Applied Machine Learning

Multilayer Perceptron

Siamak Ravanbakhsh

COMP 551 (winter 2020)

Learning objectives

multilayer percepron:

- model
  - different supervised learning tasks
  - activation functions
  - architecture of a neural network
- its expressive power
- regularization techniques

Adaptive bases

several methods can be classified as *learning these bases adaptively*

$$f(x) = \sum_d w_d \phi_d(x; v_d)$$

- decision trees
- generalized additive models
- boosting
- neural networks ←

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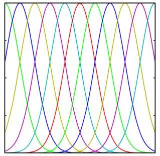
- neural networks
  - consider the adaptive bases in a general form (contrast to decision trees)
  - use gradient descent to find good parameters (contrast to boosting)
  - create more complex adaptive bases by combining simpler bases
    - leads to **deep neural networks**

Adaptive Radial Bases



$\phi_d(x) = e^{-\frac{(x-\mu_d)^2}{s^2}}$

Gaussian bases, or radial bases

non-adaptive case

model: $f(x; w) = \sum_d w_d \phi_d(x)$

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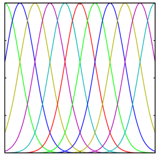

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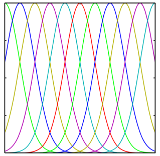

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the model is linear in its parameters

the cost is convex in w (unique minimum)

even has a closed form solution

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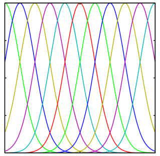

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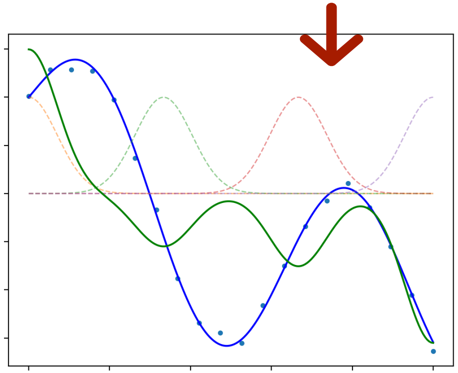

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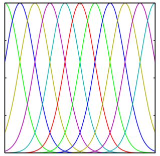

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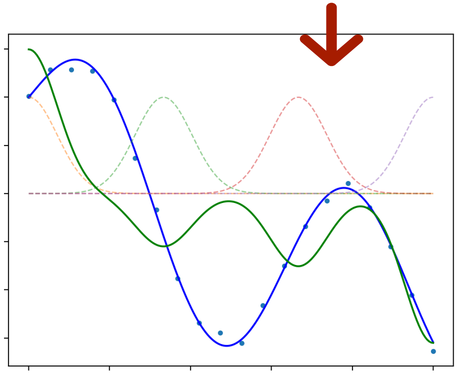

adaptive case

we can make the bases adaptive by learning these centers

model: $f(x;w,\mu) = \sum_d w_d \phi_d(x;\mu_d)$

how to minimize the cost?

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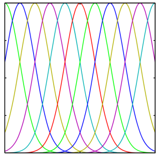

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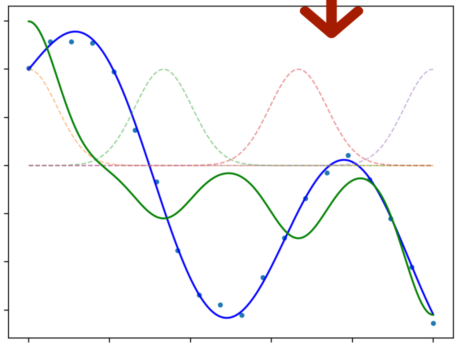

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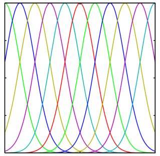

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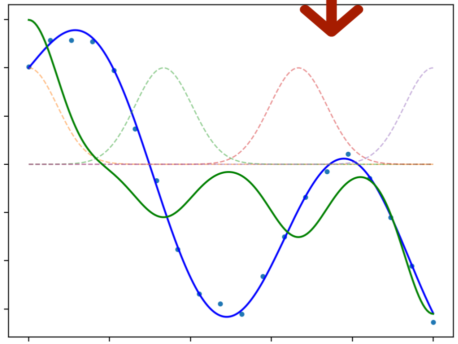

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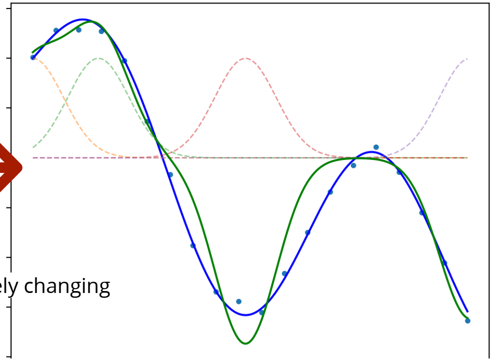
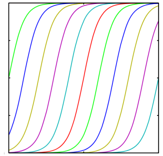


note that the basis centers are adaptively changing



$$\phi_d(x) = \frac{1}{1+e^{-(\frac{x-\mu_d}{s_d})}}$$

Sigmoid Bases

using adaptive sigmoid bases gives us a neural network

non-adaptive case

μ_d

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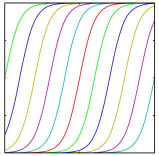
Sigmoid Bases



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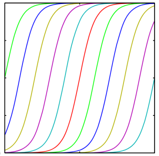

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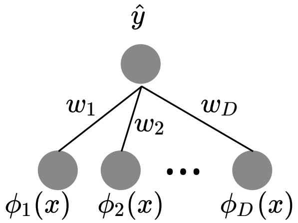


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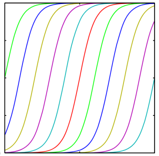

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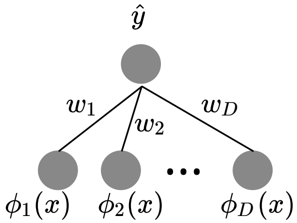

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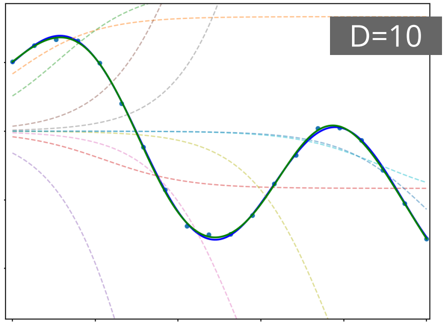

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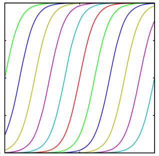

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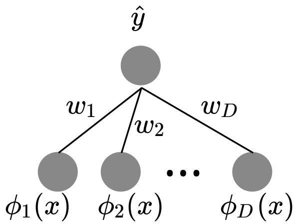

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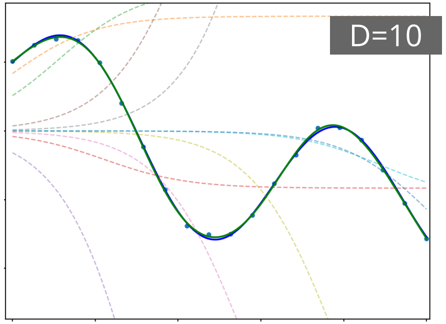

