Fields Machine Learning Course
Lecture 1: Basic Concepts

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Overview

- Today's lecture: some key concepts used throughout the course
  - Linear regression and classification
  - Gradient descent
  - Multilayer perceptrons
  - Backpropagation
- If you have taken CSC411/2515 or CSC321/421/2516, you can skip today's lecture since it's all review.

What is machine learning?

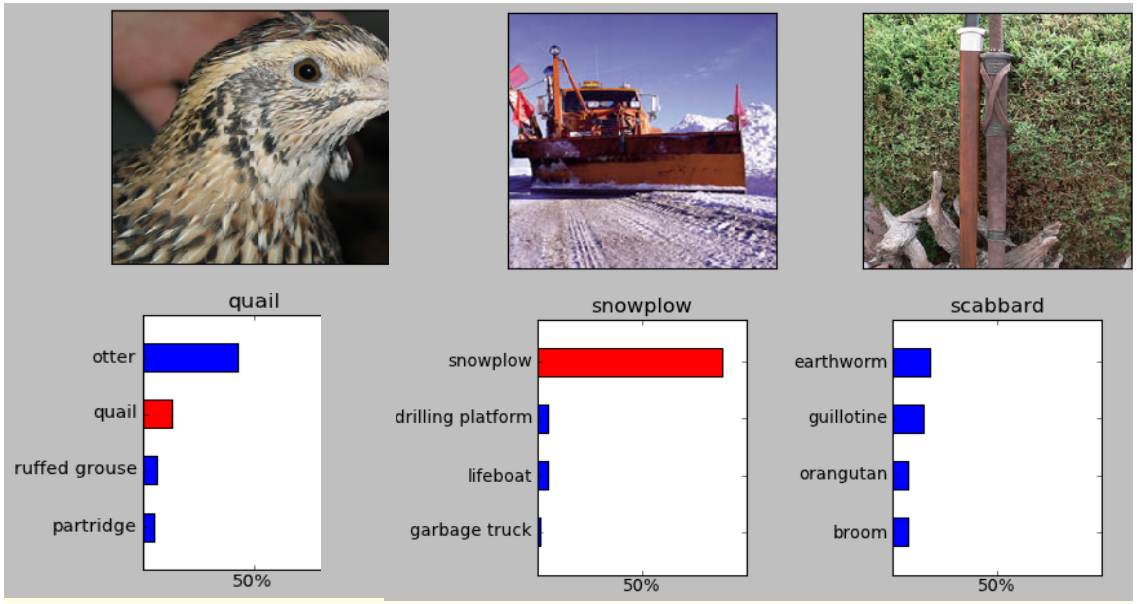
- For many problems, it's difficult to program the correct behavior by hand
  - recognizing people and objects
  - understanding human speech
- Machine learning approach: program an algorithm to automatically learn from data, or from experience
- Some reasons you might want to use a learning algorithm:
  - hard to code up a solution by hand (e.g. vision, speech)
  - system needs to adapt to a changing environment (e.g. spam detection)
  - want the system to perform *better* than the human programmers
  - privacy/fairness (e.g. ranking search results)

What is machine learning?

- Types of machine learning
  - **Supervised learning:** have labeled examples of the correct behavior
  - **Reinforcement learning:** learning system receives a reward signal, tries to learn to maximize the reward signal
  - **Unsupervised learning:** no labeled examples – instead, looking for interesting patterns in the data

Supervised learning examples

Object recognition



(Krizhevsky and Hinton, 2012)

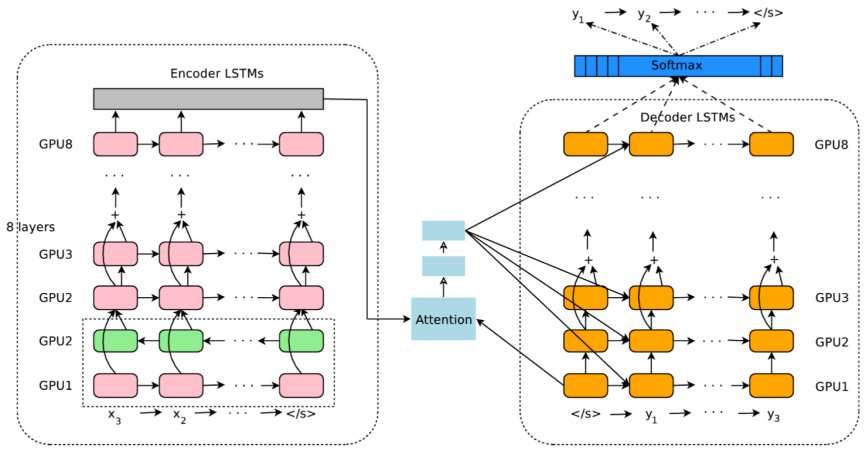
ImageNet dataset: thousands of categories, millions of labeled images

Lots of variability in viewpoint, lighting, etc.

Error rate dropped from 26% to under 4% over the course of a few years!

Supervised learning examples

Neural Machine Translation



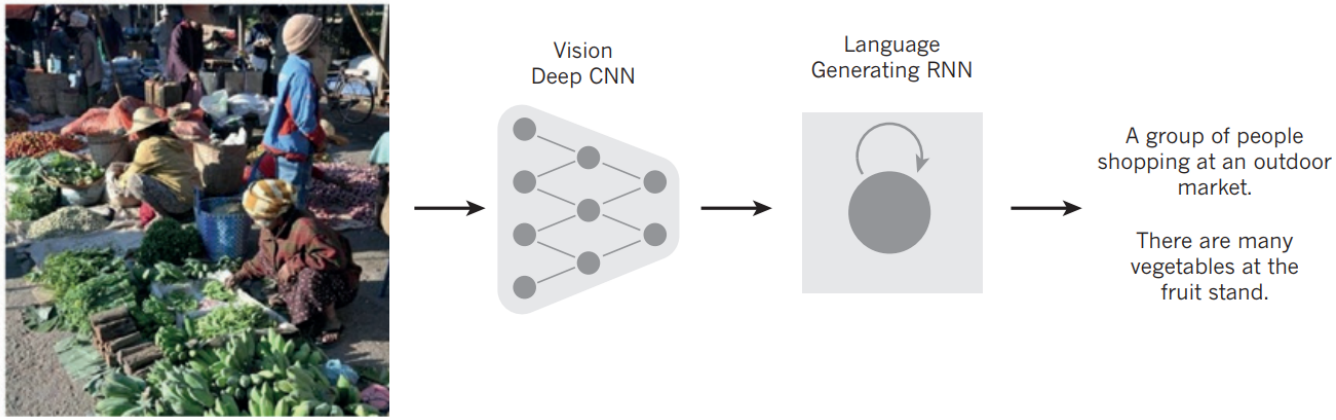
(Wu et al., 2016)

Input sentence:	*Translation (PBMT):*	*Translation (GNMT):*	*Translation (human):*
李克強此行將啟動中加總理年度對話機制，與加拿大總理杜魯多舉行兩國總理首次年度對話。	Li Keqiang premier added this line to start the annual dialogue mechanism with the Canadian Prime Minister Trudeau two prime ministers held its first annual session.	Li Keqiang will start the annual dialogue mechanism with Prime Minister Trudeau of Canada and hold the first annual dialogue between the two premiers.	Li Keqiang will initiate the annual dialogue mechanism between premiers of China and Canada during this visit, and hold the first annual dialogue with Premier Trudeau of Canada.

Now the production model on Google Translate

Supervised learning examples

Caption generation



A woman is throwing a **frisbee** in a park.

A **dog** is standing on a hardwood floor.

A **stop** sign is on a road with a mountain in the background

(Xu et al., 2015)

Given: dataset of Flickr images with captions

More examples at `http://deeplearning.cs.toronto.edu/i2t`

Unsupervised learning examples

- In **generative modeling**, we want to learn a distribution over some dataset, such as natural images.
- We can evaluate a generative model by sampling from the model and seeing if it looks like the data.
- These results were considered impressive in 2014:

Denton et al., 2014, Deep generative image models using a Laplacian pyramid of adversarial networks

Unsupervised learning examples

- Fast-forward to 2017:

Unsupervised learning examples

- Recent exciting result: a model called the CycleGAN takes lots of images of one category (e.g. horses) and lots of images of another category (e.g. zebras) and learns to translate between them.

https://github.com/junyanz/CycleGAN

Reinforcement learning

- An **agent** interacts with an **environment** (e.g. game of Breakout)
- In each time step,
  - the agent receives **observations** (e.g. pixels) which give it information about the **state** (e.g. positions of the ball and paddle)
  - the agent picks an **action** (e.g. keystrokes) which affects the state
- The agent periodically receives a **reward** (e.g. points)
- The agent wants to learn a **policy**, or mapping from observations to actions, which maximizes its average reward over time

Reinforcement learning

DeepMind trained neural networks to play many different Atari games

- given the raw screen as input, plus the score as a reward
- single network architecture shared between all the games
- in many cases, the networks learned to play better than humans (in terms of points in the first minute)

`https://www.youtube.com/watch?v=V1eYniJ0Rnk`

Reinforcement learning for control

Learning locomotion control from scratch

- The reward is to run as far as possible over all the obstacles
- single control policy that learns to adapt to different terrains

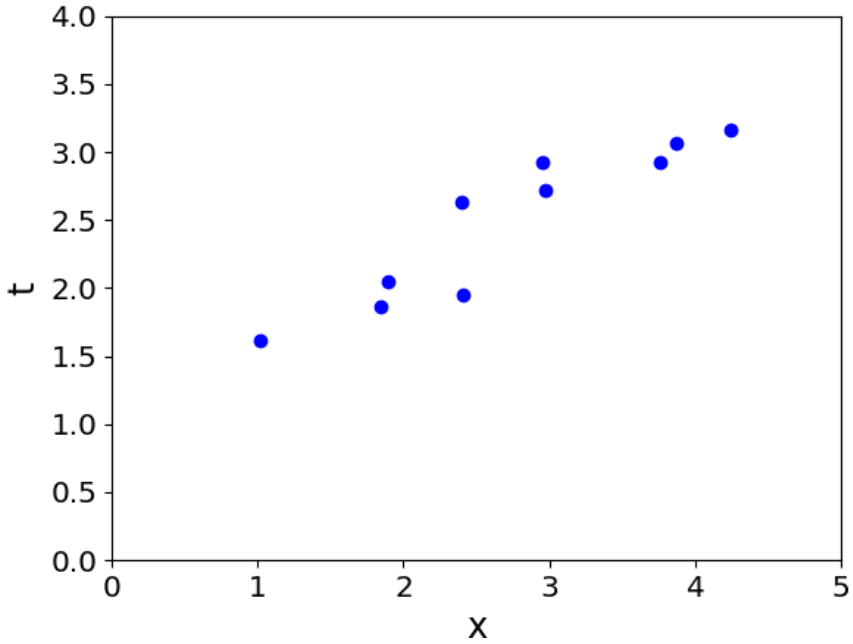
`https://www.youtube.com/watch?v=hx_bgoTF7bs`

Linear Models

Overview

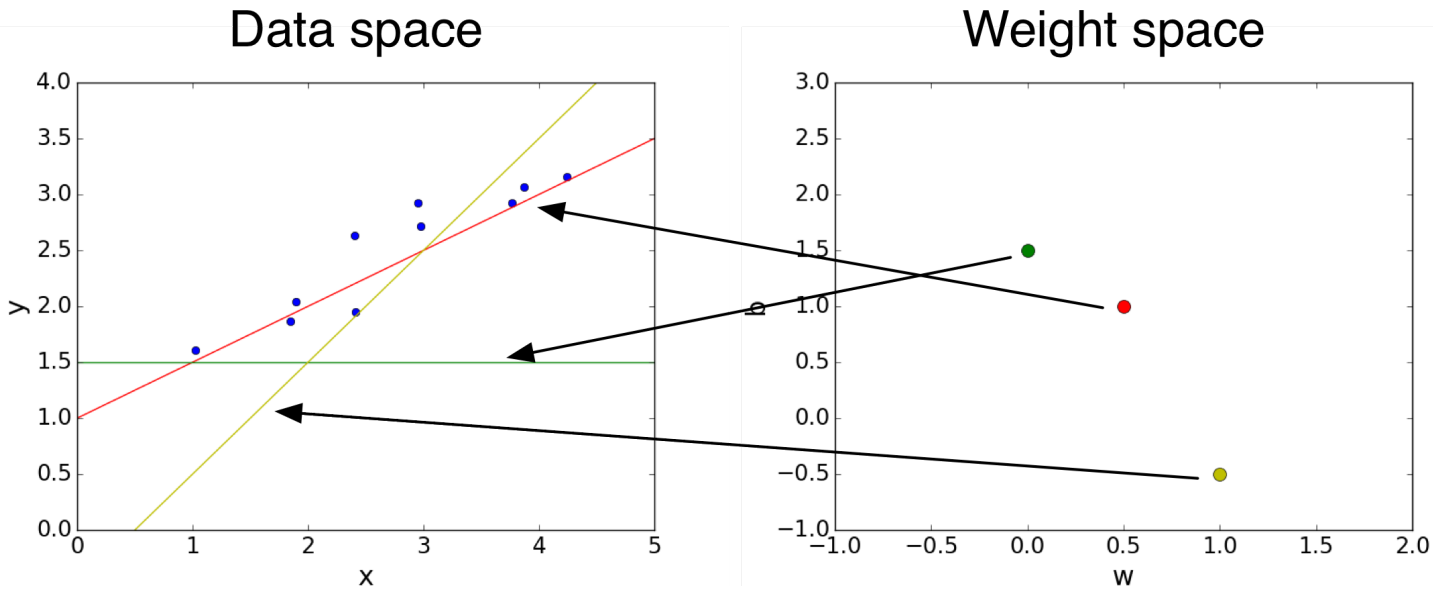
- Some canonical supervised learning problems:
  - Regression: predict a scalar-valued target (e.g. stock price)
  - Binary classification: predict a binary label (e.g. spam vs. non-spam email)
  - Multiway classification: predict a discrete label (e.g. object category, from a list)
- A simple approach is a linear model, where you decide based on a linear function of the input vector.

