

# Mixtures

- *Mixture of  $f$  and  $g$ :*

$$p(x) = \eta f(x) + (1 - \eta)g(x)$$

Simplest, most common kind of latent variable model

- *Hidden variable representation:* Define  $Z \sim \text{Bernoulli}(\eta)$  and

$$p(x) = \sum_{z=0,1} p(x|z) p(z)$$

with  $p(x|0) = f(x)$ ,  $p(x|1) = g(x)$ ,  $p(z) = \eta^z(1 - \eta)^{(1-z)}$ .

# Bayesian Inference

The parameter  $\theta$  of a model is viewed as a random variable.  
Inference usually carried out as follows:

- Choose a *generative model*  $p(x | \theta)$  for the data.
- Choose a *prior distribution*  $\pi(\theta)$  that expresses beliefs about the parameter before seeing any data.
- After observing data  $\mathcal{D}_n = \{x_1, \dots, x_n\}$ , update beliefs and calculate the *posterior distribution*  $p(\theta | \mathcal{D}_n)$ .

# Bayes' Theorem

The posterior distribution can be written as

$$p(\theta | x_1, \dots, x_n) = \frac{p(x_1, \dots, x_n | \theta)\pi(\theta)}{p(x_1, \dots, x_n)} = \frac{\mathcal{L}_n(\theta)\pi(\theta)}{c_n} \propto \mathcal{L}_n(\theta)\pi(\theta)$$

where  $\mathcal{L}_n(\theta) = \prod_{i=1}^n p(x_i | \theta)$  is the *likelihood function* and

$$c_n = p(x_1, \dots, x_n) = \int p(x_1, \dots, x_n | \theta)\pi(\theta)d\theta = \int \mathcal{L}_n(\theta)\pi(\theta)d\theta$$

is the normalizing constant, which is also called *evidence*.

## Example

$X \sim \text{Bernoulli}(\theta)$  with data  $\mathcal{D}_n = \{x_1, \dots, x_n\}$ . Prior  $\text{Beta}(\alpha, \beta)$  distribution

$$\pi_{\alpha, \beta}(\theta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \theta^{\alpha-1} (1 - \theta)^{\beta-1}$$

Let  $s = \sum_{i=1}^n x_i$  be the number of “successes.”

Posterior distribution  $\theta \mid \mathcal{D}_n$  is  $\text{Beta}(\alpha + s, \beta + n - s)$ . Posterior mean is a mixture:

$$\bar{\theta} = \frac{\alpha + s}{\alpha + \beta + n} = \left( \frac{n}{\alpha + \beta + n} \right) \hat{\theta} + \left( \frac{\alpha + \beta}{\alpha + \beta + n} \right) \theta_0$$

where  $\hat{\theta} = s/n$  is the MLE and  $\theta_0 = \alpha/(\alpha + \beta)$  is the prior mean.

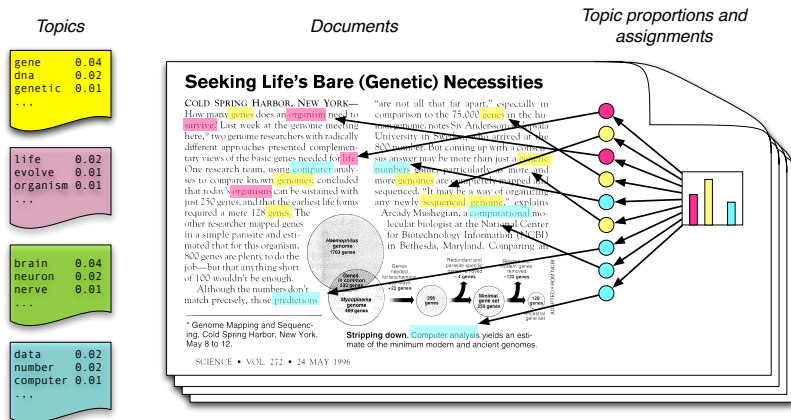
# Dirichlet

Multinomial model with Dirichlet prior is generalization of the Bernoulli/Beta model.

