EE147: Neural Networks and Deep Learning

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Contents

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- deep learning has many modern applications:
  - Google search
  - Youtube video recommendations
  - Yelp restuarant best foods
  - Instagram feeds
  - very smart image recognition:
    - what makes a car a car?
    - cannot classify purely based on physical attributes such as size or number of wheels
    - image may be obscured or obfuscated
  - fraud detection
  - cancer treatment
  - self driving car:
    - many concerns eg. traffic cones, school buses, pedestrian signals, police cars
    - much expressive capacity is required
  - AlphaGo, Deepmind's AI that plays Go:
    - there are more Go board configurations than atoms in the universe
    - cannot do something as simple as a tree search
    - although AlphaGo was trained off of *"big data"* from Go experts:
      - its successor AlphaGo Zero uses deep reinforcement learning, *without* using any human data
      - algorithm rather than data based
  - brain-machine interfaces

History

- the concept of neural networks have been around for a long time, since McCulloch and Pitts in 1943:
  - has only become relevant as of recently
  - this early model was inspired by the nervous system activity (and did not have the capacity to learn ie. update its own parameters):
    1. all or none: a brain neuron either fires or not ie. 1 or 0
    2. synapses can sum together to trigger a neuron
- in 1958, Rosenblatt proposed the first **NN (neural network)** that could learn:
  - called the **perceptron**, it had a learning rule to train it to perform clas-

sifications
  - had m neurons or inputs, m weights, a bias b, and a value v
    - where $v = w_1 x_1 + ... + w_m x_m + b$
  - this early perceptron had a **hard-limiter** function φ st. the output $y = \varphi(v)$ and $\varphi(x)$ outputs 1 if $x > 0$ and otherwise 0
    - inspired by the all or none observation
  - the perceptron could act as a linear classifier with one layer
    - but this single layer failed for nonlinear classifications, such as the XOR problem
  - thus, there was a lot of pessimism towards researching multilayer neural networks around this time

- researchers would continue to use biological inspiration for developing neural networks:
  - in 1962, Hubel and Wiesel published research on the cat V1 visual neural system
  - Fukushima's neocognitron from 1982 used the insights from these visual system in a new neural network architecture
- in 1986, Rumelhart used **backpropagation** to finally train multilayer neural networks
  - a new way to train multilayer perceptrons by essentially using the chain rule to pass partial derivatives
- in 1989, LeCun and researchers at Bell Labs used neural networks to recognize handwritten zipcodes from the MNIST dataset
- in 1998, LeCun introduced LeNet, the modern **CNN (convolutional neural network)**, similarly inspired by visual cortex experiments:
  - took inspiration from spatial independence and simple linear composition of neurons in the V1 system
  - but still just a loose inspiration, eg. neurons in brains have probabilistic rather than static weights
- why didn't CNNs and backpropagation develop widespread use then?
  - backpropagation was still only good for shallow neural networks
    - as networks are deeper, the propagated derivative becomes more inaccurate
  - in addition, neural networks are data hungry
- modern era of deep learning:
  - the famous large ImageNet dataset with over 1000 classes of images held a yearly competition

    - within a decade, deep learning teams improved drastically in the ImageNet competition, from a 25% error rate to less than 5%
- driven by the massive amount of data we have access to and computation power to process it
    - GPU hardware have accelerated the training of NNs
- trend of more and more layers used in neural networks

Basics of Machine Learning

- **machine learning** uses statistical tools to estimate ie. *learn* functions of many different types, some of which may be fairly complex:
  - **classification** produces a discrete output representing the category given an input vector $x \in \mathbb{R}^n$:
    - ie. which of k categories x belongs to
    - eg. classifying whether an image is a cat or dog
  - **regression** produces an analog output predicting the value given an input
    - eg. predicting housing prices from square footage, controlling position and velocity of a cursor through brain signals
  - **synthesis and sampling** generate new examples that resemble a training data
    - eg. used in generative adversarial networks (GANs)
  - **data imputation** fills in missing values of a vector
    - eg. Netflix predicting if you will like a show or movie
  - **denoising** takes a corrupt data sample and outputs a cleaner sample
    - eg. used in variational autoencoders
  - other types
- in **supervised learning**, input vectors x and their target vectors y are known:
  - the goal is to learn function $y = f(x)$ that predicts y given x
  - eg. takes in a dataset D of n tuples of data
- in **unsupervised learning**, goal is to discover structure in input vectors, absent of knowledge of target vectors
  - eg. finding similar input vectors in clustering, distributions of the inputs, visualization, etc.
- in **reinforcement learning**, goal is to find suitable actions in certain scenarios to maximize a given reward R
  - discovers policies through trial and error
- in this class, we will focus on supervised learning:
  - using the CIFAR-10 dataset for an image classification problem:
    - 10 possible image categories
    - 32 by 32 pixel images, represented as 32 by 32 by 3 data values (RGB colors)
    - ie. input vector $x \in \mathbb{R}^{3072}$
  - want to find a function $f(x)$ that outputs one of the 10 categories

Supervised Learning Example

- for a problem of renting a home in Westwood, we want to know if we were getting a good deal:
  - given the square footage of a house, output how much monthly rent we should expect to reasonably pay based on the training data we have
- first, we should determine how we model data:
  1. determine inputs and outputs
     - input x is the square footage, and the output y is the rent
  2. what model should we use?
     - try a linear model $y = ax + b$
       - a, b are the **parameters** that must be learned ie. found in this chosen model
     - a different model could have been chosen eg. a nonlinear, higher order polynomial
       - many more parameters to tune with
  3. how do we assess how good our model is?
     - we need a **loss function** that *scores* how good the model is
     - for a prediction $\hat{y}_i = f(x_i)$ and actual sample output y_i, we can use a least squares loss function:

$$\textit{loss} = \textit{cost} = \sum_i (y_i - \hat{y}_i)^2$$

       - note that using least squares rather than absolute value puts higher weight on outlilers
- transforming with vectors:
  - writing the model using vectors where $\theta = \begin{bmatrix} a \\ b \end{bmatrix}$ and $\hat{x} = \begin{bmatrix} x \\ 1 \end{bmatrix}$:

$$\begin{aligned} \hat{y} &= ax + b \\ &= \theta^T \hat{x} \end{aligned}$$

  - writing the cost function using vectors where k is a normalization constant:

$$\begin{aligned} L(\theta) &= k \sum_i (y_i - \hat{y}_i)^2 \\ &= k \sum_i (y_i - \theta^T \hat{x}_i)^2 \end{aligned}$$

- we want to make loss $L(\theta)$ as *small* as possible, since θ represents the parameters we can control:
  - in this case, $L(\theta)$ will look like a parabola since it is squared
    - can solve for its minimum using optimization
  1. calculate $\frac{dL}{d\theta}$
     - tells us the slope of the tangent lines with respect to θ

2. solve for θ such that $\frac{\partial L}{\partial \theta} = 0$
   - however, θ is a vector, so how do we take derivatives with respect to it?
     - these derivatives are typically called **gradients** eg. $\frac{\partial y}{\partial x}$ or $\nabla_x y$
     - can be done with respect to vectors or matrices
- rewriting the cost function:

$$
\begin{aligned}
L &= \frac{1}{2}\sum_{i=1}^{N}(y_i - \theta^T \hat{x}_i)^2 \\
&= \frac{1}{2}\sum_{i=1}^{N}(y_i - \theta^T \hat{x}_i)^T(y_i - \theta^T \hat{x}_i) \\
&= \frac{1}{2}\sum_{i=1}^{N}(y_i - \hat{x}_i^T \theta)^T(y_i - \hat{x}_i^T \theta) \\
&= \frac{1}{2}(\begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} - \begin{bmatrix} \hat{x}_1^T \\ \vdots \\ \hat{x}_N^T \end{bmatrix} \theta)^T(\begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} - \begin{bmatrix} \hat{x}_1^T \\ \vdots \\ \hat{x}_N^T \end{bmatrix} \theta) \\
&= \frac{1}{2}(Y - X\theta)^T(Y - X\theta) \\
&= \frac{1}{2}(Y^T - \theta^T X^T)(Y - X\theta) \\
&= \frac{1}{2}[Y^T Y - Y^T X\theta - \theta^T X^T Y + \theta^T X^T X\theta] \\
&= \frac{1}{2}[Y^T Y - 2Y^T X\theta + \theta^T X^T X\theta]
\end{aligned}
$$

   - where $Y \in \mathbb{R}^{N\times 1}$ and $X \in \mathbb{R}^{N\times 2}$
     - note that $\theta^T \hat{x}_i = \hat{x}_i^T \theta$ and $Y^T X\theta = \theta^T X^T Y$ since they are all scalars and inner product is commutative
   - we used **vectorization** to move from summation to a sum expressed as an equivalent inner product of vectors
- now we can take derivatives to optimize the cost function:

$$
\begin{aligned}
\frac{\partial L}{\partial \theta} &= \frac{1}{2}[0 - 2X^T Y + [X^T X + X^T X]\ \theta] \\
&= -X^T Y + X^T X\theta\ [=]\ 0 \\
X^T Y &= X^T X\theta \\
\theta &= (X^T X)^{-1} X^T Y \\
&\triangleq X^\dagger Y
\end{aligned}
$$

   - recall that $\frac{\partial z^T \theta}{\partial \theta} = z$ and $\frac{\partial \theta^T A\theta}{\partial \theta} = (A + A^T)\theta$
     - $Y^T X$ can be considered as a vector z^T
   - this solution $\theta = X^\dagger Y$ is called the **least-squares solution**

    - gives us the best parameters θ to minimize the least-squares cost
- alternatively, using the chain rule to optimize the cost function:

$$\begin{aligned} f(z) &= z^2 \\ \frac{\partial f}{\partial z} &= 2z \\ g(\theta) &= y_i - \theta^T x_i \\ \frac{\partial g}{\partial \theta} &= -x_i \end{aligned}$$

$$\begin{aligned} \frac{\partial f}{\partial \theta} &= \frac{1}{2}\sum_{i=1}^{N} \frac{\partial}{\partial \theta} f(z(\theta)) \\ &= \frac{1}{2}\sum_{i=1}^{N} -x_i \cdot 2(y_i - \theta^T x_i) \\ &= \sum_{i=1}^{N} -x_i(y_i - \theta^T x_i) \\ &= -\sum_{i=1}^{N} x_i(y_i - \theta^T x_i) \\ &= -X^T(Y - X\theta) \end{aligned}$$

  - critically, whenever we see the pattern of a vector-scalar multiply within a summation, a vectorization can be performed
  - ie. the product within the summation is equal to:

$$[x_1 \dots x_N] \begin{bmatrix} y_1 - \theta^T x_1 \\ \vdots \\ y_N - \theta^T x_N \end{bmatrix} = X^T(Y - X\theta)$$

    - since $X = \begin{bmatrix} x_1^T \\ \vdots \\ x_N^T \end{bmatrix}$ is usually represented as a matrix of data rows
    - to vectorize $\theta^T x_i$, we can equivalently multiply data rows of X with the column vector θ
- does our current least-squares formula allow for learning nonlinear polynomial fits of the form:

$$y = b + a_1 x_1 + a_2 x^2 + \dots + a_n x^n$$

  - yes, we just have to redefine the input vectors:

$$\hat{x} = \begin{bmatrix} 1 \\ x \\ x^2 \\ \vdots \\ x^n \end{bmatrix}, \quad \theta = \begin{bmatrix} b \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}$$

  - a higher degree polynomial will *always* fit the training data *no worse* than a lower degree polynomial
    * encapsulates lower degree polynomials and can implement them by just setting the necessary coefficients to 0
  - but do we always want the highest possible degree polynomial?
    * eg. for housing price example, the linear model performs best for new inputs
    * the fundamental problem is that more complex models may not *generalize* as well if the data came from a different model
      · ie. relying on fitting the training data instead of generalizing

Maximum Likelihood Optimization

- note that there are alternative types of optimization rather than minimizing a mean-square error for the loss function:
  - in **maximum likelihood optimization**, we want to instead *maximize* the probability of having *observed* the data
  - others eg. MAP estimation, KL divergence
    * important to arrive at an appropriate model and cost function, and then *optimize* it
  - in these examples, we could differentiate and set the derivative equal to zero
    * in more complex models, there are more general ways to learn model parameters
- ex. Given a weighted coin and a sequence of flips, want to find the coin's weight θ:
  - consider the example training data of `HTHHTTHT`
  1. if $\theta = 1$, the probability of observing the data is 0
  2. if $\theta = 0.75$, the probability of observing the data is $0.75^4 0.25^4 = 0.00124$
  3. if $\theta = 0.5$, the probability of observing the data is $0.5^4 0.5^4 = 0.0039$
  - thus we would want to choose model (3) since it maximizes the likelihood of seeing the data

- ex. Given a set of N paired data $\{x_i, y_i\}$ where the coordinate $x_i \in \mathbb{R}^2$ has a class y_i belongs to one of three classes, want to be able to estimate the class of a new coordinate:
  - say that each of the classes follows a normal / Gaussian distribution ie. $x_i|y_i = j \sim N(\mu_j, \Sigma_j)$
  - the μ, Σ are the parameters θ we can choose to match the data as close as possible
  - need to make some important assumptions:
    - all classes are equally probable a priori ie. $p(y_i) = \frac{1}{3} = k$
    - each data point is *independent* given the parameters:

$$p(\{x_i, y_i\}, \{x_j, y_j\}|\theta) = p(x_i, y_i|\theta)p(x_j, y_j|\theta)$$

      - very useful assumption, prevents dealing with a long expansion of the probability chain rule
      - does not completely hold in reality eg. pictures data may have both cars and dogs, time series can cause dependencies
- want to maximize the likelihood of having seen the dataset:

$$\begin{aligned} L &= p(\{x_1, y_1\}, \dots, \{x_N, y_N\}|\theta) \\ &= \prod_{i=1}^{N} p(x_i, y_i|\theta) \end{aligned}$$

$$\begin{aligned} log(L) &= \sum_{i=1}^{N} log(p(x_i, y_i|\theta)) \\ &= \sum_{i=1}^{N} log(p(y_i|\theta)p(x_i|y_i, \theta)) \\ &= \sum_{i=1}^{N} log(p(y_i|\theta)) + log(p(x_i|y_i, \theta)) \\ &= Nlog(k) + \sum_{i=1}^{N} log(p(x_i|y_i, \theta)) \end{aligned}$$

  - using a log-likelihood technique to convert a product into a sum
  - results in a function of θ, so we can optimize θ to make the log function as large as possible
- optimizing:
  - after solving $\frac{\partial logL}{\partial \mu_i} = 0$ we find that the optimal μ_i is the empirical mean of the samples
  - similarly, we can find that the optimal Σ_i is the sample covariance

- with a new coordinate, how do we find the class x_{new} belongs to:

$$\begin{aligned} argmax_j \ p(j|x_{new}) &= argmax_j \ \frac{p(j, x_{new})}{p(x_{new})} \\ &= argmax_j \ \frac{p(j)p(x_{new}|j)}{p(x_{new})} \\ &= argmax_j \ p(j)p(x_{new}|j) \\ &= argmax_j \ p(x_{new}|j) \end{aligned}$$

  - ie. calculating the probability of it belonging to each of the distributions
  - simplifications occur since $p(x_{new})$ does not depend on j and $p(j)$ is uniform in this example
    - omitting that the probabilities are given θ

Generalizing the Model

- dangers of overfitting / underfitting:
  - **training data** is data that is used to learn the parameters of the model
  - **validation data** is the data used to optimize the hyperparameters of the model:
    - **hyperparameters** are the design choices of the model, eg. the order of the fitted polynomial
    - avoids the potential of overfitting to nuances in the testing dataset
  - **testing data** is data that is excluded in training and used to score the model
    - a "pristine" dataset used to score the final model with set parameters and hyperparameters
  - all datasets should follow the same distributions
  - the phenomenon where a model has very low training error but high testing error is called **overfit**
    - beyond a certain point, model begins to overfit the data
  - addressing overfitting:
    - more data helps ameliorate the issue of overfitting
      - may be appropriate to use more complex models when given much more data
    - regularization is another useful technique
- picking a best model:
  1. assess its generalization ie. validation error
  2. pick a setting of the parameters that results in minimal losses

  - there are some scenarios where the database size is so limited that it is better to utilize model selection techniques
    - ie. penalizes the model for being overly complex
- evaluating generalization error:
  - in a common scenario, we are given a training and testing dataset
  - to train a model while validating hyperparameters, one common approach is k-fold **cross validation**:
    - split training data into k equal sets called **folds**, each with $\frac{N}{k}$ examples
    - $k-1$ folds are training datasets, while the remaining fold is a validation dataset
    - for each hyperparameter eg. polynomial order we are trying to validate
      - run k validation tests using each of the folds as a validation set, take the average as an overall validation error
    - note that class balance should be maintained across folds eg. using a stratified k-fold
  - after using cross validation to finalize hyperparameters, we can train a single model based on the entire training data

Supervised Classification

- supervised learning techniques are useful for classification, as well as some neural networks developments
  - a new renaissance in supervised learning due to the boom in computer vision applications
  - in classification, want to classify an input image x as one of several possible categories y
    - images are input into a computer vision algorithm as a $width \times height \times 3$ array representing RGB values from $[0, 255]$
- problems that arise in image classification:
  - viewpoint variation
    - cannot simply compare pixel values at certain locations
  - illumination that adjusts the RGB values
  - deformation
    - eg. different visible *features* of a cat depending on the image
  - occlusion
  - background clutter
  - intraclass variation
- different possible approaches to classifying an image:
  - have experts come in and manually craft important features of image classes
    - impossible to scale
  - instead, use a data driven approach:
    1. expose a machine learning algorithm to a lot of *data*
    2. *learns* a function mapping the image to class
    - these deep neural nets learn parameters that represent features useful for classifying the image well
      - developing their *own* features for image classes that may be difficult to interpret
    - then, test how the neural net performs on predicting the class of new images

k-Nearest Neighbors

- given a training set of input vectors $x_1, \ldots, x_m$ and their corresponding classes $y_1, \ldots, y_m$, want to estimate the class of a new data point x_{new}:
  - we previously found a way to classify through a probabilistic model where we had to learn parameters
    - is there a simpler way to classify without very much ML machin-

ery?

- in the k-**nearest neighbors** algorithm:
  - find the k closest points or neighbors in the training set according to an appropriate metric
  - each of these neighbors then vote according to what class it is in, and x_{new} is assigned to be the class with the most votes
  - k and the distance metric are hyperparameters
    - can test hyperparameters to find the settings with lowest errors and lower variances
  - an example of **instance-based classification** where similar instances will have similar classification
- k-nearest neighbors more formally:
  1. choose an appropriate distance metric $d(x, y)$ ie. just Euclidian distance where $d(x, y) = ||x - y||_2$
  2. choose the number of nearest neighbors k
  3. calculate $d(x_{new}, x_i) \ \forall \ i = 1, \dots, m$
  4. classify x_{new} as the class that occurs most frequently among the corresponding classes of the k closest neighbors
- how do we train the classifier?
  - just have to cache the entire dataset so it can run the algorithm on testing data
  - *pros*:
    - fast in $O(1)$ and simple
      - no need to copy, can just use pointers or references to point to data
  - *cons*:
    - memory intensive since we have to store all of the training data
    - memory scales with the number of training examples
      - vs. the MLE algorithm, which needs to store a constant number of parameters regardless of training examples
- how do we test a new data point?
  - have to calculate the distances from every point in the training set, and sort them
  - *pros*:
    - simple
  - *cons*:
    - takes a long time, scales with the amount of data given in $O(N)$
  - want the *reversed* complexity times for training and testing:
    - testing should be $O(1)$, while it is more acceptable for training to be slower
    - eg. in computer vison, want instantaneous results
- why might this algorithm fail for image classification?
  - calculating distance between the inputs doesn't have a semantic mean-

ing correlating to image similarity:
    * eg. shifted vs. tinted vs. images overlaid with boxes would have similar distances from the original although the boxed images may look very different than the tinted or shifted versions
  - the *"curse of dimensionality"*:
    * the number of dimensions starts to scale exponentiality given larger, more complex input data
    * as feature space gets larger, the feature vectors become sparser ie. *farther* apart
      · the notion of similarity thus begins to break down in higher dimensions
    * ie. distances in different dimensions may start to mean different things other than similarities

Softmax Classifier

- a better approach may be to develop a score for an image coming from each class and then select the class with the largest score:
  - based on **linear classification**, which consists of two major components:
    1. a *linear* score function that maps the raw data to class scores
    2. a loss function that measures how good the scoring functions is at predicting the labels
  - linear classifiers are a building block for neural networks
    * each layer of a neural network is a linear classifier that is then passed through nonlinearity
- consider a matrix $W \in \mathbb{r}^{c \times N}$ where $W = \begin{bmatrix} w_1^T \\ \vdots \\ w_c^T \end{bmatrix}$:
  - with c number of classes
  - $y = Wx + b$ is a vector of scores where its ith element corresponds to the score of x being in class i:

$$y = \begin{bmatrix} W_1^T x + b_1 \\ \vdots \\ W_c^T x + b_c \end{bmatrix}$$

    * b is a vector of bias terms
      · $b, y \in \mathbb{R}^{10}$ in CIFAR
    * x has dimensions $x \in \mathbb{R}^{3072}$ in CIFAR
  - the output will be the index of the highest score in y
    * ie. $a_i(x)$ is the ith entry of y
  - note that due to the dot product, when w_i^T is *similar* to x, the score will be higher

    - thus each w_i, when recomposed as in image, acts as a template for the *average* image in that class
- so what is a linear classifier actually doing?

$$\begin{aligned} w_i^T x &= ||w_i||\ \ ||x|| cos\theta \\ &= ||x|| cos\theta \end{aligned}$$

  - assuming $||w_i|| = 1$
  - in 2D, any point x that lies on the same line *perpendicular* to w_i has the *same score*:
    - since $||x|| cos\theta = ||x|| \frac{||adjacent||}{||hypotenuse||} = ||adjacent||$
    - ie. taking x and calculating its *projection* onto every weight vector
    - the *intersection* of these perpendicular lines indicates a **linear decision boundary** between different weights
  - eg. in binary classification in 2 dimensions, the boundary is the single line on the $\mathbb{R}^2$ plane that divides up the points into two classes
  - eg. in higher dimensions and multi-class classification, the boundaries become defined by *multiple* hyperplanes:
    - either side of each hyper plane can be interpreted as whether one of two possible classes is more likely
  - ie. linear classifiers break up space into regions bounded by hyperplanes
- where might linear classifiers fail?
  - when data is not linearly separable
    - eg. the XOR problem
  - *however*, can sometimes use tricks using change of bases:
    - eg. *radial* data can be expressed in polar to become linearly separable
    - this is a foreshadowing of what neural networks do
      - ie. finding features that make the data linearly separable themselves
- collecting the received scores into a loss function:
  - we can use the **softmax** function to transform the scores into a probability

$$softmax_i(x) = \frac{e^{a_i(x)}}{\sum_{j=1}^{c} e^{a_j(x)}}$$

    - ie. normalizes the scores to probabilities while handling negative or very large scores
      - thus all the softmax probabilities will add up to 100%
    - note that the choice of $softmax$ for loss gives a smoother curve that is much easier to optimize compared to $argmax$ or $distance$
  - $softmax_i(x)$ can be interpreted as the probability x belongs to class i:

$$Pr(y_j = i | x_j, \theta) = softmax_i(x_j)$$

    - where $\theta = \{w_j, b_j\} \ \forall \ j \in \{1, ..., c\}$
  - optimizing softmax loss function ie. the **cross-entropy loss** with respect to θ:

$$p(x_1, ..., x_m, y_1, ..., y_m|\theta) = \prod_{i=1}^{m} p(x_i, y_i|\theta) = \prod_{i=1}^{m} p(x_i|\theta)p(y_i|x_i, \theta)$$

$$\begin{aligned} argmax_\theta \prod_{i=1}^{m} p(x_i|\theta)p(y_i|x_i, \theta) &= argmax_\theta \prod_{i=1}^{m} p(y_i|x_i, \theta) \\ &= argmax_\theta \sum_{i=1}^{m} log(softmax_{y_i}(x_i)) \\ &= argmax_\theta \sum_{i=1}^{m} log[\frac{e^{a_{y_i}(x_i)}}{\sum_j e^{a_j(x_i)}}] \\ &= argmax_\theta \sum_{i=1}^{m} [a_{y_i}(x_i) - log(\sum_{j=1}^{c} e^{a_j(x_i)})] \\ &= argmin_\theta \sum_{i=1}^{m} [log(\sum_{j=1}^{c} e^{a_j(x_i)}) - a_{y_i}(x_i)] \end{aligned}$$

