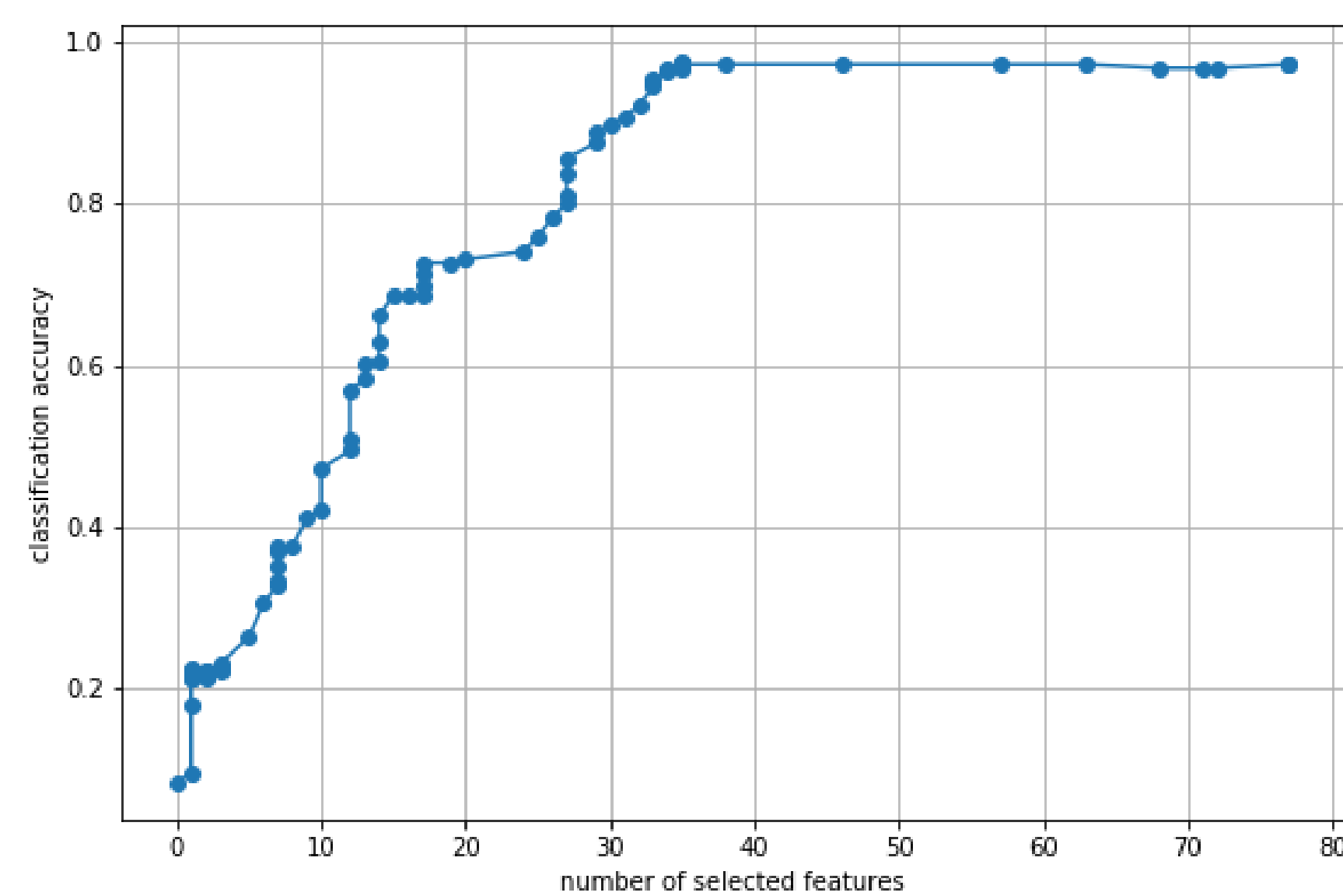


## Summary

- Much work has been done recently to make neural networks more **interpretable**, and one approach is to arrange for the network to use only a subset of the available features.
- We introduce **LassoNet**, a neural network framework with global feature selection.
- Our approach enforces a hierarchy: specifically a feature can participate in a hidden unit only if its linear representative is active.
- Unlike other approaches to feature selection for neural nets, our method delivers an **entire path** of solutions with a **range of feature sparsity**.
- The method uses projected proximal gradient descent, and generalizes directly to deep networks.
- It can be implemented by adding just a few lines of code to a standard neural network.

