Neural Networks

Introduction, multilayer perceptron, optimization techniques

Machine Learning and Data Mining, 2024

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National Research University Higher School of Economics

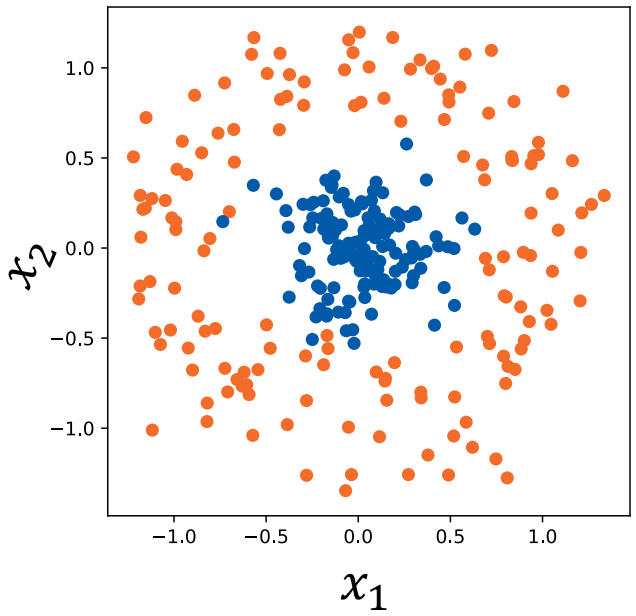
November 20, 2024

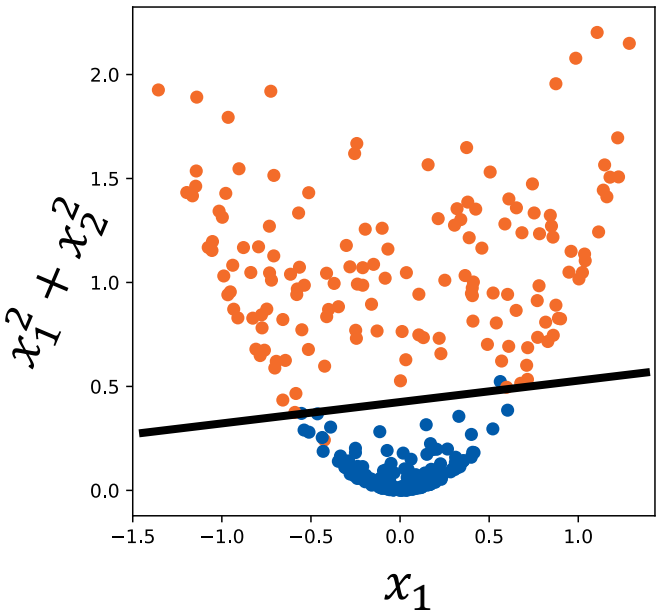
From linear model to a neural network

Linear models + feature expansion recap

Recall how, for linear models, we introduced **new features** to make the model **more powerful**

Finding good features (aka feature engineering) is a **highly non-trivial task**





Linear models + feature expansion recap

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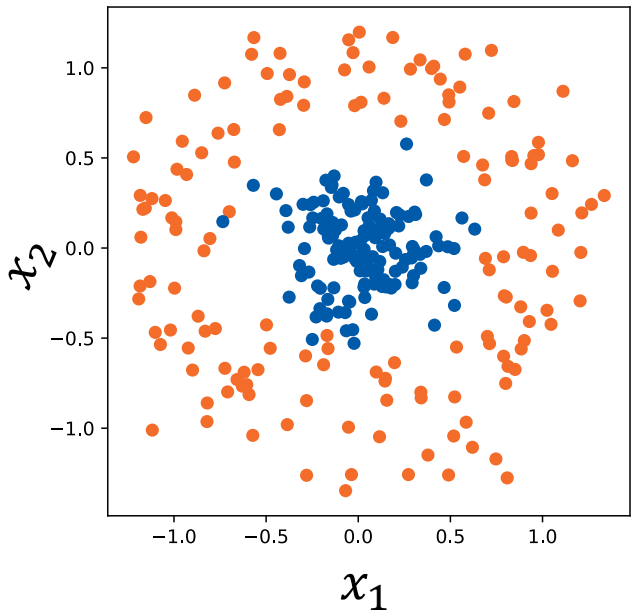
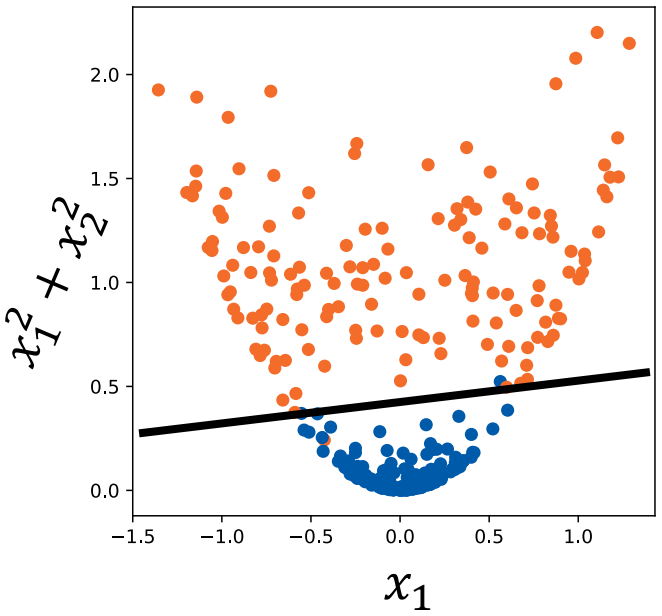
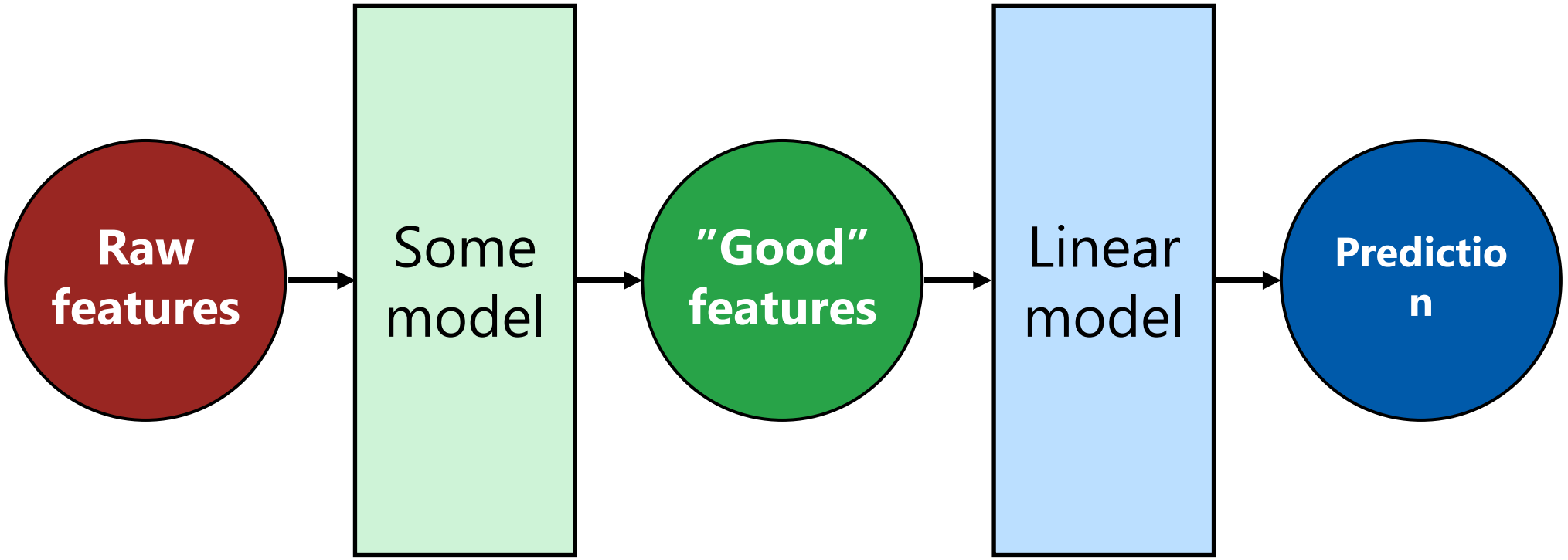
Finding good features (aka feature engineering) is a **highly non-trivial task**





Can we automate feature engineering? ☺

Idea: add another model



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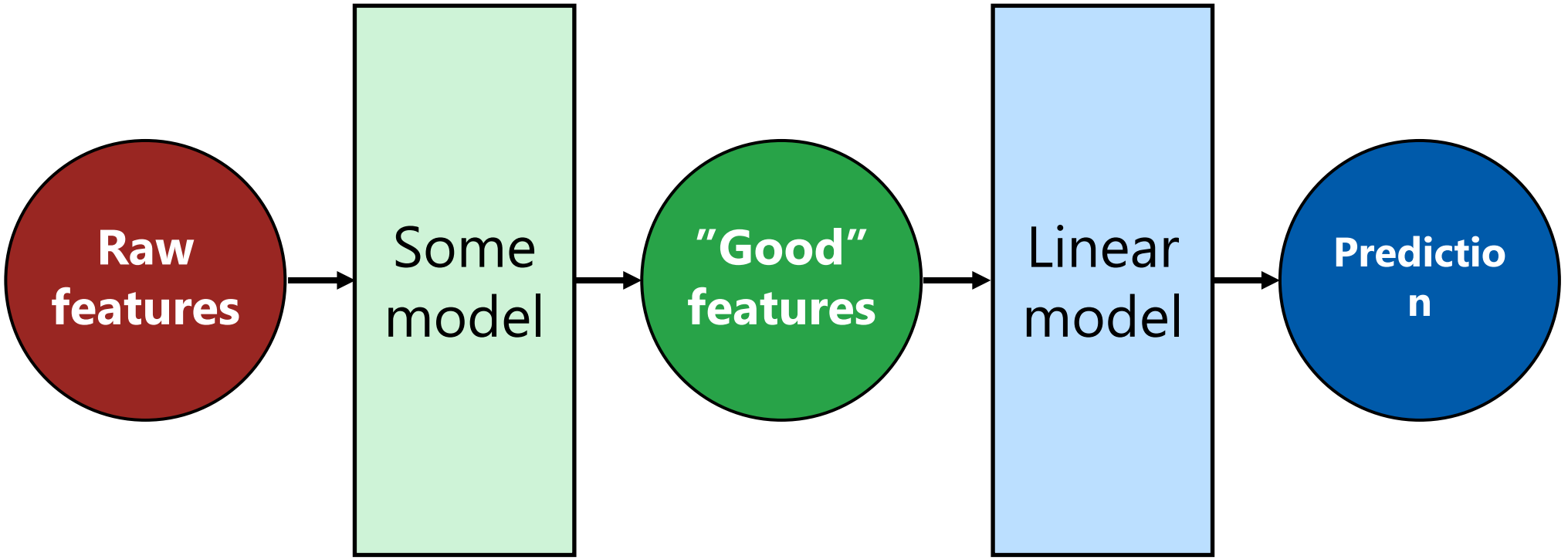

Add another model

Train everything simultaneously

- Can use gradient descent if both models are **differentiable**

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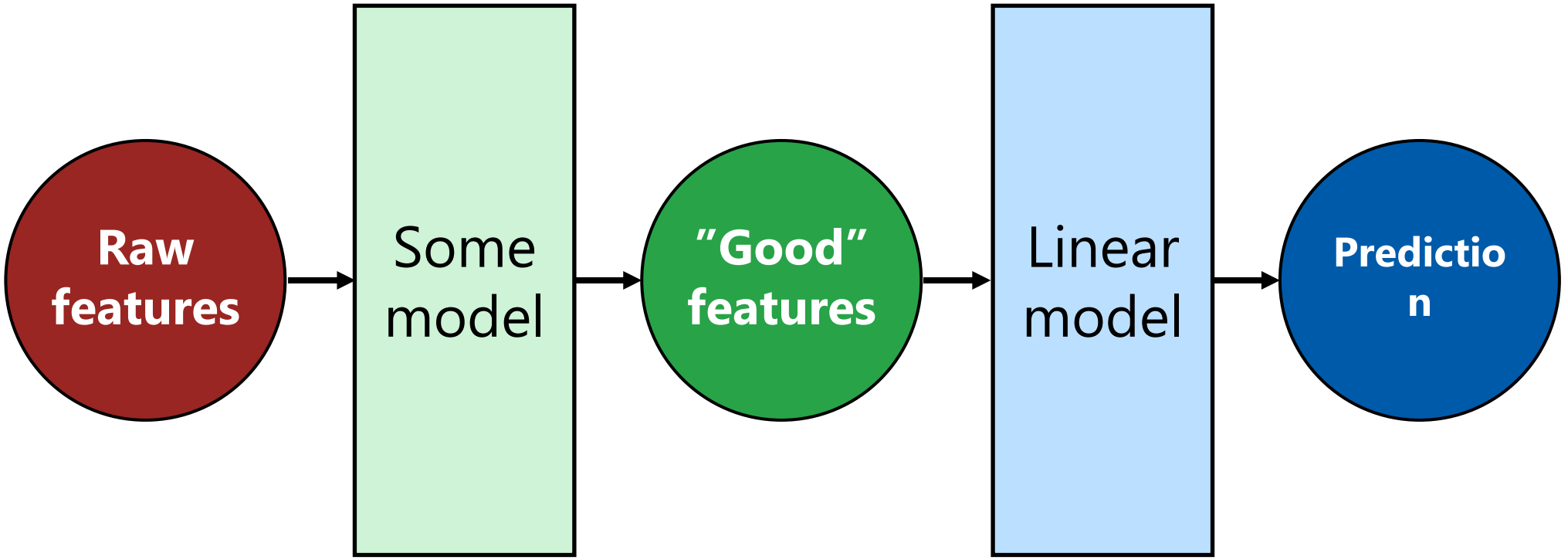