Problem Setup



- Want to predict a scalar t as a function of a vector $\mathbf{x}$
- Given a dataset of pairs $\{(\mathbf{x}^{(i)}, t^{(i)})\}_{i=1}^{N}$
- The $\mathbf{x}^{(i)}$ are called input vectors, and the $t^{(i)}$ are called targets.

Problem Setup



- **Model:** y is a linear function of x:

$$y = \mathbf{w}^\top \mathbf{x} + b$$

- y is the prediction
- $\mathbf{w}$ is the weight vector
- b is the bias
- $\mathbf{w}$ and b together are the parameters
- Settings of the parameters are called hypotheses

Problem Setup

- **Loss function:** squared error

$$\mathcal{L}(y, t) = \frac{1}{2}(y - t)^2$$

- $y - t$ is the residual, and we want to make this small in magnitude
- The $\frac{1}{2}$ factor is just to make the calculations convenient.

Problem Setup

- **Loss function:** squared error

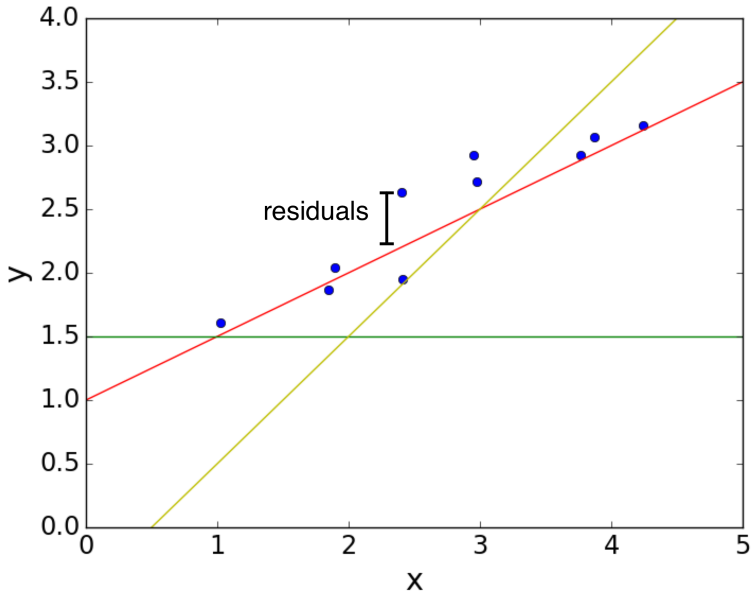
$$\mathcal{L}(y, t) = \frac{1}{2}(y - t)^2$$

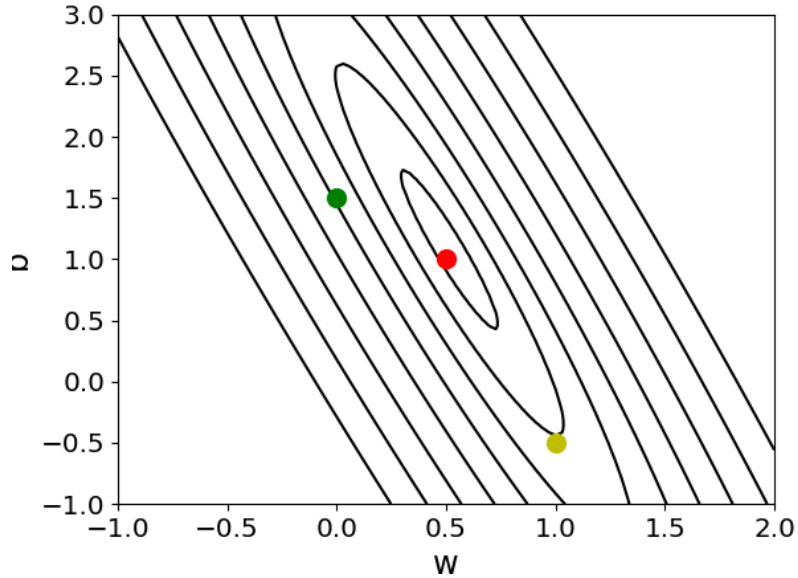
- $y - t$ is the residual, and we want to make this small in magnitude
- The $\frac{1}{2}$ factor is just to make the calculations convenient.
- **Cost function:** loss function averaged over all training examples

$$\begin{aligned}\mathcal{J}(w, b) &= \frac{1}{2N}\sum_{i=1}^{N}\left(y^{(i)} - t^{(i)}\right)^2 \\ &= \frac{1}{2N}\sum_{i=1}^{N}\left(\mathbf{w}^\top \mathbf{x}^{(i)} + b - t^{(i)}\right)^2\end{aligned}$$

Problem Setup

Visualizing the contours of the cost function:





Vectorization

- We can organize all the training examples into a matrix $\mathbf{X}$ with one row per training example, and all the targets into a vector $\mathbf{t}$.

one feature across all training examples

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}^{(1)\top} \\ \mathbf{x}^{(2)\top} \\ \mathbf{x}^{(3)\top} \end{pmatrix} = \begin{pmatrix} 8 & 0 & 3 & 0 \\ 6 & -1 & 5 & 3 \\ 2 & 5 & -2 & 8 \end{pmatrix}$$

one training example (vector)

- Computing the predictions for the whole dataset:

$$\mathbf{X}\mathbf{w} + b\mathbf{1} = \begin{pmatrix} \mathbf{w}^\top \mathbf{x}^{(1)} + b \\ \vdots \\ \mathbf{w}^\top \mathbf{x}^{(N)} + b \end{pmatrix} = \begin{pmatrix} y^{(1)} \\ \vdots \\ y^{(N)} \end{pmatrix} = \mathbf{y}$$

Vectorization

- Computing the squared error cost across the whole dataset:

$$\mathbf{y} = \mathbf{X}\mathbf{w} + b\mathbf{1}$$

$$\mathcal{J} = \frac{1}{2N}\|\mathbf{y} - \mathbf{t}\|^2$$

- In Python:

```
y = np.dot(X, w) + b
cost = np.sum((y - t) ** 2) / (2. * N)
```

Solving the optimization problem

- We defined a cost function. This is what we'd like to minimize.
- Recall from calculus class: the minimum of a smooth function (if it exists) occurs at a critical point, i.e. point where the partial derivatives are all 0.
- Two strategies for optimization:
  - Direct solution: derive a formula that sets the partial derivatives to 0. This works only in a handful of cases (e.g. linear regression).
  - Iterative methods (e.g. gradient descent): repeatedly apply an update rule which slightly improves the current solution. This is how the vast majority of machine learning models are trained.

Computing partial derivatives

- Partial derivatives: derivatives of a multivariate function with respect to one of its arguments.

$$\frac{\partial}{\partial x_1} f(x_1, x_2) = \lim_{h \to 0} \frac{f(x_1 + h, x_2) - f(x_1, x_2)}{h}$$

- To compute, take the single variable derivatives, pretending the other arguments are constant.
- Example: partial derivatives of the prediction y

$$\begin{aligned}
\frac{\partial y}{\partial w_j} &= \frac{\partial}{\partial w_j} \left[\sum_{j'} w_{j'} x_{j'} + b \right] \\
&= x_j \\
\frac{\partial y}{\partial b} &= \frac{\partial}{\partial b} \left[\sum_{j'} w_{j'} x_{j'} + b \right] \\
&= 1
\end{aligned}$$

Computing partial derivatives

- Chain rule for derivatives:

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial w_j} &= \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y}\frac{\partial y}{\partial w_j} \\ &= \frac{\mathrm{d}}{\mathrm{d}y}\left[\frac{1}{2}(y-t)^2\right] \cdot x_j \\ &= (y-t)x_j \\ \frac{\partial \mathcal{L}}{\partial b} &= y - t\end{aligned}$$

- We will give a more precise statement of the Chain Rule later in this lecture. It's actually pretty complicated.
- Cost derivatives (average over data points):

$$\frac{\partial \mathcal{J}}{\partial w_j} = \frac{1}{N}\sum_{i=1}^{N}(y^{(i)} - t^{(i)})\, x_j^{(i)}$$

$$\frac{\partial \mathcal{J}}{\partial b} = \frac{1}{N}\sum_{i=1}^{N} y^{(i)} - t^{(i)}$$

Direct solution

- The minimum must occur at a point where the partial derivatives are zero.

$$\frac{\partial \mathcal{J}}{\partial w_j} = 0 \qquad \frac{\partial \mathcal{J}}{\partial b} = 0.$$

- If $\partial \mathcal{J} / \partial w_j \neq 0$, you could reduce the cost by changing w_j.
- This turns out to give a system of linear equations, which we can solve efficiently.
- Optimal weights:

$$\mathbf{w} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{t}$$

```
w, _ = np.linalg.lstsq(X, t)
```

- Linear regression is one of only a handful of models in this course that permit direct solution.

Gradient descent

- Gradient descent is an iterative algorithm, which means we apply an update repeatedly until some criterion is met.
- We initialize the weights to something reasonable (e.g. all zeros) and repeatedly adjust them in the direction of steepest descent.
- The gradient descent update decreases the cost function for small enough α:

$$w_j \leftarrow w_j - \alpha \frac{\partial \mathcal{J}}{\partial w_j}$$

$$= w_j - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)}) \, x_j^{(i)}$$

- α is a learning rate. The larger it is, the faster $\mathbf{w}$ changes.
  - We'll see later how to tune the learning rate, but values are typically small, e.g. 0.01 or 0.0001

Gradient descent

- This gets its name from the gradient:

$$\nabla \mathcal{J}(\mathbf{w}) = \frac{\partial \mathcal{J}}{\partial \mathbf{w}} = \begin{pmatrix} \frac{\partial \mathcal{J}}{\partial w_1} \\ \vdots \\ \frac{\partial \mathcal{J}}{\partial w_D} \end{pmatrix}$$

  - This is the direction of fastest increase in $\mathcal{J}$.

Gradient descent

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  - This is the direction of fastest increase in $\mathcal{J}$.
- Update rule in vector form:

$$\begin{aligned} \mathbf{w} &\leftarrow \mathbf{w} - \alpha \nabla \mathcal{J}(\mathbf{w}) \\ &= \mathbf{w} - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)}) \, \mathbf{x}^{(i)} \end{aligned}$$

- Hence, gradient descent updates the weights in the direction of fastest *decrease*.

Gradient descent

Visualization:
http://www.cs.toronto.edu/~guerzhoy/321/lec/W01/linear_regression.pdf#page=21

Gradient descent

- Why gradient descent, if we can find the optimum directly?
  - GD can be applied to a much broader set of models
  - GD can be easier to implement than direct solution, especially with automatic differentiation software
  - For regression in high-dimensional spaces, GD is more efficient than direct solution (matrix inversion is an $\mathcal{O}(D^3)$ algorithm).