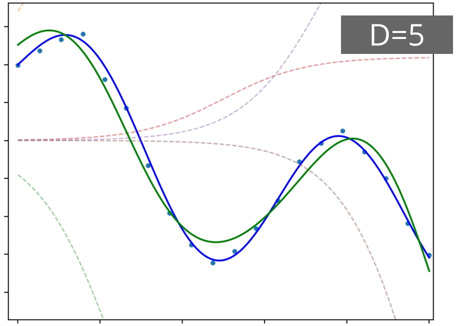

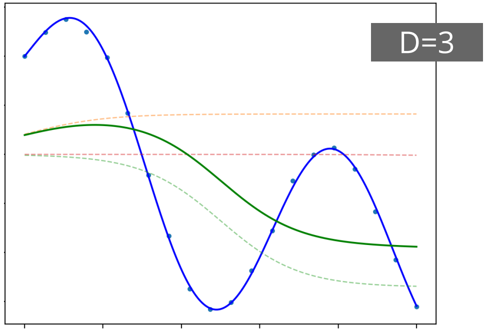

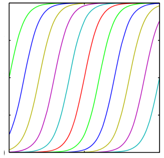

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Adaptive Sigmoid Bases

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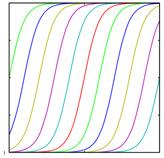

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assuming input is higher than one dimension

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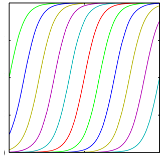

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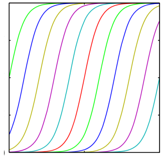

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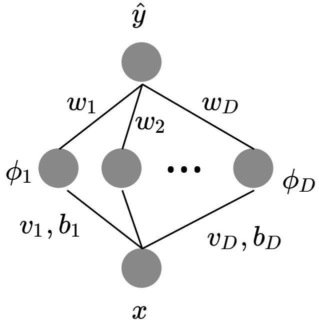

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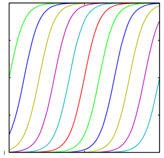

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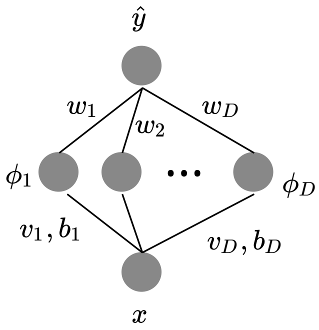
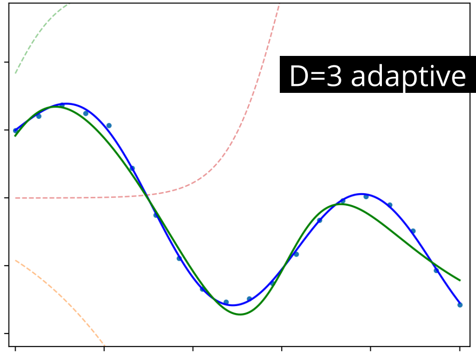
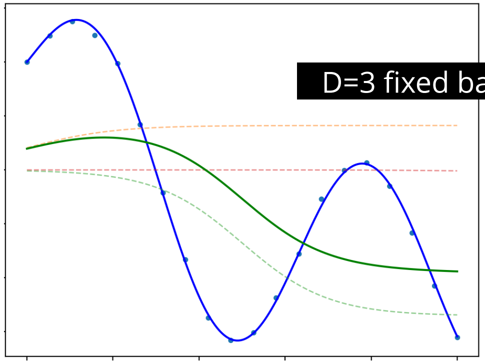


optimize using gradient descent (find a local optima)





Multilayer Perceptron (MLP)

suppose we have

- D inputs $x_1, \ldots, x_D$
- K outputs $\hat{y}_1, \ldots, \hat{y}_K$
- M hidden *units* $z_1, \ldots, z_M$

model

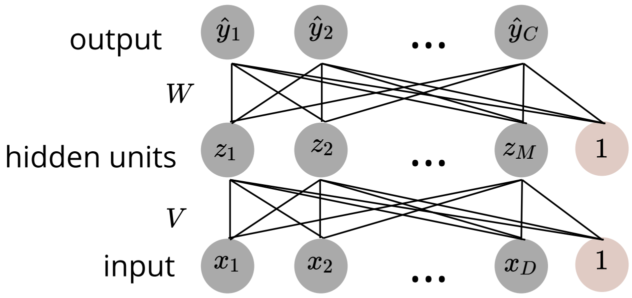
$$\hat{y}_k = g\left(\sum_m W_{k,m} h\left(\sum_d V_{m,d} x_d\right)\right)$$

nonlinearity, activation function: we have different choices

more compressed form

$$\hat{y} = g\big(W\, h(V\, x)\big)$$

non-linearities are applied elementwise



for simplicity we may drop bias terms

Regression using Neural Networks

the choice of **activation function** in the final layer depends on the task

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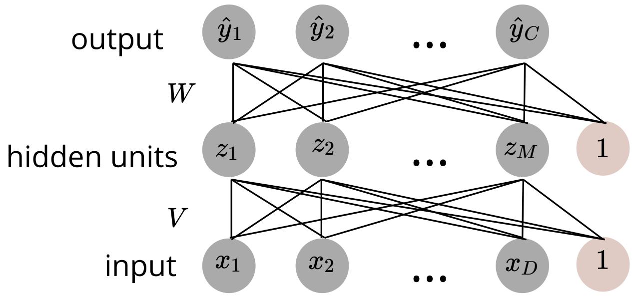

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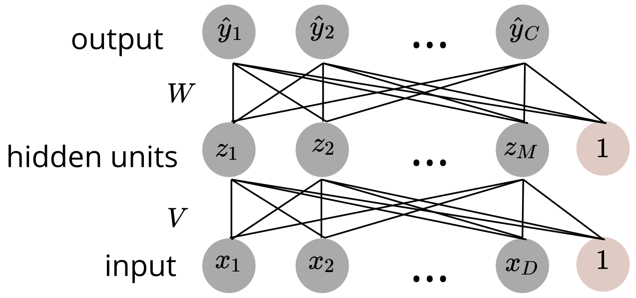
we may have one or more output variables

identity function + L2 loss : Gaussian likelihood

$L(y, \hat{y}) = \frac{1}{2}||y - \hat{y}||_2^2 = \log \mathcal{N}(y; \hat{y}, \beta \mathbf{I}) + \text{constant}$



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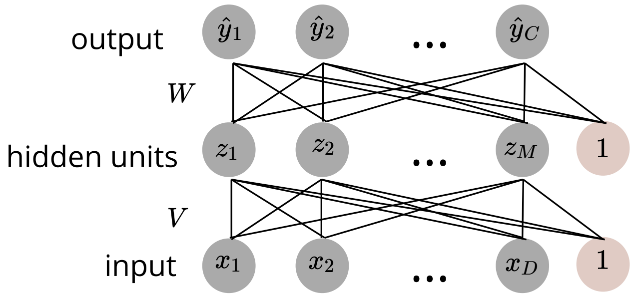
$$L(y, \hat{y}) = \tfrac{1}{2}||y - \hat{y}||_2^2 = \log \mathcal{N}(y; \hat{y}, \beta\mathbf{I}) + \text{constant}$$