$$\text{Dirichlet}_{\alpha}(\theta) = \frac{\Gamma(\sum_{j=1}^K \alpha_j)}{\prod_{j=1}^K \Gamma(\alpha_j)} \prod_{j=1}^K \theta_j^{\alpha_j-1}$$

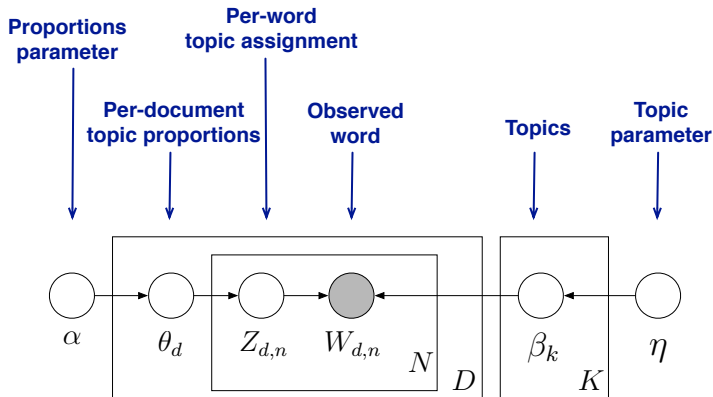
where  $\alpha = (\alpha_1, \dots, \alpha_K) \in \mathbb{R}_+^K$  is a non-negative vector.

# Generative model for LDA



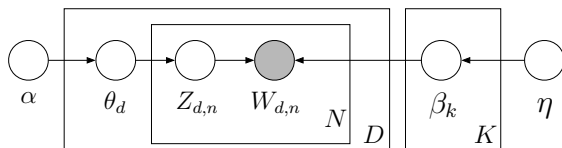
- Each **topic** is a distribution over words
- Each **document** is a mixture of corpus-wide topics
- Each **word** is drawn from one of those topics

# LDA as a graphical model



- Nodes are random variables; edges indicate dependence.
- Shaded nodes are observed.
- Plates indicate replicated variables.

# Posterior inference for LDA



- The joint distribution of the latent variables and documents is

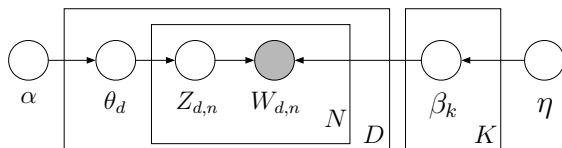
$$\prod_{i=1}^K p(\beta_i | \eta) \prod_{d=1}^D p(\theta_d | \alpha) \left( \prod_{n=1}^N p(z_{d,n} | \theta_d) p(w_{d,n} | \beta_{1:K}, z_{d,n}) \right).$$

- The posterior of the latent variables given the documents is

$$p(\beta_{1:K}, \theta_{1:D}, z_{1:D,1:N} | w_{1:D,1:N}).$$



# Posterior inference for LDA

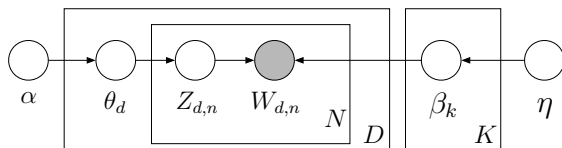


- This is equal to

$$\frac{p(\beta_{1:K}, \theta_{1:D}, \mathbf{z}_{1:D}, \mathbf{w}_{1:D})}{\int_{\beta_{1:K}} \int_{\theta_{1:D}} \sum_{\mathbf{z}_{1:D}} p(\beta_{1:K}, \theta_{1:D}, \mathbf{z}_{1:D}, \mathbf{w}_{1:D})}.$$

- We can't compute the denominator, the marginal  $p(\mathbf{w}_{1:D})$ .
- This is the crux of the inference problem.

