Neural Networks

Introduction, multilayer perceptron, optimization techniques

Machine Learning and Data Mining, 2020

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LAMBDA • HSE

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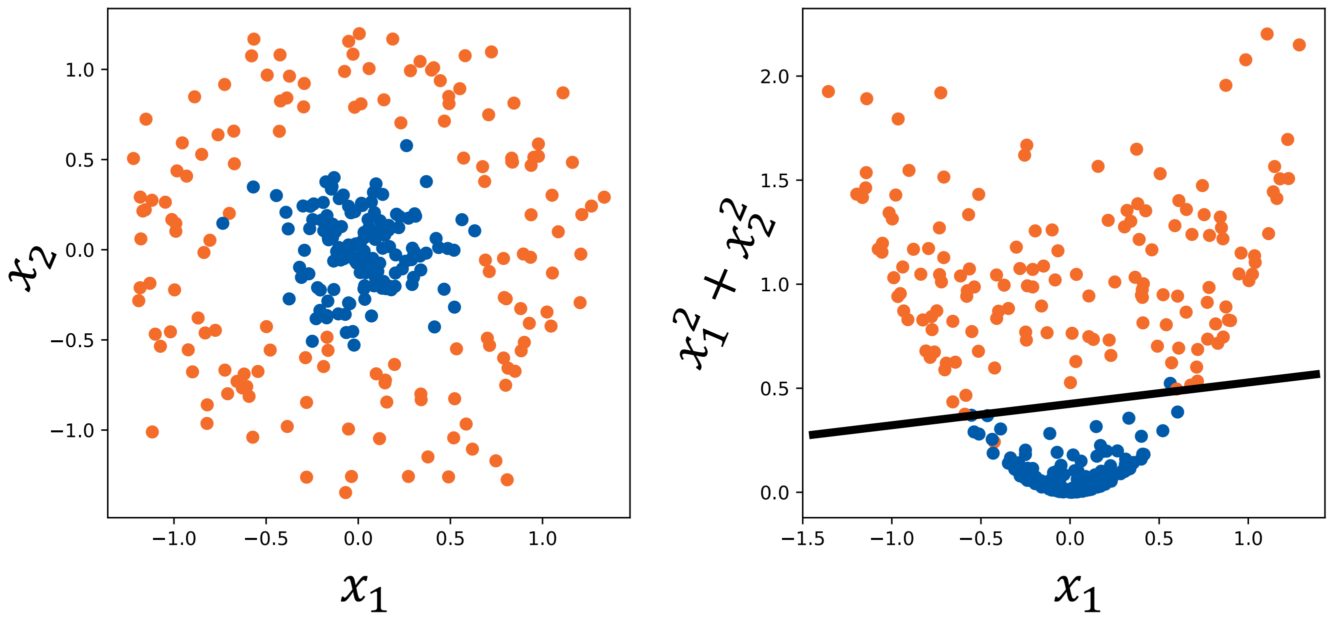
From linear model to a neural network

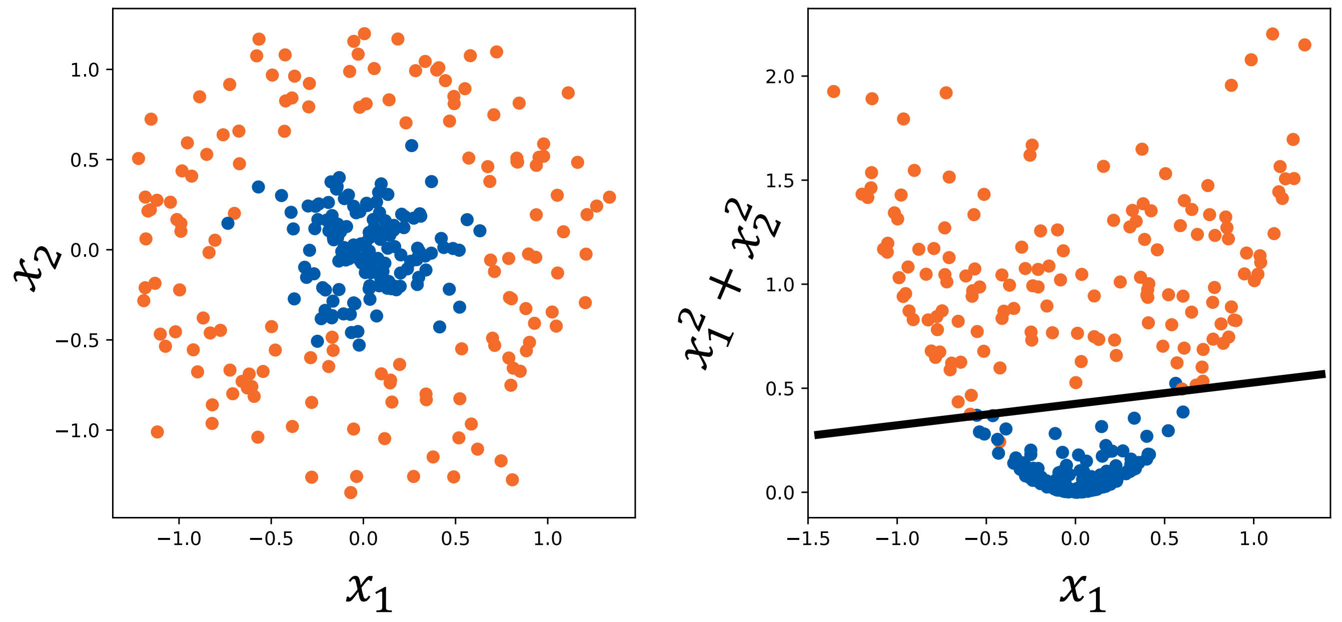
Linear models + feature expansion recap

- 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**



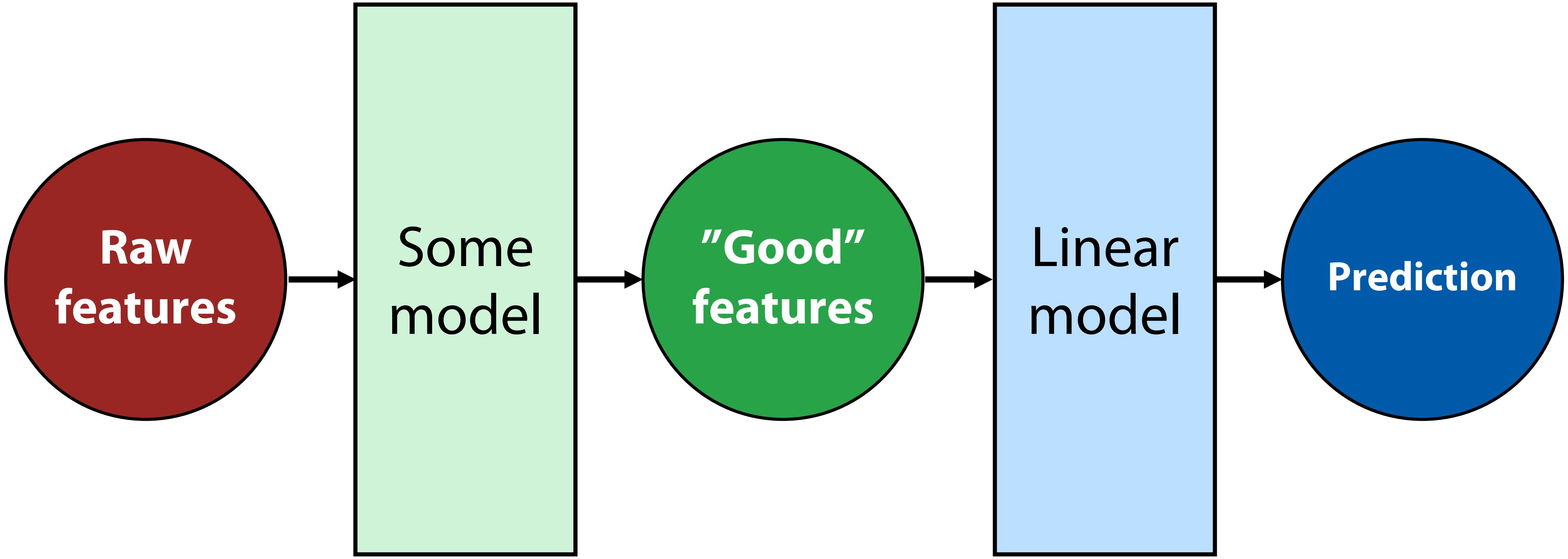
Linear models + feature expansion recap

- 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**



Can we automate feature engineering? ☺

Idea: add another model



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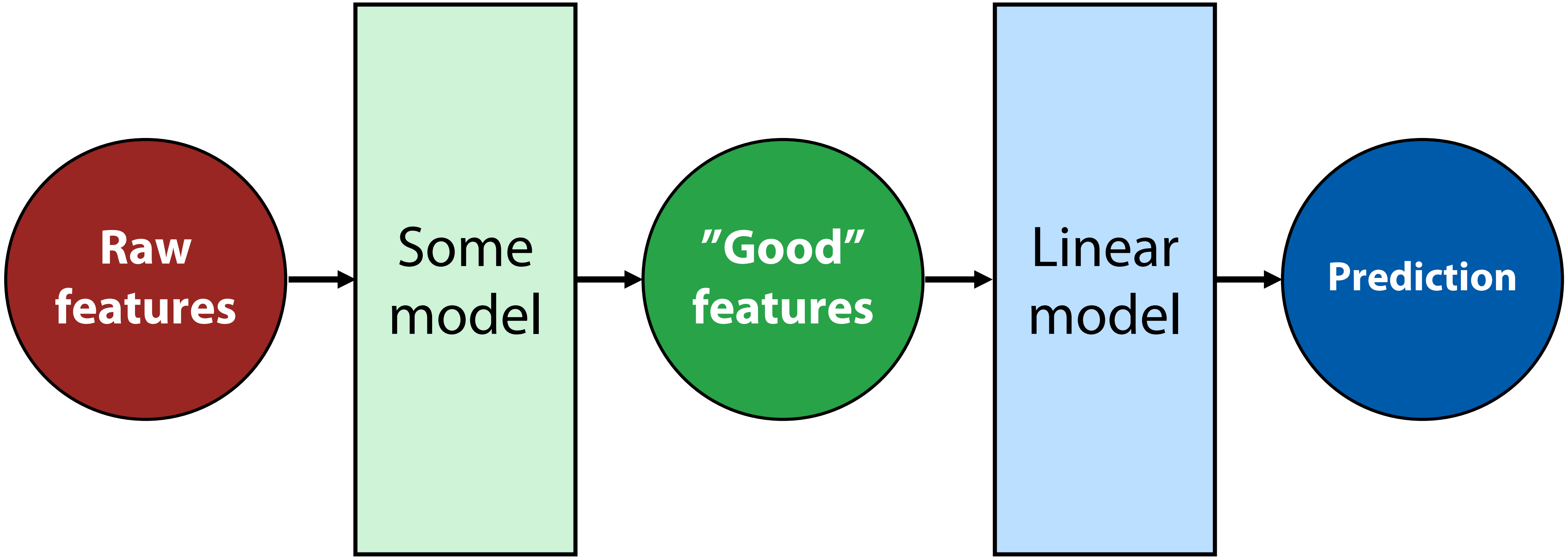

- Add another model
- Train everything simultaneously
  - Can use gradient descent if both models are **differentiable**

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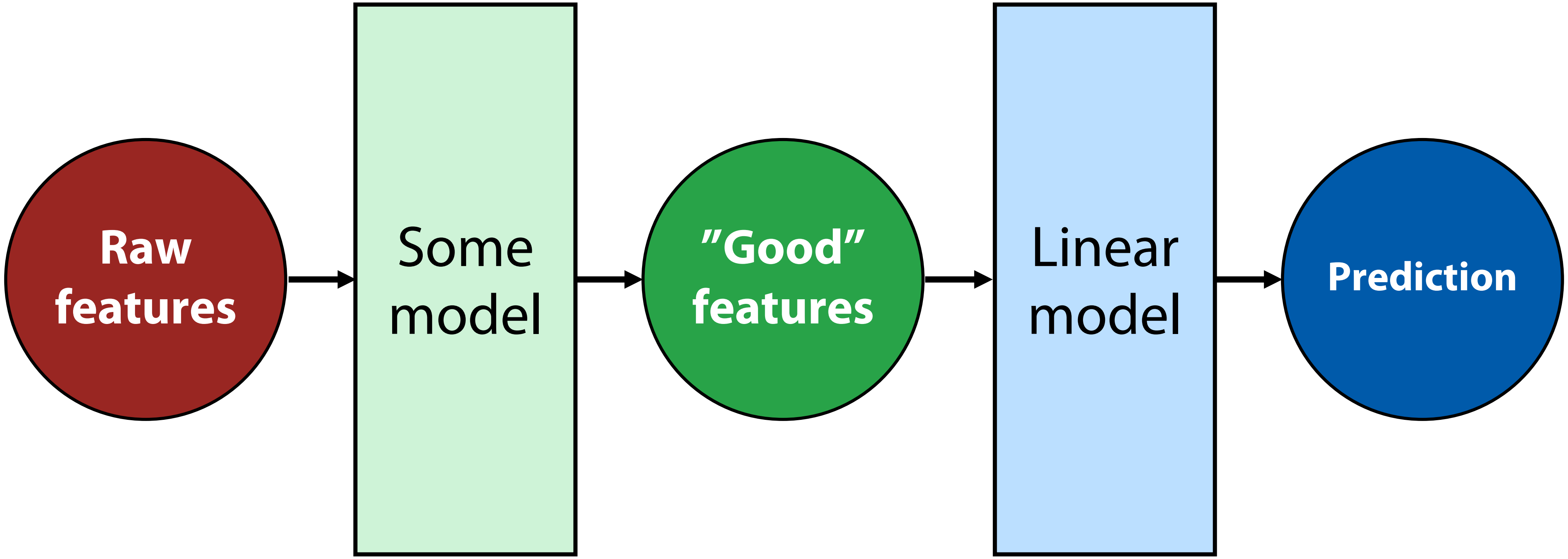