more generally

we may explicitly produce a distribution at output - *e.g.,*

- mean and variance of a Gaussian
- mixture of Gaussians

the loss will be the log-likelihood of the data under our model

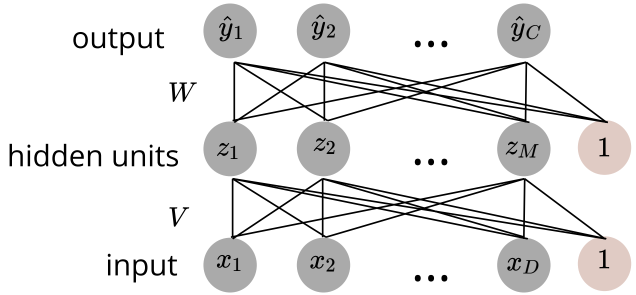
$$L(y, \hat{y}) = \log p(y; f(x))$$

neural network outputs the parameters of a distribution

Classification using neural networks

the choice of activation function in the final layer depends on the task

model $\hat{y} = g\big(W\, h(V\, x)\big)$



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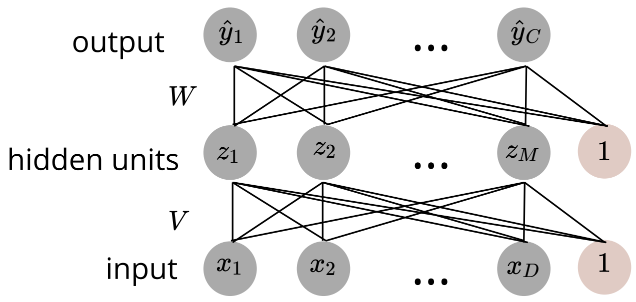
binary classification $\hat{y} = g(Wz) = \big(1 + e^{-Wz}\big)^{-1}$

scalar output C=1

logistic sigmoid + CE loss: Bernouli likelihood

$$L(y, \hat{y}) = y \log \hat{y} + (1-y)\log(1-\hat{y}) = \log \mathrm{Bernouli}(y; \hat{y})$$



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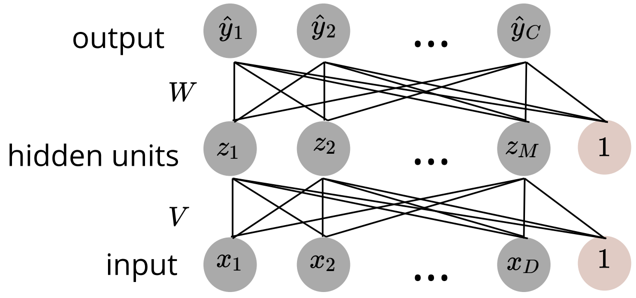

multiclass classification $\hat{y} = g(Wz) = \mathrm{softmax}(Wz)$

C is the number of classes

softmax + multi-class CE loss: categorical likelihood

$L(y, \hat{y}) = \sum_k y_k \log \hat{y}_k = \log \mathrm{Categorical}(y; \hat{y})$

Activation function

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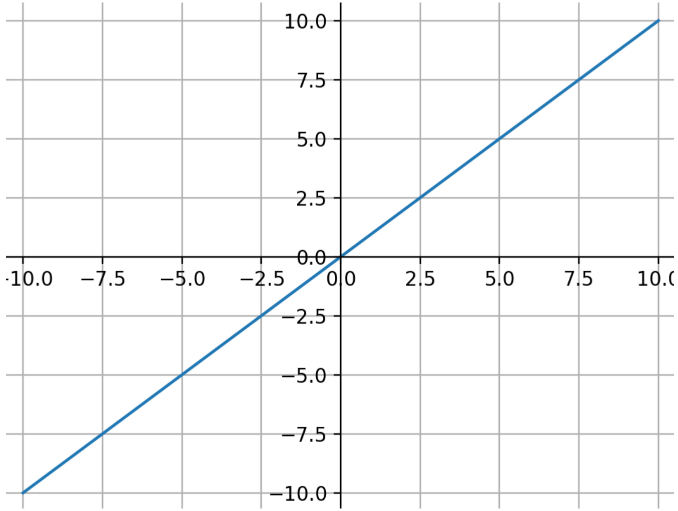

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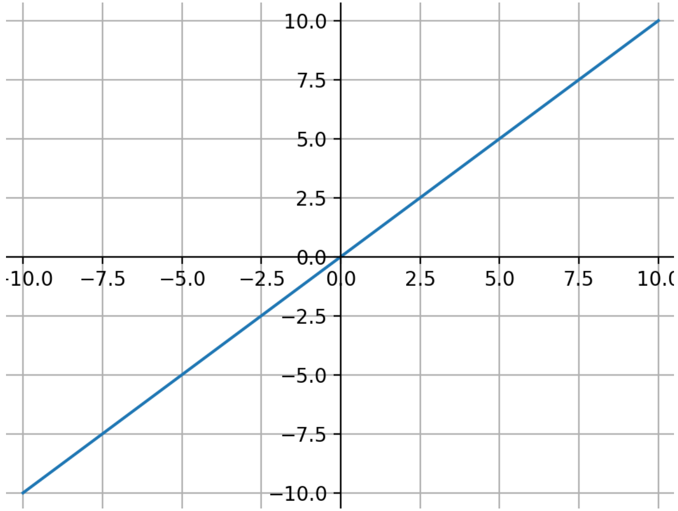

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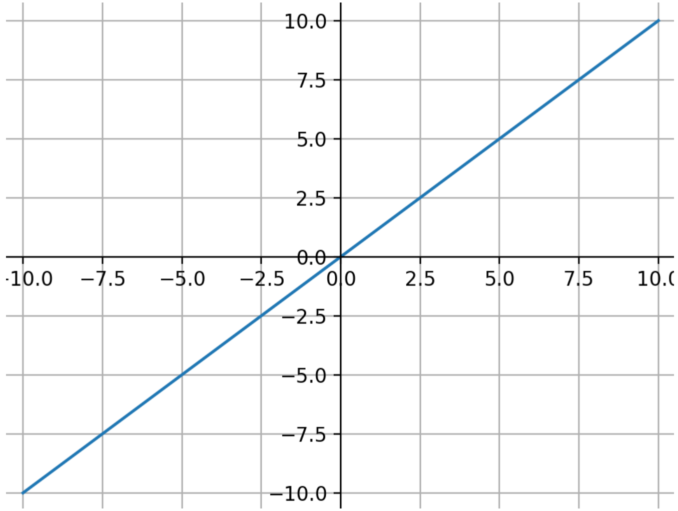

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so nothing is gained (in representation power) by stacking linear layers

exception: if $M < \min(D, K)$ then the hidden layer is compressing the data (W' is low-rank)

this idea is used in dimensionality reduction (later!)

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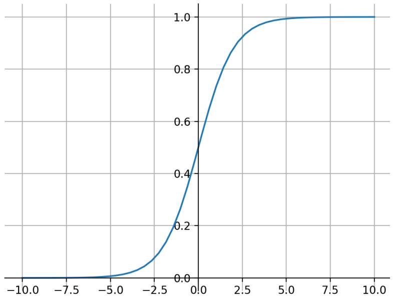

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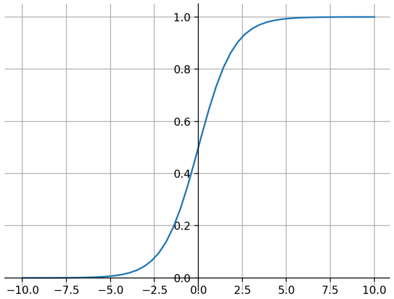

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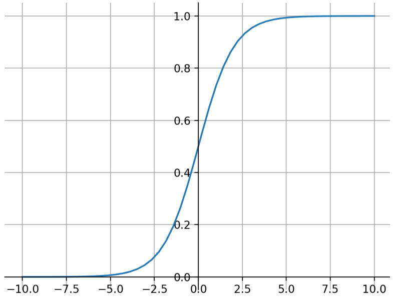