# Posterior inference for LDA

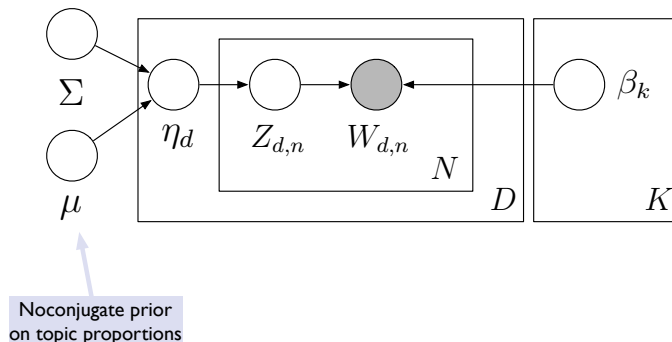


- There is a large literature on approximating the posterior.
- We will focus on
  - Gibbs sampling
  - Mean-field variational methods (batch and online)

# Modeling richer assumptions

- Correlated topic model
- Dynamic topic model

# The correlated topic model (CTM) (Blei and Lafferty, 2007)



- Draw topic proportions from a logistic normal, where topic occurrences can exhibit correlation.
- Use for:
  - Providing a “map” of topics and how they are related
  - Better prediction via correlated topics

# Language models

- A language model is a way of assigning a probability to any sequence of words (or string of text)

$$p(w_1, \dots, w_n)$$

- By the basic rules of conditional probability we can factor this as

$$p(w_1, \dots, w_n) = p(w_1)p(w_2 | w_1) \dots p(w_n | w_1, \dots, w_{n-1})$$

- The number of *histories* grows as  $V^{n-1}$ . Number of parameters in model grows as  $V^n$ , where  $V$  is number of words in vocabulary.
- What are some ways of reducing the number of parameters?

# Grouping histories

- We need to group histories.
- Let  $\pi_n : V^n \rightarrow \mathcal{C}$  be a mapping from word sequences of length  $n$  to some finite set.
- Our model becomes

$$p(w_{n+1} \mid w_1, \dots, w_n) = p(w_{n+1} \mid \pi_n(w_1, \dots, w_n))$$

- Number of parameters:  $O(V \cdot |\mathcal{C}|)$
- What are some example groupings?

# Grouping histories

- Unigrams:  $\pi(w_1, \dots, w_n) = \emptyset$ .
- Bigrams:  $\pi(w_1, \dots, w_n) = w_n$ .
- Trigrams:  $\pi(w_1, \dots, w_n) = (w_{n-1}, w_n)$ .
- Number of parameters grows as  $O(V)$ ,  $O(V^2)$ , and  $O(V^3)$ , respectively.
- Number of parameters in topics for latent Dirichlet allocation:

$$O(K \cdot V)$$

# Estimating parameters

- The maximum likelihood estimate of a trigram model:

$$\hat{p}(w_3 | w_1, w_2) = \frac{\text{count}(w_1, w_2, w_3)}{\text{count}(w_1, w_2)}$$

- What are some problems with this model?



# Bayesian inference

- The posterior mean under a Dirichlet prior would be

$$\hat{p}(w_3 \mid w_1, w_2, \text{corpus}) \propto \text{count}(w_1, w_2, w_3) + \eta$$

# Good-Turing

- Suppose we have a corpus of 500 million words. I count trigrams and find that 50 million of them are unique.
- When I see a new trigram, 10% of the time it won't have been seen before. (This is a typical number.)
- This means that the MLE is zero, and the probability that my model predicts the next word will be zero.
- The MLE is supported on the observed data. We need to spread out the probability over unseen events.

# Class-based bigram model

- Model takes form

$$\begin{aligned} p(w_2 | w_1) &= p(\text{class}(w_2) | \text{class}(w_1)) p(w_2 | \text{class}(w_2)) \\ &= p(c_2 | c_1) p(w_2 | c_2) \end{aligned}$$

- Use bottom-up agglomerative clustering to group the words.
- In each step, merge the pair of classes that gives the smallest reduction in likelihood of the data. (The MLE bigram model has the greatest likelihood.)
- $O(V^5)$  complexity to go down to  $O(1)$  classes.
- $V$  is number of words in vocabulary

# Group globally, compute locally

- Clusters contain syntactic and semantic elements
- Surprising, since use local statistics only
- “A word is known by the company it keeps”

# Perplexity

“perplexity” is evaluated as

$$\text{Perplexity}(\theta) = \left( \prod_{i=1}^N p_{\theta}(w_i | w_{1:i-1}) \right)^{-1/N}$$

If perplexity is 100, then the model predicts, on average, as if there were 100 equally likely words to follow.