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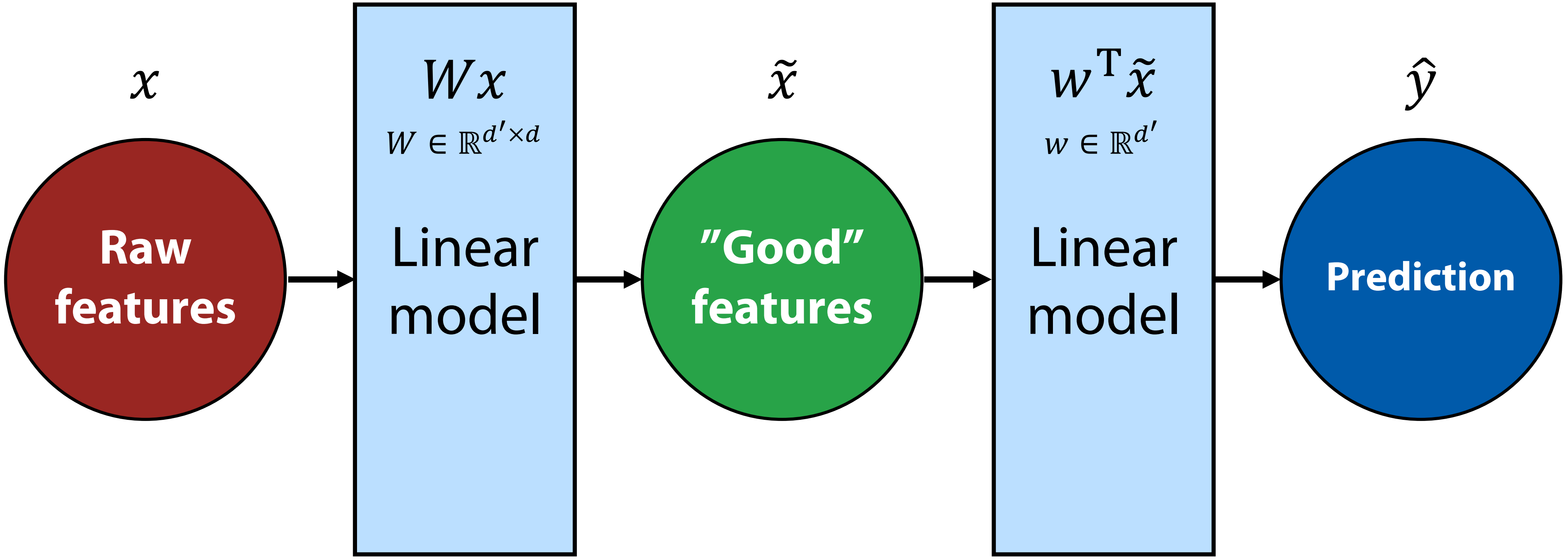
- Train everything simultaneously
  - Can use gradient descent if both models are **differentiable**

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

Can it be another linear model?



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

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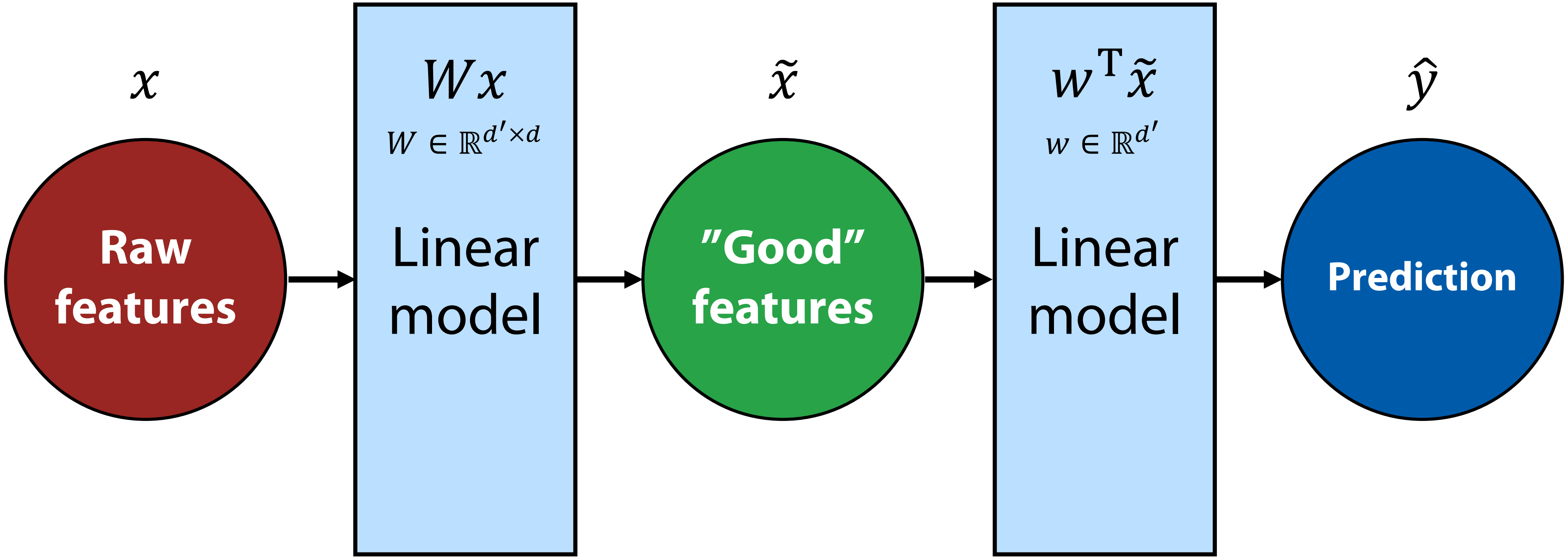

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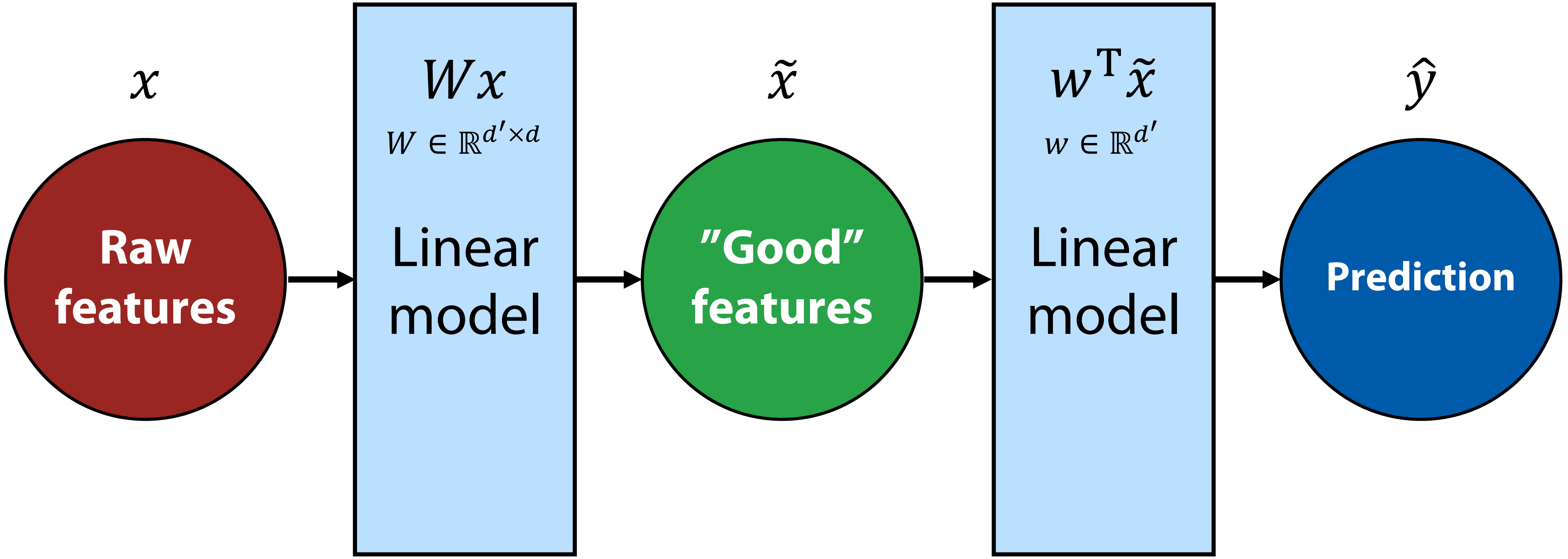

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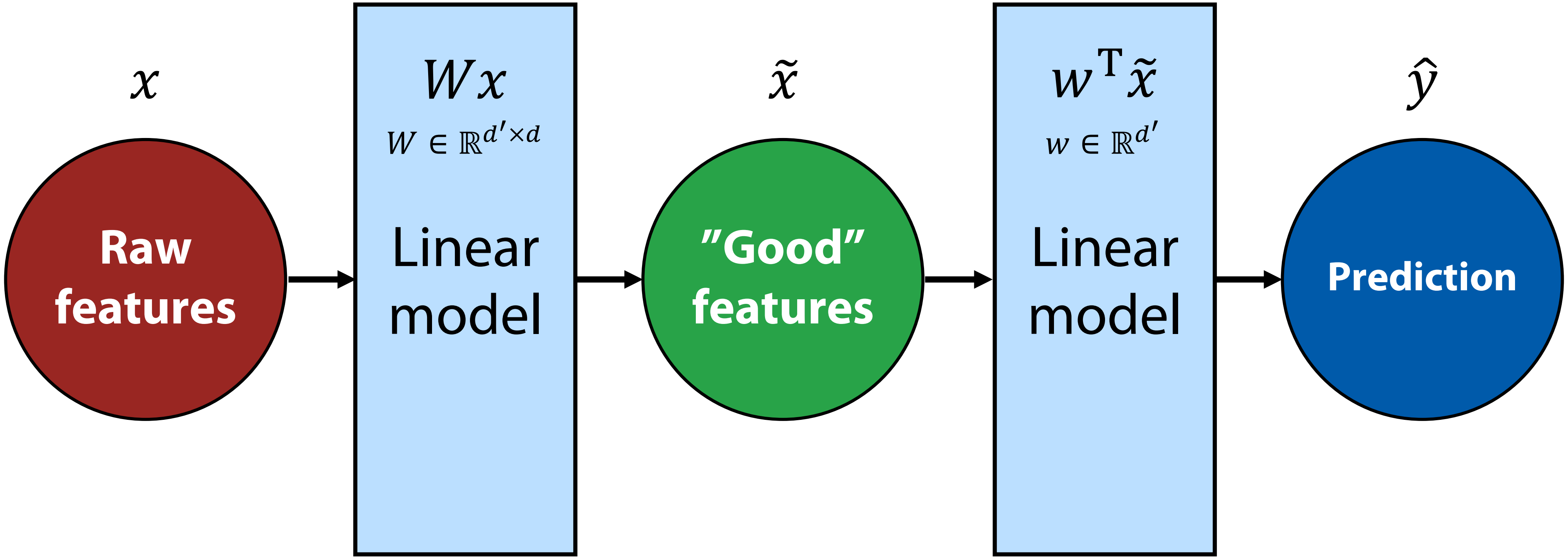
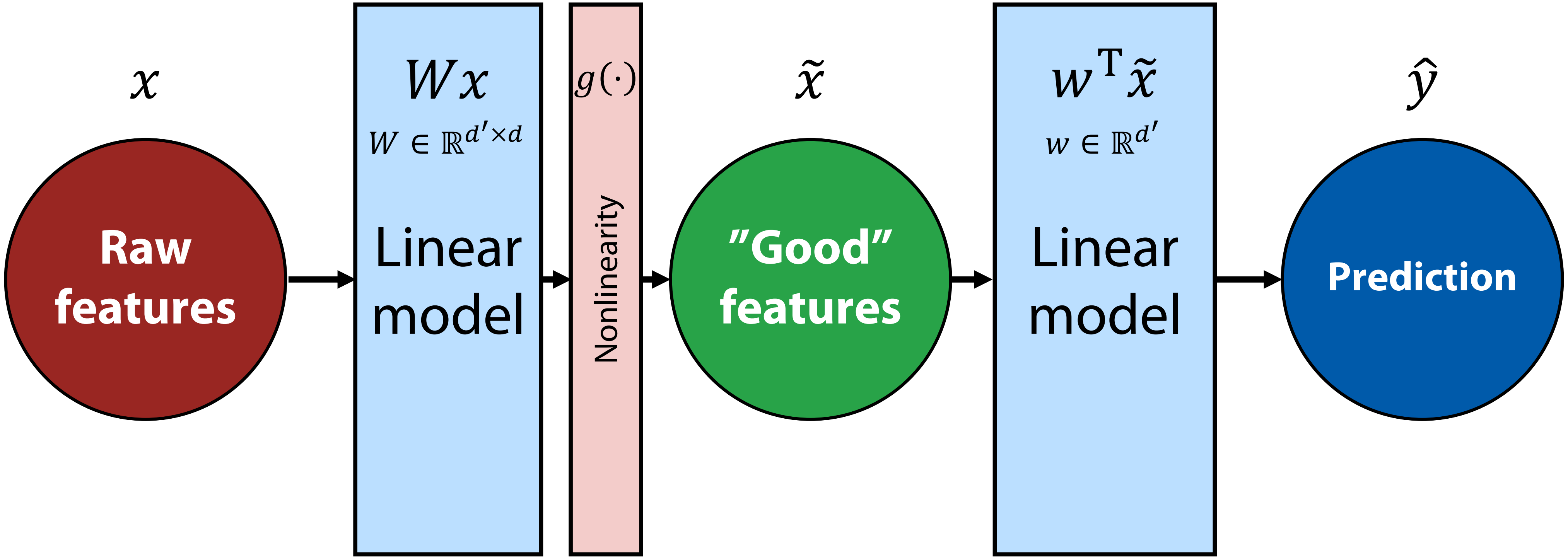


$$\hat{y} = w^{\mathrm{T}}\tilde{x} = w^{\mathrm{T}}(Wx) = \left(w^{\mathrm{T}}W\right)x = w'^{\mathrm{T}}x$$