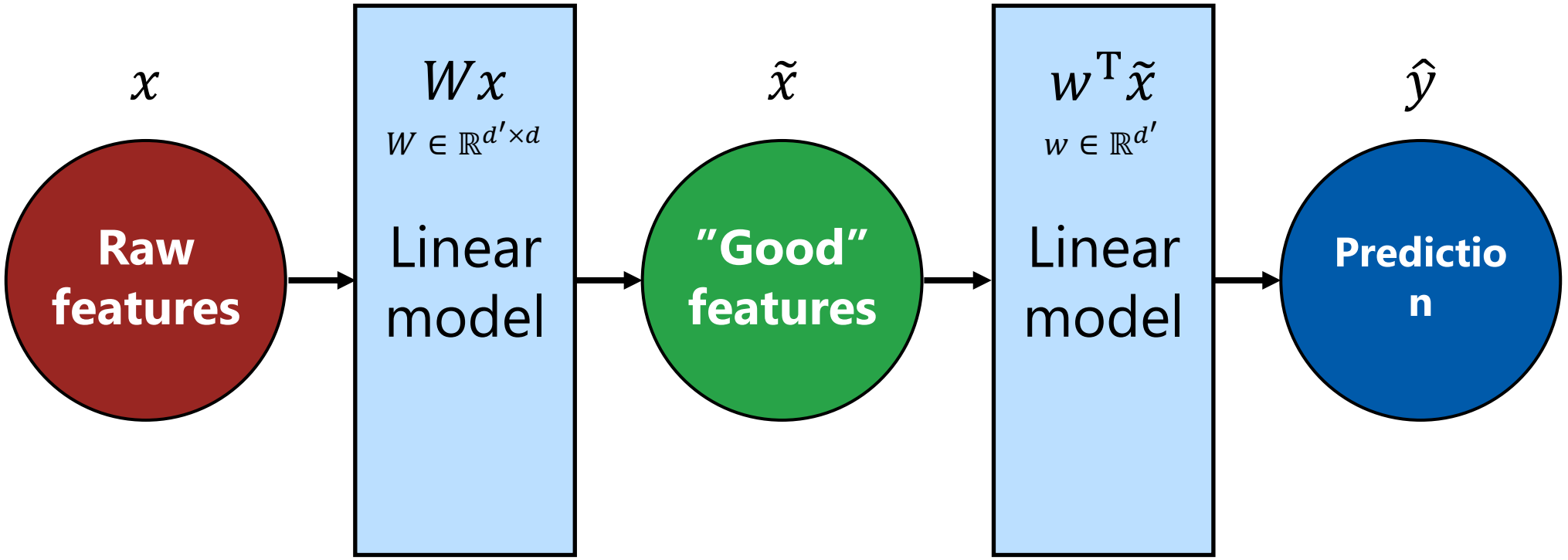
Add another model

Train everything simultaneously

- Can use gradient descent if both models are **differentiable**

Note: stacking models like this likely makes the problem non-convex
⇒ **no convergence guarantees**

Can it be another linear model?



$$\hat{y} = w^{\mathrm{T}}\tilde{x}$$

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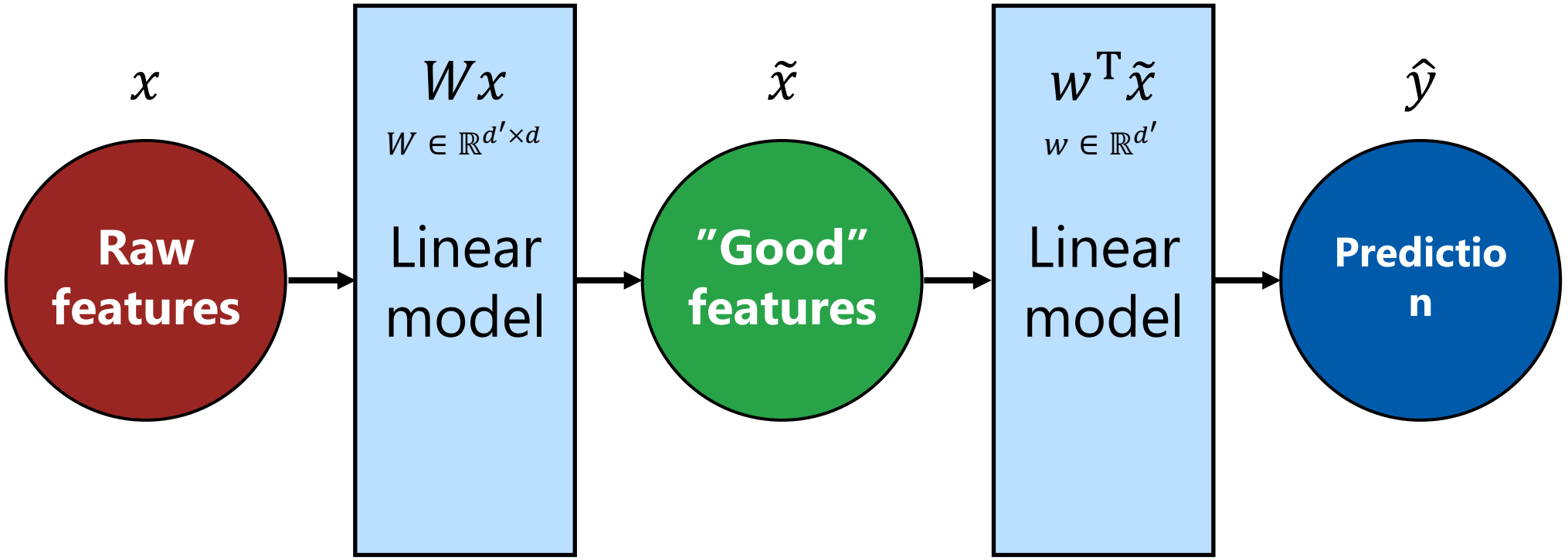

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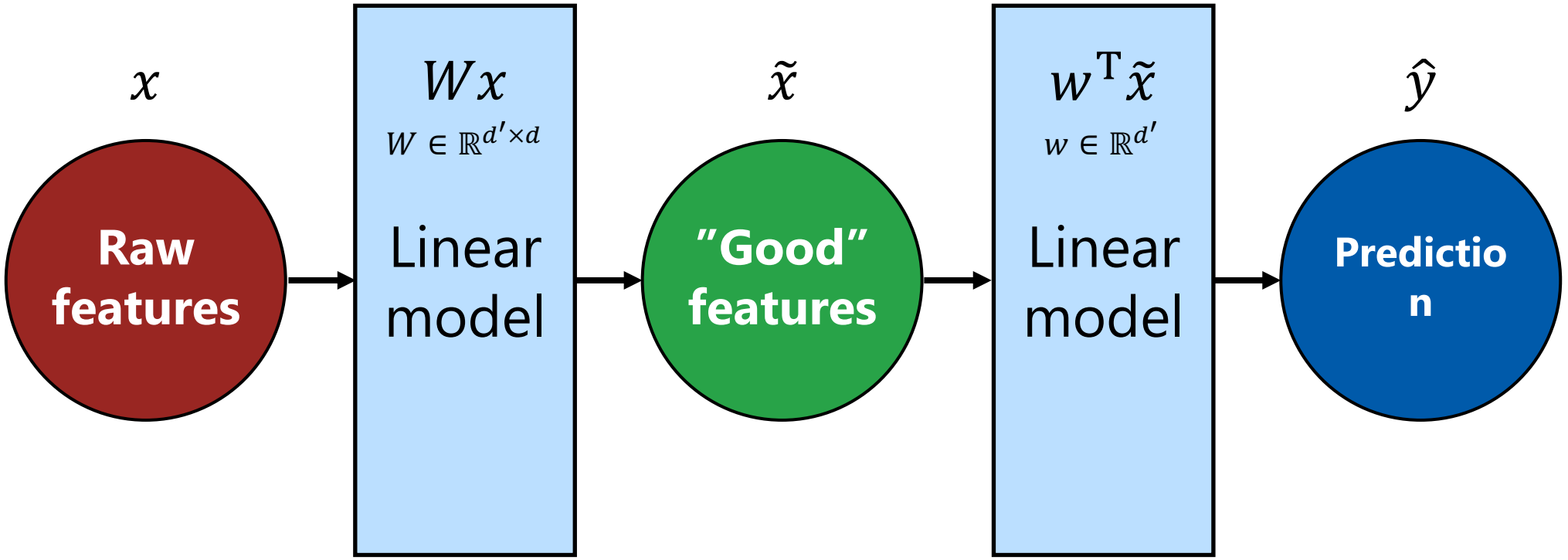

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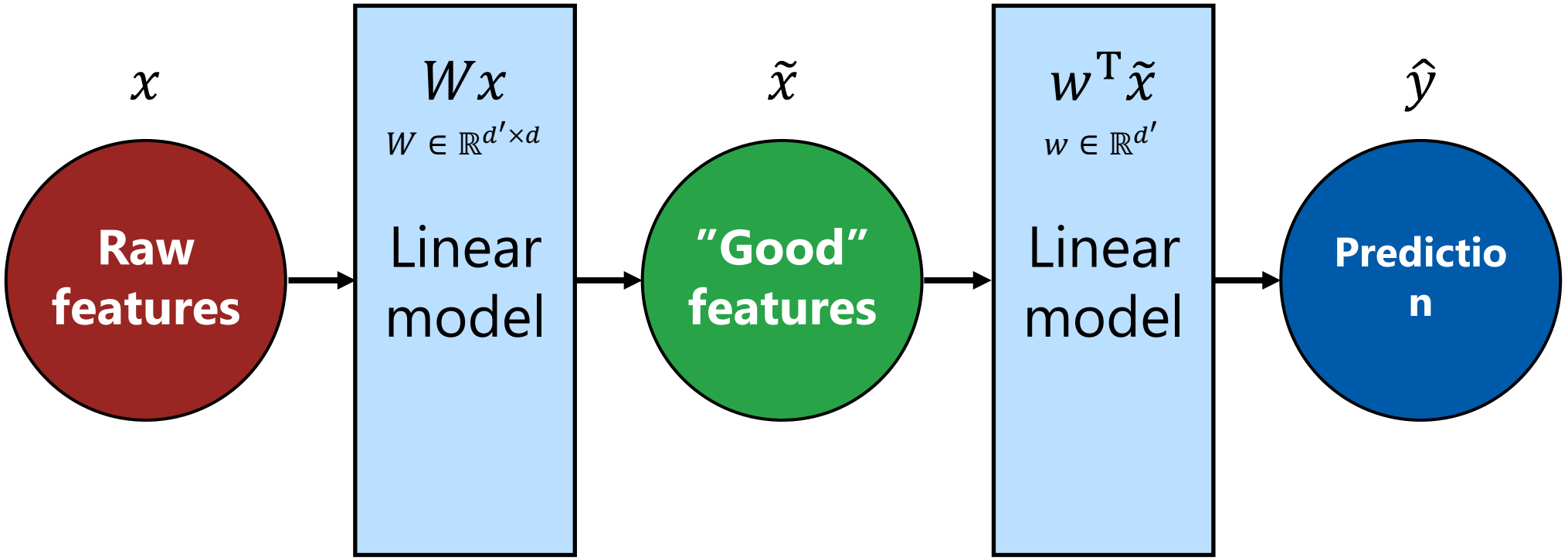
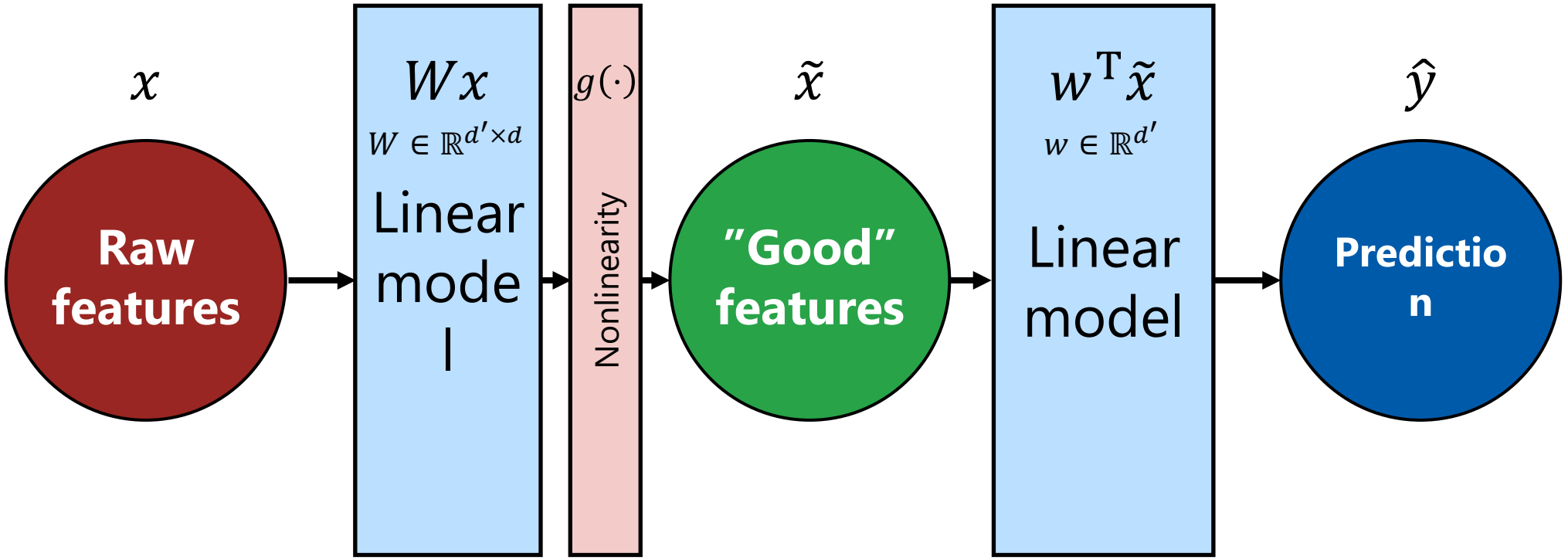


$$\hat{y} = w^{\mathrm{T}}\tilde{x} = w^{\mathrm{T}}(Wx) = \left(w^{\mathrm{T}}W\right)x = w'^{\mathrm{T}}x$$