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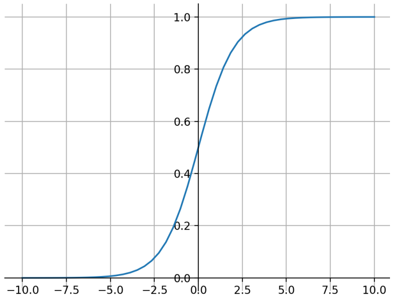

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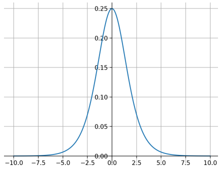

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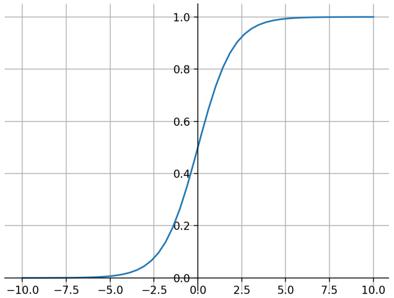

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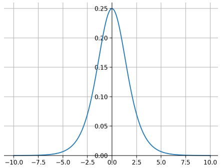

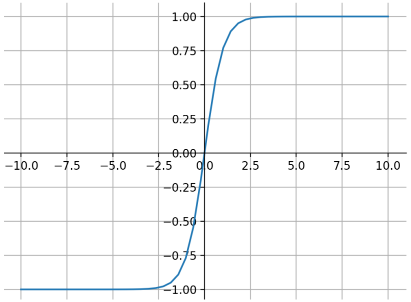

$h(x) = 2\sigma(x) - 1 = \frac{e^{x}-e^{-x}}{e^{x}+e^{-x}}$ **hyperbolic tangent**

similar to sigmoid, but symmetric

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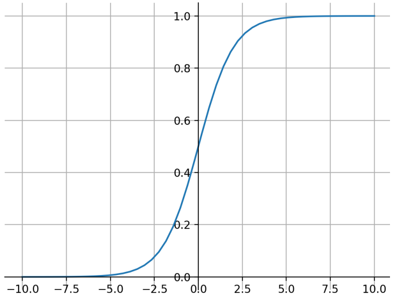

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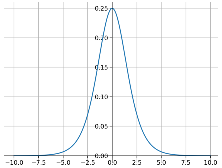

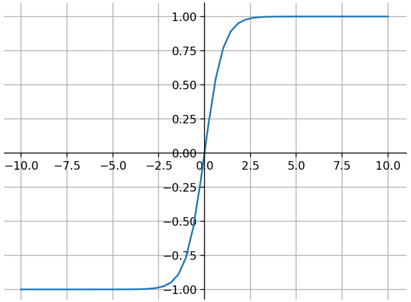

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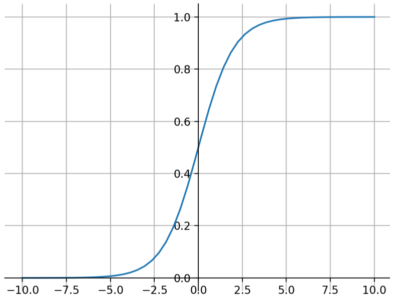

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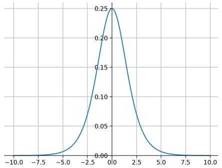

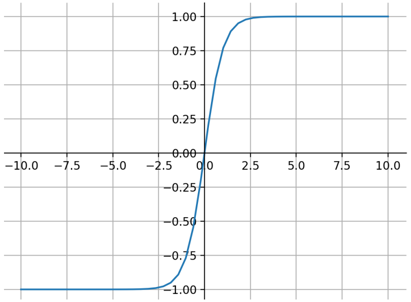

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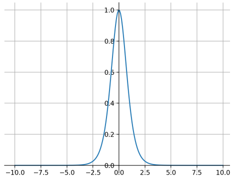

$\frac{\partial}{\partial x}\tanh(x) = 1 - \tanh(x)^2$

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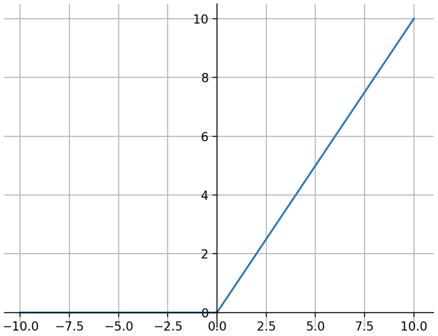

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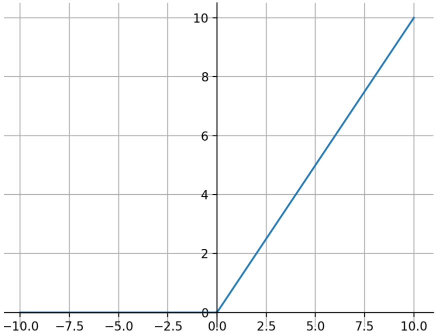

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replacing logistic with ReLU significantly improves the training of deep networks

zero derivative if the unit is "inactive"
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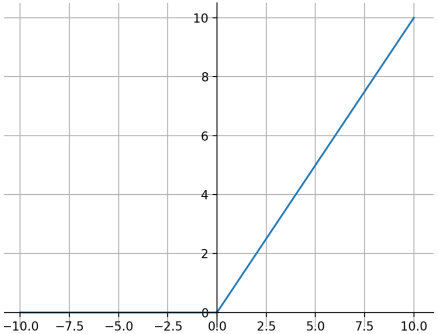

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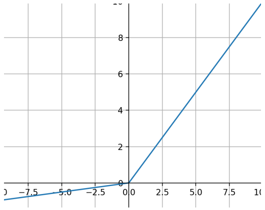

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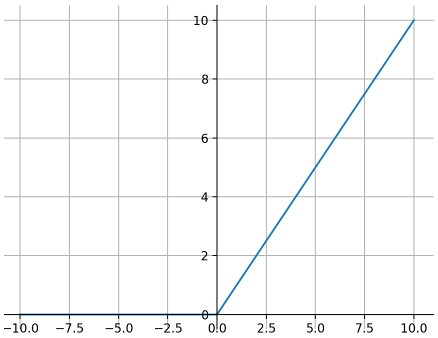

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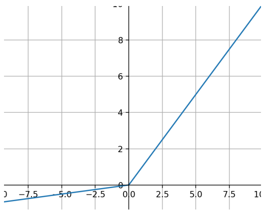

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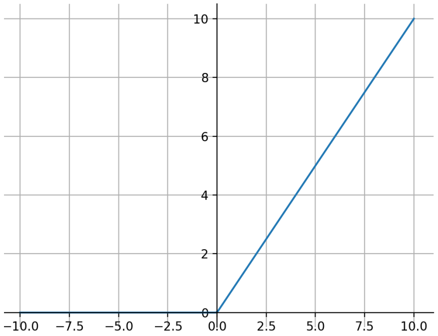

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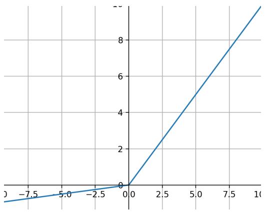