– turns everything into just a single linear model

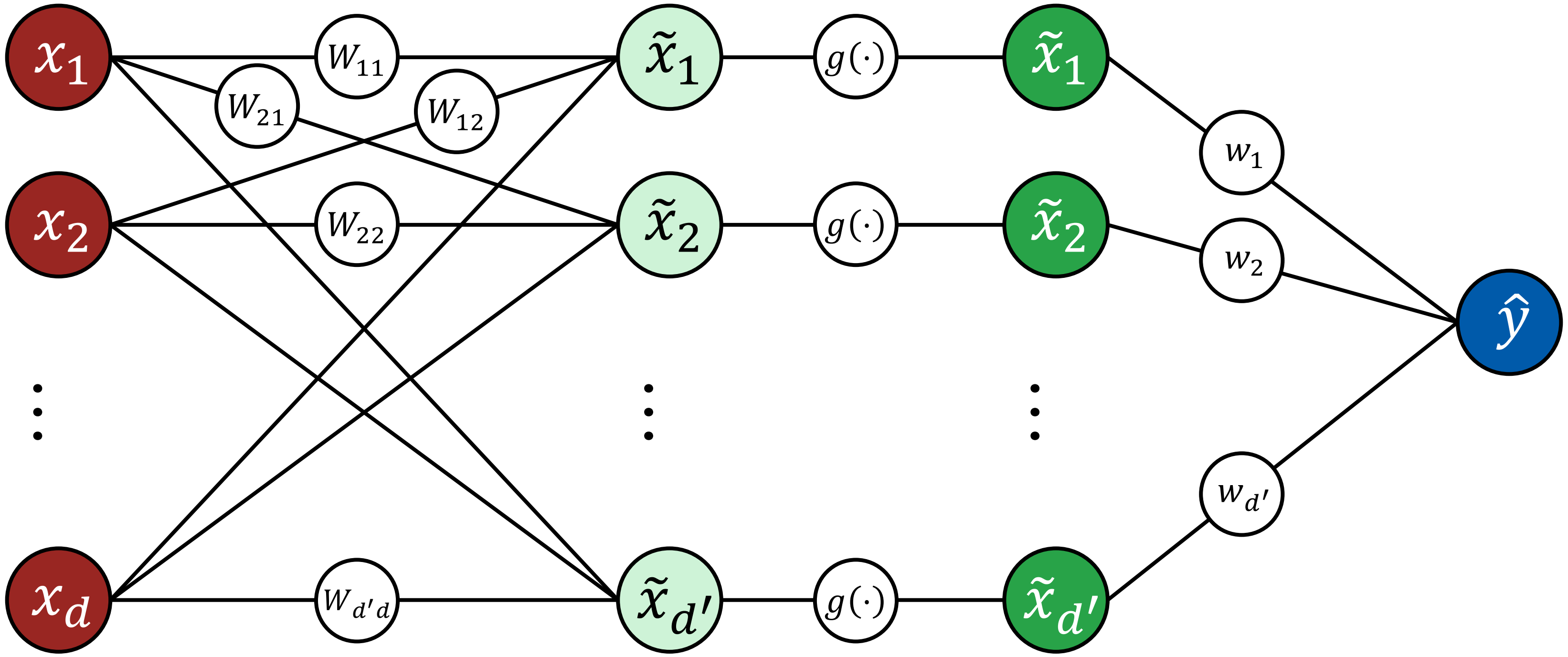
Fix: just introduce a nonlinearity



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

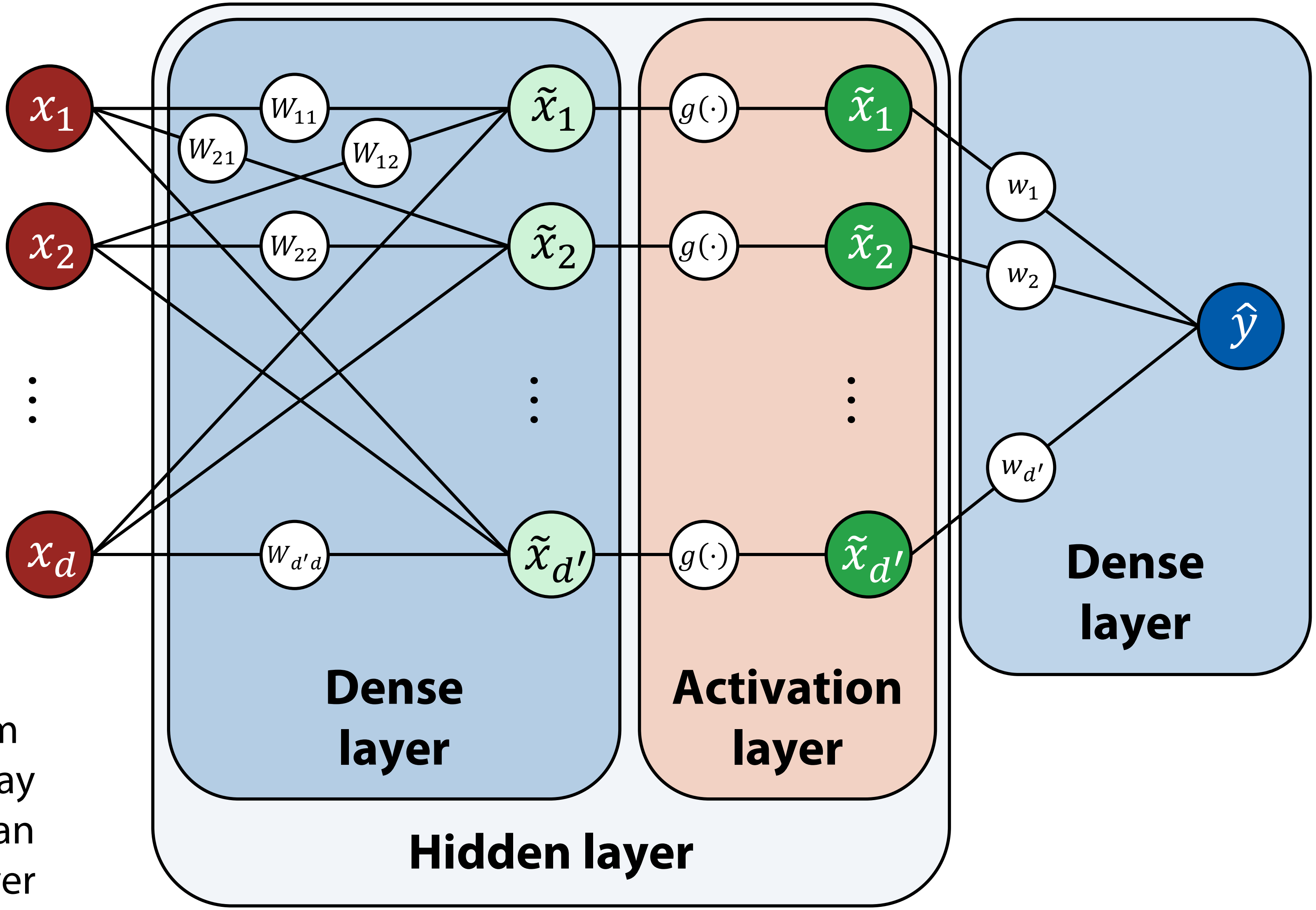
$g(\cdot)$ – some **nonlinear** scalar function (applied elementwise)

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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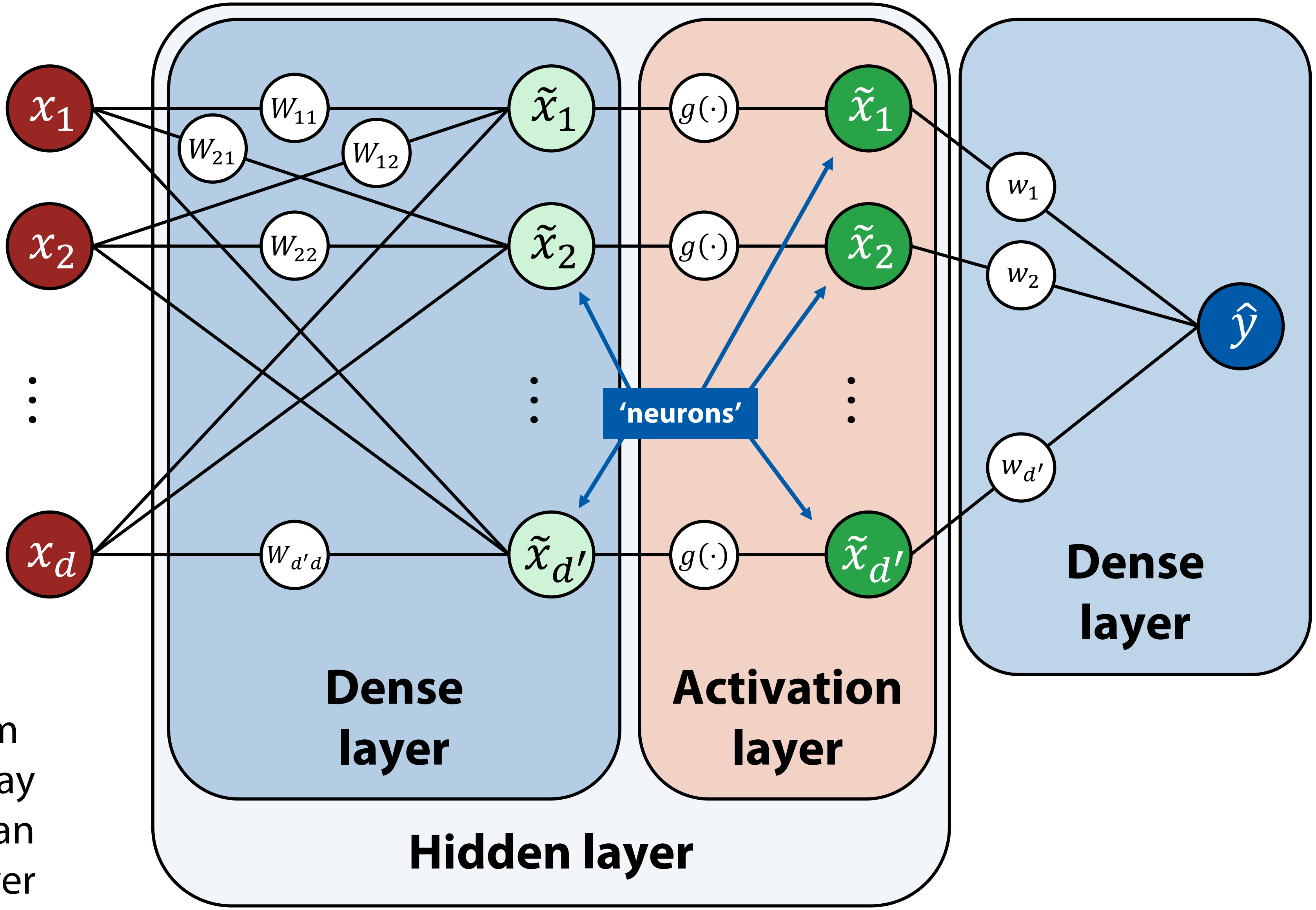

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Activation functions

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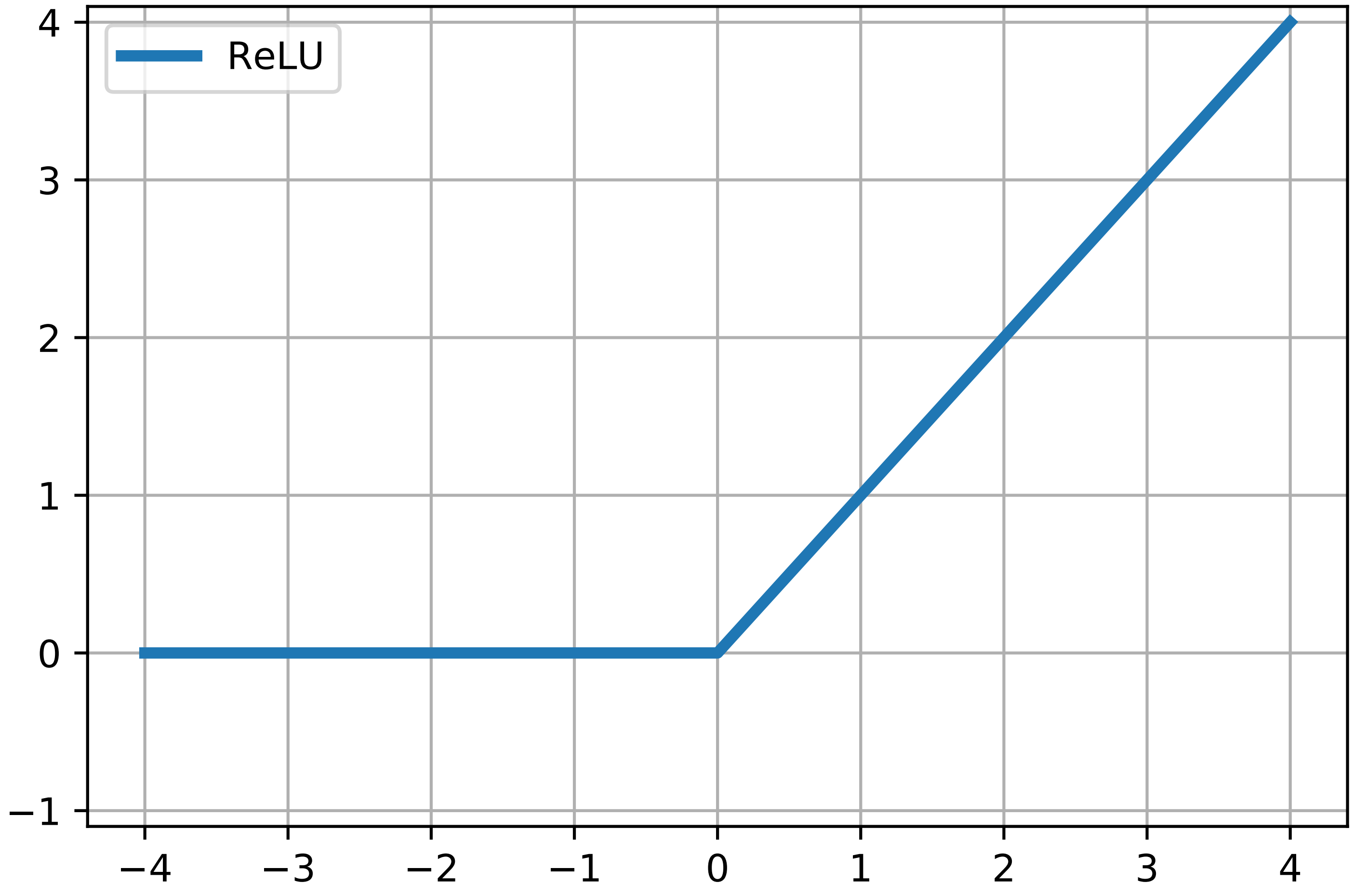