Feature maps

- We can convert linear models into nonlinear models using feature maps.

$$y = \mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x})$$

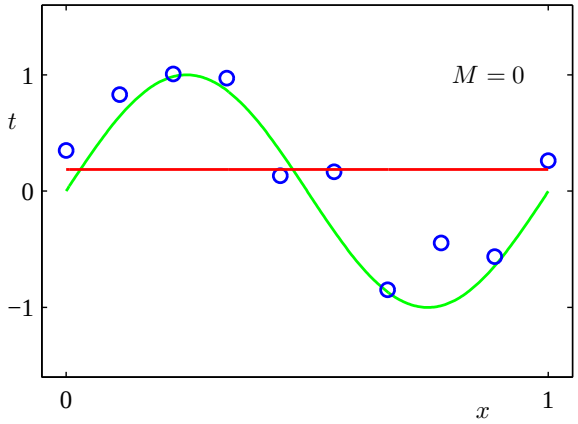
- E.g., if $\boldsymbol{\psi}(x) = (1,\ x,\ \cdots, x^D)^\top$, then y is a polynomial in x. This model is known as polynomial regression:

$$y = w_0 + w_1 x + \cdots + w_D x^D$$

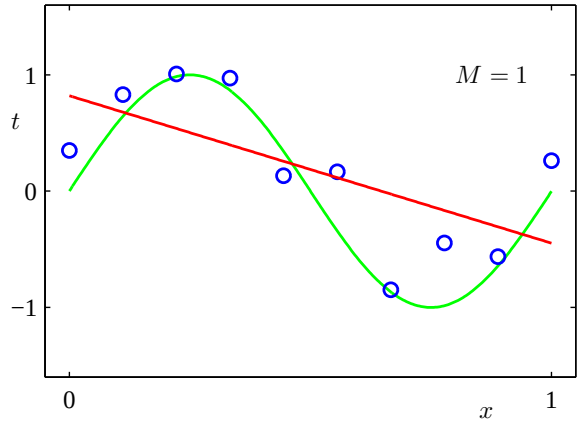
- This doesn't require changing the algorithm — just pretend $\boldsymbol{\psi}(x)$ is the input vector.
- We don't need an expicit bias term, since it can be absorbed into $\boldsymbol{\psi}$.
- Feature maps let us fit nonlinear models, but it can be hard to choose good features.
  - Before deep learning, most of the effort in building a practical machine learning system was feature engineering.

Feature maps

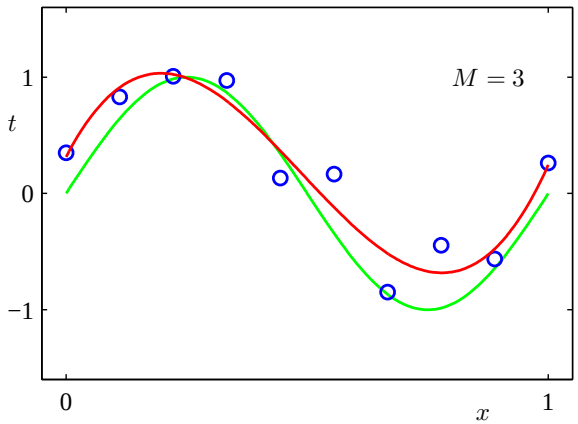
$y = w_0$



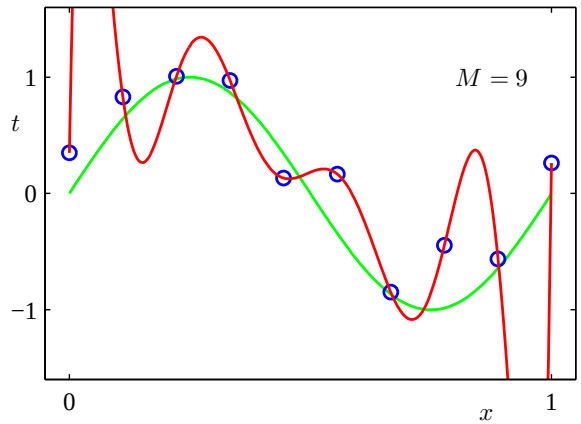
$y = w_0 + w_1 x$



$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$



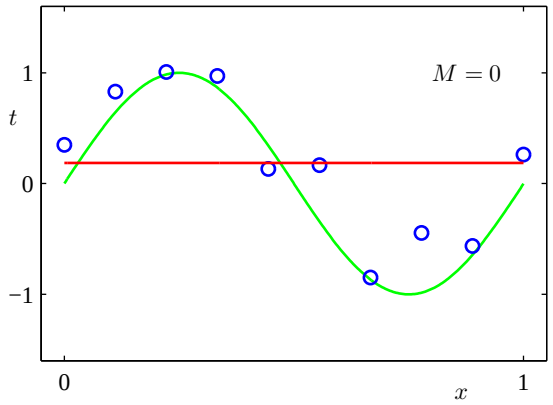
$y = w_0 + w_1 x + \cdots + w_9 x^9$



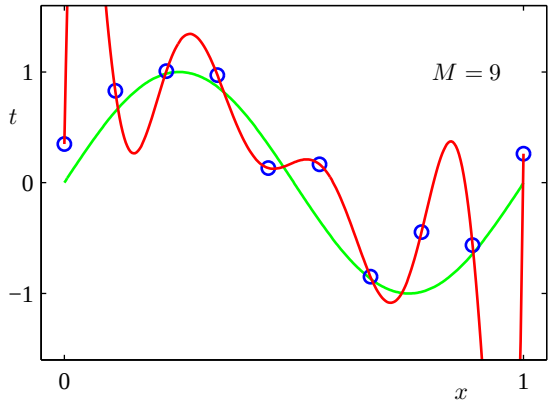
-Pattern Recognition and Machine Learning, Christopher Bishop.

Generalization

Underfitting : The model is too simple - does not fit the data.

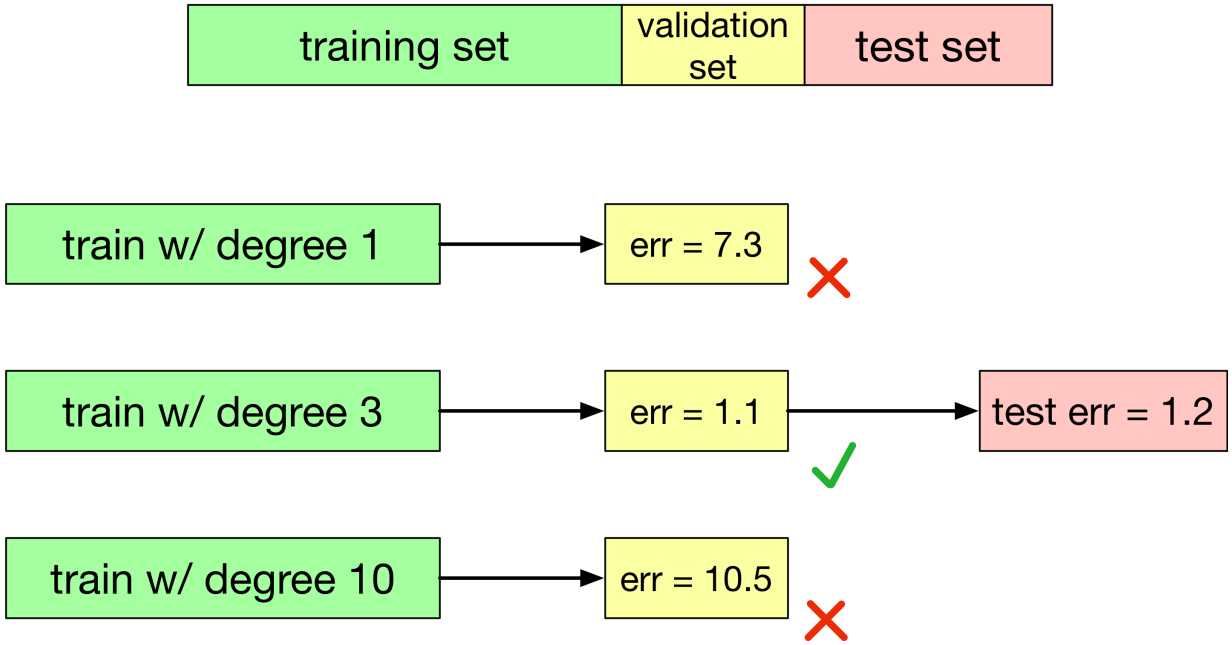


Overfitting : The model is too complex - fits perfectly, does not generalize.



Generalization

- We would like our models to generalize to data they haven't seen before
- The degree of the polynomial is an example of a hyperparameter, something we can't include in the training procedure itself
- We can tune hyperparameters using a validation set:



Linear Classification

Classification

Binary linear classification

- **classification:** predict a discrete-valued target
- **binary:** predict a binary target $t \in \{0, 1\}$
  - Training examples with $t = 1$ are called positive examples, and training examples with $t = 0$ are called negative examples. Sorry.
- **linear:** model is a linear function of $\mathbf{x}$, thresholded at zero:

$$z = \mathbf{w}^T \mathbf{x} + b$$

$$\text{output} = \begin{cases} 1 & \text{if } z \geq 0 \\ 0 & \text{if } z < 0 \end{cases}$$

Logistic Regression

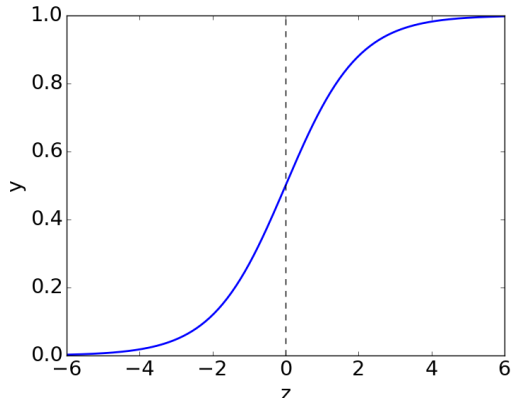
- We can't optimize classification accuracy directly with gradient descent because it's discontinuous.
- Instead, we typically define a continuous surrogate loss function which is easier to optimize. Logistic regression is a canonical example of this, in the context of classification.
- The model outputs a continuous value $y \in [0, 1]$, which you can think of as the probability of the example being positive.

Logistic Regression

- There's obviously no reason to predict values outside [0, 1]. Let's squash y into this interval.

- The logistic function is a kind of sigmoidal, or S-shaped, function:

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$



- A linear model with a logistic nonlinearity is known as log-linear:

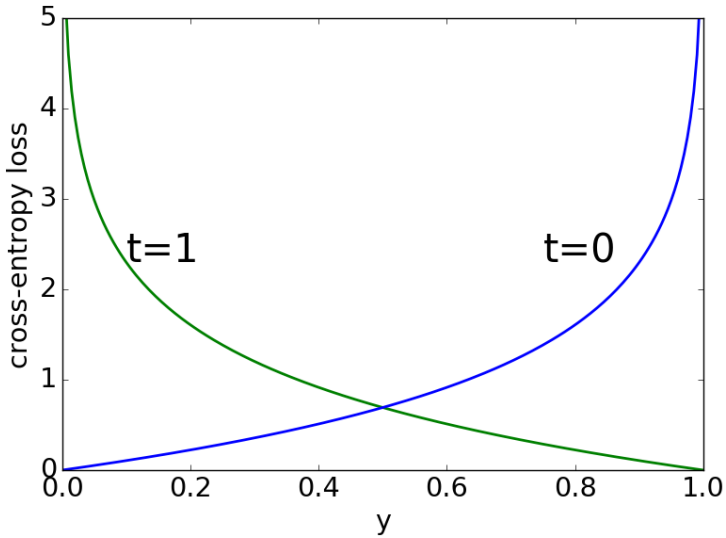
$$z = \mathbf{w}^\top \mathbf{x} + b$$
$$y = \sigma(z)$$

- Used in this way, σ is called an activation function, and z is called the logit.

Logistic Regression

- Because $y \in [0, 1]$, we can interpret it as the estimated probability that $t = 1$.
- Being 99% confident of the wrong answer is much worse than being 90% confident of the wrong answer. Cross-entropy loss captures this intuition:

$$\begin{aligned}\mathcal{L}_{\text{CE}}(y, t) &= \begin{cases} -\log y & \text{if } t = 1 \\ -\log(1 - y) & \text{if } t = 0 \end{cases} \\ &= -t \log y - (1 - t) \log(1 - y)\end{aligned}$$

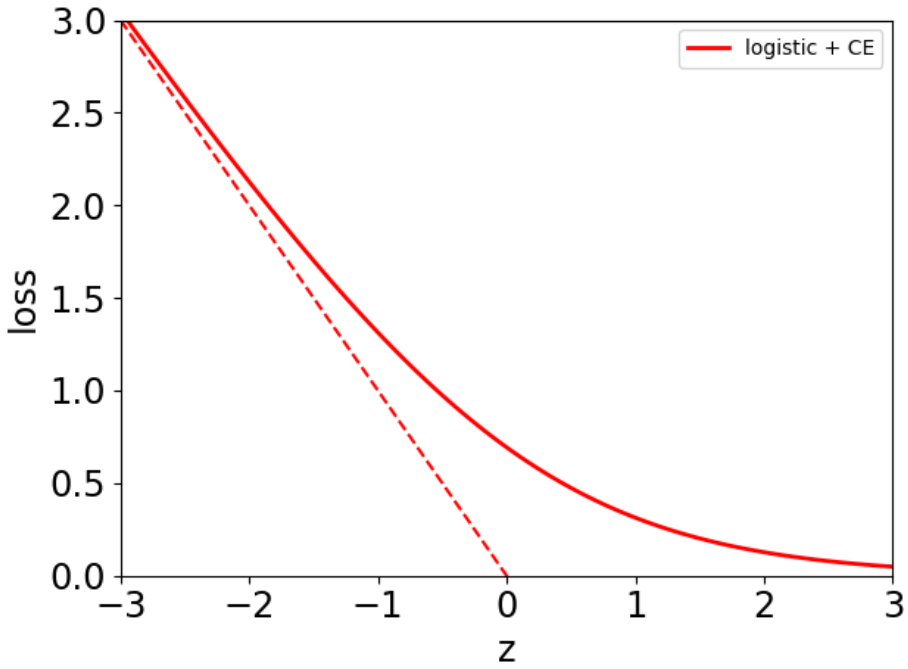


- Aside: why does it make sense to think of y as a probability? Because cross-entropy loss is a proper scoring rule, which means the optimal y is the true probability.

