CSCI 567: Machine Learning

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Lecture 6, Sep 29

USC University of Southern California

Administrivia

- Quiz 1 next week during lecture hours (5pm-7:20pm)
- In-person. Please go to your respective room as follows:
  Last name from A-L: THH 201
  Last name from M-Z: SGM 123
- Quiz will be closed-book.
- Based on material covered till last time (so up to and including SVMs).

- HW1 grades will be released on Monday.

- HW3 will be released a few days after Quiz 1.

Multiclass classification

1.1 Setup

Recall the setup:

- input (feature vector): $\boldsymbol{x} \in \mathbb{R}^d$
- output (label): $y \in [\mathsf{C}] = \{1, 2, \cdots, \mathsf{C}\}$
- goal: learn a mapping $f : \mathbb{R}^d \to [\mathsf{C}]$

Examples:

- recognizing digits ($\mathsf{C} = 10$) or letters ($\mathsf{C} = 26$ or 52)
- predicting weather: sunny, cloudy, rainy, etc
- predicting image category: ImageNet dataset ($\mathsf{C} \approx 20K$)

1.2 Linear models: Binary to multiclass

Step 1: *What should a linear model look like for multiclass tasks?*

Note: a linear model for binary tasks (switching from $\{-1, +1\}$ to $\{1, 2\}$)

$$f(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \geq 0 \\ 2 & \text{if } \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} < 0 \end{cases}$$

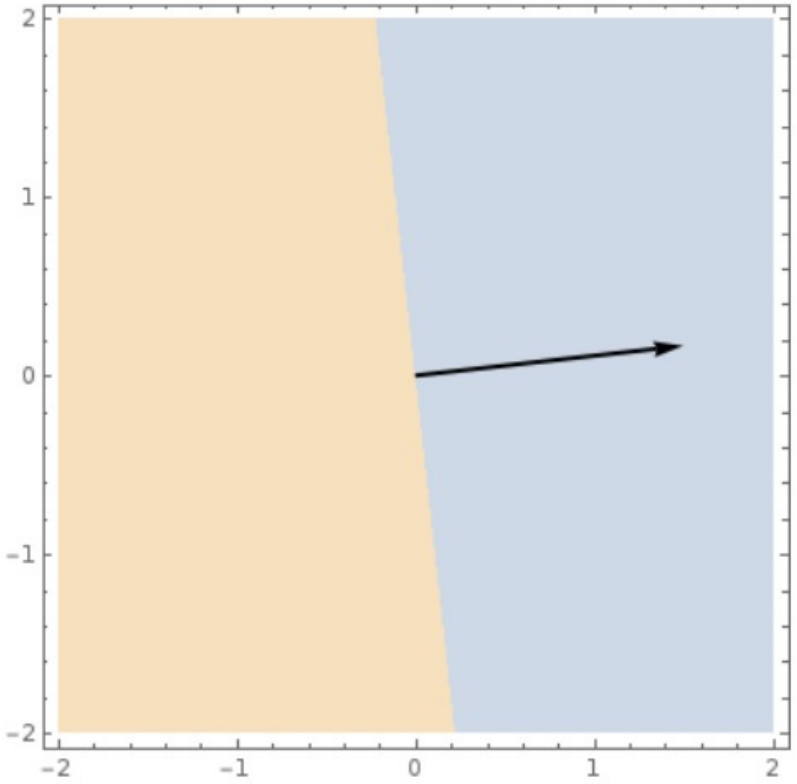
can be written as

$$f(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{w}_1^{\mathrm{T}}\boldsymbol{x} \geq \boldsymbol{w}_2^{\mathrm{T}}\boldsymbol{x} \\ 2 & \text{if } \boldsymbol{w}_2^{\mathrm{T}}\boldsymbol{x} > \boldsymbol{w}_1^{\mathrm{T}}\boldsymbol{x} \end{cases}$$
$$= \underset{k \in \{1,2\}}{\operatorname{argmax}} \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}$$

for any $\boldsymbol{w}_1, \boldsymbol{w}_2$ s.t. $\boldsymbol{w} = \boldsymbol{w}_1 - \boldsymbol{w}_2$

Think of $\boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}$ as **a score for class** k.

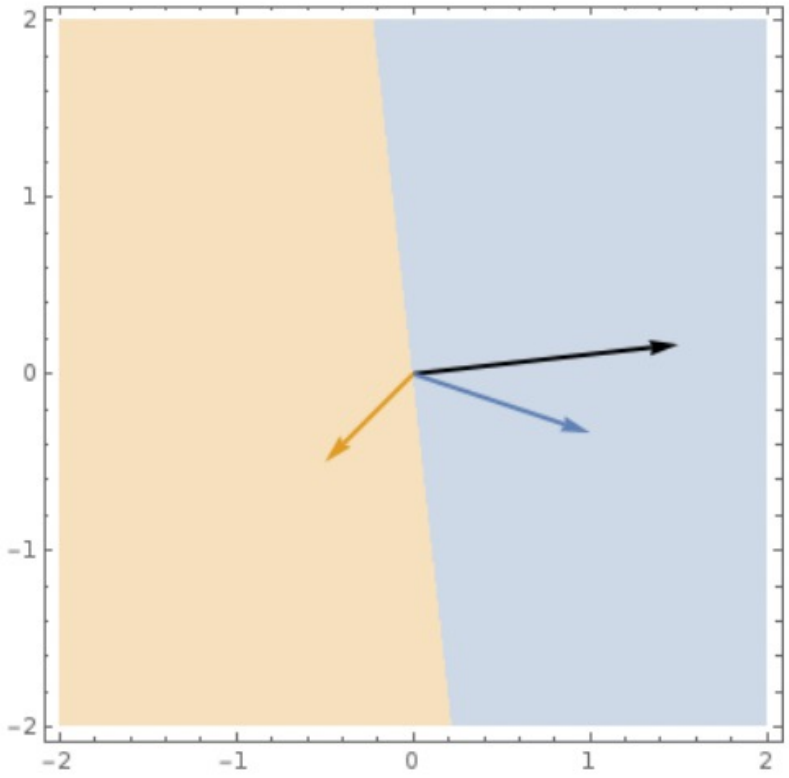
Linear models: Binary to multiclass



$$\boldsymbol{w} = (\tfrac{3}{2}, \tfrac{1}{6})$$

- Blue class:
  $\{\boldsymbol{x} : \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \geq 0\}$
- Orange class:
  $\{\boldsymbol{x} : \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} < 0\}$

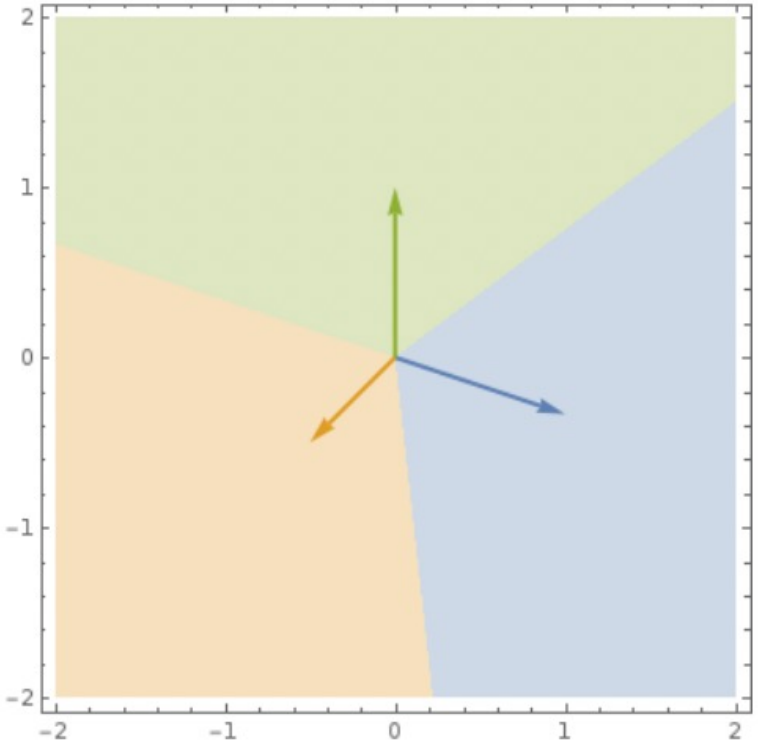
Linear models: Binary to multiclass



$$\boldsymbol{w} = (\tfrac{3}{2}, \tfrac{1}{6}) = \boldsymbol{w}_1 - \boldsymbol{w}_2$$
$$\boldsymbol{w}_1 = (1, -\tfrac{1}{3})$$
$$\boldsymbol{w}_2 = (-\tfrac{1}{2}, -\tfrac{1}{2})$$

- Blue class:
  $\{\boldsymbol{x} : 1 = \operatorname{argmax}_k \boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x}\}$
- Orange class:
  $\{\boldsymbol{x} : 2 = \operatorname{argmax}_k \boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x}\}$

Linear models: Binary to multiclass



$$\boldsymbol{w}_1 = (1, -\tfrac{1}{3})$$
$$\boldsymbol{w}_2 = (-\tfrac{1}{2}, -\tfrac{1}{2})$$
$$\boldsymbol{w}_3 = (0, 1)$$

- Blue class:
  $\{\boldsymbol{x} : 1 = \operatorname{argmax}_k \boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x}\}$
- Orange class:
  $\{\boldsymbol{x} : 2 = \operatorname{argmax}_k \boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x}\}$
- Green class:
  $\{\boldsymbol{x} : 3 = \operatorname{argmax}_k \boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x}\}$

1.3 Function class: Linear models for multiclass classification

$$\mathcal{F} = \left\{ f(\boldsymbol{x}) = \operatorname*{argmax}_{k \in [\mathsf{C}]} \ \boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x} \mid \boldsymbol{w}_1, \ldots, \boldsymbol{w}_{\mathsf{C}} \in \mathbb{R}^d \right\}$$

$$= \left\{ f(\boldsymbol{x}) = \operatorname*{argmax}_{k \in [\mathsf{C}]} \ (\boldsymbol{W}\boldsymbol{x})_k \mid \boldsymbol{W} \in \mathbb{R}^{\mathsf{C} \times d} \right\}$$

Next, lets try to generalize the loss functions. Focus on the logistic loss today.

1.4 Multinomial logistic regression: a probabilistic view

Observe: for binary logistic regression, with $\boldsymbol{w} = \boldsymbol{w}_1 - \boldsymbol{w}_2$:

$$\Pr(y = 1 \mid \boldsymbol{x}; \boldsymbol{w}) = \sigma(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}}} = \frac{e^{\boldsymbol{w}_1^{\mathrm{T}}\boldsymbol{x}}}{e^{\boldsymbol{w}_1^{\mathrm{T}}\boldsymbol{x}} + e^{\boldsymbol{w}_2^{\mathrm{T}}\boldsymbol{x}}} \propto e^{\boldsymbol{w}_1^{\mathrm{T}}\boldsymbol{x}}$$

Naturally, for multiclass:

$$\Pr(y = k \mid \boldsymbol{x}; \boldsymbol{W}) = \frac{e^{\boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}}}{\sum_{k \in [\mathsf{C}]} e^{\boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}}} \propto e^{\boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}}$$

This is called the *softmax function*.