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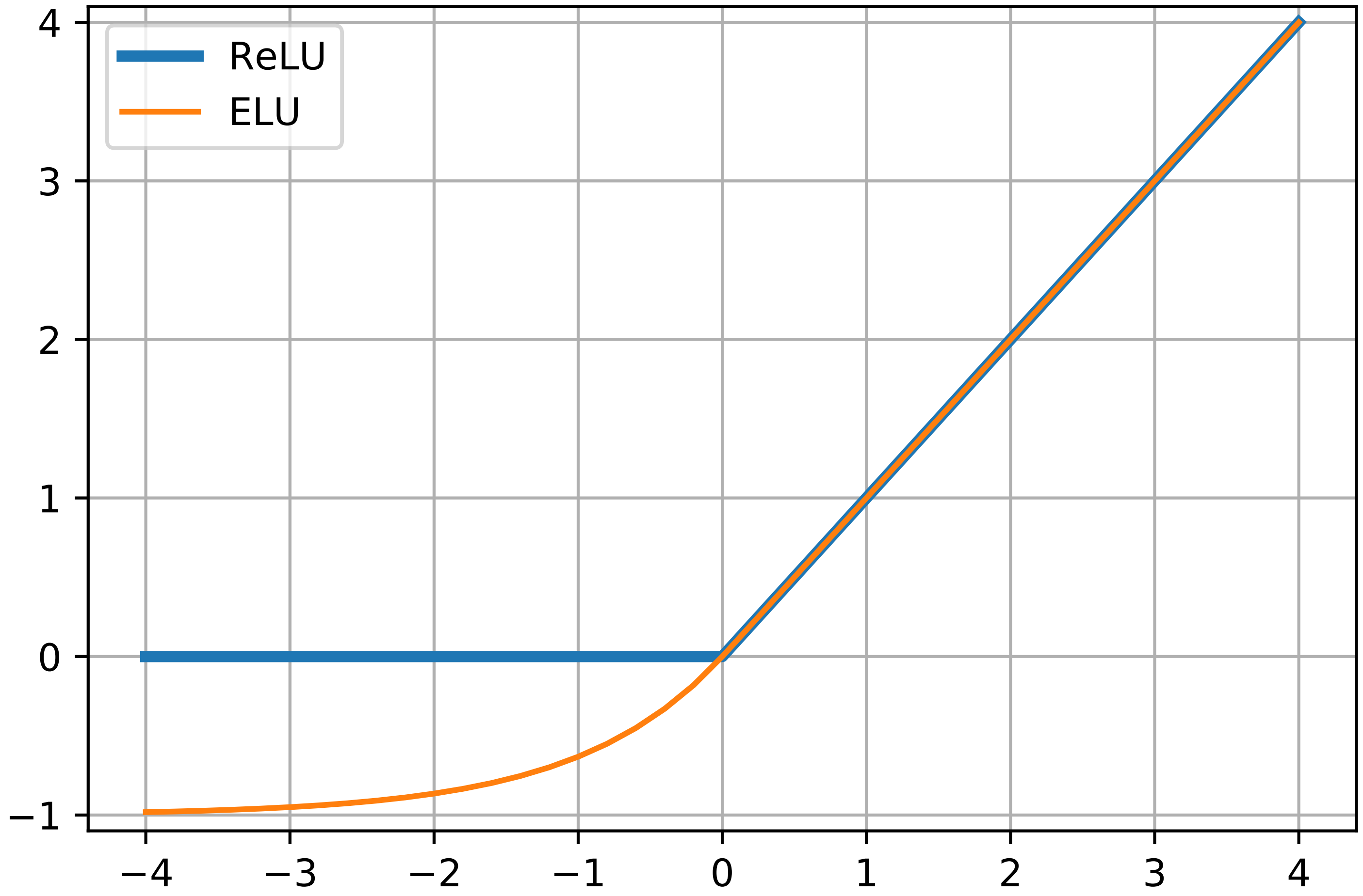

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$$\mathrm{ELU}(x) = \begin{cases} x & x \geq 0 \\ e^x - 1 & x < 0 \end{cases}$$

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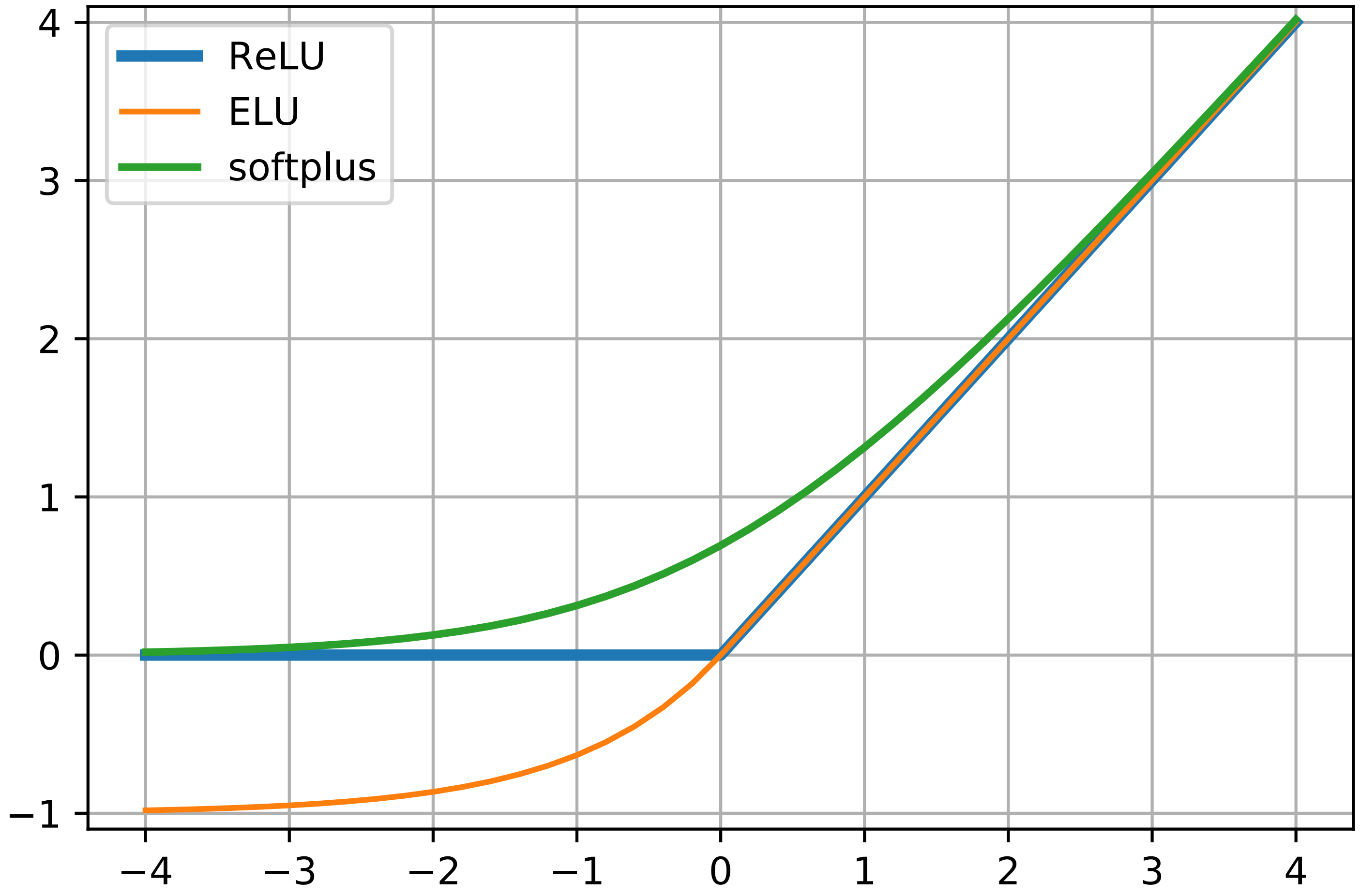

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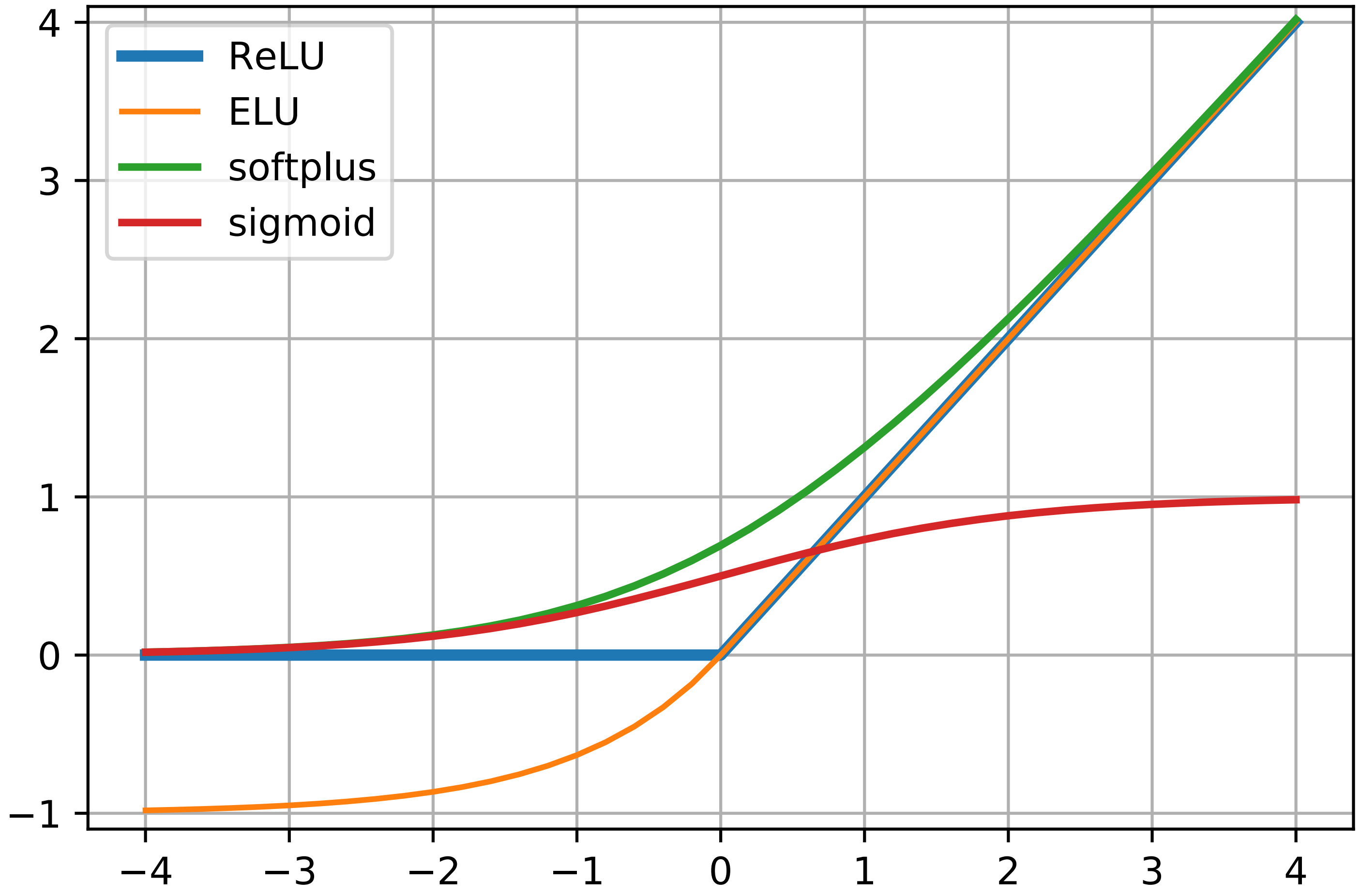

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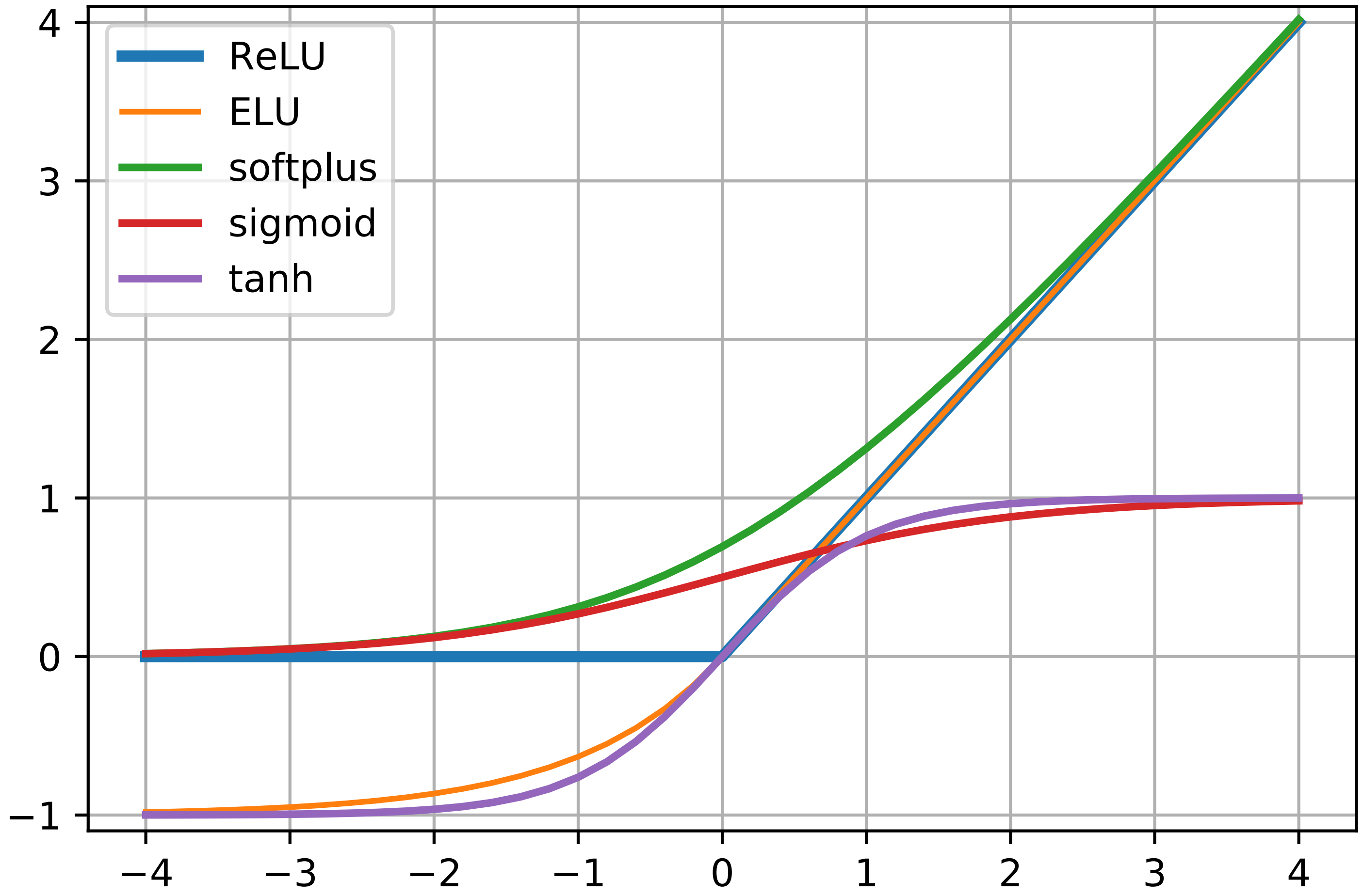