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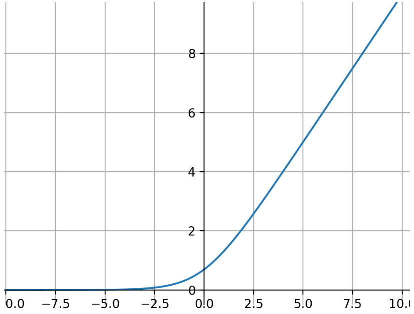
Softplus (differentiable everywhere) $h(x) = \log(1 + e^{x})$



it doesn't perform as well in practice

Network architecture

architecture is the overall structure of the network

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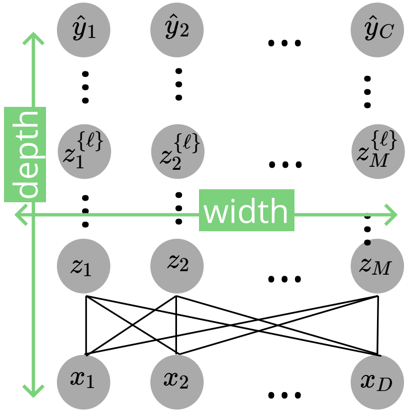
feedforward network (aka multilayer perceptron)

- can have many layers
- # layers is called the **depth** of the network



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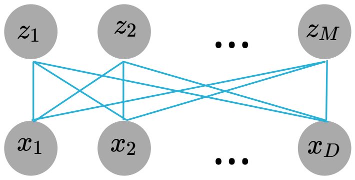

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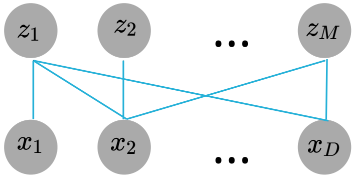

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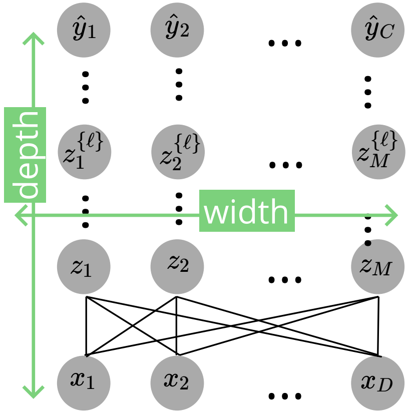

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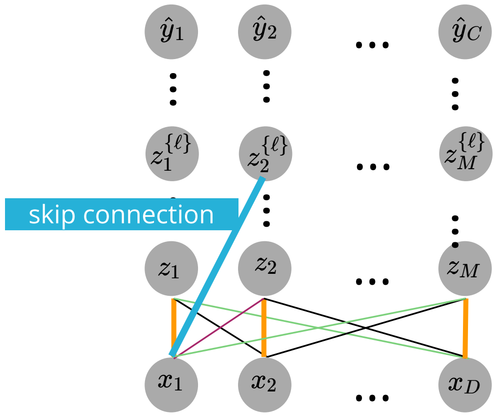

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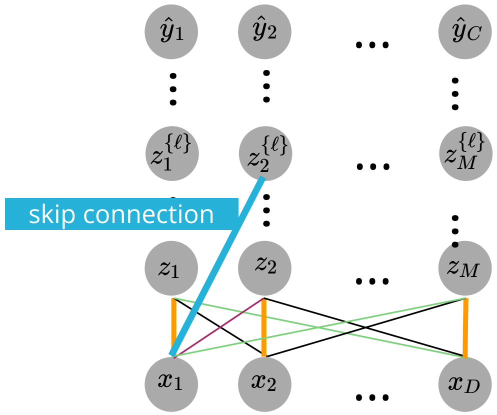

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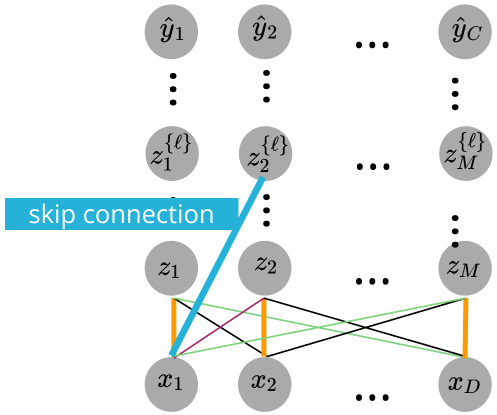

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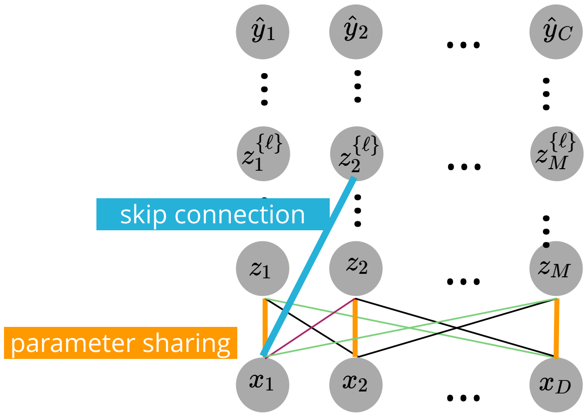

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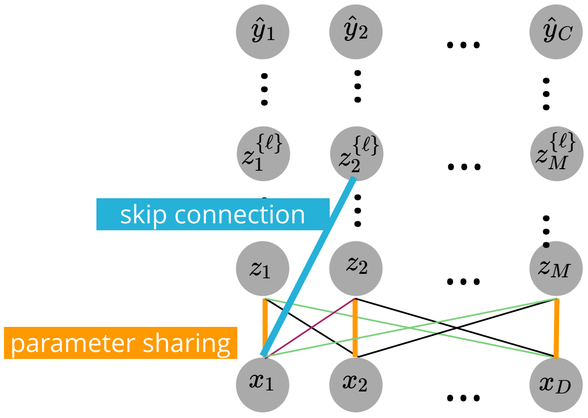

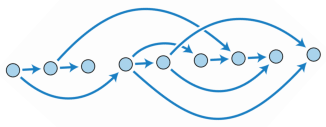

more generally a directed acyclic graph (DAG) expresses the feed-forward architecture

Expressive power

universal approximation theorem

an MLP with single hidden layer can approximate any continuous function with arbitrary accuracy

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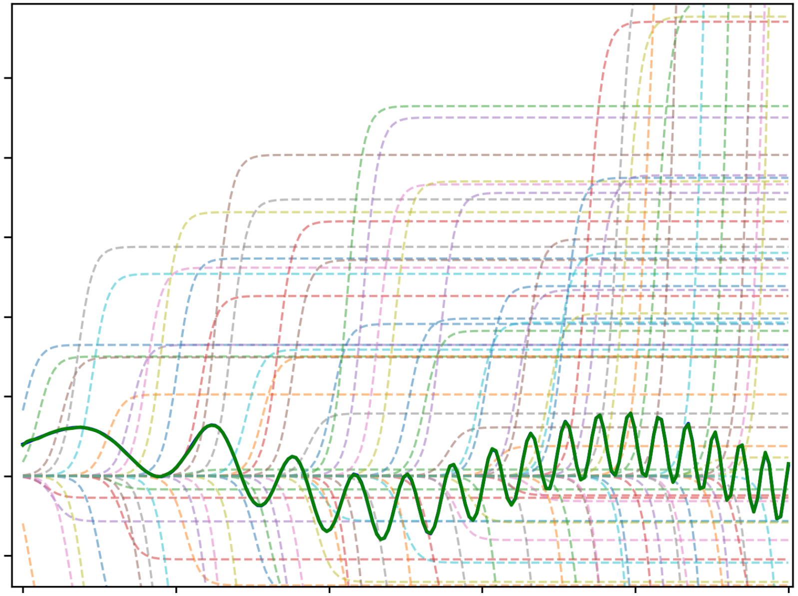

for 1D input we can see this even with **fixed bases**

M = 100 in this example

the fit is good (hard to see the blue line)