1.5 Let's find the MLE

Maximize probability of seeing labels $y_1, \ldots, y_n$ given $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$

$$P(\boldsymbol{W}) = \prod_{i=1}^{n} \Pr(y_i \mid \boldsymbol{x}_i; \boldsymbol{W}) = \prod_{i=1}^{n} \frac{e^{\boldsymbol{w}_{y_i}^{\mathsf{T}} \boldsymbol{x}_i}}{\sum_{k \in [\mathsf{C}]} e^{\boldsymbol{w}_k^{\mathsf{T}} \boldsymbol{x}_i}}$$

By taking **negative log**, this is equivalent to minimizing

$$F(\boldsymbol{W}) = \sum_{i=1}^{n} \ln \left(\frac{\sum_{k \in [\mathsf{C}]} e^{\boldsymbol{w}_k^{\mathsf{T}} \boldsymbol{x}_i}}{e^{\boldsymbol{w}_{y_i}^{\mathsf{T}} \boldsymbol{x}_i}} \right) = \sum_{i=1}^{n} \ln \left(1 + \sum_{k \neq y_i} e^{(\boldsymbol{w}_k - \boldsymbol{w}_{y_i})^{\mathsf{T}} \boldsymbol{x}_i} \right)$$

This is the *multiclass logistic loss*. It is an upper-bound on the 0-1 misclassification loss:

$$\mathbb{I}[f(\boldsymbol{x}) \neq y] \leq \log_2 \left(1 + \sum_{k \neq y} e^{(\boldsymbol{w}_k - \boldsymbol{w}_y)^{\mathsf{T}} \boldsymbol{x}} \right)$$

When $\mathsf{C} = 2$, multiclass logistic loss is the same as binary logistic loss (let's verify).

Relating binary and multiclass logistic loss

1.6 Next, optimization

Apply **SGD**: what is the gradient of

$$F(\boldsymbol{W}) = \ln\left(1 + \sum_{k \neq y_i} e^{(\boldsymbol{w}_k - \boldsymbol{w}_{y_i})^{\mathrm{T}} \boldsymbol{x}_i}\right)?$$

It's a $\mathsf{C} \times d$ matrix. Let's focus on the k-th row:

If $k \neq y_i$:

$$\nabla_{\boldsymbol{w}_k^{\mathrm{T}}} F(\boldsymbol{W}) = \frac{e^{(\boldsymbol{w}_k - \boldsymbol{w}_{y_i})^{\mathrm{T}} \boldsymbol{x}_i}}{1 + \sum_{k \neq y_i} e^{(\boldsymbol{w}_k - \boldsymbol{w}_{y_i})^{\mathrm{T}} \boldsymbol{x}_i}} \boldsymbol{x}_i^{\mathrm{T}} = \frac{e^{\boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x}_i}}{e^{\boldsymbol{w}_{y_i}^{\mathrm{T}} \boldsymbol{x}_i} + \sum_{k \neq y_i} e^{\boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x}_i}} \boldsymbol{x}_i^{\mathrm{T}} = \Pr(y = k \mid \boldsymbol{x}_i; \boldsymbol{W}) \boldsymbol{x}_i^{\mathrm{T}}$$

else:

$$\nabla_{\boldsymbol{w}_k^{\mathrm{T}}} F(\boldsymbol{W}) = \frac{-\left(\sum_{k \neq y_i} e^{(\boldsymbol{w}_k - \boldsymbol{w}_{y_i})^{\mathrm{T}} \boldsymbol{x}_i}\right)}{1 + \sum_{k \neq y_i} e^{(\boldsymbol{w}_k - \boldsymbol{w}_{y_i})^{\mathrm{T}} \boldsymbol{x}_i}} \boldsymbol{x}_i^{\mathrm{T}} = \frac{-\left(\sum_{k \neq y_i} e^{\boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x}_i}\right)}{e^{\boldsymbol{w}_{y_i}^{\mathrm{T}} \boldsymbol{x}_i} + \sum_{k \neq y_i} e^{\boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x}_i}} \boldsymbol{x}_i^{\mathrm{T}} = \left(\Pr(y = y_i \mid \boldsymbol{x}_i; \boldsymbol{W}) - 1\right) \boldsymbol{x}_i^{\mathrm{T}}$$

SGD for multinomial logistic regression

Initialize $\boldsymbol{W} = \mathbf{0}$ (or randomly). Repeat:

1. pick $i \in [n]$ uniformly at random
2. update the parameters

$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \begin{pmatrix} \Pr(y = 1 \mid \boldsymbol{x}_i; \boldsymbol{W}) \\ \vdots \\ \Pr(y = y_i \mid \boldsymbol{x}_i; \boldsymbol{W}) - 1 \\ \vdots \\ \Pr(y = \mathsf{C} \mid \boldsymbol{x}_i; \boldsymbol{W}) \end{pmatrix} \boldsymbol{x}_i^{\mathrm{T}}$$

Think about why the algorithm makes sense intuitively.

1.7 Probabilities -> Prediction

Having learned $\boldsymbol{W}$, we can either

- make a *deterministic* prediction $\operatorname{argmax}_{k \in [\mathsf{C}]} \ \boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x}$
- make a *randomized* prediction according to $\Pr(y = k \mid \boldsymbol{x}; \boldsymbol{W}) \propto e^{\boldsymbol{w}_k^{\mathrm{T}} \boldsymbol{x}}$

1.8 Beyond linear models

Suppose we have any model f (not necessary linear) which gives some score $f_k(\boldsymbol{x})$ for the datapoint $\boldsymbol{x}$ having the k-th label.

How can we convert this score to probabilities? Use the *softmax function*!

$$\tilde{f}_k(\boldsymbol{x}) = \Pr(y = k \mid \boldsymbol{x}; f) = \frac{e^{f_k(\boldsymbol{x})}}{\sum_{k' \in [\mathsf{C}]} e^{f_{k'}(\boldsymbol{x})}} \propto e^{f_k(\boldsymbol{x})}$$

Once we have probability estimates, what is suitable loss function to train the model? Use the *log loss*. Also known as the *cross-entropy loss*.

Log Loss/Cross-entropy loss: Binary case

Let's start with binary classification again. Consider a model which predicts $\tilde{f}(\boldsymbol{x})$ as the probability of label being 1 for labelled datapoint $(\boldsymbol{x}, y)$. The log loss is defined as,

$$\begin{aligned}\text{LogLoss} &= \mathbf{1}(y=1)\ln\left(\frac{1}{\tilde{f}(\boldsymbol{x})}\right) + \mathbf{1}(y=-1)\ln\left(\frac{1}{1-\tilde{f}(\boldsymbol{x})}\right) \\ &= -\mathbf{1}(y=1)\ln(\tilde{f}(\boldsymbol{x})) - \mathbf{1}(y=-1)\ln((1-\tilde{f}(\boldsymbol{x}))).\end{aligned}$$

When the model is linear, this reduces to the logistic regression loss we defined before!

Log Loss/Cross-entropy loss: Multiclass case

This generalizes easily to the multiclass case. For datapoint $(\boldsymbol{x}, y)$, if $\tilde{f}_k(\boldsymbol{x})$ is the predicted probability of label k,

$$\begin{aligned}\text{LogLoss} &= \sum_{k=1}^{\mathsf{C}} \mathbf{1}(y=k) \ln\left(\frac{1}{\tilde{f}_k(\boldsymbol{x})}\right) \\ &= -\sum_{k=1}^{\mathsf{C}} \mathbf{1}(y=k) \ln\Big(\tilde{f}_k(\boldsymbol{x})\Big).\end{aligned}$$

When the model is linear, this also reduces to the multiclass logistic regression loss we defined earlier today.

Log Loss/Cross-entropy loss: Multiclass case

By combining the softmax and the log-loss, we have a general loss $\ell(f(\boldsymbol{x}), y)$ which we can use to train a multi-class classification model which assigns scores $f_k(\boldsymbol{x})$ to the k-th class. (These scores $f_k(\boldsymbol{x})$ are sometimes referred to as logits).

$$\begin{aligned}
\ell(f(\boldsymbol{x}), y) &= -\sum_{k=1}^{\mathsf{C}} \mathbf{1}(y = k) \ln\left(\tilde{f}_k(\boldsymbol{x})\right) \\
&= \ln\left(\frac{\sum_{k\in[\mathsf{C}]} e^{f_k(\boldsymbol{x})}}{e^{f_y(\boldsymbol{x})}}\right) \\
&= \sum_{i=1}^{n} \ln\left(1 + \sum_{k\neq y} e^{f_k(\boldsymbol{x}) - f_y(\boldsymbol{x})}\right).
\end{aligned}$$

Multiclass logistic loss: Another view

1.8 Other techniques for multiclass classification

Cross-entropy is the most popular, but there are other *black-box techniques* to convert multiclass classification to binary classification.

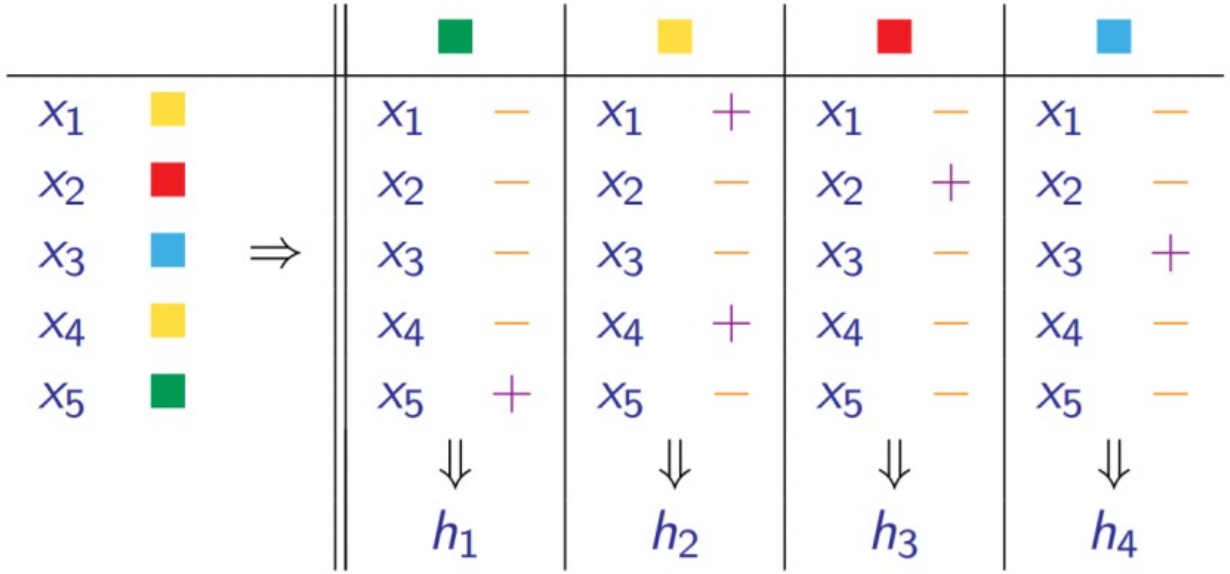
- **one-versus-all** (one-versus-rest, one-against-all, etc.)
- **one-versus-one** (all-versus-all, etc.)
- **Error-Correcting Output Codes** (ECOC)
- **tree-based reduction**

1.9 One-versus-all

Idea: train C binary classifiers to learn "**is class k or not?**" for each k.

Training: for each class $k \in [\mathsf{C}]$,

- relabel examples with class k as $+1$, and all others as -1
- train a binary classifier h_k using this new dataset



Picture credits link

1.9 One-versus-all

Idea: train C binary classifiers to learn "**is class k or not?**" for each k.

Prediction: for a new example $\boldsymbol{x}$

- ask each h_k: **does this belong to class k?** (i.e. $h_k(\boldsymbol{x})$)
- randomly pick among all k's s.t. $h_k(\boldsymbol{x}) = +1$.

