldots, e_{d_j})$, all possible directions $s \in S^{d_j-1}$ are used,
2. instead of the typical smoothing spline regularization $\int_{\mathbb{R}} \| \varphi_s(r)'' \|_2^2 \, dr$, an $L^1$-regularization $\int_{\mathbb{R}} \| \varphi_s(r)'' \|_2 \, dr$ (for $d_j = 1$) is applied and
3. the first derivative additionally gets regularized.

Equation (11) is a natural extension of Equation (12) to higher dimensional outputs. Equation (7) imposes a qualitatively similar regularization on the learned function as eq. (11), with the exception that also the zeroth derivative gets slightly regularized and the second derivative gets penalized more strongly far away from the origin $0 \in \mathbb{R}^{d_{in}}$ than close to it. However, even if one does not regularize the biases explicitly, the obtained functions will in practice have some qualitative aspects of eq. (7), since gradient descent initialized close to zero can implicitly regularize the bias too.

**Remark 8** (Random hidden layers Heiss et al. (2019)). Comparing eq. (7) to Heiss et al. (2019), where the first-layer weights and biases $v$ and $b$ are not trained but chosen randomly, one can see that the main difference is that the integrand $\frac{\| \varphi_s(r)'' \|_2}{g(r)}$ replaced the integrand $\| \varphi_s(r)'' \|_2$ (lifted to multi-dimensional in- and output), i.e., the integrand in eq. (7) takes the square root of the numerator and also the weighting function $g$ does not depend on the distribution of $v$ and $b$ anymore (since $v$ and $b$ are trainable now too). If one still sampled $v^{(j)}$ and $b^{(j)}$ randomly without training them, one could plug in the corresponding regularizing functional for $P_j$ in eq. (6).

4. Discussion of Multi-task Learning

4.1 Multi-task Learning for Single Stacks and GPs

Already for neural networks with a single hidden layer one can see that the regularizing functional from the previous section induces multi-task learning. In this case, we have
The main idea of the proof is the following: Squaring the Euclidean norm cancels the square root, adjustments in this second derivative \( \varphi_s(r)'' \) have a much lower effect on \( \| \varphi_s(r)'' \|_2 \) for this direction \( s \) than for others. In other words, the marginal regularization costs for second derivative of any other \( \hat{k} \)th component of \( \varphi_s(r) \) are much smaller for these directions \( s \) than for other directions, because of the strict concavity of the square root-function.

Consequently, the output \( f_k \) trained to perform the \( \hat{k} \)th task will prefer functions which mainly vary in those directions in which also the other outputs that were trained to perform other tasks vary a lot. In this way, different outputs can learn from each other which directions tend to be more important. Note that the model \( \mathcal{M}(L) = \arg \min_{f \in F} L(f) + \lambda P(f) \) is still universal and thus is also able to learn functions \( f \) where different components \( f_k \) vary in very different directions if there is enough evidence in the data (i.e., in \( L \)) to do so.

Already for one-dimensional input, the square-root can lead to multi-task learning: If some outputs \( f_k \) have stronger second derivative \( |f_k''(x)| \) or even kinks at some positions \( x \), other outputs \( f_k \) will also prefer to have stronger second derivative or even kinks at these positions \( x \).

In line with Remark 8 and the following proposition, shallow NNs with random first layer, and where only the terminal layer is trained are not capable of multi-task learning.

**Proposition 9.** The model \( \mathcal{M}^{L^2}(L) := \arg \min_f \left( L(f) + \lambda \int \| f''(x) \|_2^2 dx \right) \) is not capable of benefiting from multi-task learning (see Definition 4).

**Proof** The main idea of the proof is the following: Squaring the Euclidean norm cancels the square root that connects the outputs to each other. Without the square-root, learning a separate function \( f_k \) for each task would result exactly in the same functions \( f_k \) as training them all together, since

\[
\int \| f''(x) \|_2^2 dx = \int \sum_{k=1}^{d_{out}} \left( f_k''(x) \right)^2 dx = \sum_{k=1}^{d_{out}} \int \left( f_k''(x) \right)^2 dx.
\]

8. We say that \( f_k \) “varies” a lot in a direction \( s \), when changing the input \( x \) in the direction of \( s \) the output \( f_k(x) \) changes a lot, possibly very non-linearly with very strong second derivative in this direction \( s \). We say that \( f_k \) does almost not vary in other directions when changing the input in other directions has little influence on the output, i.e., the output in these other directions is mostly linear and very flat (i.e., it has low first derivative and very low second derivative in these directions).

9. The marginal costs \( \frac{\partial}{\partial a} \| a \|_2 \) of increasing one component of a vector \( a \) are inversely proportional to the euclidean norm of all the components of a vector. E.g., if \( \varphi_s(r)'' = (0, 100, 100)^T \) then replacing it by \((1, 100, 100)^T \) increases \( \| \varphi_s(r)'' \|_2 \) by only \( \| (1, 100, 100)^T \|_2 - \| (0, 100, 100)^T \|_2 \approx 0.0035 \) but if \( \varphi_s(r)'' = (0, 0, 0)^T \), replacing it by \((1, 0, 0)^T \) increases \( \| \varphi_s(r)'' \|_2 \) by \( \| (1, 100, 100)^T \|_2 - \| (0, 0, 0)^T \|_2 = 1. \)
Therefore,
\[
L(f) + \lambda \int \left\| f''(x) \right\|_2^2 \, dx = \sum_{k=1}^{d_{\text{out}}} \left( L_k(f) + \lambda \int \left( f_k''(x) \right)^2 \, dx \right),
\]

\[
\left( \mathcal{M}^{L^2}(L) \right)_k = \left( \text{arg min}_f \left( L(f) + \lambda \int \left\| f''(x) \right\|_2^2 \, dx \right) \right)_k
\]

\[
= \text{arg min}_{f_k} \left( \sum_{i \in I_k} (f_k(x_i^{\text{train}}) - y_i^{\text{train}})^2 + \lambda \int \left( f_k''(x) \right)^2 \, dx \right) = \left( \mathcal{M}^{L^2}(L_k) \right)_k.
\]

(Note that all other components of \( \mathcal{M}^{L^2}(L_k) \) are the zero function.)

By contrast, this is not the case if the square-root appears in the regularizing functional, since
\[
\int \left\| f''(x) \right\|_2^2 \, dx = \int \sqrt{\sum_{k=1}^{d_{\text{out}}} (f_k''(x))^2} \, dx
\]
is in general not equal to \( \sum_{k=1}^{d_{\text{out}}} f_k''(x) \, dx \). Therefore, we see that already a single hidden layer is sufficient to get the effect of multi-task learning for \( \lim_{\lambda \to 0^+} \mathcal{NN}_{f,\lambda} \) when \( \mathcal{NN}_{f,\lambda} \) are trained with \( \ell^2 \)-regularization.

**Proposition 10.** The model \( \mathcal{M}^P(L) := \arg \min_f (L(f) + \lambda P(f)) \), with \( P = P_1 \) from eq. (7), induces multi-task learning (without the need for any finite bottleneck layer).

**Proof** Consider \( L \) as in (3) with \( d_{\text{out}} = 2 \) tasks. Let training data be given as

\[
((x_{1,1}^{\text{train}}, x_{1,2}^{\text{train}}, y_1^{\text{train}}) = (2, 2, 2),
((x_{2,1}^{\text{train}}, x_{2,2}^{\text{train}}, y_2^{\text{train}}) = (-2, 2, 2),
((x_{3,1}^{\text{train}}, x_{3,2}^{\text{train}}, y_3^{\text{train}}) = (-2, -2, -2),
((x_{4,1}^{\text{train}}, x_{4,2}^{\text{train}}, y_4^{\text{train}}) = (2, -2, -2),
((x_{5,1}^{\text{train}}, x_{5,2}^{\text{train}}, y_5^{\text{train}}) = (0, -3, -3),
((x_{6,1}^{\text{train}}, x_{6,2}^{\text{train}}, y_6^{\text{train}}) = (0, 3, 3),
\]
for \( I_1 = \{ 1, 2, 3, 4, 5, 6 \} \) and

\[
((x_{7,1}^{\text{train}}, x_{7,2}^{\text{train}}, y_7^{\text{train}}) = (1, 2, 1),
((x_{8,1}^{\text{train}}, x_{8,2}^{\text{train}}, y_8^{\text{train}}) = (-1, -2, -1),
((x_{9,1}^{\text{train}}, x_{9,2}^{\text{train}}, y_9^{\text{train}}) = (2, 4, 2),
((x_{10,1}^{\text{train}}, x_{10,2}^{\text{train}}, y_{10}^{\text{train}}) = (-2, -4, -2),
\]
for \( I_2 = \{ 7, 8, 9, 10 \} \). Then, one can calculate the sets of minimizers as

\[
\left\{ \left( f_1 : (x_1, x_2) \mapsto x_2, f_2 : (x_1, x_2) \mapsto \frac{x_2}{2} \right) \right\} = \lim_{\lambda \to 0^+} \arg \min_{f \in \mathcal{F}} (L(f) + \lambda P(f)),
\]

\[
\left\{ \left( \tilde{f}_1 \equiv 0, \tilde{f}_2 : (x_1, x_2) \mapsto \frac{x_1 + 2x_2}{5} \right) \right\} = \lim_{\lambda \to 0^+} \arg \min_{f \in \mathcal{F}} (L_2(f) + \lambda P(f)).
\]

10
Therefore, (because of continuity arguments) for small values of $\lambda$,

$$(\mathcal{M}^P(L))_2 \neq (\mathcal{M}^P(L_1))_2.$$  

Intuitively speaking, the second output has learned from the training of the first output that $x_2$ is a more important feature than $x_1$. This is one simple example that is sufficient to prove Proposition 10 in the sense of Definition 4.

Crucially however, the limits corresponding to exactly the same NN-architecture that are discussed in Jacot et al. (2018); Neal (1996); Lee et al. (2018) result in a GP-regression with absolutely no multi-task learning benefits, because of the fixed, data-independent kernel. The prior GPs considered there have completely independent outputs. Consequently, calculating the max a posteriori (MAP) of all outputs jointly results in exactly the same function as if calculating the MAP for every output separately. Thus, it is mathematically impossible that any transfer of knowledge from one task to another can happen, as we note in the following proposition.

**Proposition 11.** Let $\mathcal{M}^{GP}(L) := \arg \min_f \left( L(f) + \|f\|^2_{RKHS} \right)$, where $\| \cdot \|_{RKHS}$ is the reproducing kernel Hilbert space norm of one of the kernels suggested in Jacot et al. (2018); Neal (1996); Lee et al. (2018) or any other kernel with independent outputs, then $\mathcal{M}^{GP}$ cannot benefit from multi-task learning according to Definition 4. ($\mathcal{M}^{GP}(L)$ corresponds to the MAP with respect to the GP prior by interpreting $L$ as the log-likelihood modulo a constant, which is also equal to the mean a posteriori.)

**Proof** Trivial, because then $\| \cdot \|_{RKHS}$ splits into a sum such as in the proof of Proposition 9.

### 4.2 Multi-task Learning for Deep Stacked NNs

Increasing the number of stacks $\#\text{stacks} > 1$ further strengthens the multi-task learning effects, because not only does the square-root in each $P_j$ enforce multi-task learning for each $h_j$, but all the functions $h_j$ for $j \in \{1, \ldots, \#\text{stacks} - 1\}$ are shared among all the outputs as well. Thus, $H := \tilde{\sigma} \circ h_{\#\text{stacks} - 1} \circ \cdots \circ \tilde{\sigma} \circ h_1$ has to be learned to transform inputs $x$ into a vector representation $H(x)$ that allows jointly for all functions $(\ell \circ f)_k$ to be nicely representable as $h_{\#\text{stacks},k} \circ H$ such that $P_{\#\text{stacks}}(h_{\#\text{stacks}})$ is not too large. In Appendix D, we visualize multi-task learning of a deep stacked NN on two simple examples.

The multi-task learning behavior enforced by the inductive bias $P$ of deep NNs (i.e., $\#\text{stacks} > 1$) is clearly different from the inductive bias $P_1$ of a shallow neural network (i.e., $\#\text{stacks} = 1$). Firstly, deep NNs allow to share arbitrarily complicated features among different tasks, and the outputs can approximate any continuous task-specific function in terms of these features (see Appendix E.3). Secondly, deep NNs allow to share different levels of abstractions among different subgroups of tasks (see Appendix E.4).

---

10. The MAP of a GP is always interpreted in a Cameron-Martin sense (Cameron and Martin, 1944) in this paper. This is equivalent to taking the point-wise MAP for posterior marginals at every single point.
5. Connection to Bayesian Neural Networks (BNNs)

The solution $\theta^{*\lambda}$ of eq. (4) is the max a posteriori (MAP) on parameter space of a Gaussian BNN, when the ratio of Gaussian i.i.d. data noise variance and the variance of the Gaussian i.i.d. prior of parameters is $\lambda$.

In this paper we study the limit in function space of $\mathcal{NN}_{\theta^{*\lambda}}$ as the number of hidden neurons goes to infinity (see Theorem 5). We even show that resulting function $\mathcal{NN}_{\theta^{*\lambda}} = \lim_{n \to \infty} \mathcal{NN}_{\theta^{*\lambda}}$ already reaches the limit when $n_j \geq n_j^*$ for all $j \in \{1, \ldots, \#\text{stacks}\}$, where $n_j^* \leq d_j \cdot N + 1$ (see Corollary 6). From this we derive that arbitrarily wide $\mathcal{NN}_{\theta^{*\lambda}}$ can benefit from multi-task learning by representation-learning (even if $n_j \gg d_j \cdot N$ and even a single hidden layer is sufficient, i.e., for $\#\text{stacks} \geq 1$).

In contrast, the MAP of a GP is not capable of benefiting from multi-task learning or representation learning because of the fixed data-independent kernel (see Proposition 11 and its discussion).

This might sound contradicting since an insufficient summary of Neal (1996) could be naively formulated as “Infinitely wide Gaussian BNNs are equivalent to shallow GPs”.

The solution to this paradox is that exchanging the order of taking the MAP, going from parameter space to function space, and taking the limit of width $n$ to infinity vastly changes the behavior of the obtained function: Neal (1996) shows that the prior of a very wide BNN is similar to a GP. However, Neal (1996) never claims that the MAP $\theta^{*\lambda}$ on the parameter space of a very wide BNN is, as a function $\mathcal{NN}_{\theta^{*\lambda}}$, close to the MAP of the corresponding GP. In fact, we show in Theorem 5 and propositions 10 and 11 that a sufficiently wide $\mathcal{NN}_{\theta^{*\lambda}}$ as given in eq. (4) is typically not close at all to the MAP of the corresponding GP. This result is important since the gradient descent-based algorithms typically used in practice aim to approximate eq. (4), and thus solutions found in practice are not accurately described by the GP’s MAP.

5.1 Is Poor Man’s Bayes Better Than Optimal Bayes?

Mathematically, in a correct Bayesian regression setting, the mean a posteriori on function space is the best possible model in terms of expected mean squared error (MSE) on a test set. The MAP (on the parameter space) is not optimal in this sense, but it can be cheaper to compute and is often a reasonable approximation of the mean a posteriori. Therefore, the MAP is called “poor man’s Bayes”.

One consequence of our result is the following plot-twist: One would expect the exact mean a posteriori of a wide BNN (given by $\mathcal{M}^{\text{GP}}(L)$) to perform even better in terms of expected test MSE than its poor approximation $\mathcal{NN}_{\theta^{*\lambda}}$ (where $\theta^{*\lambda}$ is the MAP on the parameter space). However, our results suggest that $\mathcal{NN}_{\theta^{*\lambda}}$ can generalize better than $\mathcal{M}^{\text{GP}}(L)$: While Proposition 10 shows that $\mathcal{NN}_{\theta^{*\lambda}}$ allows for multi-task learning, $\mathcal{M}^{\text{GP}}(L)$ does not (Proposition 11). Paradoxically, this suggests that the poor man’s approximation has lower expected test MSE than the theoretical optimum.

The Solution to the Paradox. When the true prior is a wide Gaussian BNN, the mean a posteriori $\mathcal{M}^{\text{GP}}(L)$ is better than $\mathcal{NN}_{\theta^{*\lambda}}$ in terms of expected MSE. However, if the

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11. In section 5 we assume that $L$ is the squared loss as given in eq. (3), while outside section 5 all results hold for more general losses too.
Gaussian BNN prior is not close enough to the true prior, this statement does not hold anymore. We conclude that the improved generalization behavior of $\mathcal{N}^{\theta, \lambda}$ over $\mathcal{M}^{GP}(L)$ does not contradict with Bayesian theory; it simply suggests that Gaussian BNNs are quite far from the true prior and that $\mathcal{N}^{\theta, \lambda}$ is better in approximating the mean a posteriori of the unknown true prior than $\mathcal{M}^{GP}(L)$.

6. Conclusion

In this paper, we gave an exact characterization for infinite-width deep $\ell^2$-regularized ReLU NNs. Further, we gave a mathematical definition of multi-task learning on function space and showed that, based on our characterization, infinitely wide, $\ell^2$-regularized ReLU NNs are capable of multi-task learning. We highlighted in particular, that many infinite-width limits of NNs previously derived in the literature, like shallow GPs are not capable of multi-task-learning. These observations enabled us to explain two paradoxical contrasts between infinite-width $\ell^2$-regularized NNs and infinite-width Gaussian BNNs: First, the optimal infinite-width $\ell^2$-regularized NN does not correspond to the MAP of the corresponding GP. Second, the two errors of poor man’s approximation of the mean a posteriori BNN and of the poor choice of the prior partially cancel out and this results in an estimator that better approximates the mean a posteriori of some other unknown prior. In particular, the latter observation could give further insights into the much discussed phenomenon of cold posteriors of Gaussian BNNs Wenzel et al. (2020). We will investigate this further in future work.