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$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

Universal approximator

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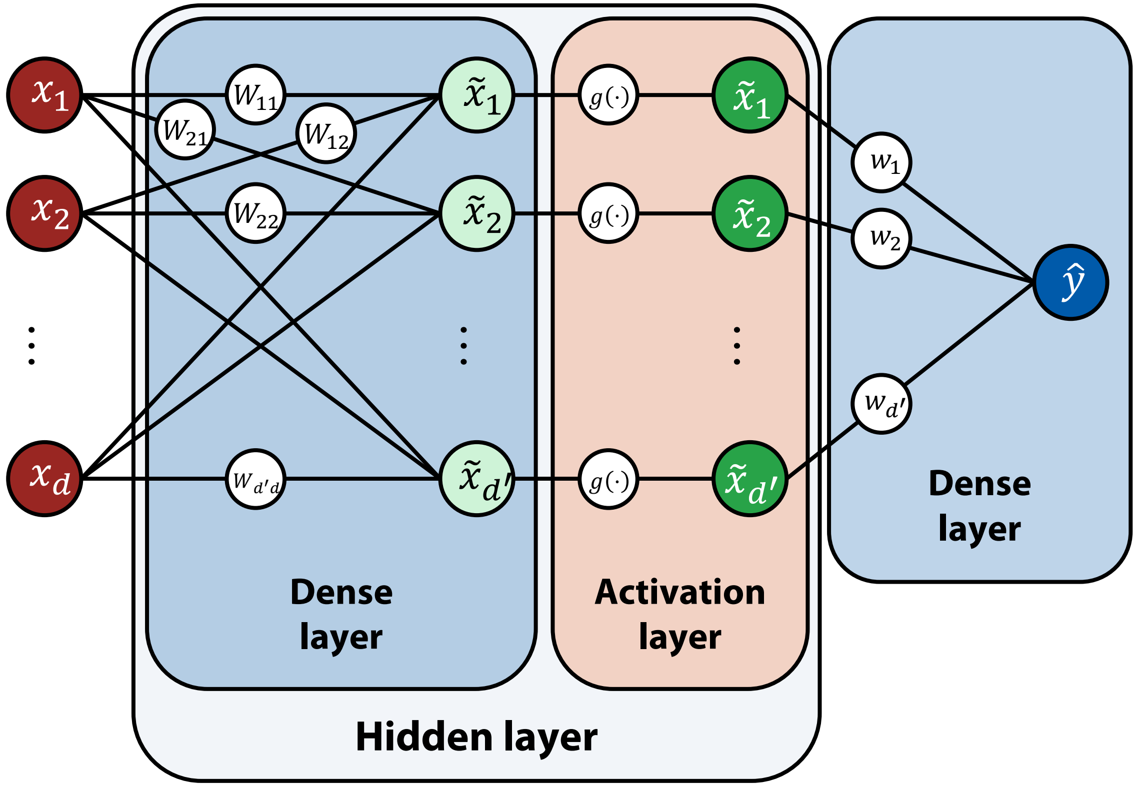
- Just a single hidden layer with a nonlinearity makes this model a universal approximator



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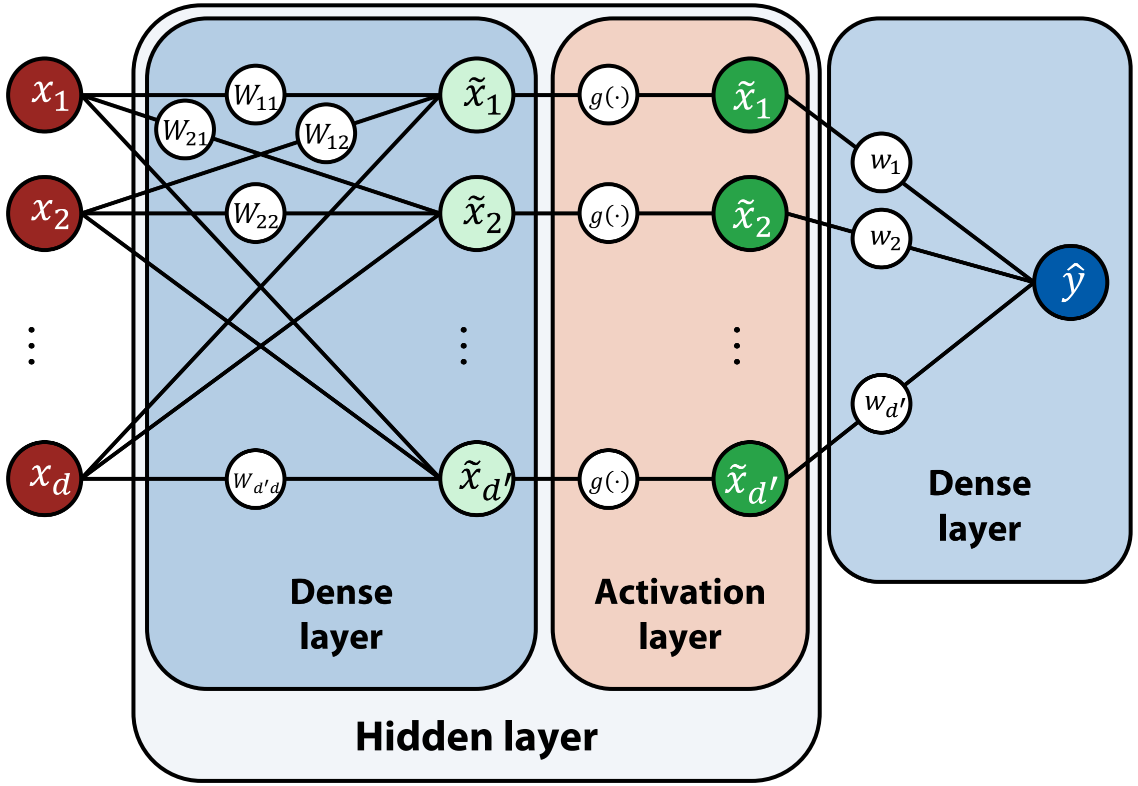
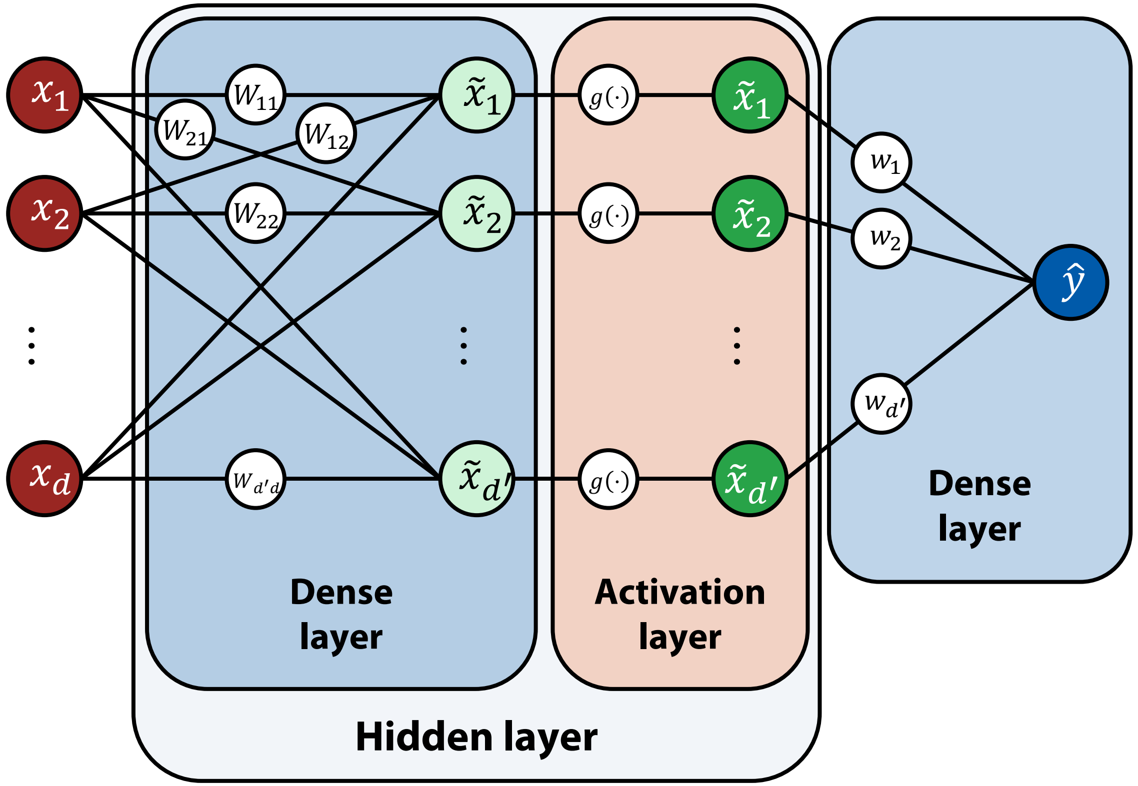
- Just a single hidden layer with a nonlinearity makes this model a universal approximator
  - any function can be approximated **arbitrarily close** given wide enough hidden layer (large enough d')

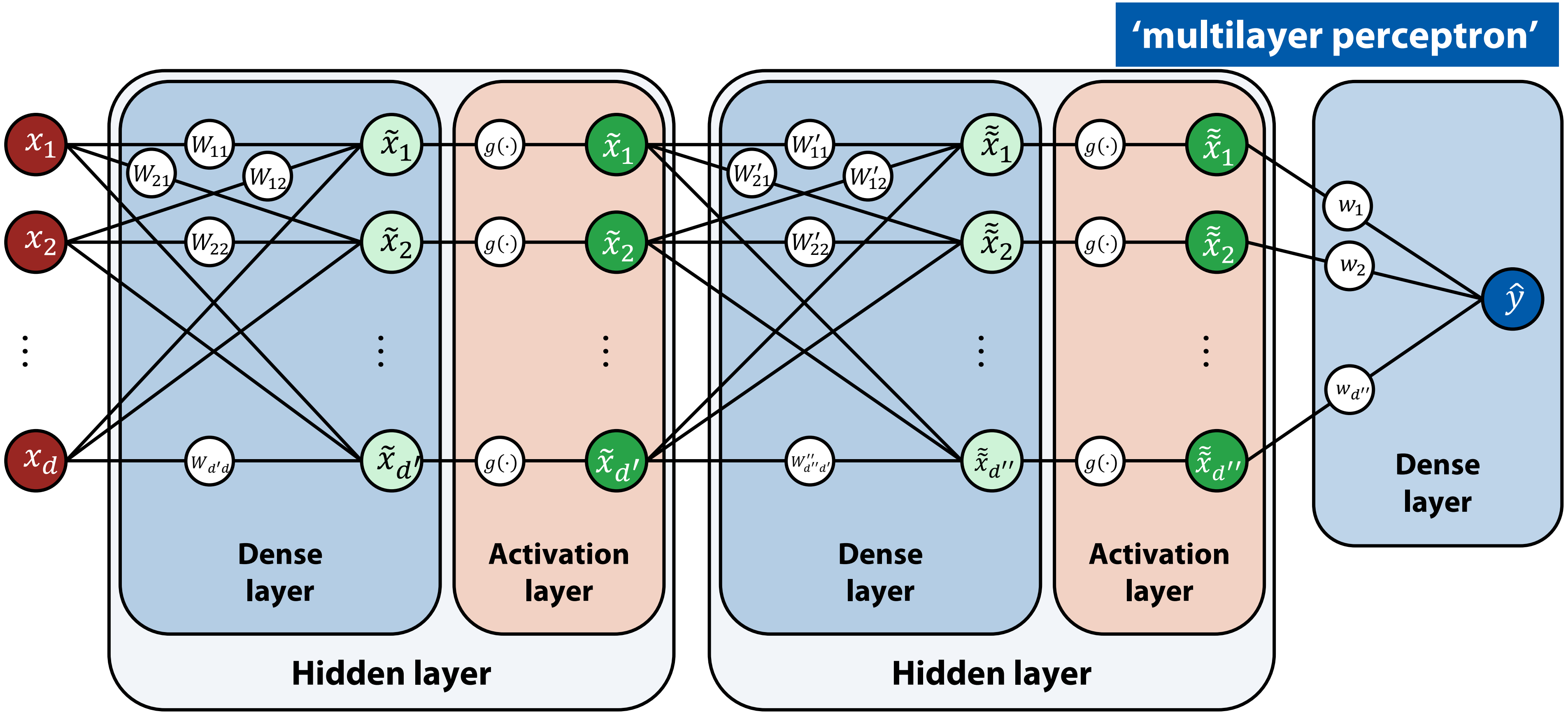


Universal approximator

- 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



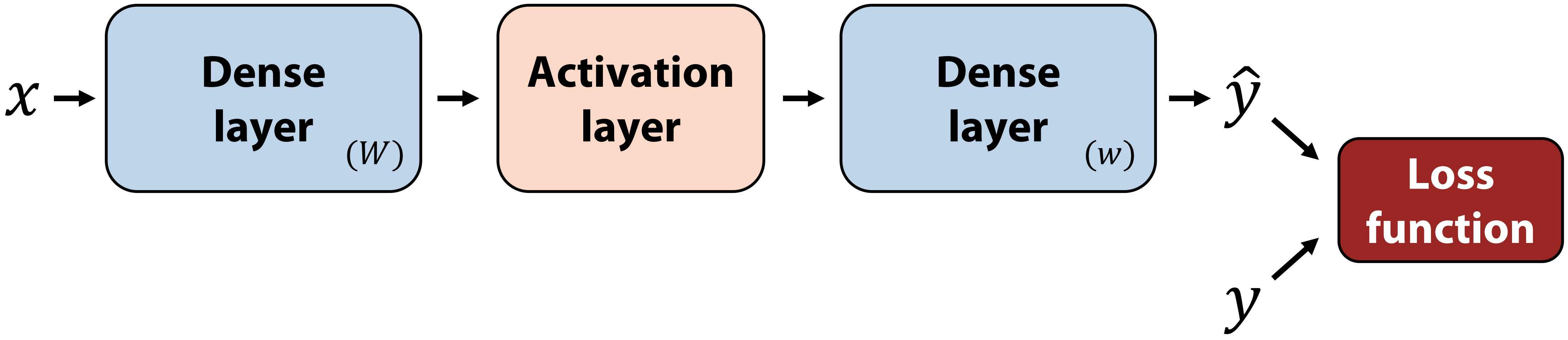
Deeper nets



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

Backpropagation

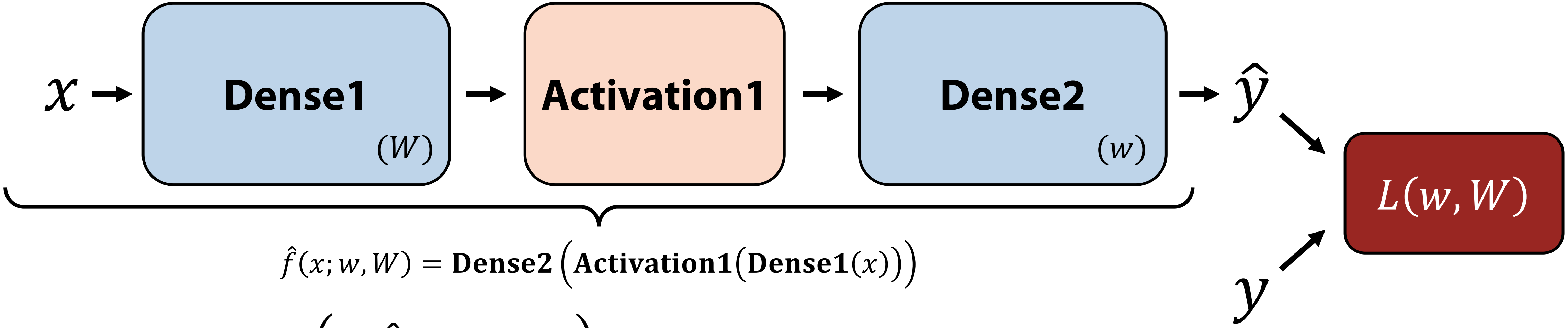
Loss function



- 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



$$\hat{f}(x; w, W) = \mathbf{Dense2}\left(\mathbf{Activation1}\left(\mathbf{Dense1}(x)\right)\right)$$