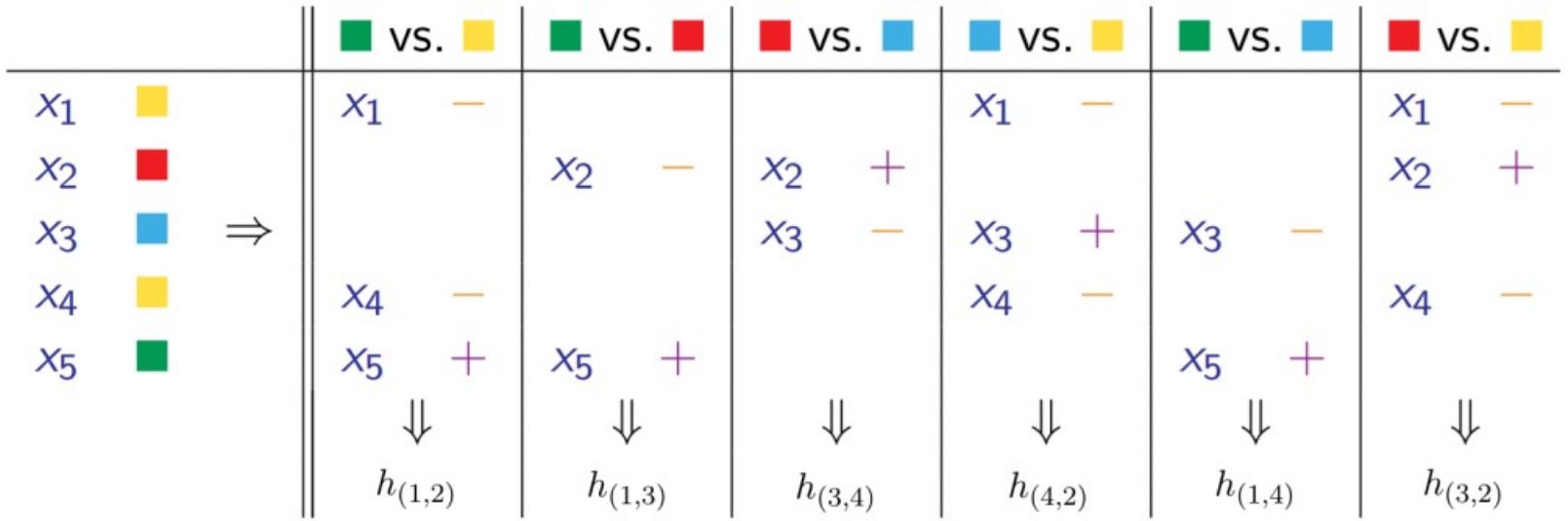
Issue: will (probably) make a mistake *as long as one of h_k errs*.

1.10 One-versus-one

Idea: train $\binom{C}{2}$ binary classifiers to learn "**is class k or k'?**".

Training: for each pair (k, k'),

- relabel examples with class k as $+1$ and examples with class k' as -1
- *discard all other examples*
- train a binary classifier $h_{(k,k')}$ using this new dataset



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1.10 One-versus-one

Idea: train $\binom{C}{2}$ binary classifiers to learn "**is class k or k'?**".

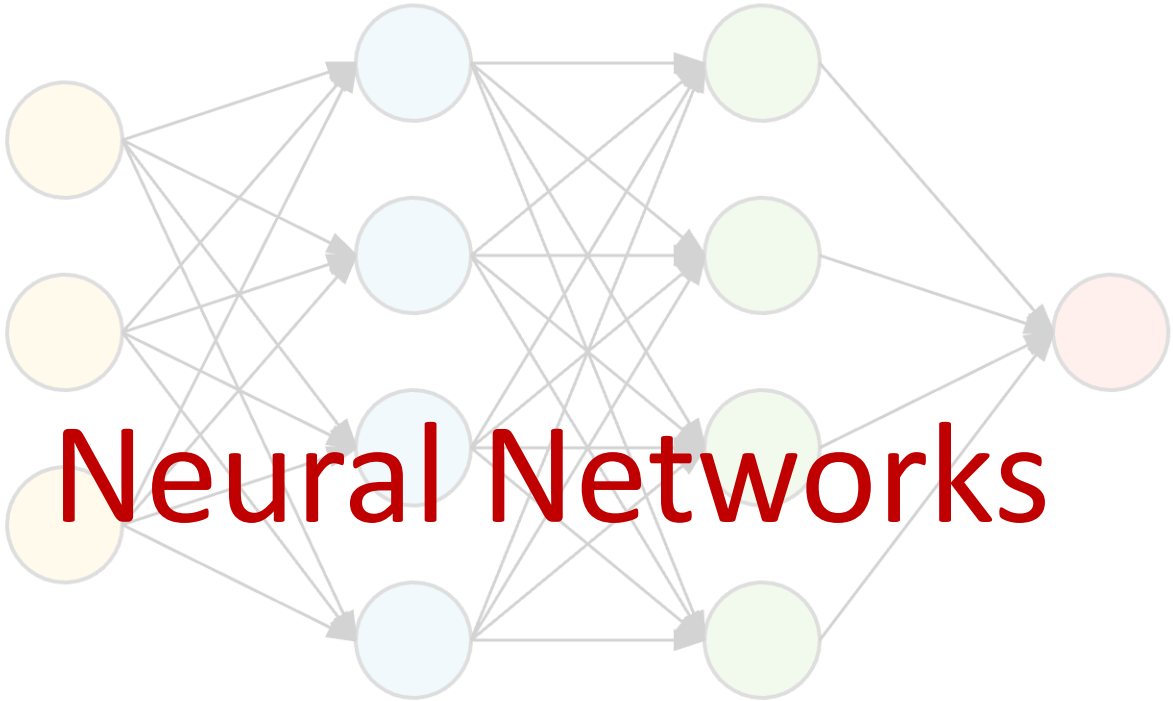
Prediction: for a new example $\boldsymbol{x}$

- ask each classifier $h_{(k,k')}$ to **vote for either class k or k'**
- predict the class with the most votes (break tie in some way)

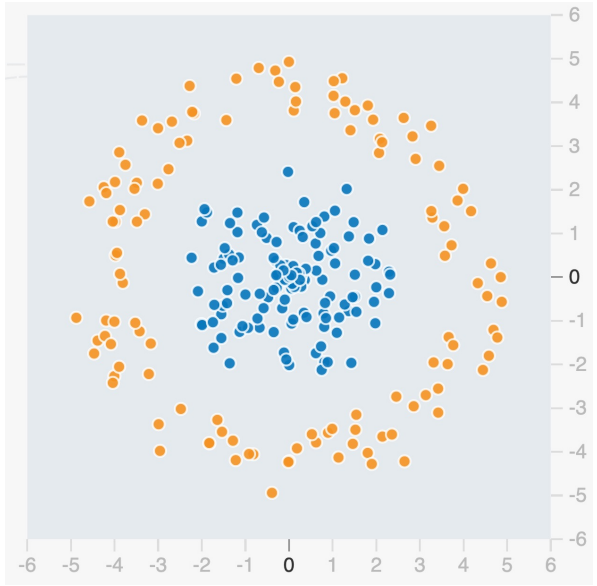
More robust than one-versus-all, but *slower* in prediction.

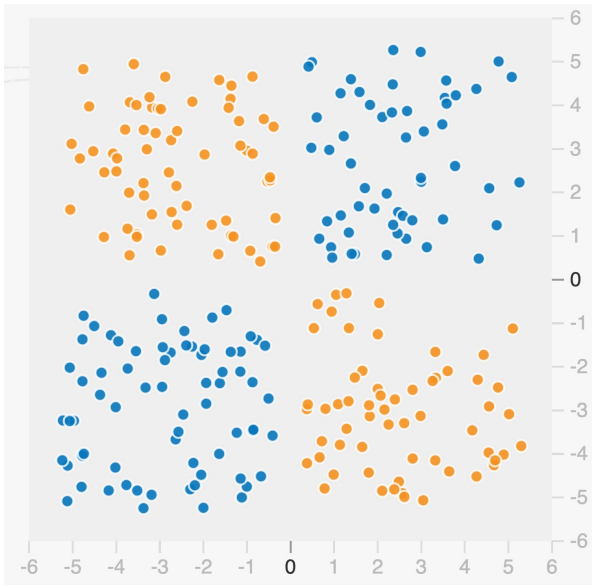
Other techniques such as tree-based methods and error-correcting codes can achieve intermediate tradeoffs.

Neural Networks



Linear -> Fixed non-linear -> **Learned non-linear map**





Linear models aren't always enough. As we discussed, we can use a nonlinear mapping and learn a linear model in the feature space:

$$\boldsymbol{\phi}(\boldsymbol{x}) : \boldsymbol{x} \in \mathbb{R}^d \rightarrow \boldsymbol{z} \in \mathbb{R}^M$$

But what kind of nonlinear mapping $\boldsymbol{\phi}$ should be used?

Can we just learn the nonlinear mapping itself?

Supervised learning in one slide

Loss function: What is the right loss function for the task?

Representation: What class of functions should we use?

Optimization: How can we efficiently solve the empirical risk minimization problem?

Generalization: Will the predictions of our model transfer gracefully to unseen examples?

All related! And the fuel which powers everything is data.

2.1 Loss function

For model which makes predictions $f(\boldsymbol{x})$ on labelled datapoint $(\boldsymbol{x}, y)$, we can use the following losses.

Regression:

$$\ell(f(\boldsymbol{x}), y) = (f(\boldsymbol{x}) - y)^2 .$$

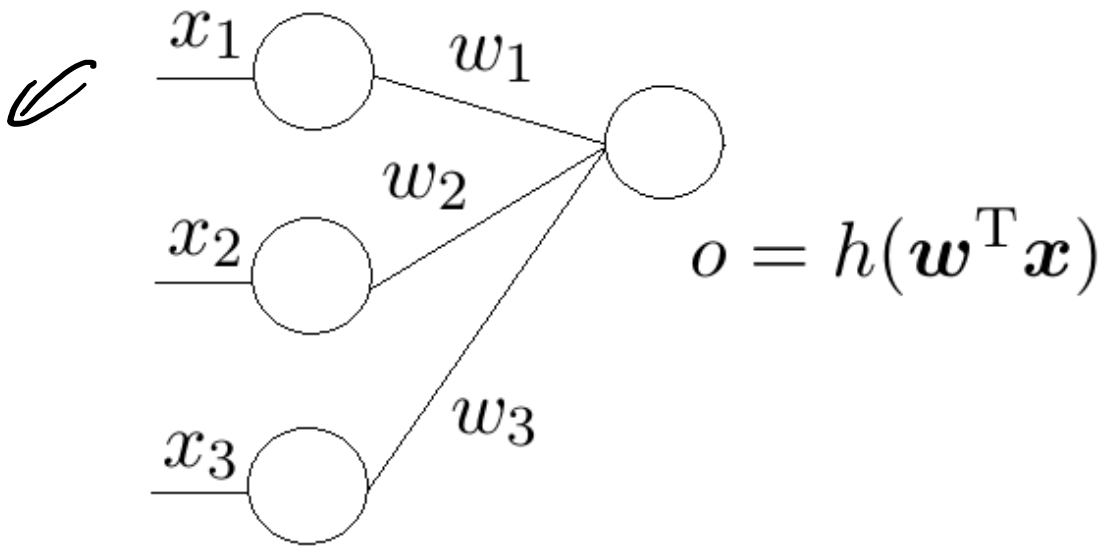
Classification:

$$\ell(f(\boldsymbol{x}), y) = \ln\left(\frac{\sum_{k\in[\mathsf{C}]} e^{f_k(\boldsymbol{x})}}{e^{f_y(\boldsymbol{x})}}\right) = \sum_{i=1}^{n} \ln\left(1 + \sum_{k\neq y} e^{f_k(\boldsymbol{x}) - f_y(\boldsymbol{x})}\right) .$$

There maybe other, more suitable options for the problem at hand, but these are the most popular for supervised problems.