- turns everything into just a single linear model

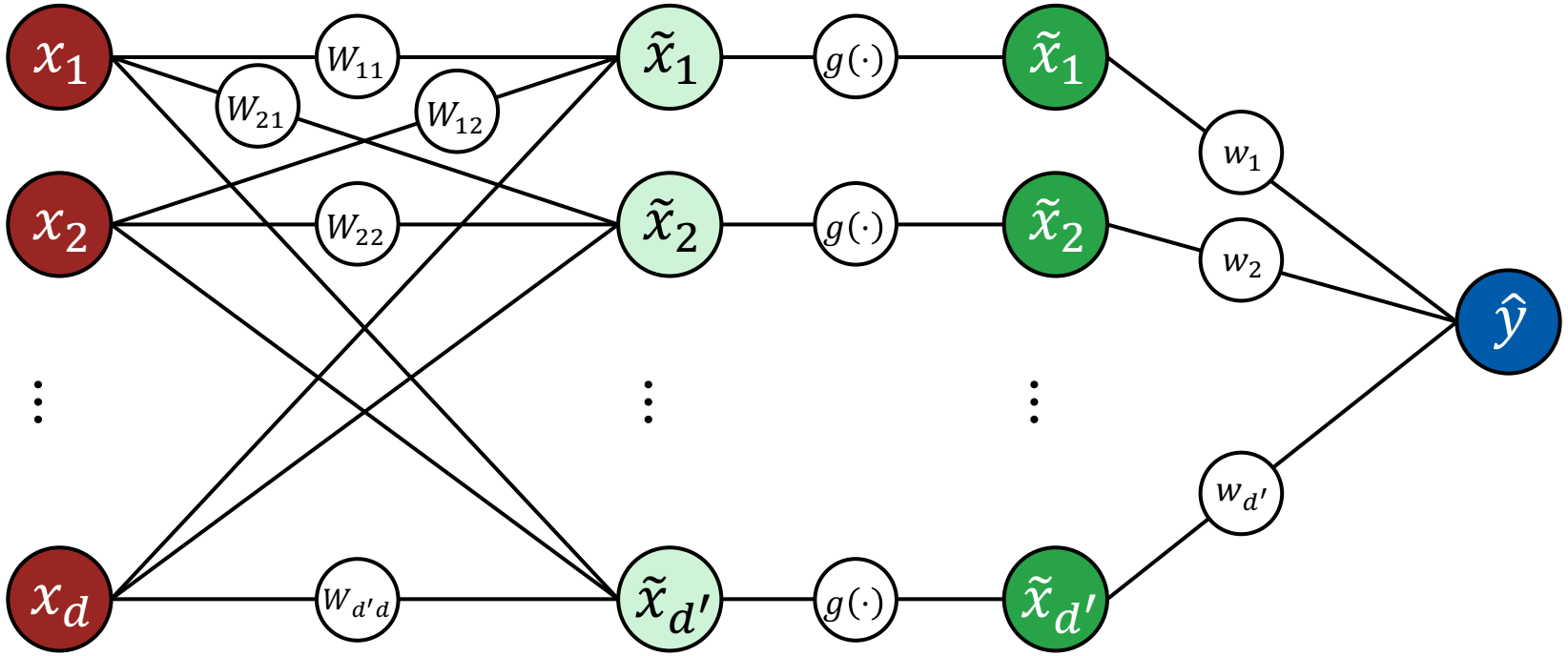
Fix: just introduce a nonlinearity



$$\hat{y} = w^{\mathrm{T}}\tilde{x} = w^{\mathrm{T}} g(Wx)$$

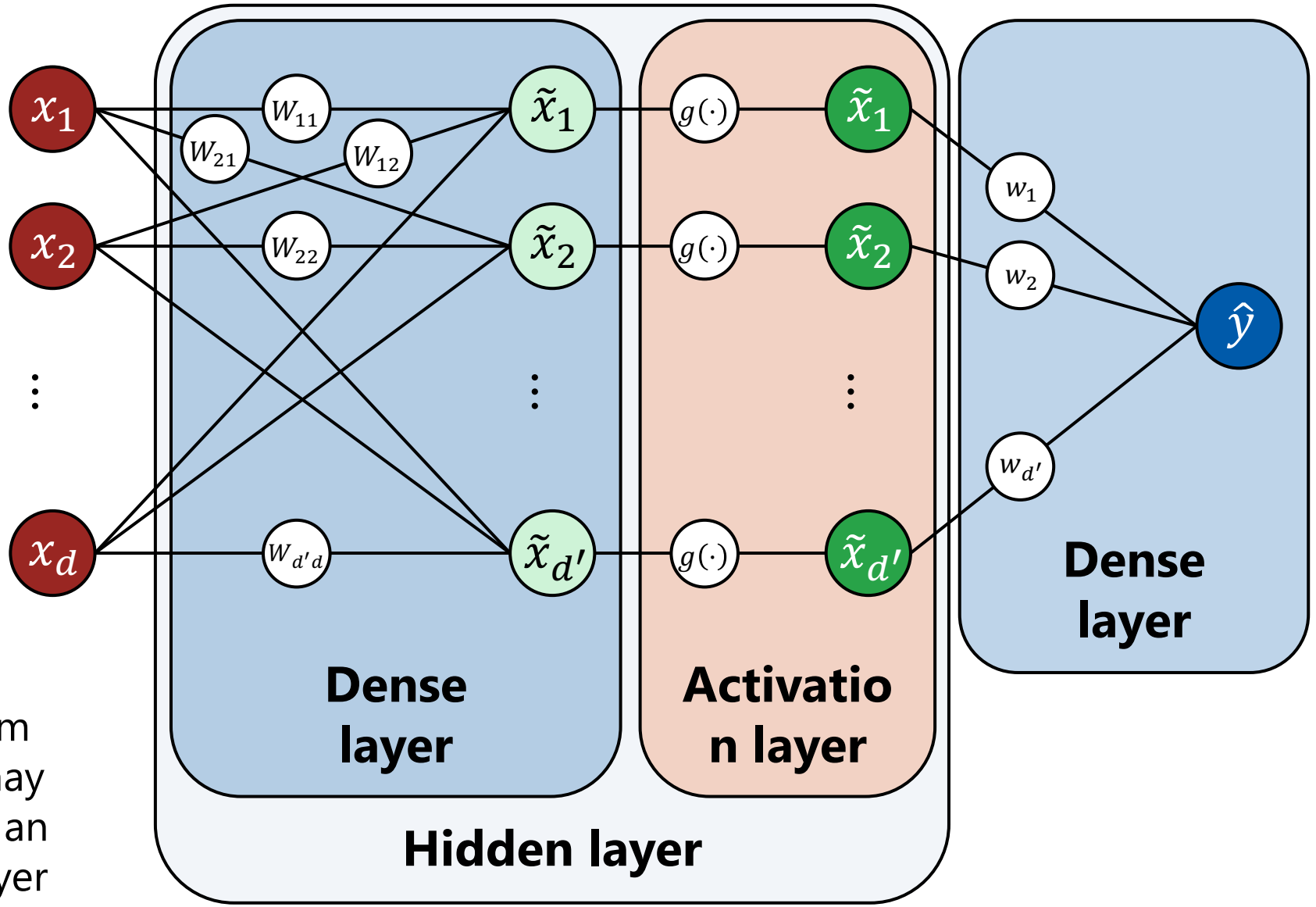
$g(\cdot)$ – some **nonlinear** scalar function (applied elementwise)

In greater detail



$$\hat{y} = w^{\mathrm{T}}\tilde{x} = w^{\mathrm{T}} g(Wx) = \sum_j \left[w_j g\left(\sum_i W_{ji} x_i \right) \right]$$

Some terminology



Note: the term "activation" may also stand for an output of a layer

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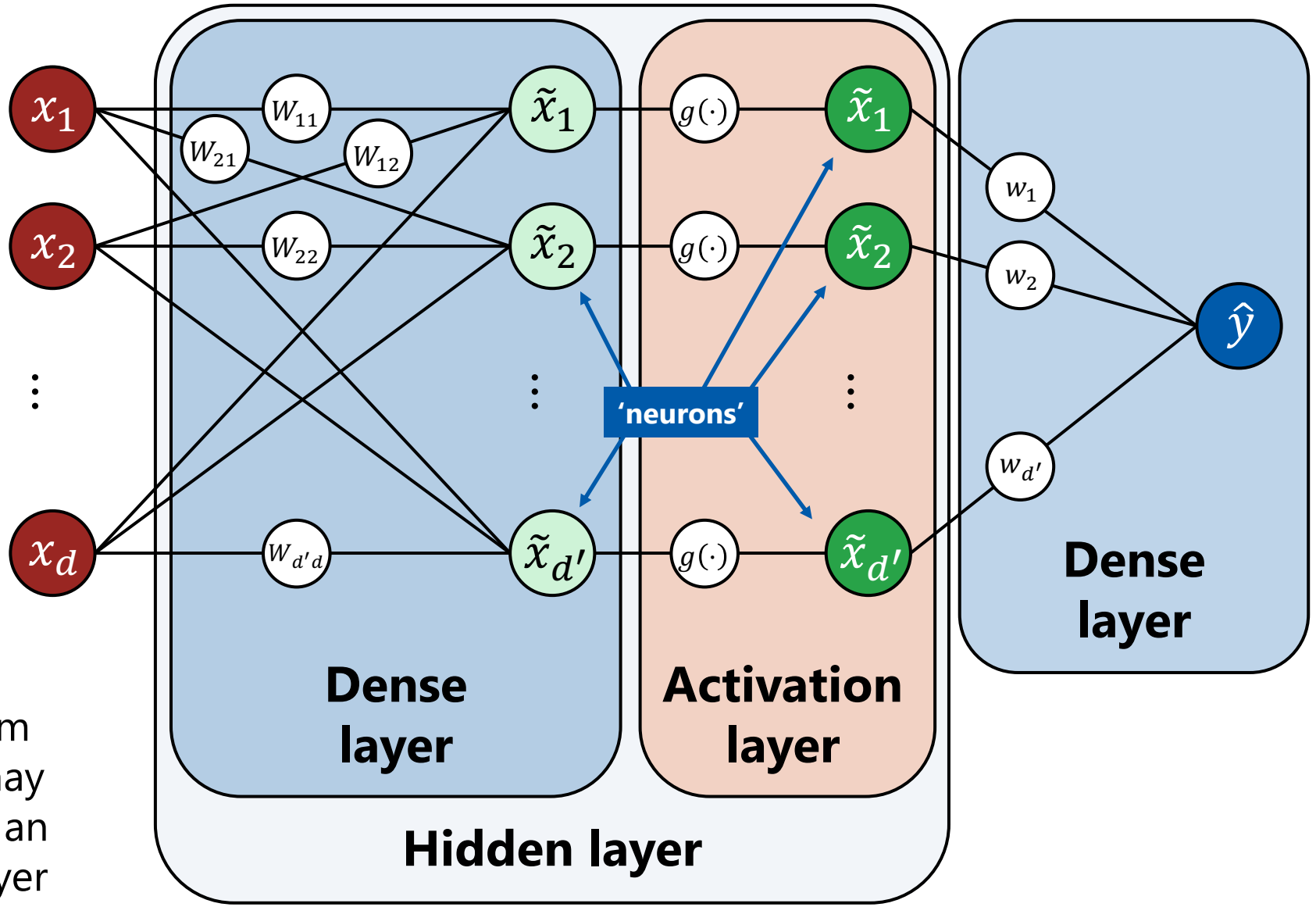

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Activation functions

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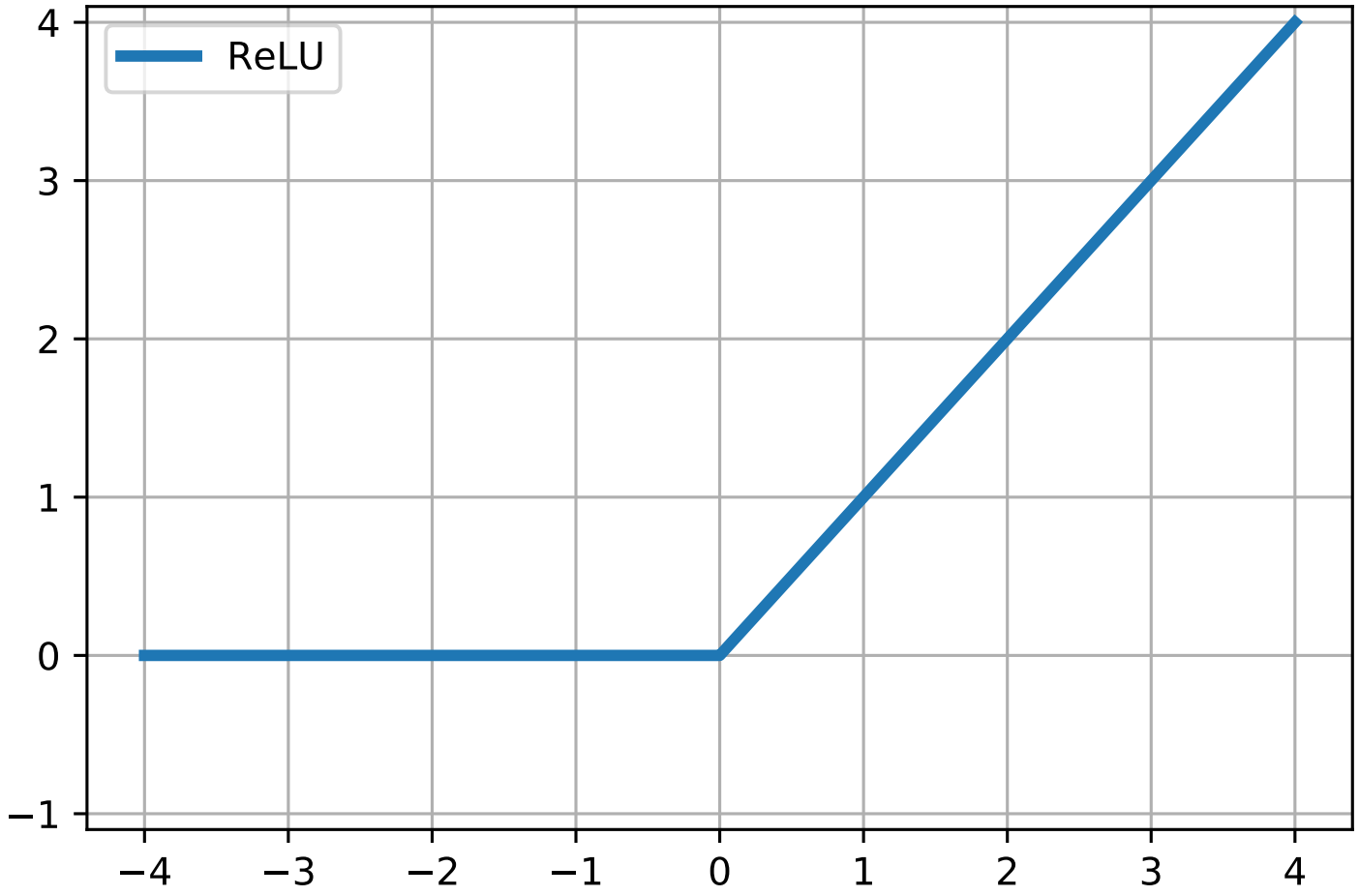

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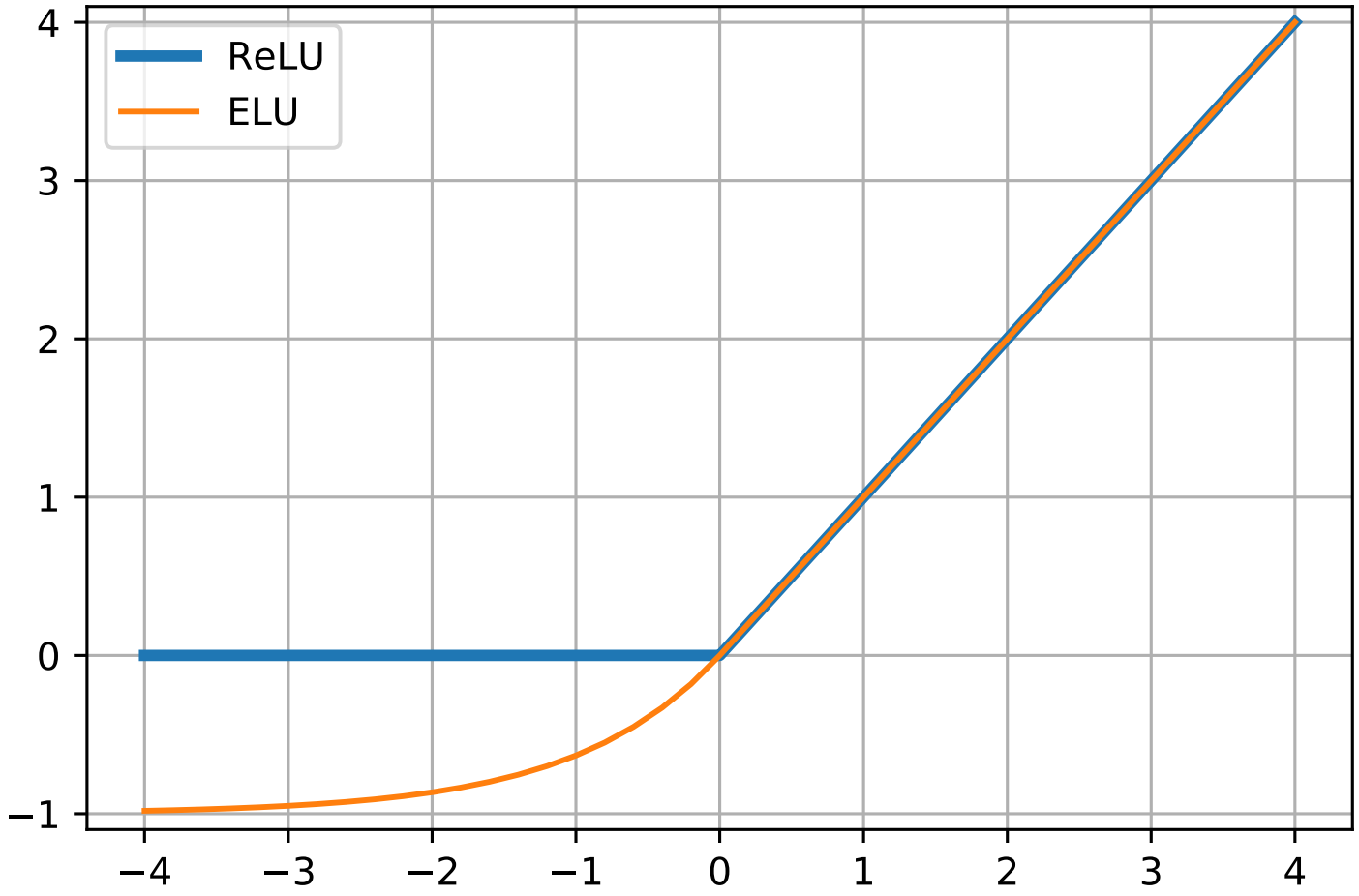
Activation functions