  - note that $p(x_i|\theta)$ is *independent* of θ ie. not dependent of chosen parameters, so it can be taken out of the $argmax_\theta$
  - in addition, $argmax_\theta f(\theta) = argmin_\theta \ -f(\theta)$
- intuition behind the name of the softmax classifier:
  - the output of the softmax can be interpreted as the probability of a class and is typically considered together with log ie. the **log likelihood**

$$\begin{aligned} log(Pr(y = i|x)) &= log(softmax_i(x)) \\ &= a_i(x) - log(\sum_{j=1}^{c} e^{a_j(x)}) \end{aligned}$$

  - the latter term can be approximated by $max_j a_j(x)$ since the biggest a_j dominates
  - if $a_i(x)$ produces the largest score, then the log likelihood is approximately 0
  - if $a_j(x)$ produces the largest score for $j \neq i$, then $a_i(x) - a_j(x)$ is negative, and the log likelihood is negative
  - ie. in cross-entropy, want to minimize the *negative* log likelihood of the correct class
- a potential problem when implementing a softmax classifier is overflow:
  - if $a_i(x) \gg 0$, then $e^{a_i(x)}$ may overflow

  - thus it is standard practice to normalize the softmax function as follows:

$$\tilde{a}_i(x) = a_i(x) + logk = \frac{ke^{a_i(x)}}{k\sum_j e^{a_j(x)}} = \frac{e^{a_i(x)+logk}}{\sum_j e^{a_j(x)+logk}}$$

    * we usually set $logk = -max_i\ a_i(x)$, which makes the maximal argument of the exponent 0

- softmax **temperature** is a scaling constant T used for tuning the softmax classifier:

$$softmax_i(x) = \frac{e^{\frac{a_i(x)}{T}}}{\sum_{j=1}^{c} e^{\frac{a_j(x)}{T}}}$$

  - affects the distribution of softmax probabilities
    * change in T is analogous to a change in base
  - as $T \to \infty$, $softmax_i(x) \to \frac{1}{c}$ ie. approaches a uniform distribution
  - as $T \to 0$, the max scores gets close to 1, and all others go to 0
  - temperature can be used to perform **knowledge distillation** that reduces the number of parameters used in a classifier:
    * uses a teacher model that outputs a softmax probability distribution to a fresh student model
    * here, temperature adjustment is important to improve efficiency of the distillation

Support Vector Machine

- another common decision boundary classifier is the **support vector machine (SVM)**:
  - the SVM finds a boundary that maximizes the margin or *gap* between the boundary and the data points
  - if a point is *further* away from the decision boundary, there ought to be greater *confidence* in classifying that point
- informally, to calculate the loss of a chosen boundary:
  - points very close to the boundary should incur small losses, even if they are correctly classified:
    * while different classifiers would not penalize these points at all
    * encourages the model to find a boundary with a large margin
  - misclassified data points that are incorrect should have a very large loss though they may be close to the boundary
  - points past a certain margin of the boundary should incur no loss
- the **hinge loss** function:
  - standardly defined for a binary output $y \in \{-1, 1\}$

  - when $y_i = 1$, want $w^T x_i + b$ to be large and positive, while when $y_i = -1$, want $w^T x_i + b$ to be large and negative

$$hinge_{y_i}(x_i) = max(0, 1 - y_i(w^T x_i + b))$$

  - when $y_i = 1$ and $w^T x_i + b \gg 1$, the hinge loss is 0
    - zero error if signs match and there is a large margin
  - when $y_i = 1$ and $w^T x_i + b = 0.3$, the hinge loss is 0.7
    - nonzero error if signs match, but there is a small margin
  - when $y_i = 1$ and $w^T x_i + b = -1$, the hinge loss is 2
    - larger error when signs do not match
  - here, 1 acts as the margin value
    - note that we can set it as 1 without a loss of generality, since a change in the margin could be compensated by changing the weights
- hinge loss extension to multiple classes:

$$hinge_{y_i}(x_i) = \sum_{j \neq y_i} max(0, 1 + a_j(x_i) - a_{y_i}(x_i))$$

  - given c classes where 1 is correct and $c - 1$ are incorrect, and $a_j(x_i) = w_j^T x_i + b_j$
  - when the correct class achieves the highest score:

$$a_{y_i}(x_i) \geq a_j(x_i), \;\; 0 \leq hinge_{y_i}(x_i) \leq c - 1$$

  - when the correct class is much higher than the other scores:

$$a_{y_i}(x_i) \gg a_j(x_i) + 1, \;\; hinge_{y_i}(x_i) = 0$$

  - when the correct class achieves an equal score:

$$a_{y_i}(x_i) = a_j(x_i), \;\; hinge_{y_i}(x_i) = c - 1$$

  - when an incorrect class achieves the highest score:

$$a_{y_i}(x_i) < a_j(x_i), \;\; a_j(x_i) - a_{y_i}(x_i) \geq 0$$

    - has the potential to be large
  - in general, the model is encouraged to make correct margins larger and incorrect margins smaller
- softmax vs. SVM intuition:
  - the softmax is a maximum likelihood loss function:
    - change the parameters to optimize having seen the data
    - cross-entropy is the most common loss function typically used

  - the hinge loss is a human-constructed heuristic:
    * bound the loss at zero, and calculate a margin from a difference of scores
    * the margin in the SVM may help more with noisy data and outliers
    * thus SVM could be more useful empirically in some scenarios
- optimizing the SVM cost function:

$$argmin_\theta \ \frac{1}{m}\sum_{i=1}^{m} hinge_{y_i}(x_i)$$

$$argmin_\theta \ \frac{1}{m}\sum_{i=1}^{m}\sum_{j\neq y_i} max(0, 1 + a_j(x_i) - a_{y_i}(x_i))$$

  - where $a_j(x_i) = W_j^T x_i + b$, $\theta = \{W, b\}$, $W = \begin{bmatrix} W_1^T \\ \vdots \\ W_c^T \end{bmatrix}$

Gradient Descent

- from calculus, the derivative of a function tells us its slope at a point:

$$f(x + \epsilon) \approx f(x) + zf'(x)$$

  - when the derivative is 0, we are at a stationary or critical point of the function:
    * may be a local or gobal maximimum or minimum, or a saddle point
    * however, when f contains nonlinear or non-differentiable functions, cannot simply set the derivative equal to 0
    * instead want to iteratively approach a critical point via **gradient descent**
  - in this class, need to optimize f with respect to vectors and matrices
- terminology:
  - a **global minimum** x_g achieves the absolute lowest values of f, ie. $f(x) \geq f(x_g) \ \forall \ x$
  - a **local minimum** x_l is a critical point that is lower than its neighboring points, however, $f(x_l) > f(x_g)$
    * analogous definitions for maximums
  - a **saddle point** is a critical point that is not a not local maximum or minimum
    * local neighbors are larger and smaller on either side
- the gradient is a vector that tells us how small changes in Δx affects $f(x)$ through:

$$f(x + \Delta x) \approx f(x) + \Delta x^T \nabla_x f(x)$$

  - to find how $f(x)$ changes in some direction of a unit vector u:

$$u^T \nabla_x f(x)$$

- to minimize $f(x)$, want to find the direction in which $f(x)$ decreases the fastest:

$$\begin{aligned} min_{u,||u||=1} u^T \nabla_x f(x) &= min_{u,||u||=1} ||u||\ ||\nabla_x f(x)||\ cos(\theta) \\ &= min_u\ ||\nabla_x f(x)||\ cos(\theta) \end{aligned}$$

  - this quantity is minimzed for u pointing in the opposite direction of the gradient such that $cos(\pi) = -1$
  - thus to update x as to minimize $f(x)$, we repeatedly calculate:

$$x \leftarrow x - \epsilon \nabla_x f(x)$$

    * ϵ is known as the **learning rate**, and may change over iterations
- how to pick the right step size ie. learning rate:
  - when the step size is too large, the linear approximation of the gradient will fail and the descent may keep overshooting its target
  - if the step size is smaller, the linear approximation of the gradient should hold
    * but with too small a step size, computation time greatly increases
  - with more and more dimensions, should we step in every direction at the same rate?
    * in a **first-order method**, we take steps in every direction at equal rates
    * in a **second-order method**, we compute the curvature of the surface in every direction to calculate how much to step in each direction
      · but this is prohibitively expensive to calculate
    * first-order methods with heuristics may be a better alternative
  - can empirically test learning rate by examining the cost function at each iteration:
    * want the loss to quickly and smoothly decrease
    * abnormalities or a plateau may indicate too high a step size
    * a slowly decreasing loss may indicate too small a step size
- why not instead use a numerical gradient as follows:

$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

  - with millions of parameters represented by h, we would have to calculate the loss at many settings of h
    * extremely slow

Hinge Loss Gradient

- want to find the gradient for the hinge loss:

$$\begin{aligned} L(\theta) &= \frac{1}{m}\sum_{i=1}^{m}\sum_{j\neq y_i} max(0, 1 + w_j^T x_i - w_{y_i}^T x_i) \\ L_i &= \sum_{j\neq y_i} max(0, 1 + w_j^T x_i - w_{y_i}^T x_i) \\ &= \sum_{j\neq y_i} max(0, z_j) \end{aligned}$$

$$\begin{aligned} \nabla_{W_j} L_i &= \begin{cases} 0 & z_j \leq 0 \\ x_i & z_j > 0 \end{cases} = \mathbb{1}(z_j > 0)x_i \\ \nabla_{W_{y_i}} L_i &= -\sum_{j\neq y_i} \mathbb{1}(z_j > 0)x_i \end{aligned}$$

  - where $W = \begin{bmatrix} W_1^T \\ \vdots \\ W_c^T \end{bmatrix}$
  - notes:
    - the biases are dropped for simplicity
    - the gradient can be applied on the inside of the averaging term since the gradient is a linear operator
      - ie. the gradient is taken over every training example and then averaged
    - manually setting the derivative at 0 to 0 using the concept of sub-gradients, though it is technically undefined
    - the indicator function $\mathbb{1}$ returns 0 if its argument ≤ 0 and 1 otherwise
- in the previous gradient descent step, we know the function f exactly and can calculate the gradient at that point exactly:
  - in optimization, we instead differentiate the cost function with respect to the parameters
    - thus this gradient is a *function* of the training data
  - ie. each data point provides a noisy estimate of the gradient at that point
  - however, it's expensive to calculate the gradient with *every* example in the set
- instead, there are alternatives approaches to calculating the gradient:
  - in a batch algorithm, use all m examples in the training set to calculate the gradient
  - in a minibatch algorithm, approximate the gradient by calculating it with k examples where $m > k > 1$

        - typically used in deep learning
    - in a stochastic algorithm, approximate the gradient by calculating it over a single example
    - the smaller the batch size, the more steps we can take in the same amount of calculation time:
        - though more noise may be introduced into the gradient estimation
        - however, more noise may be beneficial in acting as regularization
            - ie. generalizing the model better to avoid overfitting by making the loss surface *smoother*
- to find the gradient on the softmax loss, take the chain rule with the gradient of the softmax function itself

Neural Networks

- the inspiration from **neural networks** is from neural science:
  - neurons are the main signaling units of the nervous system, with 3 main parts:
    1. the dendrites are a tree like structure that receive input signals
       - each dendrite may have a synaptic weight associated with it
    2. the axon hillock is an *integration center* for summing propagated input signals
       - an *all-or-nothing* rather than analog spike for triggering some action potential
    3. axons are long tubular structures for carrying output signals
       - connects to other downstream neurons
  - in the brain, spiking responses are probabilistic:
    - exact spikes are different even for the same trials
    - instead, we can track of the *rate* at which spikes occur per second
    - this rate is what neural networks attempt to encode
- the neural network neuron vs. real neuron:
  - receives various inputs $x_1, \dots, x_N$ that act as dendrites, each with a unique fixed weight $w_1, \dots, w_N$
    - each input may be an output of prior neurons
  - has a summation computation that sums up the "dendritic-processed" signals $w_i x_i$ and a bias:

$$f(\sum_i w_i x_i + b)$$

    - performs a sum and passes it through a nonlinearity f
    - like the spike threshold, there is a new aspect of nonlinearity for the neuron to fire
- some differences between artificial and real neurons:
  - synaptic transmission are probabilistic, nonlinear, and dynamic
  - dendritic integration is probabilistic and may be nonlinear
  - there are many different cell and neuron types
  - in general, though neural networks are inspired by biology, they approximate biological computation at a fairly crude level
- nomenclature:
  - the first layer is an **input layer** typically represented with the variable x
  - the last layer is the **output layer** typically represented with the variable z
    - typically the output of the entire neural network are a processed version of z eg. sent through softmax as $softmax(z)$

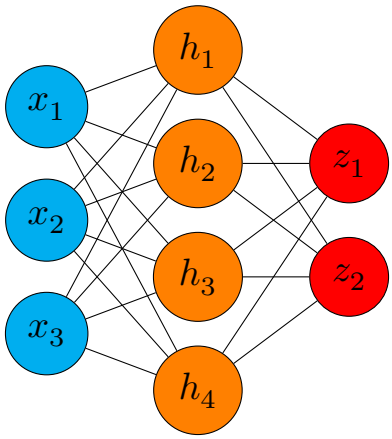


Figure 1: 2-Layer Neural Network

  - intermediate layers are known as the **hidden layers** represented by the variable h:
    - generally, these layers are extracting some kind of features from the input data
    - they are able to learn which features make the data linearly separable so that the processing softmax classifier can classify them
    - importantly, these features do not have to be handcrafted
  - when we specify a network has N layers, this does not include the input layer

- in the 2-layer network from Figure 1:
  - layers are the input, hidden, and output layer
  - $x \in \mathbb{R}^3$ inputs are processed into a four dimensional intermediate representation $h \in \mathbb{R}^4$
    - this representation is then transformed into a two dimensional output $z \in \mathbb{R}^2$
  - can express the outputs of each layer:

$$\begin{bmatrix} h_1 \\ \vdots \\ h_4 \end{bmatrix} = f\left(\begin{bmatrix} w_{11} & w_{12} & w_{13} \\ \vdots & \vdots & \vdots \\ w_{41} & w_{42} & w_{43} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + b_1 \right)$$

$$h = f(W_1 x + b_1)$$

$$z = W_2 h + b_2$$

    - applying f to a vector applies the function elementwise
  - $W_1 \in \mathbb{R}^{4\times 3}$, $W_2 \in \mathbb{R}^{2\times 4}$, $b_1 \in \mathbb{R}^4$, and $b_2 \in \mathbb{R}^2$
  - network has 6 neurons not counting the input, 20 weights, and 6 biases
    - for a total of 26 learnable parameters
  - convolutional neural networks typically have on the order of hundreds of millions of parameters

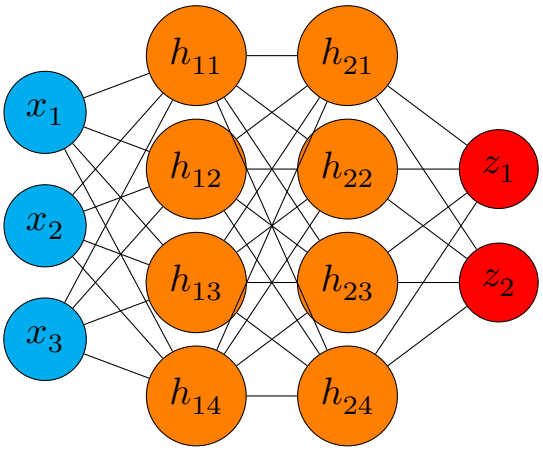


Figure 2: 3-Layer Neural Network

    - with more hidden layers, can potentially extract even more features and make the data more linearly separable

- in the 3-layer network from Figure 2:
  - we now have two hidden layers h_1, h_2 and three sets of weights w_1, w_2, w_3
  - this network is a **fully connected network (FC network)** where all neurons of one layer are connected to all neurons of the next
    - AKA a **multi-layer perceptron (MLP)** or a **feed-forward network**
  - outputs at layers:

$$h_1 = f(W_1 x + b_1)$$
$$h_2 = f(W_2 x + b_2)$$
$$z = W_3 h_2 + b_3$$

  - network has 10 neurons, 36 weight, and 10 biases

Defining the 3-layer network in Python:

```
f = lambda x: x * (x > 0)
h1 = f(np.dot(W1, x) + b1)
h2 = f(np.dot(W2, h1) + b2)
z  = np.dot(W3, h2) + b3
```

Nonlinear Activation Functions

- what if we set f to just be the identity function ie. another linear operation:
  - then, each layer can be composed linearly of the previous one eg. $h_2 = W_2(W_1 x + b_1) + b_2$

    - but in this, case we simply have yet another linear mapping $h_2 = \tilde{W}x + \tilde{b}$ where $\tilde{W} = W_2W_1$ and $\tilde{b} = W_2b_1 + b_2$
  - ie. any composition of linear functions can be reduced to a single linear function:

$$\tilde{W} = W_N ... W_2W_1$$
$$\tilde{b} = b_N + W_Nb_{N-1} + ... + W_N ... W_2b_1$$

  - this severely limits the computations we can perform, so we should not set f to be linear
    - eg. cannot solve the XOR problem
  - however, this may be useful in some contexts:
    - eg. when $dim(h) \ll dim(x)$, this corresponds to finding a low-rank representation of the inputs
    - ie. performing **dimensionality reduction** to compress the features of the input into fewer ones
- instead we want to introduce nonlinearity to increase the network capacity:
  - introduce the nonlinearity f at the output of each artifical neuron
  - f is also called the **activation function**
  - f is not typically applied on the output layer z:
    - z can be interpreted as scores that a softmax or SVM classifier will use to classify the input data
    - eg. the final hidden layer output h_{N-1} acts as the input vector into $softmax(z')$ where $z' = z = W_Nh_{N-1} + b_N$
  - "one recurring theme through neural network design is that the gradient of the cost function ($\frac{\partial L}{\partial W}$) should be large and predictable enough to serve as a good guide for the learning algorithm" — Goodfellow et al.
    - important consideration when choosing nonlinears ie. activation functions

- **sigmoid** activation function:

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

$$\frac{d\sigma(x)}{dx} = \sigma(x)(1 - \sigma(x))$$

  - *pros*:
    - around $x = 0$, the unit behaves linearly
    - is differentiable everywhere
  - *cons*:
    - at extremes, the unit *saturates* and thus has zero gradient:
      - leads to slower or no learning in these areas

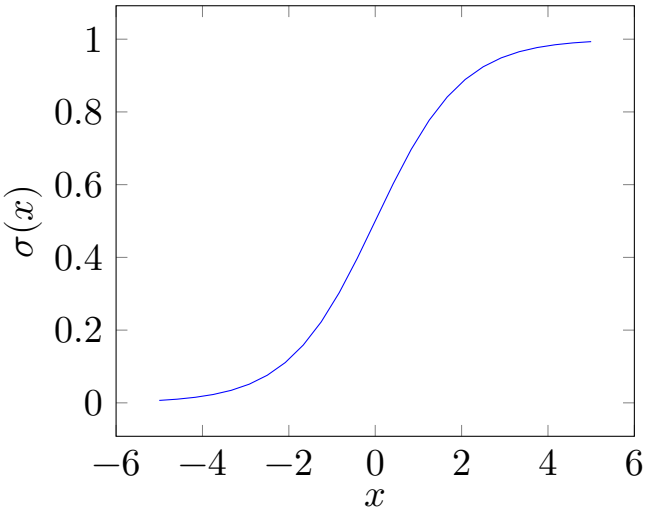


Figure 3: Sigmoid Function

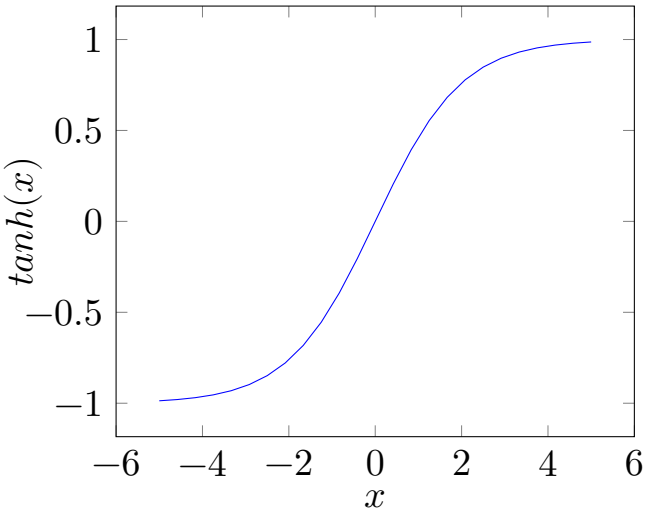


Figure 4: Hyperbolic Tangent Function

  - even if you scale ϵ to be larger, the gradient is still near zero or is not as informative for meaningful learning
* the sigmoid is centered around 0.5 and not zero-centered, causing the **zig-zagging problem** during gradient descent:
  - occurs because the sigmoid is always non-negative
  - the elements of the gradient are all ≥ 0, so $\frac{\partial L}{\partial W}$ will have either *all* entries positive or negative causing the descent to go back and forth
  - in practice, zig-zagging not very much of a problem

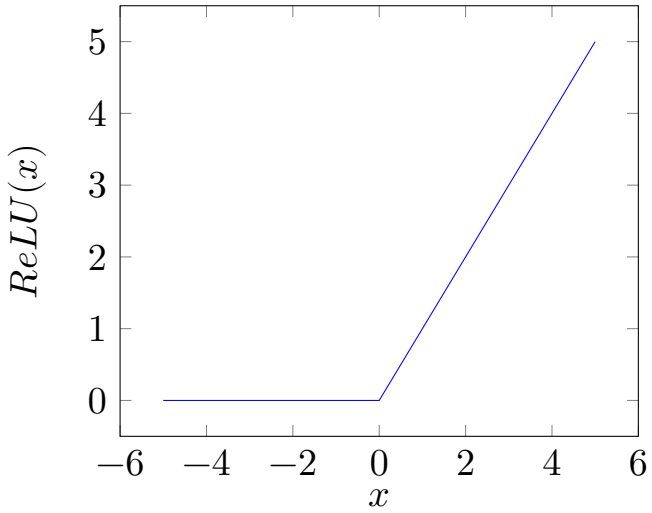


Figure 5: ReLU Function

- **hyperbolic tangent** activation function:

$$tanh(x) = 2\sigma(x) - 1$$

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

  - essentially a zero-centered sigmoid
  - *pros*:
    - around $x = 0$, the unit behaves linearly
    - is differentiable everywhere
    - is zero-centered
  - *cons*:
    - at extremes, also saturates

- **rectified linear unit (ReLU)** activation function:

$$ReLU(x) = max(0, x)$$

$$\frac{dReLU(x)}{dx} = \mathbb{1}(x)$$

  - though this function is nonlinear, it is essentially a piecewise linear function, so is this enough to give modeling capacity?
    - yes, is *still* a nonlinearity
  - ReLU is not differentiable at $x = 0$, but we can set its subgradient there to be either the left or right gradient 0 or 1
  - *pros*:
    - in practice, learning with ReLU converges faster than sigmoid and $tanh$

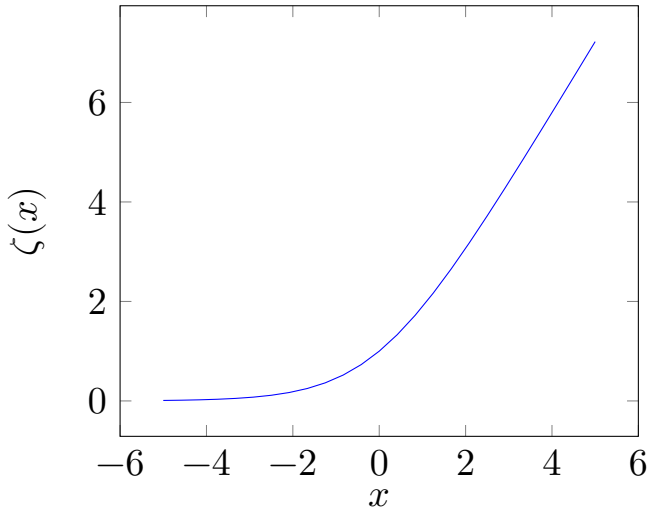


Figure 6: Softplus Function

    - derivative is always 0 or 1
    - there is no saturation if $x > 0$
  - *cons*:
    - not zero-centered and zigzags
    - not differentiable at x = 0
      - in practice, the subgradient estimation here is reasonable given digital computation is already subject to numerical error
    - learning does not happen for examples with zero activation
      - can be fixed by using a leaky ReLU or a maxout unit

- **softplus** activation function:

$$\zeta(x) = log(1 + e^x)$$

$$\frac{d\zeta(x)}{dx} = \sigma(x)$$

  - intuitively, softplus resembles ReLU and is differentiable everywhere
  - however, empirically, performs worse than ReLU