2.2 Representation: Defining neural networks

Linear model as a one-layer neural network:



For a linear model, $h(a) = a$.

To create non-linearity, can use some nonlinear (differentiable) function:

- Rectified Linear Unit (**ReLU**): $h(a) = \max\{0, a\}$
- Sigmoid function: $h(a) = \frac{1}{1+e^{-a}}$
- Tanh: $h(a) = \frac{e^{a}-e^{-a}}{e^{a}+e^{-a}}$
- many more

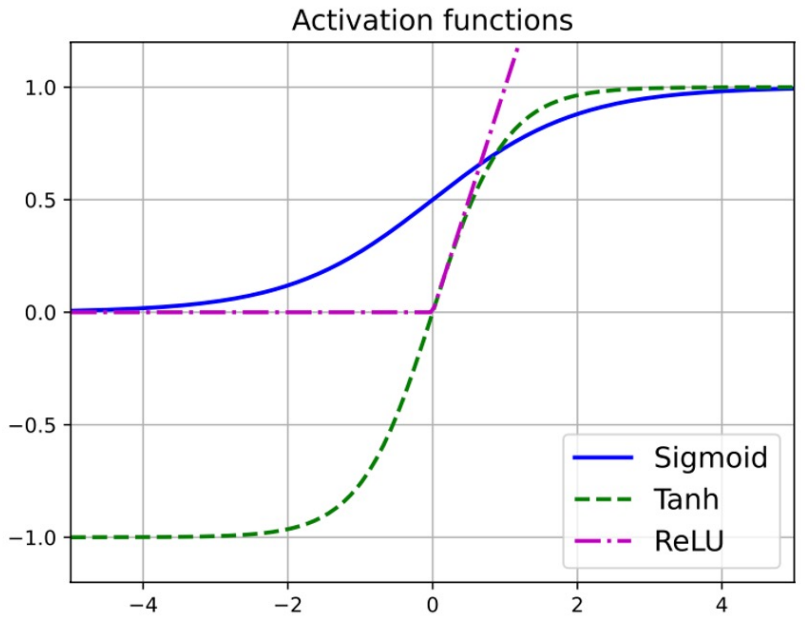
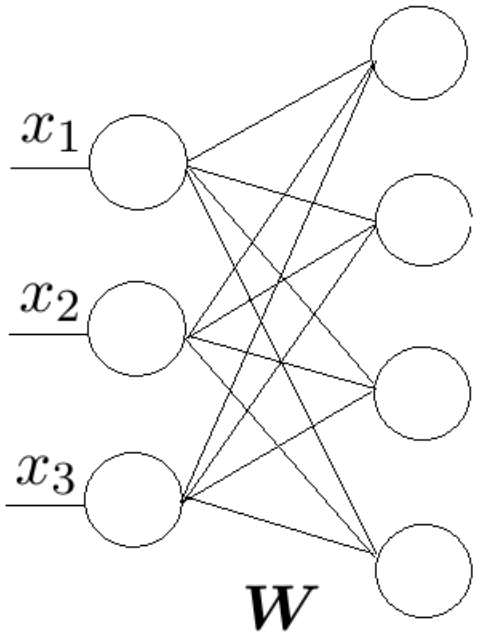


Figure 13.2 from PML

Adding a layer



$$\boldsymbol{o} = \boldsymbol{h}(\boldsymbol{W}\boldsymbol{x})$$

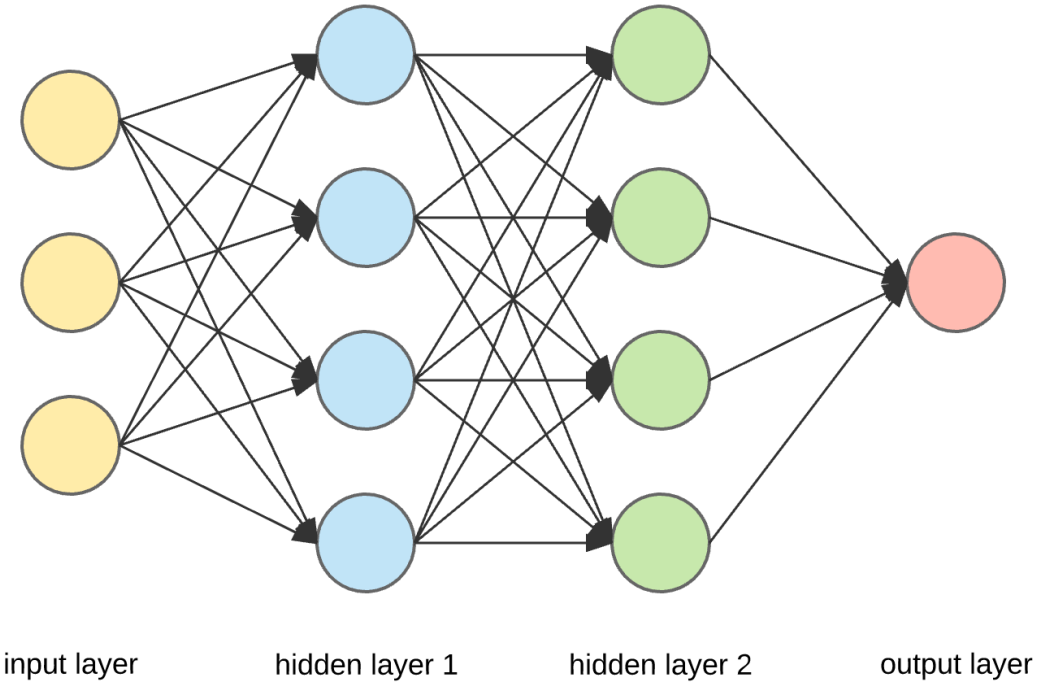
$\boldsymbol{W} \in \mathbb{R}^{4\times 3}$, $\boldsymbol{h} : \mathbb{R}^4 \to \mathbb{R}^4$ so $\boldsymbol{h}(\boldsymbol{a}) = (h_1(a_1), h_2(a_2), h_3(a_3), h_4(a_4))$

Can think of this as a nonlinear mapping: $\boldsymbol{\phi}(\boldsymbol{x}) = \boldsymbol{h}(\boldsymbol{W}\boldsymbol{x})$

Putting things together: a neural network

We now have a network:

- each node is called a **neuron**
- $\boldsymbol{h}$ is called the **activation function**
  - can use $h(a) = 1$ for one neuron in each layer to incorporate bias term
  - output neuron can use $h(a) = a$
- #layers refers to #hidden_layers (plus 1 or 2 for input/output layers)
- **deep** neural nets can have many layers and *millions* of parameters
- this is a **feedforward, fully connected** neural net, there are many variants (convolutional nets, residual nets, recurrent nets, etc.)



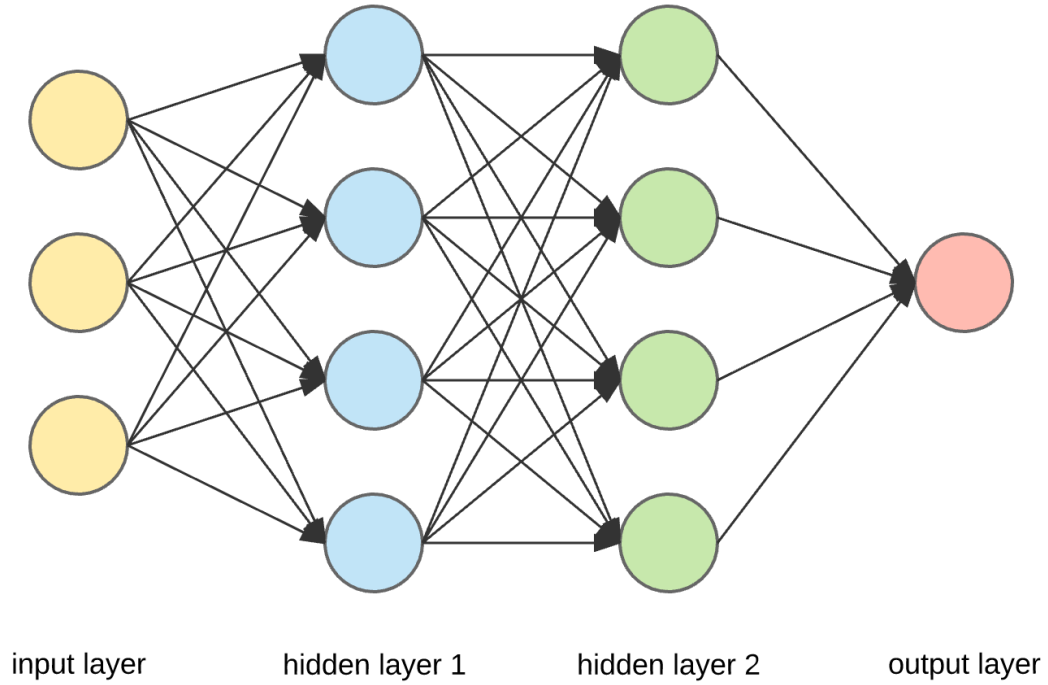
Neural network: Definition

An L-layer neural net can be written as

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{h}_{\mathsf{L}}\left(\boldsymbol{W}_{L}\boldsymbol{h}_{\mathsf{L}-1}\left(\boldsymbol{W}_{L-1}\cdots\boldsymbol{h}_{1}\left(\boldsymbol{W}_{1}\boldsymbol{x}\right)\right)\right).$$

Define

- $\boldsymbol{W}_\ell \in \mathbb{R}^{d_\ell \times d_{\ell-1}}$ is the weights between layer $\ell - 1$ and ℓ
- $d_0 = d, d_1, \ldots, d_{\mathsf{L}}$ are numbers of neurons at each layer
- $\boldsymbol{a}_\ell \in \mathbb{R}^{d_\ell}$ is input to layer ℓ
- $\boldsymbol{o}_\ell \in \mathbb{R}^{d_\ell}$ is output of layer ℓ
- $\boldsymbol{h}_\ell : \mathbb{R}^{d_\ell} \to \mathbb{R}^{d_\ell}$ is activation functions at layer ℓ



Now, for a given input $\boldsymbol{x}$, we have recursive relations:

$$\boldsymbol{o}_0 = \boldsymbol{x}, \boldsymbol{a}_\ell = \boldsymbol{W}_\ell \boldsymbol{o}_{\ell-1}, \boldsymbol{o}_\ell = \boldsymbol{h}_\ell(\boldsymbol{a}_\ell), \quad (\ell = 1, \ldots, \mathsf{L}).$$

2.3 Optimization

Our optimization problem is to minimize,

$$F(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_L) = \frac{1}{n} \sum_{i=1}^{n} F_i(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_L)$$

where

$$F_i(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_L) = \begin{cases} \|\boldsymbol{f}(\boldsymbol{x}_i) - \boldsymbol{y}_i\|_2^2 & \text{for regression} \\ \ln\left(1 + \sum_{k \neq y_i} e^{f_k(\boldsymbol{x}_i) - f_{y_i}(\boldsymbol{x}_i)}\right) & \text{for classification} \end{cases}$$

How to solve this? Apply **SGD**!

To compute the gradient efficiently, we use *backpropogation*. More on this soon.