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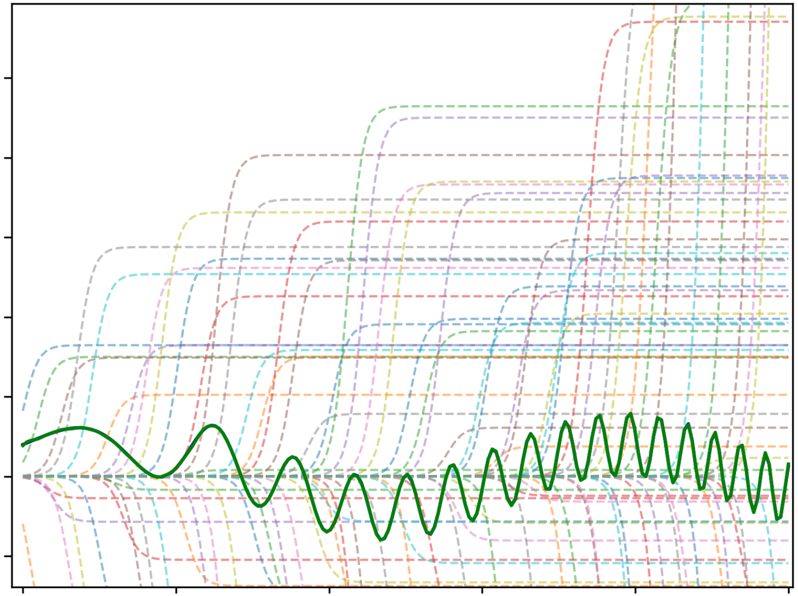

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however # bases (M) should grow exponentially with D (**curse of dimensionality**)

Depth vs Width

universal approximation theorem

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Caveats

- we may need a very wide network (large M)
- this is only about training error, we care about test error

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empirically it is observed that increasing depth is often more effective than increasing width (#parameters per layer)

assuming a compositional functional form (through depth) is a useful inductive bias

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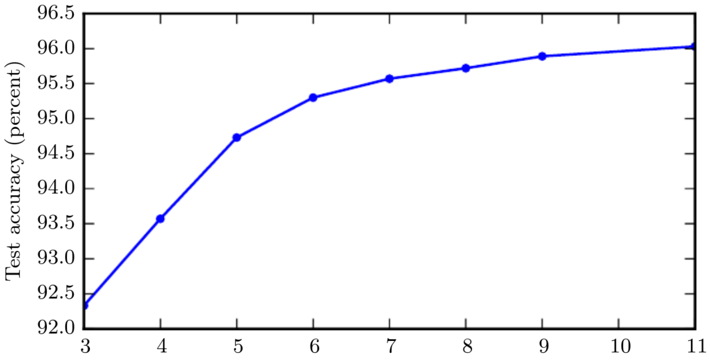

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an MLP with single hidden layer can approximate any continuous function on with arbitrary accuracy

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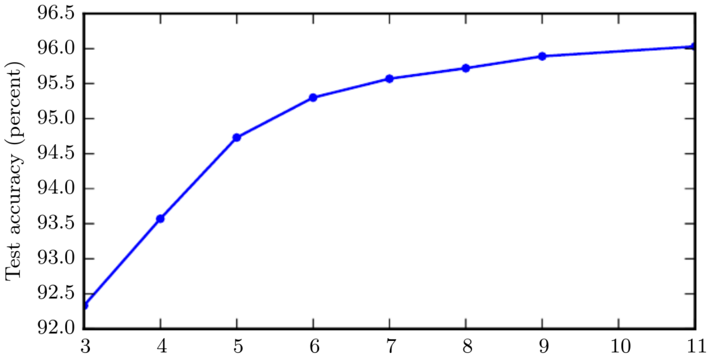

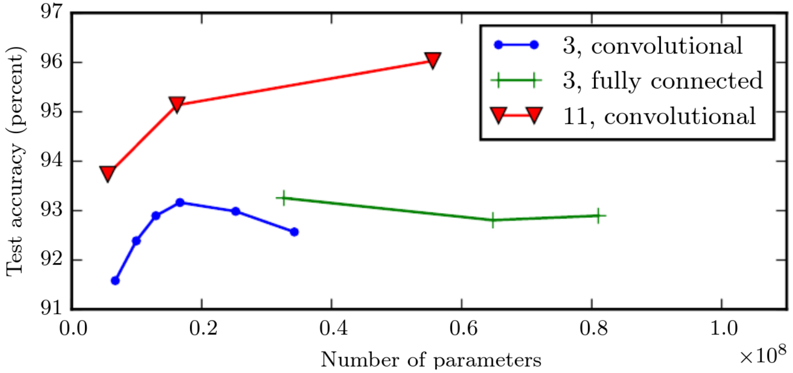

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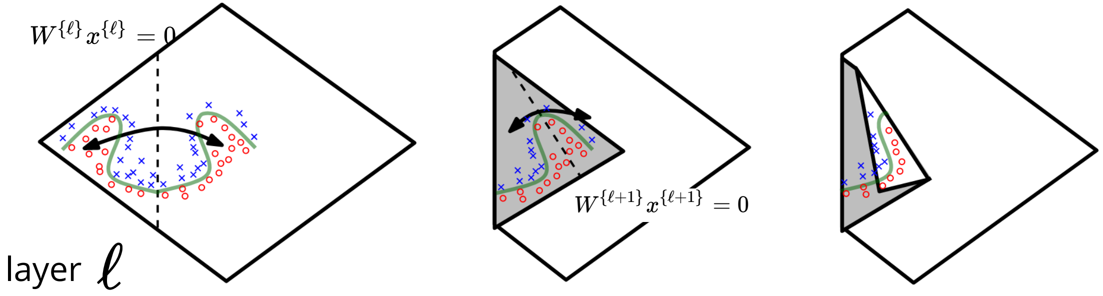
number of regions (in which the network is linear) grows exponentially with depth

simplified demonstration $h(W^{\{\ell\}}x) = |W^{\{\ell\}}x|$



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Data augmentation

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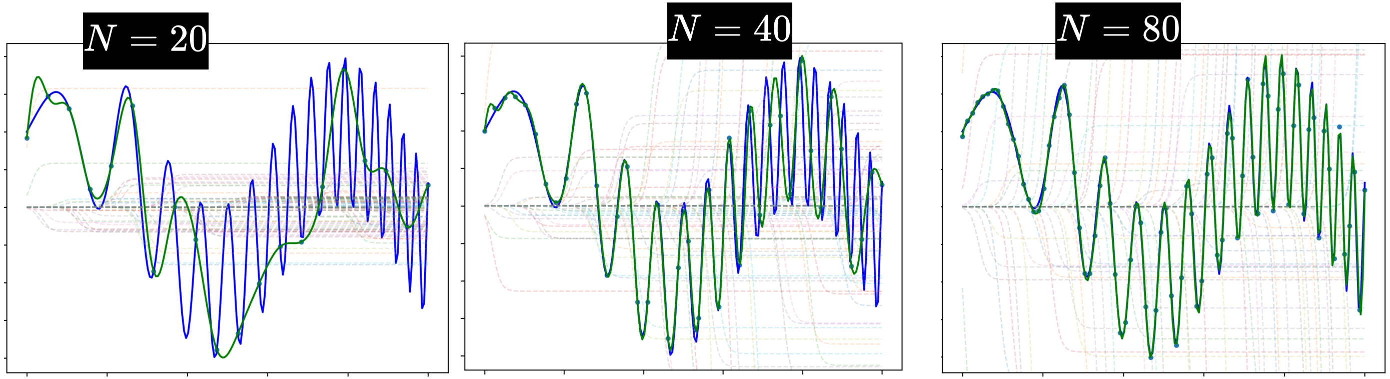
example: in all 3 examples below training error is close to zero

however, a larger training dataset leads to better generalization



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idea

increase the size of dataset by adding reasonable transformations $\tau(x)$ that change the label in predictable ways; e.g., $f(\tau(x)) = f(x)$