- **leaky ReLU** activation function:

$$f(x) = max(\alpha x, x)$$

  - *pros*:
    - leaky ReLU avoids stopping of learning when $x < 0$
  - *cons*:
    - additional parameter α
  - α can be treated as a selected hyperparameter, or even another optimizable parameter in PReLU
  - leaky RELU allows for negative values:

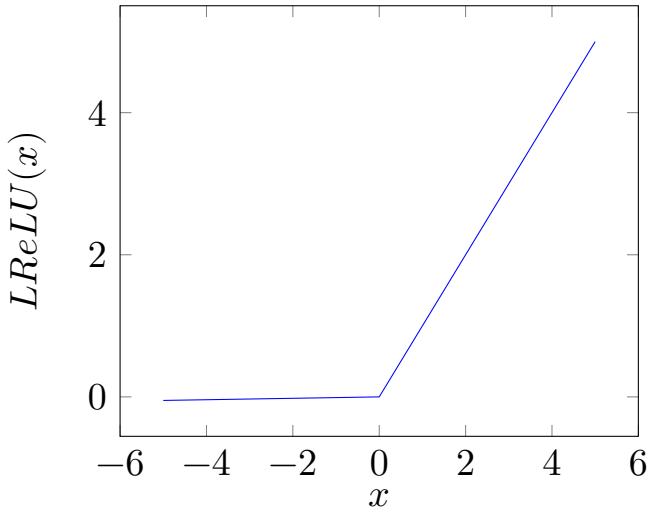


Figure 7: Leaky ReLU Function

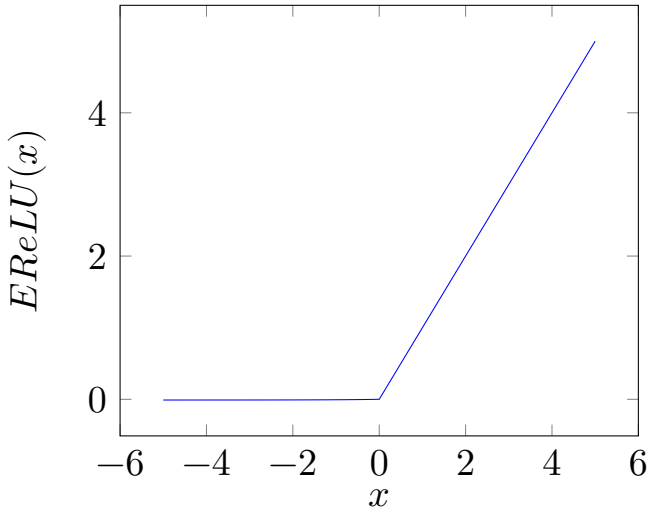


Figure 8: Exponential ReLU Function

    - the activation functions encode the probability neuron will fire
    - what does a negative rate intuitively mean?
        - want best efficiency, so we depart from the biological analogy
    - zero doesn't allow for learning, while a negative value still does

- **exponential linear unit** activation function:

$$f(x) = max(\alpha(e^x - 1), x)$$

    - *pros*:
        - again avoids stopping of learning when $x < 0$
    - *cons*:
        - requires more expensive computation of the exponential
- **maxout unit** activation function:

$$maxout(x) = max(W_1^T x + b_1, W_2^T x + b_2)$$

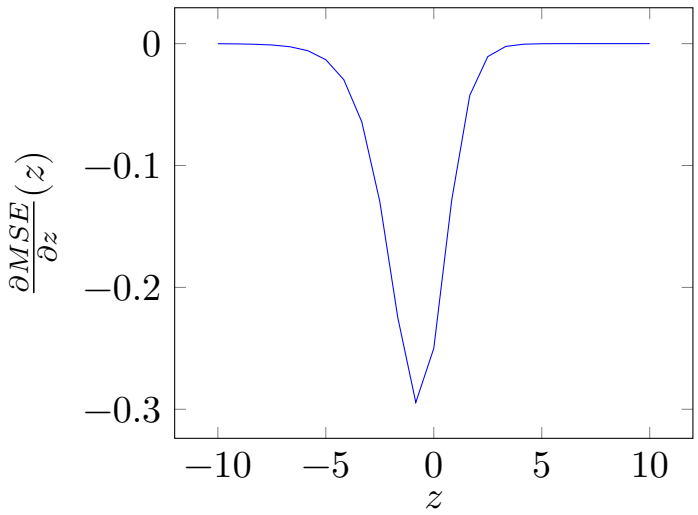


Figure 9: MSE Deriviative wrt. z_i with $y_i = 1$

  - is a generalization of ReLU and PReLU
  - *cons*:
    * doubles the number of parameters
- choosing an activation function in practice:
  - ReLU is very popular
  - sigmoid is almost never used since $tanh$ is preferred
  - leaky ReLU, PReLU, ELU, and maxout may be worth trying out for different applications

Output Activations

- there are different ways to process the output scores z to arrive at a cost function:
  - a linear output unit $\hat{y} = z$:
    * these units typically specify the conditional mean of a Gaussian distribution ie. $p(y|z) = \mathcal{N}(z, I)$
    * in this case, the maximum-likelihood estimation is equivalent to using a mean-squared error, rather than the typical cross-entropy loss
  - a sigmoid output $\hat{y} = \sigma(z)$
    * typically used in binary classification to approximate a Bernoulli distribution
  - a softmax output activation unit where $\hat{y}_i = softmax_i(z)$:
    * softmax is the generalization of the sigmoid to multiple classes
    * this the most common output activation
- ex. Consider a binary classification that outputs a single score z with the

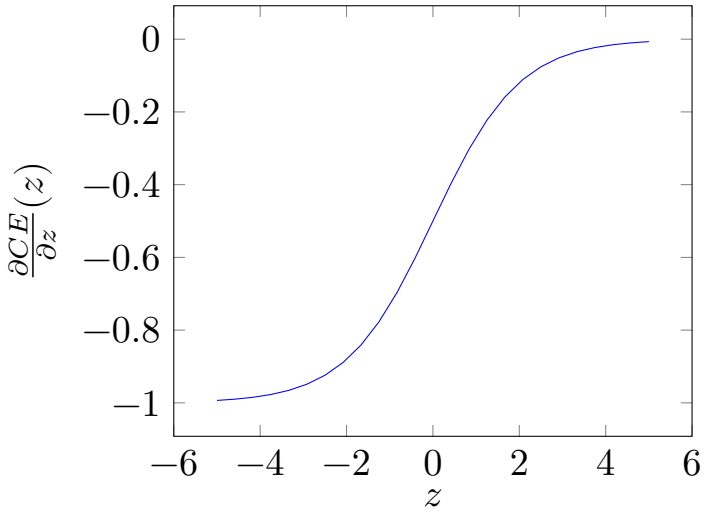


Figure 10: CE Deriviative wrt. z_i with $y_i = 1$

sigmoid chosen as the output unit:

- thus $\hat{y}_i = \sigma(z_i)$ for a training example i
  - the sigmoid function returns a score between 0 and 1 for each input x_i representing the probability x_i is in class 1
- two considerations for the cost function are mean-square error or cross-entropy (ie. MLE) specifically for binary classification:

$$MSE = \frac{1}{2}\sum_{i=1}^{n}(y_i - \sigma(z_i))^2$$

$$CE = -\sum_{i=1}^{n}[y_i log(\sigma(z_i)) + (1 - y_i)log(1 - \sigma(z_i))]$$

- a large positive z_i should indicate the data belongs to class 1, and thus $\hat{y}_i = 1$
  - while a large negative z_i should indicate the data belongs to class 0, and thus $\hat{y}_i = 0$
- consider using MSE for binary classification with some $x_i, y_i = 1$ and $z_i = -50$:

$$\begin{aligned}\frac{\partial MSE}{\partial z_i} &= \frac{\partial MSE}{\partial \sigma(z_i)} \cdot \frac{\partial \sigma(z_i)}{\partial z_i} \\ &= -2(y_i - \sigma(z_i))(\sigma(z_i)(1 - \sigma(z_i)))\end{aligned}$$

  - for this specific z_i, since $\frac{\partial \sigma(z_i)}{\partial z_i} \approx 0$, from the graph of sigmoid, we can intuitively guess that $\frac{\partial MSE}{\partial z_i}$ will be close to 0
  - in fact, we can see from the Figure 9 that when z is very negative ie. the classification is strongly incorrect, the derivative ie. the gradient saturates to 0

        - thus no learning occurs in this region!
    - however, this is where we would like *much* learning to occur ie. want the derivative to be significant to enough to move towards the right classification
        - on the other hand, it is acceptable that the gradient saturates to 0 when z is very positive since in this case the classification is correct
    - note that the term y_i appears in the derivative, which flips the graph when $y_i = 0$ so that the same issue appears for the other class
- now consider using CE for the same binary classification with x_i, y_i, z_i:

$$\frac{\partial CE}{\partial z_i} = \sigma(z_i) - 1$$

    - in this case, as seen in Figure 10, when z is very negative, learning will still occur
        - in fact the derivative is largest ie. we have the steepest change in this region
    - learning only begins to *stall* ie. take smaller gradient steps once z approaches the right answer
    - note that this calculation is specific to $c = 2$ and $y_i = 1$
        - when $y_i = 0$, the graph would similarly flip so that learning again correctly stalls when z approaches the desired answer
- thus we should *always* use cross-entropy loss when using softmax AKA sigmoid as the output unit
    - note that MSE may still be appropriate for other problems eg. regressions

Backpropagation

- now that the architecture of a neural network has been defined, including activation and output functions, how do we learn its parameters?
    - by using versions of gradient descent
    - however, these networks have several layers:
        - the parameters in the earliest layers are far removed from the loss function
        - need to use a technique called backpropagation to calculate the gradient of the loss function with respect to parameters
- **backpropagation** is an application of the chain rule for derivatives:
    - in a neural network, the weights in the earlier layers are connected to the loss function through a composition of functions:
        - ie. $h_N = f(h_{N-1}) = f(f(h_{N-2})) = ...$

    - thus computing the gradient should involve repeated applications of the chain rule
  - in **foward propagation**, we calculate the values of the hidden and output units of a neural network given an input:
    - take input x, and propagate it through each hidden unit sequentially until we get output y
    - also gives the cost function $J(\theta)$
    - the foward propagated signals are the **activations**
  - in backpropagation AKA backprop:
    - information is passed *backwards* from the cost function and outputs back to inputs
    - the backpropagated signals are the **gradients**
    - enables the calculation of gradients at every stage going back to the input layer
    - eg. want to calculate $\frac{\partial L}{\partial W_1}$ from $\frac{\partial L}{\partial W_2}$
    - note that the backprop operations requires knowing the foward propagated activation values
      - ie. perform a forward pass into a backward pass
    - can consider the cost function as a **computation graph** ie. a directed acyclic graph where each node in the graph denotes a mathematical operation
  - compared to analytical gradients:
    - evaluating analytical gradients may be computationally expensive
    - backprop is generalizable ie. modular and often inexpensive
      - eg. libraries such as Tensorflow and PyTorch can take gradients of arbitrary functions using a generalized, mechanized backprop algorithm
    - want to share repeated computations whenever possible
  - note that backprop is *not* the learning algorithm, it is only the method of computing gradients
    - the learning algorithm used with backprop is stochastic gradient descent
  - in addition, backprop is not specific to NNs, but is a general way to compute function derivatives

- from Figure 11, we can calculate backprop derivatives (in red) as follows,

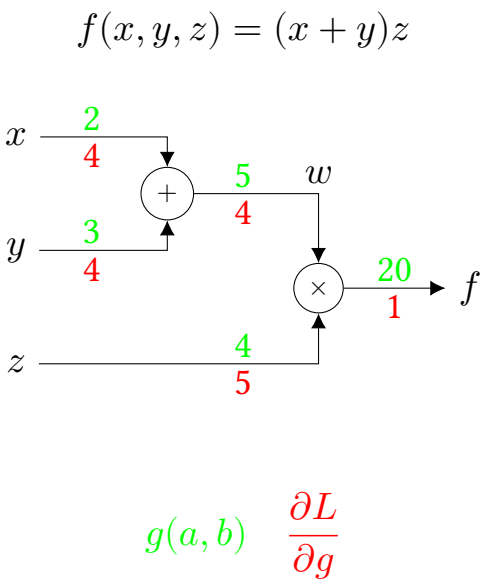


Figure 11: Simple Backprop Example

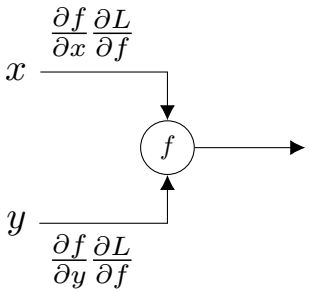


Figure 12: Backward Pass Step

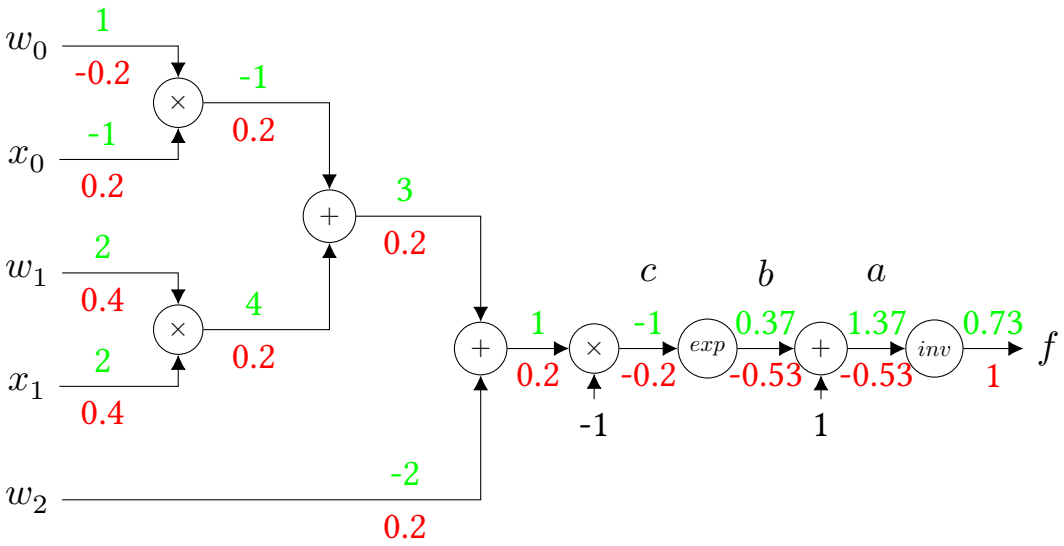
where we let $L = f$ and $\frac{\partial L}{\partial f} = 1$:

$$
\begin{aligned}
f &= w \cdot z \\
\frac{\partial f}{\partial z} &= w, \quad \frac{\partial f}{\partial w} = z \\
w &= x + y \\
\frac{\partial w}{\partial x} &= 1, \quad \frac{\partial w}{\partial y} = 1 \\
\frac{\partial L}{\partial z} &= \frac{\partial f}{\partial z}\frac{\partial L}{\partial f} = w \cdot 1 = 5 \\
\frac{\partial L}{\partial w} &= \frac{\partial f}{\partial w}\frac{\partial L}{\partial f} = z \cdot 1 = 4 \\
\frac{\partial L}{\partial x} &= \frac{\partial w}{\partial x}\frac{\partial L}{\partial w} = 1 \cdot 4 = 4, \quad \frac{\partial L}{\partial y} = \frac{\partial L}{\partial x} = 4
\end{aligned}
$$

  - in the forward pass, we simply apply a function to the node inputs to calculate the output
  - in the backwards pass, we take the **upstream derivative** and apply a **local gradient** to calculate to backpropagated derivative
    * in Figure 12, the upstream derivative is $\frac{\partial L}{\partial f}$ and the local gradients are $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial y}$
- the intuition of backprop:
  - break up the calculation into *small* and simple steps
  - each node is the graph represents a straightforward gradient calculation through multiplying an input with an application of the chain rule
    * composing the gradients together returns the overall gradient
  - with backprop, as long as we can break the computation into components where we know the local gradients, we can find the gradient of anything
  - note that in the foward pass, calculations are cached so that performing backprop is not as expensive as doing an analytic computation
- additionally, we can also interpret backpropagation as acting as different types of gradient *gates* depending on the function f:
  - an add gate distributes the gradient:

$$
\begin{aligned}
f &= x + y \\
\frac{\partial f}{\partial x} &= 1, \quad \frac{\partial f}{\partial y} = 1 \\
\frac{\partial L}{\partial x} &= \frac{\partial L}{\partial f}, \quad \frac{\partial L}{\partial y} = \frac{\partial L}{\partial f}
\end{aligned}
$$

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



$g(a,b)$ $\frac{\partial L}{\partial g}$

Figure 13: More Involved Scalar Example

– a *mult* gate switches the gradient:

$$f = x \times y$$
$$\frac{\partial f}{\partial x} = y, \quad \frac{\partial f}{\partial y} = x$$
$$\frac{\partial L}{\partial x} = y\frac{\partial L}{\partial f}, \quad \frac{\partial L}{\partial y} = x\frac{\partial L}{\partial f}$$

– a *max* gate routes the gradient:

$$f = max(x,y)$$
$$\frac{\partial f}{\partial x} = \mathbb{1}(x > y), \quad \frac{\partial f}{\partial y} = \mathbb{1}(y > x)$$
$$\frac{\partial L}{\partial x} = \mathbb{1}(x > y)\frac{\partial L}{\partial f}, \quad \frac{\partial L}{\partial y} = \mathbb{1}(y > x)\frac{\partial L}{\partial f}$$

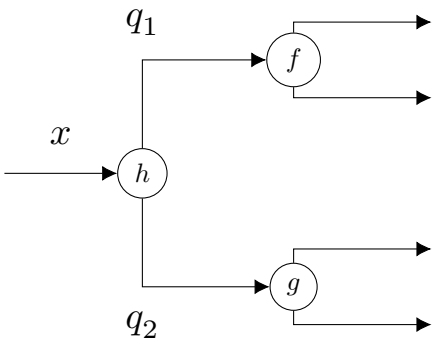


Figure 14: Converging Gradient Paths

- performing backprop on Figure 13:

$$\begin{aligned} f &= \frac{1}{a} \\ \frac{\partial f}{\partial a} &= -\frac{1}{a^2} \\ \frac{\partial L}{\partial a} &= \frac{\partial f}{\partial a}\frac{\partial L}{\partial f} = (-\frac{1}{1.37^2}) \cdot 1 = -0.53 \end{aligned}$$

$$\begin{aligned} b &= e^c \\ \frac{\partial b}{\partial c} &= e^c \\ \frac{\partial L}{\partial c} &= \frac{\partial b}{\partial c}\frac{\partial L}{\partial b} = e^{-1} \cdot -0.53 = -0.2 \end{aligned}$$

  - the rest of the calculation involves patterns with gradient gates we have already derived

- when we have converging gradient paths as in Figure 14, the calculation differs
  - by the law of total derivatives:

$$\frac{\partial L}{\partial x} = \sum_{i=1}^{n} \frac{\partial L}{\partial q_i} \cdot \frac{\partial q_i}{\partial x}$$

  - thus we have:

$$\begin{aligned} \frac{\partial L}{\partial x} &= \frac{\partial q_1}{\partial x}\frac{\partial L}{\partial q_1} + \frac{\partial q_2}{\partial x}\frac{\partial L}{\partial q_2} \\ &= \frac{\partial L}{\partial q_1} + \frac{\partial L}{\partial q_2} \end{aligned}$$

    * typically h is the identity function when gradient paths converge, so $\frac{\partial q_1}{\partial x} = 1$ and $\frac{\partial q_2}{\partial x} = 1$

$$y = softplus(x) = log(1 + e^x)$$

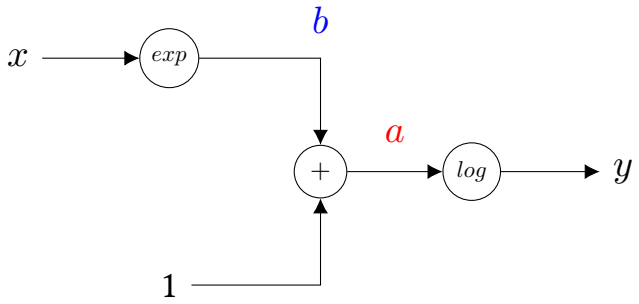


Figure 15: Backprop for Softplus

- from Figure 15, we can compute the derivative of the softplus function in two ways:
  - we can analytically find:

$$\frac{dy}{dx} = \frac{e^x}{1 + e^x}$$

  - or alternatively, we can use backprop:

$$\begin{aligned}
\frac{dy}{da} &= \frac{d}{da} log(a) = \frac{1}{a} \\
\frac{dy}{db} &= \frac{da}{db}\frac{dy}{da} = \frac{dy}{da} \\
\frac{dy}{dx} &= \frac{db}{dx}\frac{dy}{db} = e^x \frac{1}{a}
\end{aligned}$$

- to perform multivariate backpropagation, we need to use the multivariate chain rule:
  - to take the derivative of a vector with respect to a vector, construct the Jacobian J that tells us how $\Delta y \approx J\Delta x$ and $J = \nabla_x y^T$
  - eg. we will often need to take the derivative of Wx with respect to x where $W \in \mathbb{R}^{h \times n}$, $x \in \mathbb{R}^n$, and $f \in \mathbb{R}^h$:

$$\begin{aligned}
\nabla_x Wx &= \nabla_x \begin{bmatrix} w_{11}x_1 + ... + w_{1n}x_n \\ \vdots \\ w_{h1}x_1 + ... + w_{hn}x_n \end{bmatrix} \\
&= \begin{bmatrix} w_{11} \dots w_{h1} \\ \vdots \ddots \vdots \\ w_{1n} \dots w_{hn} \end{bmatrix} \\
&= W^T
\end{aligned}$$

$$h = ReLU(Wh_i + b)$$

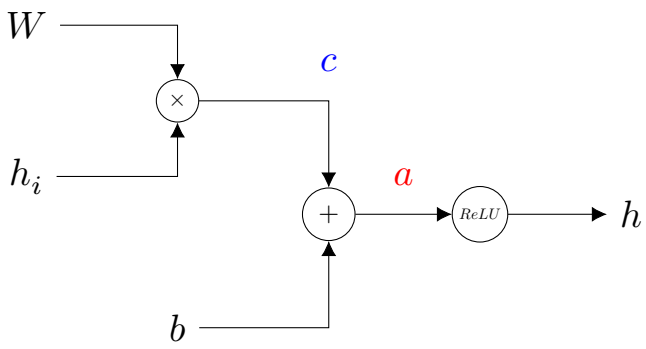


Figure 16: Backprop for a NN Layer

  * expect $\nabla_x Wx \in \mathbb{R}^{n \times h}$

- consider Figure 16, where we perform backprop on a neural network layer that is using $ReLU$ as an activation function:
  - note that $h \in \mathbb{R}^h, h_i \in \mathbb{R}^m, W \in \mathbb{r}^{h \times m}, b \in \mathbb{R}^h$
    * h_i represents the calculation of a previous layer
  - doing backprop from h given some $\frac{\partial L}{\partial h}$ that depends on the chosen loss function:

$$\begin{aligned}
\frac{\partial L}{\partial a} &= \mathbb{1}(a > 0) \bigodot \frac{\partial L}{\partial h} \\
\frac{\partial L}{\partial c} &= \frac{\partial L}{\partial b} = \frac{\partial L}{\partial a} \\
\frac{\partial L}{\partial h_i} &= \frac{\partial c}{\partial h_i}\frac{\partial L}{\partial c} = W^T \frac{\partial L}{\partial c} \\
\frac{\partial L}{\partial W} &= \frac{\partial c}{\partial W}\frac{\partial L}{\partial c} = \frac{\partial L}{\partial c} h_i^T
\end{aligned}$$

    * notes on calculation:
      · $ReLU(x) = max(0, x)$ is just a gradient gate
      · $\frac{\partial c}{\partial h_i} = \frac{\partial}{\partial h_i} Wh_i = W^T$
      · the Hadamard product $C = A \bigodot B$ performs elementwise multiplication such that $C_{ij} = A_{ij} B_{ij}$
    * sometimes derivatives will be expressed in Python as transposes to facilitate broadcasting or faster execution
      · eg. $(\frac{\partial L}{\partial h_i})^T = \frac{\partial L}{\partial c}^T W$
  - intuition behind calculating $\frac{\partial c}{\partial W}$:
    * this is a derivative of a vector with respect to a matrix, which is a tensor derivative

- however, we can use intuitively consider matrix dimensions to find the answer without a rigorous derivation as seen in the appendix