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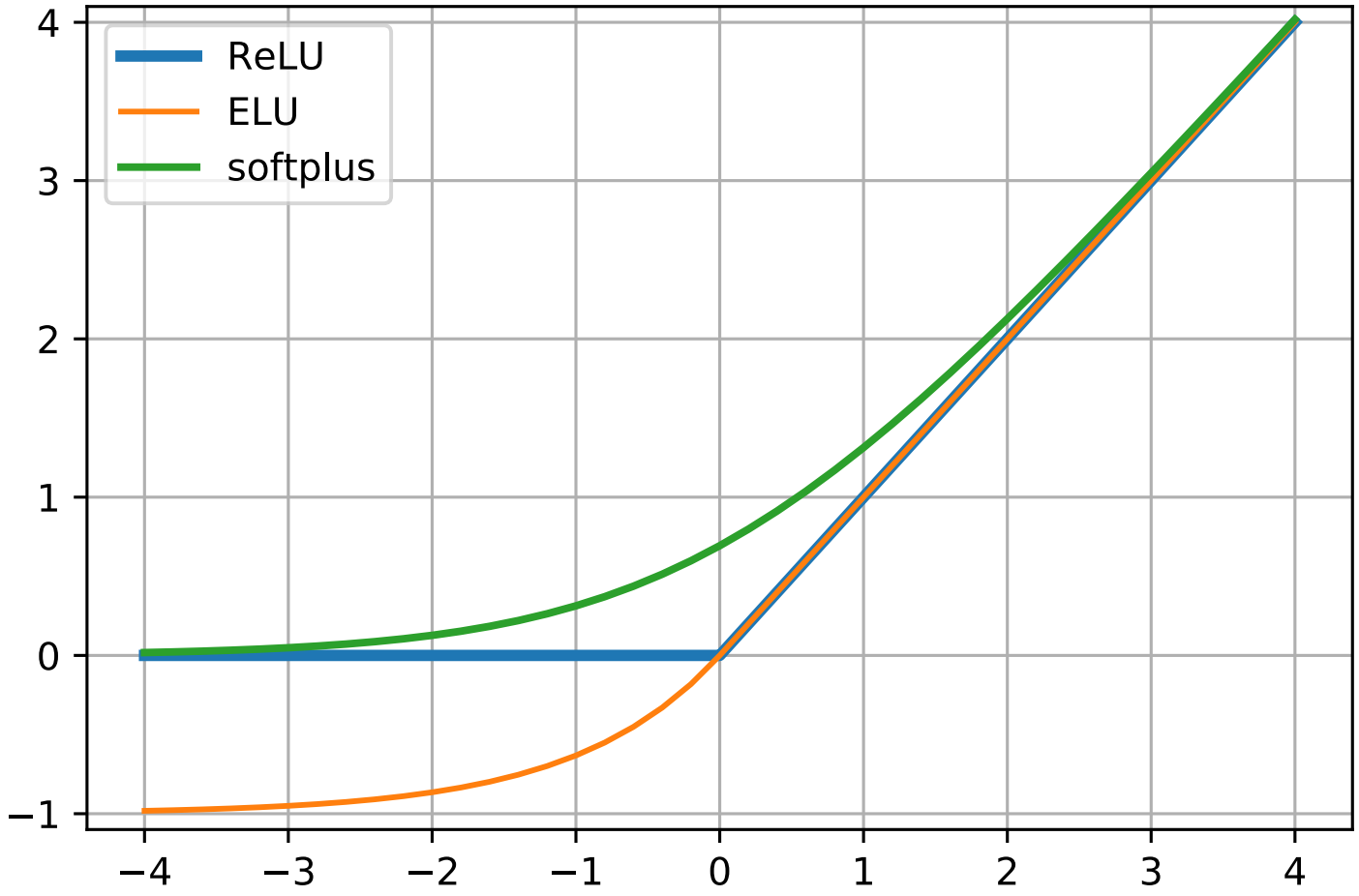

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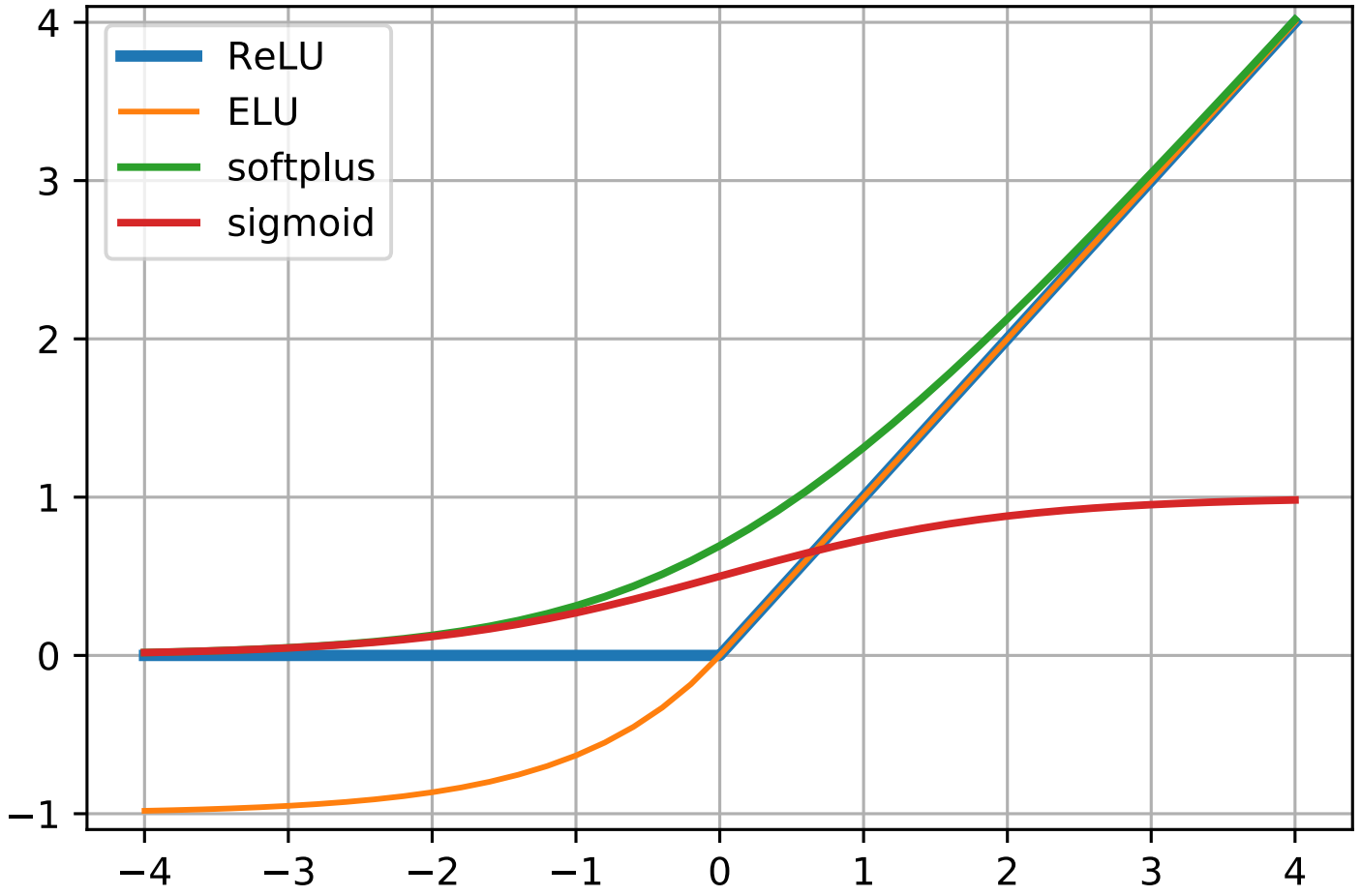

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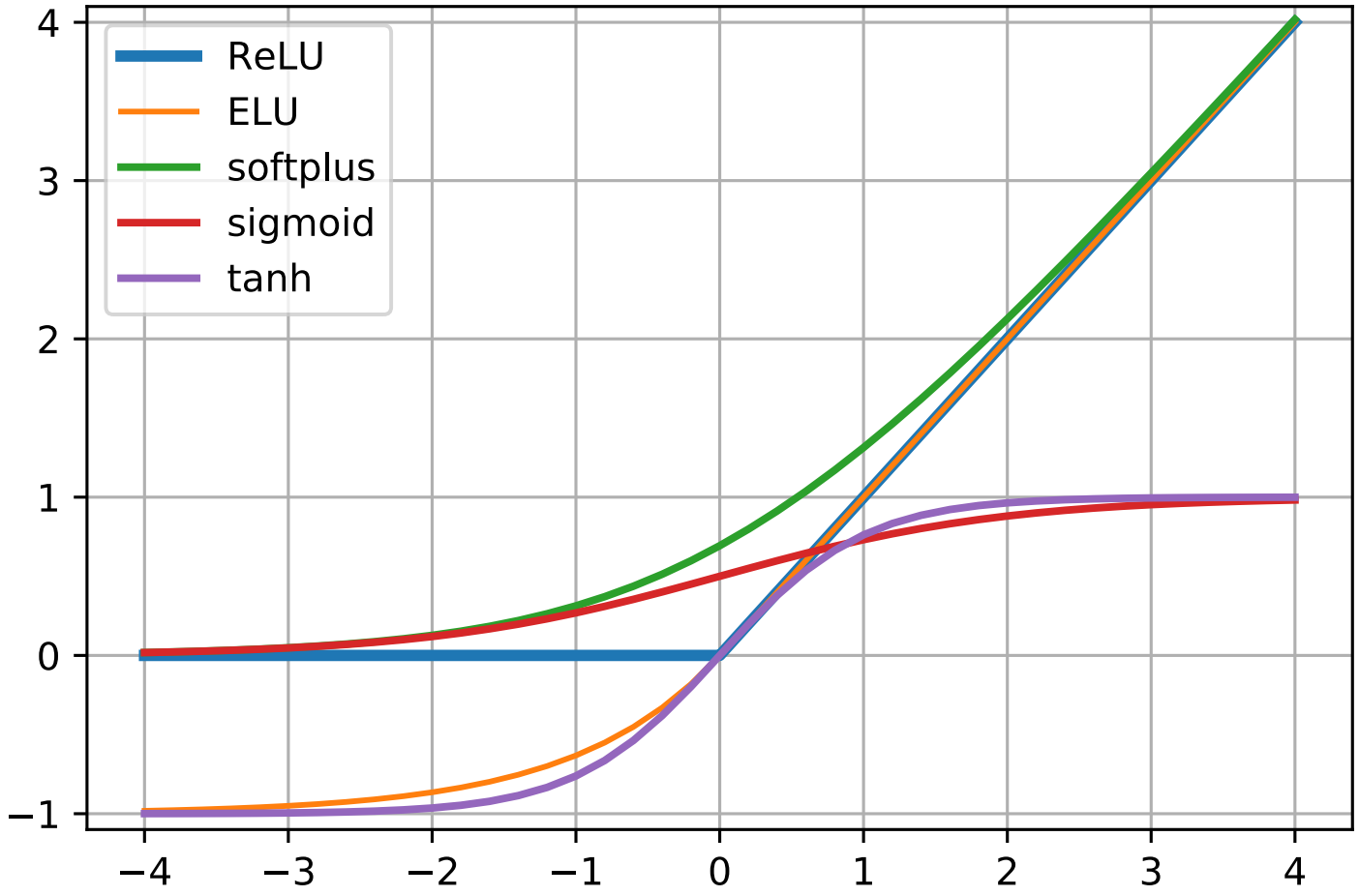

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$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

Universal approximator

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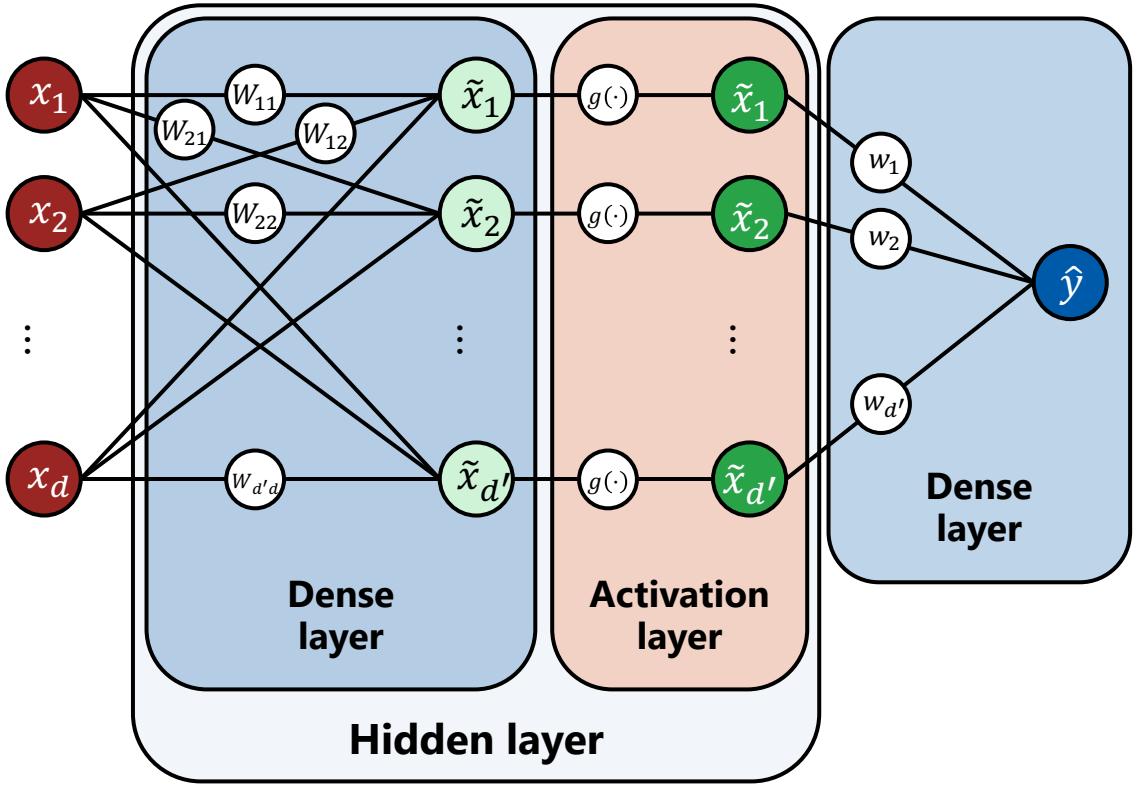
Just a single hidden layer with a nonlinearity makes this model a universal approximator