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- adding noise to the input
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sometimes we an achieve the same goal by designing the models
that are **invariant** to a given set of transformations

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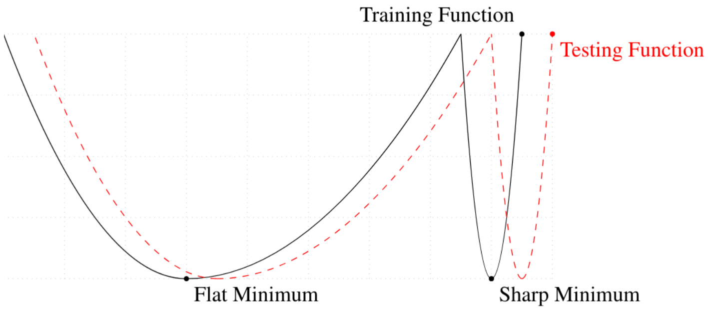

image credit: Keshkar et al'17

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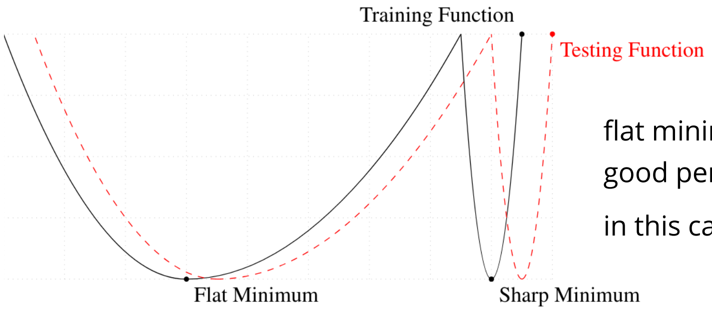

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good performance of SGD using small minibatch is attributed to flat minima

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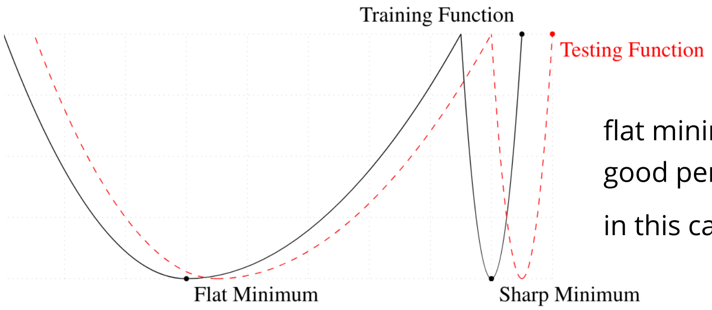

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in this case, SGD regularizes the model due to **gradient noise**

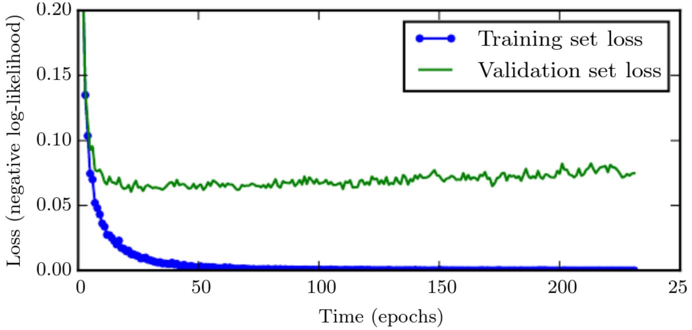
output (avoid overfitting, specially to wrong labels)

a heuristic is to replace hard labels with "soft-labels" label smoothing

e.g., $[0, 0, 1, 0] \rightarrow [\frac{\epsilon}{3}, \frac{\epsilon}{3}, 1-\epsilon, \frac{\epsilon}{3}]$

image credit: Keshkar et al'17

Early stopping



the **test loss**-vs-**time step** is "often" U-shaped

use validation for early stopping

also saves computation!

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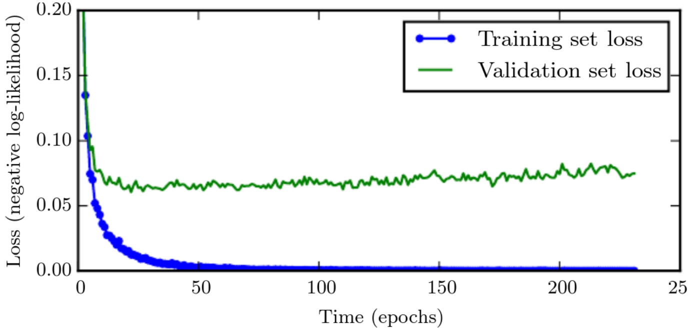

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early stopping bounds the region of the parameter-space that is reachable in T time-steps

assuming

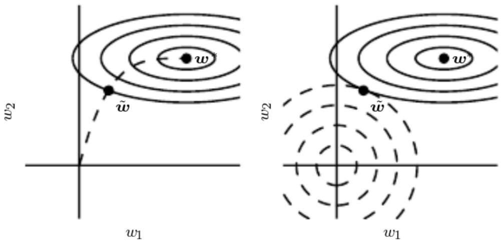
bounded gradient

starting with a small w

it has an effect similar to L2 regularization

we get the regularization path (various λ)

we saw a similar phenomena in boosting



Bagging

several sources of variance in neural networks, such as

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  - initialization
  - randomness of SGD
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use bagging or even averaging without bootstrap to reduce variance

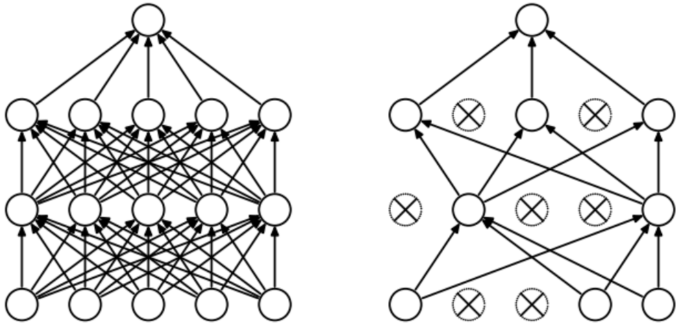
issue: computationally expensive

Dropout

idea

randomly remove a subset of units during training

as opposed to bagging a single model is trained



(a) Standard Neural Net (b) After applying dropout.