# Pointwise mutual information (PMI)

Related statistic is “pointwise mutual information” (PMI)

$$\log \left( \frac{p_{\text{near}}(w_1, w_2)}{p(w_1)p(w_2)} \right)$$

- How likely are specific words/clusters to co-occur together within some window, compared to if they were independent?

# Shortcomings of word clusters

- Clusters are still “categorical”
- Can't use vector space operations
- “One hot” representation wasteful
- These are addressed with *distributed representations* (next)

# Insight of embeddings

- Use PMI-like scores to get embedding vectors.
- Can be applied whenever have large amounts of cooccurrence data.
- We'll go further into this next time



# Pointwise mutual information (PMI)

Average mutual information

$$I(W_1, W_2) = \sum_{w_1, w_2} p(w_1, w_2) \log \frac{p(w_1, w_2)}{p(w_1)p(w_2)}$$

Pointwise mutual information (PMI)

$$\log \left( \frac{p_{\text{near}}(w_1, w_2)}{p(w_1)p(w_2)} \right)$$

- How likely are specific words/clusters to co-occur together within some window, compared to if they were independent?

# Core idea of embeddings

- Form a language model but replace classes by vectors, one for each word
- Use PMI-like scores to fit the vectors
- Can be applied whenever have cooccurrence data.

# Embedding LM

Model is

$$p(w_2 | w_1) = \frac{\exp(\phi(w_2)^T \phi(w_1))}{\sum_w \exp(\phi(w)^T \phi(w_1))}.$$

As before,

$$\begin{aligned}\ell(\phi) &= \sum_{w_1, w_2} p(w_1, w_2) \log p(\phi_2 | \phi_1) p(w_2 | \phi_2) \\ &= I(\Phi_1, \Phi_2) - H(W)\end{aligned}$$

Thus, we want embedding vectors with high mutual information.

# Constructing embeddings

Carry out stochastic gradient descent over the embedding vectors  $\phi \in \mathbb{R}^d$  (where  $d \approx 50\text{--}100$  is chosen by trial and error)

This is what Mikolov et al. (2014, 2015) did at Google. With a couple of heuristics:

# Constructing embeddings

Heuristics used:

- Skip-gram: predict surrounding words from current word
- An issue with this is that it “over generates” the data. With text  
the lazy brown fox jumped **we** will have  $p(\text{brown} | \text{lazy})$   
and  $p(\text{brown} | \text{fox})$
- Second is computational. The bottleneck is computing the denominator in the logistic (softmax) probability.
- Use “negative sampling”: Approximation

$$\begin{aligned} & \sum_w \exp(\phi(w)^T \phi(w_1)) \\ & \approx \exp(\phi(w_2)^T \phi(w_1)) + \sum_{\text{random } w} \exp(\phi(w)^T \phi(w_1)) \end{aligned}$$

# Analogies

These heuristics enable training on very large text collections. Leads to vector representations of words with interesting properties.

For example, analogies:

king is to man as ? is to woman

Paris is to France as ? is to Germany

$$\phi(\text{king}) - \phi(\text{man}) \stackrel{?}{\approx} \phi(\text{queen}) - \phi(\text{woman})$$

$$\hat{w} = \arg \min_w \|\phi(\text{king}) - \phi(\text{man}) + \phi(\text{woman}) - \phi(w)\|^2$$

Does  $\hat{w} = \text{queen}$ ?

# GloVe

Shortly after: Stanford group introduced a computational expedient (with attempt to give a “principled” motivation)

$$\mathcal{O}(\phi) = \sum_{w_1, w_2} f(c_{w_1, w_2}) \left( \phi(w_1)^T \phi(w_2) - \log c_{w_1, w_2} \right)^2$$

where  $c_{w, w'}$  are cooccurrence counts.