2.4 Generalization

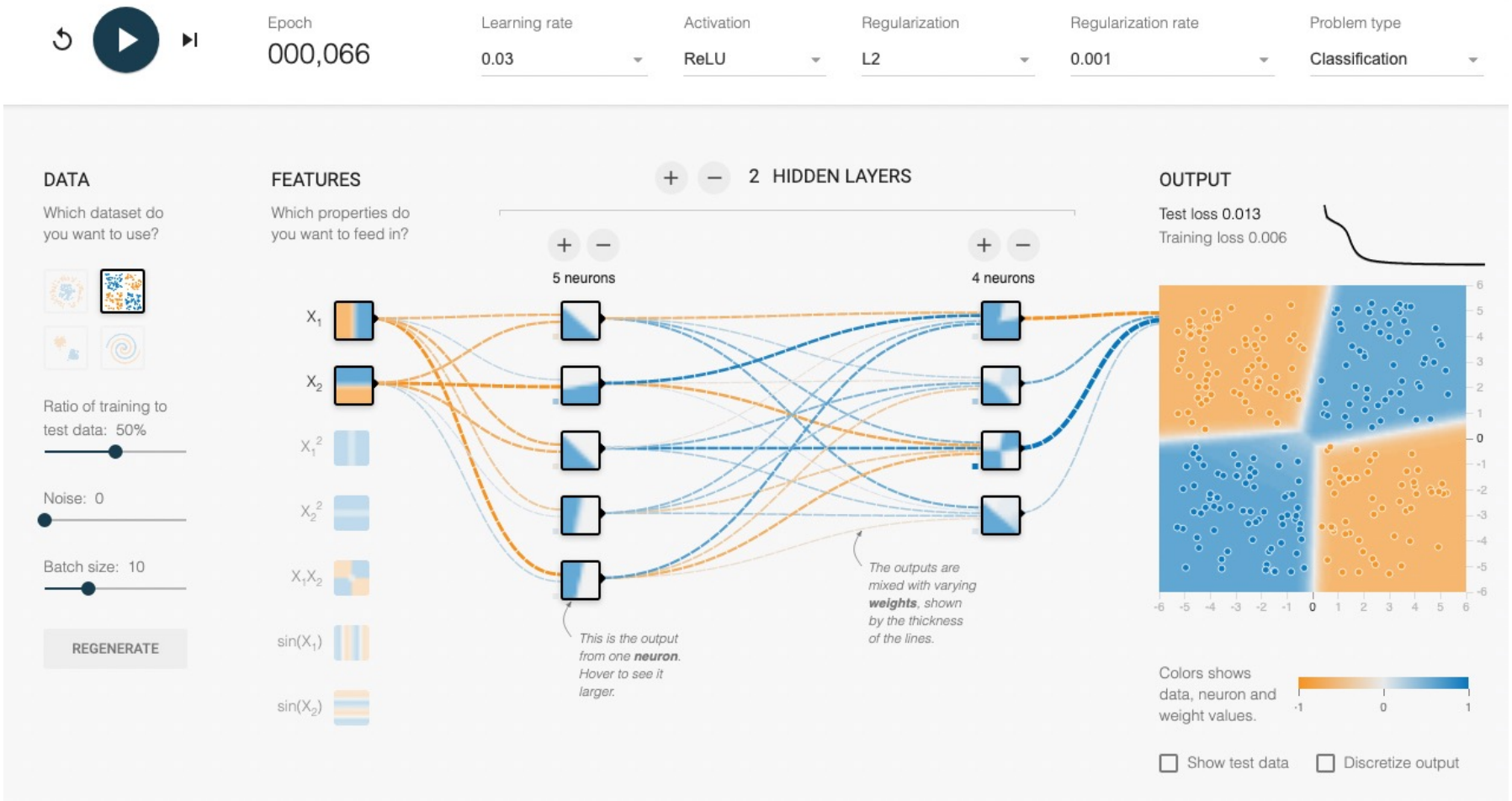
Overfitting is a concern for such a complex model, but there are ways to handle it.

For example, we can add ℓ_2 regularization.

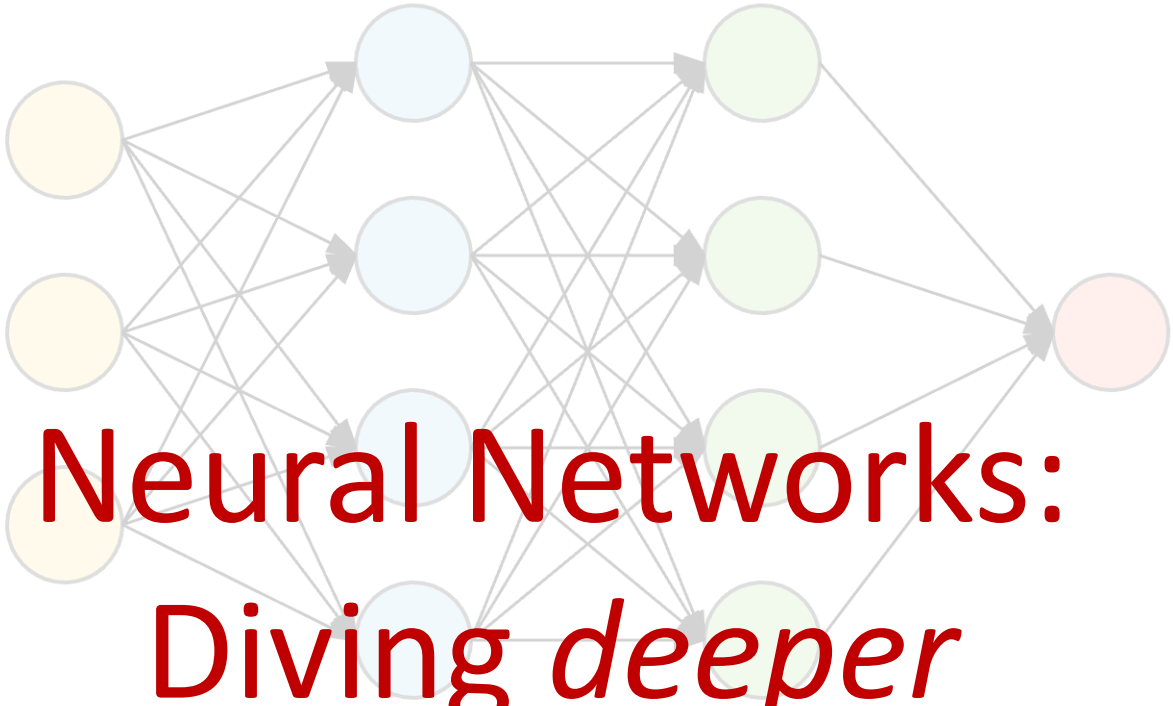
ℓ_2 **regularization**: minimize

$$G(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_L) = F(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_L) + \lambda \sum_{\substack{\text{all weights } w \\ \text{in network}}} w^2$$

Demo



http://playground.tensorflow.org/



Neural Networks: Diving *deeper*

3.1 Representation: Very powerful function class!

Universal approximation theorem (Cybenko, 89; Hornik, 91):

A feedforward neural net with a single hidden layer can approximate any continuous function.

It might need a huge number of neurons though, and *depth helps!*

Choosing the network architecture is important.

- for feedforward network, need to decide number of hidden layers, number of neurons at each layer, activation functions, etc.

Designing the architecture can be complicated, though various standard choices exist.

3.2 Optimization: Computing gradients efficiently using Backprop

To run SGD, need gradients of $F_i(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_\mathsf{L})$ with respect to all the weights in all the layers. How do we get the gradient?

Here's a naive way to compute gradients. For some function $F(w)$ of a univariate parameter w,

$$\frac{dF(w)}{dw} = \lim_{\epsilon \to 0} \frac{F(w+\epsilon) - F(w-\epsilon)}{2\epsilon}$$

Backprop

Backpropogation: A very efficient way to compute gradients of neural networks using an application of the chain rule (similar to dynamic programming).

Chain rule:

- for a composite function $f(g(w))$

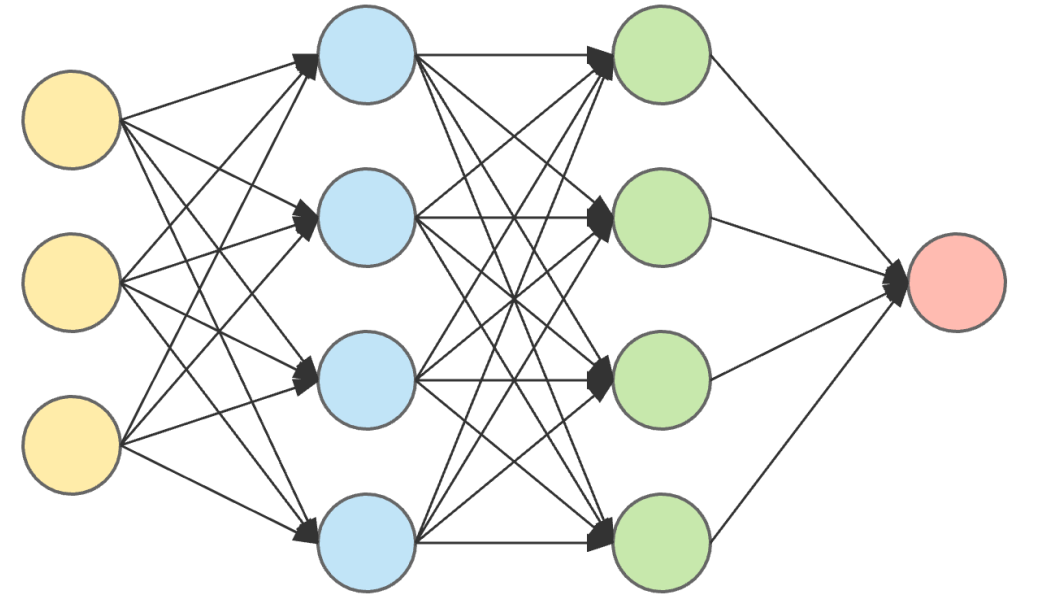
$$\frac{\partial f}{\partial w} = \frac{\partial f}{\partial g}\frac{\partial g}{\partial w}$$

- for a composite function $f(g_1(w), \ldots, g_d(w))$

$$\frac{\partial f}{\partial w} = \sum_{i=1}^{d} \frac{\partial f}{\partial g_i}\frac{\partial g_i}{\partial w}$$

  the simplest example $f(g_1(w), g_2(w)) = g_1(w)g_2(w)$

Backprop: Intuition

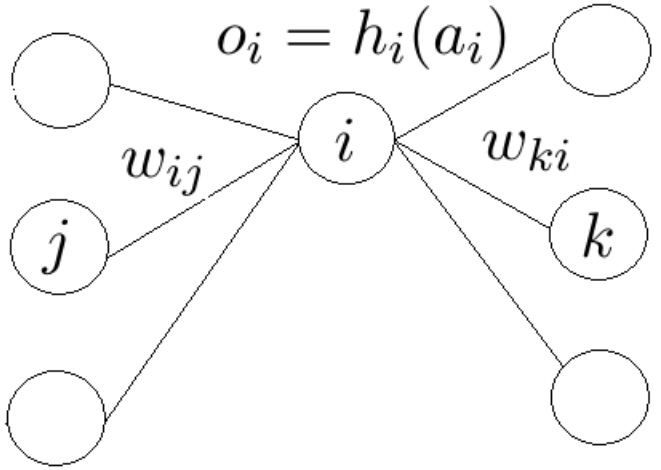


Backprop: Derivation

Drop the subscript ℓ for layer for simplicity. For this derivation, refer to the loss function as F_m (instead of F_i) for convenience.