Logistic Regression

- Logistic regression combines the logistic activation function with cross-entropy loss.

$$
\begin{aligned}
z &= \mathbf{w}^\top \mathbf{x} + b \\
y &= \sigma(z) \\
&= \frac{1}{1 + e^{-z}} \\
\mathcal{L}_{\text{CE}} &= -t \log y - (1 - t) \log(1 - y)
\end{aligned}
$$

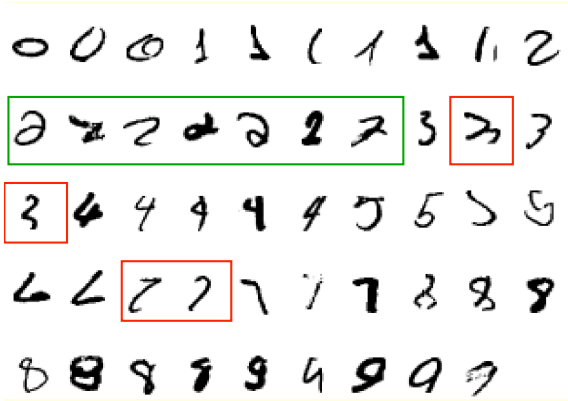


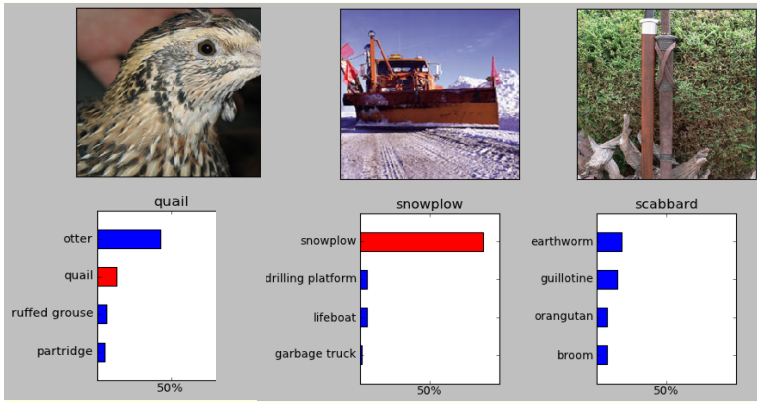
- Interestingly, the loss asymptotes to a linear function of the logit z.

Multiclass Classification

Multiclass Classification

- What about classification tasks with more than two categories?





Multiclass Classification

- Targets form a discrete set $\{1, \ldots, K\}$.
- It's often more convenient to represent them as one-hot vectors, or a one-of-K encoding:

$$\mathbf{t} = \underbrace{(0, \ldots, 0, 1, 0, \ldots, 0)}_{\text{entry } k \text{ is } 1}$$

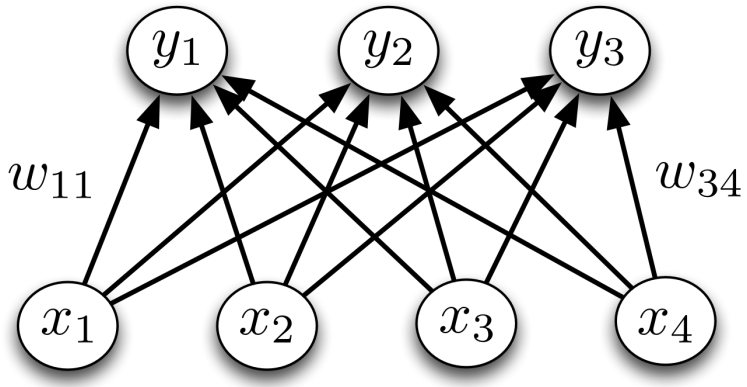
Multiclass Classification

- Now there are D input dimensions and K output dimensions, so we need $K \times D$ weights, which we arrange as a weight matrix $\mathbf{W}$.
- Also, we have a K-dimensional vector $\mathbf{b}$ of biases.
- Linear predictions:

$$z_k = \sum_j w_{kj} x_j + b_k$$

- Vectorized:

$$\mathbf{z} = \mathbf{W}\mathbf{x} + \mathbf{b}$$



Multiclass Classification

- A natural activation function to use is the softmax function, a multivariable generalization of the logistic function:

$$y_k = \mathrm{softmax}(z_1, \ldots, z_K)_k = \frac{e^{z_k}}{\sum_{k'} e^{z_{k'}}}$$

- The inputs z_k are called the logits.
- Properties:
  - Outputs are positive and sum to 1 (so they can be interpreted as probabilities)
  - If one of the z_k's is much larger than the others, $\mathrm{softmax}(\mathbf{z})$ is approximately the argmax. (So really it's more like "soft-argmax".)
  - **Exercise:** how does the case of $K = 2$ relate to the logistic function?
- Note: sometimes $\sigma(\mathbf{z})$ is used to denote the softmax function; in this class, it will denote the logistic function applied elementwise.

Multiclass Classification

- If a model outputs a vector of class probabilities, we can use cross-entropy as the loss function:

$$\begin{aligned}\mathcal{L}_{\text{CE}}(\mathbf{y}, \mathbf{t}) &= -\sum_{k=1}^{K} t_k \log y_k \\ &= -\mathbf{t}^\top (\log \mathbf{y}),\end{aligned}$$

  where the log is applied elementwise.

- Just like with logistic regression, we typically combine the softmax and cross-entropy into a softmax-cross-entropy function.

Multiclass Classification

- Softmax regression, also called multiclass logistic regression:

$$\mathbf{z} = \mathbf{W}\mathbf{x} + \mathbf{b}$$
$$\mathbf{y} = \mathrm{softmax}(\mathbf{z})$$
$$\mathcal{L}_{\mathrm{CE}} = -\mathbf{t}^\top (\log \mathbf{y})$$

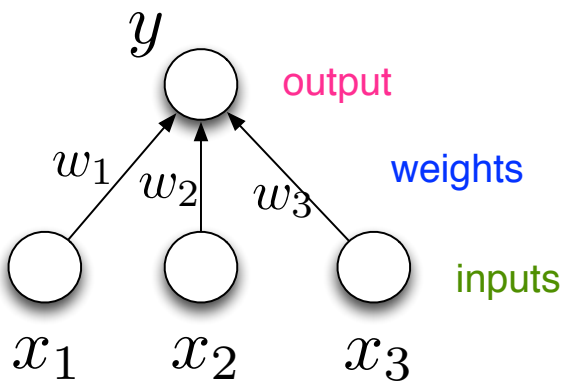
- It's possible to show the gradient descent updates have a convenient form:

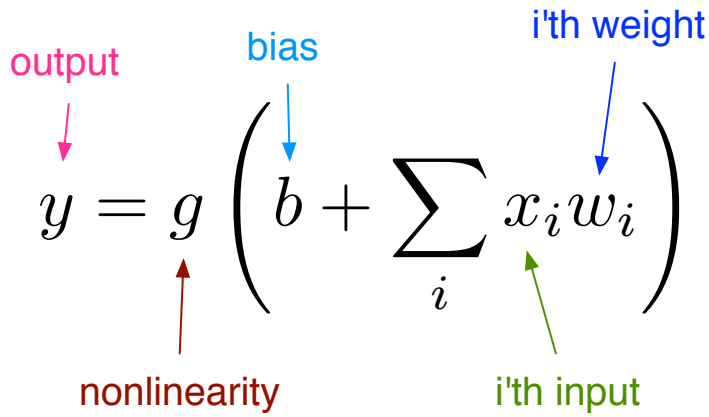
$$\frac{\partial \mathcal{L}_{\mathrm{CE}}}{\partial \mathbf{z}} = \mathbf{y} - \mathbf{t}$$

Multilayer Perceptrons

What are neural networks?

- Most of the biological details aren't essential, so we use vastly simplified models of neurons.
- While neural nets originally drew inspiration from the brain, nowadays we mostly think about math, statistics, etc.

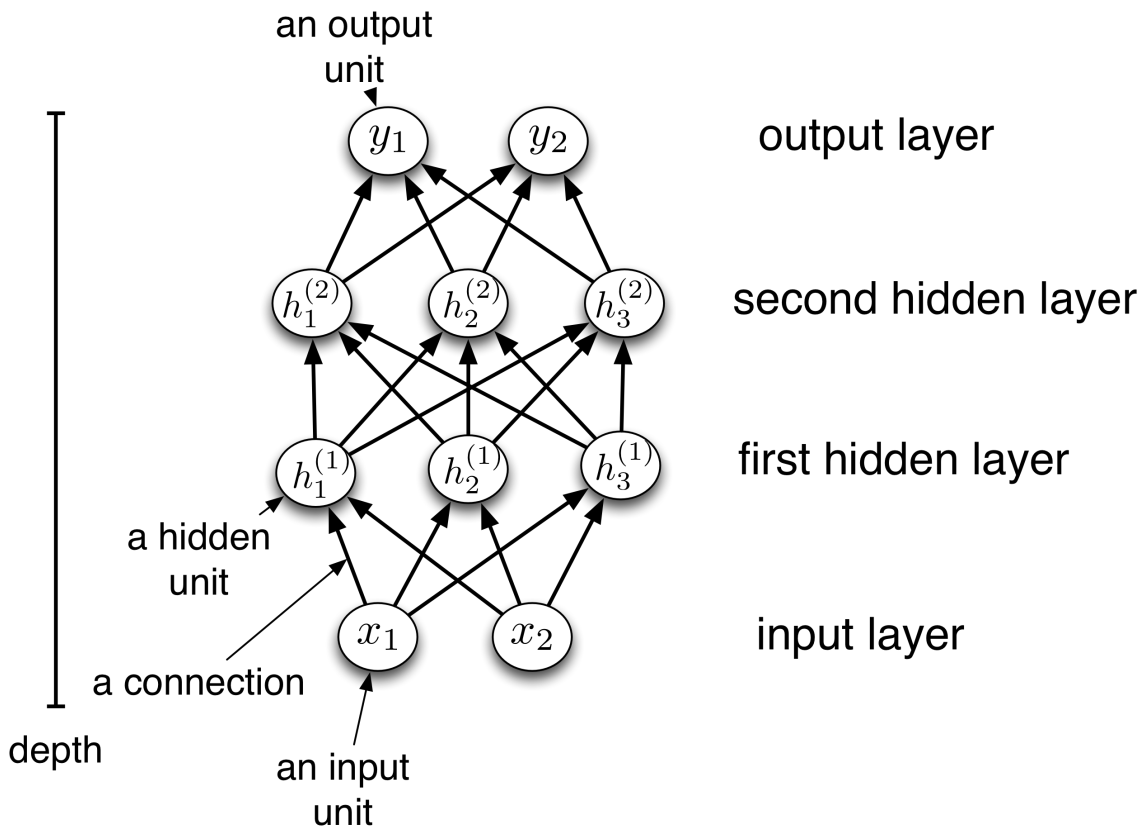




- Neural networks are collections of thousands (or millions) of these simple processing units that together perform useful computations.

Multilayer Perceptrons

- We can connect lots of units together into a directed acyclic graph.
- This gives a feed-forward neural network. That's in contrast to recurrent neural networks, which can have cycles. (We'll talk about those later.)
- Typically, units are grouped together into layers.