We mathematically proved in section 4 that different outputs of infinitely-wide $\ell^2$-regularized ReLU NNs can influence each other in the infinite width limit. We hope that our characterization of the infinite-width limit can also provide some intuition on how they influence each other, how this influence can be beneficial in terms of generalization, and how it explains representation learning, feature learning, metric learning or transfer learning. In future work, we provide empirical evidence and more discussions on the beneficial effects of multi-task learning and on its relation to model uncertainty (Heiss et al. 2021, Desiderata D4).

Our results always consider NNs that are optimal with respect to an $\ell^2$-regularized loss. In future work, we compare them to NNs trained using standard (gradient descent based) optimization algorithms with and without $\ell^2$-regularization, and compare to the results of Yang and Hu (2021). Finally, we extend our results to other architectures.

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12. Aitchison (2020) only partially solves the paradox explained in Wenzel et al. (2020).
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A. Network Architectures and Their P-functionals

Figure 2: Schematic representation of a shallow neural network, which corresponds to one stack in the main paper.

Figure 3: Schematic representation of a shallow neural network with a trainable linear skip connection.

Figure 4: Schematic representation of a shallow neural network where many \((n_j)\) hidden nodes have a ReLU activation and some \((\min(d_{j-1}, d_j))\) hidden nodes have a linear (identity) activation function. Compared to Figure 3 the linear skip connection is factorized into two matrices.

Figure 5: Schematic representation of 
\#stacks = 3 stacks of Figure 3.

Figure 6: Schematic representation of 
\#stacks = 3 stacks of Figure 4.
In a future version of this paper, we will discuss $P$-functionals for modifications of the NN architecture. For architectures of the type of Figures 3 and 5, for instance, $P_j$ (and $T_j$) are given with the same abuse of notation as in the main paper (treating distributions as if they were functions) as

$$P_j(h_j) := \min_{\varphi \in T_j, c \in \mathbb{R}^d, \mathcal{A} \in \mathbb{R}^{d_j 	imes d_j}} \left( 2 \int_{S^{d_j-1}} \left\| \varphi_s(r)'' \right\|_2 dr ds + 2 \rho(\|c\|_2 + \|A\|_2^2) \right),$$

where $\|A\|_2$ is the Frobenius norm of $A$ and $T_j := \{ \varphi = (\varphi_s)_{s \in S^{d_j-1}} \mid \forall s \in S^{d_j-1}, \varphi_s : \mathbb{R} \rightarrow \mathbb{R}^{d_j}, x \mapsto \varphi_s(x) = 0 \text{ and } x \mapsto \frac{\partial}{\partial x} \varphi_s(x) = 0 \}$. For an architecture of the type of Figures 4 and 6 one gets:

$$P_j(h_j) := \min_{\varphi \in T_j, c \in \mathbb{R}^d, \mathcal{A} \in \mathbb{R}^{d_j 	imes d_j}} \left( 2 \int_{S^{d_j-1}} \left\| \varphi_s(r)'' \right\|_2 dr ds + 2 \rho(\|c\|_2 + \|A\|_{\text{Schatten}1}^2) \right),$$

where $\|A\|_{\text{Schatten}1}$ is the Schatten 1-norm (or Schatten–von-Neumann 1-norm) of $A$, i.e., the sum of the absolute values of the singular values of $A$.

## B. Equivalent Formulations of Regularization Functionals $P$

In this section, we state equivalent formulations of regularizing functional $P$. See Appendix F.1 for proofs of their equivalence. Moreover, we set $g(r) := \frac{1}{\sqrt{1 + r^2}}$ as in the main paper.

We start with some basic definitions.

**Definition 12.** Let $\Omega \subseteq \mathbb{R}$ be an open set. We define the Banach-space $BV^2(\Omega; \mathbb{R}^{d_j})$ as the set of functions $f \in W^{1,1}(\mathbb{R}; \mathbb{R}^{d_j})$ which second distributional derivative $D^2f = \mu$ is a bounded $\mathbb{R}^{d_j}$-valued Radon-measure, i.e., $\int f \phi'' = \int \phi \mu$ for all $\phi \in C^2_c$, with norm

$$\|f\|_{BV^2} = \|f\|_{L^1} + \|f'\|_{L^1} + |D^2f|,$$

where\(^\text{13}\)\(^\text{14}\)

$$|\mu| := |\mu|(\Omega) := \sup_{(E_1), \ldots, n \text{ is partition of } \Omega, n \in \mathbb{N}} \sum_{i=1}^n |\mu(E_i)|_2.$$
We define a “point-wise Radon–Nikodym density” analogously to the classical Radon–Nikodym density 

\[ M \]

Definition 15. Without any notational ambiguities: and therefore the following mathematical definition can also deal precisely with these atoms \( \mu \) has a BV \( \| \cdot \|_g \) measure theory point of view is that second distributional derivative \( D^2 f = \mu \) is a locally bounded \( \mathbb{R}^d \)-valued Radon-measure (i.e. \( \int f \phi'' = \int \phi d\mu \forall \phi \in C_c^2 \)). For the remainder of the paper, we will often just write \(BV^2_{\text{loc}}(\mathbb{R}; \mathbb{R}^d)\) as a short notation for \( BV^2_{\text{loc}}(\mathbb{R}; \mathbb{R}^d)\).

In other words \(BV^2_{\text{loc}}(\mathbb{R}; \mathbb{R}^d)\) consists of functions \( f \in W^{1,1}_{\text{loc}}(\mathbb{R}; \mathbb{R}^d)\) such that the weak derivative \( f' \) is in \(BV^2_{\text{loc}}(\mathbb{R}; \mathbb{R}^d)\) where \(BV^2_{\text{loc}}(\mathbb{R}; \mathbb{R}^d)\) is defined as in Leoni (2017, p. 188).

Throughout the paper, it is \( g(r) := \frac{1}{\sqrt{1+r}} \) as in (7), as it is also in the following definition:

**Definition 14. Based on Definition 13 we define**

\[
BV^2_{0-}(\mathbb{R}; \mathbb{R}^d) := \left\{ f \in BV^2_{\text{loc}}(\mathbb{R}; \mathbb{R}^d) \mid \lim_{r \to -\infty} f(r) = 0 = \lim_{r \to -\infty} \frac{\partial}{\partial r} f(r), |D^2 f|_g < \infty \right\}
\]

We equip this space with the norm \( |D^2(\cdot)|_g \) where

\[
|\mu|_g := |\mu|_g(\mathbb{R}) := \sup_{(E_i)_{i=1}^n \text{ is partition of } \mathbb{R}, n \in \mathbb{N}} \sum_{i=1}^n \left\| \int_{E_i} g(r) d\mu(r) \right\|_2.
\]

(This is a norm because of the boundary conditions.) (We will sometimes write \( |\mu|_{g_{\text{loc}}} \) instead of \( |\mu|_g \).) For the remainder of the paper, we will often just write \( BV^2_{0-} \) as a short notation for \( BV^2_{0-}(\mathbb{R}; \mathbb{R}^d)\).

The following Definition 15 is the most straightforward mathematically precise interpretation of eq. (7), where we interpret the “function” \( \varphi \) as a distribution, which is mathematically a \(BV^2_{\text{loc}}\)-valued bounded Radon measures \( \mu \) on \( S^{d_j-1} \) (for the jth stack). This \( \mu \) has a \(BV^2_{0-}\)-valued Radon–Nikodym density \( \varphi := \varphi_{\mu} := \frac{d\mu}{d|\mu|} : S^{d_j-1} \to BV^2_{0-}, s \mapsto \varphi_s \) which is actually a classical function in the strict mathematical sense. The advantage of the measure theory point of view is that \( \mu \) and thus \( |\mu| \) can also have atoms (Dirac impulses) and therefore the following mathematical definition can also deal precisely with these atoms without any notational ambiguities:

**Definition 15.** \( \mathcal{M}^{BV^2_{0-} (S^{d_j-1})} \) is the set of all \(BV^2_{0-}\)-valued bounded Radon measures on \( S^{d_j-1} \) for some stack \( j \) for which the \(BV^2_{0-}\)-valued point-wise Radon–Nikodym density \( \varphi := \varphi_{\mu} := \frac{d\mu}{d|\mu|} : S^{d_j-1} \to BV^2_{0-}, s \mapsto \varphi_s \) exists. Then we define

\[
P_j(h_j) := \min_{\substack{\mu_j \in \mathcal{M}^{BV^2_{0-} (S^{d_j-1}), \ \mu_{d_j-1} = \mu_j \downharpoonright S^{d_j-1-1}, \ c \in \mathbb{R}^{d_j} \ s.t. \ \forall x \in \mathbb{R}^{d_j-1}, \ h_j(x) = c + \int_{S^{d_j-1-1}} \phi_{\mu_j}((s,x)) d|\mu_j|(s)}} \left( 2 \rho \|\|_2 + 2 \int_{S^{d_j-1-1}} |D^2 \varphi_s|_g d|\mu_j|(s) \right)
\]

15. We define a “point-wise Radon–Nikodym density” analogously to the classical Radon–Nikodym density except replacing the Banach space topology used in the definition of the Bochner integral by the topology of point-wise convergence ptw.

16. Out of context, it should be clear that \( |\mu| \) refers to the total variation measure \( |\mu| : \mathcal{B}(S^{d_{\text{dim}}-1}) \to \mathbb{R}_{\geq 0} \), while \( |D^2 \varphi_s|_g \) is a short notation of \( |D^2 \varphi_s|_g(\mathbb{R}) \) (see Definition 14).
Moreover,

\[ \mathcal{F} := \left\{ f = \ell^{-1} \circ h_{\# \text{stacks}} \circ \cdots \circ h_1 \mid \forall j \in \{1, \ldots, \# \text{stacks}\} : \exists \mu_j \in \mathcal{M}^{BV_{\infty}}(S^{d_j-1}), c(j) \in \mathbb{R}^{d_j} : \right. \\
\left. \forall x \in \mathbb{R}^{d_j-1} : h_j(x) = c(j) + \int_{S^{d_j-1}} \varphi_j(s, x) d|\mu_j|(s) \right\}. \]

Note, that \( \mathcal{F} \) is dense in the continuous functions \( C(\mathbb{R}^{d_{in}}; \mathbb{R}^{d_{out}}) \) with respect to the maximum norm on every compact set, if \( d \geq \min(d_{in}, d_{out}) \). (This can be easily derived from the universal approximation theorem in Hornik (1991); Cybenko (1989).)

**Definition 16.** For \( f \in \mathcal{F} \) as in Definition 15, we define

\[
\tilde{F}_{\text{measure}}(f) = \min_{(h_1, \ldots, h_{\# \text{stacks}}, \text{s.t. } f = \ell^{-1} h_{\# \text{stacks}} \circ \cdots \circ h_1)} \left( \tilde{F}_1^{\text{measure}}(h_1) + \tilde{F}_2^{\text{measure}}(h_2) + \cdots + \tilde{F}_{\# \text{stacks}}^{\text{measure}}(h_{\# \text{stacks}}) \right),
\]

with

\[
\tilde{F}_j^{\text{measure}}(h_j) = \min \left\{ 2|\mu| + \|c\|^2 : \mu_j \in \mathcal{M}(S^{d_j-1} \times S^{d_j-1}) , \right. \\
\left. \forall x \in \mathbb{R}^{d_j-1} : h_j(x) = c + \int_{S^{d_j-1} \times S^{d_j-1}} w \sigma((v, x) - r) d\mu((v, r), w) \right\},
\]

where \( \mathcal{M}(S^{d_j-1} \times S^{d_j-1}) \) is the set of bounded Radon measures on \( S^{d_j-1} \times S^{d_j-1} \).

Moreover, we state two further (equivalent, as we will see in Appendix F.1) reformulations of regularizing functional \( P_j \) on the \( j \)th stack.

**Definition 17.**

\[
P_j^{\text{measureVer}}(h_j) = \min \left\{ 2|\mu| + \|c\|^2 : \mu_j \in \mathcal{M}^d(S^{d_j-1-1} \times \mathbb{R}), \right. \\
\left. \forall x \in \mathbb{R}^{d_j-1} : h_j(x) = c + \int_{S^{d_j-1-1} \times \mathbb{R}} \sigma((v, x) - r) d\mu(v, r) \right\},
\]

with \( \mathcal{M}^d(S^{d_j-1-1} \times \mathbb{R}) \) the set of bounded \( \mathbb{R}^d \)-valued Radon measures on \( S^{d_j-1-1} \times \mathbb{R} \) and

\[
|\mu|_{\frac{1}{|S|}} := |\mu|_{\frac{1}{|S|}}(S^{d_j-1-1} \times \mathbb{R}) := \sup_{(E_i)_{1, \ldots, n} \text{ is partition of } S^{d_j-1-1} \times \mathbb{R}, n \in \mathbb{N}} \sum_{i=1}^{n} \left\| \int_{E_i} \frac{1}{g(r)} d\mu(v, r) \right\|_2.
\]

**Definition 18.**

\[
\tilde{F}_j^{\text{measureG}}(h_j) = \min \left\{ 2 \int \frac{1}{g(r)} d\mu(v, r, w) + 2\rho(\|c\|_2) : \mu \in \mathcal{M}(S^{d_j-1-1} \times \mathbb{R} \times S^{d_j-1}), \right. \\
\left. \forall x \in \mathbb{R}^{d_j-1} : h_j(x) = c + \int_{S^{d_j-1-1} \times \mathbb{R} \times S^{d_j-1}} w \sigma((v, x) - r) d\mu(v, r, w) \right\}
\]
C. Required Number of Neurons

In the case of linear $\tilde{\sigma}$, a possible choice of $n^*$ and $d^*$ is always $n_j^* = \sum_{i=0}^{#\text{stacks} - j - 1} N^i$ and $d_j^* = \sum_{i=0}^{#\text{stacks} - j} N^i$ independent of $x^{\text{train}}, y^{\text{train}}$ and $\lambda$. A smaller choice can be made in the case of letting some $d_j$ stay small and only letting $d_j$ tend to infinity for some indices $j$. This smaller choice can be written down recursively: $d^*_j = \text{out} = d_{\text{out}}, n^*_j = 1 + N$, and $d_j^* = \min(d_j, n_j^* + 1)$ and $n_j^* = 1 + N \cdot d_j^*$ for $j \in \{1, \ldots, #\text{stacks} - 1\}$.

In the case of $\tilde{\sigma} = \text{ReLU}$, a possible choice of $n^*$ and $d^*$ is always $n_j^* = \sum_{i=0}^{2(#\text{stacks} - j) + 1} N^i$ and $d_j^* = \sum_{i=0}^{2(#\text{stacks} - j) - 1} N^i$ independent of $x^{\text{train}}, y^{\text{train}}$ and $\lambda$. A smaller choice can be made in the case of letting some $d_j$ stay small and only letting $d_j$ tend to infinity for some indices $j$. This smaller choice can be written down recursively: $d^*_j = \text{out} = d_{\text{out}}, n^*_j = 1 + N$, and $d_j^* = \min(d_j, 1 + N \cdot n_j^* + 1)$ and $n_j^* = 1 + N \cdot d_j^*$ for $j \in \{1, \ldots, #\text{stacks} - 1\}$.

See Appendix F.4 for proof of these statements.

D. Visualizing Multi-task Learning

In this section, we present a simple example of a data-generating function $f$ with $d_{\text{out}} = 7$ outputs which are all periodic with the same periodicity $\frac{2}{3}$ and input dimension $d_{\text{in}} = 1$.

The knowledge that the outputs are periodic is not given to the network a priori and we hope that the network with $#\text{stacks} = 3, n \gg N, d_1 = d_2 = 1, \tilde{\sigma} = id, \ell^{-1} = id$ (with architecture as in Figure 1) is able to find a periodic representation $H$ by itself, as this would be helpful for all 7 outputs. In all figures below, we show $\mathcal{NN}_y^{(j)}$ instead of $h_j$, since we have obtained $\theta$ from actually training a NN with gradient descent (that can get stuck in local minima) for a a finite time instead of calculating the perfect solution. In Figures 7 and 8, we visualize what each stack has learned: Figure 7 visualizes how the hidden stacks learn a shared representation $H = \mathcal{NN}_y^{(2)} \subset \mathcal{NN}_y^{(1)}$ and Figure 8 visualizes how this can be useful for the different tasks.

In this case the benefits from multi-task learning are not too big, since all tasks share exactly the same input training data points. Nonetheless, there are still small benefits from multi-task learning in that the model can better filter out data noise.

Next we will show an example for the same 7 tasks but with a different training set. This time we have less data for the first task – in particular we only have training data for $x \in [-2, 0]$ for the first task, while for the other 6 tasks we also have $y$ values corresponding to input training data points $x \in [-2, 2]$. If one were to train the first task separately only on the input training data $x < 0$, it would be extremely hard for the neural network to extrapolate to input testing data $x > 0$, but with the help of the multi-task learning induced by $P$, the network can extrapolate very well to input testing data $x > 0$ as shown in Figure 9. Note that for this experiment we use wide bottlenecks, i.e. $d_1 = d_2 = 2048$, to also experimentally validate Corollary 6 by showing that multi-task learning does not vanish for large bottleneck dimensions. The detailed experimental setup is #stacks = 3, $n_1 = n_2 = n_3 = 2048, \lambda = 0.0005, \tilde{\sigma} = \text{ReLU}, \ell^{-1} = id$. Note that The training data and the learned functions for the 6 tasks that have training input data $x \in [-2, 2]$ are shown in Figure 10. For the plots we used a neural network $\mathcal{NN}_y$ which was trained with gradient descent on the objective (4), which is probably not a perfect approximation of
(a) 1\textsuperscript{st} stack: $\mathcal{N}_{\theta(1)}$ in green and its (distributional) second derivative $\sum_{i=1}^{n_1} v_i^{(1)} w_i^{(1)} \delta_{\xi_i^{(1)}}$ (visualized by yellow dots $(\xi_i^{(1)}, v_i^{(1)} w_i^{(1)})$), where $\xi_i^{(1)} = -\frac{h_i^{(1)}}{v_i^{(1)}}$, and a smoothed version of it (yellow dashed line). The smooth second derivative was obtained from a convolution using a Gaussian kernel.