* consider the following previous vector-matrix derivatives we have calculated:

$$\nabla_h h^T y = y$$
$$\nabla_h W h = W^T$$

- thus $\frac{\partial}{\partial W} W h_i$ should *look like* h_i^T

* note that $\frac{\partial L}{\partial W} \in \mathbb{R}^{h \times m}$ and $\frac{\partial L}{\partial c} \in \mathbb{R}^{h \times 1}$, and we can construct the desired matrix of dimension $(h \times m)$ by multiplying a column vector $(h \times 1)$ with a row vector of dimension $(1 \times m)$
* thus by shuffling dimensions:

$$\frac{\partial L}{\partial W} = \frac{\partial L}{\partial c} h_i^T$$

- with dimensions $(h \times 1)(1 \times m) = (h \times m)$

Optimizing Neural Networks

- several techniques can be used to aid training of neural networks
  - eg. weight initialization, batch normalization, regularizations, dataset augmentation

Weight Initialization

- how do we determine what values our weights should start at?
  - generally want to use some sort of Gaussian distribution for each layer, but what should the variances of the distribution be?
    - eg. small vs. large, using some heuristic, etc.
  - note that handling initializations only affects the early iterations, and doesn't deal with other issues with training that may arise in later iterations
- using *small* random weight initializations:
  - motivated by the fact that we don't want large initial values that may bias training
  - empirically, with ReLU nonlinearities, this initialization causes all activations to *decay* to zero
    - activations are the outputs of each layer ie. later layers output approach zero
  - when we consider backprop with a small weight initialization:
    - backpropagating over later layers gives a gradient ≈ 0
    - must propagate through a multiplication gate that multiplies by layers where $h_n \approx 0$
  - other activations such as $tanh$ have these same undesired properties as ReLU with small weight initializations
  - may be appropriate in much smaller neural networks
- using *large* random weight initializations:
  - empirically, this initialization coupled with ReLU causes the units to explode in magnitude
    - gradients become much too large, leading to zig-zagging
  - for $tanh$, leads to highly saturated activation regions with small gradients and thus little to no learning
- in **Xavier initialization**:
  - argues that the variance of all units across all layers ought to be the same:
    - similarly for backpropagated gradients
    - motivated by the assumption that the input itself has equal variance

across all dimensions
  - concretely, for any unit in the ith layer h_i
    * $\mathbb{E}(h_i) = \mathbb{E}(h_j)$, $var(h_i) = var(h_j)$, and $var(\nabla_{h_i} J = \nabla_{h_j} J)$
- then we can argue the following, where n_{in} is the number of units in the previous $(i-1)$th layer:

$$\begin{aligned} h_i &= \sum_{j=1}^{n_{in}} w_{ij} h_{i-1,j} \\ var(wh) &= \mathbb{E}^2(w) var(h) + \mathbb{E}^2(h) var(w) + var(w) var(h) \\ &= var(w) var(h) \end{aligned}$$

$$var(h_i) = var(h_{i-1}) \cdot \sum_{j=1}^{n_{in}} var(w_{ij})$$

$$\sum_{j=1}^{n_{in}} var(w_{ij}) = \frac{var(h_i)}{var(h_{i-1})} = 1$$

$$n_{in} \cdot var(w_{ij}) = 1$$

$$var(w_{ij}) = \frac{1}{n_{in}}$$

  - assumptions:
    * all units are linear
    * $\mathbb{E}(w) = \mathbb{E}(h) = 0$
      · only works for $tanh$ since ReLU does not have an expected value of 0
    * w_{ij} and h_{i-1} are independent, allowing their variances to be separated
    * we want all weights to become identically distributed
  - the same argument can be made for the backpropagated gradients to argue that $var(w_{ij}) = \frac{1}{n_{out}}$
    * where n_{out} is the number of units in the next layer
  - thus, we have the following:

$$n_{avg} = \frac{n_{in} + n_{out}}{2}$$

$$var(w_{ij}) = \frac{1}{n_{avg}}$$

    * ie. initialize each weight in layer i to be drawn from $\mathcal{N}(0, \frac{2}{n_{in}+n_{out}})$
- however, as previously mentioned, this Xavier initialization typically leads to dying ReLU units:

  - in the He initialization, an additional normalizer factor of 2 is used with ReLU
  - motivated by the intuitiion that half of linear activations should be killed by ReLU, which should decrease the variance by half
  - ie. set the variance of each unit to $var(w_{ij}) = \frac{2}{n_{avg}}$

Normalization

- two large subsets of samples of the same class may lie in *different* regions of the feature space:
  - this difference in distribution within the same class is called **covariate shift**
  - empirically, if there is covariate shift in the chosen minibatches used for training, training is very slow
    - when the minibatches have their images uniformly sampled from the entire distribution, there is *neglible* covariate shift
  - thus covariate shift on the *input* layer alone can be addressed by randomizing by randomizing the data before creating minibatches
    - but how do we address this covariate shift as we move *deeper* into the network?
- normalization is motivated by the related problem of internal covariate shift:
  - an obstacle to standard training is that the distribution of inputs to each layer changes as learning occurs in *previous* layers:
    - thus the unit activations can be very variable, especially for later layers
    - ie. every time there is an update of weights for earlier layers, the *distribution* of later layers changes
      - this is exactly the phenomenon of **internal covariate shift**
  - in addition, when we do gradient descent, we calculate how to update each parameter *assuming* the other layers do not change:
    - but these layers may change drastically
    - ie. $\frac{\partial L}{\partial W_i}$ tells how L changes if W_i *alone* is "wiggled"
  - *cons*:
    - learning rates may be forced to be smaller than if the distributions were not so variable
      - training is thus very slow
    - networks are more sensitive to initializations
    - difficulties in networks that saturate, where learning will no longer occur
  - one technique may be to only change a single W_i at a time, but this will drastically increase the training time by a factor of the number of layers

  - internal covariate shift can be solved by normalizing the inputs for each layer over a minibatch through batch-normalization
- but more recently, there are studies that show that batch-norm regularization is effective for another signifcant reason other than just addressing internal covariate shift:
  - the K-**Lipschitz** value expresses how *smooth* a function is:
    * essentially calculated as change in output over change in input
    * ie. gives a *cone* on each point of the function that indicates areas the function cannot cross through
      · slope of the cone tells how much "wiggle" room it has
    * a smaller K indicates the function is more smooth
      · ie. the cone is wider and the output thus doesn't vary dramatically
  - when a function is β-smooth, its gradient ∇f is β-Lipschitz:
    * constrains how dramatically the derivative can change
      · ie. how smooth the loss surface is
    * the smoother the loss function, the bigger steps we can take with respect to its gradient
      · ie. derivatives are more reliable
  - batch-norm makes the gradient smoother by increasing its β-smoothness
    * recent studies show that batch-norm does not really even address its purpoted issue of internal covariate shift
- the idea of **batch-normalization** is to normalize the output of each layer to have unit statistics:
  - learning then becomes simpler because parameters in the lower layers do not change the statistics of the input to a given layer
    * note that we are not *changing* layers, but instead *standardizing* (to unit variance and mean 0) ie. *transforming* them to a different area of the feature space
  - ie. for a layer $h_i = relu(x_i)$, want $\mathbb{E}(x_i) = 0$ and $var(x_i) = 1$
  - the batch-norm component can be placed in different positions:
    * in the original paper, the batch-norm was performed after the affine unit but before the ReLU such that $h_i = f(batchnorm(W_i h_{i-1} + b_i))$
      · note that putting this batch-norm before ReLU will actually initially kill off half the activations
    * more recently, it has become common practice to perform batch-norm after the activation to improve performance
  - another issue with batch-norm is that it may force features to be learned a certain way ie. with unit mean and variance:
    * batch-norm will thus provide an alternative way to change the mean and variance as extra parameters through rescaling and

shifting
    - allows network to undo batch-norm for specific features
  - thus batch-norm with parameters *encourages* the network to start with unit statistics, but gives a way to *undo* the normalization in case the network finds a more optimal way to learn
    - empirically, allows higher learning rates to be used and reduces strong dependence on initialization
  - relatively modern technique, introduced by a paper in 2015 by Google researchers Ioffe and Szegedy
  - *pros*:
    - higher learning rates since gradients do not saturate ie. explode or vanish as easily
      - also makes gradient propagation more stable
    - brings in a regularization effect
      - allows dropout regularization to be dropped or reduced in strength
    - allows saturating non-linearities to be used
    - more robust ie. less sensitive to hyperparameters and initialization
    - empirically, initial and converged validation accuracy is improved with batch-norm
      - in addition, convergence is faster
- in practice, to implement batch-norm, we can do the following:

$$\hat{x}_i = \frac{x_i - \mu_i}{\sqrt{\sigma_i^2 + \varepsilon}}$$
$$\mu_i = \frac{1}{m}\sum_{j=1}^{m} x_i^{(j)}$$
$$\sigma_i^2 = \frac{1}{m}(x_i^{(j)} - \mu_i)^2$$
$$y_i = \gamma_i \hat{x}_i + \beta_i$$

  - batch-norm is done over each minibatch where m is the number of examples in the minibatch:
    - note that if the minibatch is size 1, the gradient with respect to the input will disappear, since $\mu_i = x_i$
    - typically, minibatches of size power 2 are used eg. 64
  - scaling is done on a *per unit* rather than a per layer basis for computational efficiency:
    - the i subscript indicates the unit of the network ie. $x_i^{(j)}$ represents the jth example on the ith unit
    - to normalize the entire layer, we would have to use covariance matrix multiplication ie. $\Sigma^{\frac{-1}{2}}(x - \mu)$

$$y_j = batchnorm(x_j, \varepsilon)$$

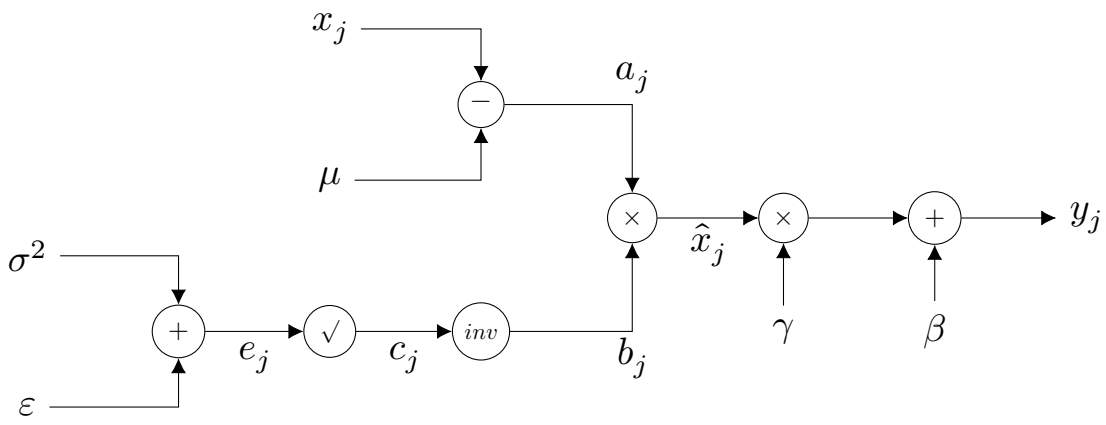


Figure 17: Backprop for Batch-Norm

  - · requires expensive matrix inversion and multiplication to backprop through
- scaling and shifting parameters γ_i, β_i are applied *per unit* in order to allow the network to rescale the activations and thus undo the normalization
  - * note that these are parameters to be learned jointly with other model parameters, ie. are not hyperparameters
- ε is a small hyperparameter to avoid division by zero

- calculating the backprop of batch-norm from the computational graph in Figure 17, for a single unit i (the i subscript is dropped from the calculation for

simplicity):

$$\begin{aligned}
\frac{\partial L}{\partial \beta} &= \sum_{j=1}^{m} \frac{\partial L}{\partial y_j} \\
\frac{\partial L}{\partial \gamma} &= \sum_{j=1}^{m} \frac{\partial L}{\partial y_j} \hat{x}_j \\
\frac{\partial L}{\partial \hat{x}_j} &= \frac{\partial L}{\partial y_j} \gamma \\
\frac{\partial L}{\partial a_j} &= \frac{1}{\sqrt{\sigma^2 + \varepsilon}} \frac{\partial L}{\partial \hat{x}_j} \\
\frac{\partial L}{\partial \mu} &= -\frac{1}{\sqrt{\sigma^2 + \varepsilon}} \sum_{j=1}^{m} \frac{\partial L}{\partial \hat{x}_j} + \frac{\partial \sigma^2}{\partial \mu} \frac{\partial L}{\partial \sigma^2} \\
&= -\frac{1}{\sqrt{\sigma^2 + \varepsilon}} \sum_{j=1}^{m} \frac{\partial L}{\partial \hat{x}_j} - \frac{\partial L}{\partial \sigma^2} \frac{2}{m} \sum_{j=1}^{m} (x_j - \mu) \\
\frac{\partial L}{\partial b_j} &= (x_j - \mu) \frac{\partial L}{\partial \hat{x}_j} \\
\frac{\partial L}{\partial c_j} &= -\frac{1}{\sigma^2 + \varepsilon} (x_j - \mu) \frac{\partial L}{\partial \hat{x}_j} \\
\frac{\partial L}{\partial e_j} &= -\frac{1}{2} \frac{1}{(\sigma^2 + \varepsilon)^{\frac{3}{2}}} (x_j - \mu) \frac{\partial L}{\partial \hat{x}_j} \\
\frac{\partial L}{\partial \sigma^2} &= \sum_{j=1}^{m} \frac{\partial L}{\partial e_j}
\end{aligned}$$

- note that the law of total derivatives used to sum up all the gradients over all m training examples
- now, σ^2 and μ are both dependent on x, so we can use the law of total derivatives again:

$$\begin{aligned}
\frac{\partial L}{\partial x_j} &= \frac{\partial L}{\partial a_j} + \frac{\partial \sigma^2}{\partial x_j} \frac{\partial L}{\partial \sigma^2} + \frac{\partial \mu}{\partial x_j} \frac{\partial L}{\partial \mu} \\
&= \frac{1}{\sqrt{\sigma^2 + \varepsilon}} \frac{\partial L}{\partial \hat{x}_j} + \frac{2(x_j - \mu)}{m} \frac{\partial L}{\partial \sigma^2} + \frac{1}{m} \frac{\partial L}{\partial \mu}
\end{aligned}$$

Regularization

- **regularization** is any modification we make to a learning algorithm that is intended to reduce its generalization error but not its training error:
  - ie. used to improve the *generalizability* of the model and reduce overfitting
  - it may be appropriate to choose a large model while regularizing it, without worrying about the danger of overfitting that comes with increased complexity
- there are many different forms of regularization:
  1. adding a soft constraint on parameter values in the objective function:
     - to account for prior knowledge eg. parameters have a bias
     - to prefer simpler model classes that promote generalization
     - to make an undetermined problem determined
  2. dataset augmentation
  3. ensemble methods ie. essentially combining the output of several models
  4. some training algorithms themselves can be seen as a type of regularization
- one common regularization approach is using parameter norm penalties:
  - ie. modifying the cost function with a **parameter norm penalty**, typically denoted $\Omega(\theta)$
    - not specific to neural networks eg. commonly used in linear regression
  - results in a new cost function of the form:

$$L(\theta, X, y) + \alpha\Omega(\theta)$$

    - where $\alpha \geq 0$
  - α is a hyperparameter that weights the contribution of the norm penalty:
    - with $\alpha = 0$, no regularization is being done
    - as $\alpha \to \infty$, the cost function becomes irrelevant and the model will set parameters to minimize $\Omega(\theta)$
    - choice of α can strongly affect generalization performance
- a common parameter norm regularization is to penalize the size of the weights:
  - promotes models with parameters that are closer to 0 and thus "simpler"
  - this is known as L^2 regularization AKA **ridge regression** or Tikhonov regression
  - the regularization is expressed as:

$$\Omega(\theta) = \frac{1}{2}||w||_2^2 = \frac{1}{2}w^T w$$

    - for matrices, we would use the Frobenius norm

  - calculating the gradient:

$$\tilde{L}(w, X, y) = J(w, X, y) + \frac{\alpha}{2} w^T w$$
$$\nabla_w \tilde{J}(w, X, Y) = \alpha w + \nabla_w J(w, X, y)$$

    * in the gradient step, we set w to $(1 - \varepsilon\alpha)w - \varepsilon J(w, X, Y)$
      · the $(1 - \varepsilon\alpha)$ term is known as the weight decay
  - equivalent to maximum a-posteriori inference, where the prior on the parameters has a unit Gaussian distribution ie. $w \sim \mathcal{N}(0, \frac{1}{\alpha} I)$
  - when performing this regularization, the component of w aligned with the ith eigenvector of the Hessian is rescaled by a factor $\frac{\lambda_i}{\lambda_i + \alpha}$
  - in linear regression, the least squares solution becomes:

$$w = (X^T X L + \alpha I)^{-1} X^T y$$

    * scales the variance of each input feature
- other similar forms of L^2 regularization include:
  - instead of a soft constraint that the parameters be small, we may have prior knowledge that w is close to some value b:

$$\Omega(\theta) = ||w - b||_2$$

  - alternatively, we may have prior knowledge two parameters w_1, w_2 ought to be close to each other:

$$\Omega(\theta) = ||w_1 - w_2||_2$$

- in L^1 regularization, we instead define the parameter norm penalty as:

$$\Omega(\theta) = ||w||_1 = \sum_i |w_i|$$

  - also intuitively causes the weights to be small
  - however, the subgradient of $||w||_1$ is $sign(w)$, which makes the gradient the same regardless of the size of w, unlike in L^2 regularization:
    * thus typically results in sparse solutions where $w_i = 0$ for several i
    * in L^2 regularization, due to the squared factor, the gradient when L is small, eg. $\ll 1$, is less emphasized
  - can be useful for **feature selection** where features corresponding to zero weight may be discarded
  - equivalent to to maximum a-posteriori inference, where the prior on the parameters has an isotropic Laplace distribution ie. $w_i \sim Laplace(0, \frac{1}{\alpha})$
  - instead of having sparse parameters, it may be appropriate to have sparse *representations*:
    * ie. in hidden layers h_i, set $\Omega(h_i) = ||h_i||_1$
    * allows certain units h_i to be removed, instead of only weights

Dataset Augmentation

- neural networks achieved much popularity when they were applied for computer vision:
  - **dataset augmentation** is a technique used often in computer vision to improve performance:
    - eg. the same cat in an image is still a cat when the image is fliped, croped, rotated, has brightness adjusted, etc.
    - creates *multiple* data samples from a single training image
    - training on these adjusted images should make the model *more* generalizable and robust
      - can be interpreted as adding additional noise into the network in order to make the loss surface smoother
  - augmentation can be done specifically to target certain desired features we want the network to be robust towards
  - typically, there are heuristics used in order to keep the input sizes the same
    - eg. sampling smaller patches when resizing or scaling
- other types of dataset augmentation:
  - injecting noise into the network
    - can be done at various levels eg. perturbing pixels of the image or perturbing weights and biases
  - in **label smoothing**, instead of having a one-hot representation of the correct class, each class for a training example has an associated probability:
    - eg. one class may have probability 0.9 and the remaining classes a uniform probability distribution of 0.011
    - the correct label-smoothed probability eg. 0.9 can be a hyperparameter
    - helps decrease the error rate of networks

Smarter Learning and Ensembling

- in **multitask learning**, we can have the model trained to perform multiple tasks:
  - intiutively, multiple tasks may share common factors that explain variations in the data
    - ie. solve multiple tasks using similar features
  - pass the input through an encoder that generates shared features for multiple decoders that each perform a task

  - eg. in computer vision, could split into the following tasks:
    * labeling the class of every pixel
    * label all instances of a class
    * determining the depth of an object
  - useful when we know specific sub-tasks the network should work on
  - then we can calculate a *multi-task* loss by summing together the losses from each specific task
    * could weight each task in the overall multi-task loss using a hyper-parameter or even a learnable parameter
  - the entire model need not be shared across different tasks
- in **transfer learning**:
  - we can take neural networks trained in one context and use them in another with little additional training
    * if the tasks are similar enough, then the features at later layers of the network ought to be good features for the *new* task
  - useful when little training data is available, but tasks are similar
    * may need to only train a *single* new linear layer at the output of the *pre-trained* network
  - if more data is available, it may still be a good idea to use transfer learning and tune more of the layers
  - eg. use natural features on MRI images to detect specific pathologies for those medical images
- another way to get a boost in performance for very little cognitive work is to use **ensemble** methods:
  1. train multiple different models
     - models don't have to use the same hyperparameters or even belong to the same class
  2. average their results together at test time
  - almost always increases performance by substantial amounts eg. a few percentage improvment
  - intuitively, want to average out the natural errors that occur when training on a single individual network
    * if models are independent, they will usually not all make the *same* errors on the test set
  - with k independent models, the average model error will decrease by a factor $\frac{1}{k}$:

$$\begin{aligned}\mathbb{E}[(\frac{1}{2}\sum_{i=1}^{k}\varepsilon_i)^2] &= \frac{1}{k^2}\sum_{i=1}^{k}\mathbb{E}\varepsilon_i^2 \\ &= \frac{1}{k}\mathbb{E}\varepsilon_i^2\end{aligned}$$

    * assuming models are independent and $\mathbb{E}(\varepsilon_i, \varepsilon_j) = \mathbb{E}(\varepsilon_i)\mathbb{E}(\varepsilon_j)$

        - in addition assuming $\mathbb{E}\varepsilon_i = 0$ and the error statistics are the same across all models
    - even if the models are not independent, the calculated average model error will still be less than or equal of the error of a single model:

$$\frac{1}{k}\mathbb{E}\varepsilon_i^2 + \frac{k-1}{k}\mathbb{E}(\varepsilon_i\varepsilon_j)$$

- one implementation of ensemble methods is via **bagging** AKA bootstrap aggregation:
    1. construct k datasets using the bootstrap:
        - set a dataset size N
        - draw with replacement from the orignal dataset to get N samples
        - repeat k times
    2. train k different models using the k datasets
    - handles the problem of ensembling that if models are trained on exactly the same datasets, they are probably not completely independent:
        * by bagging with replacement, the datasets will be similar, but still noticeably different from one another
        * however, given different initializations and hyperparameters, models will still tend to produce partially independent errors, even if they are trained from the same dataset
    - very expensive computationally for neural networks, since the time to train models can be very large
- avoiding computational expense:
    1. take snapshots at the model at different local minima and average the results all together
    2. use a technique called dropout
- **dropout** is a computationally inexpensive yet effective method for generalization:
    - can be viewed as approximating the bagging procedure for exponentially many models, while only optimizing a *single* set of parameters
    - to use the dropout regularizer:
        1. on a single given training iteration, sample a binary mask for all input and hidden units in the network:
            * mask elements will be 1 with probability p and 0 with probability $1 - p$ ie. using a Bernoulli hyperparameter p
            * p represents the probability that a unit in the network will remain active for an iteration
            * each iteration, a new mask is generated
        2. apply ie. elementwise multiply the mask to all units
        3. during prediction, mutliply each hidden unit by the Bernoulli mask parameter p as a scaling factor
    - how does dropout emulate model ensembling?

        - considering a neural nework with a different configuration each iteration
            - there are 2^N configurations where N is the number of neurons
        - essentially want the randomly chosen active features to be robust in as many configurations ie. contexts as possible
            - ie. robust enough to work in almost a different network
        - each config should be good at predicting the output
        - dropout may cause units to encode redundant features for robustness
            - eg. recognizing a cat by fur, ears, and a tail
    - but we are changing our loss surface on every iteration, so shouldn't this warp the learning?
        - p is typically around 0.8 and 0.9, so only some units are dropped and the surface isn't radically changing
        - so dropout can be interpreted as generalizing the loss even further so the model performs better
    - training will take longer since generally the number of neurons will be increased
    - the dropout calculation must be backpropagated
        - just multiplciation, so have to cache the masks
- at test time, we need to multiply all units by the Bernoulli probability:
    - the contribution of a single unit to the output should be p times its output
        - ie. over many iterations, the contribution of $w_i h_i$ to the output h_{out} is just $pw_i h_i$
    - thus in test time, there is no additional complexity unlike true ensembling
        - with m ensemble models, testing time evaluation would have scaled by $o(m)$
    - in practice, we can perform **inverted dropout** where the scaling by $\frac{1}{p}$ is already done during training:
        - going from 0 and 1s on the mask to 0 and $\frac{1}{p}$s
        - thus testing will look the same irrespective of if we used dropout or not

Optimizing Gradient Descent

- initialization, regularization, and data augmentation can be used to improve performance of neural networks
    - how do we improve the performance with respect to the chosen optimizer, stochastic gradient descent?