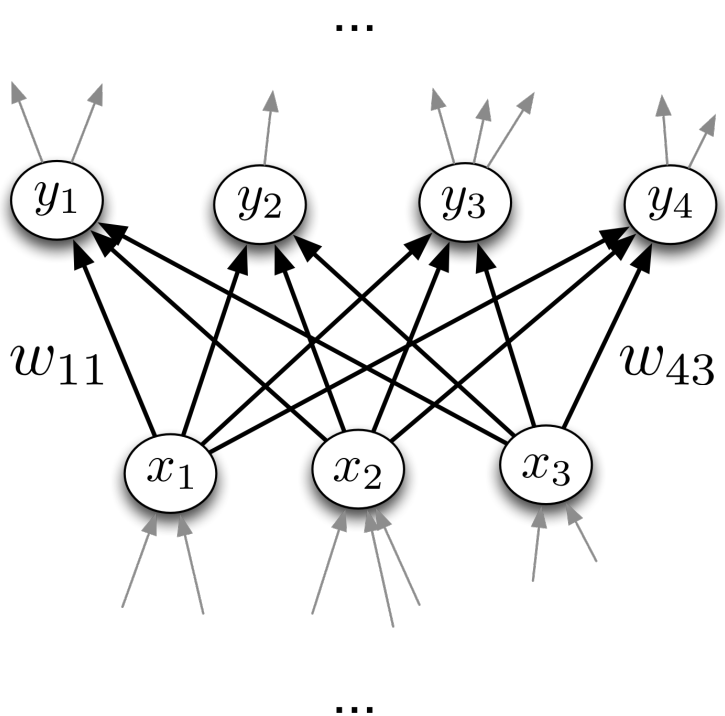
Multilayer Perceptrons

- Each layer connects N input units to M output units.
- In the simplest case, all input units are connected to all output units. We call this a fully connected layer. We'll consider other layer types later.
- Note: the inputs and outputs for a layer are distinct from the inputs and outputs to the network.

- Recall from multiway logistic regression: this means we need an $M \times N$ weight matrix.
- The output units are a function of the input units:

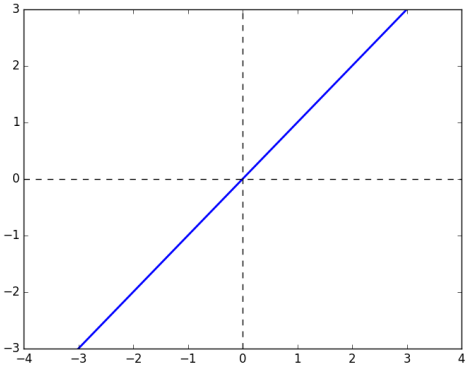
$$\mathbf{y} = f(\mathbf{x}) = \phi(\mathbf{W}\mathbf{x} + \mathbf{b})$$

- A multilayer network consisting of fully connected layers is called a multilayer perceptron. Despite the name, it has nothing to do with perceptrons!



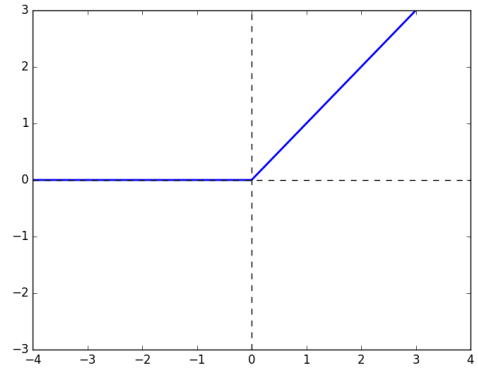
Multilayer Perceptrons

Some activation functions:



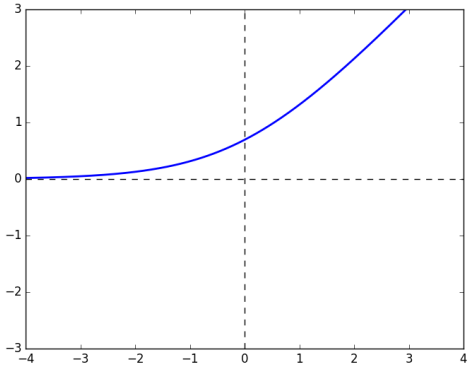
Linear

$$y = z$$



Rectified Linear Unit (ReLU)

$$y = \max(0, z)$$

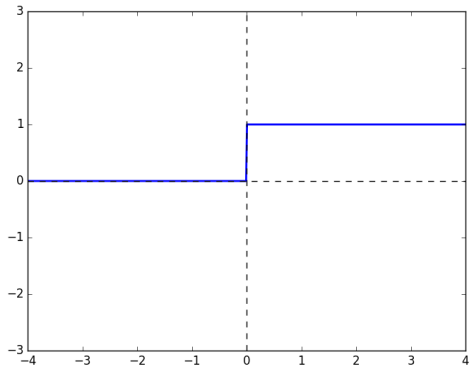


Soft ReLU

$$y = \log 1 + e^z$$

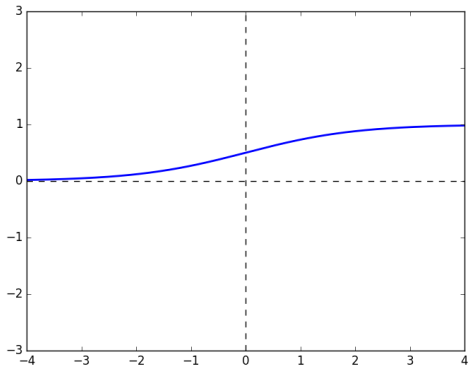
Multilayer Perceptrons

Some activation functions:



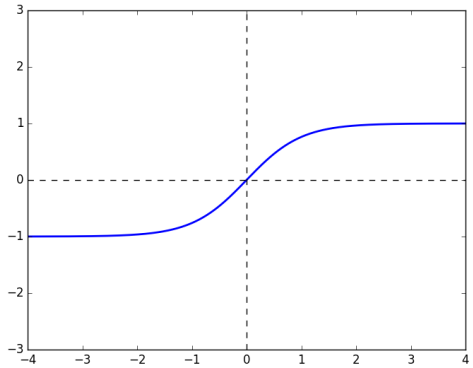
Hard Threshold

$$y = \begin{cases} 1 & \text{if } z > 0 \\ 0 & \text{if } z \leq 0 \end{cases}$$



Logistic

$$y = \frac{1}{1 + e^{-z}}$$



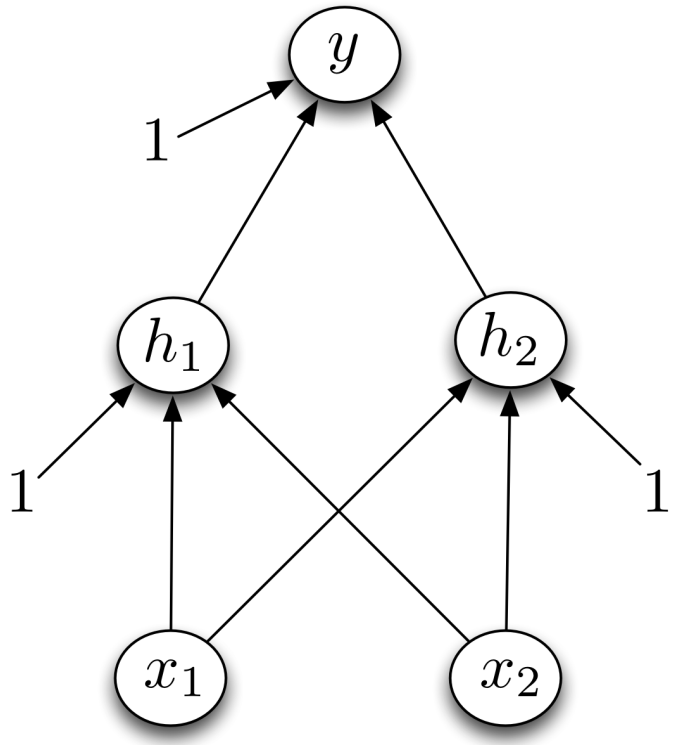
Hyperbolic Tangent (tanh)

$$y = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

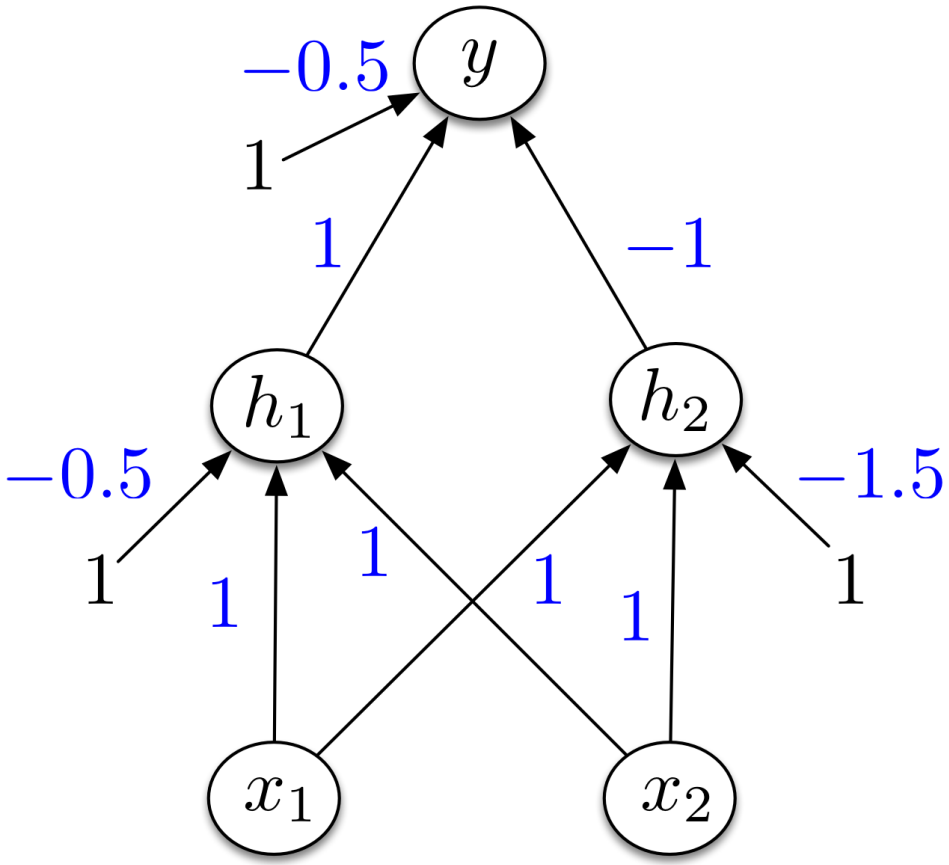
Multilayer Perceptrons

Designing a network to compute XOR:

Assume hard threshold activation function



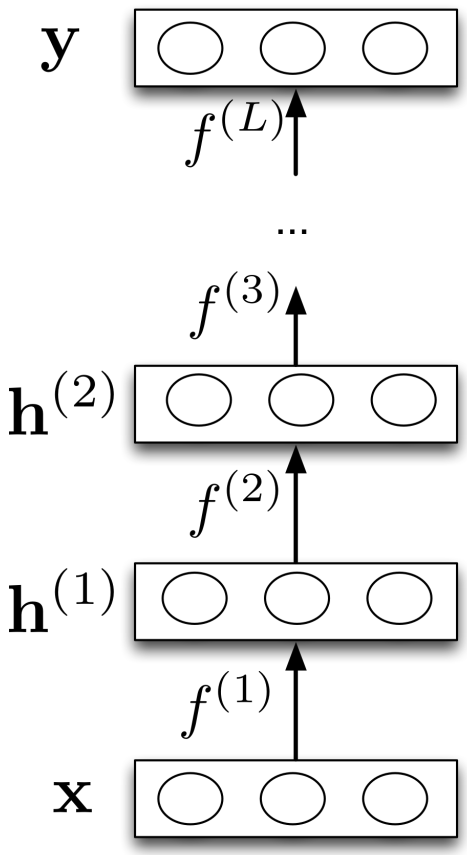
Multilayer Perceptrons



Multilayer Perceptrons

- Each layer computes a function, so the network computes a composition of functions:

$$\mathbf{h}^{(1)} = f^{(1)}(\mathbf{x})$$
$$\mathbf{h}^{(2)} = f^{(2)}(\mathbf{h}^{(1)})$$
$$\vdots$$
$$\mathbf{y} = f^{(L)}(\mathbf{h}^{(L-1)})$$



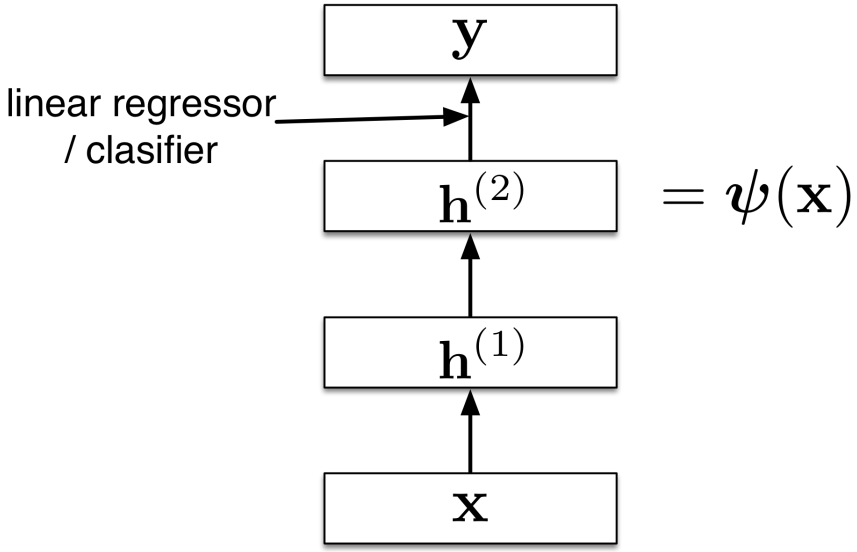
- Or more simply:

$$\mathbf{y} = f^{(L)} \circ \cdots \circ f^{(1)}(\mathbf{x}).$$

- Neural nets provide modularity: we can implement each layer's computations as a black box.