(b) 2\textsuperscript{nd} stack: $\mathcal{N}_{\theta(2)}$ in green and $H := \mathcal{N}_{\theta(2)} \circ \mathcal{N}_{\theta(1)}$ in red and the (distributional) second derivative $h_i'' = \sum_{i=1}^{n_2} v_i^{(2)} w_i^{(2)} \delta_{\xi_i^{(2)}}$ (visualized by yellow dots $(\xi_i^{(2)}, v_i^{(2)} w_i^{(2)})$), where $\xi_i^{(2)} = -\frac{h_i^{(2)}}{v_i^{(2)}}$ and a smoothed version of it (yellow dashed line) as in Figure 7a.

Figure 7: The hidden stacks learn a periodic shared representation $H = \mathcal{N}_{\theta(2)} \circ \mathcal{N}_{\theta(1)}$.

$\mathcal{N}_{\theta,\lambda}$, but good enough to show the qualitative behavior of $f^*\lambda$. (For high dimensional $d_1 = d_2 = 2048$ the learned hidden representation cannot be visualized as easily as for the previous experiment. This is why we do not have an analogous plot to Figure 7 for this experiment.)

Without multi-task learning neural networks would not extrapolate the function periodically. If one would train the same model only on the first task without any additional task, the model would just extrapolate with as little second derivative as possible as can be seen (approximately again because of gradient descent) in Figure 11.

E. Discussion of Multi-Task Learning and Definition 4

Mathematically one cannot judge a priori if multi-task learning is beneficial or not, because this depends on whether or not one’s prior belief (or inductive bias) matches with the true prior.\textsuperscript{17}

One can however very precisely define a notion capturing that learning multiple tasks at once does not result in different estimators than when learning them separately (see

\textsuperscript{17} If the data comes from a function that was actually sampled from a GP with independent outputs, then multi-task-learning will not be beneficial.
Figure 8: The last stack can easily learn the different tasks based on the representation from the hidden representation. The hidden stacks learn a periodic representation $H = \mathcal{N}_{\theta(1)} \circ \mathcal{N}_{\theta(2)}$ (see Figure 7). The (distributional) second derivatives are visualized in yellow as in Figure 7.
Figure 9: For the first task we only observe training input data $x \leq 0$, but $\hat{f}_1 := (\mathcal{NN}_\beta)_1$ learns to extrapolate well to $x > 0$, because of the multi-task benefits of being trained together with 6 other tasks (see Figure 10).

Figure 10: The last stack can easily learn the different tasks based on the representation from the hidden representation $H$. The hidden stacks learn a periodic representation $H = \mathcal{NN}_{\beta(2)}^{(2)} \circ \mathcal{NN}_{\beta(1)}^{(1)}$. 
Definition 4). And if learning different tasks jointly does not make any difference (in terms of generalization), one can obviously not benefit (in terms of generalization) from learning them jointly. If however, the generalization behaviours of different outputs trained jointly to perform different tasks influence each other, these outputs can also benefit from it depending on one’s prior belief.

Some intuition for what kind of influence among tasks is desirable for real-world applications according to a common sense prior is given in Caruana et al. (1997). Intuitively, it is not beneficial if different outputs just influence each other randomly. With our formulation of $P$, the discussion in section 4 and the visualizations in Appendix D, we see that this influence is not random for $\ell^2$-regularized NNs (or $\mathcal{M}^P$). Instead, training NNs with weight-decay enforces multi-task learning due to the shared representation $H$, which corresponds to the intuitively beneficial multi-task learning described in Caruana et al. (1997). Moreover, from an empirical point of view, in various applications, training multiple tasks jointly has outperformed separate training of the individuals tasks (Caruana et al., 1997; Ruder, 2017; Fifty et al. 2021; Tran et al. 2021; Aribandi et al. 2021).
E.1 Connection to Representation Learning, Feature Learning, Metric Learning and Transfer Learning

In this subsection we will explain that multi-task learning, representation learning, feature learning, metric learning and transfer learning are highly related phenomena. In this paper we focused on multi-task learning, because the absence of multi-task learning can be rigorously defined for models $M$ in functions space (see Definition 4).

But $P$ defined in eqs. (6) and (7) also intuitively reveals the ability of wide deep $\ell^2$-regularized NNs to perform representation learning, feature learning, metric learning and transfer learning. For example$^{18}$, we can interpret $H(x) = \tilde{\sigma} \circ h_{\#\text{stacks} - 1} \circ \cdots \circ \tilde{\sigma} \circ h_1(x)$ as the learned representation of $x$. Then we can interpret the coordinates $H_k(x)$ as the learned features of $x$. Further we can interpret $d_H(x, \tilde{x}) := \|H(x) - H(\tilde{x})\|_2$ as the learned metric on the input space $\mathbb{R}^{d_n}$. Since the hidden representation $H$ is shared among all tasks, it enforces multi-tasking. If one does not train all task simultaneously, one can first train some tasks to obtain $H$ and then afterwards train further tasks with fixed $H$ (or by only slightly varying $H$) to achieve transfer learning.

Multi-task learning, representation learning, feature learning, metric learning and transfer learning can not be achieved via Gaussian process regression with a fixed kernel.

E.2 Adaptivity vs Multi-task Learning

Bach (2017); Chizat and Bach (2020) have shown that wide $\ell^2$-regularized NNs with one hidden layer are adaptive to hidden linear low-dimensional structures in terms of generalization. This means: If the unknown true function $f$ can be expressed as $f(x) = \hat{f}(Vx)$, where $V \in \mathbb{R}^{r \times d_n}$ is a projection matrix on a $r$-dimensional subspace, then the generalization bound of the NN asymptotically only depends on $r$ instead of $d_n$ under mild smoothness conditions on $f$. In other words, this means that the curse of dimensionality can be avoided (asymptotically) if $r \ll d_n$. The same holds true, if they chose the first layer weights $v$ and biases $b$ randomly$^{19}$ and only train the output weights $w$ and biases $c$ with $\ell^1$-regularization. In function space training both layers with $\ell^2$-regularization corresponds to $P = P_1$ introduced in eq. (7)$^{20}$, while only training the output layer with $\ell^1$-regularization corresponds to$^{21}

$$
\hat{P}^{\ell^1}(f) := \min_{\varphi \in T_1, c \in \mathbb{R}^{d_{out}} \text{ s.t.} \int_{S^q_{d_{in}-1}} \varphi(s) ds + c} \left( 2 \int_{S^q_{d_{in}-1}} \int_{\mathbb{R}} \left\| \varphi_s(r)'' \right\|_1 g(r) dr ds + 2 \|c\|_1 \right),
$$

18. A reasonable alternative point of view would be to see $\hat{H}(x) = \left( \max(0, b_k^{\#\text{stacks}}) + \langle v_k^{\#\text{stacks}}, H(x) \rangle \right)_{k \in \{1, \ldots, \#\text{stacks} \}}$ as the learned representation of $x$. The representation $\hat{H}(x)$ captures the learned hidden representation up to the last hidden layer, but $H$ can be studied more conveniently on function space.

19. We assume that the support of the distribution of $(v, b)$ is $S^{d_{in}}$, e.g., $(v, b) \sim \mathcal{U}(S^{d_{in}})$ can be distributed uniformly on the sphere $S^{d_{in}}$.

20. If we have only 1 hidden layer (i.e., $\#\text{stacks} = 1$) and the identity as final non-linearity $\ell^{-1} = \text{id}$, then $P$ from eq. (6) is obviously equal to $P_1$ from eq. (7).

21. For eq. (16) we use the same abuse of notation as for eq. (7) (treating distributions as if they were functions).
where the main difference between $\tilde{P}^{d_1}$ and $P$ is that the norm inside the inner integral is an $\ell^1$-norm instead of an Euclidean $\ell^2$-norm. In other words, we have an $L^1(\mathbb{R}; (\mathbb{R}^{d_{out}}, \| \cdot \|_1))$-norm for $\tilde{P}^{d_1}$ instead of the $L^1(\mathbb{R}; (\mathbb{R}^{d_{out}}, \| \cdot \|_2))$-norm that we had for $P$. As we have an $L^1$-norm in both cases, the models $\mathcal{M}\tilde{P}^{d_1}, L \mapsto \mathcal{M}\tilde{P}^{d_1}(L) := \arg\min_f \left( L(f) + \lambda \tilde{P}^{d_1}(f) \right)$ and $\mathcal{M}P$ both are adaptive to hidden linear low-dimensional structures in terms of generalization.

However, while $\mathcal{M}P$ cannot benefit from multi-task learning (see Proposition 10), $\mathcal{M}\tilde{P}^{d_1}$ cannot benefit from multi-task learning as the following proposition shows.

**Proposition 19.** The model $\mathcal{M}\tilde{P}^{d_1}$ (where $\mathcal{M}\tilde{P}^{d_1}(L) := \arg\min_f \left( L(f) + \lambda \tilde{P}^{d_1}(f) \right)$ is defined as above based on eq. (16)) is not capable of benefiting from multi-task learning (see Definition 4).

**Proof** The proof is trivial, since $\tilde{P}^{d_1}$ splits into a sum as in the proof of Proposition 9: Without the square-root, learning a separate function $f_k$ for each task would result exactly in the same functions $f_k$ as training them all together, since

$$
\int \left\| f''(x) \right\|_1 dx = \int \sum_{k=1}^{d_{out}} \left| f''_k(x) \right| dx = \sum_{k=1}^{d_{out}} \int \left| f''_k(x) \right| dx.
$$

Therefore,

$$
L(f) + \lambda \tilde{P}^{d_1}(f) =
= \sum_{k=1}^{d_{out}} \left( L_\varsigma(f) + \lambda \min_{\varphi \in \mathcal{T}^{d_{in}:1} \subset \mathbb{R}^{d_1}} \min_{f_k = \int_{S^{d_{in}-1}} \varphi_s((s,cdot)) ds + c} \left( 2 \int_{S^{d_{in}-1}} \int_{\mathbb{R}} \frac{\|\varphi_s(r)''\|}{g(r)} dr ds + 2|c| \right) \right),
$$

where $\mathcal{T}^{d_{in}:1}$ is defined as $\mathcal{T}_1$ with the only difference that $d_1$ is replaced by 1.22

$$
\left( \mathcal{M}\tilde{P}^{d_1}(L) \right)_k = \left( \arg\min_f \left( L(f) + \lambda \tilde{P}^{d_1}(f) \right) \right)_k = \left( \mathcal{M}\tilde{P}^{d_1}(L_\varsigma) \right)_k.
$$

(Note that all its other components of $\mathcal{M}\tilde{P}^{d_1}(L_\varsigma)$ are the zero function.)

So we can see that adaptivity to hidden linear low-dimensional structures in terms of generalization (as introduced by Bach, 2017); Chizat and Bach (2020)) does not imply the ability for benefiting from multi-task learning, representation learning, feature learning, metric learning or transfer learning.

Therefore, the ability to benefit from multi-task learning can be seen as an extension/continuation of “quest for adaptivity” by Bach.

22. Following this notation $\mathcal{T}_j = \mathcal{T}^{d_{j-1}:d_j}$ and $\mathcal{T}^{d_{in}:1}$ is defined as

$$
\mathcal{T}^{d_{in}:1} := \left\{ \varphi = (\varphi_s)_{s \in S^{d_{in}-1}} \mid \forall s \in S^{d_{j-1}-1} : \varphi_s : \mathbb{R} \rightarrow \mathbb{R}^1, \lim_{r \rightarrow -\infty} \varphi_s(r) = 0 = \lim_{r \rightarrow -\infty} \frac{\partial}{\partial r} \varphi_s(r) \right\}.
$$
E.3 Universal Features and Universal “Readout”

In terms of universality, there are two aspects in which deep stacked NNs (i.e., \#stacks > 1) differs from the shallow NNs (i.e., \#stacks = 1).

First, for \#stacks > 1 the representation \( H(x) \) can approximate any (continuous) function in \( x \) by universal approximation theorems (Hornik, 1991; Cybenko, 1989). This is important since in applications of modern deep learning, representations \( H(x) \) shared among different tasks can be a highly non-linear functions of \( x \). In Figure 7b, we see such a non-trivial representation \( H \) learned by a neural network. A shallow ReLU NN however cannot learn such a representation within its shared hidden layer.

Second, for \#stacks > 1 the last stack \( h_{\#stacks} \) can be seen as a universal non-linear readout. A shallow NN only consists of one hidden layer that learns the shared representation, and one linear task-specific readout layer. In contrast, deep NNs are able to learn non-linear task-specific readout functions \( h_{\#stacks,k} \) for the different tasks (see Figure 8). This is not possible for methods such as linear group-Lasso regression (on non-linear fixed features). The latter we refer to as “shallow multi-task learning”.

For the generalization behavior shown in Figure 10c of Appendix D both universal representation and universal readout is needed, since seven components of the function \( f \) are very different highly non-linear functions composed with the highly non-linear sine function. Thus, in this example, the most important shared feature should be somehow related to a sine function and different non-linear readouts are needed for the different tasks in order to obtain such strong benefits from multi-task learning as in Figure 10c. There is no single shared feature, such that all functions could be represented as linear functions of this shared feature.

E.4 Different Levels of Abstraction

In practice it is often observed that low level features (such as edges for images) are important across many different tasks (for example even tasks based on different types of images, such as natural images and X-ray images share edges as important features). According to our formulation of \( P \) for \#stacks > 1, a first stack \( h_1 \) is preferred that mainly learns features that can be shared among as many tasks as possible instead of learning different features for different tasks in order to keep \( P_1(h_1) \) as low as possible even when \( d_1 \gg 1 \) is very large. Then medium-low level features \( h_2 \circ h_1 \) share the property that they can be represented by a rather “flat” (in terms of \( P_2 \)) function \( h_2 \) on top of the shared low-level features \( h_1 \). \( P \) still prefers to learn features \( h_2 \circ h_1 \) which are helpful\(^{23} \) for all tasks. However, depending on how unrelated the tasks are, also some task-specific features can be learned for the cost of higher regularisation costs. And as the stack-index \( j \) increases, more of the higher-level features \( (h_j \circ \cdots \circ \hat{\sigma} \circ h_1)_k \) become mainly relevant for smaller subsets of tasks and only \( f \) of the high level features are relevant for all tasks (depending on how related they are). A similar effect has been studied empirically in Neyshabur et al. (2020), where the performance on one task was improved by reusing features learned from a different task.

\(^{23} \) Mathematically speaking a feature \( (h_j \circ \cdots \circ \hat{\sigma} \circ h_1)_k \) is not helpful (or irrelevant) for the \( l \)-th task if the function \( (\ell^{-1} \circ h_{\#stacks} \circ \cdots \circ \hat{\sigma} \circ h_{j+1})_l \) is constant with respect to its \( k \)-th input dimension. (In practice it is more a continuum of helpfulness/relevance if the function is almost constant with respect to certain input dimensions.)
How Infinitely Wide Neural Networks Can Benefit from Multi-task Learning

Table 1: Various infinite width limits, their inductive bias in function space and their ability to benefit from multi-task learning.

| Model | Multi-task Learning | Inductive Bias in Function Space |
|-------|---------------------|----------------------------------|
| Kernel ridge regression with fixed kernel (e.g., NTK, Gaussian BNN kernel, random feature kernel) | No (Propositions 9 and 11) | $L^2(\ell_2)$-typed regularization |
| Kernel lasso regression with fixed kernel (i.e., linear $\ell_1$ regression) | No (Proposition 19) | $L^1(\ell_1)$-typed regularization |
| Kernel group-lasso regression with fixed kernel (i.e., linear group-lasso regression) | “shallow” | $L^1(\ell_2)$-typed regularization |
| $\mathcal{NN}_{\text{m,3}}$ (i.e., our setting) | one hidden layer (i.e., #stacks = 1) | “shallow” | Regularization functional $P_1$ given in eq. (6) ($L^1(\ell_2)$-typed) |
| | multiple hidden layers (i.e., #stacks > 1) | “deep” | Regularization functional $P$ given in eq. (6) |
| Multiplying a hard-coded, non-trainable matrix on the outputs of a model (that itself is not able to benefit from multi-task learning) | Weak form of “shallow” multi-task learning | Handcrafted inductive bias favoring a certain sign of correlation |

where especially in the first hidden layer a lot of features could be reused and the number of features that could be reused decreased from low level layers to high level layers.

See Table 1 in Appendix E.5 for an overview which methods allows for “deep” multi-task learning and which do not.

E.5 On Multi-task Learning Induced by Regularization

In this paper, we show that the function space regularization $P$ induced by $\ell_2$-regularization on the parameters of NNs enables them to benefit from multi-task learning. We like to highlight that the induced regularization does not involve the $L^2$-norm in function space. We show that the $\ell_2$-regularization in parameter space induces an $L^1(\ell_2)$-regularization $P_1$ of the second derivative in function space in the case of 1 hidden layer. (Here, we call a norm $L^p(\ell_q)$-typed if inside the integral there is a $\|\cdot\|_{\ell_q}^p$-term. This can be seen as a $L^p(\mathbb{R}; (\mathbb{R}^{d_{\text{out}}}; \|\cdot\|_q))$-norm as in Appendix E.2.)