- in typical stochastic gradient performance we compute the gradient over the examples as:

$$g = \frac{1}{m} \sum_{i=1}^{m} \nabla_\theta L(\theta)$$
$$\theta \leftarrow \theta - \varepsilon g$$

- gradient descent terminology:
  - given an arbitrary function, a point at which the gradient is the zero vector is called a **critical point**:
    - in a one-dimensional cost function, can have minima, maxima, and saddle points
    - however for a cost function in d-dimensional space, we can "slice" through a critical point on d different axes
      - to be a local minima, it must appear as a minima in *every* one of the slices
    - ie. *exponentially* more rare for a minima to be a local minima as d, the size of the parameter space, increases
- non-convex cost functions have multiple optima, only one of which is the global optimum
  - cost functions in deep learning are mostly non-convex, and thus it may be difficult for SGD to converge to the global optimum
- optimization of gradient descent should address the following general challenges:
  1. learning rate selection:
     - a small learning rate has slower convergence
     - a large learning rate leads to overshooting and we might not converge
  2. avoiding poor local minimas
     - difference from the global minimum may be large
  3. avoid drastic changes to the loss surface:
     - ie. if training data has a very different distribution than testing data, the loss surface will be very different, since the loss surface is a function of the data distribution
     - want to ensure that the training and test data is a representation of the total distribution
  4. difficulty finding local minima in higher dimensions
  5. exploding and vanishing gradients:
     - sometimes the cost function can have "cliffs" where small changes drastically change the cost function:

        - usually happens if parameters are multiplied repeatedly together, as in recurrent neural networks
        - can be ameloriated using **gradient clipping**, which bounds the maximum gradient norm through $g\frac{clip}{||g||}$
    - on the other hand, repeated multiplication of a matrix W can cause vanishing gradients, since the gradient may shrink by a factor of λ_i^t along its eigenvector u_i when multiplied t times
        - can be dealt with through architectural decisions and appropriate regularization

- can we address the oscillations that occur with high curvature loss surfaces in plain gradient descent?
    - oscillations slow down conversion:
        - they generally move SGD in the right direction, but along a slower, unideal path
        - want to *dampen* oscillations
    - using **momentum**, we maintain an exponentially decaying running average of the gradients, which then updates the parameters
        - add a measure of *resistance* ie. inertia that resists the change in direction

1. initialize $v = 0$ and $\alpha \in [0, 1]$, typically 0.9 or 0.99
2. until stopping criterion is met:

$$v \leftarrow \alpha v - \varepsilon g$$
$$\theta \leftarrow \theta + v$$

    - essentially augments the gradient with the running average of previous gradients
        - using momentum helps to *average* away the zig-zagging components
    - ie analogous to a gradient momentum
    - we can calculate the first several v values as follows:

$$v_0 = 0$$
$$v_1 = -\varepsilon g_1$$
$$v_2 = \alpha v_1 - \varepsilon g_2 = -\varepsilon(\alpha g_1 + g_2)$$
$$v_3 = \alpha v_2 - \varepsilon g_3 = -\varepsilon(\alpha^2 g_1 + \alpha g_2 + g_3)$$

- does momentum help with finding local optima?
    - momentum moves *ahead* of ordinary gradient descent:
        - thus gradient considering momentum may not be zero where gradient descent may have saturated to zero at some local gradient

        - due to the gradient carrying previous momentum, it may converge at different local minima that could be better
    - momentum tends to find *shallow* local optima, ie. very flat at the bottom such that the momentum *slows* down:
        - this is desired, since a shallow local optima indicates the loss is not very sensitive to changes in the weights in this region of the loss surface
            - vs. deeper local optima are much more sensitive to weight changes
        - thus we can intuitively predict that shallower local optima should generalize better

- **Nesterov momentum** is an extension on momentum:
    - similar to momentum, except the gradient is calculated *after* taking a step along the direction of the momentum:

$$v \leftarrow \alpha v - \varepsilon \nabla_\theta L(\theta + \alpha v)$$
$$\theta \leftarrow \theta + v$$

        - ie. step in the overall momentum first and then upgrade the parameters based on gradient descent
    - tends to work better than normal momentum
        - looks ahead to prevent momentum carrying too far
    - but this requires an additional complex backprop step due to the changed loss function:
        - we can instead perform a change of variables from $\theta + \alpha v$ to $\tilde{\theta}$ to simplify the Nesterov momentum calculation
        - no need to compute the extra gradient
    - Nesterov momentum with change of variables:

$$v_{new} = \alpha v_{old} - \varepsilon \nabla_{\tilde{\theta}_{old}} L(\tilde{\theta}_{old})$$
$$\tilde{\theta}_{new} = \tilde{\theta}_{old} + v_{new} + \alpha(v_{new} - v_{old})$$
$$v_{old} \leftarrow v_{new}$$
$$\tilde{\theta}_{old} \leftarrow \tilde{\theta}_{new}$$

- adaptive gradient methods:
    - choosing ε judiciously can be important for learning
    - in the beginning, a larger learning rate is typically better since bigger updates in parameters accelerate learning
        - in addition, it may not be appropriate to have the same learning rate for all parameters
            - may want to step different distances in different directions

  - however, as time goes on, ε may need to be small to make appropriate updates to the parameters
  - sometimes, the we can perform **annealing** on the learning rate to apply a decay rule on it
    * common practice to anneal the learning rate is to do so manually when the loss plateaus, or to anneal it after a set number of epochs of gradient descent
  - instead, we can update the learning base adaptively based on the *history* of gradients
    * appropriately modify the learning rate over the span of learning to improve convergence properties

- in **Adagrad** or adaptive gradient:
  - the learning rate is decreased through division by the historical gradient norms:
    * uses a variable a denoting a running sum of squares of gradient norms
    * ie. want to bias the direction of the gradient towards directions where not as many large steps have been historically taken

  1. initialize $a = 0$ and set v to a small value to avoid division by zero eg. 1×10^{-7}
  2. until stopping criterion is met:

$$a \leftarrow a + g \odot g$$
$$\theta \leftarrow \theta - \frac{\varepsilon}{\sqrt{a} + v} \odot g$$

  - however, this history of gradients grows very quickly, monotonically, without decreasing:

$$a_0 = 0$$
$$a_1 = g_1^2$$
$$a_2 = g_1^2 + g_2^2$$
$$a_3 = g_1^2 + g_2^2 + g_3^2$$

    * learning rate thus *decays* very quickly
    * another issue is that all historical gradients are weighed equally

- **RMSProp** augments Adagrad by making the gradient accumulator an exponentially weighted moving average:
  - allows the average to *not* monotonically increase and reduces the influence of older gradients:
    * allows the learning rate to grow again when a becomes especially small

    - vs. the learning rate of Adagrad can only ever decay
  - note that there is a "hiccup" in the early stages of gradient descent since the mean is not being correctly estimated with very few samples

1. initialize $a = 0$, set v to a small value, and set β between 0 and 1, typically 0.99
2. until stopping criterion is met:

$$a \leftarrow \beta a + (1 - \beta) g \bigodot g$$
$$\theta \leftarrow \theta - \frac{\varepsilon}{\sqrt{a} + v} \bigodot g$$

  - affect of the moving average:

$$a_0 = 0$$
$$a_1 = (1 - \beta) g_1^2$$
$$a_2 = \beta(1 - \beta) g_1^2 + (1 - \beta) g_2^2$$
$$a_3 = \beta^2(1 - \beta) g_1^2 + \beta(1 - \beta) g_2^2 + (1 - \beta) g_3^2$$

- RMSProp can also be combined with momentum:

1. initialize $a = 0$, set v to a small value, and set α, β between 0 and 1
2. until stopping criterion is met:

$$a \leftarrow \beta a + (1 - \beta) g \bigodot g$$
$$v \leftarrow \alpha v - \frac{\varepsilon}{\sqrt{a} + v} \bigodot g$$
$$\theta \leftarrow \theta + v$$

  - a holds the accumulated gradient while v holds the averaged gradient

  - it is also possible to do RMSProp with Netserov momentum

- however, there is a more principled way to combine RMSProp together with momentum using **Adam** or the adaptive moments optimizer:
  - one of the most commonly used and robust, eg. to hyperparameters, optimizers
  - Adam is composed of a momentum-like step, followed by an Adagrad/RMSProp-like step

- Adam without a bias correction:

1. initializations:
   - set $v = 0$ as the "first" moment and $a = 0$ as the "second" moment
   - set β_1, β_2 to be between 0 and 1, typically 0.9 and 0.999, respectively

   - set ν to be small
2. until stopping criterion is met:

$$
\begin{aligned}
v &\leftarrow \beta_1 v + (1-\beta_1) g \\
a &\leftarrow \beta_2 a + (1-\beta_2) g \bigodot g \\
\theta &\leftarrow \theta - \frac{\varepsilon}{\sqrt{a} + \nu} \bigodot v
\end{aligned}
$$

- Adam incorporates a bias correction on the moments:
  - intuition is to account for initialization:
    - since the bias corrections amplify the second moments, extremely large steps are not taken at the start of the optimization
    - ie. running means are inaccurate for early terms since $v \approx (1-\beta_1)g$ and $a \approx (1-\beta_2) g \bigodot g$, so we can try inflating the values using a bias correction
- Adam with bias correction:
  1. initializations:
     - set $v = 0$ as the "first" moment and $a = 0$ as the "second" moment
     - set β_1, β_2 to be between 0 and 1, typically 0.9 and 0.999, respectively
     - set ν to be small and $t = 0$
  2. until stopping criterion is met:

$$
\begin{aligned}
t &\leftarrow t + 1 \\
v &\leftarrow \beta_1 v + (1-\beta_1) g \\
a &\leftarrow \beta_2 a + (1-\beta_2) g \bigodot g \\
\tilde{v} &= \frac{1}{1-\beta_1^t} v \\
\tilde{a} &= \frac{1}{1-\beta_2^t} a \\
\theta &\leftarrow \theta - \frac{\varepsilon}{\sqrt{\tilde{a}} + \nu} \bigodot \tilde{v}
\end{aligned}
$$

- first order vs. second order methods:
  - SGD and its various optimizers are all first order methods and use the learning rate as a hyperparameter
  - a **first order method** refers to the fact that we only use the first derivative ie. the gradient, and take linear steps along the gradient
  - while **second order methods** use the **curvature** of the cost function to know how to take steps:
    - the second derivative ie. Hessian is used to asses the curvature and thus take appropriate sized steps in each dimension

    - with low curvature, want to take larger steps, while large steps would be damaging with a high curvature
    - make a quadratic approximation at θ_t, and then minimize the step along that parabola AKA take a Hessian step
        - ie. actually solving a quadratic optimization problem on each iteration

- the most widely used second order method is **Newton's method**:
    - consider the Taylor series expansion of $J(\theta)$ around θ_0 up to the second order terms:

$$J(\theta) \approx J(\theta_0) + (\theta - \theta_0)^T \nabla_\theta J(\theta_0) + \frac{1}{2}(\theta - \theta_0)^T H(\theta - \theta_0)$$

    - if this were a second order function, we can minimize it by taking its derivative and setting it to zero:

$$\begin{aligned}\nabla_\theta g &= \nabla_\theta [\theta^T g + \frac{1}{2}(\theta - \theta_0)^T H(\theta - \theta_0)] \\ &= g + \frac{1}{2}(H + H^T)(\theta - \theta_0) \\ &= g + H(\theta - \theta_0) \\ [=]\ 0\end{aligned}$$

    - this gives us the Newton step:

$$\theta = \theta_0 - H^{-1} g$$

        - has the inverse of curvature in the step calculation, so the parameters are updated depending on the curvature
        - note that when the Hessian has negative eigenvalues, it may be necessary to regularize the Hessian as $(H + \alpha I)^{-1}$
    - *pros*:
        - Newton's method does not require a learning rate
    - *cons*:
        - very memory intensive to store the Hessian
        - computational intensive to compute the inverse of the Hessian on the order of $O(n^3)$, at every iteration
        - Hessian typically requires a large batch to adequately estimate

- there are quasi-Newton methods that avoid some of the computational issues with the Hessian inversions:
    - in the **BFGS update**, instead of computing and inverting the Hessian at each iteration, the inverse H_o^{-1} is initalized and then resursively updated as follows:

$$H_k^{-1} \leftarrow (I - \frac{sy^t}{y^t s}) H_{k-1}^{-1} (I - \frac{ys^T}{y^T s}) + \frac{ss^T}{y^T s}$$

    - where $s = \theta_k - \theta_{k-1}$ and $y = g_k - g_{k-1}$
    - this update allows the inverse of any Hessian to be reconstructed from the sequence of s_k, y_k, but requires iterating over k examples
- can also use the **limited memory BFGS (L-BFGS)** where the inverse Hessian is just computed using the last m examples
- quasi-Newton methods usually require a full batch or very large mini-batches since errors in estimating the inverse Hessian can result in poor steps
- **conjugate gradient (CG)** methods find search directions that are *conjugate* with respect to the Hessian ie. $g_k^T H g_{h-1} = 0$
    - can also calculate derivatives iteratively this way through a recurrence relation

Convolutional Neural Networks

- the **convolutional neural network (CNN)** has played a large role in the latest *revival* of neural networks:
  - around the last 8 years, from the early 2010s
  - CNNs have been around since the 1990s
    - LeCun introduced LeNet in 1998 which set the architecture for the modern CNN
- biological motivating principles for CNNs:
  - attempting to replicate 3 key properties from the primary cat visual cortex, specifically the V1 neurons in the cortex:
    1. V1 has a retinotopic map
       - the neurons in a CNN are *spatially* organized, so that nearby cells act on nearby parts of the input image
    2. V1 is composed of simple cells that can be adequately described by a linear model in a spatially localized receptive field
       - CNNs use linear filters with a thresholding
    3. V1 is composed of complex cells that respond to similar features as simple cells, but are largely invariant to the position of the feature
       - CNNs use pooling units to incorporate invariance to shifts of the position of the feature
  - there is *some* correspondence between the feature computations done in a CNN with the visual system
  - however, there are many limitations of these biological analogies:
    - CNNs have no feedback connections while neural populations are recurrently connected
    - the brain does more than just image category classification
    - modern CNNs have hundred of layers, so it is challenging to correlate these layers to neural layers
- another motivation for CNNs:
  - for images, fully connected networks (what we have previously been designing) require many parameters:
    - in CIFAR-10, each neuron has 3072 weights
    - for more normal sized images, neurons in just the first layer would require 120,000 weights
    - would take long to train and be prone to overfitting

Convolution

- the **convolution** of two functions f, g is given by:

$$(f * g)(t) = \int_{-\infty}^{\infty} f(\tau)g(t-\tau)d\tau$$

- in discrete time, the convolution is given by:

$$(f * g)(n) = \sum_{m=-\infty}^{\infty} f(m)g(n-m)$$

- in CNN, we generally do not use convolution and instead use **cross-correlation**:

$$(f * g)(n) = \sum_{m=-\infty}^{\infty} f(m)g(n+m)$$

  - colloquially, instead of performing a "flip-and-drag", CNNs only "drag"
  - by the convention in the field, this operation is still generally called convolution

- the convolution in two dimensions is given by:

$$(f * g)(i,j) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} f(m,n)g(i+m, j+n)$$

  - generalizes to higher dimensions as well
  - note these convolutions are *not* commutative
  - can be interpreted as dragging the kernel g across f and performing a scale and sum over the overlapping squares
    - technically the kernel may be partially overlapped, but in practice we will only consider *valid* convolutions where the kernel is fully overlapped
  - in the valid convolution case, the resulting output of the convolution has dimensions $(w - w_f + 1, h - h_f + 1)$
    - note the output will always be smaller than the input if the filter is greater than (1×1), so sometimes we will zero-pad the input so that the output is the same

- to perform padding on the image, we add pad layers of zeros around all sides of the input:

  - output dimension is now $(w - w_f + 1 + 2 \cdot pad, h - h_f + 1 + 2 \cdot pad)$
  - thus by padding, we can avoid shrinking outputs if our filter size is relatively small

- another variable to control is the **stride** of the convolution:

  - defines how much the filter moves in the convolution
    - stride is normally set to 1, which denotes the filter is dragged across every part of the input
  - eg. a (7×7) input with a (3×3) filter has output with dimensions (5×5) with stride 1
    - with stride 2, the output becomes (3×3)
  - output dimension is $(\frac{w-w_f+2 \cdot pad}{stride} + 1, \frac{h-h_f+2 \cdot pad}{stride} + 1)$ with padding as well
  - note that the stride value should allow for valid convolutions, otherwise the input may have to be zero padded

CNN Layers

- the **convolutional layer** of a CNN:
  - the convolution operation defines this layer of the CNN
    - typically done in 3D, since images have a width, height, and *depth* for RGB channels
  - given the following dimensions:
    - input with dimensionality $(w \times h \times d)$
    - filter with dimensionality $(w_f \times h_f \times d)$:
      - depth is *matched* to that of the input
      - never have to "drag" only the depth dimensions, summing across the depth as well
    - $w_f < w$ and $h_f < d$
    - each filter will also have a bias term that is added to the convolution
    - after performing the convolution, the output dimension is $(w - w_f + 1, h - h_f + 1)$
      - not a tensor, unlike the filter
  - convolutional layer defines a collection of filters or activation maps, each with the same dimension:
    - ie. multiple filters from the single layer that may correspond to different feature maps:
      - each element in a feature map can be interpreted as an artificial neuron
      - whereas each filter can be interpreted as weights for neurons in different layers
    - convolving with each filter gives an output that is a matrix *slice*
    - the output slices from each filter are composed together to form a tensor of k depth, where k is the number of filters
  - output tensor is then passed through an activation nonlinearity and passed as input into the next layer

- in theory FC layers can converge to the perform the same calculation as a convolutional layer:
  - the convolution operation is just performing a special linear operation on the input data
    - the transformation could be expressed as a matrix
  - however, there too many parameters and intialiations to handle, so it would not naturally converge to perform convolution
  - the convolution layer *constrains* the solutions ie. regularizes the solution and empirically improves performance
- a large component of the CNN is then made up of *composed* convolutional layers:
  - convolutional layers have sparse interactions ie. sparse connectivity:
    - unlike in fully connected layers where every neuron is connected to every neuron in the next layer
    - in a convolutional layer, one neuron is only connected to its *nearby* neighbors:
      - based on how the convolution operation is performed and also from how a feature map becomes *stacked* in the output and then passed to the next convolutional layer
      - draws from the motivation of spatial connectivity
  - sparse interactions reduce computational memory:
    - in a FC layer, each neuron has $w \cdot h \cdot d$ weights
    - in a convolutional layer, each neuron has $w_f \cdot h_f \cdot d$ weights
      - in addition, every output neuron in a slice of a convolutional layer has the same weights
  - sparse interactions reduce computation time:
    - in a FC layer with m inputs and n outputs, a FC layer would take $O(mn)$ to compute
    - in a convolutional layer, if each output is connected to $k = w_f \cdot h_f \cdot d$ inputs, the layer would require $O(kn)$ operations to compute the output
  - a concern of sparse interactions is that information from different parts of the input may not interact:
    - eg. a self-driving car should know where obstacles are from all over the image
    - this motivates that networks should be composed of more layers, since units in deeper layers will indirectly interact with larger portions of the input
      - ie. has a larger receptive field
- convolutional layers have shared parameters or *tied* weights:
  - in every output neuron in a given slice uses the same set of parameters in the filter
  - ex. Given an input that is $(32 \times 32 \times 3)$, find the number of neurons

and parameters:
    * in the FC architecture, there are 500 output neurons at the first layer
    * in the convolutional net, there are 4 filters that are all $(4 \times 4 \times 3)$:
        · each filter gives a (29×29) slice
        · overall output is a $(29 \times 29 \times 4)$ tensor
        · thus we have $(29 \times 29 \times 4)$ output neurons in the CNN
    * FC has $(32 \times 32 \times 3 + 1) \cdot 500 = 1.5$ million parameters
        · additional 1 parameter for the bias
    * CNN only has $(4 \times 4 \times 3 + 1) \cdot 4 = 196$ parameters
- convolutional layers can handle variable sized inputs:
  - unlike in a FC layer, the input and output dimensions are defined by the W, b parameters
  - in a convolutional layer:
    * if the input changes in size, the convolution operation can still be performed
    * if the output dimensions are required to be a fixed size, we can perform modifications such as pooling to create the correct output size
- the **pooling layer** applies an operation to all elements within the filtering extent
  - pooling filter has dimensions $(w_p \times h_p)$ and is applied with a given stride
    * output has dimensions $(\frac{w-w_p}{stride} + 1, \frac{h-h_p}{stride} + 1)$
  - most common to use max as the pooling operation
  - effects on the network:
    * effectively performs downsampling
    * pooling layers introduce no additional parameters
    * pooling layers introduce small spatial invariances between units in the same filtering area
        · motivated by complex cells with spatial invariances in biological neurons
- **receptive fields (RFs)** in CNNs is the region in the input space that a feature from a particular CNN is looking at:
  - indicates the extent of the scope of the input data a neuron in a layer can be exposed to:
    * the field can be described by the center location along with the size ie. radius
    * receptive field is defined by the filter size, stride, and padding size
  - note that the closer a pixel is to center of the receptive field, the more it contributes to the calculation of the output feature
  - neurons within a layer are tasked with learning visual features from a small region of the input data:
    * since lower layers have a smaller RF, they learn low level features

such as lines, edges, contours, etc.
    * highler layers learn more abstract features of the images such as shapes
        · have a larger receptive field made up of the accumulated RFs of lower layers

CNN Examples

- typical CNN architectures:
  - several paired convolutional-ReLU layers
    * typically cascaded together, ending with a max pooling layer
  - CNN may end with a FC-ReLU layer, followed by a final softmax
  - eg. m conv-ReLU layers followed by a maxpool form a unit that is then repeated n times:
    * followed by k FC-ReLU layers
    * concluded by a final softmax layer

LeNet 1998

- input size was 32x32, in two dimensions, for grey-scale images
- C1 contains six 5x5 convolutional filters applied at stride 1 and pad 0:
  - feature maps ie. output is dimension 28x28x6
    * $6 \cdot 28 \cdot 28 \cdot (5 \cdot 5 + 1) = 122,804$ connections
  - $(5 \cdot 5 + 1) \cdot 6 = 156$ parameters
- S2 is a 2x2 pooling layer applied at stride 2:
  - output is dimension 14x14x6
  - no parameters
  - instead of a max pool operation, pooling layer added all elements, multiplied by a trainable coefficient, and then passed through sigmoid
- C3 contains 16 5x5 convolutional filters applied at stride 1 and pad 0:
  - filter dimensions are really 5x5x6 to match the depth of the previous convolutional layer
  - output is dimension 10x10x16

1. [28x28x6] CONV: 6 convolutional 5x5 filters
2. [14x14x6] POOL: 2x2 pool with stride 2
3. [10x10x16] CONV: 16 convolutional 5x5 filters
4. [5x5x16] POOL: 2x2 pool with stride 2
5. [120] CONV: 120 convolutional 5x5 filters
6. [84] FC: 84x120 layer
7. [10] OUT: MSE against a template for each digit

- overall structure can be described as `[CONV-POOL]x2 - CONV - FC - OUT`

AlexNet 2012

- image processing:
  - ImageNet has variable sized images
  - AlexNet downsampled each image, given a rectangular input:
    - crop so shorter side is 256 pixels, take central 256x256 image
    - actual input to the CNN was smaller, at 224x224x3, to allow for dataset augmentation
      - reported as 224x224 in the paper, but would have to be 227x227 to fit with the architecture in the paper
  - subtracted mean image over the trainings set from each pixel
    - regularize the weights by centering the image
- data augmentation:
  - perform image translations and horizontal reflections
  - at test time, extract 5 random 224x224 patches and their horizontal reflections and average the predictions of their 10 output softmax scores
    - test averaging reduced error rate by 1.5%
  - perform color augmentation by scaling the principal components of colors
    - captures different levels of illumination and intensities
- input size was 227x227x3

1. [55x55x96] CONV: 96 convolutional 11x11 filters with stride 4
   - filters have matched depth, so there are $96 \times (11 \times 11 \times 3 + 1) = 34,944$ parameters
2. [27x27x96] POOL: 3x3 pool with stride 2
3. [27x27x96] NORM: normalization layer
4. [27x27x256] CONV: 256 convolutional 5x5 filters with stride 1, pad 2
5. [13x13x256] POOL: 3x3 pool with stride 2
6. [13x13x256] NORM: normalization layer
7. [13x13x384] CONV: 384 convolution 3x3 filters at stride 1, pad 1
8. [13x13x384] CONV: 384 convolution 3x3 filters at stride 1, pad 1
9. [13x13x256] CONV: 256 convolution 3x3 filters at stride 1, pad 1
10. [6x6x256] POOL: 3x3 pool with stride 2
11. [4096] FC: Fully connected layer with 4096 units
12. [4096] FC: Fully connected layer with 4096 units
13. [1000] FC: Fully connected layer with 1000 units ie. class scores
14. [1000] OUT: Softmax layer