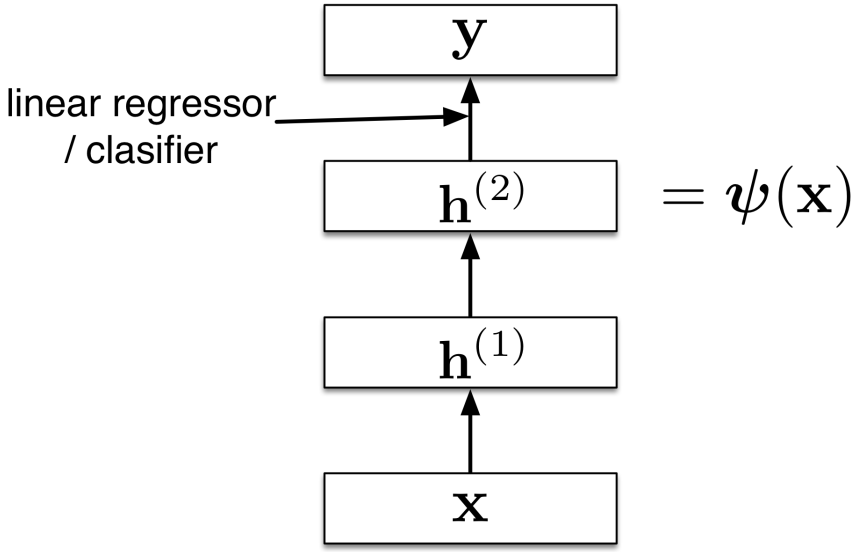
Feature Learning

- Neural nets can be viewed as a way of learning features:

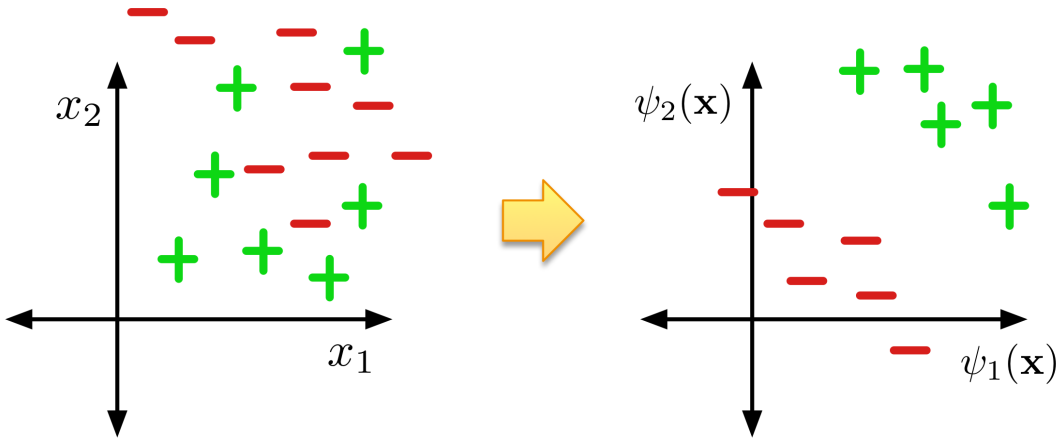


Feature Learning

- Neural nets can be viewed as a way of learning features:

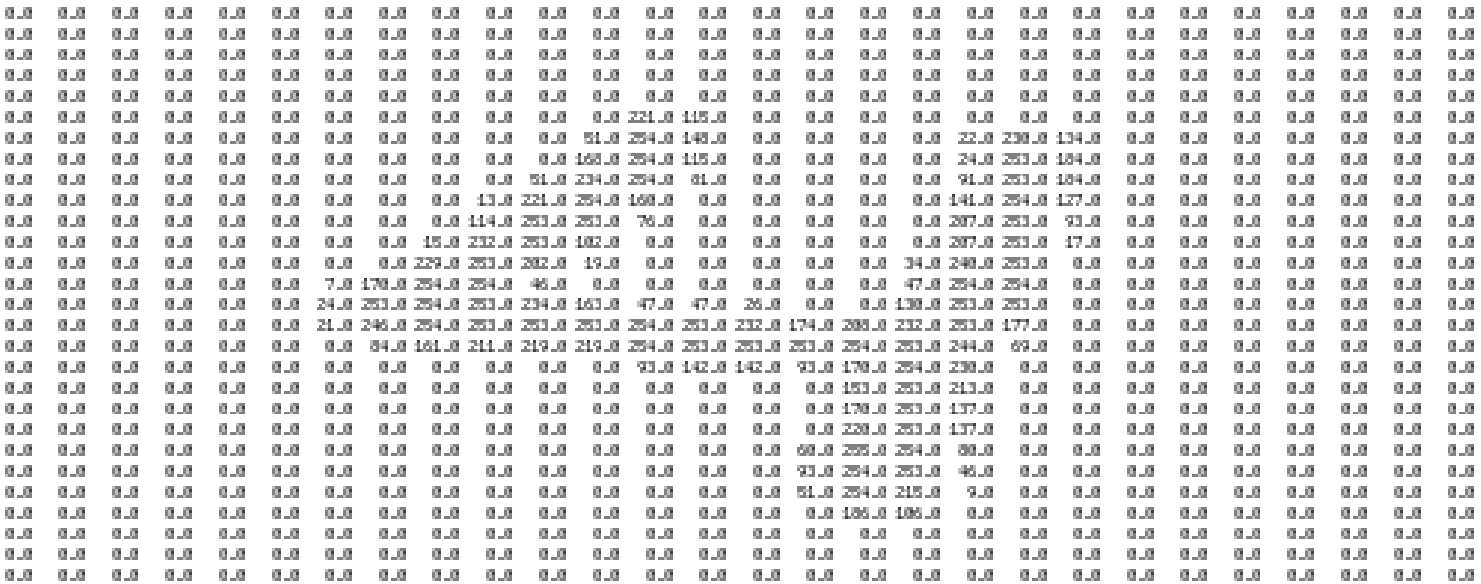


- The goal:



Feature Learning

Input representation of a digit : 784 dimensional vector.



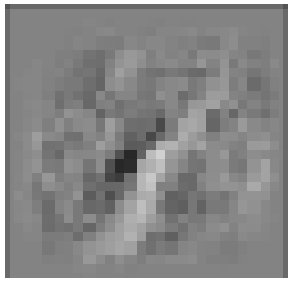
Feature Learning

Each first-layer hidden unit computes $\sigma(\mathbf{w}_i^T \mathbf{x})$

Here is one of the weight vectors (also called a feature).

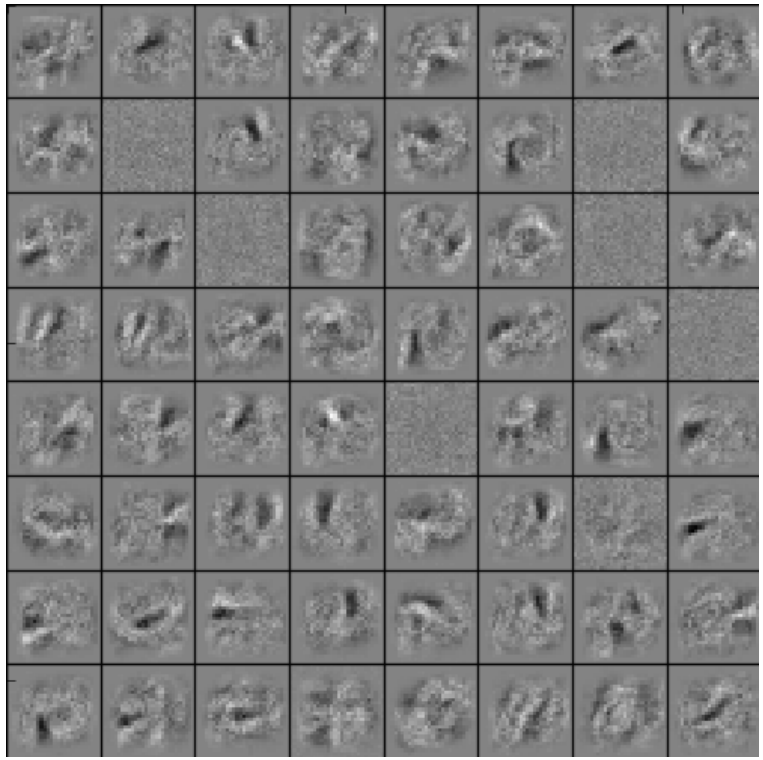
It's reshaped into an image, with gray $= 0$, white $= +$, black $=$ -.

To compute $\mathbf{w}_i^T \mathbf{x}$, multiply the corresponding pixels, and sum the result.



Feature Learning

There are 256 first-level features total. Here are some of them.



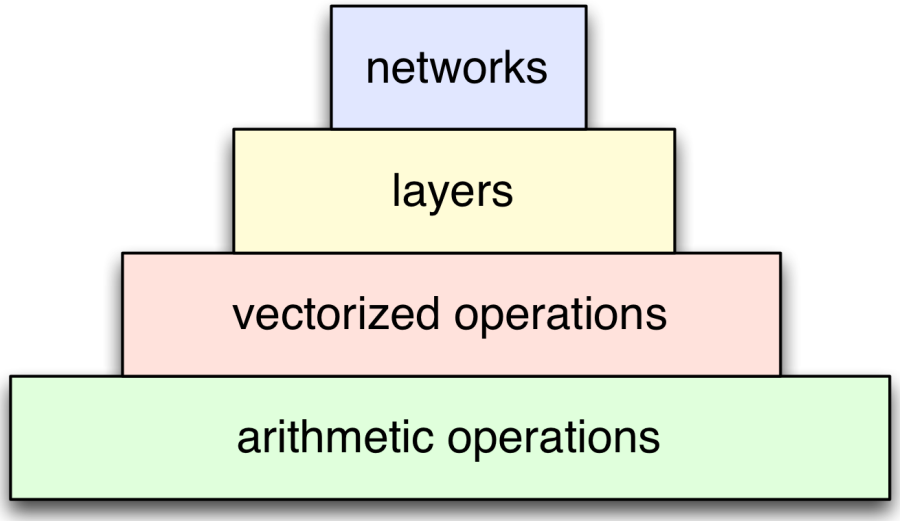
Levels of Abstraction

The psychological profiling [of a programmer] is mostly the ability to shift levels of abstraction, from low level to high level. To see something in the small and to see something in the large.

– Don Knuth

Levels of Abstraction

When you design neural networks and machine learning algorithms, you'll need to think at multiple levels of abstraction.



Expressive Power

- We've seen that there are some functions that linear classifiers can't represent. Are deep networks any better?
- Any sequence of *linear* layers can be equivalently represented with a single linear layer.

$$\mathbf{y} = \underbrace{\mathbf{W}^{(3)}\mathbf{W}^{(2)}\mathbf{W}^{(1)}}_{\triangleq \mathbf{W}'}\mathbf{x}$$

  - Deep linear networks are no more expressive than linear regression!
  - Linear layers do have their uses — stay tuned!