Find the **derivative of F_m w.r.t. to w_{ij}**

$$\frac{\partial F_m}{\partial w_{ij}} = \frac{\partial F_m}{\partial a_i}\frac{\partial a_i}{\partial w_{ij}} = \frac{\partial F_m}{\partial a_i}\frac{\partial (w_{ij}o_j)}{\partial w_{ij}} = \frac{\partial F_m}{\partial a_i}o_j$$



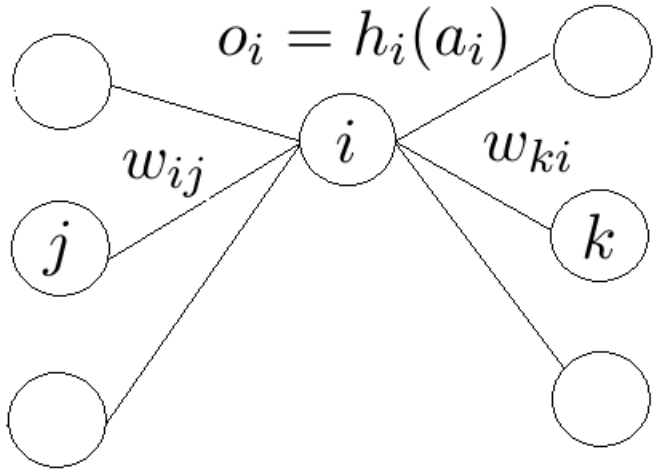
$$\frac{\partial F_m}{\partial a_i} = \frac{\partial F_m}{\partial o_i}\frac{\partial o_i}{\partial a_i} = \left(\sum_k \frac{\partial F_m}{\partial a_k}\frac{\partial a_k}{\partial o_i}\right) h_i'(a_i) = \left(\sum_k \frac{\partial F_m}{\partial a_k} w_{ki}\right) h_i'(a_i)$$

Backprop: Derivation

Adding the subscript for layer:

$$\frac{\partial F_m}{\partial w_{\ell,ij}} = \frac{\partial F_m}{\partial a_{\ell,i}} o_{\ell-1,j}$$

$$\frac{\partial F_m}{\partial a_{\ell,i}} = \left(\sum_k \frac{\partial F_m}{\partial a_{\ell+1,k}} w_{\ell+1,ki} \right) h'_{\ell,i}(a_{\ell,i})$$



For the last layer, for square loss

$$\frac{\partial F_m}{\partial a_{\mathsf{L},i}} = \frac{\partial (h_{\mathsf{L},i}(a_{\mathsf{L},i}) - y_{n,i})^2}{\partial a_{\mathsf{L},i}} = 2(h_{\mathsf{L},i}(a_{\mathsf{L},i}) - y_{n,i}) h'_{\mathsf{L},i}(a_{\mathsf{L},i})$$

Exercise: try to do it for logistic loss yourself.

Backprop: Derivation

Using **matrix notation** greatly simplifies presentation and implementation:

$$\frac{\partial F_m}{\partial \boldsymbol{W}_\ell} = \frac{\partial F_m}{\partial \boldsymbol{a}_\ell} \boldsymbol{o}_{\ell-1}^{\mathsf{T}} \in \mathbb{R}^{d_\ell \times d_{\ell-1}}$$

$$\frac{\partial F_m}{\partial \boldsymbol{a}_\ell} = \begin{cases} \left(\boldsymbol{W}_{\ell+1}^{\mathsf{T}} \frac{\partial F_m}{\partial \boldsymbol{a}_{\ell+1}} \right) \circ \boldsymbol{h}_\ell'(\boldsymbol{a}_\ell) & \text{if } \ell < \mathsf{L} \\ 2(\boldsymbol{h}_\mathsf{L}(\boldsymbol{a}_\mathsf{L}) - \boldsymbol{y}_n) \circ \boldsymbol{h}_\mathsf{L}'(\boldsymbol{a}_\mathsf{L}) & \text{else} \end{cases}$$

where $\boldsymbol{v}_1 \circ \boldsymbol{v}_2 = (v_{11}v_{21}, \cdots, v_{1d}v_{2d})$ is the element-wise product (a.k.a. Hadamard product).

Verify yourself!

The backpropagation algorithm (Backprop)

Initialize $\boldsymbol{W}_1, \ldots, \boldsymbol{W}_{\mathsf{L}}$ randomly. Repeat:

1. randomly pick one data point $i \in [n]$
2. **forward propagation**: for each layer $\ell = 1, \ldots, \mathsf{L}$
   - compute $\boldsymbol{a}_\ell = \boldsymbol{W}_\ell \boldsymbol{o}_{\ell-1}$ and $\boldsymbol{o}_\ell = \boldsymbol{h}_\ell(\boldsymbol{a}_\ell)$ $\qquad (\boldsymbol{o}_0 = \boldsymbol{x}_i)$
3. **backward propagation**: for each $\ell = L, \ldots, 1$
   - compute

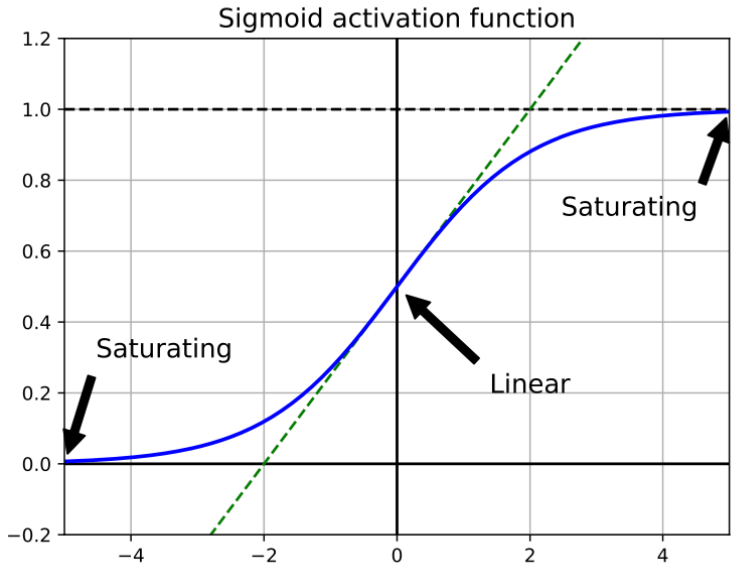
$$\frac{\partial F_i}{\partial \boldsymbol{a}_\ell} = \begin{cases} \left(\boldsymbol{W}_{\ell+1}^{\mathsf{T}} \frac{\partial F_i}{\partial \boldsymbol{a}_{\ell+1}}\right) \circ \boldsymbol{h}_\ell'(\boldsymbol{a}_\ell) & \text{if } \ell < \mathsf{L} \\ 2(\boldsymbol{h}_{\mathsf{L}}(\boldsymbol{a}_{\mathsf{L}}) - \boldsymbol{y}_n) \circ \boldsymbol{h}_{\mathsf{L}}'(\boldsymbol{a}_{\mathsf{L}}) & \text{else} \end{cases}$$

   - update weights

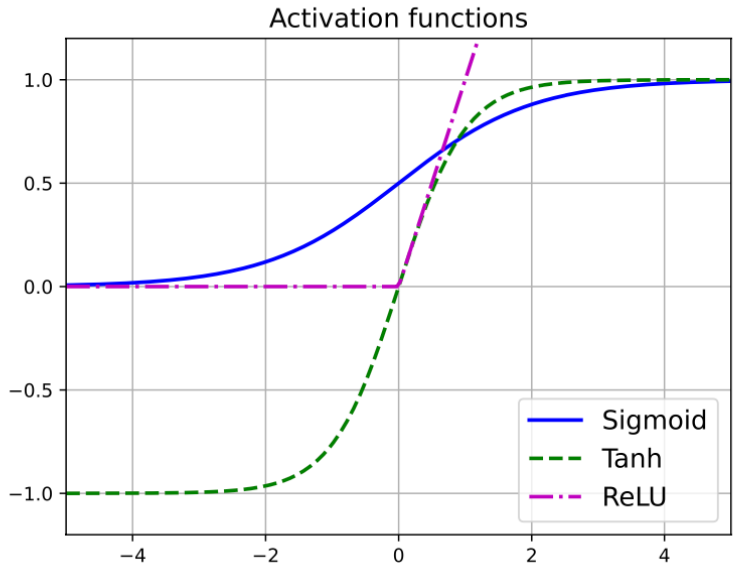
$$\boldsymbol{W}_\ell \leftarrow \boldsymbol{W}_\ell - \eta \frac{\partial F_i}{\partial \boldsymbol{W}_\ell} = \boldsymbol{W}_\ell - \eta \frac{\partial F_i}{\partial \boldsymbol{a}_\ell} \boldsymbol{o}_{\ell-1}^{\mathsf{T}}$$

(Important: *should $\boldsymbol{W}_\ell$ be overwritten immediately in the last step?*)

Non-saturating activation functions



(a)

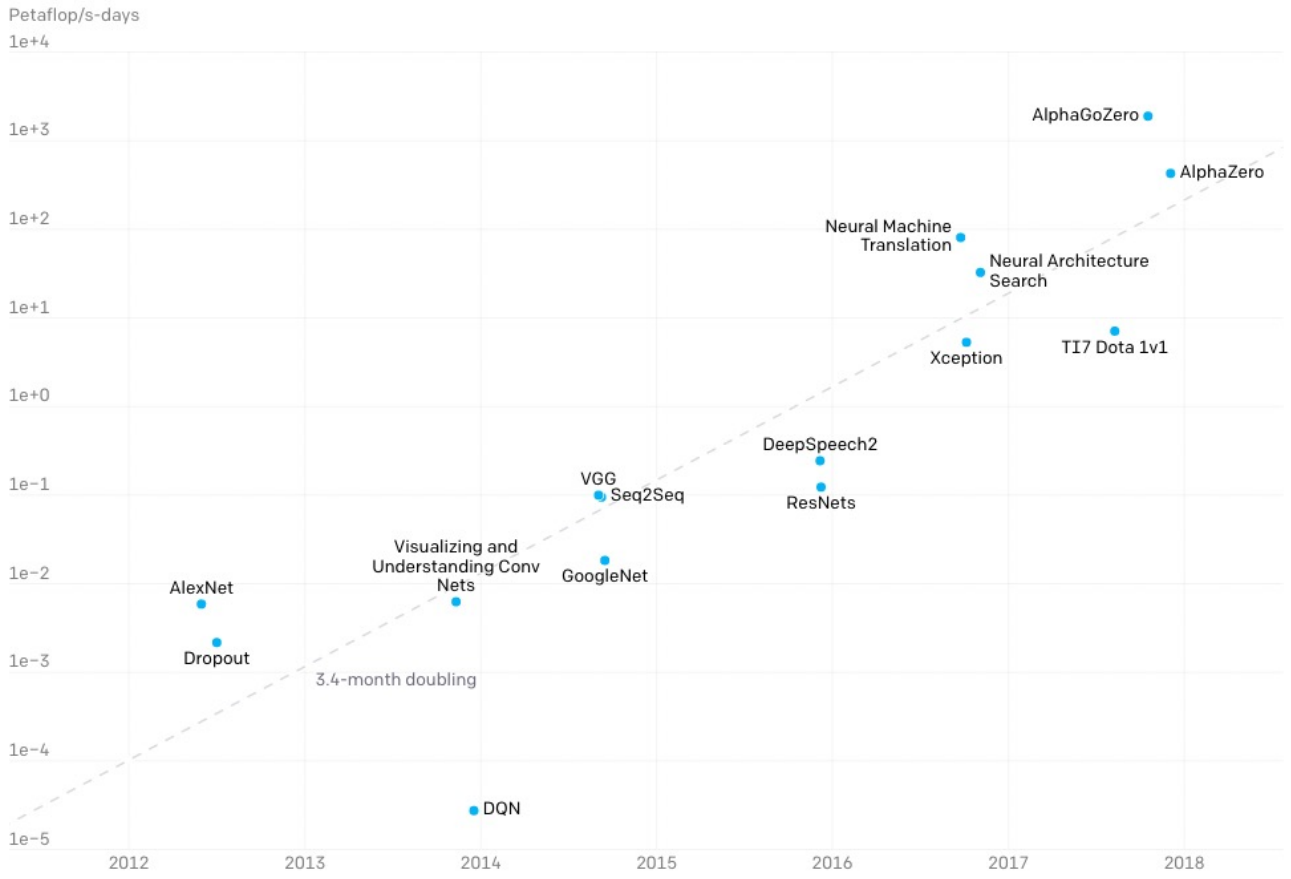


(b)

Figure 13.2 from PML

Modern networks are huge, and training can take time

Y-axis: Petaflop/s-day (pfs-day) consists of performing 10^{15} neural net operations per second for one day, or a total of about 10^{20} operations.