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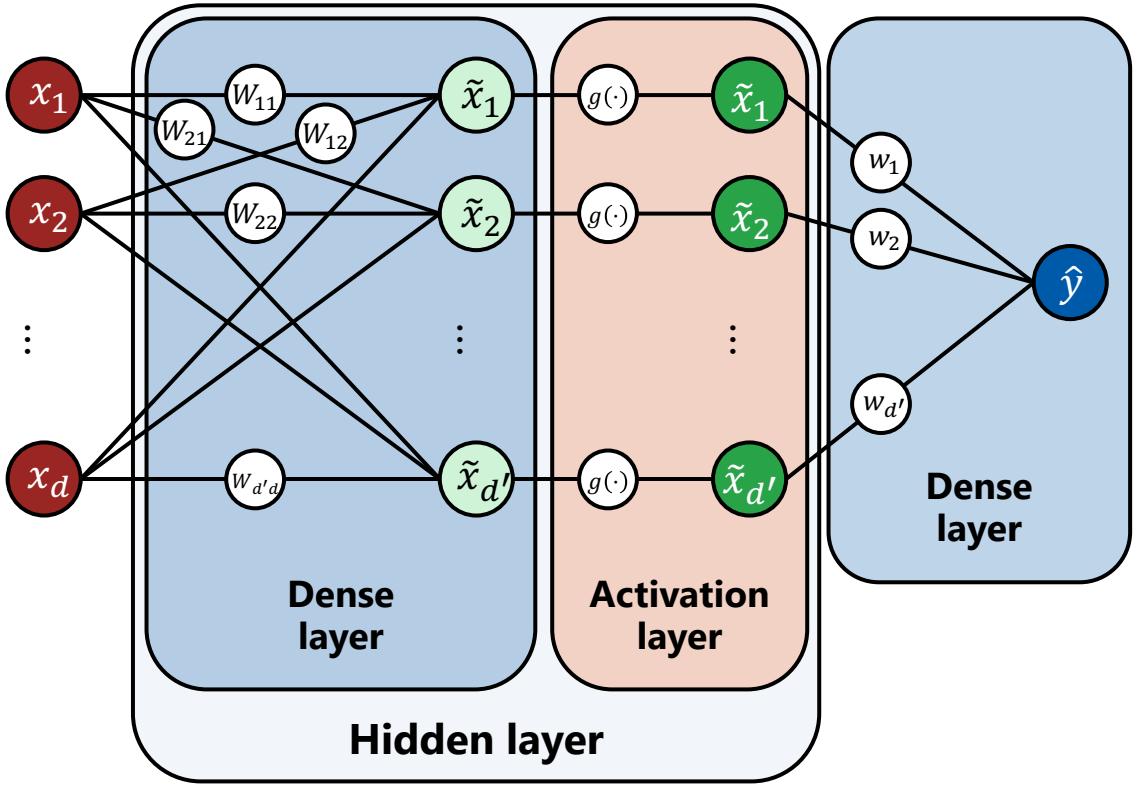
Just a single hidden layer with a nonlinearity makes this model a universal approximator

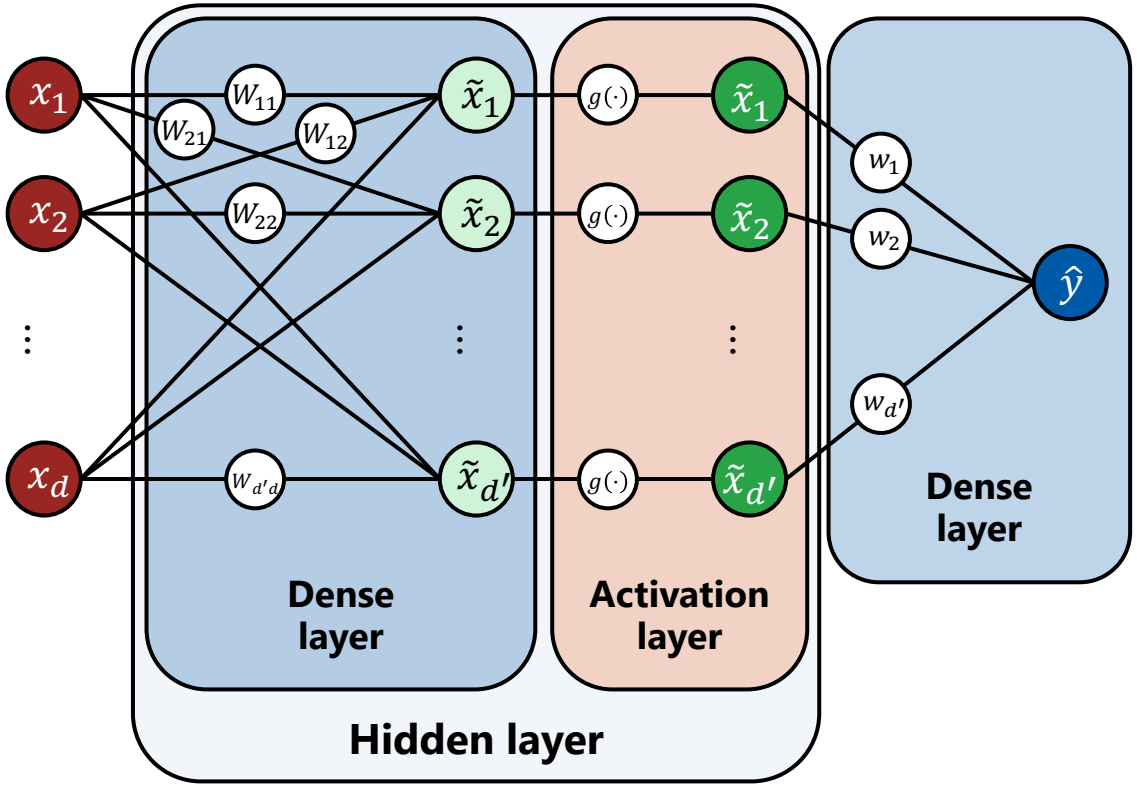
- any function can be approximated **arbitrarily close** given wide enough hidden layer (large enough d')



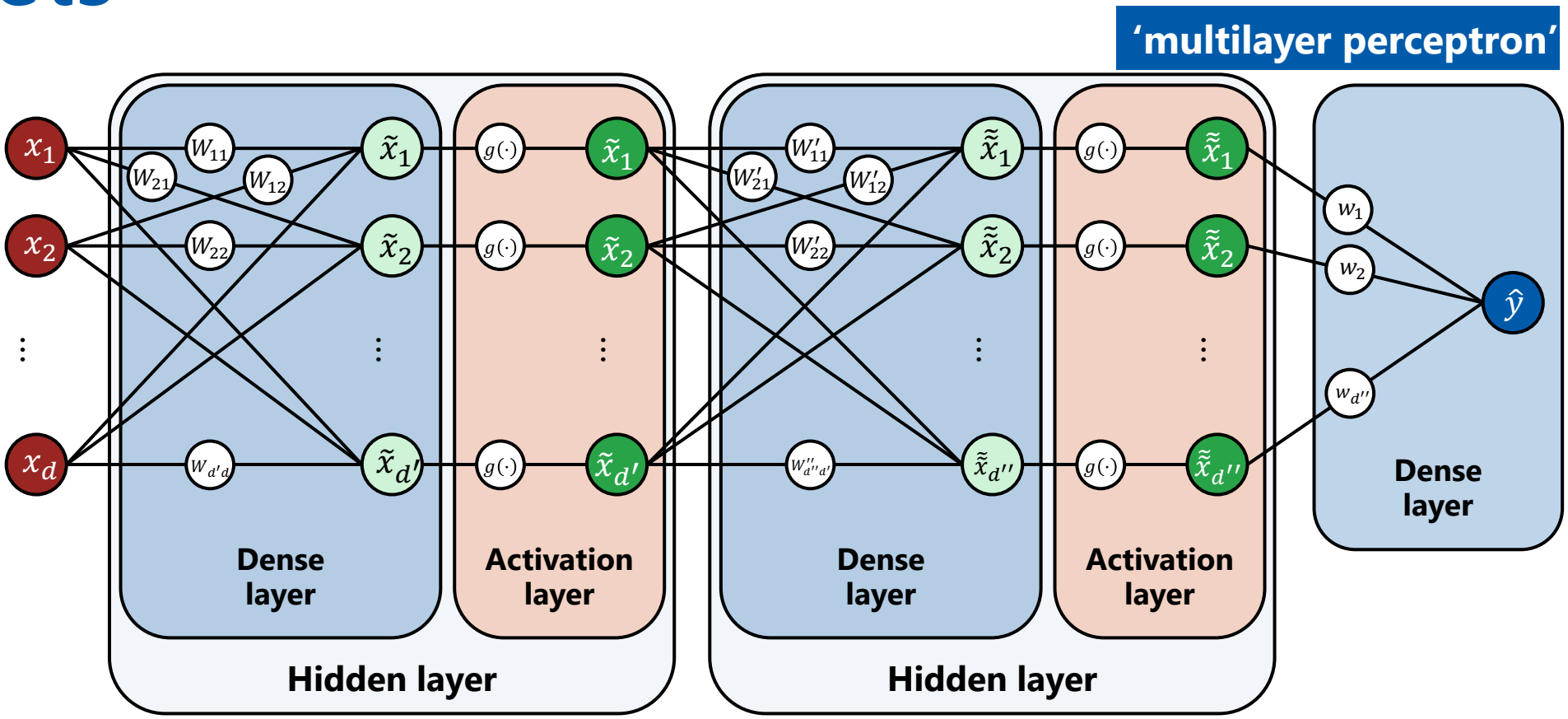
Universal approximator

Just a single hidden layer with a nonlinearity makes this model a universal approximator

- any function can be approximated **arbitrarily close** given wide enough hidden layer (large enough d')
- Note: in practice we might not be able to find this approximation
  - e.g. due to heavily non-convex loss function, infeasibly large d', overfitting



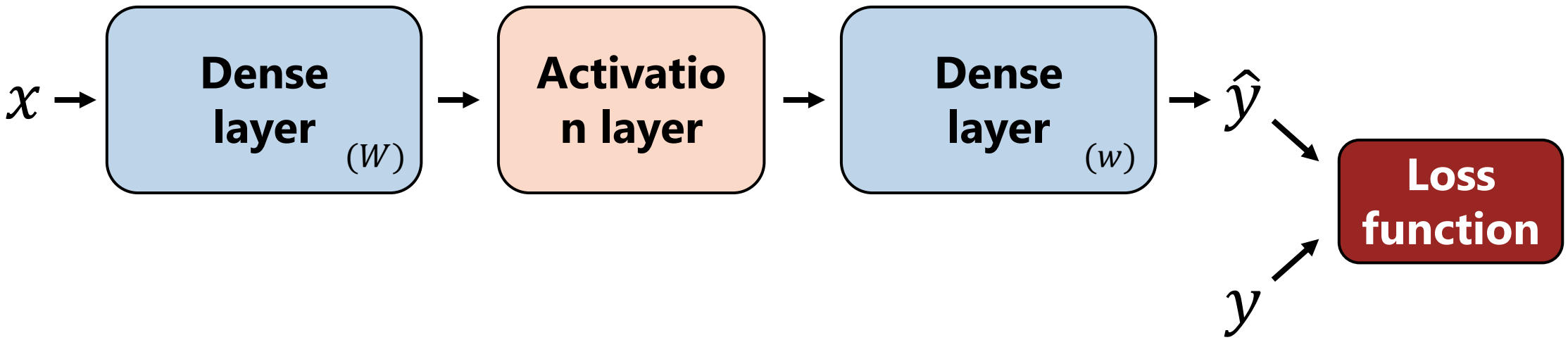
Deeper nets



In practice, stacking more hidden layers often reduces the number of neurons required to represent a given function

Backpropagation

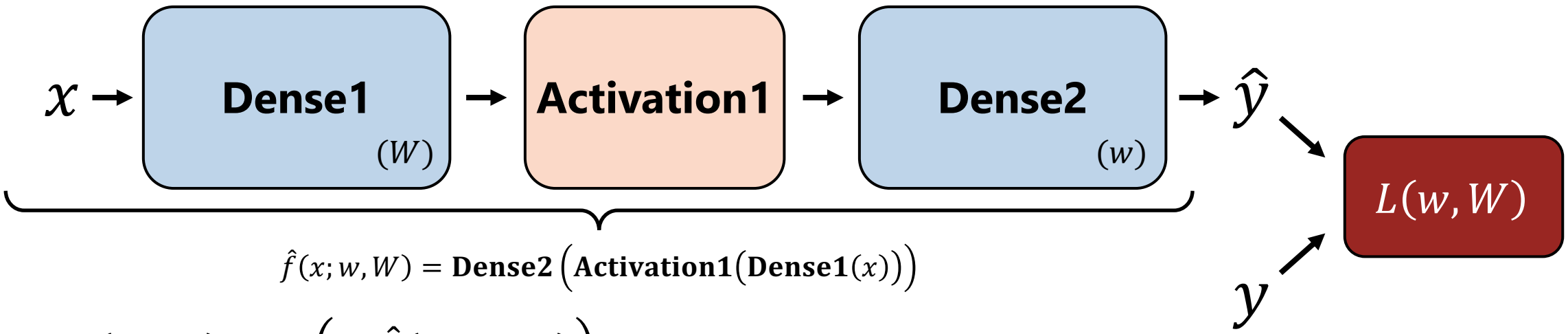
Loss function



E.g. mean squared error:

$$L = \frac{1}{N} \sum_{i=1 \ldots N} \left(y_i - w^{\mathrm{T}} g(W x_i) \right)^2$$

Calculating derivatives



$$L(w, W) \equiv L\left(y, \hat{f}(x; w, W)\right)$$

$$\frac{\partial L}{\partial W} = \frac{\partial L(y, \hat{f})}{\partial \hat{f}} \cdot \frac{\partial \hat{f}}{\partial W} =$$

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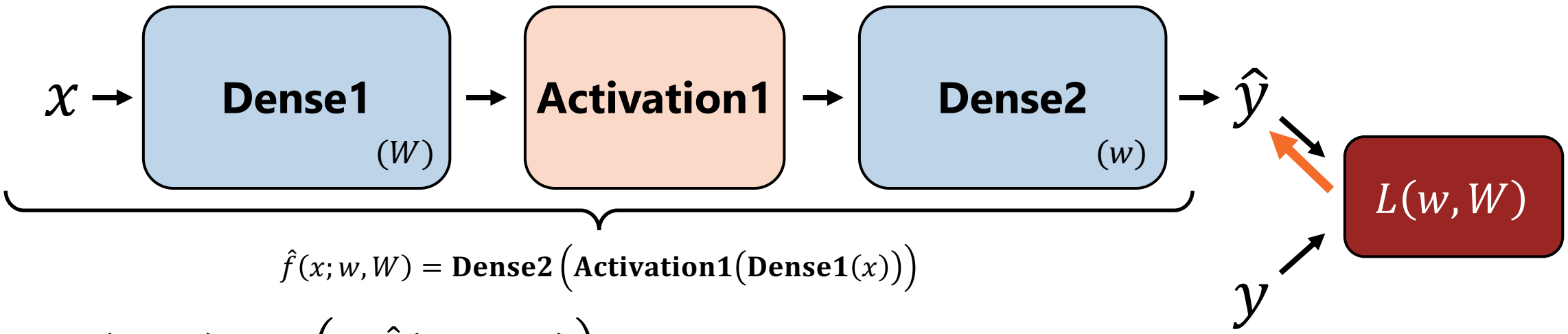