Expressive Power

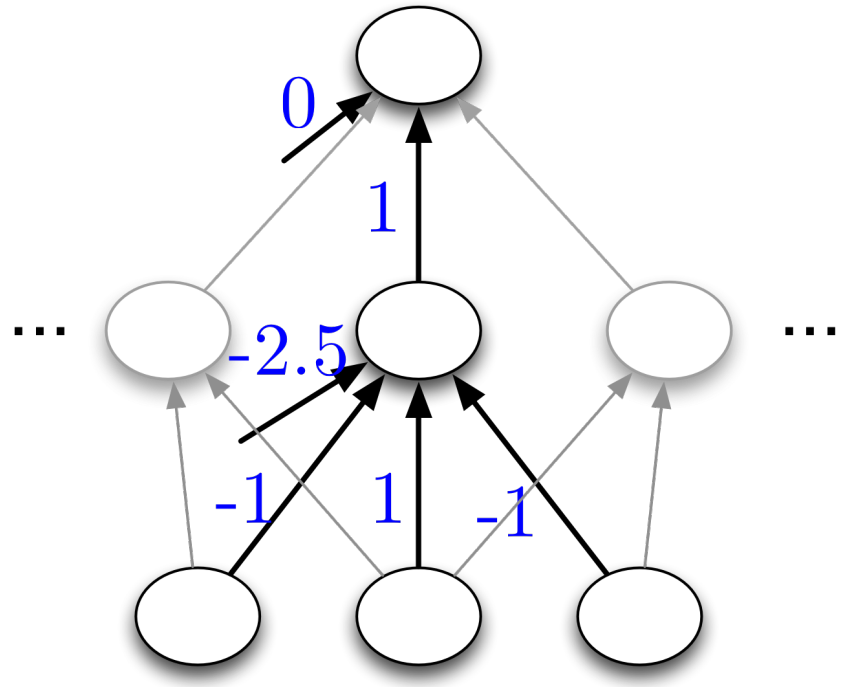
- Multilayer feed-forward neural nets with *nonlinear* activation functions are universal approximators: they can approximate any function arbitrarily well.
- This has been shown for various activation functions (thresholds, logistic, ReLU, etc.)
  - Even though ReLU is "almost" linear, it's nonlinear enough!

Expressive Power

Universality for binary inputs and targets:

- Hard threshold hidden units, linear output
- Strategy: 2^D hidden units, each of which responds to one particular input configuration

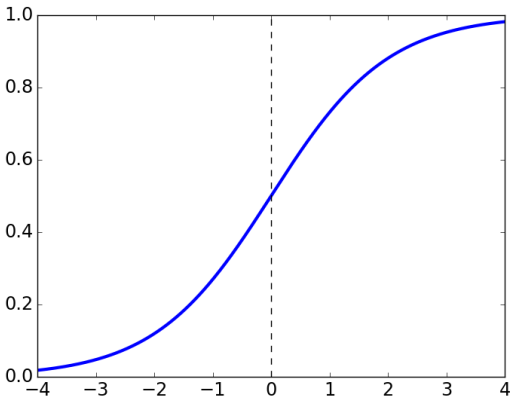
x_1	x_2	x_3	t
	$\vdots$		$\vdots$
-1	-1	1	-1
-1	1	-1	1
-1	1	1	1
	$\vdots$		$\vdots$



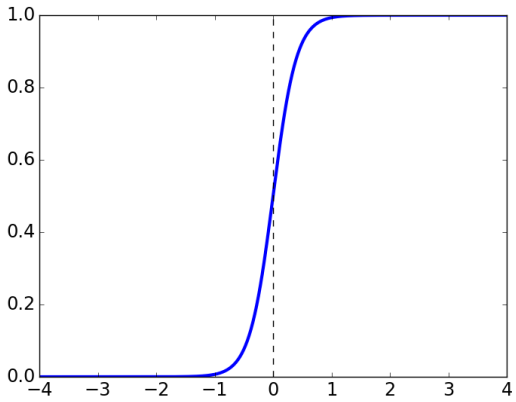
- Only requires one hidden layer, though it needs to be extremely wide!

Expressive Power

- What about the logistic activation function?
- You can approximate a hard threshold by scaling up the weights and biases:



$y = \sigma(x)$



$y = \sigma(5x)$

- This is good: logistic units are differentiable, so we can tune them with gradient descent. (Stay tuned!)

Expressive Power

- Limits of universality

Expressive Power

- Limits of universality
  - You may need to represent an exponentially large network.
  - If you can learn any function, you'll just overfit.
  - Really, we desire a *compact* representation!

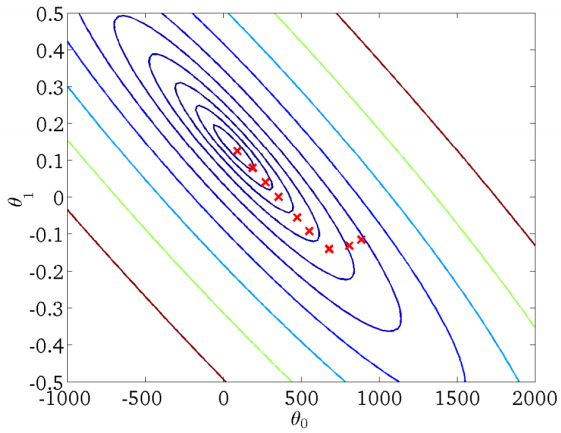
Expressive Power

- Limits of universality
  - You may need to represent an exponentially large network.
  - If you can learn any function, you'll just overfit.
  - Really, we desire a *compact* representation!
- We've derived units which compute the functions AND, OR, and NOT. Therefore, any Boolean circuit can be translated into a feed-forward neural net.
  - This suggests you might be able to learn *compact* representations of some complicated functions

Backpropagation

Recap: Gradient Descent

- **Recall:** gradient descent moves opposite the gradient (the direction of steepest descent)



- Weight space for a multilayer neural net: one coordinate for each weight or bias of the network, in *all* the layers
- Conceptually, not any different from what we've seen so far — just higher dimensional and harder to visualize!
- We want to compute the cost gradient $\nabla \mathcal{J}(\mathbf{w})$, which is the vector of partial derivatives.
  - This is the average of $\mathrm{d}\mathcal{L}/\mathrm{d}\mathbf{w}$ over all the training examples, so in this lecture we focus on computing $\mathrm{d}\mathcal{L}/\mathrm{d}\mathbf{w}$.

Univariate Chain Rule

- We've already been using the univariate Chain Rule.
- Recall: if $f(x)$ and $x(t)$ are univariate functions, then

$$\frac{\mathrm{d}}{\mathrm{d}t} f(x(t)) = \frac{\mathrm{d}f}{\mathrm{d}x} \frac{\mathrm{d}x}{\mathrm{d}t}.$$

Univariate Chain Rule

Recall: Univariate logistic least squares model

$$z = wx + b$$
$$y = \sigma(z)$$
$$\mathcal{L} = \frac{1}{2}(y - t)^2$$

Let's compute the loss derivatives.

Univariate Chain Rule

How you would have done it in calculus class

$$\mathcal{L} = \frac{1}{2}(\sigma(wx+b)-t)^2$$

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial w} &= \frac{\partial}{\partial w}\left[\frac{1}{2}(\sigma(wx+b)-t)^2\right] \\
&= \frac{1}{2}\frac{\partial}{\partial w}(\sigma(wx+b)-t)^2 \\
&= (\sigma(wx+b)-t)\frac{\partial}{\partial w}(\sigma(wx+b)-t) \\
&= (\sigma(wx+b)-t)\sigma'(wx+b)\frac{\partial}{\partial w}(wx+b) \\
&= (\sigma(wx+b)-t)\sigma'(wx+b)x
\end{aligned}$$

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial b} &= \frac{\partial}{\partial b}\left[\frac{1}{2}(\sigma(wx+b)-t)^2\right] \\
&= \frac{1}{2}\frac{\partial}{\partial b}(\sigma(wx+b)-t)^2 \\
&= (\sigma(wx+b)-t)\frac{\partial}{\partial b}(\sigma(wx+b)-t) \\
&= (\sigma(wx+b)-t)\sigma'(wx+b)\frac{\partial}{\partial b}(wx+b) \\
&= (\sigma(wx+b)-t)\sigma'(wx+b)
\end{aligned}$$

What are the disadvantages of this approach?

Univariate Chain Rule

A more structured way to do it

Computing the loss:

$$z = wx + b$$
$$y = \sigma(z)$$
$$\mathcal{L} = \frac{1}{2}(y - t)^2$$

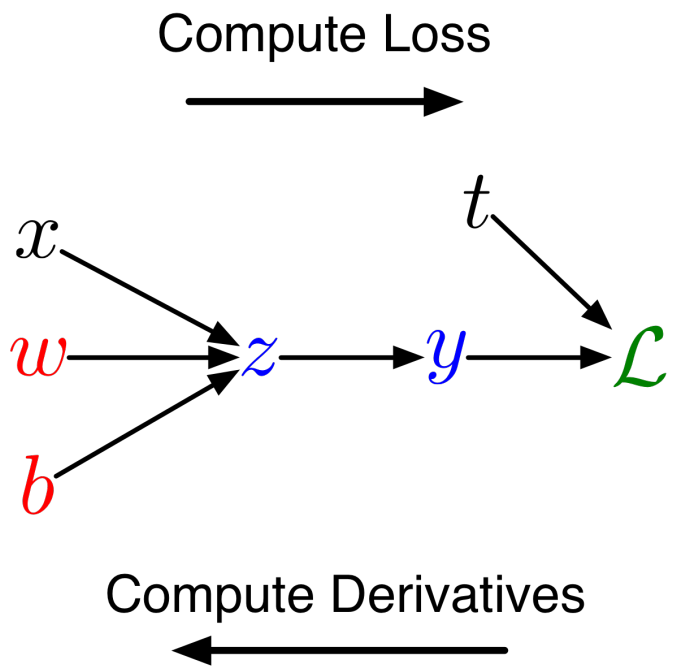
Computing the derivatives:

$$\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y} = y - t$$
$$\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}z} = \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y}\sigma'(z)$$
$$\frac{\partial\mathcal{L}}{\partial w} = \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}z}x$$
$$\frac{\partial\mathcal{L}}{\partial b} = \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}z}$$

Remember, the goal isn't to obtain closed-form solutions, but to be able to write a program that efficiently computes the derivatives.

Univariate Chain Rule

- We can diagram out the computations using a computation graph.
- The nodes represent all the inputs and computed quantities, and the edges represent which nodes are computed directly as a function of which other nodes.



Univariate Chain Rule

A slightly more convenient notation:

- Use $\overline{y}$ to denote the derivative $\mathrm{d}\mathcal{L}/\mathrm{d}y$, sometimes called the error signal.
- This emphasizes that the error signals are just values our program is computing (rather than a mathematical operation).
- This is not a standard notation, but I couldn't find another one that I liked.

Computing the loss:

$$z = wx + b$$
$$y = \sigma(z)$$
$$\mathcal{L} = \frac{1}{2}(y - t)^2$$

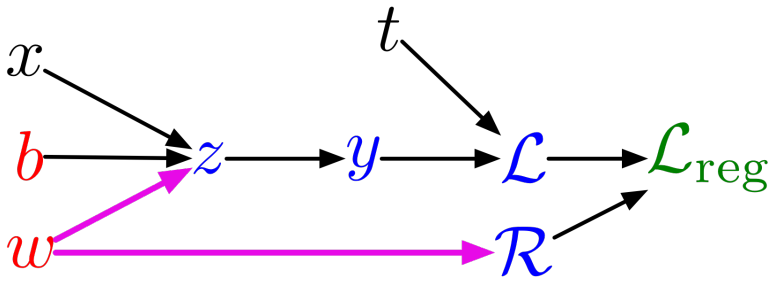
Computing the derivatives:

$$\overline{y} = y - t$$
$$\overline{z} = \overline{y}\,\sigma'(z)$$
$$\overline{w} = \overline{z}\,x$$
$$\overline{b} = \overline{z}$$

Multivariate Chain Rule

Problem: what if the computation graph has fan-out > 1?
This requires the multivariate Chain Rule!