The total amount of compute, in petaflop/s-days,[2] used to train selected results that are relatively well known, used a lot of compute for their time, and gave enough information to estimate the compute used.

..since 2012, the amount of compute used in the largest AI training runs has been increasing exponentially with a 3.4-month doubling time (by comparison, Moore's Law had a 2-year doubling period). Since 2012, this metric has grown by more than 300,000x (a 2-year doubling period would yield only a 7x increase).

From https://openai.com/blog/ai-and-compute/

Modern networks are huge, and training can take time

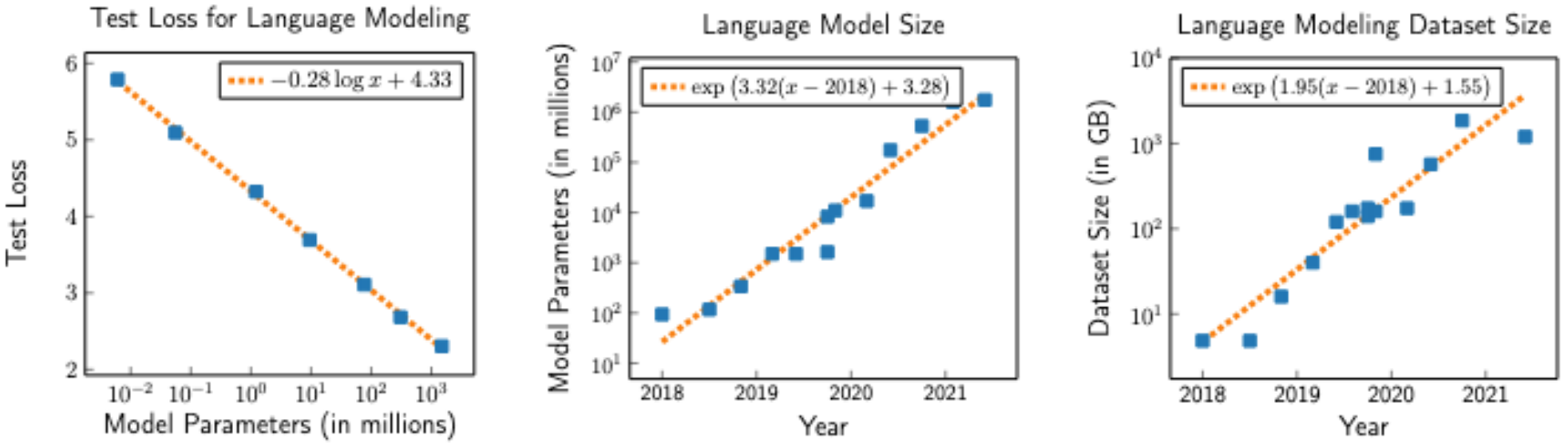


Figure 1.3: Scaling of neural language models over 2018-2022. **Left**: As the model size increases across orders of magnitude, the performance of the model at language modeling, as measured by the cross entropy on unseen data, consistently improves. The numbers are taken from (Kaplan et al., 2020). **Center & Right**: The size of the recent neural language models (center) and the amount of data they were trained on (right) have consistently increased across orders of magnitude.

Optimization: Variants on SGD

- **mini-batch**: randomly sample a batch of examples to form a stochastic gradient (common batch size: 32, 64, 128, etc.)

Mini-batch

Consider $F(\boldsymbol{w}) = \sum_{i=1}^{n} F_i(\boldsymbol{w})$, where $F_i(\boldsymbol{w})$ is the loss function for the i-th datapoint.

Recall that any $\nabla \tilde{F}(\boldsymbol{w})$ is a stochastic gradient of $F(\boldsymbol{w})$ if

$$\mathbb{E}[\nabla \tilde{F}(\boldsymbol{w})] = \nabla F(\boldsymbol{w}).$$

Mini-batch SGD (also known as mini-batch GD): sample $S \subset \{1, \ldots, n\}$ at random, and estimate the average gradient over these batch of $|S|$ samples:

$$\nabla \tilde{F}(\boldsymbol{w}) = \frac{1}{|S|} \sum_{j \in S} F_j(\boldsymbol{w}).$$

Common batch size: 32, 64, 128, etc.

Optimization: Variants on SGD

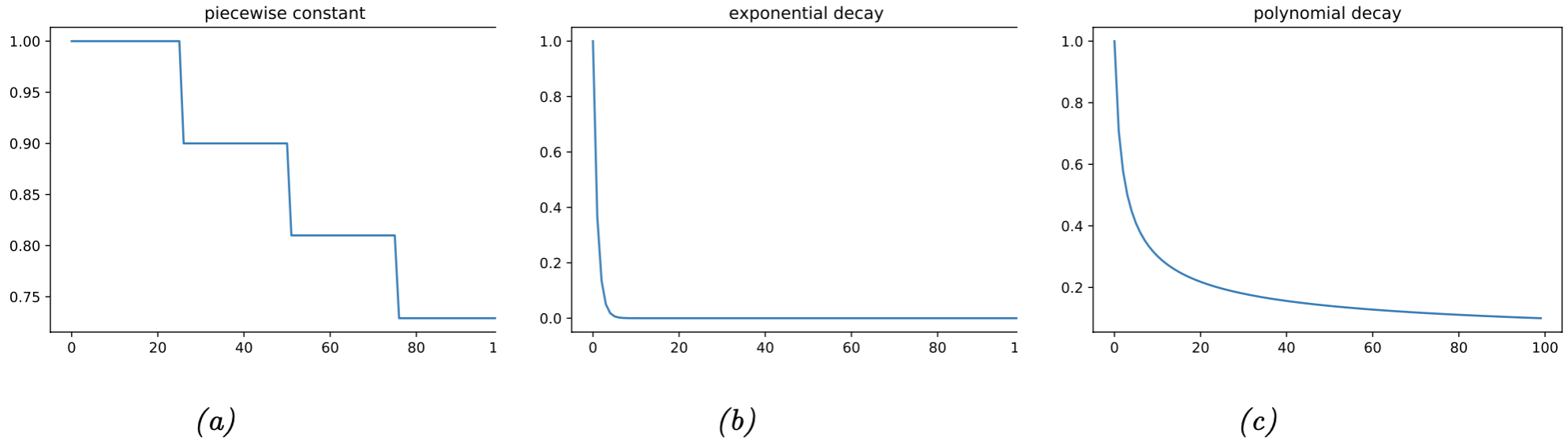
- **mini-batch**: randomly sample a batch of examples to form a stochastic gradient (common batch size: 32, 64, 128, etc.)

- **adaptive learning rate tuning**: choose a different learning rate for each parameter (and vary this across iterations), based on the magnitude of previous gradients for that parameter (used in Adagrad, RMSProp)

Adaptive learning rate tuning

``The learning rate is perhaps the most important hyperparameter.
If you have time to tune only one hyperparameter, tune the learning rate."
-Deep learning (Book by Goodfellow, Bengio, Courville)

We often use a **learning rate schedule**.



Some common learning rate schedules (figure from PML)

Adaptive learning rate methods (Adagrad, RMSProp) scale the learning rate of each parameter based on some moving average of the magnitude of the gradients.

Optimization: Variants on SGD

- **mini-batch**: randomly sample a batch of examples to form a stochastic gradient (common batch size: 32, 64, 128, etc.)

- **adaptive learning rate tuning**: choose a different learning rate for each parameter (and vary this across iterations), based on the magnitude of previous gradients for that parameter (used in Adagrad, RMSProp)

- **momentum**: add a "momentum" term to encourage model to continue along previous gradient direction

Momentum

"move faster along directions that were previously good, and to slow down along directions where the gradient has suddenly changed, just like a ball rolling downhill." [PML]

Initialize $\boldsymbol{w}_0$ and (velocity) $\boldsymbol{v} = \mathbf{0}$

For $t = 1, 2, \ldots$

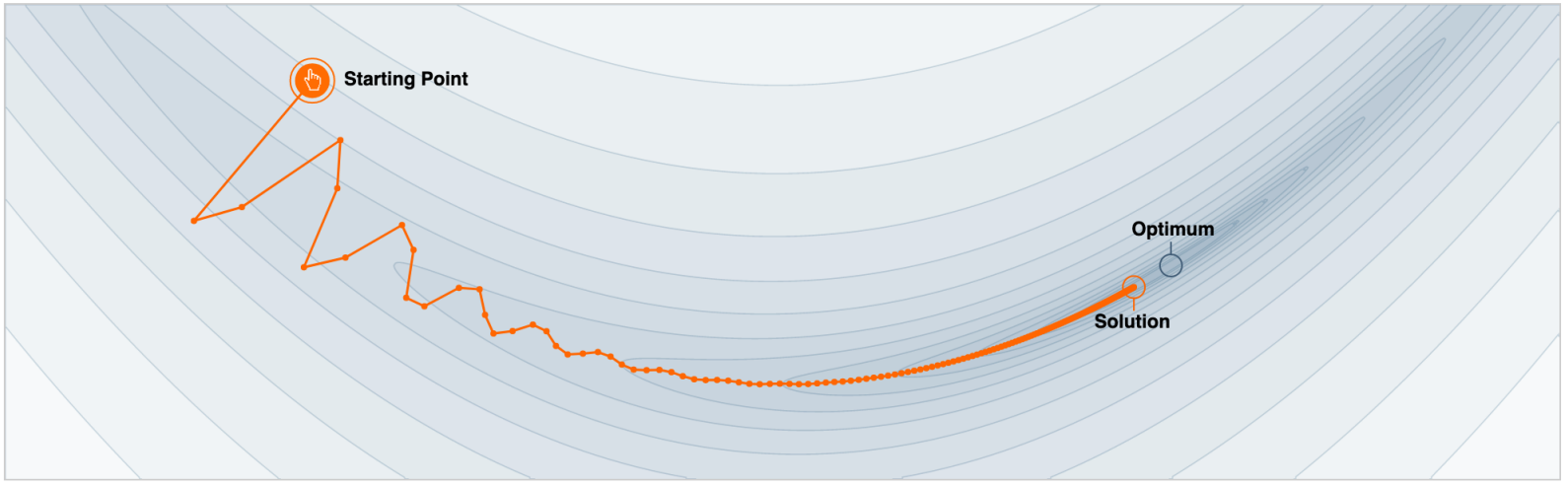
- estimate a stochastic gradient $\boldsymbol{g}_t$
- update $\boldsymbol{v} \leftarrow \alpha \boldsymbol{v} + \boldsymbol{g}_t$ for some discount factor $\alpha \in (0, 1)$
- update weight $\boldsymbol{w}_t \leftarrow \boldsymbol{w}_{t-1} - \eta \boldsymbol{v}$

Updates for first few rounds:

- $\boldsymbol{w}_1 = \boldsymbol{w}_0 - \eta \boldsymbol{g}_1$
- $\boldsymbol{w}_2 = \boldsymbol{w}_1 - \alpha\eta \boldsymbol{g}_1 - \eta \boldsymbol{g}_2$
- $\boldsymbol{w}_3 = \boldsymbol{w}_2 - \alpha^2\eta \boldsymbol{g}_1 - \alpha\eta \boldsymbol{g}_2 - \eta \boldsymbol{g}_3$
- $\ldots$

Momentum

Why Momentum Really Works



Step-size α = 0.02

0 0.003 0.006

Momentum β = 0.99

0.00 0.500 0.990

We often think of Momentum as a means of dampening oscillations and speeding up the iterations, leading to faster convergence. But it has other interesting behavior. It allows a larger range of step-sizes to be used, and creates its own oscillations. What is going on?