- implementation details:
  - used ReLU as a nonlinearity, much faster than sigmoid or $tanh$ unit
    - applied at output of every convolution and FC layer
  - dropout with $p = 0.5$ substantially reduced overfitting
    - took twice as long to rain

  - took 5 to 6 days to train:
    * the architecture was replicated to allow for training on two separate GTX 580 GPUs
    * stored the 1.2 million images on GPUs to avoid slower memory accesses
  - SGD with regular momentum of 0.9 and L^2 decay of 0.0005, no adaptive gradients
  - batch size of 128
  - learning rate initially 0.01, but was manually decreased when validation error stopped improving
  - ensembled with up to 7 similar CNNs
    * accuracy improved from 18 to 15 percent through ensembling
  - used local response normalization
  - used pooling with overlapping ie. the stride was not the pool width
- ZFNet from 2013 was the same as AlexNet, but with better hyperparameters:
  - decreased error rate from 11.7% down to 7.3%
    * approximately a 30% error reduction
  - architecture differences:
    * reduced 11x11 filters at stride 4 to 7x7 filters at stride 2
    * increased number of subsequent convolution layeres to 512, 1024, and 512
  - takeaways:
    * smaller filters applied at smaller strides appears to help
    * having more fitlers later on in deeper layers appears to help

VGGNet

- use small 3x3 convolution filters and an extended architecture depth:
  - instead of only 8 layers, increased the network architecture to 16-19 layers
  - all convolution filters are uniform at 3x3 with stride 1, pad 1
  - all pool filters are max pools and uniform at 2x2 wtih stride 2
  - overall structure is `[CONVx2-POOL]x3 - [CONVx3-POOL]x2 - FCx3 - SOFTMAX`
  - decreased error rate from 11.7% down to 7.3%
    * approximately a 40% error reduction
  - altogether has 138 million parameters, but the FC nets contribute 122 million of those parameters
    * requires around 100 MB to cache forward passes
- considerations of using a smaller filter?
  - *pros*:
    * smaller filters dramatically reduce the number of parameters, with a smilar effective receptive field
      · parameters of three 3x3 CONV layers halves the parameters of

one 7x7 CONV layer
        - in practice, with more depth, we allow for more nonlinearities and thus potentially more express features
    - *cons*:
        - with a small filter, the receptive field of neighboring layers is reduced
        - can be addressed by using more convolutional layers together:
            - increases the effective receptive field
            - this is why VGGNet has a deeper architecture than its predecessors
        - more memory is used, since there are more layers of activations to store
            - not a major downside
- input size was 224x224x3

1. [224x224x64] 64 CONV
2. [224x224x64] 64 CONV
3. [112x112x64] POOL
4. [112x112x128] 128 CONV
    - the number of filters is doubled every time after a pooling layer so that the number of operations in each layer remains the same
        - since pooling layers halve the input sizes
5. [112x112x128] 128 CONV
6. [56x56x128] POOL
7. [56x56x256] 256 CONV
8. [56x56x256] 256 CONV
9. [56x56x256] 256 CONV
10. [28x28x256] POOL
11. [28x28x512] 512 CONV
12. [28x28x512] 512 CONV
13. [28x28x512] 512 CONV
14. [14x14x512] POOL
15. [14x14x512] 512 CONV
16. [14x14x512] 512 CONV
17. [14x14x512] 512 CONV
18. [7x7x512] POOL
19. [4096] FC
20. [4096] FC
21. [1000] FC

- implementation details:
    - images were global mean-subtracted
        - also performed flips, crops, and RGB shifts
    - disposed of the local response normalization layers from AlexNet

  - batch size of 256 and SGD with momentum 0.9
  - L^2 regularization of 0.0005
  - dropout on the first two FC layers
  - manual learning rate adjustment as in AlexNet
  - used Xavier initialization
  - training took 2-3 weeks on a 4 GPU machine
  - ensembled the output of 7 networks

GoogLeNet

- take-home points:
  - from the same year as VGGNet
    - 6.7% error rate instead of VGGNet's 7.3%
  - another deeper architecture with 22 layers
  - introduces a new inception module
  - gets rid of FC layers
  - has only 5 million parameters, which is 12x less than AlexNet and 27x less than VGGNet
  - created with the goal of keeping the computational budget low
- why not just go deeper and use more neurons?
  - increases the number of parameters
    - should lead to more overfitting and more learning
  - dramatically increases the computational expenses
- GoogLeNet's new **inception modules** leverage an idea called "network-in-network":
  - allow the network to pick out the most important features of the data
  - feed the activations from a layer in *parallel* through different layer types:
    - ex. GoogLeNet uses 1x1 convolutions, 3x3 convolutions, 5x5 convolutions, and a 3x3 max pool
      - the number of each filter type controls how weighted each type is towards the next layer
    - each part of the module extracts different features of the data
  - the filters outputs are then concatenated together and fed on to the next layer:
    - note that the width and height for each filter type must be equal to perform concatenation
    - each layer needs to padded
  - note that after the concatenation, the depth dimension may be quite large depending on the number of filters:
    - eg. if a max pool is always part of the inception module, the concatenation depth will always be at *least* as deep as the input
      - leads to an exploding number of neurons and operations

        * to solve this, place an F-deep 1x1 convolution filter *before* the 3x3 and 5x5 convolution layers and after pooling layers to substantially reduce the number of operations
            · although this leads to some loss of information, dramatically limits the depths of the incoming activations and reducing operations by a factor of 4
        * GoogLeNet uses an F of 64
    - thus each inception layer has two layers of convolutions
- overall structure is:
    - `CONV-POOL-CONVx2-POOL-INCEPx2-POOL-INCEPx5-POOL-INCEPx2-AVGPOOL-LINEAR-SOFTMAX`
    - 22 total layers
    - such a deep network may lead to exploding or vanishing issues when backpropagating, even with batchnorm:
        * GoogLeNet uses *auxiliary* networks that lead off of the 11th and 17th layers of the network
        * reduces the distance backpropagation has to be performed, eg. 14 instead of 22 layers
        * the auxiliary losses are discarded at inference time
- implementation details:
    - SGD with 0.9 momentum
    - decrease learning rate by 4% every 8 epochs
    - used 144 crops per image
    - averaged results of 7 GoogLeNets
    - did not use GPUs to train, due to smaller number of parameters

ResNet

- from 22 layers all the way to 152 layers:
    - dropped error from 6.7% down to 3.57%
    - why not just keep adding layers, as seen in the evolution from AlexNet to VGGNet and GoogLeNet?
        * when increasing parameters, complexity increases and can lead to more overfitting without regularization
        * but empirically, with more layers, networks generally cannot even *overfit* the data as well
            · training error is worse than it would be with fewer layers, and testing error also suffers since network is not learning as well overall
        * this result is nonintuitive, since similarly to increasing parameters, we should be able to copy the parameters of a network with fewer layers and just force the identity matrix on the remaining layers
            · but the network does not naturally learn the identity matrix for its weights and arrive here

- "The degradation problem suggests that the solvers might have difficulties approximating identity mappings by multiple nonlinear layers" — He et al.
  - the goal in ResNet is to change the architecture so that it is *easier* to learn the identity mapping
    - facilitate the network training by causing each layer to learn a residual to add to the input
  - use a **residual layer** where $h_i = h_{i-1} + F(h_{i-1})$ rather than $h_i = F(h_{i-1})$
  - to emulate an identity layer, just have to drive the weights down towards zero, rather than learning the entire identity matrix
  - these identity transformations are also known as **skip connections** that easily allow a layer to just pass through previous activations:
    - skip connections converge on an addition gradient gate
    - when backpropagating through a network full of skip connections, we have a gradient *"highway"*
      - avoids possible vanishing or exploding gradients from backpropagating through many convolutional layers
  - in addition, we can use a similar idea to inception and use 1x1 filters in order to reduce the input depth and thus computational complexity
- without the residual layers, increasing the number of layers, the training error does not improve:
  - however, using the ResNet architecture with increased layers *does* give better training and validation error
  - up to a certain point, cannot arbitrarily keep increasing layers towards infinity
- network architecture and implementation details:
  - follows design rules of VGGNet:
    - all convolution layers are 3x3 filters
    - if the feature map size is halved by a pool, the number of channels is doubled
    - output ends with an average pooling and then a linear 1000 layer to a softmax
  - performed data augmentation with image scaling and different crops
  - batch size of 256 and SGD with momentum 0.9
  - L^2 regularization of 0.0001
  - learning rate starts off at 0.1 and is decreased by an order of magnitude when the error plateaus
  - no dropout
- **Fractal Networks** were motivated by the idea that the residual representations were not fundamental to the success of deep CNNs:
  - instead, theorized that the network's ability to transform from effectively shallow to deeper networks made it perform well with more layers

    - ie. the identity connections do not matter, but rather the reduced effective depth of the network
  - a layer's effective depth may be smaller than its actual depth due to skip connections that are used in the layer
    - fractal nets are made up of extremely deep layers with a shallow effective depth that allows for skipping of many of the convolution operations
  - fractal nets perform just as well as ResNet architectures
  - by reducing the effective depth of the network, we shorten the longest path from the output loss to the network input
    - helps avoid the fundamental problem of deep learning of vanishing, exploding, and noisy gradients

Modern Developments

- in the Inception-v4 architecture, we have inception style layers used along with residuals
- with wide ResNets, many more filters are used in the convolutions
- with ResNeXt, more paths of convolutions in the inception layers
  - increasing width as well as cardinality
- performing dropout on ResNet residual layers

Recurrent Neural Networks

- a key missing feature of FC and convolutional neural networks is that they lack *recurrent* connectivity and thus they have no dynamics:
  - ie. there are no *feedback* connections since the activations always feed forward
  - incorporating feedback connections would lead to more complex behavior
  - in biology, neurons are known to be recurrently connected that define a dynamical system
- a motivating thought experiment is to attempt train a neural network to perform character prediction:
  - if the network was a CNN that only takes in a *single* character, the CNN would *not* be able to differentiate between the context of different strings
    - eg. the same character would be predicted for `"th"` vs. `"though"`
  - due to the feedforward and fixed connection nature of the CNN, it will *always* give the same outputs for a given input
  - could we instead pass in a history of previous words into the CNN?
    - grows very quickly in dimensionality by a factor of the history siez
    - CNNs are thus not the ideal architecture for **natural language processing (NLP)**
  - this leads to the problem of **state**:
    - in some cases our data will have a temporal structure
    - eg. classifying videos and generating text, where the past *matters*
- state captures, usually in a succinct matter, what has happened in the past:
  - say we want to infer some output z_t from a history of inputs $x_1, \dots, x_t$
  - one approach is to define a function that takes all the history ie. $z_t = f(x_1, \dots, x_t)$
    - has an issue of scaling input size depending on the history
  - instead, introduce a state variable $s_t = f(s_{t-1}, x_t)$:
    - this state update defines the recurrent connections of a RNN
    - making the Markov assumption that all relevant information about past inputs is stored in the current state
      - ie. encapsulating all the history into this state variable
    - note that s_t will be optimized to perform the task at hand
    - then, we can predict the next output $z_t = g(s_{t-1}, x_t)$
- famous RNN examples:
  - RNN learning to spell out `"hello"` given a single seed of `"h"`
    - explicitly shows how the state variable affects output compared to a CNN

  - RNN learning to type out Shakespeare
    - generating Wikipedia articles, algebraic geometry
  - GPT-2 can generate text with reasonable semantic meaning
- at a high level, the RNN can be broken into three major weight components:
  - W_{in} transforms an input x_t into activations
  - W_{rec} defines recurrent connections for each artificial neuron
    - together with W_{in}, we can calculate neuron activations as $h_t = relu(W_{rec}h_{t-1} + b + W_{in}x_t)$
  - W_{out} linearly maps the artificial neuron activations to the output $z_t = W_{out}h_t + b_{out}$
    - can then be passed to a softmax classifier
  - loss functions are straightforward:
    - for regression, can perform mean-square error across all time

$$\sum_t ||\hat{y}_t - y_t||^2$$

    - for classification, can minimize the sum of softmax losses across all time

$$\sum_t L_t$$

    - sometimes, we only care about the output after some time τ

$$\sum_{t \geq \tau} L_t$$

      - only calculate the loss over these certain outputs
- how do we train an RNN?
  - we can perform a forward pass and a loss
  - but do we know how to take gradients of the weight matrices?
    - the application of backpropagation in RNNs differs from feedforward networks
  - the upstream gradients at any given time come from units who are themselves potentially receiving inputs from the node we are calculating the gradient of
    - in addition the activations at any given node for an input depends on time
  - instead, we can consider the RNN as a computational graph *through time*:
    - ie. will look like a feedforward network if we unroll the RNN in time
    - makes backpropagation possible
- ex. Unrolling the computational graph for an RNN with 4 units:
  - if $h_t \in \mathbb{R}^4$, $W_{rec} \in \mathbb{R}^{4 \times 4}$

  - W_{rec} describes how each of the 4 units of h_t is weighted in each unit of the next output h_{t+1}:
    * each layer in time, when unrolled, performs the same affine computation based on W_{rec}
    * feedforward as well as feedbackward connections
  - backpropagation through this unrolled graph is called **backpropagation through time (BPTT)**
    * since loss is summed across time, there are multiple gradient paths from the loss through each time slice
      · each time slice can also backpropagate through its previous neighbor
  - in general, we have:

$$\frac{\partial L}{\partial h_{t-1}} = W_{rec}^T \mathbb{1}(W_{rec} h_{t-1} > 0) \bigodot \frac{\partial L}{\partial h_t}$$

    * note that to go back many time steps, we end up multiplying the gradient by W_{rec}^T many times
      · based on the eigendecomposition of the multiplication, we can see that along the eigenvectors of W_{rec}^T, the gradients will be attenuated to zero or grow exponentially depending on the eigenvalue
    * thus with RNNs, vanishing and exploding gradients causes major problems for gradient descent at earlier layers
- addressing vanishing and exploding gradients in RNNs:
  - even if gradients backpropagated through many time steps of the future may vanish, shouldn't the network still learn from prior gradients closer in time that did not explode or vanish through multiple time steps?
    * ie. directly through only a couple time steps instead of much longer time paths
    * defeats the purpose of RNNs since we are no longer considering state far away in time to learn distant features
      · can never learn dependencies past a certain distance
  1. a general way is to perform *truncated* backpropagation through time
     - instead of backpropagating all gradients back to the activations at time 1, we only backpropagate through p layers of time
  2. perform gradient clipping for exploding gradients
  3. can use regularization to address vanishing gradients:

$$\Omega = \sum_t \left(\frac{\left|\left|\frac{\partial h_{t+1}}{\partial h_t}\frac{\partial L}{\partial h_{t+1}}\right|\right|}{\left|\left|\frac{\partial L}{\partial h_{t+1}}\right|\right|} - 1\right)^2$$

  - want neighboring layers in time to have similar statistics

Long Short-Term Memory

- the **long short-term memory (LSTM)** is a particular RNN architecture that solves the issues RNNs face with exploding and vanishing gradients:
  - one of the most commonly used RNN architectures today
  - name refers to ability to store *short-term* memory for a *long* period of time
- the standard LSTM is defined as follows:

$$
\begin{aligned}
f_t &= \sigma(W_f \begin{bmatrix} h_{t-1} \\ x_t \end{bmatrix} + b_f) \\
i_t &= \sigma(W_i \begin{bmatrix} h_{t-1} \\ x_t \end{bmatrix} + b_i) \\
v_t &= tanh(W_v \begin{bmatrix} h_{t-1} \\ x_t \end{bmatrix} + b_v) \\
o_t &= \sigma(W_o \begin{bmatrix} h_{t-1} \\ x_t \end{bmatrix} + b_o) \\
c_t &= f_t \bigodot c_{t-1} + i_t \bigodot v_t \\
h_t &= o_t \bigodot tanh(c_t)
\end{aligned}
$$

- the key idea behind LSTM is it introduces a new variable c_t called the **cell state**:
  - this is the central component that has memory in the LSTM:
    - however, we can alter this cell state
    - ie. can *update* the cell state and then *read* out from the cell state to update H_t
  - cell state operations:
    1. forget information
    2. write-in information
    3. read-out information
  - to forget information, the LSTM usees the forget gate f_t:
    - comprises the update $c_t = C_{t-1} \bigodot f_t$
    - if f_t is close to 1, then $c_t \approx c_{t-1}$
      - ie. when the forget gate is large, most of the information is remembered
    - if f_t is close to 0, then $c_t \approx 0$
      - ie. when the forget gate is small, most of the information is forgotten
    - f_t takes in the last output h_{t-1} which reflects the current cell state, as well as the current input x_t

            - thus reflects both local and global information
    - to write in information, the LSTM needs to compute two values:
        - comprises the update $c_t = c_{t-1} + i_t \bigodot v_t$
        - the value gate v_t that takes on values between -1 and 1, and tells us the value we want to add to the cell state
        - the input gate i_t tells us how much of the value gate to write to the cell state
        - if either gate is zero, we write no information to the cell state
            - if i_t is close to 1, we update the cell with v_t
    - to read out information:
        - comprises the update $h_t = o_t \bigodot tanh(c_t)$
        - $tanh$ on c_t gives us a value, and the output gate o_t tells us how much of the cell state is going to be read out to the hidden state

- backpropagating through an LSTM:
    - write in stage passes through the gradient due to the addition
    - the product at the forget stage could zero out the gradient, is this acceptable?
        - yes, zeroing out the gradient occurs if the forget gate is close to 0, which is desired functionality
    - why the LSTM works well:
        - the cell state during backpropagation has almost uninterrupted gradient flow, analagous to gradient highways in ResNets
            - ie. the addition operation passes the gradient backwards
        - the gradient can be attenuated through the forget gate

- in practice:
    - LSTMs are easily to train than vanilla RNNs using first-order gradient descent techniques
    - however, has four times the number of parameters of a vanilla RNN

Gated Recurrent Unit

- the **gated recurrent unit (GRU)** solves the problems of exploding number of

parameters an LSTM has, and is defined as follows:

$$
\begin{aligned}
r_t &= \sigma(W_r \begin{bmatrix} h_{t-1} \\ x_t \end{bmatrix} + b_r) \\
u_t &= \sigma(W_u \begin{bmatrix} h_{t-1} \\ x_t \end{bmatrix} + b_u) \\
\tilde{h_t} &= tanh(W_h \begin{bmatrix} r_t \bigodot h_{t-1} \\ x_t \end{bmatrix} + b_h) \\
h_t &= u_t \bigodot h_{t-1} + (1 - u_t) \bigodot \tilde{h_t}
\end{aligned}
$$

- unlike the LSTM, the GRU has no cell state, which reduces the number of parameters
- the update gate u_t tells us how the hidden state updates:
  - comprises the update $h_t = u_t \bigodot h_{t-1} + (1 - u_t) \bigodot \tilde{h_t}$
  - if the update gate is close to 1, then the hidden state stays approximately constant
  - if the update gate is close to 0, then the hidden state forgets its previous value and adopts the candidate activation $\tilde{h_t}$
  - hence the GRU uses the hidden state as memory as opposed to instantiating a new cell state
- the reset gate r_t controls the candidate hidden state $\tilde{h_t}$:
  - comprises the subcalculation $\tilde{h_t} = tanh(W_h \begin{bmatrix} r_t \bigodot h_{t-1} \\ x_t \end{bmatrix} + b_h)$
  - if reset gate is close to 1, then the candidate hidden state looks like a standard vanilla RNN update
  - if it is close to 0, then the value is completely set by the input
  - intuition is that if the reset gate is close to 0, it'll be as if the GRU was being reset, only looking at the input
- much like the LSTM the GRU is able to learn long term dependencies since there is a gradient highway on the hidden states h_t
  - when the update gate is close to 1, the gradient will flow back in time through h_{t-1}
- in this formulation of the GRU, it has three times as many parameters of a vanilla RNN:
  - in a minimal GRU, only twice as many parameters as a vanilla RNN are used
  - GRU uses less memory and computation than the LSTM, since it doesn't maintain a cell state

  - GRUs have been empirically observed to train faster than LSTMs
  - LSTMs ought to be able to remember longer sequences by using a dedicated cell state
  - GRUs empirically tend to perform better than LSTMs

- since RNNs tend to have less units, second order methods may be more plausible
  - eg. conjugate or approximation gradient methods with second order methods may perform especially well

- approaches for training RNNs:
  1. use a vanilla RNN with gradient clipping and Pascanu's regularization
     - or alternatively truncated BPTT
  2. use an LSTM
  3. use a GRU
  4. use some other gating unit variant
  5. consider using second order optimization methods

  - can add depth by stacking multiple RNN units
  - may also be helpful to batch normalize the cell state of the LSTMs
    * as well as applying dropout to recurrent units

Unsupervised Learning

- neural networks can also be used for modeling data via generative models:
  - allows for expressive techniques to model distributions of the data as well as more sophisticated unsupervised learning
  - why unsupervised learning?
    - data can be quite large
    - learn key features or structure in the data without labels
    - simple linear techniques include PCA, FA and linear techniques include LLE, tSNE
- ex. Dimensionality reduction on motor neuron responses:
  - draw a trajectory through space through the estimated firing rates for each neuron through time
    - but with very many neurons, it is difficult to *visualize* such a trajectory in above a 3D space
  - it is possible to find *projections* of activity where the neural signal exists into fewer dimensions
    - ie. the trajectory will not occupy very much space along certain dimensions
  - creates a low-dimensional time series by identifying the principal dimensions along which the date evolves
    - essential for big data that take up an exploding number of dimensions

Autoencoders and Variational Autoencoders

- both **autoencoders** and **variational autoencoders (VAEs)** produce a lower-dimensional representation of the input data:
  - produces a lower-dimensionality set of features h that are sufficient toe reconstruct the important features of x
    - eg. $x \in \mathbb{R}^n$ and $h \in \mathbb{R}^d$ where $d << n$
  - VAEs are probabilistic, which allow them to be generative models
  - we can pass h into a decoder that produces a reconstruction $\hat{x} \in \mathbb{R}^n$
    - formally, we have an encoder f and decoder g such that $\hat{x} = g(f(x))$
  - loss function can simply be the squared loss ie. $L = ||x - \hat{x}||^2$
    - note that we did not use labels in this network, so this is an example of unsupervised learning
- PCA can be modeled as an autoencoder as follows:

  - with $h = f(x) = W^T x$ and $g(h) = Wh$, we have a loss function:
$$L = ||x - WW^T x||^2$$
  - this autoencoder learns a W that is the singular value decomposition of x, ie. spans the same subspace as performing PCA on x
- in general, we want to implement f, g as neural networks to perform nonlinear dimensionality reduction:
  - eg. in the simplest form, $f(x) = tanh(Wt)$ and $g(h) = tanh(Wh)$
  - in general, f, g could be deep neural networks, and it is straightforward to train with SGD using backpropagation
- a sparse autoencoder is one that is regularized not only to minimize the loss but to also incorporate sparse features:
  - ie. using an L^1 penalty
  - useful when we are unsure what dimensions to reduce to
    * when the outputs corresponding to a certain dimension are close to zero, we can reduce the dimension
- a denoising autoencoder is one that is robust to noise:
  - can generate noise ε and add it to the input x so that $\tilde{x} = x + \varepsilon$
  - then the loss function of the autoencoder would have loss $L(x, g(f(\tilde{x})))$
    * here the autoencoder would learn to denoise $\tilde{x}$ to reproduce x in its reconstruction
- a contractive autoencoder is one where the features are robust:
  - ie. a small change in x produces only a small change in h
  - can be accomplished by regularizing the Frobenius norm of the Jacobian matrix
    * loss function becomes $L(x, \hat{x}) + \lambda||\nabla_x h||_F^2$
  - names comes from the fact that the features can be seen as a contraction of the inputs of f in the neighborhood of examples from the data-generating distributions p
- variational autoencoders learn *distributions* of the features given the input and the input given the activations:
  - ie. learning probabilistic versions of f and g
  - concretely, the VAE will learn:
    * $p(h|x)$, the distribution of the features given the input used by the encoder
    * $p(x|h)$, the distribution of the input given the features used by the decoder
    * typically, z is used to denote the features h
  - these distributions are parametrized by neural networks, meaning that they can express nonlinear transformations and be trained via SGD
  - why learn distributions?
    * often times, the data is noisy, so the model of the distribution may be more useful