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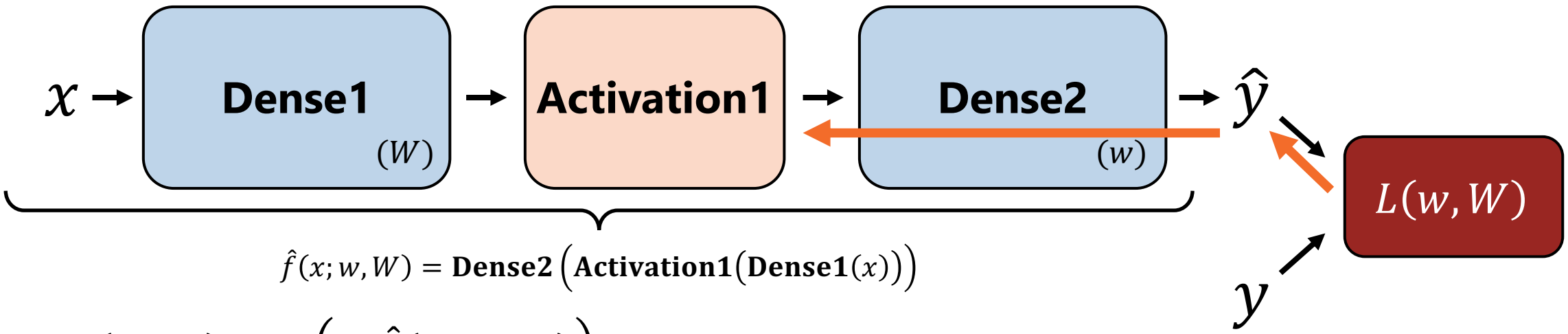

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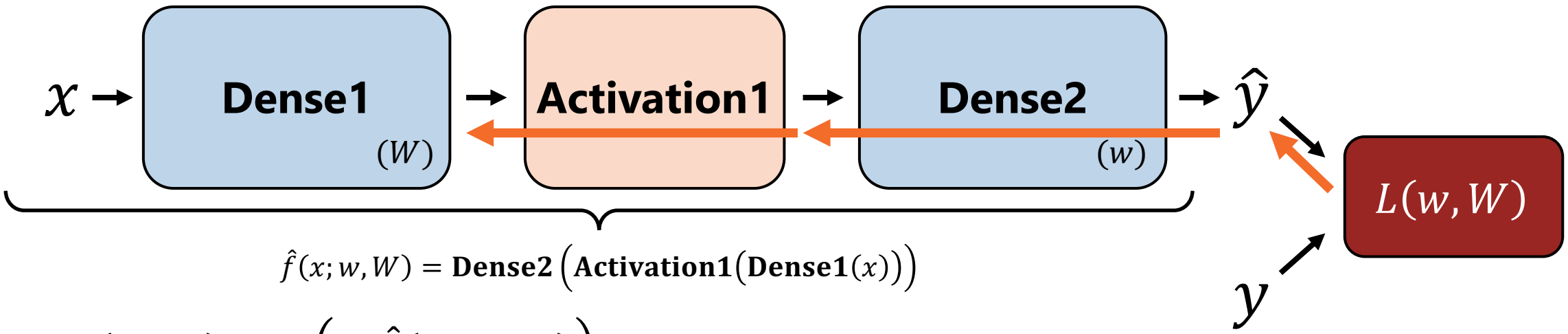

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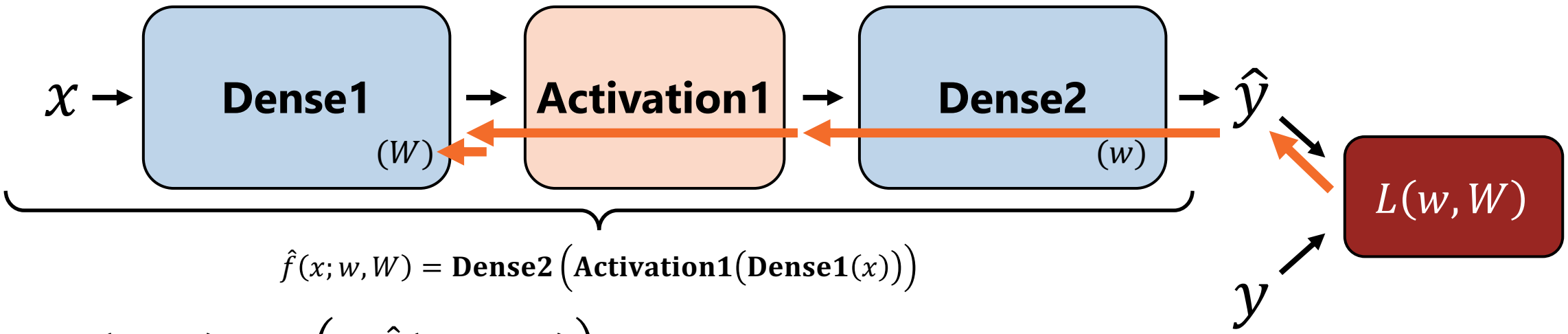

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Backpropagation algorithm ≈ applying the chain rule

- The actual algorithm states how to do it efficiently

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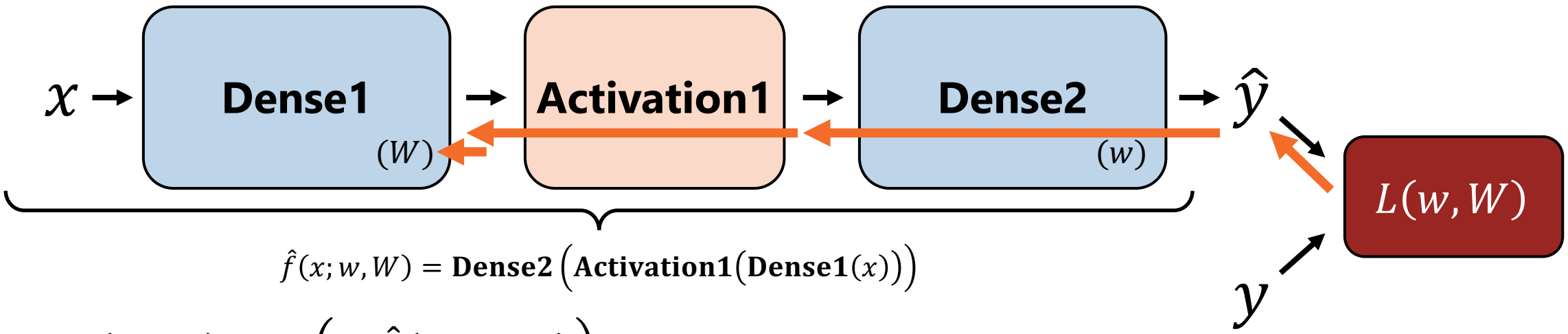

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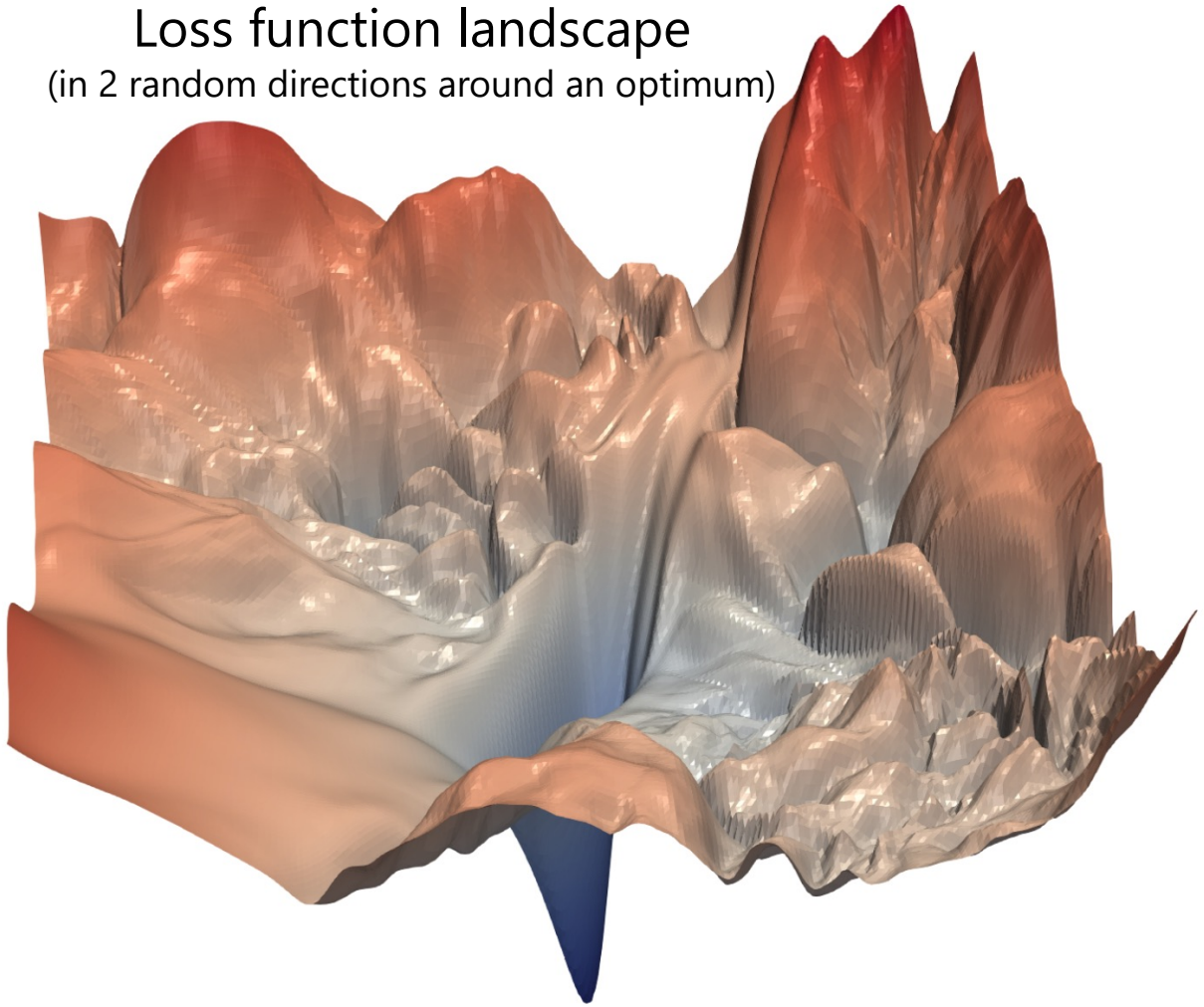
Optimization techniques

How to optimize such functions?

Loss function landscape
(in 2 random directions around an optimum)



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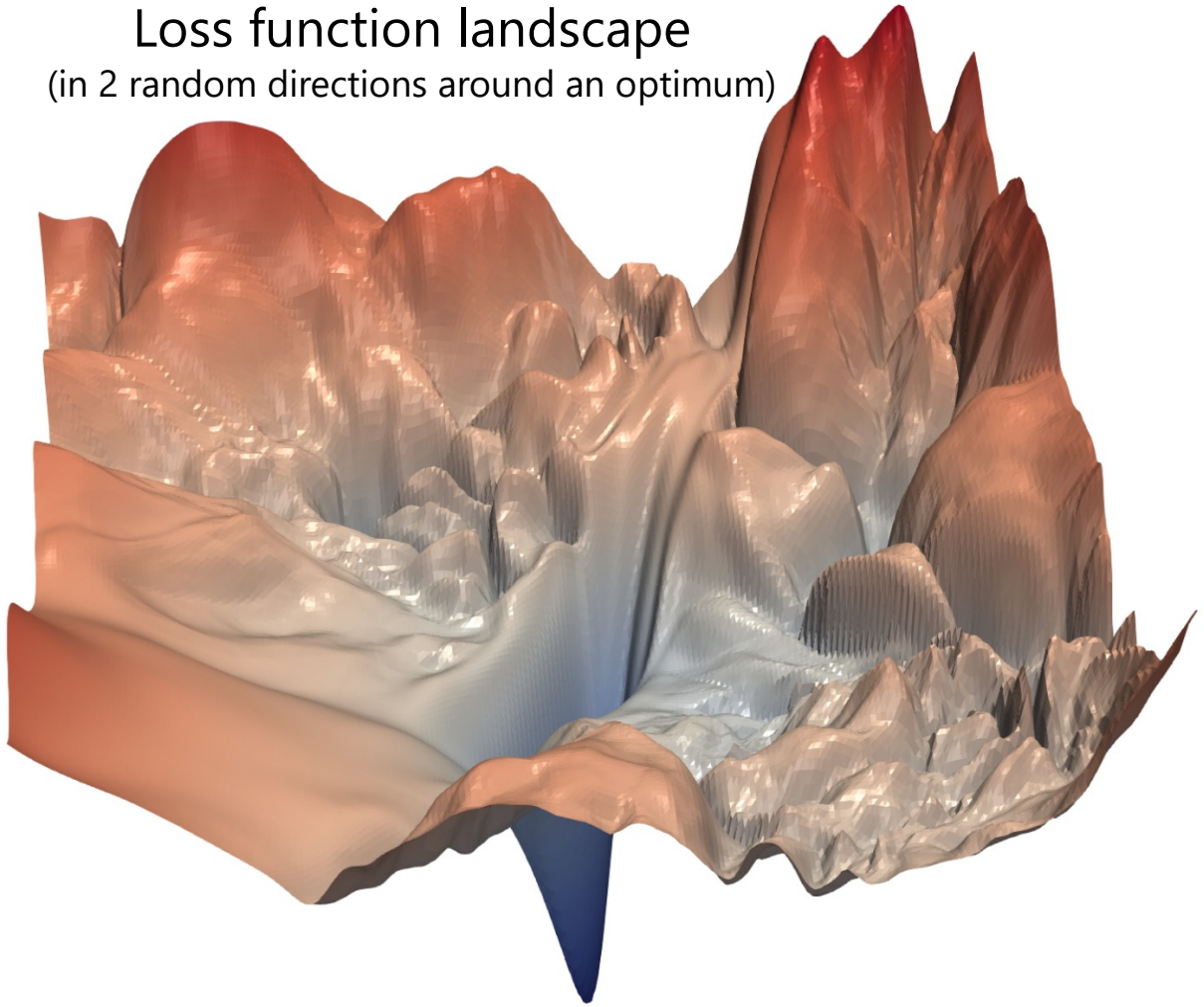