GABRIEL GOH
UC Davis

April. 4
2017

Citation:
Goh, 2017

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

Optimization: Variants on SGD

- **mini-batch**: randomly sample a batch of examples to form a stochastic gradient (common batch size: 32, 64, 128, etc.)

- **adaptive learning rate tuning**: choose a different learning rate for each parameter (and vary this across iterations), based on the magnitude of previous gradients for that parameter (used in Adagrad, RMSProp)

- **momentum**: add a "momentum" term to encourage model to continue along previous gradient direction

- Many other variants and tricks such as **batch normalization**: normalize the inputs of each layer over the mini-batch (to zero-mean and unit-variance; like we did in HW1)

3.3 Generalization: Preventing Overfitting

Overfitting can be a major concern since neural nets are very powerful.

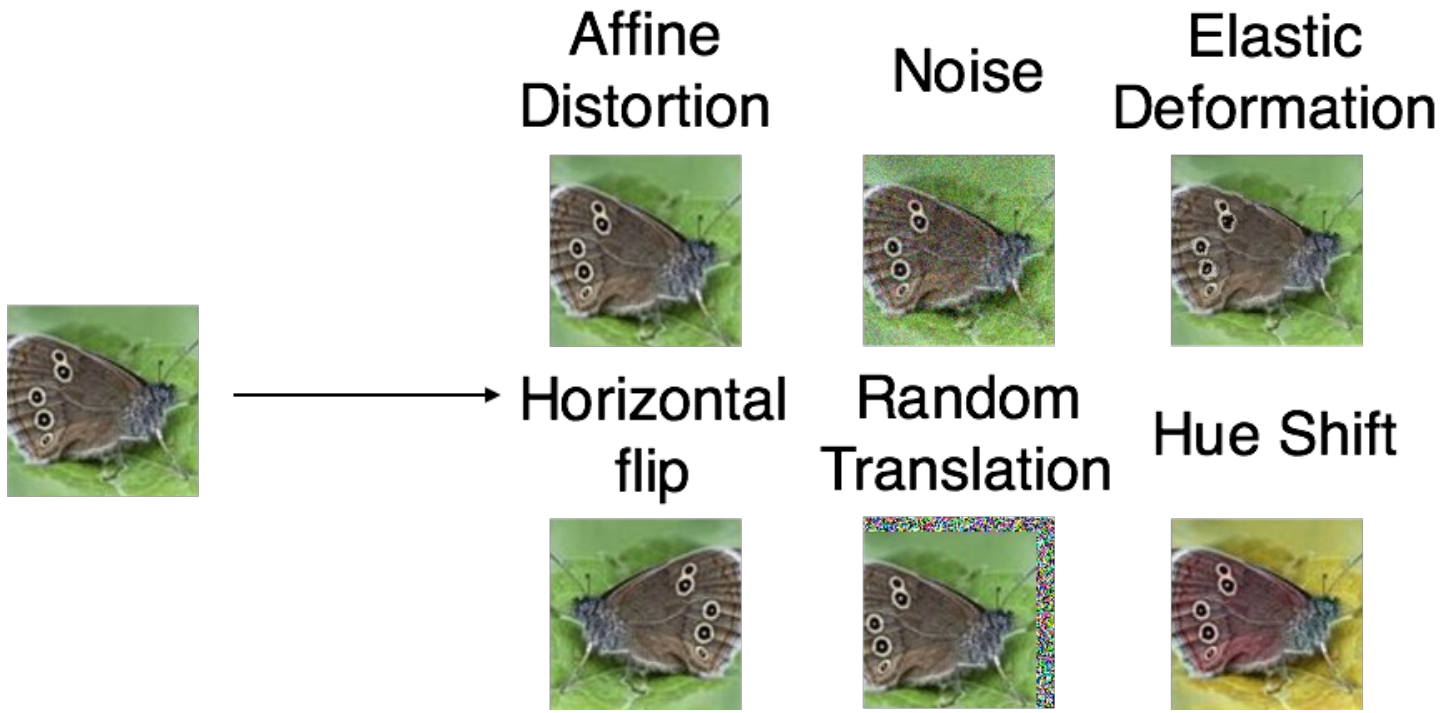
Methods to overcome overfitting:

- data augmentation
- regularization
- dropout
- early stopping
- . . .

Preventing overfitting: Data augmentation

The best way to prevent overfitting? Get more samples.
What if you cannot get access to more samples?

Exploit prior knowledge to add more training data:

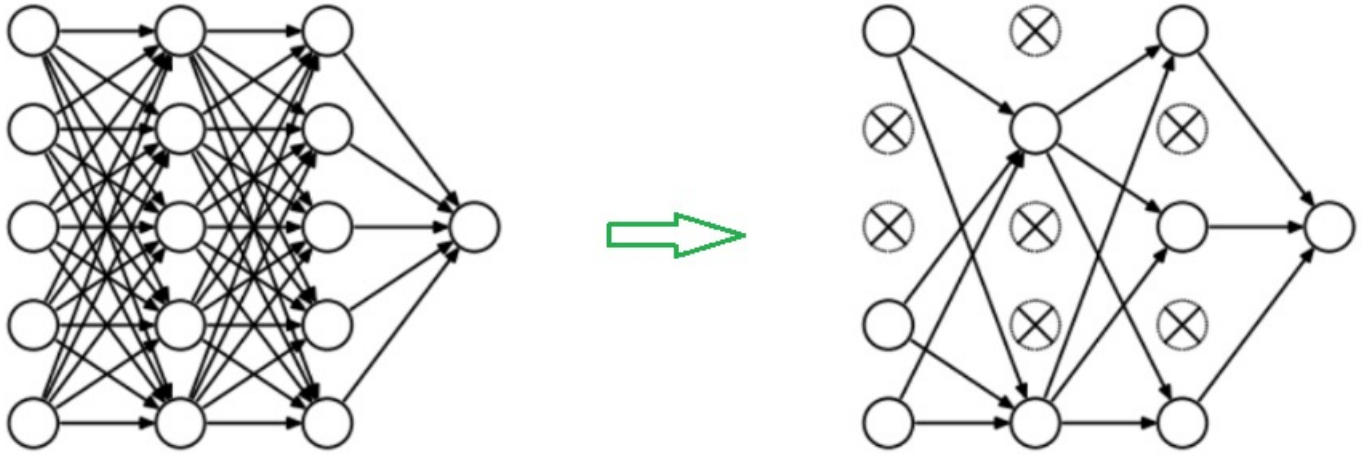


Preventing overfitting: Regularization & Dropout

We can use regularization techniques such as ℓ_2 regularization.
ℓ_2 regularization: minimize

$$G(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_L) = F(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_L) + \lambda \sum_{\substack{\text{all weights } w \\ \text{in network}}} w^2$$

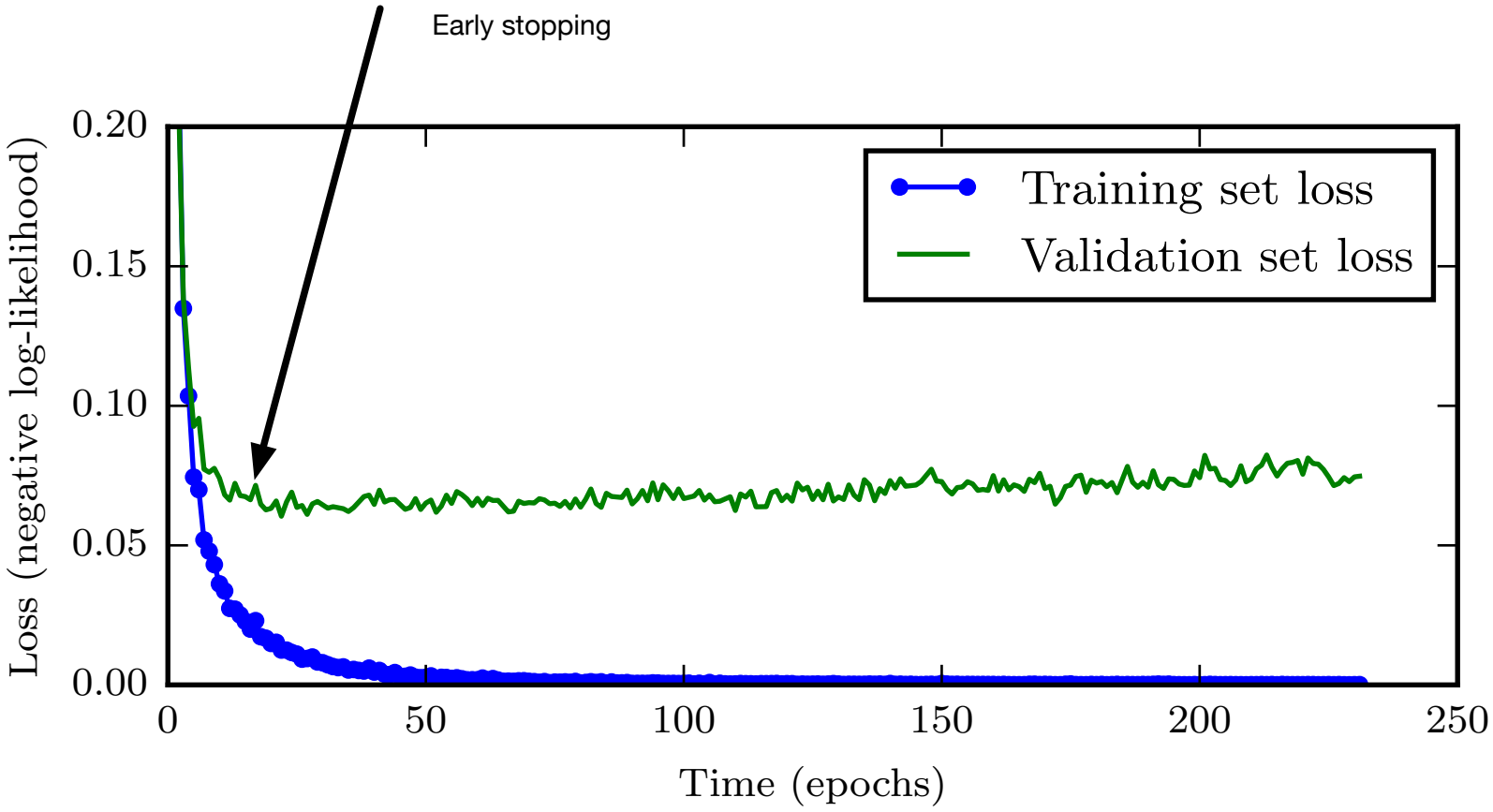
A very popular technique is **Dropout**. Here, we *independently delete each neuron* with a fixed probability (say 0.1), during each iteration of Backprop (only for training, not for testing)



Very effective and popular in practice!

Preventing overfitting: Early stopping

Stop training when the performance on validation set stops improving



There are **big mysteries** about how and why deep learning works

- Why are certain architectures better for certain problems? How should we design architectures?
- Why do gradient-based methods work on these highly-nonconvex problems?
- Why can deep networks generalize well despite having the capacity to so easily overfit?
- What implicit regularization effects do gradient-based methods provide?
- …

Picture credit: NASA/JPL-Caltech

Neural networks: Summary

Deep neural networks

- are hugely popular, achieving *best performance* on many problems
- do need *a lot of data* to work well
- can take *a lot of time* to train (need GPUs for massive parallel computing)
- take some work to select architecture and hyperparameters
- are still not well understood in theory