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

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

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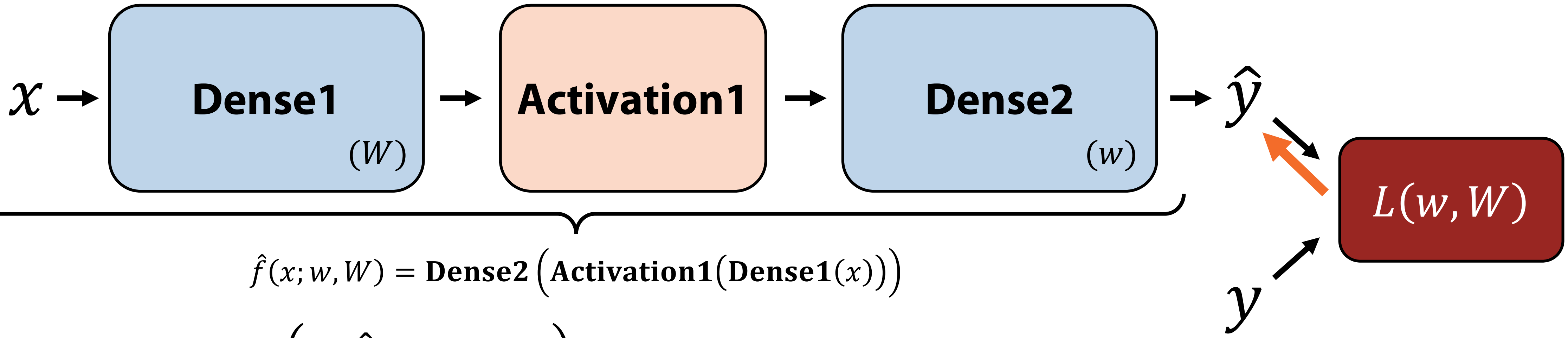

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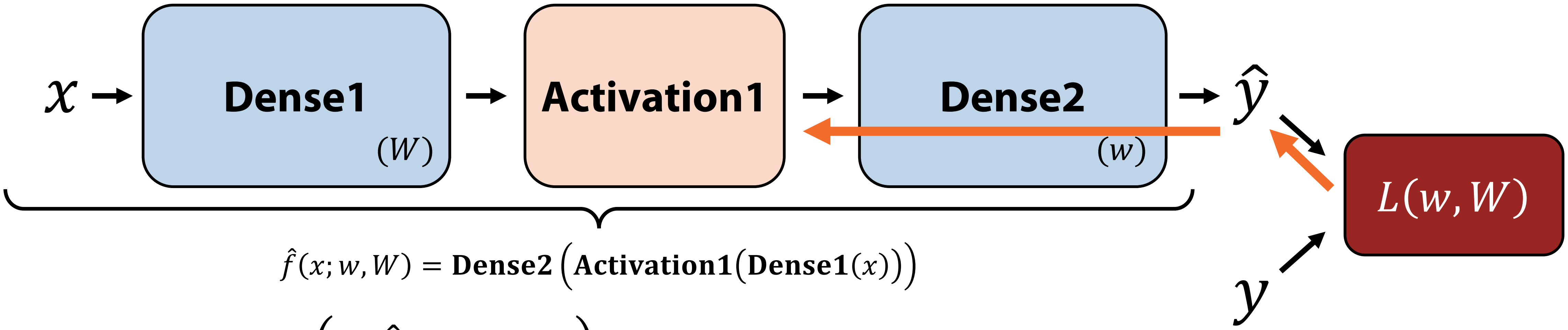

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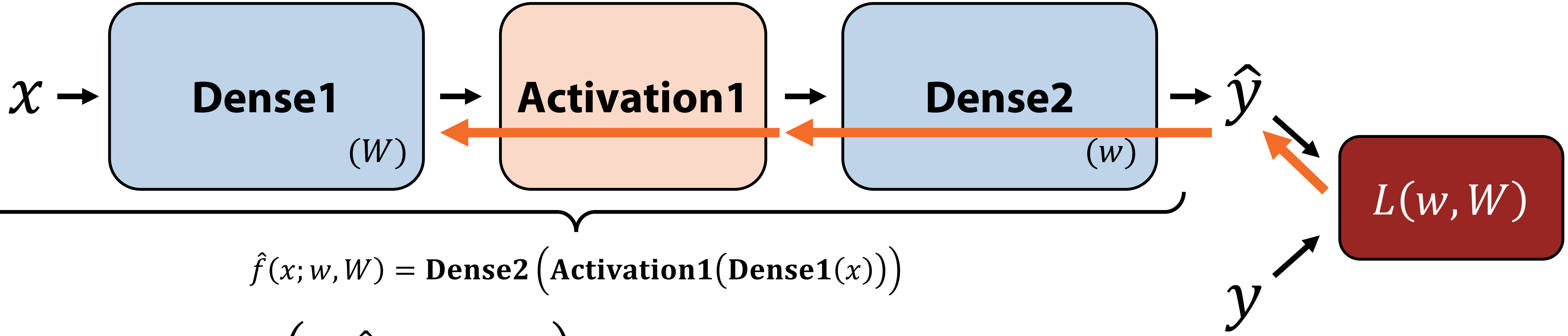

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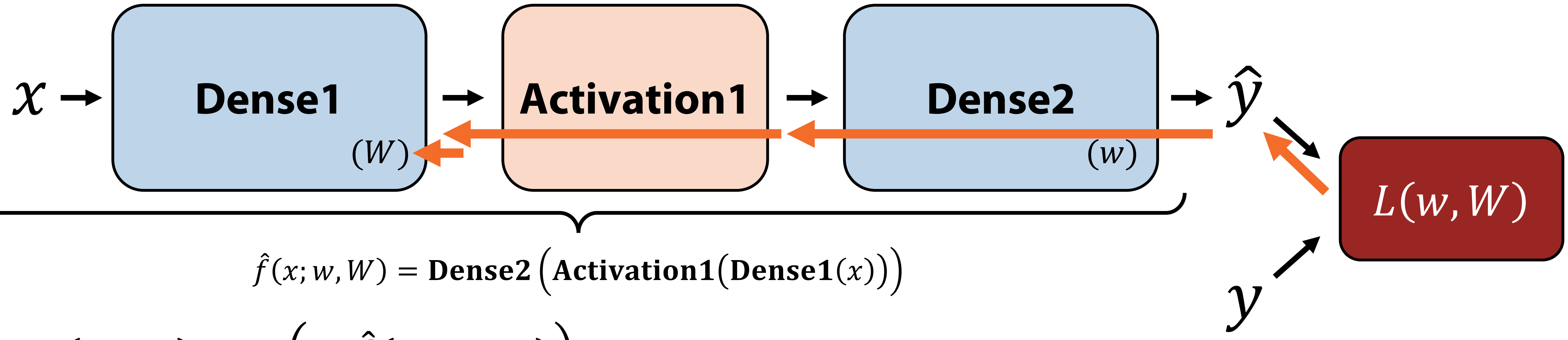

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  - The actual algorithm states how to do it efficiently

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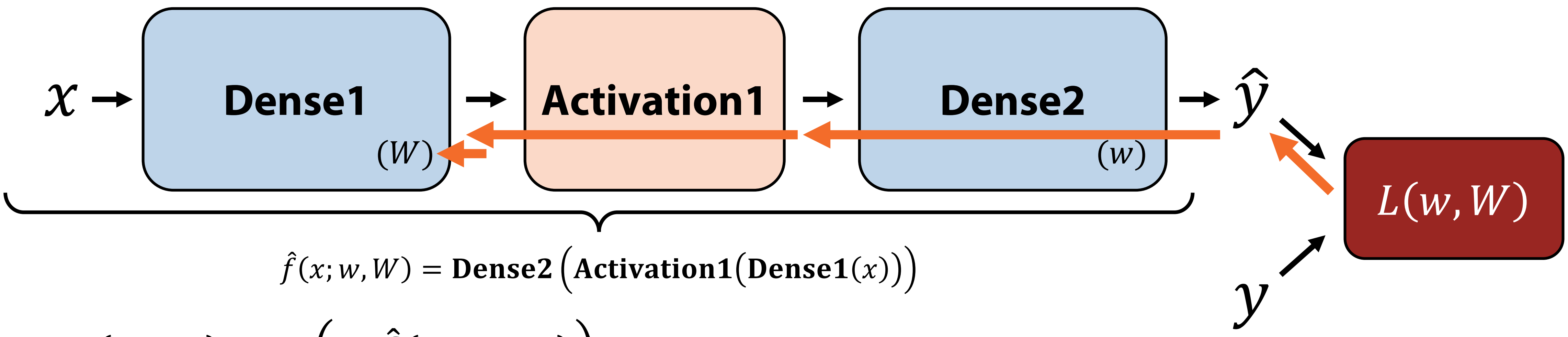

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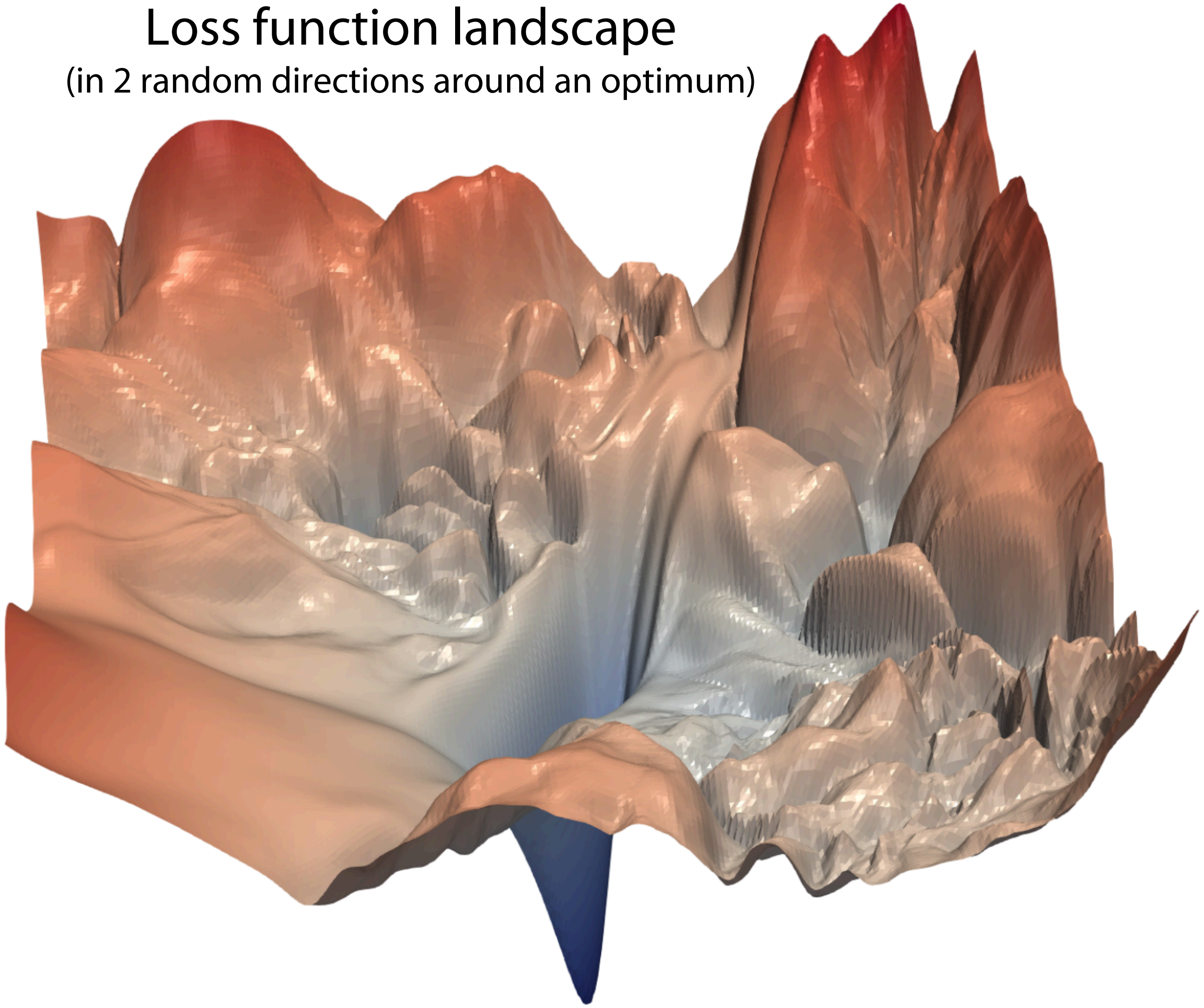
Optimization techniques

How to optimize such functions?