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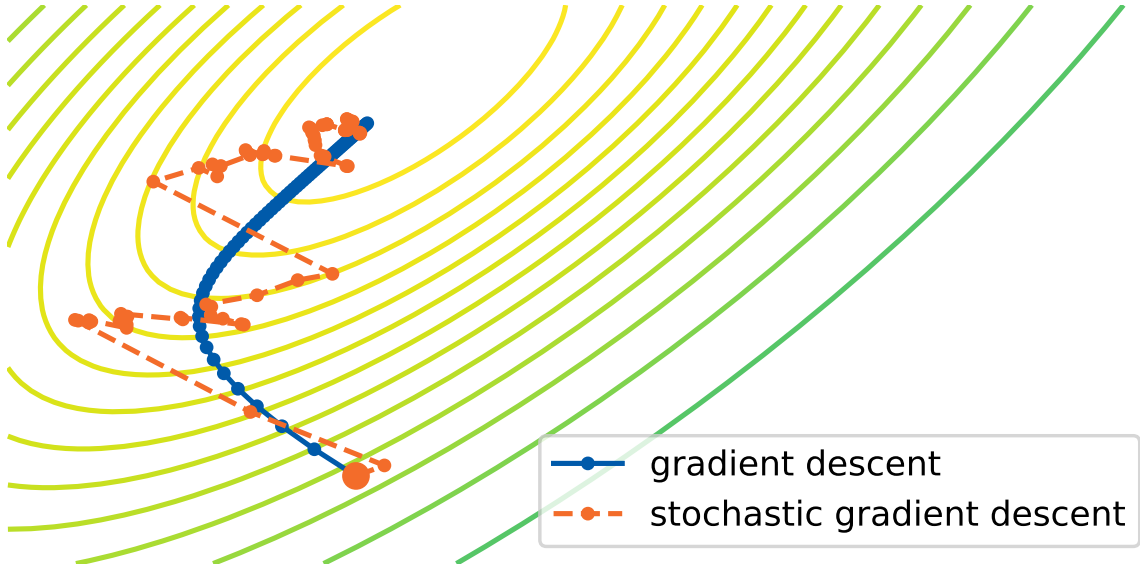
No convergence guarantees for the stochastic gradient descent

There's a number of modifications to improve training

SGD on mini-batches

SGD:

- At each step k pick $l_k \in \{1, \dots, N\}$ at random, then update:
- $\theta^{(k)} \leftarrow \theta^{(k-1)} - \eta \nabla_\theta \mathcal{L}\left(y_{l_k}, \widehat{f}_\theta\left(x_{l_k}\right)\right)\Big|_{\theta = \theta^{(k-1)}}$



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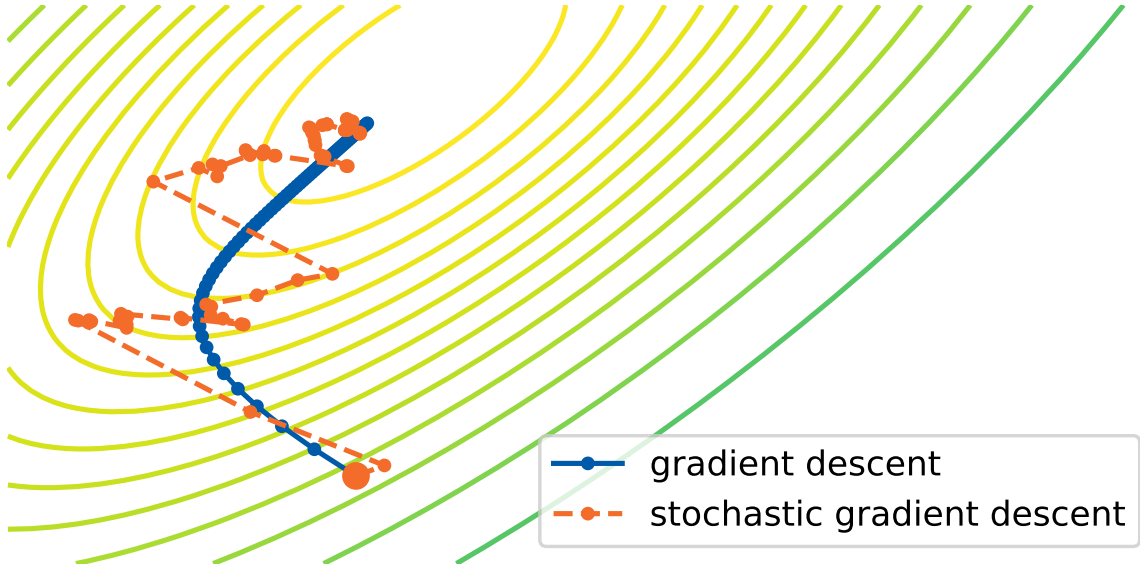
Mini-batch SGD:

- Shuffle the training set, then iterate through it in chunks (batches) of fixed size



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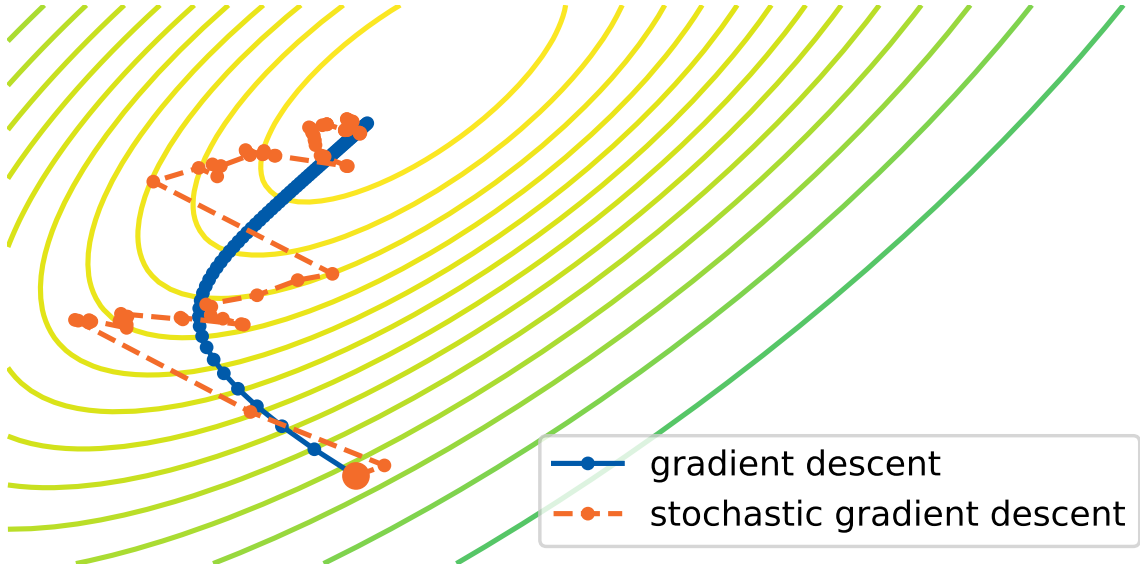

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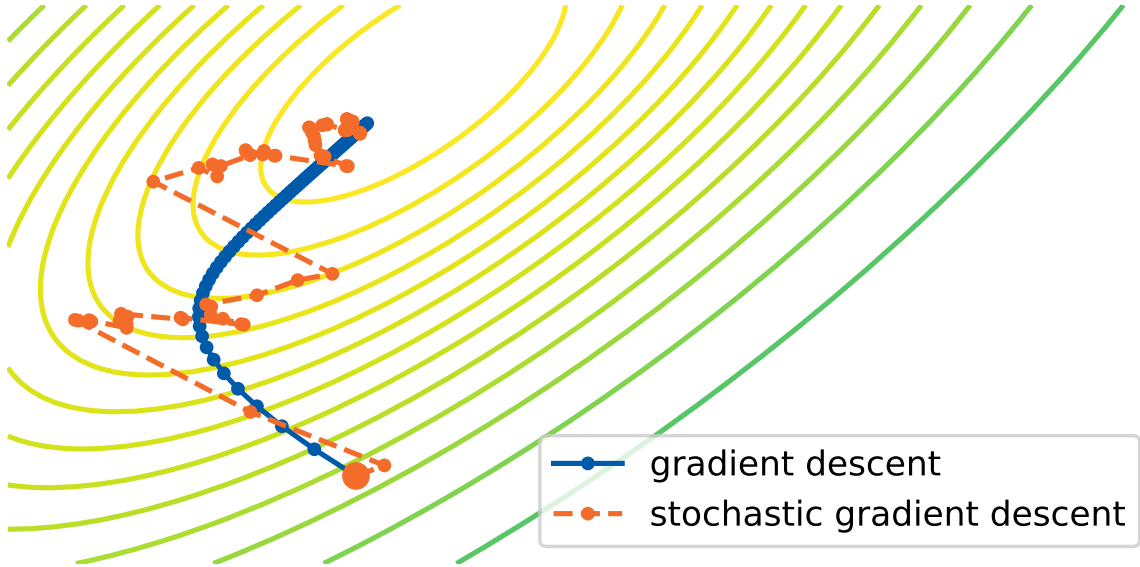
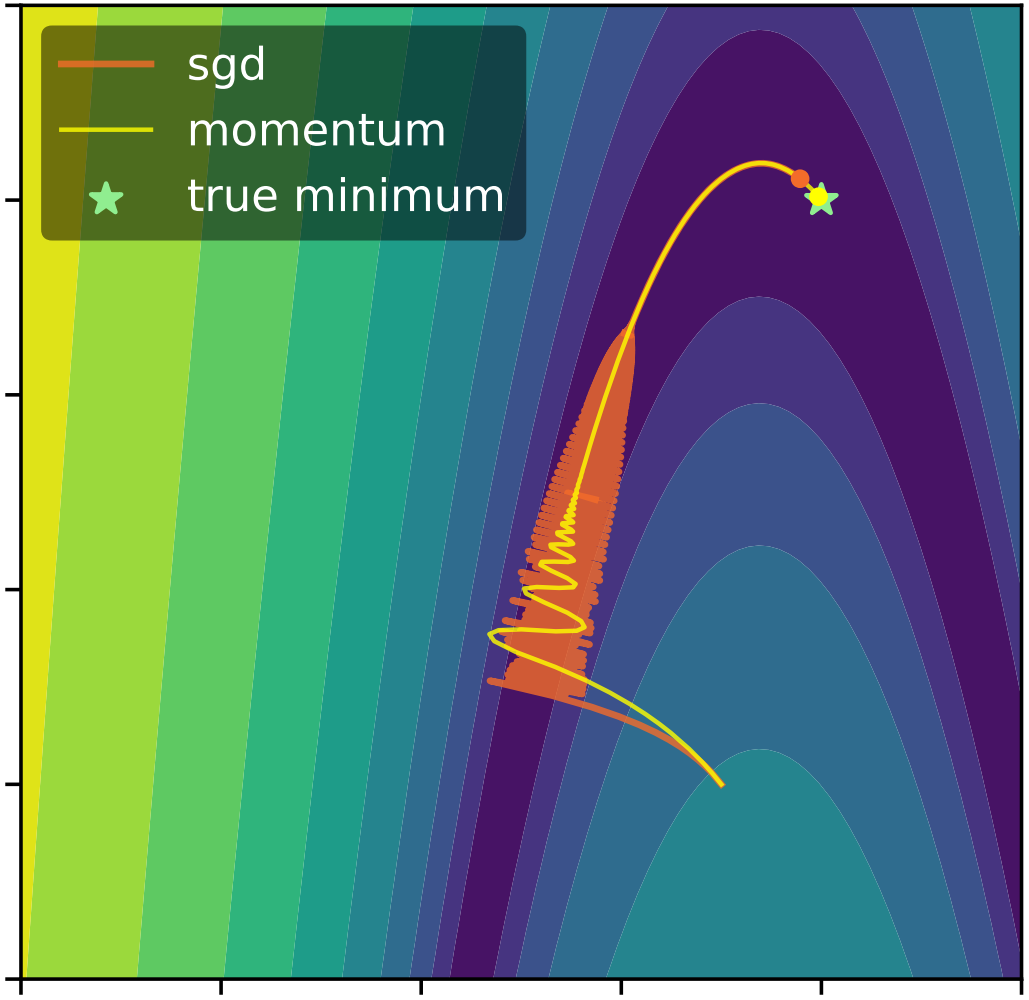
- Update the model parameters: $\theta^{(k)} \leftarrow \theta^{(k-1)} - \eta \cdot g$



Momentum SGD



Idea: introduce inertia (like a ball rolling down a hill)

$$m^{(k)} \leftarrow \beta \cdot m^{(k-1)} + (1-\beta) \cdot \left.\frac{\partial L}{\partial \theta}\right|_{\theta=\theta^{(k-1)}}$$

$$\theta^{(k)} \leftarrow \theta^{(k-1)} - \eta \cdot m^{(k)}$$

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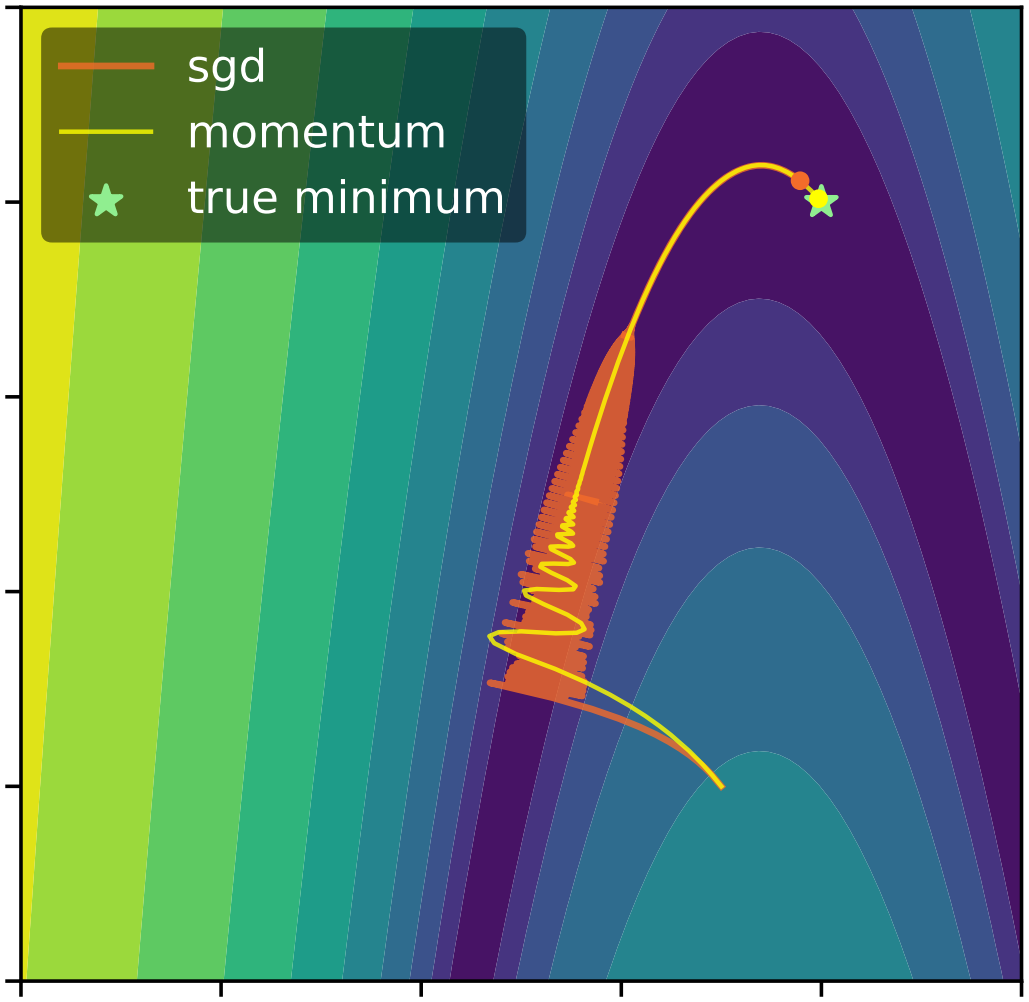