        - the VAE is generative, since it is possible to sample z and then sample x
    - instead of inferring $p(x)$ directly, we can use what are called **latent variable models**:
        - latent variables model the data x as *arising* from a latent ie. unobserved variable z
        - it may be easier to choose some distribution for the latent variable $p(z)$ with standard statistics and instead model $p(x|z)$
        - intuitively, this means that we model how x arises from some latent variable z that *itself* has certain variability?
    - to generate samples from $p(x)$:
        1. generate a sample z_s randomly from $p(z)$
        2. generate a sample x_s from $p(x|z = z_s)$
            - this sample x_s comes from $p(x)$
- modeling a distribution with a latence variable:
    - say we want to model $x \sim N(\mu, \Sigma)$
    - to use a latent variable model, we can define some latent variable z
        - if $z \sim N(v, \Lambda)$, then $x = Az + b$ has the distribution:

$$x \sim N(Av + b, A\Lambda A^T) = N(b, AA^T)$$

    - since x is normal, we can always set $z \sim N(0, I)$ and define:

$$x = \mu + \Sigma^{\frac{1}{2}} z$$

        - this gives us samples of x as desired
- designing the prior distribution $p(z)$:
    - in almost all cases, we will set z to have unit statistics
    - is this too strong a constraint on the distribution of the latent variables?
        - no, even if z has a simple distribution, if $x|z$ is expressive enough and incorporates nonlinear transformations, we can put *all* of our work into optimizing $x|z$
    - ie. we can generate nonlinear transformations that map a $N(0, I)$ distribution to arbitrarily complex distributions
    - to draw samples x, first draw samples z and then apply $x = \mu_\theta(z) + \Sigma_\theta(z)^{\frac{1}{2}} z$
    - in general:
        - x is generally not normal
        - z is defined to be normal
        - $x|z$ is normal, but has a nonlinear dependence on z
- overview of the VAE:
    - the VAE learns the distribution $q(z|x) = N(\mu_\phi(x), \Sigma_\phi(x))$:
        - uses two networks to learn the mean and covariance of the input data

        - then, we *sample* from this distribution to obtain a latent representation z that follows $N(0, I)$
            - need to be able to backprop through this sampling step
    - the VAE then learns another distribution $p(x|z) = N(\mu_\theta(z), \Sigma_\theta(z))$:
        - uses two additional neural networks
        - this distribution can again be sampled to create a new $\hat{x}$ of the same dimensionality of x that can be compared
    - note that this is computationally expensive, since a single VAE requires four neural networks
- how do we find the parameters θ?
    - need to define a loss function and calculate its gradient
    - the most natural loss function to optimize is to maximize the likelihood of observing the data:

$$\prod_{i=1}^{m} p_\theta(x_i)$$

        - note that we cannot break down $p(x)$ into $p(z)p(x|z)$ because $p(x|z)$ has a nonlinear dependence
        - thus $p(x)$ cannot be calculated explicitly, and we *cannot* use a maximum-likelihood loss function
    - this leads to the VAE loss function, which is typically called the **evidence lower bound (ELBO)**:
        - if we can't formulate the maximum likelihood, instead derive a lower bound on it
            - if the lower bound is tractable, then we can optimize the parameters with respect to the lower bound
        - if we are making the lower bound larger, we are making the likelihood larger
        - similar to expectation maximization
    - the issue is that $p(z|x)$ is still intractable
        - need to make an approximation of this distribution
        - we take a similar approach to when we defined the likelihood to say z given x should be a nonlinear function ie a neural network that has nromally distributed statistics
    - the **Kullback-Liebler (KL) divergence** of two distributions is a measure of how similar the distributions are:

$$KL(q||p) = -\sum_s q(z) log \frac{p(z)}{q(z)}$$

        - in general, KL divergence is not commuitative
        - KL divergence is nonnegative for any q, p
        - KL divergence is zero only if the distributions are identical

  - the ELBO is:

$$log\ \ p_\theta(x) \geq \mathbb{E}_z log\ \ p(x|z) - KL(q(z|x)||p(z))$$

    * this encapsulates the penalty in estimating the log-likelihood of the data from using $q(z|x)$ to approximate $p(z|x)$
  - the ELBO gives us the lower bound for a loss function that is tractable:
    * $log\ \ p(x|z)$ can be approximated using minibatches
    * KL divergence has a closed form when the distributions are Gaussian
  - to backpropagate through a sampling step, a reparameterization trick can be done with another sampling step during backprop

Generative Adversarial Networks

- **generative adversarial networks (GANs)** are a generative model that does even better at generating images:
  - no probability density has to be estimated
    * unlike VAEs that sample from an *inferred* distribution
  - uses game theory, by pitting two *adversary* neural networks against each other:
    * one network attempts to generate images that look real
    * a discriminator netowkr attempts to distinguish between the generated and real images
  - predicting the future in MSE vs. adversarial approaches:
    * MSE attempts to *average* together the possible future results in an attempt to minimize the loss
      · leads to a general blurring of image futures
    * while an adversarial approach tries to select a single sample from its distribution
  - applications include:
    * upscaling images
    * interpolation between images
    * image to image style translation eg. labels to street scene, black and white to color, edges to photo

Deep Learning Libraries

- deep learning libraries provide APIs to train a diversity of deep neural networks:
  - these libraries also allow us to easily implement training on GPUs
  - may be applicable for other contexts eg. taking gradients
- basic idea of deep learning libraries:
  - write code that builds a computational graph
  - the libraries then implementation backpropagation, so that after the graph is built, there is no need to manually implement the backward pass
  - provide a straightforward API to train on GPUs

PyTorch

- **PyTorch** is a deep learning framework designed for Python
- *pros*:
  - easy to get started
  - pythonic with a consistent API
    - shares many commands with NumPy
  - good documentation
  - easy to install
- cons
  - relatively slower than Tensorflow
- in PyTorch, **tensors** area speecialized data structure similar to arrays and matrices:
  - use tensors to encode the inputs and outputs of a model, as well as its parameters
  - `torch.tensor(data)` creates a tensor directly from data, and `torch.from_numpy(np_array)` creates a tensor from a NumPy array

Building a computational graph:

```
import torch
from torch.autograd import variable

num_in, num_hidden = 10, 50
```

```
x = torch.randn(num_in, requires_grad=True) # x, W, b are all PyTorch tensors
W = torch.randn(num_in, num_hidden, requires_grad=True)
b = torch.randn(num_hidden, requires_grad=True)

z = torch.matmul(x, W) + b
h = torch.max(z, torch.zeros(num_hidden))

loss = (torch.sum(h)-1).pow(2)
loss.backward() # takes the loss function and stores the gradient wrt. loss
                # for every variable with requires_grad
print(x.grad.data, W.grad.data, b.grad.data)
```

- `requires_grad=True` tells PyTorch to *store* the gradients of the tensor `x` with respect to the loss function in `x.grad.data`

Using Torch modules to build networks:

```
import torch
import torch.nn as nn
import torch.nn.functional as F

class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.conv1 = nn.Conv2d(1, 6, 3)   # 1 input, 6 output, 3x3 square conv
        self.conv2 = nn.Conv2d(6, 16, 3)
        self.fc1 = nn.Linear(16*6*6, 120) # affine operation y=mx+b
        self.fc2 = nn.Linear(120, 84)
        self.fc3 = nn.Linear(84, 10)
        # nn.Parameter can be used to initialize a learnable parameter
        self.fc1.weight = nn.Parameter(torch.zeros(16*6*6, 120))
        self.fc1.bias = nn.Parameter(torch.ones(120))
        # ... remaining inits ...

    def forward(self, x):
        x = F.max_pool2d(F.relu(self.conv1(x)), (2, 2)) # max pool over 2x2 window
        x = F.max_pool2d(F.relu(self.conv2(x)), 2)
        x = x.view(x.shape[0], -1)
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        x = self.fc3(x)
        return x
```

```
net = Net()
```

- `net.parameters` gives the learnable parameters of a network

Training a neural network:

```
import torch.optim as optim
net = Net()
criterion = nn.MSELoss()
input = torch.randn(1, 1, 32, 32)

optimizer = optim.SGD(net.parameters(), lr=0.01)

output = new(input)
loss = criterion(output, target)

optimizer.zero_grad() # zero out the previous gradient step
loss.backward()
optimizer.step()
```

Using Torch with GPUs:

```
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
print('device type is {}'.format(device))
x_tensor = x_tensor.to(device) # copy the tensor to device
print('x_tensor is {}'.format(x_tensor))
net = Net().to(device) # copy network to device
```

- important tips:
  - we can use `with torch.no_grad()` to disable grad during inference and testing
    - reduces memory consumption for computations that would otherwise have `requires_grad` enabled
  - if we want to copy parameters from one network to the other, we can use `net.clone()`
  - the variable `loss` contains references to the entire computational graph, so we need to use `loss.item()` to get the actual numeric value of the loss

Keras

- **Keras** is a high-level API for TensorFlow

- *pros*:
  - works directly with NumPy
  - high-level, less explicit
  - automatic GPU usage
- *cons*:
  - less flexible
  - static computational graph
  - difficult to manipulate gradients

Standard Keras imports:

```
import tensorflow as tf
from tensorflow import keras
import tensorflow.keras.models as models
import tensorflow.keras.layers as layers
import tensorflow.keras.regularizers as reg
```

Sequential model in Keras:

```
hidden_dim = 20
model = models.Sequential()
model.add(layers.Permute((2, 1), input_shape=(22. 1000))) # permute dimensions
model.add(layers.SimpleRNN(hidden_dim))
model.add(layers.Dense(4, activation='softmax', kernel_regularizer=reg.L1(0.01)))
model.compiles('adam', 'sparse_categorical_crossentropy', metrics=['acc'])
model.summary() # print network summary
```

- can also concatenate layers together using `layers.Concatenate` and `layers.Flatten`
- Keras also supports a functional API that passes one layer to the next:
  - requires an extra explicit input layer
  - allows intermediate models to be compiled

Training a model in Keras:

```
tensorboard_callback = keras.callbacks.TensorBoard(log_dir='logs') # visualizer

loss_hist = model.fit(Xtrain, ytrain,
                      validation_data=(Xval, yval),
                      epochs=5,
                      callbacks=[tensorboard_callback])
hist = loss_hist.history # another way to access the history
```

Example convolutional network in Keras using functional API:

```
inputs = layers.Input(shape=(22, 1000))
r1 = layers.Reshape((22, 1000, 1))(inputs)
c1 = layers.Conv2D(40, (1, 25), activation='elu', data_format='channels_last')(r1)
p1 = layers.Permute((2, 1, 3))(c1)
r2 = layers.Reshape((976, 22*40))(p1)
d1 = layers.Dense(40, activation='elu')(r2)
sq1 = layers.Activation(Ksquare)(d1)
ap1 = layers.AveragePooling1D(75, strides=15)(sq1)
log1 = layers.Activation(Klog)(ap1)
f1 = layers.Flatten()(log1)
outputs = layers.Dense(4, activation='softmax')(f1)

model = models.Model(inputs=inputs, outputs=outputs, name='shallow_convenet')
model.compile('adam', 'sparse_categorical_crossentropy', metrics=['acc'])
```

Appendix

Python Libraries

NumPy

- linera algebra:
  - `linalg.inv(m)` inverts matrix `m`
  - `ndarray.dot(b)` takes the dot product of two arrays
  - `ndarray.T` gives the transpose of the array
  - `vstack(tuple)` stacks the arrays in `tuple` in sequence vertically
    - useful for constructing transposed matrices
- building arrays and distributions:
  - `arange(start, stop, step)` returns evenly spaced values within an interval given a step size
  - `linspace(start, stop, num)` returns `num` evenly spaced numbers over an interval given a number of steps
  - `ones(shape)` returns a new array of shape filled with ones
  - `ones_like(a)` returns an array of ones with the same shape and type as given array `a`
  - `random.uniform(low, high, size)` draws `size` samples from a uniform distribution between `low` and `high`
  - `random.normal(loc, scale, size)` draws `size` samples from a normal distribution with mean `loc` and standard deviation `scale`
  - `flatnonzero(a)` returns indices that are non-zero in the flattened version of `a`
  - `random.choice(a, size, replace)` generates a random sample from `a`
  - `split(a, sections, axis)` divides an array into `sections` subarrays along a specified axis
- other methods:
  - `concatenate` joins a sequence of arrays along an existing axis
  - `count_nonzero(a)` counts the number of non-zero values in the array `a`

MatPlotLib

- `plt.figure` creates a new figure
- `Figure.gca` gets the current axes of a figure

- `Axes.plot(x, y, fmt)` plots a figure with points or line nodes given by x, y
  - `fmt` is a format string eg. `'ro'` for red circles, `'.'` for dots, `'x'` for crosses
- `Axes.set_xlabel(lbl)` and `Axes.set_ylabel(lbl)` sets the labels for the axes
- `Axes.legend()` places a legend on the axes

Linear Algebra Review

Vectors

- $x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$ is a **column vector** with n elements
- $z = \begin{bmatrix} z_1 z_2 \dots z_n \end{bmatrix}$ is a **row vector** with n elements
- the **transpose** of a column vector is a row vector, and vice versa
  - eg. $x = \begin{bmatrix} x_1 x_2 \dots x_n \end{bmatrix}^T$
- the **dot product** of two column vectors is given by:

$$x^T y = \sum_{i=1}^{n} x_i y_i$$

  - the dot product of two vectors is commutative
- the **norm** of a vector measures its length
- the **p-norm** of a vector is given by the following, where $p \geq 1$:

$$||x||_p = (\sum_{i=1}^{n} |x_i|^p)^{\frac{1}{p}}$$

- the **Euclidian norm** is the 2-norm, and can also be writen as:

$$||x|| = ||x||_2 = \sqrt{x^T x}$$

  - the 2-norm is often more convenient to work with
  - a **unit vector** is a vector with $||x||_2 = 1$

- the dot product can also be written as the following, where θ is the angle between the vectors:
$$x^T y = ||x||||y||cos\theta$$
- x and y are **orthogonal** if $x^T y = 0$:
  - if both vectors have nonzero norm, than they are at a 90 degree angle to each other
  - in $\mathbb{R}^n$ at most n vectors may be mutually orthogonal with nonzero norm
  - if the vectors are orthogonal and also have unit norm, they are **orthonormal**
- a **linear combination** of vectors is a summation of those vectors scaled by a constant:
$$\sum_i c_i v_i$$
  - the **span** of a set of vectors is the set of all points obtainable by linear combinations of the vectors

Matrices

- $A = \begin{bmatrix} a_{11} \dots a_{1n} \\ \vdots \quad \ddots \quad \vdots \\ a_{m1} \dots a_{mn} \end{bmatrix}$ is an $m \times n$ **matrix**
- the product operation of two matrices $C = AB$ is defined by:
$$C_{ij} = \sum_k A_{ik} B_{kj}$$
  - matrix multiplication is distributive and associative
  - however, it is *not* commutative
- matrix multiplication is usually used to write down a system of linear equations, where $A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m, x \in \mathbb{R}^n$:
$$Ax = b$$
$$A_1 x = b_1$$
$$A_2 x = b_2$$
$$\dots$$
$$A_m x = b_m$$
  - this system can be solved using **matrix inversion** where $A^{-1}A = I_n$

and I_n is the $n \times n$ **identity matrix**:

$$\begin{aligned} Ax &= b \\ A^{-1}Ax &= A^{-1}b \\ I_n x &= A^{-1}b \\ x &= A^{-1}b \end{aligned}$$

  - however, $Ax = b$ may not always have a solution:
    * the **column space** is the span of the columns of A
    * to have a solution for all values of $b \in \mathbb{R}^m$, the column space of A must be all of $\mathbb{R}^m$
    * thus A should have at least m columns or $m > n$:
      · however, some of the columns may be redundant ie. **linearly dependent** as well
      · in addition, we need each equation to have at *most* one solution for each value of b, so A can also have at most m columns
    * therefore, the system will have a solution if it is square and all the columns are **linearly independent** ie. no vector in the columns is a linear combination of the other vectors
      · a square matrix with linearly dependent columns is **singular**
    * the **rank** of a matrix is the number of linearly independent columns it has

- the **determinant** of a square matrix $det(A)$ is a function that maps matrices to real scalars:
  - the determinant is equal to the product of all eigenvalues of a matrix
  - thus, since eigenvalues measure the scaling of eigenvectors, the absolute value of the determinant is a measure of how much the matrix expands or contracts space
  - if the determinant is 0, then space is contracted *completely* along at least one dimension, losing all its volume

- the **transpose** of a matrix satisfies:

$$A_{ij} = (A^T)_{ji}$$

  - a matrix is **symmetric** if $A = A^T$

- if the matrix is square ie. $m = n$ with rank n, then the **inverse** of a matrix satisfies the following, where I is the $n \times n$ **identity** matrix:

$$A^{-1}A = AA^{-1} = I$$

- the **trace** of a matrix is the sum of its diagonal elements:

$$tr(A) = \sum_{i=1}^{n} a_{ii}$$

  - the trace operator is invariant to transposition:

$$tr(A) = tr(A^T)$$

  - the trace operator is invariant to cyclic permutations of its input (even if the resulting product has different shapes):

$$tr(ABC) = tr(CAB) = tr(BCA)$$

  - the trace operator is linear:

$$tr(aX + bY) = atr(X) + btr(Y)$$

- the **Frobenius norm** of matrix $A \in \mathbb{R}^{m \times n}$ is:

$$||A||_F = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^2} = \sqrt{tr(AA^T)}$$

- a **diagonal** matrix consists of only nonzero entries along the main diagonal:
  - ie. $D_{ij} = 0 \ \forall \ i \neq j$
  - eg. the identity matrix
  - useful properties of diagonal matrices:
    - multiplying by a diagonal matrix is computationally efficient
      - to find Dx, we just need to scale each element x_i by D_{ii}
    - to compute the inverse of a square diagonal matrix where each element on the diagonal is nonzero, just take the reciprocal $\frac{1}{D_{ii}}$ on the diagonal
    - nonsquare diagonal matrices do not have inverses, but can still be multiplied cheaply
- a **symmetric** matrix is one that is equal to its own transpose $A = A^T$
- given a symmetric matrix A:
  - A is called **positive definite** if $x^T Ax > 0 \ \forall \ x$
  - if $x^T Ax \geq 0$, A is **positive semidefinite**
  - similarly for **negative definite** and **negative semidefinite** matrices
- an **orthogonal matrix** is a square matrix whose rows are mutually orthonormal and whose columns are mutually orthonormal:

$$A^T A = AA^T = I$$

$$A^{-1} = A^T$$

  - thus the inverse of these matrices are easily computed

Decomposition

- an **eigenvector** u_i and its corresponding **eigenvalue** λ_i of a square matrix $A \in \mathbb{R}^{n \times n}$ satisfy:

$$Au_i = \lambda_i u_i$$

  - the eigenvalues can be found by solving:

$$det(A - \lambda I) = 0$$

- collecting all of A's eigenvectors and eigenvalues into the following matrices gives the following **eigendecomposition** of A:

$$U = [u_1 u_2 ... u_n] \quad \Lambda = \begin{bmatrix} \lambda_1 & 0 & ... & 0 \\ 0 & \lambda_2 & ... & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & ... & \lambda_n \end{bmatrix}$$

$$A = U\Lambda U^{-1}$$

  - this decomposes square matrices in a *unique*, guaranteed way that show us information about their fundamental functional properties
  - tells us that these transformations *scale* space by eigenvalue λ_i in the direction of eigenvector v_i
  - in addition, makes the calculation of A^p easier, since $A^p = U\Lambda^p U^{-1}$

- specifically, if U's columns are an orthonormal set of the eigenvectors:

$$A = U\Lambda U^T$$

- the eigendecomposition can be derived as follows from the definition of an eigenvector:

$$\begin{aligned} Au_1 &= \lambda_2 u_1 \\ Au_2 &= \lambda_2 u_2 \\ A[u_1 u_2] &= [u_1 u_2] \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} \\ AU &= U\Lambda \\ A &= U\Lambda U^{-1} \end{aligned}$$

- if A is **normal**, then its eigenvectors are **orthonormal**:

$$u_i^T u_j = 0 \ \ \forall \ \ i \neq j, \quad u_i^T u_i = 1$$

- the **singular value decomposition (SVD)** of a matrix $A \in \mathbb{R}^{m \times n}$ is:

$$A = U\Sigma V^T$$

  - where U is an $m \times m$ matrix with orthonormal columns and V is an $n \times n$ matrix with orthonormal columns
    - the columns of U are the **left singular vectors** of A and are the orthonormal eigenvectors of AA^T
    - the columns of V are the **right singular vectors** of A and are the orthonormal eigenvectors of A^TA
  - Σ is a diagonal $m \times n$ matrix with σ_i as its ith diagonal element
    - σ_i is called the ith **singular value** of A and can be calculated as:

$$\sigma_i = \lambda_i^{\frac{1}{2}}(A^TA) = \lambda_i^{\frac{1}{2}}(AA^T)$$

  - essentially factorizing a matrix into singular vectors and singular values by performing an eigendecomposition for A^TA
  - unlike an eigendecomposition, SVD is applicable to nonsquare matrices as well eg. can solve $Ax = b$ for nonsquare and perform **principal component analysis (PCA)**

Mathematical Tools

- useful properties of common functions:
  1. the **logistic sigmoid**:

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

     - commonly used to produce the probability parameter of a Bernoulli distribution
     - its range is $(0, 1)$, and saturates when its argument is very positive or negative
  2. the **softplus function**:

$$\zeta(x) = log(1 + e^x)$$

     - useful for producing the $\sigma = \frac{1}{\beta}$ parameter of a normal distribution
     - its range is $(0, \infty)$

Probability

- notation note:
  - $Pr(E)$ is the probability of the event E

  - $Pr(X = x)$ or equivalent shorthand $p(x)$ is the probability of random variable X taking on the value x

- manipulating probabilities revolves around two main rules:

  1. the **law of total probability** ie. sum rule:

$$p(x) = \sum_y p(x, y), \quad x, y \text{ discrete}$$

$$p(x) = \int_y p(x, y)dy, \quad x, y \text{ continuous}$$

  - more particularly, if $A_1, \dots, A_n$ forms a partition of the sample space S, then the probability of an event B is:

$$Pr(B) = \sum_{i=1}^{n} Pr(B \cap A_i)$$

  - alternatively, using the conditional probability definition:

$$Pr(B) = \sum_{i=1}^{n} Pr(B|A_i)Pr(A_i)$$

  2. the **probability chain rule** ie. product rule:

$$\begin{aligned} Pr(E_1, E_2) &= Pr(E_1)Pr(E_2|E_1) \\ &= Pr(E_2)Pr(E_1|E_2) \end{aligned}$$

  - used to break up a joint probability into a product probability
  - can be further decomposed as follows:

$$\begin{aligned} p(w, x, y, z) &= p(w, x)p(y, z|w, x) \\ &= p(x)p(w|x)p(y, z|w, x) \\ &= p(x)p(w|x)p(z|w, x)p(y|z, w, x) \end{aligned}$$

    * any event that has been in front of the conditioning bar must be behind the conditioning bar for all other probability expressions
    * ie. assuming a random variable *has* taken on a value, and evaluating the remaining events
  - can also represent conditional independencies in graphical models
  - generalized for a joint probability over many variables:

$$p(x_1, \dots, x_n) = p(x_1) \prod_{i=2}^{n} p(x_i|x_1, \dots, x_{i-1})$$

    - could be proved through induction

- chain rule examples:

$$\begin{aligned} p(b,c|d,e) &= \frac{q}{p(d)p(e|d)} \\ p(d)p(e|d)p(b,c|d,e) &= q \\ q &= p(b,c,d,e) \end{aligned}$$

$$\begin{aligned} p(d,e)q &= \frac{p(a,b,c,d,e)}{p(a|b,c,d,e)} \\ p(d,e)p(a|b,c,d,e)q &= p(a,b,c,d,e) \\ q &= p(b,c|d,e) \end{aligned}$$

- **Bayes' rule** gives the following relationship:

$$p(x|y) = \frac{p(y|x)p(x)}{\sum_x p(y|x)p(x)}$$

- an intuition on **Bayesian inference**, which appears frequently in machine learning:
    - let x represent model parameters we wish to infer denoted θ and y correspond to data we have observed D:

$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{\sum_x p(D|\theta)p(\theta)}$$

    - $p(\theta|D)$ is the **posterior distribution**, ie. the probability distribution of model parameters given the data
    - $p(D|\theta)$ is the **likelihood** of the data, ie. the probability of having seen the data given a chosen set of model parameters
    - $p(\theta)$ are **prior parameters**, ie. the probabilities of the model parameters *absent* of any data
        - we can consider that the prior is *updated* by the likelihood to arrive at the posterior distribution on the parameters
    - in Bayesian inference, we calculate $p(\theta|D)$, giving a distribution over the model parameters given the data we observed
        - concretely gives us all the parameters of our model
    - in **Frequentist inference** or **maximum-likelihood estimation**, we calculate $p(D|\theta)$, wanting to infering the θ that makes the data most likely to have been observed
        - ie. we choose the parameters that maximize the likelihood of the data