The $L^1(\ell_2)$-regularization is able to benefit from multi-task learning (see Proposition 10). This is in contrast to the regularizations $L^1(\ell_1)$ (see eq. (16)) and $L^2(\ell_2)$, which are both not able to benefit from multi-task learning (see Propositions 9 and 19). Note also that for deep NNs, $P$ (see eq. (6)) is more intricate than $P_j$ (see eq. (7)). In contrast to $P_j$, $P$ is not a norm anymore, and thus $P$ promotes much more interesting forms of “deep” multi-task learning (see Appendices E.3 and E.4).

To highlight once more the differences between various models in terms of multi-task learning and regularization in function space, we have compiled Table 1.

F. Proofs

See Definitions 12–14 for definitions of the function spaces (such as $BV^2_{0-}$) that we consider.

Lemma 20. The normed vector space $BV^2_{0-}(\mathbb{R}; \mathbb{R}^{d_j})$ is a Banach space.

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Proof It suffices to consider the case $d = 1$. Completeness of $BV^2_{0-}(\mathbb{R};\mathbb{R})$ can be seen through the following inequalities: firstly, we observe that
\[
\sup_{r \in \mathbb{R}} |f'(r)| \leq |D^2 f|_{\frac{1}{g}} \tag{17}
\]
by the fact that $\frac{1}{g} \geq 1$ and the $f'(-\infty) = 0$.

Secondly, it follows from integration by parts that
\[
|f(c)| = \left| \int_{-\infty}^{c} f'(a) da \right| = \left| \int_{-\infty}^{c} D^2 f((-\infty,a]) da \right| 
\leq \left| D^2 f|_{(-\infty,c]} \right|_{c-(\cdot)} 
\leq \left| D^2 f|_{(-\infty,c]} \right|_{\frac{1+\max(0,c)}{g}} \leq \left| D^2 f \right|_{\frac{1}{g}} \cdot (1 + \max(0, c)), \tag{18d}
\]
where we used that $|c - (\cdot)| \leq \frac{1+\max(0,c)}{g}$. Analogously, one can derive the same bound for $\|f'|_{(-\infty,c]}\|_{L^1}$. Obviously, we have for $a \leq b \leq 0$ that
\[
|f(b) - f(a)| \leq \int_{a}^{b} |f'(r)| dr.
\]
Therefore, we can conclude that a Cauchy sequence $(f_n)$ in $BV^2_{0-}(\mathbb{R};\mathbb{R})$ defines a limiting measure of bounded variation $\mu$, a limiting function $u$ being $L^1$ limit of $(f'_n)$ on any interval $(-\infty,a]$ for any real $a$ and a function $h$ being the limit of $(f_n)$ uniformly on $(-\infty,a]$ for any real $a$. Whence there exists $f \in W^{1,1}_{\text{loc}}(\mathbb{R};\mathbb{R})$ such that $f = h$, $f' = u$ and $D^2 f = \mu$. Additionally, $h(-\infty) = 0$ (because of (18)) and $f'(-\infty) = 0$ (by (17)) hold true as well as $|D^2 f|_{\frac{1}{g}} < \infty$. \hfill \blacksquare

Definition 21. Let $j \in \{1, \ldots, \#\text{stacks}\}$, $\mathcal{M}_j := \mathcal{M}(K_j) \times \mathbb{R}^{d_j}$ with $K_j := S^{d_j-1} \times S^{d_j-1}$. We then define

1. the set of functions
\[
\mathcal{F}_{K_j} := \left\{ f : \mathbb{R}^{d_j-1} \to \mathbb{R}^{d_j} \mid \exists (\nu, c) \in \mathcal{M}_j \forall x \in \mathbb{R}^{d_j-1} : f(x) = c + \int_{K_j} w \sigma((v,x) - r) d\nu((v,r),w) \right\},
\]

2. and the set of function representations
\[
\mathcal{E}^f_{K_j} := \left\{ (\mu, c) \in \mathcal{M}_j \mid \forall x \in \mathbb{R}^{d_j-1} : f(x) = c + \int_{K_j} w \sigma((v,x) - r) d\mu((v,r),w) \right\},
\]
of a given \( f \in \mathcal{F}_{K_j} \).

F.1 Proofs of Equivalences of \( P \)

**Lemma 22.** Let \( f : \mathbb{R} \to \mathbb{R}^d \) be any function and \( g(r) := \frac{1}{\sqrt{1+r^2}} \) as in the main paper. Then, the following equivalence holds

1. \( P_{measureVec1}^j(f) < \infty \)
2. \( f \in BV_{0-}^2 \)

with

\[
P_{measureVec1}^j(f) := \inf \left\{ |\mu|_{\frac{1}{g}} : \mu \in \mathcal{M}_{d_j}(\mathbb{R}), \forall r \in \mathbb{R} : f(r) = \int_{\mathbb{R}} \sigma(r - \xi) d\mu(\xi) \right\}.
\]

In this case (if 1 or 2 holds):

\[
P_{measureVec1}^j(f) = |D^2 f|_{\frac{1}{g}}
\]

**Proof** First, assume \( \exists \mu \in \mathcal{M}_{d_j}(\mathbb{R}) : \forall r \in \mathbb{R} : f(r) = \int_{\mathbb{R}} \sigma(r - \xi) d\mu(\xi) \). Then:

\[
\forall \mu \in \mathcal{M}_{d_j}(\mathbb{R}) : D^2 \int_{\mathbb{R}} \sigma(r - \xi) d\mu(\xi) = \mu
\]

\[
\implies D^2 f = \mu, \text{ if } \forall r \in \mathbb{R} : f(r) = \int_{\mathbb{R}} \sigma(r - \xi) d\mu(\xi)
\]

This implies that \( |\mu|_{\frac{1}{g}} = |D^2 f|_{\frac{1}{g}} < \infty \), for all \( \mu \in \mathcal{M}_{d_j}(\mathbb{R}) \), that fulfill the integral equality \( f(r) = \int_{\mathbb{R}} \sigma(r - \xi) d\mu(\xi) \). Moreover, by Monotone Convergence Theorem, we have

\[
\lim_{r \to -\infty} f(r) = \lim_{r \to -\infty} \int_{\mathbb{R}} \sigma(r - \xi) d\mu(\xi) = 0
\]

\[
\lim_{r \to -\infty} \frac{\partial}{\partial r} f(r) = \lim_{r \to -\infty} \int_{\mathbb{R}} 1_{r-\xi > 0} d\mu(\xi) = 0.
\]

Now, assume on the other hand that we have 2. We set \( u := \frac{\partial}{\partial r} f \) as the weak derivative of \( f \) and \( \mu := D^2 u = D^2 f \). Then, using the boundary conditions of 2, we get

\[
\int_{\mathbb{R}} \sigma(r - \xi) d\mu(\xi) = -\int_{\mathbb{R}} 1_{[0,\infty)}(r - \xi) u(\xi) d\xi = \int_{\mathbb{R}} \delta_0(r - \xi) f(\xi) d\xi = f(r).
\]

Thus, \( \mu \) fulfills all conditions of \( P_{measureVec1}^j \), and since eq. (19) shows the uniqueness of such \( \mu \), we get \( P_{measureVec1}^j(f) = |D^2 f|_{\frac{1}{g}} < \infty \).

**Lemma 23.**

\[
P_j = P_{measureVec}^j
\]
Proof

1. $P_j \leq P_j^{\text{measure Vec}}$

Let $\mu \in M^{d_j}(S^{d_j-1} \times \mathbb{R}), c \in \mathbb{R}^{d_j}$ such that $\forall x \in \mathbb{R}^{d_j-1} : f(x) = c + \int_{S^{d_j-1} \times \mathbb{R}} \sigma(\langle v, x \rangle - r) d\mu(v,r)$ and $|\mu|_{\frac{1}{g(r)}} < \infty$. Then we define $\nu \in M^{\text{BV}_{0-}}(S^{d_j-1})$ as

$$\nu(B)(x) := \int_{B \times \mathbb{R}} \sigma(x - r) d\mu(v, r), \quad \forall B \in \mathcal{B}(S^{d_j-1}), \forall x \in \mathbb{R}.$$ 

Let us decompose $|\mu|(dv, dr) = k(v, dr)a(dv)$, where $a$ is the marginal measure of $|\mu|$ on $S^{d_j-1}$. With this in mind we can calculate the total variation measure of $|\nu|$, namely

$$|\nu|(B) := \int_{B} \int_{\mathbb{R}} \frac{1}{g(r)} k(v, dr) a(dv), \quad \forall B \in \mathcal{B}(S^{d_j-1}).$$

Denote additionally $\tilde{k}(v, dr) := \frac{d\mu}{d|\mu|}(v, r) k(v, dr)$ the $\mathbb{R}^{d_j}$-valued kernel representing $\mu$ via $a$, i.e.

$$\mu(dv, dr) = \frac{d\mu}{d|\mu|}(v, r) |\mu|(dv, dr) = \frac{d\mu}{d|\mu|}(v, r) k(v, dr) a(dv) = \tilde{k}(v, dr) a(dv).$$

This then allows to calculate the point-wise Radon Nikodym derivative of $\nu$ with respect to $|\nu|$ and introduce the notation $\varphi = \frac{d\nu}{d|\nu|} : S^{d_j-1} \to \text{BV}_{0-}, v \mapsto \varphi_v$, such that

$$\varphi_v(x) = \frac{\int_{\mathbb{R}} \sigma(x - r) \tilde{k}(v, dr)}{\int_{\mathbb{R}} \frac{1}{g(r)} k(v, dr)}, \quad \forall x \in \mathbb{R}.$$ 

Then we get that

- for every $x \in \mathbb{R}^{d_j-1}$:

$$f(x) = c + \int_{S^{d_j-1} \times \mathbb{R}} \sigma(\langle v, x \rangle - r) \mu(dv, dr)$$

$$= c + \int_{S^{d_j-1}} \int_{\mathbb{R}} \sigma(\langle v, x \rangle - r) \tilde{k}(v, dr) a(dv)$$

$$= c + \int_{S^{d_j-1}} \left( \frac{\int_{\mathbb{R}} \sigma(\langle v, x \rangle - r) \tilde{k}(v, dr)}{\int_{\mathbb{R}} \frac{1}{g(r)} k(v, dr)} \right) \int_{\mathbb{R}} \frac{1}{g(r)} k(v, dr) a(dv)$$

$$= c + \int_{S^{d_j-1}} \varphi_v(\langle \langle v, x \rangle \rangle) |\nu|(dv).$$
• Finally, we obtain $P_j \leq P_j^{\text{measure Vec}}$ from

$$
\int_{S^{d_j-1}} |D^2 \varphi_v| \frac{1}{g(r)} |\nu|(dv) = \int_{S^{d_j-1}} \left| \frac{\hat{k}(v, \cdot)}{g(r)} \right| \frac{1}{g(r)} |\nu|(dv)
$$

$$
= \int_{S^{d_j-1}} \frac{1}{g(r)} k(v, dr) |\nu|(dv)
$$

$$
= \int_{S^{d_j-1}} \int_{R} \frac{1}{g(r)} k(v, dr) a(dv)
$$

$$
= \int_{S^{d_j-1} \times R} \frac{1}{g(r)} |\mu|(dv, dr) = |\mu| \frac{1}{g(r)}.
$$

\[ \text{2. } P_j \geq P_j^{\text{measure Vec}} \]

Let $\nu \in M^{BV}_{d_j}(S^{d_j-1})$, $c \in \mathbb{R}^{d_j}$. Then, we define $\mu \in M^d(S^{d_j-1} \times \mathbb{R})$ as

$$
\mu(B, dr) := D^2(\nu(B))(dr).
$$

Analogously to before, we have $\forall x \in \mathbb{R}^{d_j-1} : f(x) := c + \int_{S^{d_j-1}} \varphi_v(\langle v, x \rangle) |\nu|(dv) = c + \int_{S^{d_j-1} \times \mathbb{R}} \sigma(\langle v, x \rangle - r) \mu(dv, dr)$ and

$$
|\mu| \frac{1}{g} = \int_{S^{d_j-1}} |D^2 \varphi_v| \frac{1}{g(r)} d|\nu|(s).
$$

\[ \text{Lemma 24.} \]

$$
P_j^{\text{measure Vec}} = \tilde{P}_j^{\text{measure G}}
$$

**Proof** Similarly to Chizat and Bach (2018), we define an operator $T$ mapping a bounded Radon measure on $S^{d_j-1} \times \mathbb{R} \times S^{d_j-1}$ onto an $\mathbb{R}^{d_j}$-valued, bounded Radon measure on $S^{d_j-1} \times \mathbb{R}$ as

$$
T : M(S^{d_j-1} \times \mathbb{R} \times S^{d_j-1}) \rightarrow M^d(S^{d_j-1} \times \mathbb{R})
$$

$$
\nu \mapsto T(\nu), T(\nu)(B) := \int_{B \times S^{d_j-1}} w \, dv((v, r), w), \quad \forall B \in \mathcal{B}(S^{d_j-1} \times \mathbb{R}).
$$

• $\tilde{P}_j^{\text{measure G}} \geq P_j^{\text{measure Vec}}$

Then, for every $\nu \in M(S^{d_j-1} \times \mathbb{R} \times S^{d_j-1})$ s.t.

$$
f(x) = c + \int_{S^{d_j-1} \times \mathbb{R} \times S^{d_j-1}} w \sigma(\langle v, x \rangle - r)dv(v, r, w),
$$

the above defined $T(\nu)$ fulfills

$$
f(x) = c + \int_{S^{d_j-1} \times \mathbb{R} \times S^{d_j-1}} w \sigma(\langle v, x \rangle - r)dv(v, r, w)
$$

$$
= c + \int_{S^{d_j-1} \times \mathbb{R}} \sigma(\langle v, x \rangle - r)dT(\nu)(v, r),
$$

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and

\[
\left| T(\nu) \right| = \sup_{(E_i)_{1,\ldots,n} \text{ is partition of } S_{d_j-1}^{d_j-1} \times \mathbb{R}, n \in \mathbb{N}} \sum_i \left\| \int_{E_i} \frac{1}{g(r)} dT(\nu)(v, r) \right\|_2
\]

\[
= \sup_{(E_i)_{1,\ldots,n} \text{ is partition of } S_{d_j-1}^{d_j-1} \times \mathbb{R}, n \in \mathbb{N}} \sum_i \left\| \int_{E_i \times S_{d_j-1}^{d_j-1}} w \frac{1}{g(r)} d\nu(v, r, w) \right\|_2
\]

\[
\leq \int_{S_{d_j-1}^{d_j-1} \times \mathbb{R} \times S_{d_j-1}^{d_j-1}} \left\| w \right\|_2 \frac{1}{g(r)} d\nu(v, r, w)
\]

\[
= \int_{S_{d_j-1}^{d_j-1} \times \mathbb{R} \times S_{d_j-1}^{d_j-1}} \frac{1}{g(r)} d\nu(v, r, w)
\]

• \( P_{\text{measureVec}} \geq P_{\text{measureG}} \)

Conversely, for every \( \mu \in \mathfrak{M}^d_j(S_{d_j-1}^{d_j-1} \times \mathbb{R}) \) of bounded variation, there exists a \( h : S_{d_j-1}^{d_j-1} \times \mathbb{R} \to \mathbb{R}_j \) such that

\[
\mu(B) = \int_B hd|\mu| = \int_{B \times S_{d_j-1}^{d_j-1}} wd |\mu| \left( (id \times h)(v, r, w),
\right)
\]

where the last inequality takes the pushforward measure\(^{24}\) of \( |\mu| \) under \( id \times h : S_{d_j-1}^{d_j-1} \times \mathbb{R} \to S_{d_j-1}^{d_j-1} \times \mathbb{R} \times S_{d_j-1}^{d_j-1} \).