- A type of regression estimator. Can interpret/relate this to other objectives.
- Main advantage is that SGD can be carried out much more efficiently

# GloVe

$$\mathcal{O}(\phi) = \sum_{w_1, w_2} f(c_{w_1, w_2}) \left( \phi(w_1)^T \phi(w_2) - \log c_{w_1, w_2} \right)^2$$

where  $c_{w, w'}$  are cooccurrence counts.

- Heuristic weighting function

$$f(x) = \left( \frac{x}{x_{\max}} \right)^{\alpha}$$

where  $\alpha = 3/4$  set empirically.

- So  $10^{-4} \mapsto 10^{-3}$ . Each order of magnitude down gets “boosted” by 1/4-magnitude.



# Embedding embeddings: t-SNE

- How can we visualize the embeddings?
- We're in a very high dimensional space
- Can do PCA, but this will introduce an additional projection/approximation step
- Many visualization techniques exist. A currently popular one is t-SNE: "Student-t Stochastic Neighborhood Embedding"

# t-SNE

Here's the idea behind t-SNE:

- Form a language model using the embeddings
- Scale and symmetrize, giving a matrix  $P = [P_{ij}]$
- Represent word  $i$  by  $y_i \in \mathbb{R}^2$ . Use a heavy-tailed distribution (Student-t with one degree of freedom)
- Select  $y_i$  using stochastic gradient descent

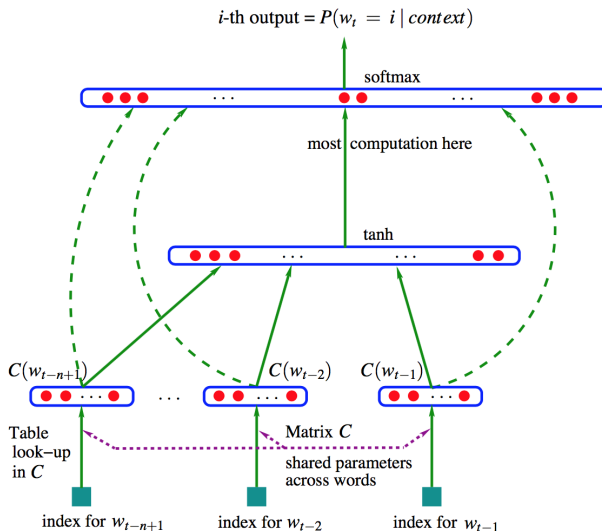
# Summary: Word embeddings

- Word embeddings are vector representations of words, learned from cooccurrence statistics
- The models can be viewed in terms of logistic regression and class-based bigram models
- Surprising semantic relations are encoded in linear relations
- Various heuristics have been introduced to get scalability
- Embeddings improve with more data
- t-SNE is an algorithm for visualizing embeddings

# Neural LM: Idea

- Associate each word in vocabulary with a feature vector  $C(w) \in \mathbb{R}^d$
- Express probabilities in terms of those vectors
- Form a big logistic regression to predict the next word. Can introduce some nonlinearities.
- Simultaneously learn vectors (word representations) and weightings (model parameters), using SGD

# Neural LM architecture



# Neural LM: Simplified further!

Suppose

$$p(w_t | w_{t-1}) = \frac{e^{y_{w_t}}}{\sum_i e^{y_i}}$$

with

$$y = b + Ax$$

$$x = C(w_{t-1})$$

$$\text{so: } y_w = b_w + A_w^T C(w_{t-1})$$

Key property is that the word representations  $C(w) \in \mathbb{R}^d$  are *learned* as part of the model.

This is the essence of the model. Note that we get two “embedding” vectors:  $A_w$  and  $C(w)$ .

# Important aspects

- Unsupervised: No labels used, discovers useful features of input
- Compression: Code reduces dimension of data
- Lossy: Input won't be reconstructed exactly
- Trained: The compression algorithm is learned for specific data

# Simple autoencoder example

Encoder network of the form

$$h = \text{ReLU}(Wx + b)$$

where  $W \in \mathbb{R}^{H \times D}$  and  $b \in \mathbb{R}^H$ , decoder network is

$$\hat{x} = \text{ReLU}(\widetilde{W}h + \widetilde{b})$$

where  $\widetilde{W} \in \mathbb{R}^{D \times H}$  and  $\widetilde{b} \in \mathbb{R}^D$ .