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



https://papers.nips.cc/paper/7875-visualizing-the-loss-landscape-of-neural-nets

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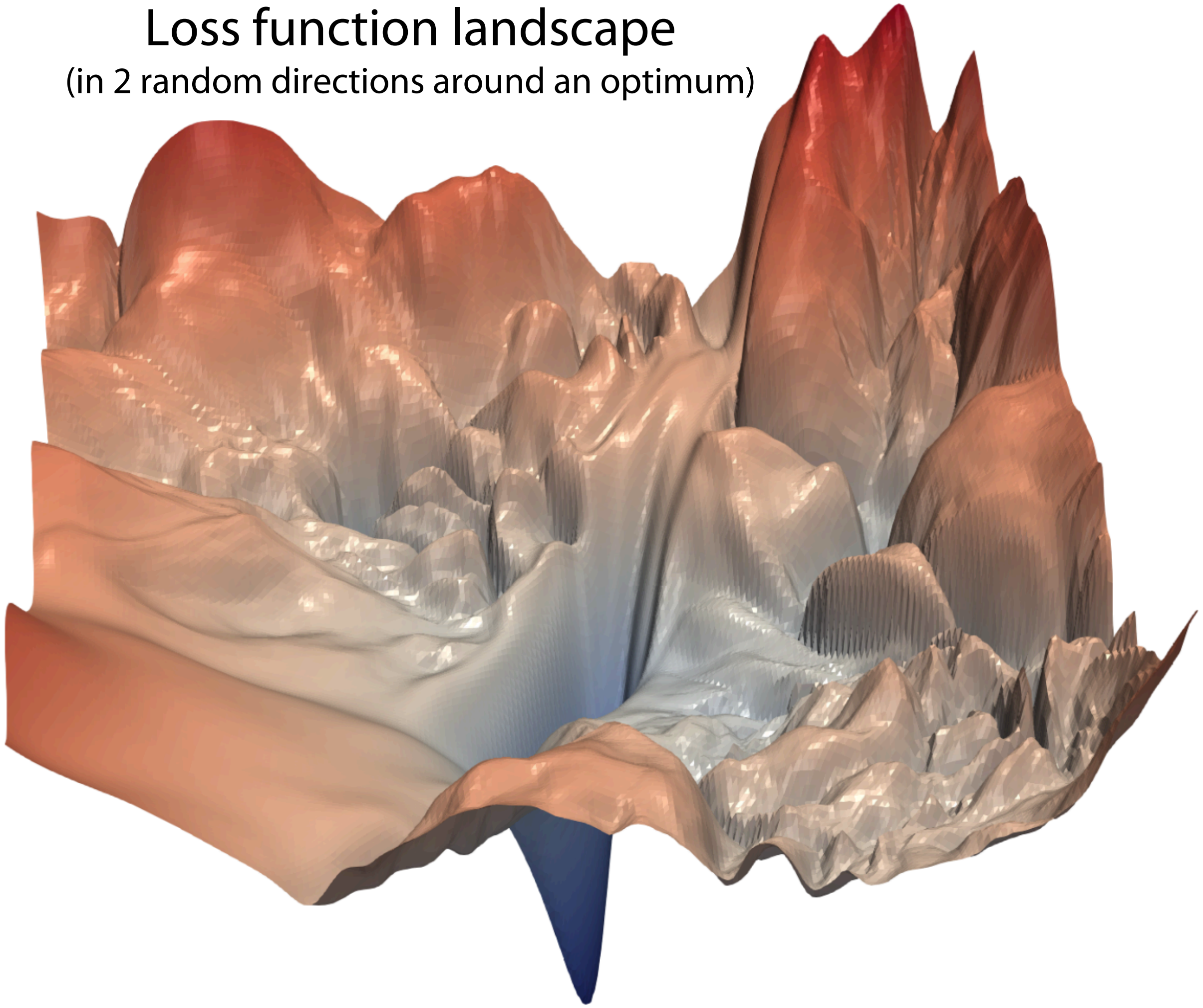

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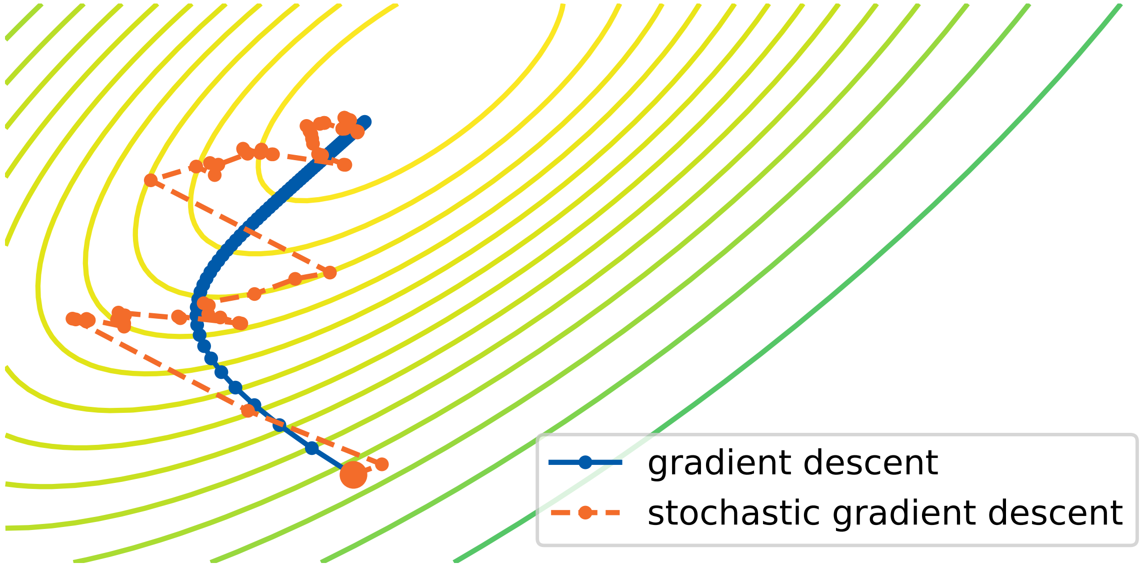
- No convergence guarantees for the stochastic gradient descent
- There’s a number of modifications to improve training

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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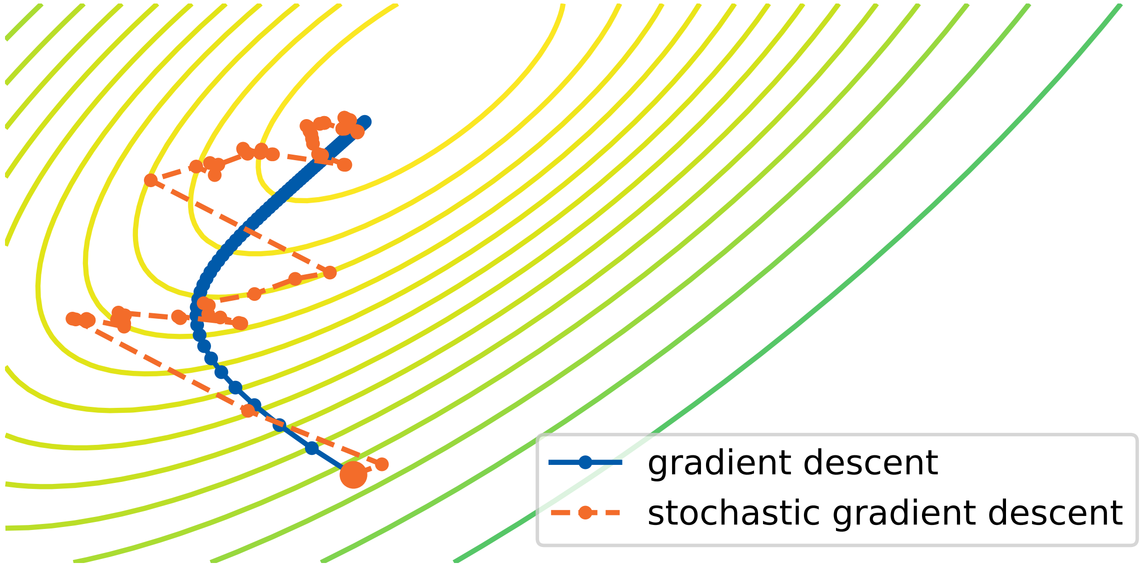

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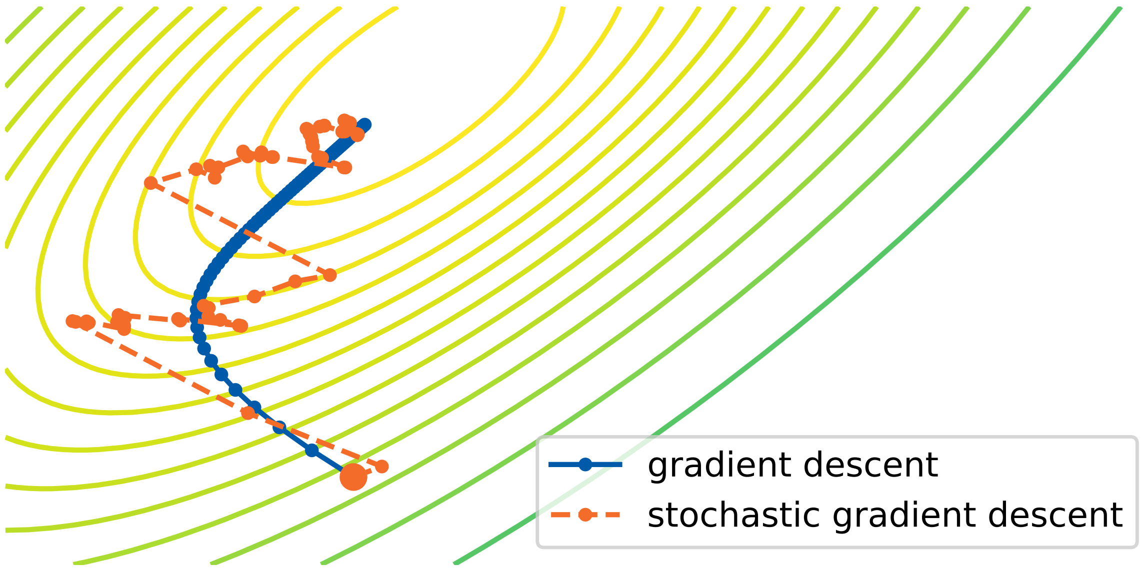

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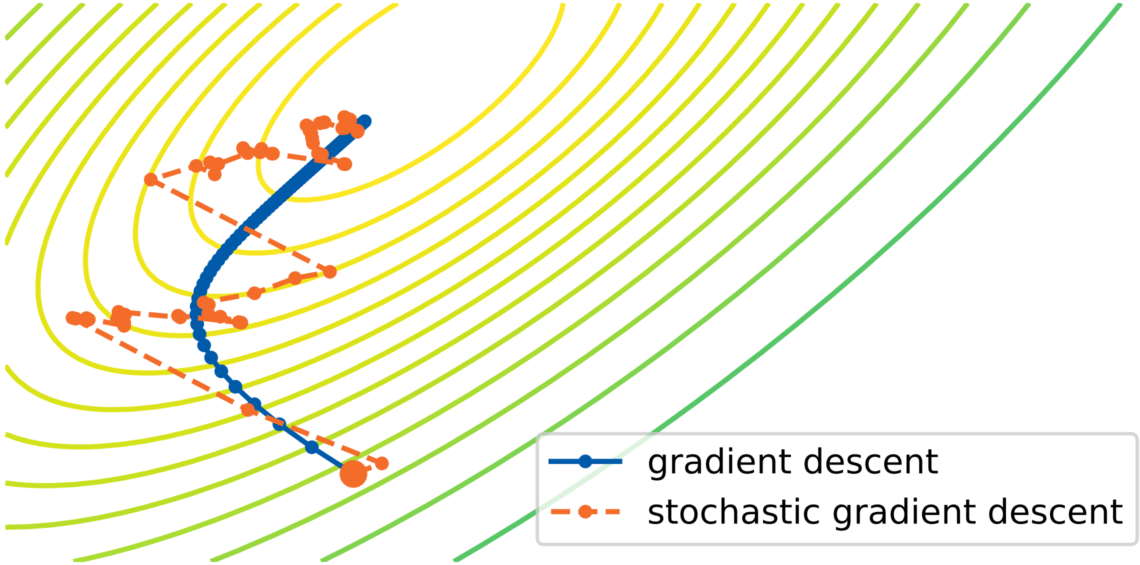

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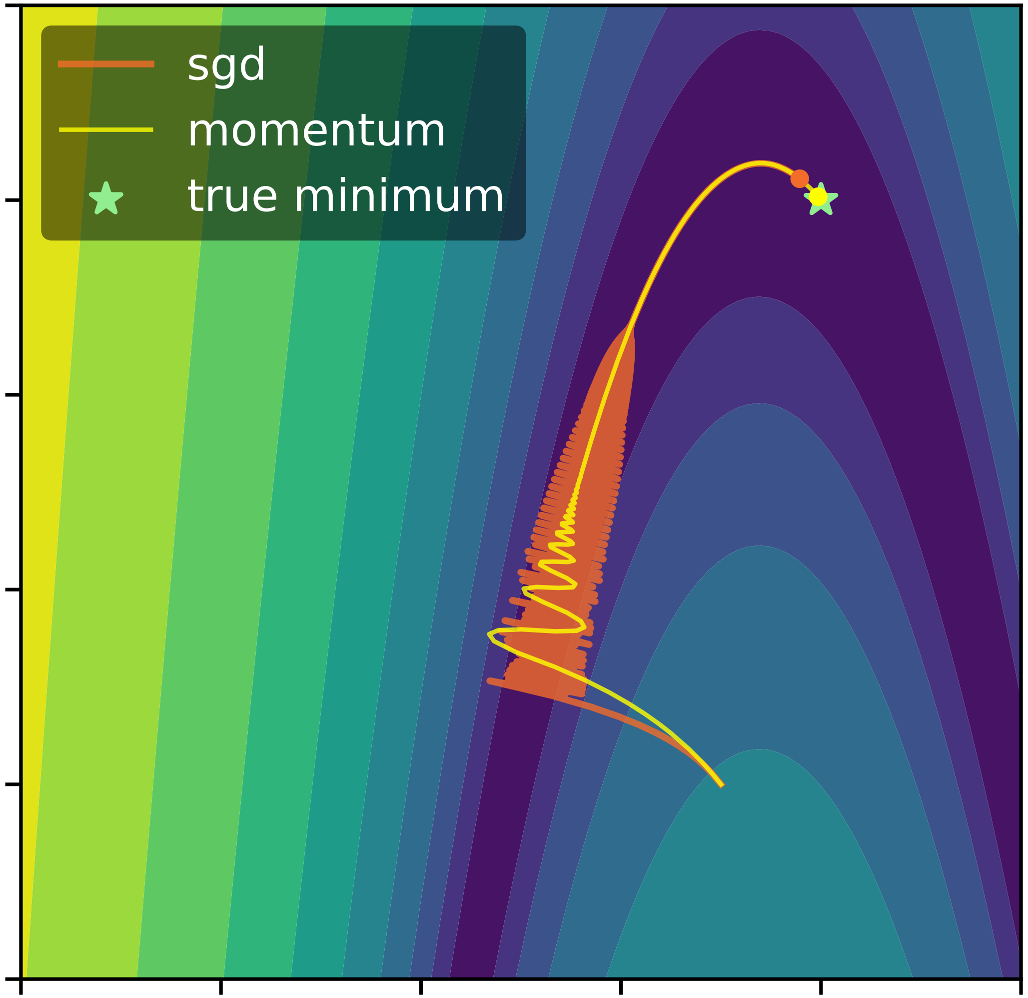
  - Update the model parameters: $\theta^{(k)} \leftarrow \theta^{(k-1)} - \eta \cdot g$