One can pull the norm inside the integral for sufficiently fine measurable partition \((E_i)\) since \( h \) is measurable:

\[
\left| \mu \right| = \sup_{(E_i)_{1,\ldots,n} \text{ is partition of } S_{d_j-1}^{d_j-1} \times \mathbb{R}, n \in \mathbb{N}} \sum_i \left\| \int_{E_i} \frac{1}{g(r)} d\mu(v, r) \right\|_2
\]

\[
= \sup_{(E_i)_{1,\ldots,n} \text{ is partition of } S_{d_j-1}^{d_j-1} \times \mathbb{R}, n \in \mathbb{N}} \sum_i \left\| \int_{E_i} \frac{1}{g(r)} hd|\mu|(v, r) \right\|_2
\]

\[
= \sup_{(E_i)_{1,\ldots,n} \text{ is partition of } S_{d_j-1}^{d_j-1} \times \mathbb{R}, n \in \mathbb{N}} \sum_i \int_{E_i} \frac{1}{g(r)} \left\| h \right\|_2 d|\mu|(v, r)
\]

\[
= \sup_{(E_i)_{1,\ldots,n} \text{ is partition of } S_{d_j-1}^{d_j-1} \times \mathbb{R}, n \in \mathbb{N}} \sum_i \int_{E_i \times S_{d_j-1}^{d_j-1}} \frac{1}{g(r)} \left\| w \right\|_2 d\nu(v, r, w)
\]

\[
= \int_{S_{d_j-1}^{d_j-1} \times \mathbb{R} \times S_{d_j-1}^{d_j-1}} \frac{1}{g(r)} \left\| w \right\|_2 d\nu(v, r, w)
\]

\[
= \int_{S_{d_j-1}^{d_j-1} \times \mathbb{R} \times S_{d_j-1}^{d_j-1}} \frac{1}{g(r)} d\nu(v, r, w)
\]

\[\text{\textsuperscript{24}. Within this argument } |\mu| \text{ denotes the total variation measure, whereas most of the time we use } |\mu| \text{ as a short notation of } |\mu|(\Omega)\]

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Moreover,

\[ f(x) = c + \int_{S^{d_j-1} \times \mathbb{R} \times S^{d_j-1}} w \sigma(\langle v, x \rangle - r) d\nu(v, r, w) \]
\[ = c + \int_{S^{d_j-1} \times \mathbb{R}} \sigma(\langle v, x \rangle - r) d\mu(v, r). \]

\[ \tilde{P}_j^{\text{measure}} \tilde{G} = \tilde{F}_j^{\text{measure}} \]

**Proof** Analogous arguments as in the proofs of Lemmas 24 and 31 prove the claim as follows.

Let \( A := S^{d_j-1} \times S^{d_j-1} \) and \( B := S^{d_j-1} \times \mathbb{R} \times S^{d_j-1} \). Also, let \( A_0 := \{(v, r, w) \in A \mid v = 0\} \) and \( A_{\not= 0} := A \setminus A_0 = \{(v, r, w) \in A \mid v \not= 0\} \), and

\[ \Psi : A_{\not= 0} \to B, \]
\[ ((v, r), w) \mapsto \left( \frac{v}{g\left(-\frac{r}{\|v\|_2}\right)}, \frac{r}{g\left(-\frac{r}{\|v\|_2}\right)}, w \right), \]

a measurable and bijective function. Additionally, let \( f \in \mathcal{F}_A \) and \( (\mu, c) \in \mathcal{C}_A \) be a minimizer of \( \tilde{P}_j^{\text{measure}}(f) \).

Next, we define the restricted measures \( \mu_{\not= 0} := \mu|_{A_{\not= 0}} \), where \( \mu|_{A_{\not= 0}}(E) := \mu(E \cap A_{\not= 0}) \), and \( \mu_0 := \mu|_{A_0} \). \(^{25}\) Then, we additionally define the measure

\[ \tilde{\mu} : B \to [0, \infty), \]
\[ \tilde{\mu}(E) := \int_E g\left(-\frac{r}{\|v\|_2}\right) d\Psi_{\not= 0}(v, r, w), \ E \in \mathcal{B}(B), \]

and the constant vector

\[ \tilde{c} := c + \int_{A_0} w d\mu_0((v, r), w) \]

\(^{25}\) Note that \( \mu(E) = \mu_{\not= 0}(E \cap A_{\not= 0}) + \mu_0(E \cap A_0) = \mu|_{A_{\not= 0}}(E \cap A_{\not= 0}) + \mu|_{A_0}(E \cap A_0) \).
where \( A_0^- := \{(0, -1), w) \mid w \in S^{d_j - 1}\} \subseteq A_0 \). For \( x \in \mathbb{R}^{d_j - 1} \) we then get
\[
  f(x) = c + \int_A \phi_x(v, r, w) \, d\mu((v, r), w)
\]
\[
  = c + \int_{A_0} \phi_x(v, r, w) \, d\mu_0((v, r), w) + \int_{A_0^\neq} \phi_x(v, r, w) \, d\mu_\neq((v, r), w)
\]
\[
  = c + \int_{A_0^-} w \, d\mu_0((v, r), w) + \int_{A_0^\neq} \phi_x(v, r, w) \, d\mu_\neq((v, r), w)
\]
\[
  = c + \int_{A_0^-} w \, d\mu_0((v, r), w) + \int_{A_0^\neq} (\phi_x \circ \Psi^{-1} \circ \Psi)(v, r, w) \, d\mu_\neq((v, r), w)
\]
\[
  = c + \int_{B} (\phi_x \circ \Psi^{-1})(v, r, w) \, d(\Psi_\#\mu_\neq)(v, r, w)
\]
\[
  = c + \int_{B} (\phi_x \circ \Psi^{-1})(v, r, w) \frac{1}{g \left( -\frac{r}{\|v\|_2} \right)} \, d\tilde{\mu}(v, r, w)
\]
\[
  = c + \int_{B} \phi_x(v, r, w) \, d\tilde{\mu}(v, r, w)
\]
where we used
(a) that in \( A_0 \) it is \( r = \pm 1 \) but in case of \( r = 1 \), we get \( \phi_x(0, 1, w) = 0 \), i.e., only the case \( r = -1 \) is of relevance where we always have \( \phi_x(0, -1, w) = w \);
(b) a change-of-variable via the pushforward measure \( \Psi_\#\mu_\neq \),
(c) the definition of \( \tilde{\mu} \) and
(d) the positive homogeneity of \( \sigma \).

Overall, we have shown that \((\tilde{\mu}, \tilde{c}) \in \mathcal{C}_B^f\).

Now, first note that
\[
  2 \int_B \frac{1}{g(r)} \, d\tilde{\mu}(v, r, w) = 2 \int_B \frac{g \left( -\frac{r}{\|v\|_2} \right)}{g(r)} \, d(\Psi_\#\mu_\neq)(v, r, w)
\]
\[
  = 2 \int_{A_0^\neq} \frac{g \left( -\frac{r}{\|v\|_2} \right)}{g \left( -\frac{r}{\|v\|_2} \right)} \, d\mu_\neq((v, r), w)
\]
\[
  = 2 \int_{A_0^\neq} \, d\mu_\neq((v, r), w) = 2 |\mu_\neq|
\]
where the last step stems from \( \mu_\neq \) being non-negative.

Next, we make a case distinction:
1. let \( \|\tilde{c}\|_2 \leq 1 \):
\[
  2\rho(\|\tilde{c}\|_2) = \|\tilde{c}\|_2^2 \leq \|c\|_2^2 + \int_{A_0} \|w\|_2^2 \, d\mu_0((v, r), w) \leq \|c\|_2^2 + |\mu_0| \leq \|c\|_2^2 + 2|\mu_0|,
\]

\[20\text{thm}\]
2. let \( \| \tilde{c} \|_2 > 1 \):

\[
2 \rho(\| \tilde{c} \|_2) = 2 \| \tilde{c} \|_2 - 1 \leq 2 \| c \|_2 + 2|\mu_0| - 1 \leq \| c \|_2^2 + 2|\mu_0|.
\]

Overall, we obtain due to (20) that

\[
2 \int_B \frac{1}{g(r)} d\tilde{\mu}(v, r, w) + 2 \rho(\| \tilde{c} \|_2) \leq 2|\mu_{\neq 0}| + 2|\mu_0| + \| c \|_2^2 = 2|\mu| + \| c \|_2^2,
\]

i.e., we have \( \tilde{P}_j^{\text{measure}}(f) \leq \tilde{P}_i^{\text{measure}}(f) \).

The case \( \tilde{P}_j^{\text{measure}}(f) \geq \tilde{P}_i^{\text{measure}}(f) \) follows in an analogous manner.

\[\blacksquare\]

**Lemma 26.** It holds that \( P_j = \tilde{P}_j^{\text{measure}}, \) for all \( j = 1 \ldots, \#\text{stacks} \), and therefore

\[
P = \tilde{P}^{\text{measure}}.
\]

**Proof** By Lemmas 23–25, we know that

\[
P_j = \tilde{P}_j^{\text{measure}}, \quad \forall j = 1 \ldots, \#\text{stacks}.
\]

Thus, for every \( f \in \mathcal{F} \)

\[
P(f) = \inf_{(h_1, \ldots, h_{\#\text{stacks}}), \text{s.t.} \atop f = \ell^{-1} o_{h_{\#\text{stacks}}} o_{\cdots} o_{\tilde{\sigma} o_{h_1}}} (P_1(h_1) + P_2(h_2) + \cdots + P_{\#\text{stacks}}(h_{\#\text{stacks}})) \tag{21}
\]

\[
= \inf_{(h_1, \ldots, h_{\#\text{stacks}}), \text{s.t.} \atop f = \ell^{-1} o_{h_{\#\text{stacks}}} o_{\cdots} o_{\tilde{\sigma} o_{h_1}}} \left( \tilde{P}_1^{\text{measure}}(h_1) + \tilde{P}_2^{\text{measure}}(h_2) + \cdots + \tilde{P}_{\#\text{stacks}}^{\text{measure}}(h_{\#\text{stacks}}) \right) \tag{22}
\]

\[
= \tilde{P}^{\text{measure}}(f). \tag{23}
\]

**F.2 Proof of Existence of Minimizers**

In Theorem 29 we prove that the minimum in eq. (15) is actually attained and in Corollary 30 we prove that the minimum in (5) is attained for the regularization functional \( \tilde{P}^{\text{measure}} \). Together with the equivalences of Appendix B, this yields the existence of minimizers in Theorem 5.

In order to prove Theorem 29 and Corollary 30, we first need some basic definitions and lemmas.

In the following, we will use the *topology of point-wise convergence* or \( \tau_{\text{ptc}} \) for short which we will denote by \( \tau_{\text{ptc}} \). For a more detailed introduction of this topology, we refer to (Munkres, 2014, § 46). For a topological vector space \( (V, \tau) \), we will also sometimes write \( (A, \tau) \) for a subset \( A \subseteq V \) if we want to emphasise the underlying topology.
Lemma 27. Let \( d_1, d_2, d_3 > 1 \) and \( A := C(\mathbb{R}^{d_1}, \mathbb{R}^{d_2}), B := \text{Lip}_{\text{Lip}}(\mathbb{R}^{d_2}, \mathbb{R}^{d_3}) \) the set of Lipschitz continuous functions with a Lipschitz constant smaller than \( L_{\text{Lip}} \) where \( \infty > L_{\text{Lip}} > 0 \), and \( Y^X \), the topological space of all functions from \( X := \mathbb{R}^{d_1} \) into \( Y := \mathbb{R}^{d_3} \), each be equipped with the \( \text{tptc} \). Then, for \( h_1 \in A \) and \( h_2 \in B \), each being \( \text{tptc} \)-continuous, with \( h_2 \) additionally being Lipschitz continuous, the concatenation

\[
\circ : ((B, \tau_{\text{tptc}}), (A, \tau_{\text{tptc}})) \rightarrow (Y^X, \tau_{\text{tptc}}), \quad (h_2 \circ h_1)(x) := h_2(h_1(x)),
\]

for \( x \in \mathbb{R}^{d_1} \), is also continuous.

Proof. First, let \( d_2 = d_3 = 1 \).

Now, let \( h := (h_1, h_2) \in A \times B \) with \( h_1 \) and \( h_2 \) being \( \text{tptc} \)-continuous and \( h_2 \) additionally being Lipschitz continuous with Lipschitz constant \( L_{h_2} < L_{\text{Lip}} \). Also, let \( x \in \mathbb{R}^{d_1} \) and \( \epsilon > 0 \). Then, the open set

\[
S(x, \epsilon) := \left\{ h \in Y^X \mid h(x) \in (h_2(h_1(x)) - \epsilon, h_2(h_1(x)) + \epsilon) \right\}
\]

forms a subbasis element about \( h_2 \circ h_1 \) at \( x \).

Next, we define

\[
U(x, \epsilon) := \left\{ (\bar{h}_1, \bar{h}_2) \in A \times B \mid \bar{h}_1(x) \in \left( h_1(x) - \frac{\epsilon}{2L_{\text{Lip}}}, h_1(x) + \frac{\epsilon}{2L_{\text{Lip}}} \right), \quad \bar{h}_2(h_1(x)) \in \left( h_2(h_1(x)) - \frac{\epsilon}{2}, h_2(h_1(x)) + \frac{\epsilon}{2} \right) \right\},
\]

(25)

which is an open set in \( (B, \tau_{\text{tptc}}) \times (A, \tau_{\text{tptc}}) \).

We first note that the set \( U(x, \epsilon) \) is not empty since \( (h_1, h_2) \in U(x, \epsilon) \).

For \( (\bar{h}_2, \bar{h}_1) \in U(x, \epsilon) \), we get

\[
\bar{h}_2(\bar{h}_1(x)) \leq \bar{h}_2(h_1(x)) + L_{\bar{h}_2} \frac{\epsilon}{2L_{\text{Lip}}} < h_2(h_1(x)) + \epsilon
\]

and, analogically,

\[
\bar{h}_2(\bar{h}_1(x)) > h_2(h_1(x)) - \epsilon,
\]

i.e., we have \( \bar{h}_2(\bar{h}_1(x)) \in S(x, \epsilon) \).

Thus, for every \( (h_1, h_2) \in A \times B \) and subbasis element \( S \) of \( h_2 \circ h_1 \), we have constructed an open neighborhood \( U \) of \( (h_1, h_2) \) such that each of its elements are mapped into \( S \) under the concatenation, i.e., the mapping in eq. (24) is continuous.

In case of \( d_2, d_3 > 1 \), we just demand each \( \bar{h}_1(x) \) and \( \bar{h}_2(h_1(x)) \) in eq. (25) to be an element of the open ball around \( h_1(x) \) with radius \( \frac{\epsilon}{2L_{\text{Lip}}} \) and \( h_2(h_1(x)) \) with radius \( \frac{\epsilon}{2} \), respectively. □
Lemma 29. Let \( j \in \{1, \ldots, \#\text{stacks}\} \), \( \mathcal{M}_j := \mathcal{M}(K_j) \times \mathbb{R}^{d_j} \) with \( K_j := S^{d_j-1} \times S^{d_j-1} \), and \( \phi_x \in C(K_j) \) with \( \phi_x(v, r) := w\sigma(v, x - r) \) for \( x \in \mathbb{R}^{d_j-1} \). Then, the surjective function

\[
\Psi_j : (\mathcal{M}_j, \tau_w) \to (\mathcal{F}_{K_j}, \tau_{\text{typc}}), \quad \Psi_j(\mu, c)(x) := c + \int_{K_j} \phi_x \, d\mu,
\]

where \( \tau_w \) denotes the weak topology, is continuous for every \( x \in \mathbb{R}^{d_j-1} \).

Proof. Let \( V \subseteq \mathcal{F}_{K_j} \) be non-empty and open, i.e., for every \( f \in V \) there exist finitely many \( x_1, \ldots, x_n \in \mathbb{R}^{d_j-1} \) and \( \epsilon > 0 \) such that

\[
V(f, n, \epsilon) := \left\{ g \in \mathcal{F}_{K_j} \mid \forall x \in \{x_1, \ldots, x_n\} : \|f(x) - g(x)\|_2 < \epsilon \right\}
\]

where \( \| \cdot \|_2 \) denotes the weak topology, is continuous for every \( w \in \mathbb{R} \).

Now, let \( (\mu, c) \in \Psi_j^{-1}(V) \), and \( \tilde{x}_1, \ldots, \tilde{x}_m \in \mathbb{R}^{d_j-1} \) and \( r > 0 \) such that \( V(\Psi_j(\mu, c), m, r) \subseteq V \). Then, we get that

\[
U((\mu, c), m, r) := \left\{ (\nu, \hat{c}) \in \mathcal{M}_j \mid \forall \tilde{x} \in \{\tilde{x}_1, \ldots, \tilde{x}_m\} : \left\| c - \hat{c} + \int_{K_j} \phi_x \, d(\mu - \nu) \right\|_2 < r \right\}
\]

i.e., we have shown that the set \( \Psi_j^{-1}(V) \) is open and, therefore, also the continuity of \( \Psi_j \). \( \blacksquare \)

Theorem 29. The infimum of \( \bar{\mathcal{F}} \mathcal{M} \mathcal{E} \mathcal{A}(\mathcal{F}) \) for every \( f \in \mathcal{F} \) is attained.

Proof. We first focus on a single stack; here, we follow a classical direct method approach:

1. \( K := S^{d_{\text{in}}} \times S^{d_{\text{out}}-1} \) and \( \mathcal{M}_0 := \mathcal{M}(K) \times \mathbb{R}^{d_{\text{out}}} \) be equipped with the norm \( |(\cdot, \cdot)| := |\cdot| + \|\cdot\|_2 \), where \( \mathcal{M}(K) \) is a closed, convex subset of the Banach space \( (\mathcal{M}_0(K), |\cdot|) \) of all finite signed Radon measures \( \mu : \mathcal{B}(K) \to \mathbb{R} \).

2. the set of functions \( \mathcal{F}_K \) and the set \( \mathcal{E}_0 := \mathcal{E}_f^K \) as in Definition 21, and

3. a minimizing sequence \( (\mu_k, c_k) \) in \( \mathcal{E}_0 \) with \( F_0(\mu_k, c_k) \to \inf_{(\mu, c) \in \mathcal{E}_0} F_0(\mu, c) \) where

\[
F_0 : \mathcal{M}_0 \to \mathbb{R}_{\geq 0}, \quad (\mu, c) \mapsto 2|\mu| + \|c\|_2^2.
\]

The set \( \mathcal{E}_0 \) is obviously convex. Additionally, it is even closed:

let \( (\tau_k, \hat{c}_k) \) be a sequence in \( \mathcal{E}_0 \) converging to \( (\tau, \hat{c}) \in \mathcal{M}_0 \). For \( \phi_x \in C(K, \mathbb{R}^{d_{\text{out}}} \) with \( \phi_x((v, r), w) := w\sigma((v, x - r) \), we then get

\[
\left\| f(x) - \hat{c} - \int_{K} \phi_x \, d\tau \right\|_2 \leq \left\| \hat{c}_k - \hat{c} + \int_{K} \phi_x \, d(\tau_k - \tau) \right\|_2 \leq \|\hat{c}_k - \hat{c}\|_2 \|\phi_x\|_\infty |\tau_k - \tau| \xrightarrow{k \to \infty} 0
\]
for all \( x \in \mathbb{R}^d \), i.e., we have \( (\tau, \hat{c}) \in \mathcal{C}_0 \) and, therefore, the set \( \mathcal{C}_0 \) is closed.