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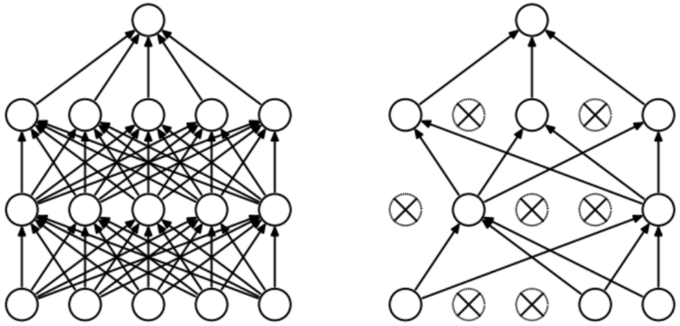

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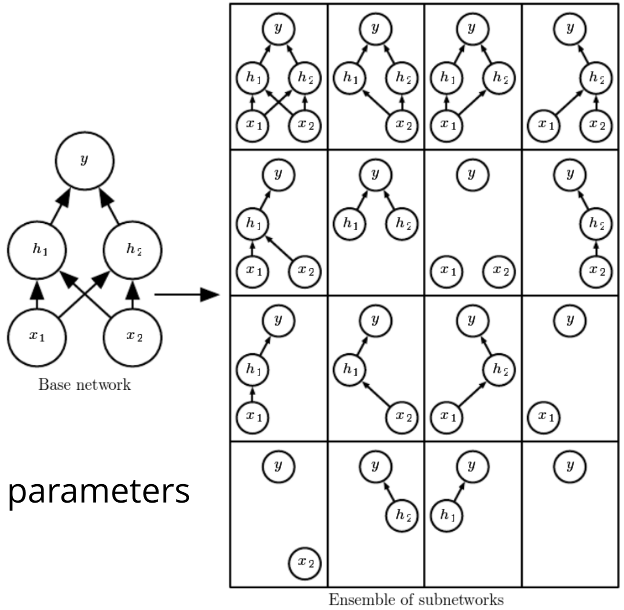

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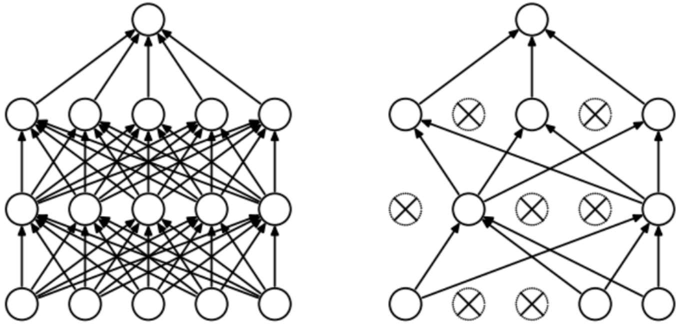

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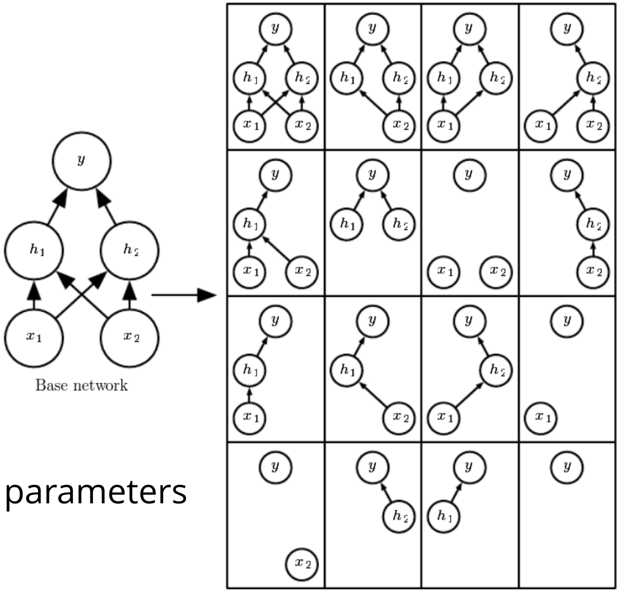

can be viewed as exponentially many subnetworks that share parameters

is one of the most effective regularization schemes for MLPs

Dropout

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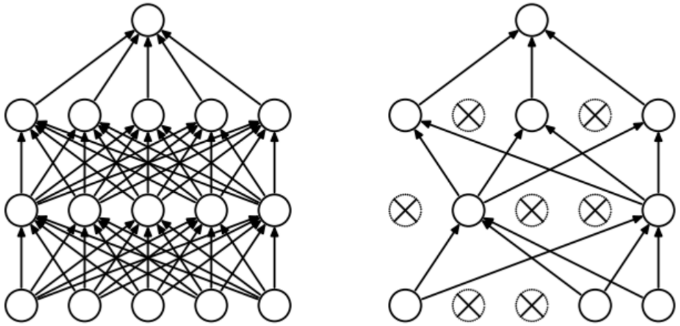

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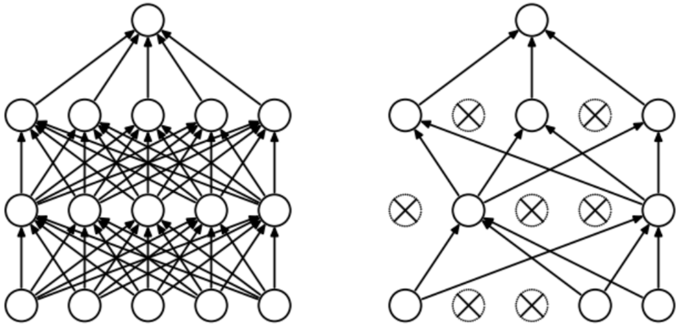
for each instance (n):

randomly dropout each unit with probability p (e.g., p=.5)

only the remaining subnetwork participates in training



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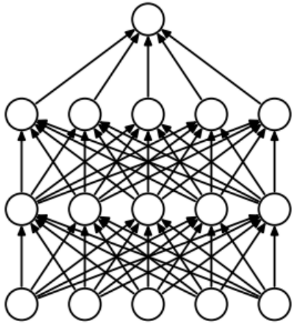

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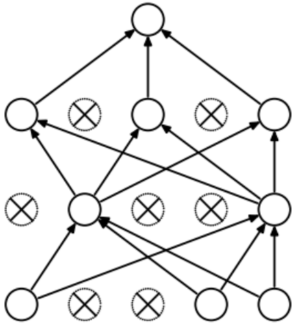

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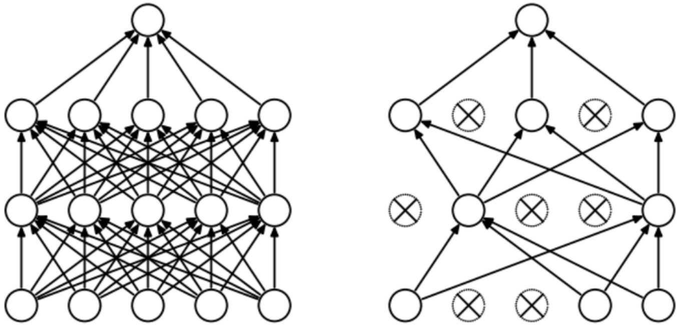

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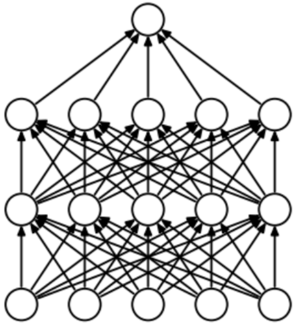

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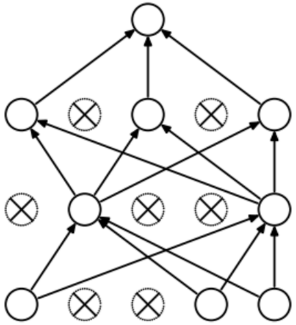

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2) weight scaling: scale the weights by **p** to compensate for dropout

e.g., for 50% dropout, scale by a factor of 2

in general this is **not** equivalent to the average prediction of the ensemble

Summary

Deep feed-forward networks learn **adaptive bases**
more complex bases at higher layers
increasing **depth** is often preferable to width
various choices of **activation function** and **architecture**
universal approximation power
their expressive power often necessitates using **regularization** schemes