## Motivating example

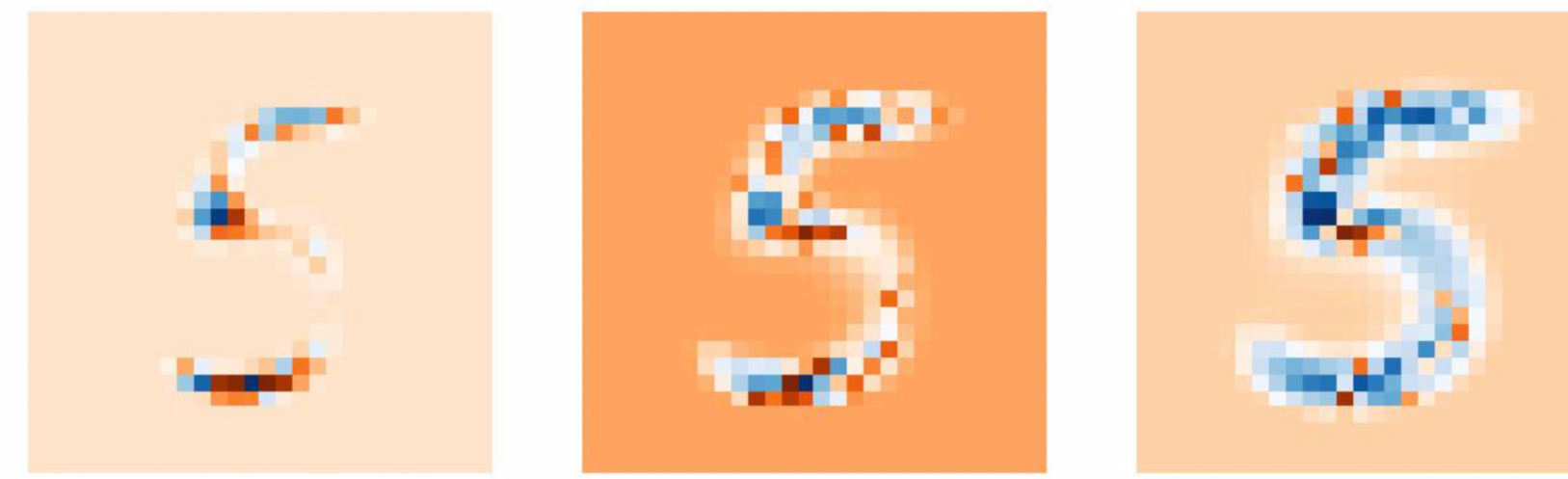
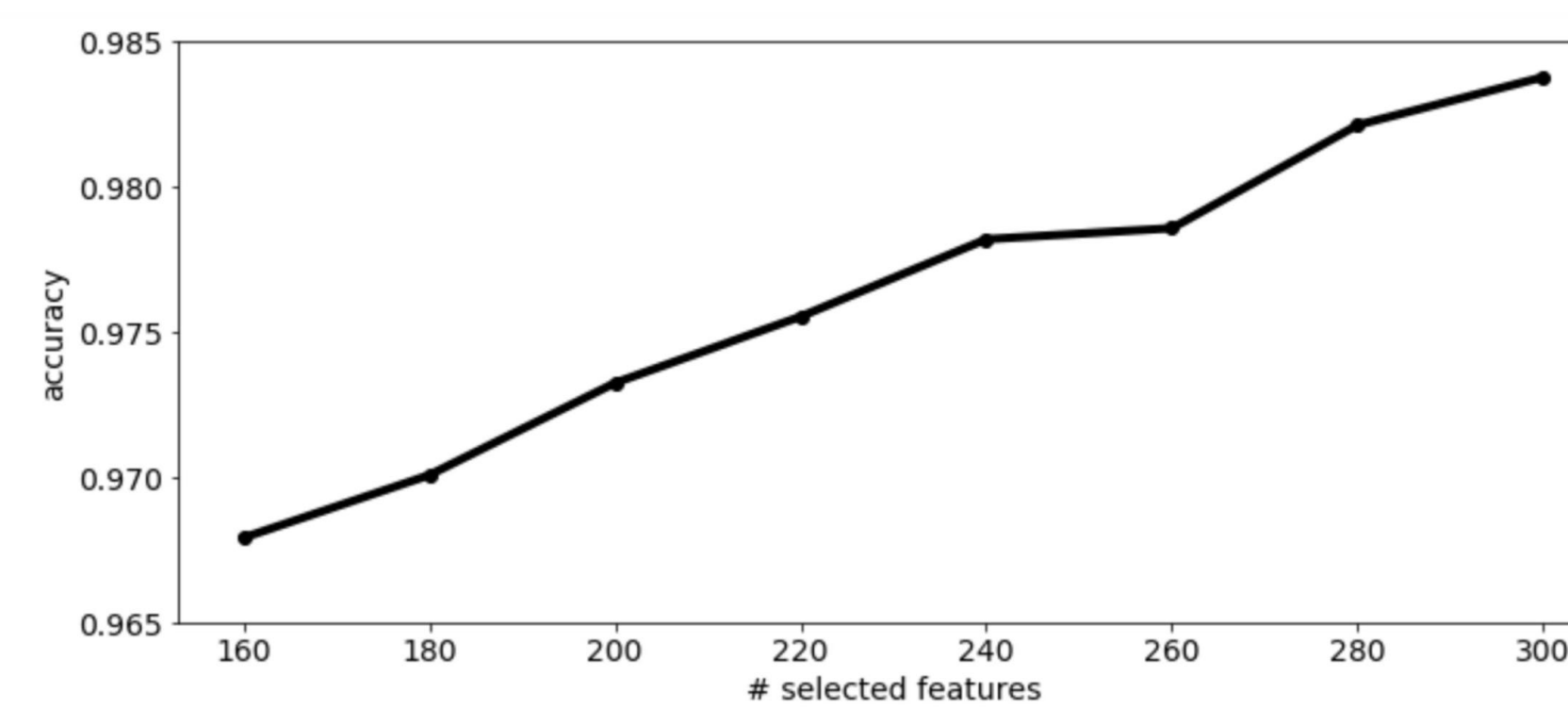
- Consider a data set that consists of the expression levels of **various proteins** across patients' tissue samples.
- Such measurements are increasingly carried out to assist with **disease diagnosis**, as biologists measure many proteins with the aim of discriminating between disease classes.
- Yet, it remains expensive to conduct all of the measurements needed to fully characterize proteomic diseases.
- The relationship between the **protein expressions** and the **outcome** is **sparse** and **highly nonlinear**.