Derivatives

- in machine learning, we want to find the *best* model according to some performance metric:
  - this requires **optimization**, in which derivatives are crucial
  - in simple cases, we can find minima and maxima by simply setting the derivative equal to 0
  - however, in more complex cases, there is no closed-form solution, but the derivative is still useful in telling us how a change in the model parameters will affect the performance
- the definition of a **derivative** of a function $f : \mathbb{R} \to \mathbb{R}$ at a point $x \in \mathbb{R}$ is:

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

  - gives how much a small change in x affects f:

$$f(x + \varepsilon) \approx f(x) + \varepsilon f'(x)$$

  - given $y = f(x)$, we denote the derivative of y with respect to x as $\frac{dy}{dx}$, such that:

$$\Delta y \approx \frac{dy}{dx} \Delta x$$

- the **scalar chain rule** states that if $y = f(x)$ and $z = g(y)$:

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$

  - ie. a small change in x will cause a small change in y that will in turn cause a small change in z as follows:

$$\begin{aligned} \Delta y &\approx \frac{dy}{dx} \Delta x \\ \Delta z &\approx \frac{dz}{dy} \Delta y \\ &= \frac{dz}{dy}\frac{dy}{dx} \Delta x \end{aligned}$$

- the **gradient** generalizes the scalar derivative to multiple dimensions:
  - if $f : \mathbb{R}^n \to \mathbb{R}$ transforms a vector to a scalar and $y = f(x)$, the gradient with respect to a vector x is :

$$\nabla_x y = \begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_n} \end{bmatrix}$$

  - the gradient is a vector that is the same size as x
  - each dimension of $\nabla_x y$ tells us how small changes in x in that dimension affect y
  - ie. after changing the ith dimension of x by a small amount affects y as follows:

$$\Delta y \approx \frac{\partial y}{\partial x_i} \Delta x_i$$

    * equivalently, $\frac{\partial y}{\partial x_i} = (\nabla_x y)_i$
  - similarly, after changing multiple dimensions of x, y is changed as follows in a dot product:

$$\begin{aligned} \Delta y &= \sum_i \frac{\partial y}{\partial x_i} \Delta x_i \\ &= (\nabla_x y)^T \Delta x \end{aligned}$$

- ex. If $f(x) = \theta^T x$, find $\nabla_x f(x)$ where $\theta, x \in \mathbb{R}^n, y \in \mathbb{R}$:
  - by rules of the gradient, $\nabla_x y \in \mathbb{R}^n$
  1. expand the dot product in $f(x)$:

$$f(x) = \theta_1 x_1 + ... + \theta_n x_n$$

  2. write out the gradient:

$$\nabla_x y = \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_n \end{bmatrix} = \theta$$

  - dimensions match up
- ex. If $f(x) = x^T A x$, find $\nabla_x f(x)$ where $A \in \mathbb{R}^{n \times n}, x \in \mathbb{R}^n, y \in \mathbb{R}$:
  - by rules of the gradient, $\nabla_x y \in \mathbb{R}^n$
  1. expand $f(x)$:

$$f(x) = \sum_i \sum_j a_{ij} x_i x_j$$

2. write out the gradient:

$$\begin{aligned}
\frac{\partial y}{\partial x_1} &= \frac{\partial (a_{11}x_1^2)}{\partial x_1} + a_{12}x_2 + ... + a_{1n}x_n + a_{21}x_2 + ... + a_{n1}x_n \\
&= 2a_{11}x_1 + \sum_{j=2}^{n} a_{1j}x_j + \sum_{i=2}^{n} a_{1i}x_i \\
&= \sum_{j=1}^{n} a_{1j}x_j + \sum_{i=1}^{n} a_{i1}x_i \\
&= (Ax)_1 + (A^T x)_1 \\
\frac{\partial y}{\partial x_i} &= (Ax)_i + (A^T x)_i \\
\frac{\partial y}{\partial x} &= \nabla_x f(x) = Ax + A^T x
\end{aligned}$$

   - an intuition check is to consider the problem in a single dimension:
     - ie. when $n = 1$, $f(x) = xax = ax^2$ and $\frac{\partial f(x)}{\partial x} = 2ax$
     - when A is symmetric, the gradient is analogously just $2Ax$

- derivative of a scalar with respect to a matrix:
  - given a scalar y and a matrix $A \in \mathbb{R}^{m \times n}$, the derivative is given by:

$$\nabla_A y = \begin{bmatrix} \frac{\partial y}{\partial a_{11}} & \cdots & \frac{\partial y}{\partial a_{1n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y}{\partial a_{m1}} & \cdots & \frac{\partial y}{\partial a_{mn}} \end{bmatrix}$$

  - like the gradient, the i, jth element of $\nabla_A y$ tells us how small changes in a_{ij} affect y
  - this layout is called **denominator layout** notation, in which the dimensions of $\nabla_A y$ and A are the same
    - in **numerator layout**, the dimensions are transposed
- derivative of a vector with respect to a vector:
  - given $y \in \mathbb{R}^n$ as a function of $x \in \mathbb{R}^m$, the derivative of y with respect to x would be used as follows:

$$\Delta y_i = \nabla_x y_i \cdot \Delta x$$

  - thus, the derivative J should be an $n \times m$ matrix as follows:

$$\begin{aligned} J &= \begin{bmatrix} (\nabla_x y_1)^T \\ \vdots \\ (\nabla_x y_n)^T \end{bmatrix} \\ &= \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_n}{\partial x_1} & \cdots & \frac{\partial y_n}{\partial x_m} \end{bmatrix} \end{aligned}$$

  - like the gradient, we can see how small changes in x affect y as follows:

$$\Delta y \approx J \Delta x$$

    * J is called the **Jacobian** matrix
  - since in the denominator layout, the denominator vector changes along rows (instead of along columns, as in the Jacobian):

$$\begin{aligned} J &= (\nabla_x y)^T \\ &= (\frac{\partial y}{\partial x})^T \\ \nabla_x y &= J^T \end{aligned}$$

- the **Hessian** matrix of a function $f(x)$ is a square matrix of second-order partial derivatives of f as follows:

$$H = \begin{bmatrix} \frac{\partial f}{\partial x_1^2} & \frac{\partial f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial f}{\partial x_1 \partial x_n} \\ \frac{\partial f}{\partial x_2 \partial x_1} & \frac{\partial f}{\partial x_2^2} & \cdots & \frac{\partial f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f}{\partial x_m \partial x_1} & \frac{\partial f}{\partial x_m \partial x_2} & \cdots & \frac{\partial f}{\partial x_m^2} \end{bmatrix}$$

  - the Hessian is denoted as $\nabla_x(\nabla_x f(x))$ or equivalently $\nabla_x^2 f(x)$

Chain Rule

- the **chain rule** for vector valued functions:
  - in the denominator layout, the chain rule runs from right to left
  - if $x \in \mathbb{R}^m$, $y \in \mathbb{R}^n$, $z \in \mathbb{R}^p$ and $y = f(x)$ for $f : \mathbb{R}^m \to \mathbb{R}^n$ and $z = g(y)$ for $g : \mathbb{R}^n \to \mathbb{R}^p$, then:

$$\begin{aligned} \nabla_x z &= \nabla_x y \nabla_y z \\ \frac{\partial z}{\partial x} &= \frac{\partial y}{\partial x} \frac{\partial z}{\partial y} \end{aligned}$$

    - $\nabla_x z$ should have dimensionality $\mathbb{R}^{m \times p}$
    - since $\nabla_x y \in \mathbb{R}^{m \times n}$ and $\nabla_y z \in \mathbb{R}^{n \times p}$, the operations are dimensionally correct
- composing the chain rule:
  - intuitively, a small change Δx affects Δz through the Jacobian $(\nabla_x z)^T$:

$$\Delta z \approx (\nabla_x z)^T \Delta x$$

  - then, through composition:

$$\Delta y \approx (\nabla_x y)^T \Delta x$$
$$\Delta z \approx (\nabla_y z)^T \Delta y$$
$$\Delta z \approx (\nabla_y z)^T (\nabla_x y)^T \Delta x$$

  - thus reduces to the right to left chain rule:

$$(\nabla_x z)^T = (\nabla_y z)^T (\nabla_x y)^T$$
$$\nabla_x z = \nabla_x y \nabla_y z$$

Tensors

- we may need to take a derivative that is more than 2-dimensional:
  - eg. the derivative of a vector with respect to a matrix would be a 3-dimensional **tensor**
    - a tensor is an array with more than two axes
  - if $y = Wx \in \mathbb{R}^m$, $x \in \mathbb{R}^n$, and $W \in \mathbb{R}^{m \times n}$ then $\nabla_W z$ is a 3-dimensional tensor with shape $\mathbb{R}^{m \times n \times n}$:
    - breaking down the vector y into scalar-matrix derivatives that we do know how to compute
    - ie. each $m \times n$ slice is the matrix derivative $\nabla_W y_i$
  - in general, can usually use intuition to calculate tensor derivatives rather than a rigorous derivation
    - actually calculating and storing tensor derivatives can be very expensive for memory and computation
- ex. Consider the squared loss function:

$$\begin{aligned} L &= \frac{1}{2} \sum_{i=1}^{N} ||y_i - W x_i||^2 \\ &= \frac{1}{2} \sum_{i=1}^{N} (y_i - W x_i)^T (y_i - W x_i) \\ &= \frac{1}{2} \sum_{i=1}^{N} z_i^T z_i \end{aligned}$$

$$\frac{\partial L}{\partial W} = \frac{\partial z}{\partial W} \frac{\partial L}{\partial z}$$

$$\begin{aligned}
\frac{\partial z_k}{\partial w} &= \frac{\partial}{\partial W}[y_k - \sum_{j=1} W_{kj}x_j] \\
\frac{\partial z_k}{\partial W_{ip}} &= -\frac{\partial}{\partial W_{ip}}[\sum_j W_{kj}x_j] \\
&= -\frac{\partial}{\partial W_{ip}}[W_{k1}x_1 + ... + W_{kn}x_n] \\
&= \begin{cases} 0 & i \neq k, \\ -x_p & i = k \end{cases}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial \varepsilon}{\partial W} &= \frac{\partial z}{\partial W}\frac{\partial \varepsilon}{\partial z} \\
&= \sum_{k=1}^{m} \frac{\partial z_k}{\partial W}\frac{\partial \varepsilon}{\partial z_k} \\
&= \frac{\partial \varepsilon}{\partial z_1}\begin{bmatrix} -x^T \\ 0 \\ \vdots \\ 0 \end{bmatrix} + ... + \frac{\partial \varepsilon}{\partial z_m}\begin{bmatrix} 0 \\ \vdots \\ 0 \\ -x^T \end{bmatrix} \\
&= \begin{bmatrix} -\frac{\partial \varepsilon}{\partial z_1}x^T \\ \vdots \\ -\frac{\partial \varepsilon}{\partial z_m}x_T \end{bmatrix} \\
&= -\frac{\partial \varepsilon}{\partial z}x^T
\end{aligned}$$

- calculation notes:
  - we drop the summation and calculate the gradient of the loss over a single example where $L_i = \varepsilon$
  - $z \in \mathbb{R}^m$, $W \in \mathbb{R}^{m \times n}$, $\frac{\partial z}{\partial W} \in \mathbb{R}^{m \times n \times m}$, and $\frac{\partial z_k}{\partial W} \in \mathbb{R}^{m \times n}$
  - the dimensionality of the gradient $\frac{\partial L}{\partial W}$ should give $(m \times n \times m)(m \times 1) = (m \times n)$
  - $\frac{\partial z_k}{\partial W}$ is a matrix where all the entries are 0, except the kth row which is equal to $-x^T$
- in lecture, we used the trace operator to circumvent the tensor derivative calculation

Discussion Problems

Linear Algebra Review

- ex. Show the following properties for matrices:
  1. if $b^T Ab > 0 \ \forall \ b \in \mathbb{R}^n$, then all eigenvalues of A are positive:

$$\begin{aligned} Av_i &= \lambda_i v_i \\ v_i^T Av_i &= \lambda_i v_i^T v_i \\ v_i^T Av_i &= \lambda_i ||v_i||_2^2 > 0 \\ &\therefore \ ||v_i||_2^2 > 0, \lambda_i > 0 \end{aligned}$$

     - this is a positive definite matrix
  2. if $A \in \mathbb{R}^{n \times n}$ is an orthogonal matrix, then all eigenvalues of A have norm 1:

$$\begin{aligned} Av_i &= \lambda_i v_i \\ A^T Av_i &= \lambda_i A^T v_i \\ v_i &= \lambda_i A^T v_i \\ ||v_i||_2^2 &= |\lambda_i|^2 ||A^T v_i||_2^2 \\ &= |\lambda_i|^2 (A^T v_i)^T (A^T v_i) \\ &= |\lambda_i|^2 v_i^T AA^T v_i \\ &= |\lambda_i|^2 ||v_i||_2^2 \\ &\therefore \ |\lambda_i| = 1 \end{aligned}$$

  3. If $A \in \mathbb{R}^{m \times n}$ is a matrix with rank r, then $\sigma_i(A) = \lambda_i^{\frac{1}{2}}(AA^T)$:

$$\Sigma\Sigma^T = diag(\sigma_1^2, \dots, \sigma_n^2)$$

$$\begin{aligned} A &= U\Sigma V^T \\ AA^T &= (U\Sigma V^T)(U\Sigma V^T)^T \\ &= U\Sigma V^T V\Sigma^T U^T \\ &= U\Sigma\Sigma^T U^T \\ &= U diag(\sigma_1^2, \dots, \sigma_n^2) U^T \\ &\therefore \ \sigma_i(A) = \lambda_i^{\frac{1}{2}}(AA^T) \end{aligned}$$

     - producing an eigendecomposition of AA^T

Vector and Matrix Derivatives

- trace has useful properties for computing derivatives:
  - the **trace** of a matrix is the sum of the diagonal entries

  - $Tr(AB) = Tr(BA)$
  - $Tr(A) = Tr(A^T)$
  - $Tr(A^T B) = \sum_i \sum_j a_{ij} b_{ij}$

- ex. $\nabla_A tr(AB)$ where $A = \begin{bmatrix} a_1^T \\ \vdots \\ a_n^T \end{bmatrix}$ and $B = [b_1 \dots b_n]$:

$$\begin{aligned} Tr(AB) &= a_1^T b_1 + \cdots + a_n^T b_n \\ &= \sum_{i=1}^{n} a_i^T b_i \\ &= \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} b_{ji} \\ [\nabla_A tr(AB)]_{ij} &= b_{ji} \end{aligned}$$

$$\nabla_A tr(AB) = B^T$$

- ex. $\nabla_A (x^T A x)$:

$$Tr(x^T A x) = x^T A x$$

$$\begin{aligned} \nabla_A (x^T A x) &= \nabla_A (Tr(x^T A x)) \\ &= \nabla_A (Tr(A x x^T)) \\ &= (x x^T)^T \\ &= x x^T \end{aligned}$$

- ex. $\nabla_z (x - z)^T \Sigma^{-1} (x - z)$ where $y = f(z) = x - z$, $r = g(y) = y^T \Sigma^{-1} y$, and Σ^{-1} is symmetric:

$$\begin{aligned} \nabla_z y &= \nabla_z (x - z) \\ &= -I \end{aligned}$$

$$\begin{aligned} \nabla_y r &= \nabla_y (y^T \Sigma^{-1} y) \\ &= \Sigma^{-1} y + (\Sigma^{-1})^T y \\ &= 2\Sigma^{-1} y \end{aligned}$$

$$\begin{aligned} \nabla_z r &= \nabla_z y \nabla_y r \\ &= -2\Sigma^{-1} y \\ &= -2\Sigma^{-1} (x - z) \end{aligned}$$

- a technique used to address the overfitting found in the normal least squares approach is called **regularization**:
  - this produces the regularized least squared problem with the following cost function where λ is a tunable regularization parameter:

$$L = \frac{1}{2}\sum_{i=1}^{N}(y_i - \theta^T \hat{x}_i)^2 + \frac{\lambda}{2}||\theta||_2^2$$

    - want a least squares solution with a smaller ie. simpler θ norm
  - optimizing L:

$$\begin{aligned} L &= \frac{1}{2}(Y - X\theta)^T(Y - X\theta) + \frac{\lambda}{2}||\theta||_2^2 \\ L(\theta) &= \frac{1}{2}[Y^TY - Y^TX\theta - \theta^TX^TY + \theta^TX^TX\theta] + \frac{\lambda}{2}\theta^T\theta \\ &= \frac{1}{2}Y^TY - Y^TX\theta + \frac{1}{2}[\theta^T(X^TX + \lambda I)\theta] \\ \nabla_\theta L(\theta) &= -\nabla_\theta[Y^TX\theta] + \frac{1}{2}\nabla_\theta[\theta^T(X^TX + \lambda I)\theta] \\ &= -X^TY + \frac{1}{2}2(X^TX + \lambda I)\theta \ \ [=] \ \ 0 \\ \theta &= (X^TX + \lambda I)^{-1}X^TY \end{aligned}$$

    - note that $X^TX + \lambda I$ is symmetric

Supervised Classification and Gradients

- examine how k-NN classifiers can be more robust to noise:
  - given two labels 0 and 1, a test point x, and its k nearest neighbors z_i where p_i is the probability the label of z_i is not equal to x
  - let $p_1 = 0.1$ and $p_i = 0.2 \ \ \forall \ \ i > 1$
  - the probability that the 1-NN classifier makes a mistake classifying is 0.1
  - the probability that the 3-NN classifier makes a mistake occurs when at least 2 of the 3 nearest neighbors have a different label than x:
    - $Pr(\textit{all different}) = 0.1 \times 0.2^2$
    - $Pr(\textit{first different, one other different}) = 0.1 \times 0.2 \times 0.8$
    - $Pr(\textit{second and third different}) = 0.9 \times 0.2^2$
    - altogether, the sum is of probabilities is 0.072
  - thus the 3-NN classifier is more robust, since it checks more neighbors
- taking the derivative of the softmax function:

$$f(z_j) = \frac{e^{z_j}}{\sum_k e^{z_k}}$$

- calculate $\nabla_{z_i} f(z_j)$ for $i = j$:

$$\begin{aligned}
\nabla_{z_i} f(z_j) &= \frac{\partial}{\partial z_i}[\frac{e^{z_i}}{e^{z_1} + ... + e^{z_c}}] \\
&= \frac{e^{z_i} \sum_k e^{z_k} - e^{z_i} \cdot e^{z_i}}{(\sum_k e^{z_k})^2} \\
&= \frac{e^{z_i}}{\sum_k e^{z_k}} - \frac{(e^{z_i})^2}{(\sum_k e^{z_k})^2} \\
&= f(z_i) - (f(z_i))^2 \\
&= f(z_i)(1 - f(z_i))
\end{aligned}$$

  - uses the quotient rule for derivatives
- calculate $\nabla_{z_i} f(z_j)$ for $i \neq j$:

$$\begin{aligned}
\nabla_{z_i} f(z_j) &= \frac{\partial}{\partial z_i}[\frac{e^{z_j}}{e^{z_1} + ... + e^{z_c}}] \\
&= \frac{0 \cdot \sum_k e^{z_k} - e^{z_j} \cdot e^{z_i}}{(\sum_k e^{z_k})^2} \\
&= \frac{-e^{z_j}}{\sum_k e^{z_k}} \frac{e^{z_i}}{\sum_k e^{z_k}} \\
&= -f(z_j) f(z_i)
\end{aligned}$$

Backpropagation

- performing backprop on the following regularized linear classification model:

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

- want to be able to update w, b using $\frac{\partial L_{reg}}{\partial w}$ and $\frac{\partial L_{reg}}{\partial b}$

- from the chain rule:

$$\begin{aligned}\frac{\partial L_{reg}}{\partial w} &= [\sigma(wx+b)-t](\frac{\partial}{\partial w}[\sigma(wx+b)-t]) + \lambda w \\ &= [\sigma(wx+b)-t]\sigma'(wx+b)\frac{\partial}{\partial w}(wx+b) + \lambda w \\ &= [\sigma(wx+b)-t]\sigma'(wx+b)x + \lambda w\end{aligned}$$

$$\frac{\partial L_{reg}}{\partial b} = [\sigma(wx+b)-t]\sigma'(wx+b)$$

  - using the full chain rule is not modular and involves redundant calculations

- using backprop on the computation graph in Figure 18:

$$\begin{aligned}\frac{\partial L_{reg}}{\partial L} &= \frac{\partial L_{reg}}{\partial R} = 1 \\ \frac{\partial L_{reg}}{\partial g} &= g \\ \frac{\partial L_{reg}}{\partial q_2} &= \lambda q_2 \\ \frac{\partial L_{reg}}{\partial g} &= g \\ \frac{\partial L_{reg}}{\partial z} &= \sigma'(z)g \\ \frac{\partial L_{reg}}{\partial b} &= \sigma'(z)g \\ &= \sigma'(wx+b)[\sigma(wx+b)-t] \\ \frac{\partial L_{reg}}{\partial m} &= \sigma'(z)g \\ \frac{\partial L_{reg}}{\partial q_1} &= x\sigma'(z)g \\ \frac{\partial L_{reg}}{\partial w} &= \frac{\partial L_{reg}}{\partial q_1} + \frac{\partial L_{reg}}{\partial q_2} \\ &= x\sigma'(z)g + \lambda q_2 \\ &= x\sigma'(wx+b)[\sigma(wx+b)-t] + \lambda w\end{aligned}$$

  - note that h is the identity function, so its gradients drop out in the law of total derivatives

Neural Network Review

1. In which of the following applications can we apply deep learning to?

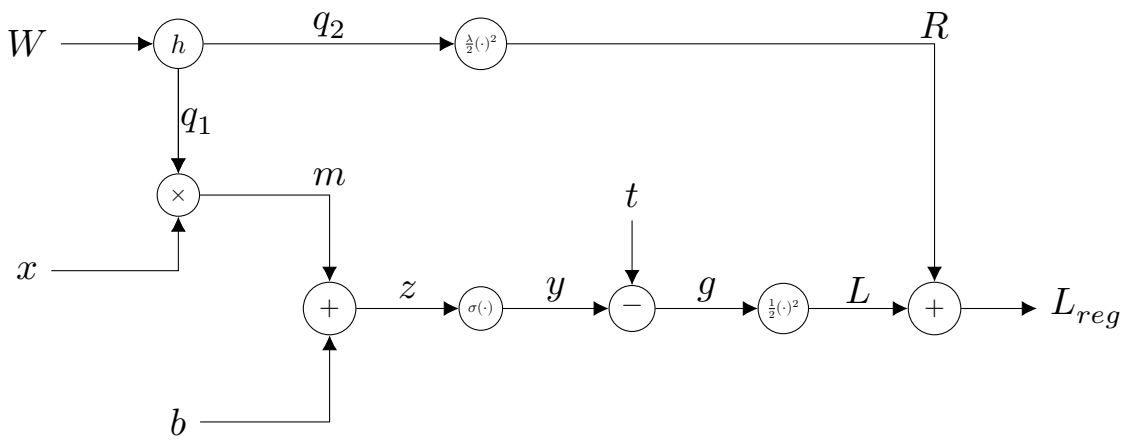


Figure 18: Backprop for a Regularized Linear Classification

a. Protein structure prediction
b. Prediction of chemical reactions
c. Detection of exotic particles
d. All of these

- D, neural networks act as a universal function approximator

2.
- Statement 1: It is possible to train a network well by initalizing all the weights as 0.
- Statement 2: It is possible to train a network well by initalizing biases as 0.
- Statement 2 can be true while Statement 1 is false
  - the gradient vanishes when the weights are 0

3. The number of nodes in the input layer is 10 and the hidden layer is 5. The maximum number of connections from the input layer to the hidden layer are:

a. 50
b. Less than 50
c. More than 50
d. It is an arbitrary value

- A, the weights are defined as connections

4. Which of the following functions can be used as an activation function in the output layer if we wish to predict the probabilities of classes such that the sum of probabilities equals to 1?

a. Softmax

b. ReLU
c. Sigmoid
d. $tanh$

- A, need to use softmax
  - sigmoid and $tanh$ output values that do not add up to 1, and ReLU ranges from 0 to infinity

5. Which of the following functions can't be used at output layer to classify an image?

   a. Softmax
   b. $tanh$
   c. ReLU
   d. None of the above

   - C, since ReLU gives continous output in range 0 to infinity, but we want a finite range of values for the output layer

6. Which of the following neural network training challenges can be solved using batch normalization?

   a. Overfitting
   b. Restrict activations to become too high or low
   c. Training is too slow
   d. All of the above

   - D

7. Assume a simple MLP model with 3 neurons and inputs 1, 2, and 3 and weights to input neurons 4, 5, and 6 respectively. Assume the activation function is a linear constant value of 3. What will be the output?

   - $(1 \times 4 + 2 \times 5 + 3 \times 6) \times 3 = 96$
   - MLP AKA multilayer perceptron indicates a fully connected model