It should also be noted that the functional \( F_0 \) is coercive and, therefore, the sequence \( (\mu_k, c_k) \) is bounded.

Next, it follows from Riesz’s representation theorem that there exists an isometric isomorphism from \( \mathcal{M}(K) \) to the closed subset of all positive linear functionals of the dual space \( C(K)^* \) (see (Elstrodt, 2018, 2.26)). Given that \( C(K)^* \) is a separable Banach space, every bounded sequence in \( C(K)^* \) has a weak*-convergent subsequence due to the Banach–Alaoglu theorem. Therefore, we can say that due to the isometric isomorphism, \( (\mu_k, c_k) \) must have a weakly convergent subsequence that weakly converges against a \( (\mu_0, c_0) \in \mathcal{M}_0 \).

Since \( \mathcal{C}_0 \) is closed and convex, it is even \( (\mu_0, c_0) \in \mathcal{C}_0 \) by the Hahn-Banach separation theorem, i.e., the set \( \mathcal{C}_0 \) is weakly closed.

Additionally, because \( F_0 \) is convex and (lower semi-)continuous, we can conclude via Mazur’s lemma (see (Rudin, 1991, 3.13 Theorem)) that \( F_0(\mu_0, c_0) = \inf_{(\mu, c) \in \mathcal{C}_0} F_0(\mu, c) \), i.e., we have \( \tilde{F}_{\text{measure}}(f) = F_0(\mu, c) \) for at least one \( (\mu, c) \in \mathcal{C}_0 \).

In case of a deep stacked NN where we use the notation \( h := (h_1, \ldots, h_{#\text{stacks}}) \), the minimization problem is

\[
\tilde{F}_{\text{measure}}(f) := \inf_{h \in \mathcal{D}^f} \sum_{j=1}^{#\text{stacks}} \tilde{F}_{\text{measure}}(h_j) \tag{26}
\]

with

\[
\mathcal{D}^f := \left\{ h \mid f = \ell^{-1} \circ h_{#\text{stacks}} \circ \cdots \circ \sigma \circ h_1, h_j : \mathbb{R}^{d_j-1} \to \mathbb{R}^{d_j}, \right. \\
\left. |h_j|_{K_j} \neq \emptyset \quad \forall j = 1, \ldots, #\text{stacks} \right\}
\]

where \( f \in \mathcal{F} \) and \( K_j := S^{d_j-1} \times S^{d_j-1} \).

We will first focus on the following problem in measure space:

\[
\inf_{(\mu, c) \in \mathcal{E}} F(\mu, c) := \inf_{(\mu, c) \in \mathcal{E}} \sum_{j=1}^{#\text{stacks}} 2|\mu_j| + \|c_j\|_2^2 \tag{27}
\]

with an appropriate closed and convex set \( \mathcal{E} \subseteq \mathcal{M}^{#\text{stacks}} := \prod_{j=1}^{#\text{stacks}} \mathcal{M}_j \) with \( \mathcal{M}_j := \mathcal{M}(K_j) \times \mathbb{R}^{d_j} \), that we will define later on, for which we will show that a minimum is being attained; from this, we will then conclude the same for eq. (26):

Let \( j \in \{1, \ldots, #\text{stacks}\} \). We first define the set

\[
\mathcal{E}_j := \left\{ (\mu, c) \in \mathcal{M}_j \left| |(\mu, c)| \leq #\text{stacks} + F(\nu, \hat{c}) \right. \right\} \supseteq \left\{ (\mu, c) \in \mathcal{M}_j \left| F(\mu, c) \leq F(\nu, \hat{c}) \right. \right\}
\]

26. The weak topology on \( \mathcal{M}(K) \) is induced by \( C(K)^* \); a sequence \( (\mu_k) \) converges against a \( \mu \) w.r.t. this also called vague topology if \( f f d\mu_k \to f f \mu \) for all \( f \in C(K) \).

We also note that the product topology consisting of each of the weak topologies equals the weak topology of the product space.
with

\[(\nu, \tilde{c}) = ((\nu_1, \tilde{c}_1), \ldots, (\nu_{\#stacks}, \tilde{c}_{\#stacks})) \in \prod_{j=1}^{\#stacks} \mathcal{C}^{h_j}_{K_j} \]

for an arbitrarily chosen \(\tilde{h} \in \mathcal{D}'\) which does exist because \(f \in \mathcal{F}\). The set \(\mathcal{S}_j\) is obviously closed and convex and, therefore, weakly closed. Because it is also bounded, any sequence in \(\mathcal{S}_j\) has a subsequence weakly convergent to a point contained in the same set as we have seen in the first part of the proof, i.e., the set is weakly sequentially compact and by the Eberlein–Šmulian theorem also weakly compact. The same then also applies to the Cartesian product \(\mathcal{S} := \prod_{j=1}^{\#stacks} \mathcal{S}_j\).

Now, given that we can choose \(L_\sigma := 1\) as a Lipschitz constant for \(\sigma\), for a fixed \((\mu, c) \in \mathcal{C}^{h_j}_{K_j}\) we then get

\[\|h_j(x) - h_j(y)\|_2 \leq |\mu| \|x - y\|_2\]

for all \(x, y \in \mathbb{R}^{d_j-1}\), i.e., we have \(h_j \in \text{Lip}_{|\mu|}(\mathbb{R}^{d_j-1}, \mathbb{R}^{d_j})\) for every \(j = 1, \ldots, \#stacks\).

Next, let \(L_{\tilde{h}} := \#stacks + F(\nu, \tilde{c})\). We define the continuous and surjective function

\[\Psi : (\mathcal{M}^{\#stacks}, \tau_w) \to (\mathcal{F}_{K_1} \times \cdots \times \mathcal{F}_{K_{\#stacks}}, \tau_{ptc}),\]

\[\Psi(\mu, c) := (\Psi_1(\mu_1, c_1), \ldots, \Psi_{\#stacks}(\mu_{\#stacks}, c_{\#stacks})),\]

with \(\Psi_j\) from lemma 28. We then have \(\Psi(\mathcal{S}) \subseteq \text{Lip}_{L_{\tilde{h}}}^{\#stacks}\) with

\[\text{Lip}_{L_{\tilde{h}}}^{\#stacks} := \text{Lip}_{L_{\tilde{h}}}(\mathbb{R}^{d_0}, \mathbb{R}^{d_1}) \times \cdots \times \text{Lip}_{L_{\tilde{h}}}(\mathbb{R}^{d_{\#stacks-1}}, \mathbb{R}^{d_{\#stacks}}).\]

Now, for \(Y^X\) with \(X := \mathbb{R}^{d_0}\) and \(Y := \mathbb{R}^{d_{\#stacks}}\), the function

\[T : (\text{Lip}_{L_{\tilde{h}}}^{\#stacks}, \tau_{ptc}) \to (Y^X, \tau_{ptc}),\]

\[(h_1, \ldots, h_{\#stacks}) \mapsto \ell^{-1} \circ h_{\#stacks} \circ \cdots \circ \tilde{\sigma} \circ h_1,\]

\[\text{(28)}\]

is continuous according to lemma 27 given that \(\ell^{-1}\) and \(\tilde{\sigma}\) are both Lipschitz continuous. Then, the set \(\Psi^{-1}(T^{-1}(\{f\}))\) is weakly closed, i.e., the intersection

\[\mathcal{C} := \Psi^{-1}(T^{-1}(\{f\})) \cap \mathcal{S} \subseteq \mathcal{C}\]

is weakly compact. We want to note that due to the domain of \(T\), the pre-image \(T^{-1}(\{f\})\) is not empty.

Given that the functional \(F\) is convex and (lower semi-)continuous and, therefore, weakly lower semi-continuous, the problem in eq. (27) attains its infimum in the aforementioned weakly compact set \(\mathcal{C}\). Let us denote by \(\mathcal{S}'\) the respective solution set.
Now, in eq. (26) we can replace \( \mathcal{D}^f \) with the (tptc-)compact set \( \Psi(\hat{\mathcal{C}}) \) because for any \( h \in \mathcal{D}^f \setminus \Psi(\hat{\mathcal{C}}) \) we have that for \((\mu, c) \in \Psi^{-1}(h)\) it is \(|(\mu_j, c_j)| > \#\text{stacks} + F(\nu, \tilde{c})\) for at least one \( j = 1, \ldots, \#\text{stacks} \), i.e., it is \( F(\mu, c) > |(\mu_j, c_j)| - \#\text{stacks} > F(\nu, \tilde{c}) \) and, therefore, it would not be in the solution set of eq. (26) anyways.

Finally, we can directly conclude that the problem in eq. (26) must also attain its infimum only in every \( \hat{h} \in \Psi(\mathcal{L}^f) \subseteq \Psi(\hat{\mathcal{C}}) \) because if we assume that there exists a minimizer \( \hat{h} \in \mathcal{D}^f \) with

\[
\sum_{j=1}^{\#\text{stacks}} \hat{F}_j \text{measure}(\hat{h}_j) < \sum_{j=1}^{\#\text{stacks}} \hat{F}_j \text{measure}(\hat{h}_j),
\]

then, following from the proof of the single stack case, there must exist a \((\hat{\mu}, \hat{c}) \in \Psi^{-1}(\hat{h})\) with

\[
F(\hat{\mu}, \hat{c}) = \sum_{j=1}^{\#\text{stacks}} \hat{F}_j \text{measure}(\hat{h}_j) < \sum_{j=1}^{\#\text{stacks}} \hat{F}_j \text{measure}(\hat{h}_j) = F(\hat{\mu}, \hat{c})
\]

for all \((\hat{\mu}, \hat{c}) \in \Psi^{-1}(\hat{h})\) which contradicts \( \Psi^{-1}(\hat{h}) \in \mathcal{L}^f \) being a minimizer.

\[ \blacksquare \]

**Corollary 30.** The infimum of \( L(f) + \lambda \hat{F}^{\text{measure}}(f) \) with \( \lambda > 0 \) over all \( f \in \mathcal{F} \) is attained.

**Proof** We will reuse objects and notations defined within the proof of theorem 29: We want to show that for \( \lambda > 0 \), the problem

\[
\inf_{f \in \mathcal{F}} G(f) := \inf_{f \in \mathcal{F}} L(f) + \lambda \hat{F}^{\text{measure}}(f)
\]

attains its infimum in \( \mathcal{F} \):

Let \( j \in \{1, \ldots, \#\text{stacks}\} \), \( \hat{h}_j \in \mathcal{F}_{K_j} \) be arbitrarily chosen, and \( g := T(\hat{h}_1, \ldots, \hat{h}_{\#\text{stacks}}) \) with \( T \) from eq. (28) (e.g., \( \hat{h} = 0 \) and, thus, \( g = 0 \)). Analogous to the proof of theorem 29, we can conclude that the Cartesian product \( \hat{\mathcal{G}} := \prod_{j=1}^{\#\text{stacks}} \hat{\mathcal{G}}_j \) with

\[
\hat{\mathcal{G}}_j := \left\{ (\mu, c) \in \mathcal{M}(K_j) \times \mathbb{R}^{d_j} \mid |(\mu, c)| \leq \#\text{stacks} + G(g)/\lambda \right\}
\]

is weakly compact.

Now, let \( L_{\hat{h}} := \#\text{stacks} + G(g)/\lambda \), \( x \in \mathbb{R}^{d_{\text{in}}} \), and the continuous point evaluation operator

\[
\delta_x : (\text{Lip}_{L^f}(\mathbb{R}^{d_{\text{in}}}, \mathbb{R}^{d_{\text{out}}}), \tau_{\text{tptc}}) \to \mathbb{R}^{d_{\text{out}}}, \ f \mapsto f(x),
\]
with $L_f := L_{f-1} \prod_{j=1}^{#stacks-1} L_{\tilde{\sigma}} \prod_{j=1}^{#stacks} L_{\tilde{h}}$.

Now, given that $x \mapsto x^2$ is continuous, we can conclude that the loss function

$$L : (\text{Lip}_{L_f}(\mathbb{R}^{d_{in}}, \mathbb{R}^{d_{out}}), \tau_{tpc}) \rightarrow \mathbb{R}_{\geq 0}, \quad L(f) := \sum_{j=1}^{N} (\delta_{x_j}^{\text{train}}(f) - y_j^{\text{train}})^2,$$

with training data $\{(x_j^{\text{train}}, y_j^{\text{train}})\}_{j=1}^{N}$ is continuous.

Next, we define the functional

$$\tilde{G} : (\tilde{\mathcal{S}}, \tau_w) \rightarrow (\mathbb{R}, \|\cdot\|_2), \quad (\mu, c) \mapsto \tilde{G}(\mu, c) := (L \circ T \circ \Phi + \lambda F)(\mu, c),$$

which is lower semi-continuous given the continuity of $L$, $T$ and $\Phi$, and the lower semi-continuity of $F$. Then, the problem

$$\inf_{(\mu, c) \in \tilde{\mathcal{S}}} \tilde{G}(\mu, c)$$

does attain its infimum. Let us denote by $\mathcal{L}^F$ the respective solution set.

Finally, we can directly conclude that eq. (29) must also attain its infimum only in every $\hat{f} \in (T \circ \Psi)(\mathcal{L}^F)$ because if we assume that there exists a minimizer $\hat{f} \in \mathcal{F} \setminus (T \circ \Psi)(\mathcal{L}^F)$ with $G(\hat{f}) < G(\hat{f})$, then there must exist a $(\hat{\mu}, \hat{c}) \in (T \circ \Psi)^{-1}(\hat{f})$ with

$$\tilde{G}(\hat{\mu}, \hat{c}) = (G \circ T \circ \Psi)(\hat{\mu}, \hat{c}) < (G \circ T \circ \Psi)(\hat{\mu}, \hat{c}) = \tilde{G}(\hat{\mu}, \hat{c})$$

for all $(\hat{\mu}, \hat{c}) \in (T \circ \Psi)^{-1}(\hat{h})$ which contradicts $(T \circ \Psi)^{-1}(\hat{f}) \in \mathcal{L}^F$ being a minimizer.

\section*{F.3 Proof of Theorem 5}

In this appendix F.3, we will first prove multiple Lemmas, that we then use to conclude the proof of Theorem 5.

For the proof we use the mathematically precise definition of $P_j$ given in Definition 15.

Similar theorems for shallow NNs with one-dimensional output have already been presented in concurrent and previous work, such as Chizat and Bach (2020); Neyshabur et al. (2014); Ongie et al. (2019); Savarese et al. (2019); Williams et al. (2019); Heiss et al. (2019). More recently, independently and in parallel to us, Parhi and Nowak (2022) have proven a theorem, which is even more similar to Theorem 5 for a slightly different regularization.

To get some intuition for Theorem 5 it is particularly important to understand the equivalence in function space of solutions to different optimization problems on parameter space (leading to different solutions in parameter space). This equivalence is shown in the following Lemma 31.
Lemma 31. Let $\mathcal{NN}_j$ be a stack (i.e., $\#$stacks $= 1$) with input dimension $d_{in}$, output dimension $d_{out}$, number of hidden neurons $n_1$, and parameters $\theta := (v, b, w, c)$. It holds that the set of solutions

$$\left\{ \mathcal{NN}_{\theta^*} \bigg| \theta^* \in \arg \min_{\theta} \left( L(\mathcal{NN}_\theta) + \lambda \|\theta\|_2^2 \right) \right\}, \quad \text{(30)}$$

$$\left\{ \mathcal{NN}_{\theta^*} \bigg| \theta^* \in \arg \min_{\theta, \text{ s.t. } \forall k \in \{1, \ldots, n_1\} : \|v_k, b_k\|_2 = 1} \left( L(\mathcal{NN}_\theta) + \lambda \left( \|c\|_2^2 + \sum_{k=1}^{n_1} 2\|w_k\|_2 \right) \right) \right\} \quad \text{(31)}$$

$$\left\{ \mathcal{NN}_{\theta^*} \bigg| \theta^* \in \arg \min_{\theta, \text{ s.t. } \forall k \in \{1, \ldots, n_1\} : \|v_k\|_2 = 1} \left( L(\mathcal{NN}_\theta) + \lambda \left( 2\rho(||c||_2) \, \text{if } w_{n_1} = 0 + 2 \sum_{k=1}^{n_1} \|w_k\|_2 \right) \right) \right\},$$

and

$$\arg \min_{f \in \mathcal{F}_n} \left( L(f) + \lambda \tilde{E}^{\text{measure}}(f) \right),$$

coincide, where $\rho(r) = \left\{ \begin{array}{ll} r^2/2 & \text{, if } |r| \leq 1 \\ |r| - 1/2 & \text{, else} \end{array} \right.$ is the Huber-loss, and

$$\mathcal{F}_n := \left\{ f \in \mathcal{F} \bigg| f = \ell^{-1} \circ h_1, \exists (\mu, c) \in \mathcal{M}_{n_1}(S^{d_0} \times S^{d_1-1}) \times \mathbb{R}^{d_1} : h_1 : \mathbb{R}^{d_0} \to \mathbb{R}^{d_1}, h_1(x) := \int_{S^{d_0} \times S^{d_1-1}} w \sigma((v, \cdot) - r) \, d\mu((v, r), w) + c \right\},$$

and $\mathcal{M}_{n_1}(S^{d_0} \times S^{d_1-1}) := \{ \mu \in \mathcal{M}(S^{d_0} \times S^{d_0-1}) : \#\text{supp}(\mu) = n_1 \}$ is the set of Radon-measures only supported on $n_1$ points.