L_2-Regularized regression



$$z = wx + b$$

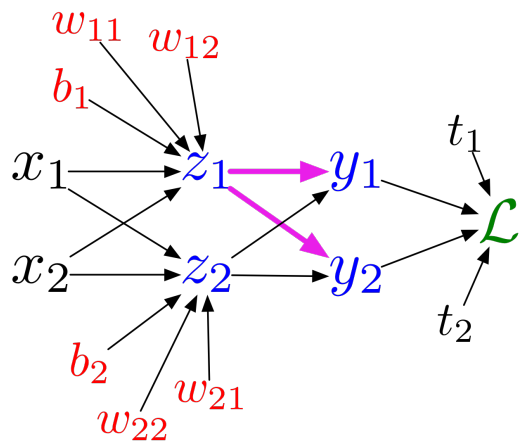
$$y = \sigma(z)$$

$$\mathcal{L} = \frac{1}{2}(y - t)^2$$

$$\mathcal{R} = \frac{1}{2}w^2$$

$$\mathcal{L}_{\text{reg}} = \mathcal{L} + \lambda\mathcal{R}$$

Multiclass logistic regression



$$z_\ell = \sum_j w_{\ell j} x_j + b_\ell$$

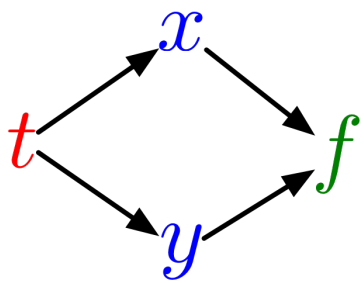
$$y_k = \frac{e^{z_k}}{\sum_\ell e^{z_\ell}}$$

$$\mathcal{L} = -\sum_k t_k \log y_k$$

Multivariate Chain Rule

- Suppose we have a function $f(x, y)$ and functions $x(t)$ and $y(t)$. (All the variables here are scalar-valued.) Then

$$\frac{\mathrm{d}}{\mathrm{d}t} f(x(t), y(t)) = \frac{\partial f}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}t}$$



- Example:

$$f(x, y) = y + e^{xy}$$
$$x(t) = \cos t$$
$$y(t) = t^2$$

- Plug in to Chain Rule:

$$\begin{aligned}\frac{\mathrm{d}f}{\mathrm{d}t} &= \frac{\partial f}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}t} \\ &= (ye^{xy}) \cdot (-\sin t) + (1 + xe^{xy}) \cdot 2t\end{aligned}$$

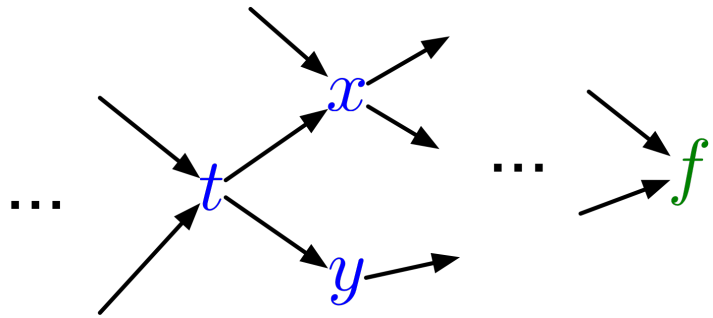
Multivariable Chain Rule

- In the context of backpropagation:

Mathematical expressions to be evaluated

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}t}$$

Values already computed by our program



- In our notation:

$$\bar{t} = \bar{x}\frac{\mathrm{d}x}{\mathrm{d}t} + \bar{y}\frac{\mathrm{d}y}{\mathrm{d}t}$$

Backpropagation

Full backpropagation algorithm:

Let $v_1, \ldots, v_N$ be a topological ordering of the computation graph (i.e. parents come before children.)

v_N denotes the variable we're trying to compute derivatives of (e.g. loss).

forward pass

For $i = 1, \ldots, N$

Compute v_i as a function of $\text{Pa}(v_i)$

backward pass

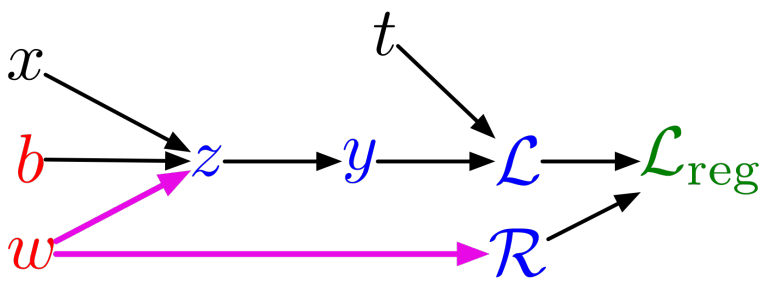
$\overline{v_N} = 1$

For $i = N - 1, \ldots, 1$

$\overline{v_i} = \sum_{j \in \text{Ch}(v_i)} \overline{v_j} \frac{\partial v_j}{\partial v_i}$

Backpropagation

Example: univariate logistic least squares regression



Forward pass:

$$
\begin{aligned}
z &= wx + b \\
y &= \sigma(z) \\
\mathcal{L} &= \frac{1}{2}(y - t)^2 \\
\mathcal{R} &= \frac{1}{2}w^2 \\
\mathcal{L}_{\text{reg}} &= \mathcal{L} + \lambda\mathcal{R}
\end{aligned}
$$

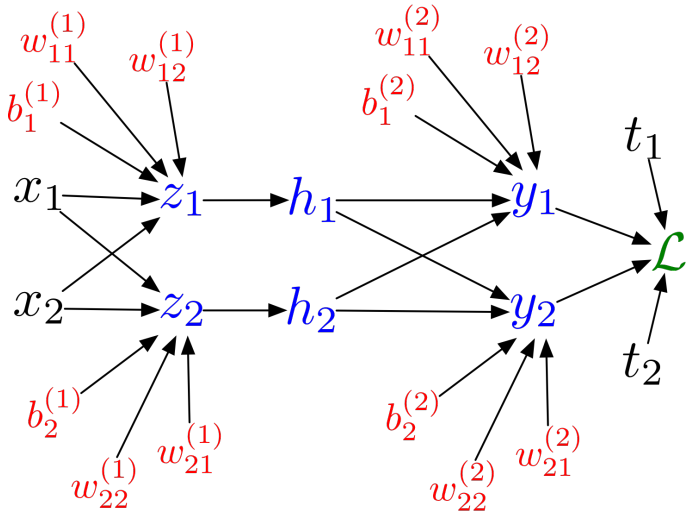
Backward pass:

$$
\begin{aligned}
\overline{\mathcal{L}_{\text{reg}}} &= 1 \\
\overline{\mathcal{R}} &= \overline{\mathcal{L}_{\text{reg}}}\,\frac{\mathrm{d}\mathcal{L}_{\text{reg}}}{\mathrm{d}\mathcal{R}} \\
&= \overline{\mathcal{L}_{\text{reg}}}\,\lambda \\
\overline{\mathcal{L}} &= \overline{\mathcal{L}_{\text{reg}}}\,\frac{\mathrm{d}\mathcal{L}_{\text{reg}}}{\mathrm{d}\mathcal{L}} \\
&= \overline{\mathcal{L}_{\text{reg}}} \\
\overline{y} &= \overline{\mathcal{L}}\,\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y} \\
&= \overline{\mathcal{L}}\,(y - t)
\end{aligned}
$$

$$
\begin{aligned}
\overline{z} &= \overline{y}\,\frac{\mathrm{d}y}{\mathrm{d}z} \\
&= \overline{y}\,\sigma'(z) \\
\overline{w} &= \overline{z}\,\frac{\partial z}{\partial w} + \overline{\mathcal{R}}\frac{\mathrm{d}\mathcal{R}}{\mathrm{d}w} \\
&= \overline{z}\,x + \overline{\mathcal{R}}\,w \\
\overline{b} &= \overline{z}\,\frac{\partial z}{\partial b} \\
&= \overline{z}
\end{aligned}
$$

Backpropagation

Multilayer Perceptron (multiple outputs):



Forward pass:

$$z_i = \sum_j w_{ij}^{(1)} x_j + b_i^{(1)}$$

$$h_i = \sigma(z_i)$$

$$y_k = \sum_i w_{ki}^{(2)} h_i + b_k^{(2)}$$

$$\mathcal{L} = \frac{1}{2} \sum_k (y_k - t_k)^2$$

Backward pass:

$$\overline{\mathcal{L}} = 1$$

$$\overline{y_k} = \overline{\mathcal{L}} (y_k - t_k)$$

$$\overline{w_{ki}^{(2)}} = \overline{y_k} \, h_i$$

$$\overline{b_k^{(2)}} = \overline{y_k}$$

$$\overline{h_i} = \sum_k \overline{y_k} w_{ki}^{(2)}$$

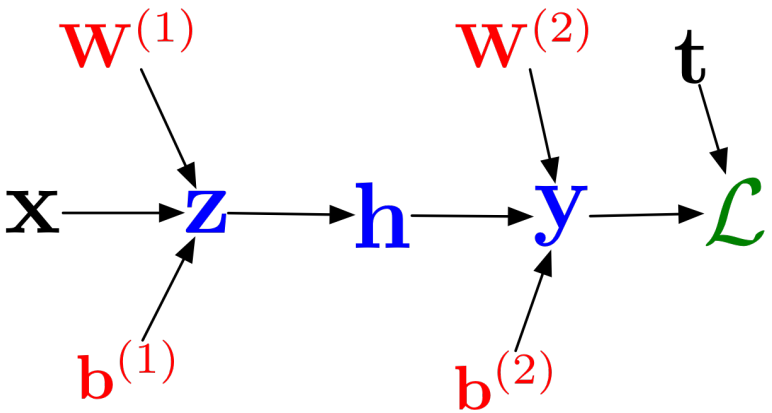
$$\overline{z_i} = \overline{h_i} \, \sigma'(z_i)$$

$$\overline{w_{ij}^{(1)}} = \overline{z_i} \, x_j$$

$$\overline{b_i^{(1)}} = \overline{z_i}$$

Backpropagation

In vectorized form:



Forward pass:

$$\mathbf{z} = \mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)}$$

$$\mathbf{h} = \sigma(\mathbf{z})$$

$$\mathbf{y} = \mathbf{W}^{(2)}\mathbf{h} + \mathbf{b}^{(2)}$$

$$\mathcal{L} = \frac{1}{2}\|\mathbf{t} - \mathbf{y}\|^2$$

Backward pass:

$$\overline{\mathcal{L}} = 1$$

$$\overline{\mathbf{y}} = \overline{\mathcal{L}}\,(\mathbf{y} - \mathbf{t})$$

$$\overline{\mathbf{W}^{(2)}} = \overline{\mathbf{y}}\mathbf{h}^\top$$

$$\overline{\mathbf{b}^{(2)}} = \overline{\mathbf{y}}$$

$$\overline{\mathbf{h}} = \mathbf{W}^{(2)\top}\overline{\mathbf{y}}$$

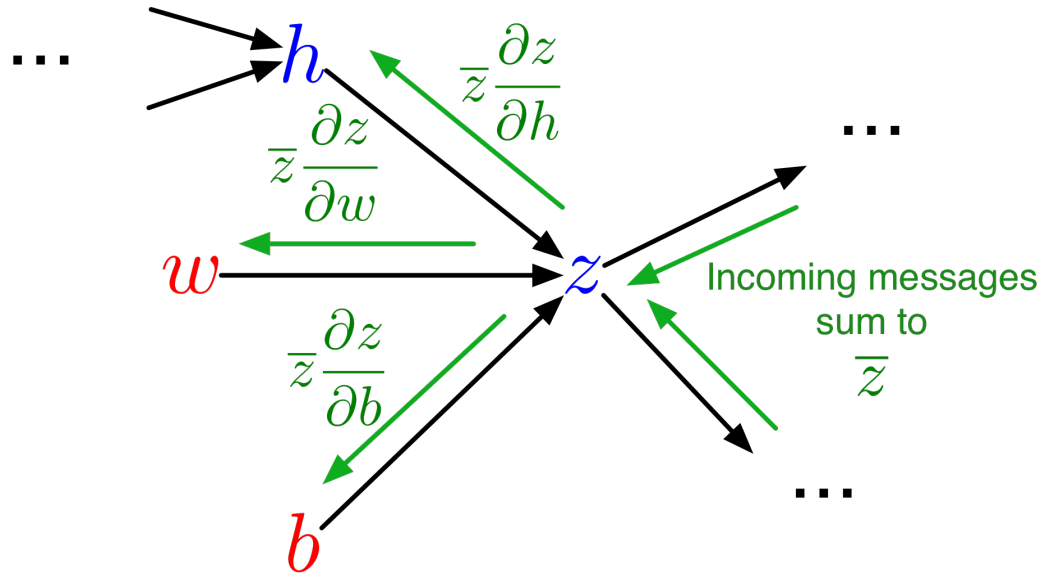
$$\overline{\mathbf{z}} = \overline{\mathbf{h}} \circ \sigma'(\mathbf{z})$$

$$\overline{\mathbf{W}^{(1)}} = \overline{\mathbf{z}}\mathbf{x}^\top$$

$$\overline{\mathbf{b}^{(1)}} = \overline{\mathbf{z}}$$

Backpropagation

Backprop as message passing:



- Each node receives a bunch of messages from its children, which it aggregates to get its error signal. It then passes messages to its parents.
- This provides modularity, since each node only has to know how to compute derivatives with respect to its arguments, and doesn't have to know anything about the rest of the graph.

Computational Cost

- Computational cost of forward pass: one add-multiply operation per weight

$$z_i = \sum_j w_{ij}^{(1)} x_j + b_i^{(1)}$$

- Computational cost of backward pass: two add-multiply operations per weight

$$\overline{w_{ki}^{(2)}} = \overline{y_k}\, h_i$$

$$\overline{h_i} = \sum_k \overline{y_k} w_{ki}^{(2)}$$

- Rule of thumb: the backward pass is about as expensive as two forward passes.
- For a multilayer perceptron, this means the cost is linear in the number of layers, quadratic in the number of units per layer.

Backpropagation

- Backprop is used to train the overwhelming majority of neural nets today.
  - Even optimization algorithms much fancier than gradient descent (e.g. second-order methods) use backprop to compute the gradients.
- Despite its practical success, backprop is believed to be neurally implausible.
  - No evidence for biological signals analogous to error derivatives.
  - All the biologically plausible alternatives we know about learn much more slowly (on computers).
  - So how on earth does the brain learn?