**Feature selection path produced by our method on the MICE Protein Dataset.** The method captures **70% of the signal** with about **20% of the features**. This allows to narrow down the list of important features, making the conclusions of the prediction task more actionable.

## Background

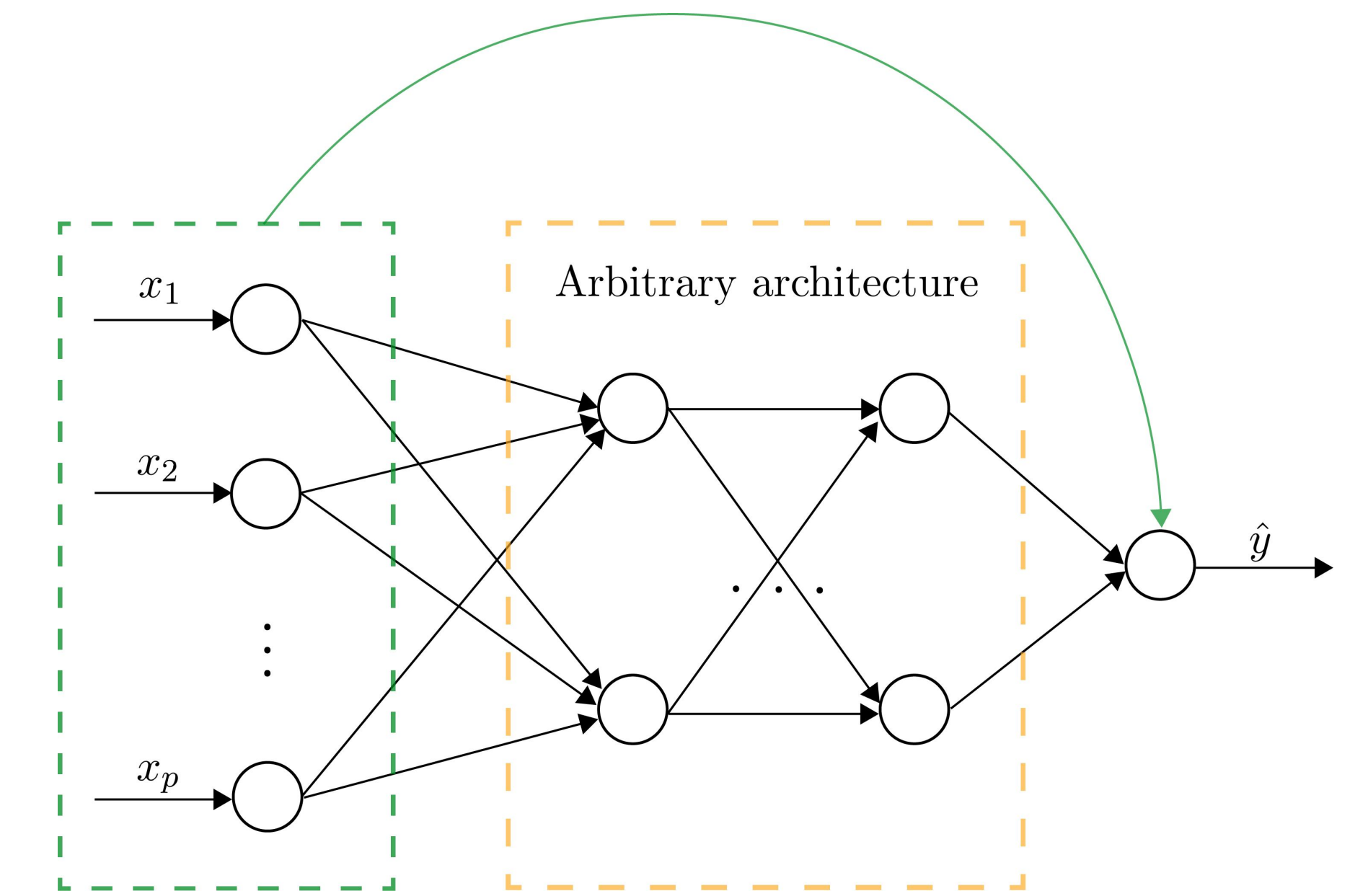
- **Lasso** (or  $\ell_1$ -regularized) regression assigns zero weights to the most irrelevant or redundant features, and is widely used in data science.
- The limitation of Lasso, however, is that it only offers solutions to **linear** models.
- We propose a new approach that **extends lasso regression** and its feature sparsity to **feed-forward neural networks**.
- The method allows to capture arbitrary nonlinearity in a nonparametric way while simultaneously performing **feature selection**.