Proof For a simpler notation we have formulated the statement for $j = 1$, but the proof works analogously for other every stack $j$, therefore we write $j$ instead of 1 within this proof. By the positive homogeneity of the ReLU, for all $x \in \mathbb{R}^{d_{in}}$ we have

$$\mathcal{NN}_\theta(x) = \sum_{k=1}^{n_j} w_k \max(0, b_k + \langle v_k, x \rangle) + c = \sum_{k=1}^{n_j} \tilde{w}_k \max(0, \tilde{b}_k + \langle \tilde{v}_k, x \rangle) + c,$$

where $\tilde{w}_k := w_k \sqrt{\|v_k, b_k\|_2^2 / \|w_k\|_2^2}$, $\tilde{v}_k := v_k \sqrt{\|w_k\|_2 / \|v_k, b_k\|_2}$, and $\tilde{b}_k := b_k \sqrt{\|w_k\|_2 / \|v_k, b_k\|_2}$. We define $\tilde{\theta} := (\tilde{v}, \tilde{b}, \tilde{w}, c)$. Then,

1. $\mathcal{NN}_\theta = \mathcal{NN}_{\tilde{\theta}}$ and thus $L(\mathcal{NN}_\theta) = L(\mathcal{NN}_{\tilde{\theta}})$,

2. with the inequality between geometric and arithmetic mean for every $\theta$

$$\frac{1}{2} \|\theta\|^2_2 = \frac{1}{2} \left( \sum_{k=1}^{n_j} \|w_k\|_2^2 + \|v_k, b_k\|_2^2 + \|c\|_2^2 \right) \geq \left( \sum_{k=1}^{n_j} \|w_k\|_2 \|v_k, b_k\|_2 \right) + \frac{1}{2} \|c\|_2^2.$$
3. and equality holds for $\tilde{\theta}$

$$
\frac{1}{2} \|\tilde{\theta}\|_2^2 = \frac{1}{2} \left( \sum_{k=1}^{n_j} \|\tilde{w}_k\|_2 + \left\| (\tilde{v}_k, \tilde{b}_k) \right\|_2^2 + \|c\|_2^2 \right)
\]
$$

$$
= \frac{1}{2} \left( \sum_{k=1}^{n_j} \|w_k\|_2 \|v_k, b_k\|_2 + \|w_k\|_2 \|v_k, b_k\|_2 \right) + \frac{1}{2} \|c\|_2^2
\]
$$

$$
= \sum_{k=1}^{n_j} \|w_k\|_2 \|v_k, b_k\|_2 + \frac{1}{2} \|c\|_2^2
\]
$$

$$
= \sum_{k=1}^{n_j} \|\tilde{w}_k\|_2 \|\tilde{v}_k, \tilde{b}_k\|_2 + \frac{1}{2} \|c\|_2^2
\]
$$

$$
= \sum_{k=1}^{k^*} \|\tilde{w}_k\|_2 \|\tilde{v}_k, \tilde{b}_k\|_2 \left[ 1 + \left( \frac{\tilde{b}_k}{\|\tilde{v}_k\|_2} \right)^2 \right] + \sum_{k=k^*+1}^{n_j} \|\tilde{w}_k\|_2 |\tilde{b}_k| + \frac{1}{2} \|c\|_2^2,
\]
$$

where we assume w.l.o.g. that there exists an index $k^* \in \{1, \ldots, n_j\}$, such that $v_k \neq 0$ for all $k \leq k^*$ and $v_k = 0$ for all $k \geq k^* + 1$. Thus, if $\theta$ is optimal with respect to (30), $\tilde{\theta}$ is optimal with respect to (30) as well and $\mathcal{N}_j \supseteq \mathcal{N}_j^\vee$.

4. Then $\tilde{\tilde{\theta}} = (\tilde{v}, \tilde{b}, \tilde{w}, c)$ with $\tilde{\tilde{w}}_k := \tilde{w}_k \|\tilde{v}_k, \tilde{b}_k\|_2$, $\tilde{\tilde{v}}_k := \tilde{v}_k \|\tilde{v}_k, \tilde{b}_k\|_2$ and $\tilde{\tilde{b}}_k := \frac{1}{\|\tilde{v}_k\|_2} \tilde{b}_k$.

Then $\tilde{\tilde{\theta}}$ is optimal with respect to (31) and $\mathcal{N}_j \supseteq \mathcal{N}_j^\vee$. Thus, (30)$\supseteq$(31). Analogously, one can prove that (30)$\supseteq$(31).

5. Analogously, one can show (30)=$(32)$ by setting $\tilde{\tilde{\theta}} = (\tilde{v}, \tilde{b}, \tilde{w}, c)$ with $\tilde{c} := c + \sum_{k=k^*+1}^{n_j} \tilde{w}_k |\tilde{b}_k|$ and $\forall k \in \{1, \ldots, k^*\}: \tilde{\tilde{w}}_k := \tilde{w}_k \|\tilde{v}_k, \tilde{b}_k\|_2$, $\tilde{\tilde{v}}_k := \tilde{v}_k \|\tilde{v}_k, \tilde{b}_k\|_2$ and $\tilde{\tilde{b}}_k := \frac{1}{\|\tilde{v}_k\|_2} \tilde{b}_k$.

$\forall k \in \{k^*+1, \ldots, n_j\}: \tilde{\tilde{w}}_k := 0$, $\tilde{\tilde{v}}_k := 0$ and $\tilde{\tilde{b}}_k := 0$. Then $\tilde{\tilde{\theta}}$ is optimal with respect to (32) and $\mathcal{N}_j \supseteq \mathcal{N}_j^\vee$. Thus, (30)$\supseteq$(32).

Analogously, one can prove that (30)$\supseteq$(32).

6. (31)=$(33)$, since we can translate parameters $\tilde{\tilde{\theta}}$ into measures $\mu := \sum_{k=1}^{n_j} \delta_{(\tilde{\tilde{v}}_k, -\tilde{\tilde{b}}_k, \tilde{\tilde{w}}_k)} \in \mathcal{M}_{n_j}(S^{d_j-1} \times S^{d_j-1})$ and vice versa.

Consequently, the sets (30), (31), (32) and (33) are equal.

---

27. We can make this assumption be without loss of generality, since the order of the neurons does not matter.
Lemma 31 has only shown the equivalence for NNs with a finite number of neurons. The remainder of this appendix F.3 will prove the infinite width limit. This proof will rely on Definition 16 and lemmas 26 and 37.

F.3.1 Proof of (8)

**Lemma 32.** It holds that for a sufficiently large\(^{28}\) number of neurons \(n\) every solution \(\mathcal{NN}_{\gamma,\lambda}\) with

\[
\theta^{\gamma,\lambda} \in \arg \min_{\theta} \left( L(\mathcal{NN}_\theta) + \lambda \|\theta\|_2^2 \right),
\]

satisfies

\[
\mathcal{NN}_{\gamma,\lambda} \in \arg \min_{f \in \mathcal{F}} \left( L(f) + \lambda \tilde{P} \right).
\]

**Proof** We will first prove the statement for \(\tilde{P}\) measure from Definition 16. By the equivalence of (30) and (33) in Lemma 31 for every stack we obtain, that the neural network \(\mathcal{NN}_{\gamma,\lambda}\) has optimal parameters according to (34) if and only if

\[
\mathcal{NN}_{\gamma,\lambda} \in \arg \min_{f \in \mathcal{F}_\gamma} \left( L(f) + \lambda \tilde{P} \right) \subseteq \arg \min_{f \in \mathcal{F}_\gamma} \left( L(f) + \lambda \tilde{P} \right),
\]

where

\[
\mathcal{F}_\gamma := \left\{ f \in \mathcal{F} \mid f = \ell^{-1} \circ h_{\# \text{stacks}} \circ \cdots \circ \tilde{\sigma} \circ h_1, \quad \forall j \in \{1, \ldots, \# \text{stacks}\} : \exists (\mu_j, c_j) \in \mathcal{M}_{n_j}(S^{d_j-1} \times S^{d_j-1}) \times \mathbb{R}^{d_j} : \right. \]

\[
h_j : \mathbb{R}^{d_j-1} \to \mathbb{R}^{d_j}, \quad h_j(x) := \int_{S^{d_j-1} \times S^{d_j-1}} w \sigma(\langle v, \cdot \rangle - r) d\mu_j((v, r), w) + c_j\]

and \(\mathcal{M}_{n_j}(S^{d_j-1} \times S^{d_j-1}) := \{ \mu \in \mathcal{M}(S^{d_j-1} \times S^{d_j-1}) : \# \text{supp}(\mu) = n_j \} \) is the set of Radon-measures only supported on \(n_j\) points.

By Lemma 37, \( \arg \min_{f \in \mathcal{F}} \left( L(f) + \lambda \tilde{P} \right) \) contains a function \( f \) that can be expressed via finite measures \( \mu_j \in \mathcal{M}_{n_j}(S^{d_j-1} \times S^{d_j-1}) \). This implies for all \( n > \tilde{n} \)

\[
\min_{f \in \mathcal{F}_\gamma} \left( L(f) + \lambda \tilde{P} \right) = \min_{f \in \mathcal{F}} \left( L(f) + \lambda \tilde{P} \right),
\]

since “\( \geq \)” obviously holds because removing restrictions cannot increase the minimum and “\( \leq \)” again holds because of Lemma 37. Therefore, (36) implies

\[
\mathcal{NN}_{\gamma,\lambda} \in \arg \min_{f \in \mathcal{F}} \left( L(f) + \lambda \tilde{P} \right) = \arg \min_{f \in \mathcal{F}} \left( L(f) + \lambda P(f) \right),
\]

where the last equality holds because of Lemma 26.

---

\(^{28}\) See appendix C for explicit bounds how many neurons are sufficient.
F.3.2 Proof of (9)

**Lemma 33.** Furthermore, it holds that for every non-empty compact \( K \subset \mathbb{R}^{d_{in}} \), \( \forall \epsilon \in \mathbb{R}_{>0} : \)

\[
\forall f^{*,\lambda} \in \arg \min_{f \in \mathcal{F}} (L(f) + \lambda P(f)) : \exists \bar{n} \in \mathbb{N} \#^{\text{stacks}} : \forall n > \bar{n} : \\
\exists \theta^{*,\lambda} \in \arg \min_{\theta} \left( L(\mathcal{N}_\lambda \mathcal{N}_\lambda) + \lambda \|\theta\|_2^2 \right) : \sup_{x \in K} \|f^{*,\lambda}(x) - \mathcal{N}_\lambda^\#^{\text{stacks},\lambda}(x)\|_\infty < \epsilon \tag{38}
\]

**Proof** We prove the statement for \( \bar{F}^{\text{measure}} \) from Definition 16 instead of \( P \), since Lemma 26 tells us that \( \bar{F}^{\text{measure}} = P \). Let \( f^{*,\lambda} \in \arg \min_{f \in \mathcal{F}} (L(f) + \lambda \bar{F}^{\text{measure}}(f)) \). We define \( p^* := \bar{F}^{\text{measure}}(f^{*,\lambda}) \). Then \( f^{*,\lambda} \) is Lipschitz-continuous with Lipschitz-constant at most \( C^{\text{Lip}} \leq \left( \frac{p^*}{2 \#^{\text{stacks}}} \right) \). (With a slightly more technical proof one can even show that \( C^{\text{Lip}} \leq \left( \frac{p^*}{2 \#^{\text{stacks}}} \right) \).

Let \( \epsilon > 0 \). Since \( K \) is compact, there exists a finite number \( N_{K,\delta} \in \mathbb{N} \) of points \( \left( x_{i,\text{train}}^{\text{train}} \right)_{i \in \{1, \ldots, N_{K,\delta}\}} \) such that for every \( x \in K \) there exists \( x_{i,\text{train}}^{\text{train}} \) with \( \|x_{i,\text{train}}^{\text{train}} - x\|_2 < \delta := \frac{\epsilon}{2 C^{\text{Lip}}} \). Lemma 37 tells us that there exists a network \( \mathcal{N}_\lambda \mathcal{N}_\lambda \) with (non-bottleneck) widths \( \bar{n} \), such that \( L(\mathcal{N}_\lambda \mathcal{N}_\lambda) = L(f^{*,\lambda}), \mathcal{N}_\lambda \mathcal{N}_\lambda(x_{i,\text{train}}^{\text{train}}) = f^{*,\lambda}(x_{i,\text{train}}^{\text{train}}) \) for all \( i \in \{1, \ldots, N_{K,\delta}\} \) and \( \bar{F}^{\text{measure}}(\mathcal{N}_\lambda \mathcal{N}_\lambda) = \bar{F}^{\text{measure}}(f^{*,\lambda}) \).

Thus, also \( \mathcal{N}_\lambda \mathcal{N}_\lambda \) has a Lipschitz-constant of at most \( C^{\text{Lip}} \leq \left( \frac{p^*}{2 \#^{\text{stacks}}} \right) \). This implies that \( \mathcal{N}_\lambda \mathcal{N}_\lambda - f^{*,\lambda} \) has a Lipschitz-constant of at most \( 2 C^{\text{Lip}} \). Consequently, \( \sup_{x \in K} \|\mathcal{N}_\lambda \mathcal{N}_\lambda - f^{*,\lambda}\|_\infty < \epsilon \).

\[ \square \]

F.4 Proof of Corollary 6

We prove a similar statement in Corollary 34. Moreover, we give further viewpoints on Corollaries 6 and 34 in Corollary 35. Then we prove Corollary 6. In the remainder of Appendix F.4 we state and prove the lemmas needed for the proof of Corollary 34.

**Corollary 34** (Corollary 6 restated). Let \( \sigma \) be ReLU or linear. For every number of training data points \( N \), there exist \( n^* \in \mathbb{N} \#^{\text{stacks}} \) and \( d^* \in \mathbb{N} \#^{\text{stacks}{-1}} \), such that for every solution \( \theta^{*,\lambda} \in \arg \min_{\theta \in \Theta(n^*,d^*)} \left( L(\mathcal{N}_\lambda \mathcal{N}_\lambda) + \lambda \|\theta\|_2^2 \right) \) with network-dimensions \( n^* \) and \( d^* \), the corresponding neural network \( \mathcal{N}_\lambda \mathcal{N}_\lambda \) is also a solution of \( \arg \min_{f \in \mathcal{F}} (L(f) + \lambda P_{(d)}(f)) \) for all bottleneck dimensions \( d \geq d^* \). I.e.,

\[
\forall N \in \mathbb{N} : \exists n^* \in \mathbb{N} \#^{\text{stacks}}, d^* \in \mathbb{N} \#^{\text{stacks}{-1}} : \forall d > d^* : \\
\forall \theta^{*,\lambda} \in \arg \min_{\theta \in \Theta(n^*,d^*)} \left( L(\mathcal{N}_\lambda \mathcal{N}_\lambda) + \lambda \|\theta\|_2^2 \right) : \mathcal{N}_\lambda \mathcal{N}_\lambda \in \arg \min_{f \in \mathcal{F}} (L(f) + \lambda P_{(d)}(f)),
\]

where \( \mathcal{N}_\lambda \mathcal{N}_\lambda \) has network dimensions \( n^* \) and \( d^* \) and \( P_{(d)} \) has bottleneck dimensions \( d \).

**Proof** According to Corollary 30, there exists a minimizer \( f^* \in \arg \min_{f \in \mathcal{F}} (L(f) + \lambda P(f)) \). By Lemma 26, \( f^* \) is also a solution of

\[
\arg \min_{f \in \mathcal{F}} \left( L(f) + \lambda \bar{F}^{\text{measure}}(f) \right)
\]
Therefore, $f^*$ admits a representation
\[ f = \ell^{-1} \circ h_{\#\text{stacks}} \circ \tilde{\sigma} \circ \ldots \circ \tilde{\sigma} \circ h_1 \]
with stacks
\[ \forall x \in \mathbb{R}^{d_j-1} : h_j(x) = c_j + \int_{S^{d_j-1} \times S^{d_j-1}} w\sigma((v, x) - r)d\mu_j((v, r), w), \]
with $c_j \in \mathbb{R}^{d_j}$ and measures $\mu_j \in \mathcal{M}(\Omega_j)$ and $\Omega_j := S^{d_j-1} \times S^{d_j}$.