Momentum SGD



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

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

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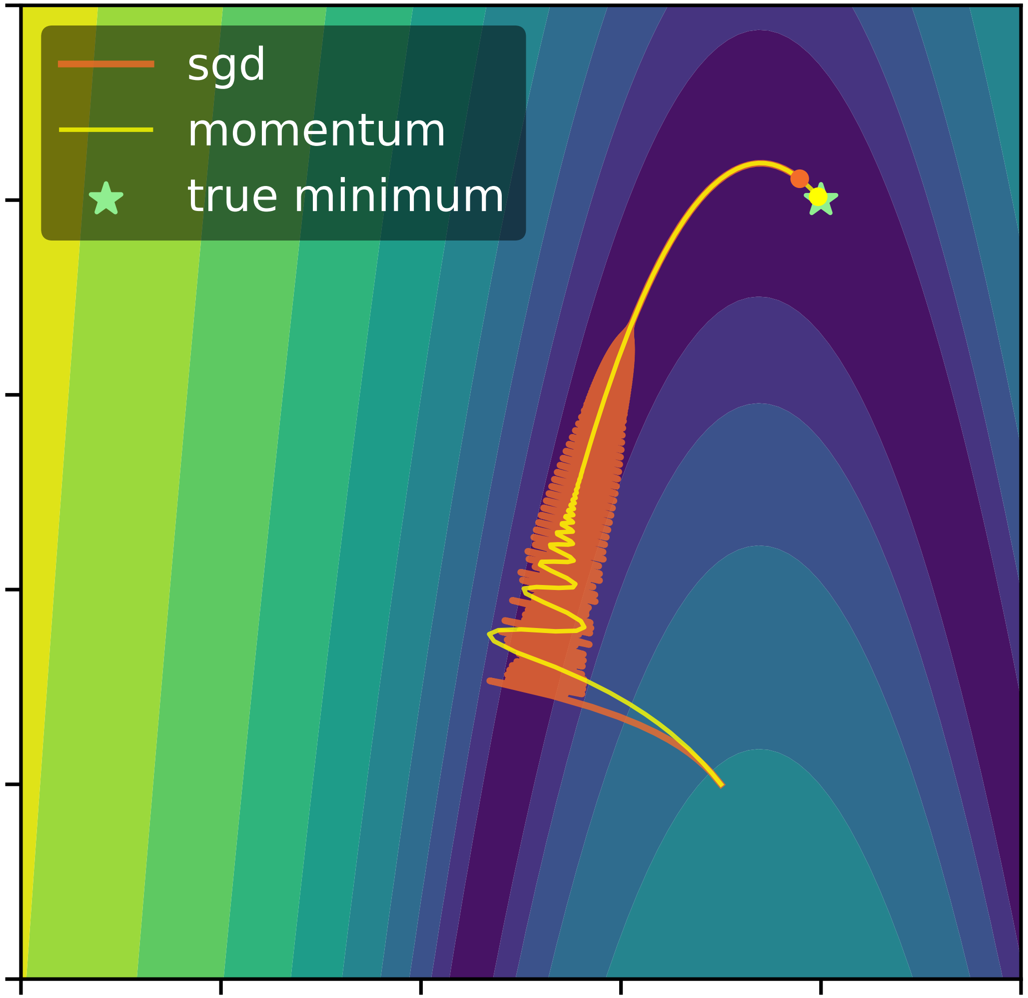
Momentum SGD



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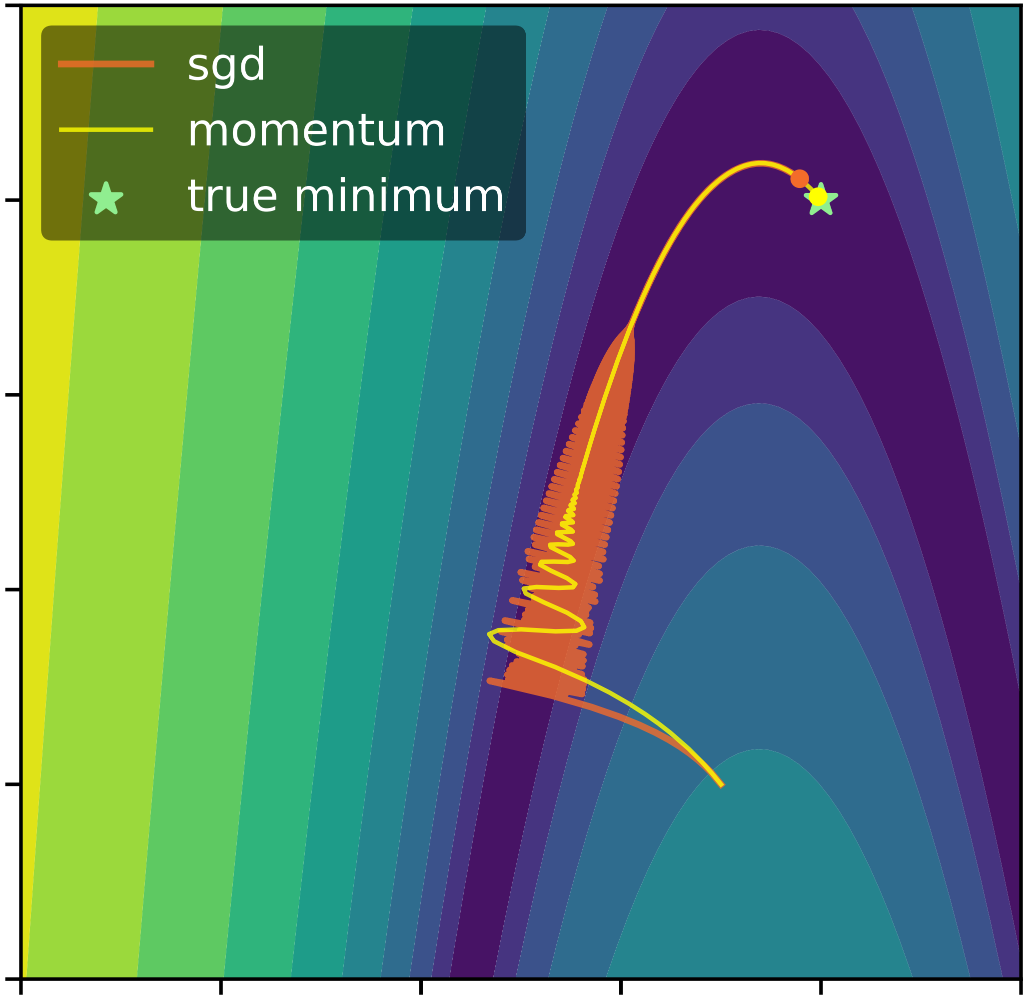

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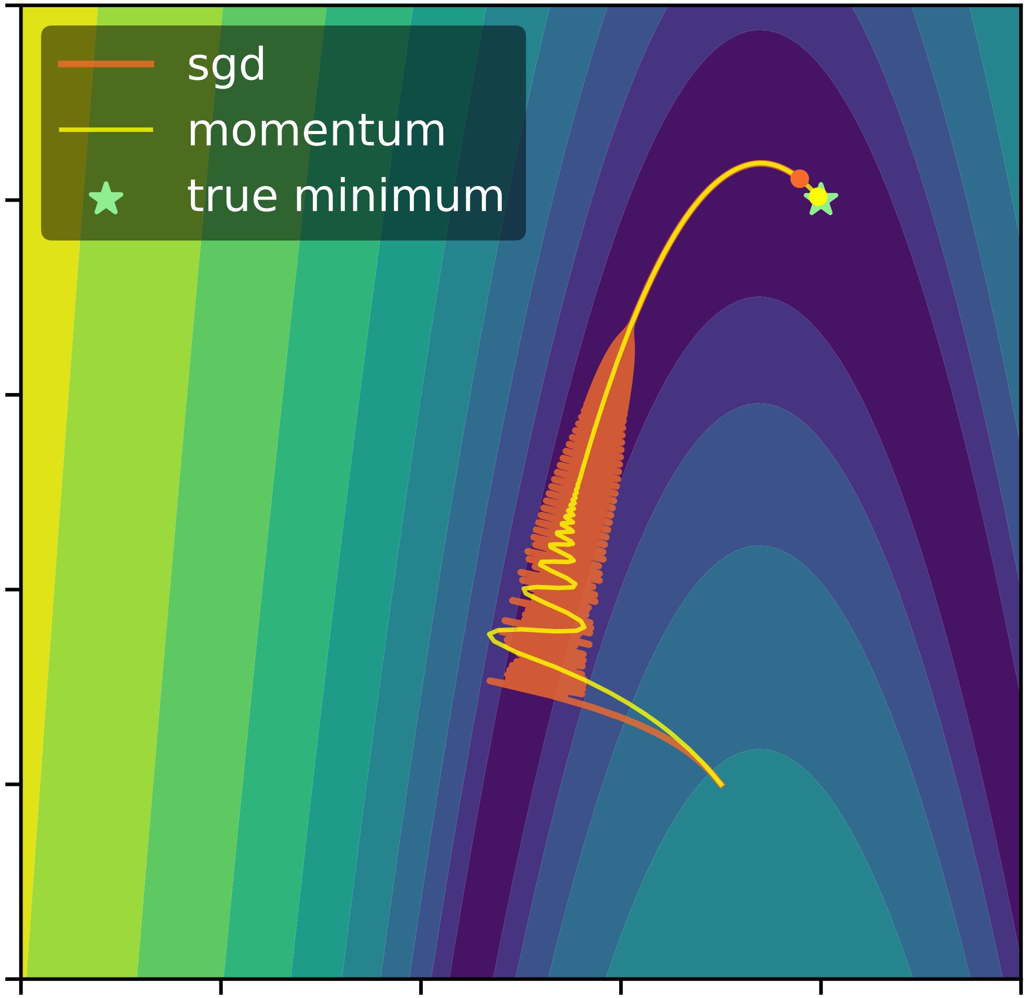

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  - Helps getting out of small local minima
  - Allows for larger range of learning rates*

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

RMSprop

- Idea: adjust learning rate separately for different components of the parameter vector
  - Gradients getting smaller ⇒ increase the learning rate (scale by inverse running RMS of the gradient)

RMSprop

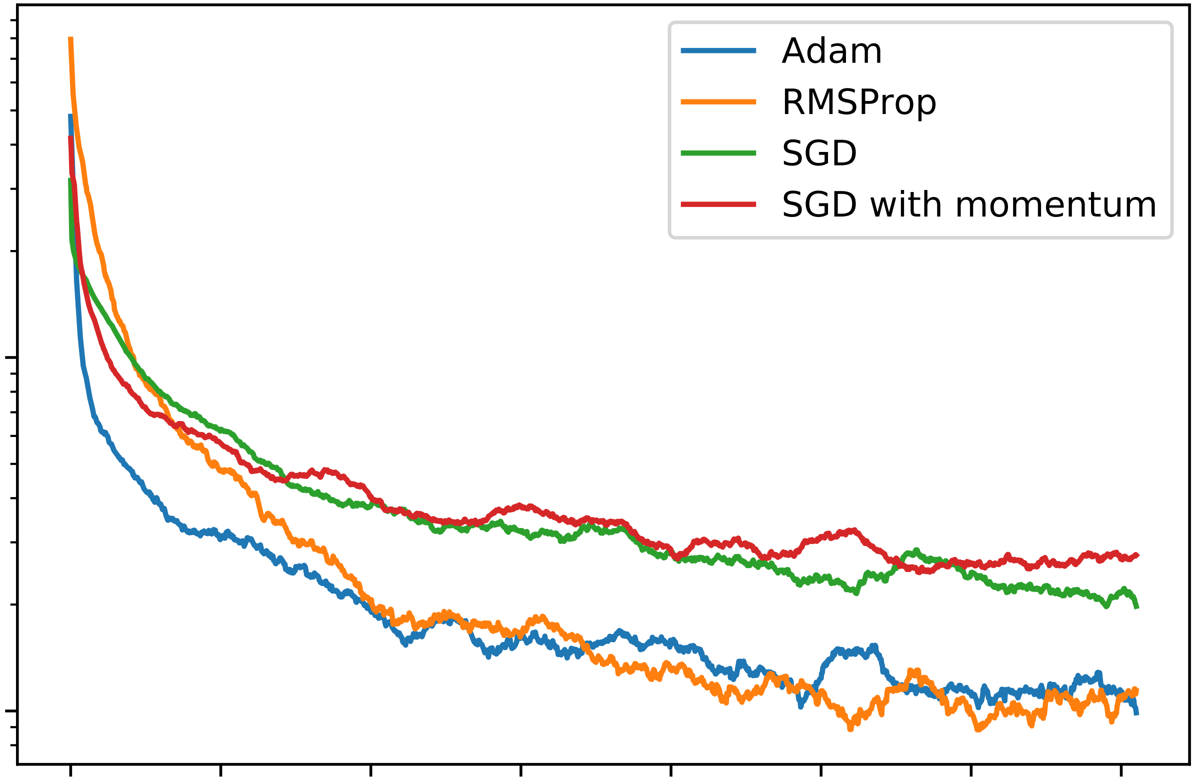
- Idea: adjust learning rate separately for different components of the parameter vector
  - Gradients getting smaller ⇒ increase the learning rate (scale by inverse running RMS of the gradient)

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

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

Adam

- Combine both ideas (momentum + RMSprop)
- Typically a good first choice for an optimizing algorithm



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

Thank you!

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