**Demonstrating LassoNet on the MNIST dataset.** Here, we show the results of using LassoNet to simultaneously select informative pixels and classify digits 5 and 6 from the MNIST dataset. *Top:* The classification accuracy by number of selected features. *Bottom:* A sample from the model with 160, 220 and 300 active features (out of the 784 features).

## Formulation of the method

- We consider the class of all fully connected feed-forward residual neural networks, abbreviated as  $\mathcal{F} = \{f : f(\mathbf{x}) = \theta^T \mathbf{x} + \text{NN}(\mathbf{x}, W)\}$ .
- **Notation:**  $W$  denotes the network parameters,  $K$  denotes the size of the first hidden layer,  $W^{(0)} \in \mathbb{R}^{d \times K}$  denotes the first hidden layer,  $x \in \mathbb{R}^d$  denotes an input data point, and  $L(\theta, W) = \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{x}_i, y_i; \theta, W)$  denotes the loss on the training data set.
- The LassoNet **objective function** is defined as
 
$$\begin{aligned} & \underset{\theta, W}{\text{minimize}} && L(\theta, W) + \lambda \|\theta\|_1 \\ & \text{subject to} && \|W_j^{(0)}\|_\infty \leq M |\theta_j|, j = 1, \dots, d. \end{aligned} \quad (1)$$
- The constraint  $|W_{jk}^{(0)}| \leq M \cdot |\theta_j|$ ,  $k = 1, \dots, K$ , **budgets** the total amount of **non-linearity** involving variable  $j$  according to the relative importance of  $X_j$  as a linear variable.
- It follows that  $W_j = 0$  as soon as  $\theta_j = 0$ . In other words, variable  $j$  is completely inactive from the model, without the need for an explicit penalty on  $W$ .
- The only **hyper-parameters** are the hierarchy coefficient,  $M$ , and the regularization strength,  $\lambda$ .



The architecture of LassoNet consists of a **single residual connection**, shown in **green**, and an **arbitrary feed-forward neural network**, shown in **black**. The residual layer and the first hidden layer are optimized jointly using a hierarchical operator.

## Efficient Numerical Optimization

- The objective is optimized using **proximal gradient descent**.
- The key novelty is a **numerically efficient algorithm** for the proximal inner-loop.
- The complexity of the algorithm is  $O(dK \cdot \log(dK))$ , where  $d \cdot K$  is the total number of the parameters being updated.
- Thus, the method's complexity is **negligible overhead** compared to the cost of computing the gradients.

## Competitive Results on Real Data

- We compare LassoNet with several supervised feature selection methods detailed in the paper.
- We measure classification accuracy by passing the selected features to an extremely randomized trees classifier, a variant of random forests that has been used with feature selection methods in prior literature.
- The results are shown here on the **ISOLET data set**, which is a widely used benchmark for feature selection.
- Overall, we find that our method is the strongest performer in the large majority of cases.