Then, by Lemma 37, there exists a NN $\tilde{f}$ whose corresponding measures $\tilde{\mu}_j$ are supported on a finite number of nodes $n^* := (\tilde{n}_1, \ldots, \tilde{n}_{\#\text{stacks}})$ and $d^* := (\tilde{d}_1, \ldots, \tilde{d}_{\#\text{stacks}-1})$, s.t. we have
\[ L(f) = L(\tilde{f}) \]
\[ c_j = \tilde{c}_j \text{ and } \mu_j(\Omega_j) = \tilde{\mu}_j(\tilde{\Omega}_j), \quad \forall j = 1, \ldots, \#\text{stacks}. \] (40)

The latter implies that $\tilde{\tilde{\mu}}^\text{measure}(f) = \tilde{\tilde{\mu}}^\text{measure}(\tilde{f})$. Thus in total,
\[ \tilde{f} \in \arg\min_{f \in \mathcal{F}} \left( L(f) + \lambda \tilde{\tilde{\mu}}^\text{measure}(f) \right). \]

By the equivalence of (30) and (33) in Lemma 31, there exists $\theta^* \in \arg\min_{\theta \in \Theta} \left( L(\mathcal{N}\mathcal{N}_\beta) + \lambda \|\theta\|_2^2 \right)$ s.t. $f = \mathcal{N}\mathcal{N}_{\theta^*}$. \( \blacksquare \)

**Corollary 35.** Let $\tilde{\sigma}$ be ReLU or linear. For every number of training data points $N$, there exist $n^* \in \mathbb{N}^{\#\text{stacks}}$ and $d^* \in \mathbb{N}^{\#\text{stacks}-1}$ such that for all bottleneck dimensions $d \geq d^*$, 30

1. and for every $n \geq n^*$,
\[ \min_{\theta \in \Theta(n^*, d^*)} \left( L(\mathcal{N}\mathcal{N}_\beta) + \lambda \|\theta\|_2^2 \right) \]
\[ = \min_{\theta \in \Theta(n, d)} \left( L(\mathcal{N}\mathcal{N}_\beta) + \lambda \|\theta\|_2^2 \right) \]
\[ = \min_{f \in \mathcal{F}} \left( L(f) + \lambda P(d^*)(f) \right) \]
\[ = \min_{f \in \mathcal{F}} \left( L(f) + \lambda P(d)(f) \right). \]

2. and for every $n \geq n^*$ there exists a solution $\mathcal{N}\mathcal{N}_{\theta^*, \lambda}$ with
\[ \theta^*, \lambda \in \arg\min_{\theta \in \Theta(n, d)} \left( L(\mathcal{N}\mathcal{N}_\beta) + \lambda \|\theta\|_2^2 \right) \]
and network-dimensions $n$ and $d$, such that the function $\mathcal{N}\mathcal{N}_{\theta^*, \lambda}$ can also be represented by a network with dimensions $n^*$ and $d^*$.

30. Note that $\mathcal{N}\mathcal{N}_\beta$ depends on $d$ and $n$ since it refers to a network with $d_j$ and $n_j$ neurons in the corresponding layers. Moreover, $d \geq d^*$ is always understood component-wise, i.e., $\forall j \in \{1, \ldots, \#\text{stacks} - 1\}$: $d_j \geq d_j^*$, while $d_0 = d_{\text{in}}$ and $d_{\#\text{stacks}} = d_{\text{out}}$ are considered constant throughout the paper.
3. there exists a solution

\[ f_{*\lambda}^{*} \in \arg\min_{f \in F} \left( L(f) + \lambda P_{(d)}(f) \right) \]

(where \( P_{(d)} \) denotes \( P \) with bottleneck-dimensions \( d_j \)).

s.t. there exist parameters

\[ \theta_{*\lambda} \in \arg\min_{\theta \in \Theta_{(n^*,d^*)}} \left( L(\mathcal{N}\theta) + \lambda \|\theta\|^2 \right) \]

with dimensions \( n^* \) and \( d^* \) such that \( \mathcal{N}\theta_{*\lambda} = f_{*\lambda}^{*} \).

4. and for every \( \tilde{n} \geq n \geq n^* \) and for every \( \tilde{d} \geq d \geq d^* \) the sets of solutions are nested:

\[ \emptyset \neq \mathcal{N}\theta_{*\lambda} : \arg\min_{\theta \in \Theta_{(n,d)}} \left( L(\mathcal{N}\theta) + \lambda \|\theta\|^2 \right) \subseteq \mathcal{N}\theta_{*\lambda} : \arg\min_{\theta \in \Theta_{(n,d)}} \left( L(\mathcal{N}\theta) + \lambda \|\theta\|^2 \right) \subseteq \mathcal{N}\theta_{*\lambda} : \arg\min_{\theta \in \Theta_{(\tilde{n},\tilde{d})}} \left( L(\mathcal{N}\theta) + \lambda \|\theta\|^2 \right) \].

5. and for every \( \tilde{d} \geq d \geq d^* \) and for every solution

\[ \theta_{*\lambda} \in \arg\min_{\theta \in \Theta_{(n^*,d^*)}} \left( L(\mathcal{N}\theta) + \lambda \|\theta\|^2 \right) \]

it holds that the sets of solutions are nested:

\[ \mathcal{N}\theta_{*\lambda} \in \arg\min_{f \in F} \left( L(f) + \lambda P_{(d^*)}(f) \right) \subseteq \arg\min_{f \in F} \left( L(f) + \lambda P_{(d)}(f) \right) \subseteq \arg\min_{f \in F} \left( L(f) + \lambda P_{(\tilde{d}^*)}(f) \right) \).

**Proof** These statements follow quite directly from Theorem 5 and corollary 34.

**Proof of Corollary 6.** Items 4 and 5 in Corollary 35 show that (10a)=(10b) and (10c)=(10d) (where both equalities would even hold without the closure).

Equation (8) in Theorem 5 implies that (10b)\( \subseteq \) (10d) (without the closure). Equation (9) in Theorem 5 implies that (10b)\( \supseteq \) (10d), because of the closure. Thus, (10b)=(10d).

Therefore, (10a)=(10b)=(10c)=(10d) holds.

The second part of Corollary 6 follows directly from Corollary 34.

**Lemma 36.** We define \( \Omega := S^{d_{in}} \times S^{d_{out}-1} \) and let \( \mu \in \mathcal{M}(\Omega) \) be a Radon-measure. Based on this measure, we define a function \( f \) as

\[ \forall x \in \mathbb{R}^{d_{in}} : f(x) = \int_{S^{d_{in}} \times S^{d_{out}-1}} w\sigma(\langle v, x \rangle - r) d\mu((v, r), w) \]

31. \( P \) always depends on the bottleneck-dimensions \( d \), but by writing \( P_{(d)} \) we make the dependency on \( d \) more explicit at this point.
Let $I_1 \cup \ldots \cup I_{d_{out}} = \{1, \ldots, N\}$. Then there exists a Radon measure $\tilde{\mu} \in \mathcal{M}_{N+1}(S^{d_{in}} \times S^{d_{out}-1})$, such that

$$\forall k \in \{1, \ldots, d_{out}\} : \forall i \in I_k : f_k(x_i^{train}) = \hat{f}_k(x_i^{train}),$$

where $\hat{f}(x) = \int_{S^{d_{in}} \times S^{d_{out}-1}} w_\sigma(\langle v, x \rangle - r)d\tilde{\mu}(\langle v, r \rangle, w)$ and

$$\mu(\Omega) = \tilde{\mu}(\Omega).$$

**Proof**

$$\forall x \in \mathbb{R}^{d_{in}} : f(x) = \mu(\Omega) \int_{\Omega} w \max(0, \langle v, x \rangle - r) \ d\tilde{\mu}(\langle v, r \rangle, w) \quad (42)$$

for a probability measure $\tilde{\mu} = \frac{\mu}{\mu(\Omega)} \in \mathcal{P}(\Omega)$.

We define $k(i) = k$, such that $i \in I_k$. By a change of measure $\tilde{\mu} := \tilde{\mu} \circ \beta \in \mathcal{P}(C)$ with

$$\beta : (v, r, w) \mapsto \left( w_{k(i)} \max(0, \langle v, x_i^{train} \rangle - r) \right)_{i \in \{1, \ldots, N\}}$$

and $C := \beta(\Omega)$, we finally obtain

$$(f_k(i)(x_i^{train}))_{i \in \{1, \ldots, N\}} = \mu(\Omega) \int_{\Omega} \beta(v, r, w) d\tilde{\mu}(\langle v, r \rangle, w) = \mu(\Omega) \int_{C} z d\tilde{\mu}(z). \quad (43)$$

Given that $C \subseteq \mathbb{R}^N$ is bounded and $\text{supp}(\tilde{\mu}) \subseteq C$, we obtain by (Rosset et al., 2007, Lemma 2 on p. 557) that $\int_{C} z d\tilde{\mu}(z) \in \text{conv}(C)$ where $\text{conv}(C)$ is the convex hull of $C$. Then by Caratheodory’s Convex Hull Theorem, the integral $\int_{C} z d\tilde{\mu}(z)$ can be expressed as a convex combination of at most $N + 1$ points $c_j \in C$, i.e., $\int_{C} z d\tilde{\mu}(z) = \sum_{j=1}^{N+1} t_j c_j$ (a shallow network of finite width). This convex combination of $N + 1$ points defines a measure $\bar{\mu} := \mu(\Omega) \sum_{j=1}^{N+1} t_j \delta_{\omega_j}$ as the convex combination of $N + 1$ Dirac-distributions at points $\omega_j \in \beta^{-1}(c_j)$. Thus, we obtain,

$$\hat{f}_k(i)(x_i^{train}) = \int_{\Omega} w_{k(i)}(v) \sigma(\langle v, x_i^{train} \rangle - r) d\tilde{\mu}(\langle v, r \rangle, w) = \int_{\Omega} \beta_{ij}(v, r, w) d\tilde{\mu}(\langle v, r \rangle, w) = \mu(\Omega) \sum_{j=1}^{N+1} t_j c_j = \left( \mu(\Omega) \sum_{j=1}^{N+1} t_j c_j \right)_{i} = \left( \mu(\Omega) \int_{C} z d\tilde{\mu}(z) \right)_{i} \hat{f}_k(i)(x_i^{train}).$$

**Lemma 37.** We define for $j = 1, \ldots, \#\text{stacks}$, the sets $\Omega_j := S^{d_{j-1}} \times S^{d_{j-1}}$ and let $\mu_j \in \mathcal{M}(\Omega_j)$ be Radon-measures. Let $f : \mathbb{R}^{d_{in}} \rightarrow \mathbb{R}^{d_{out}}$ be a function that can then be written as

$$f = \ell^{-1} \circ h_\#\text{stacks} \circ \sigma \circ \ldots \circ \sigma \circ h_1$$

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with stacks

$$\forall x \in \mathbb{R}^{d_{j-1}} : h_j(x) = \int_{S^{d_{j-1}} \times S^{d_{j-1}}} w\sigma((v, x) - r) d\mu_j((v, r), w).$$

Let $\tilde{\sigma}$ be ReLU or linear and $I_1 \cup \ldots \cup I_{d_{out}} = \{1, \ldots, N\}.$

1. Assume that the dimensions of bottleneck layers $d_j$ are kept fixed. Then there exist Radon measures $\tilde{\mu}_j \in \mathcal{M}_{\tilde{d}_j}(S^{\tilde{d}_j-1} \times S^{\tilde{d}_j-1})$ with finite support on $n_j$ points, such that

$$\forall k \in \{1, \ldots, d_{out}\} : \forall i \in I_k : f_k(x_i^{\text{train}}) = \tilde{f}_k(x_i^{\text{train}}).$$

where

$$\tilde{f} = \ell^{-1} \circ \tilde{h}_\#\text{stacks} \circ \tilde{\sigma} \circ \ldots \circ \tilde{\sigma} \circ \tilde{h}_1$$

with stacks $\tilde{h}_j(x) = \int_{S^{\tilde{d}_{j-1}} \times S^{\tilde{d}_{j-1}}} w\sigma((v, x) - r) d\tilde{\mu}_j((v, r), w)$ and

$$\mu_j(\Omega) = \tilde{\mu}_j(\Omega) \quad \forall j = 1, \ldots, \#\text{stacks}.$$

The number of required nodes is $n_j = N\tilde{d}_j + 1$ for $j = 1, \ldots, \#\text{stacks} - 1$ and $n_{\#\text{stacks}} = N + 1$ for the terminal stack.

2. a) For $\tilde{\sigma} = \text{id}$, let $\tilde{d}_j = \sum_{k=0}^{\#\text{stacks}-j} N^k$ for $j = 1, \ldots, \#\text{stacks}$, and

b) for $\tilde{\sigma} = \text{ReLU}$, let $\tilde{d}_j = \sum_{k=0}^{2(\#\text{stacks}-j)} N^k$ for $j = 1, \ldots, \#\text{stacks} - 1$.

Then, for every $d \geq \tilde{d}$ and $f$ as defined above (i.e., $h_j : \mathbb{R}^{d_{j-1}} \to \mathbb{R}^{d_j}$), there exist $\tilde{\mu}_j \in \mathcal{M}_{\tilde{d}_j}(S^{\tilde{d}_{j-1}} \times S^{\tilde{d}_{j-1}})$ with finite support on $\tilde{n}_j$ points, such that

$$\forall k \in \{1, \ldots, d_{out}\} : \forall i \in I_k : f_k(x_i^{\text{train}}) = \tilde{f}_k(x_i^{\text{train}}),$$

where

$$\tilde{f} = \ell^{-1} \circ \tilde{h}_\#\text{stacks} \circ \tilde{\sigma} \circ \ldots \circ \tilde{\sigma} \circ \tilde{h}_1$$

with stacks $\tilde{h}_j(x) = \int_{S^{\tilde{d}_{j-1}} \times S^{\tilde{d}_{j-1}}} w\sigma((v, x) - r) d\tilde{\mu}_j((v, r), w)$ and

$$\mu_j(\Omega) = \tilde{\mu}_j(\Omega) \quad \forall j = 1, \ldots, \#\text{stacks}.$$

The number of required nodes in these cases are

a) $\tilde{n}_j = \sum_{k=0}^{\#\text{stacks}-j+1} N^k$ for $j = 1, \ldots, \#\text{stacks}$, and

b) $\tilde{n}_j = \sum_{k=0}^{2(\#\text{stacks}-j)+1} N^k$, $j = 1, \ldots, \#\text{stacks}$.

**Proof** We show that $\tilde{\mu}_j$ satisfy the even stronger condition:

$$\forall i \in \{1, \ldots, N\} : h_j(x_i^{\text{train}}) = \tilde{h}_j(x_i^{\text{train}}) \in \mathbb{R}^{d_j}.$$
1. In the case of a deep stacked neural network with fixed bottleneck dimensions $d_j$ for $j = 1, \ldots, \#\text{stacks} - 1$, by Lemma 36, $n_j = N d_j + 1$ is an upper bound for the number of neurons$^{33}$ in the hidden layer of stack $j$ for $j = 1, \ldots, \#\text{stacks}$.

2. Next, we assume the bottleneck dimensions not to be fixed and $\tilde{\sigma}$ to be the identity function. Again, by Lemma 36, an upper bound for the number of neurons of the last hidden layer is $\tilde{n}_{\#\text{stacks}} := N + 1$. Additionally, Lemma 36 applied to the second-to-last stack gives a representation of the $\#\text{stacks} - 1$-th stack by a measure with finite support on $n_{\#\text{stacks}} - 1 = N d_{\#\text{stacks}} - 1 + 1$, s.t. the mapping from the hidden layer of the second-to-last to the last hidden layer is $M := V_{\#\text{stacks}} W_{\#\text{stacks} - 1} \in \mathbb{R}^{\tilde{n}_{\#\text{stacks}} \times n_{\#\text{stacks}} - 1}$ where

$$W_{\#\text{stacks} - 1} := \left( w_1^{(\#\text{stacks} - 1)} \ldots w_{\tilde{n}_{\#\text{stacks} - 1}}^{(\#\text{stacks} - 1)} \right)^t \in \mathbb{R}^{d_{\#\text{stacks} - 1} \times \tilde{n}_{\#\text{stacks} - 1}} \quad (44)$$

$$V_{\#\text{stacks}} := \left( v_1^{(\#\text{stacks})} \ldots v_{\tilde{n}_{\#\text{stacks}}}^{(\#\text{stacks})} \right)^t \in \mathbb{R}^{\tilde{n}_{\#\text{stacks}} \times d_{\#\text{stacks} - 1}}. \quad (45)$$

Now, knowing that we can write $M$ as its single value decomposition, i.e., $M = U \Sigma V$ with $p := \min\{\tilde{n}_{\#\text{stacks}}, n_{\#\text{stacks}} - 1\}$ being the number of singular values, we define $A := \sqrt{\Sigma} V_{p1} \in \mathbb{R}^{p \times \tilde{n}_{\#\text{stacks} - 1}}$ and $B := U_{p2} \sqrt{\Sigma} \in \mathbb{R}^{\tilde{n}_{\#\text{stacks}} \times p}$ where the subscripts $p$, $p_1$ and $p_2$ refer to the upper left submatrix with dimension $\mathbb{R}^{p \times p}$, the submatrix with all rows and the submatrix with all columns removed after dimension $p$, respectively, such that we get the additional decomposition $M = BA$. This allows us to limit the maximum number of necessary neurons of the last bottleneck layer to $\tilde{d}_{\#\text{stacks} - 1} := N + 1$ (since $\tilde{n}_{\#\text{stacks}} = N + 1 < N d_{\#\text{stacks} - 1} + 1 = n_{\#\text{stacks} - 1}$) and of the second-to-last hidden layer, following again from Lemma 36. to $\tilde{n}_{\#\text{stacks} - 1} := N(\tilde{d}_{\#\text{stacks} - 1} + 1) = N(N + 1) + 1$. Inductively, an upper limit of necessary neurons of the $j$-th bottleneck layer can be set at $\tilde{d}_j = \tilde{n}_{j+1}$ and for the $j$-th hidden layer at $\tilde{n}_j = \sum_{k=0}^{\#\text{stacks} + 1 - j} N^k$.

In case of $\tilde{\sigma}$ being ReLU, the architecture reduces to a regular deep neural network, i.e., respective upper bounds for the number of required neurons can be set at $\tilde{d}_j = \sum_{k=0}^{2(\#\text{stacks} - j)} N^k, j = 1, \ldots, \#\text{stacks} - 1$ and $\tilde{n}_j = \sum_{k=0}^{2(\#\text{stacks} - j) + 1} N^k, j = 1, \ldots, \#\text{stacks}.$

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$^{33}$ By the equivalence of (30) and (33) in Lemma 31, we know every measure $\tilde{\mu}_j \in \mathcal{M}_{n_j}(S^{d_j - 1} \times S^{d_j - 1})$ corresponds to a stack $\mathcal{N}_{\tilde{\mu}_j}^{(j)}$ with $\tilde{n}_j$ hidden neurons.