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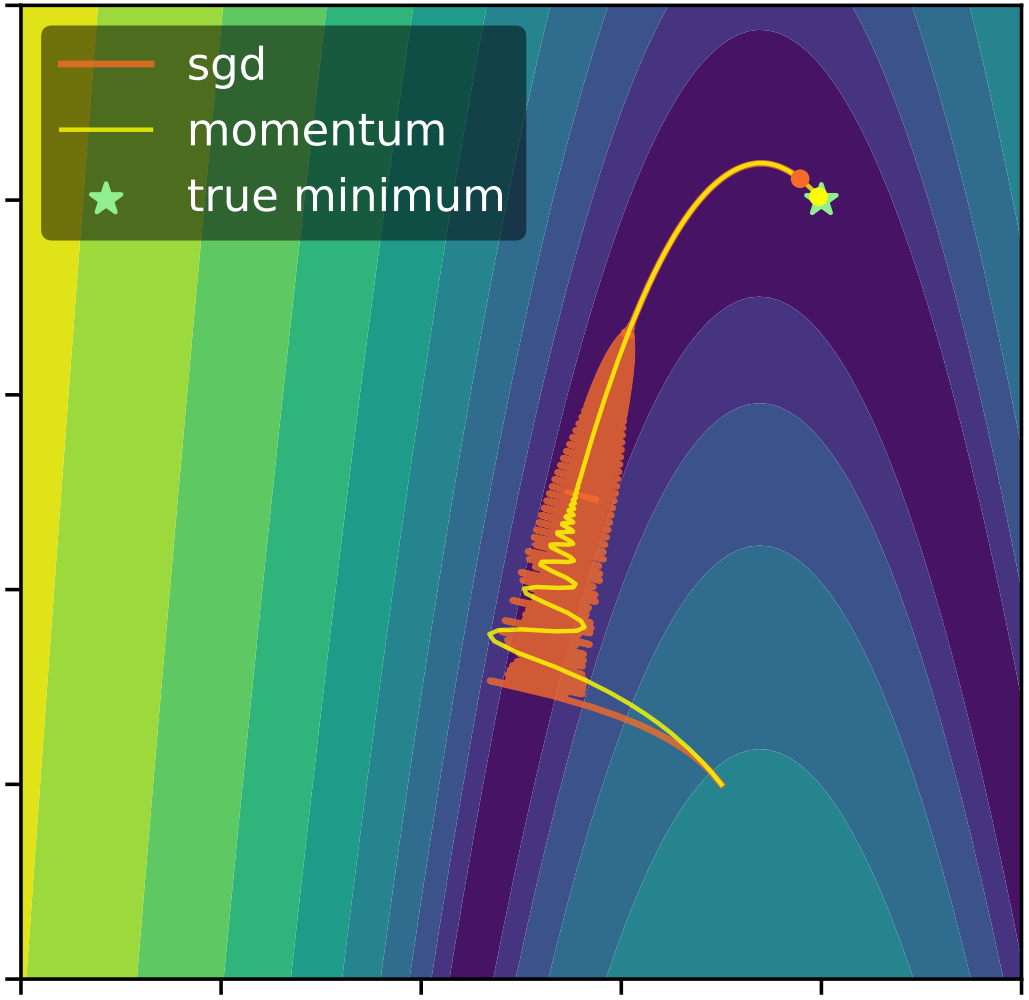

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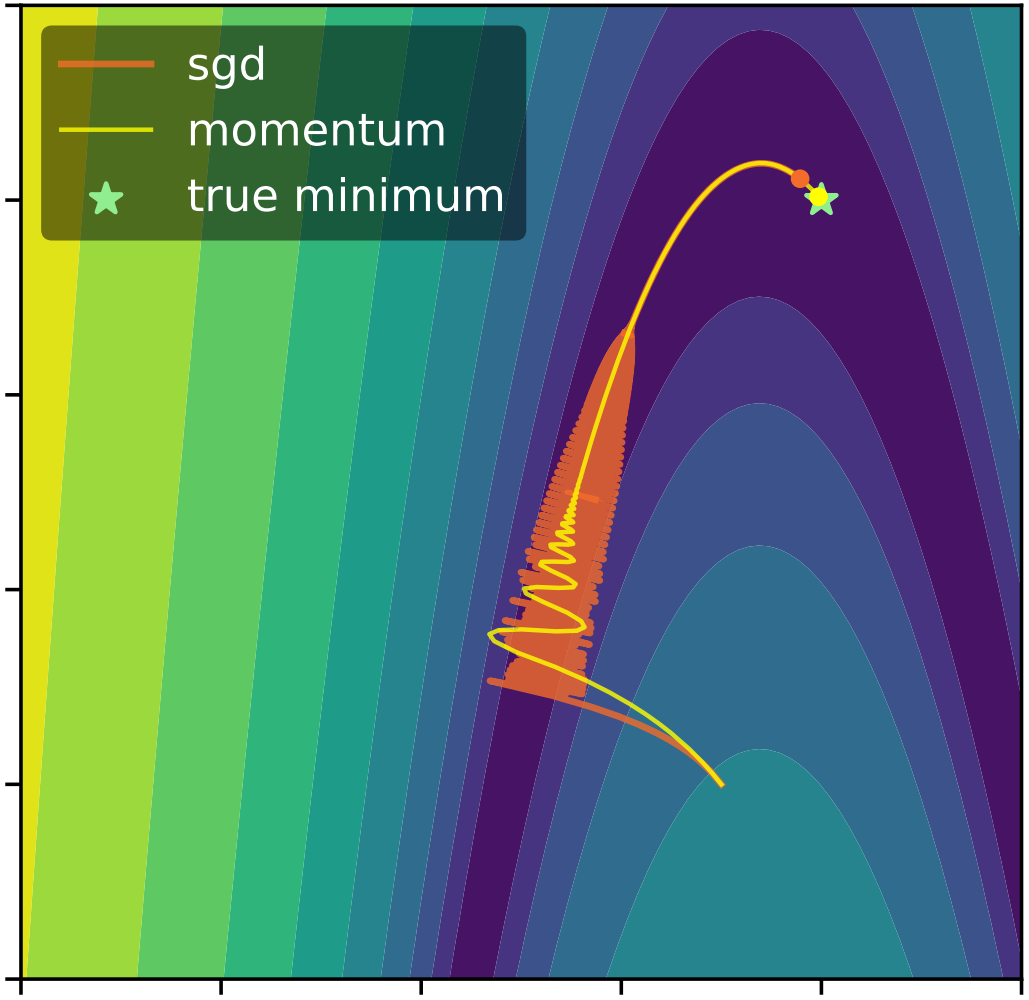

Idea: introduce inertia (like a ball rolling down a hill)

- Smooths out fast oscillations
- Helps getting out of small local minima
- Allows for larger range of learning rates*

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* https://distill.pub/2017/momentum/

RMSprop

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- Gradients getting smaller ⇒ increase the learning rate (scale by inverse running RMS of the gradient)

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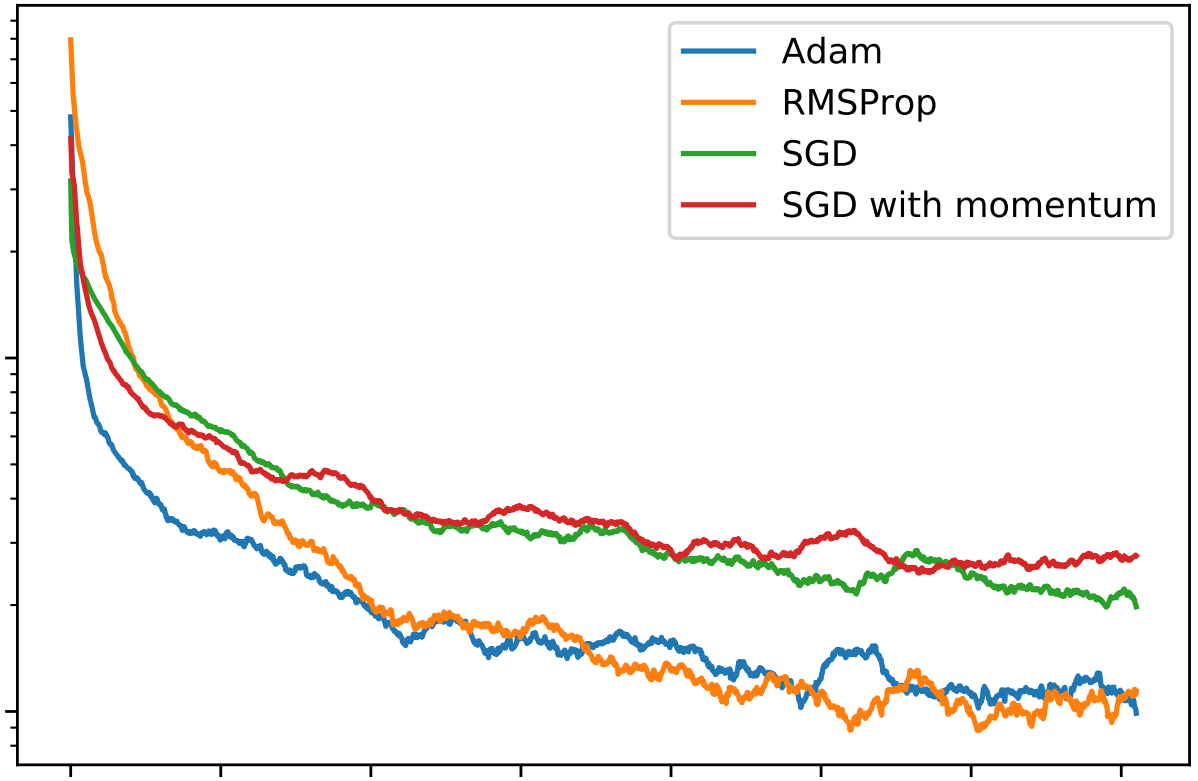
$$\mathbb{E}[g^2]_{(k)} \leftarrow \beta \cdot \mathbb{E}[g^2]_{(k-1)} + (1-\beta) \cdot \left(\frac{\partial L}{\partial \theta}\right)^2 \Bigg|_{\theta=\theta^{(k-1)}}$$

$$\theta^{(k)} \leftarrow \theta^{(k-1)} - \frac{\eta}{\sqrt{\mathbb{E}[g^2]_{(k)} + \varepsilon}} \cdot \frac{\partial L}{\partial \theta}\Bigg|_{\theta=\theta^{(k-1)}}$$

Adam

Combine both ideas (momentum + RMSprop)

Typically a good first choice for an optimizing algorithm



NN generalization

Why deep neural nets generalize well?

Number of parameters is often well above the size of the training dataset

Would expect heavy overfitting according to “classical ML” theory

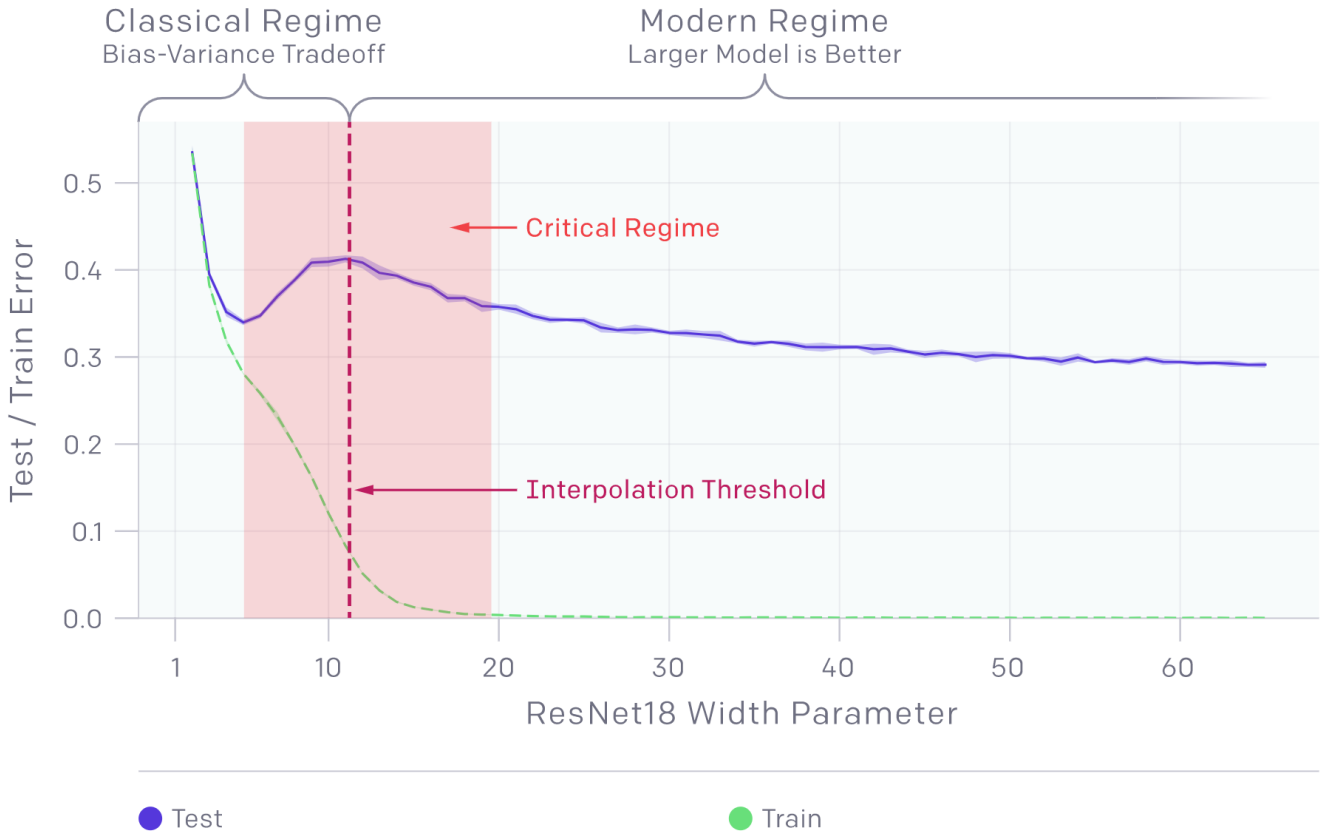
In practice, test error often decreases with the size of the model

Deep Double Descent

Img source: https://openai.com/blog/deep-double-descent/

In fact, the dependence of the test error from the model size is more complicated

Often, the effect of **double descent** is observed



Not understood well

- See this review
- Probably, cannot be explained by the implicit regularization from the optimization technique (see, e.g., 2109.14119, 2104.14421)
- Moreover: happens in simpler models, like linear regression (2109.02355)

Summary

Neural networks are essentially **stacked linear models** with scalar nonlinearities in between

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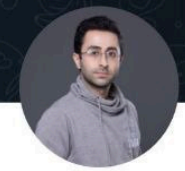
A variety of **SGD modifications** are available to mitigate this problem

Food for thought: being the 'universal approximators', can neural nets really solve every possible supervised learning problem?

Thank you!

Majid Sohrabi

msohrabi@hse.ru



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