Objective function:

$$\mathcal{L} = \frac{1}{n} \sum_{i=1}^n \|x_i - \text{ReLU}(\widetilde{W} \text{ReLU}(Wx_i + b) + \widetilde{b})\|^2.$$

$\text{ReLU}(x) = \max(0, x)$ , applied component-wise.



# Simple example – code of dimension $K$

Encoder network of the form

$$h = \text{ReLU}(W_1 x + b_1)$$

$$c = \text{ReLU}(W_2 h + b_2)$$

where  $W_1 \in \mathbb{R}^{H \times D}$  and  $b_1 \in \mathbb{R}^H$ , and  $W_2 \in \mathbb{R}^{K \times H}$  and  $b_2 \in \mathbb{R}^K$

Decoder network of the form

$$\hat{h} = \text{ReLU}(\widetilde{W}_1 c + \widetilde{b}_1)$$

$$\hat{x} = \text{Sigmoid}(\widetilde{W}_2 \hat{h} + \widetilde{b}_2)$$

where  $\widetilde{W}_1 \in \mathbb{R}^{H \times K}$  and  $\widetilde{b}_1 \in \mathbb{R}^H$ , and  $\widetilde{W}_2 \in \mathbb{R}^{D \times H}$  and  $\widetilde{b}_2 \in \mathbb{R}^D$

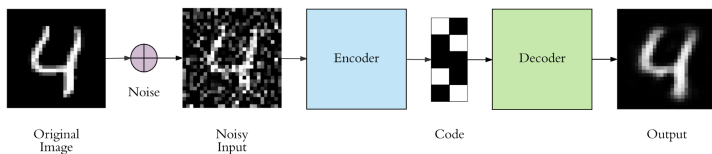
Objective function: binary cross-entropy

$$\mathcal{L} = \frac{1}{n} \sum_{i=1}^n (x_i \log \hat{x}_i + (1 - x_i) \log(1 - \hat{x}_i))$$

# Adam optimizer

- Variant of stochastic gradient descent where separate learning rate (step size) is maintained for each network weight (parameter)
- Each step size adapted as learning progresses based on moments of the derivatives

# Variant: Denoising autoencoder



- Feed in noisy data
- Train to match to denoised data

## Variant: Sparse autoencoder

- Add penalty to encourage sparsity
- Forces autoencoder to discover interesting structure in data
- Same principle as sparse coding

In Keras this is easy to do:

```
code = Dense(code_size, activation='relu',  
             activity_regularizer=l1(10e-6))(input_img)
```

# Variational autoencoders

Start with a generative model

$$z \sim N(0, I_K)$$
$$x | z \sim \text{Sigmoid}(G(z))$$

$G(z)$  is the *generator network* or *decoder*

As a simple example:

$$G(z) = A_2 \text{ReLU}(A_1 z + b_1) + b_2$$

# Déjà vu all over again

We saw this before—almost.

Simple autoencoder

$$\|x - \text{ReLU}(A \text{ReLU}(Bx + d) + b)\|^2$$

Variational autoencoder

$$\frac{1}{N} \sum_{s=1}^N \frac{1}{2} \|x - \text{ReLU}(A (\text{ReLU}(Bx + d) + \epsilon_s) + b)\|^2$$

But the perspective and thinking have changed significantly. We're back to statistics!

# Summary: What did we learn today?

- Autoencoders compress the input and then reconstruct it
- Bottleneck forces extraction of useful features
- Will overfit and “memorize” the data
- Overfitting mitigated by denoising autoencoders
- More fundamental view: Latent variable generative models and posterior inference
- Parameterize variational parameters in terms of neural networks
- Reparameterization trick allows simultaneous training of both networks

**Introductory Machine Learning**

## Some Notes on Backpropagation

Backpropagation is—at the heart of it—nothing more than the chain rule from high school calculus. It boils down to the following fact:

If  $\mathcal{L}$  is a scalar function and  $A = BC$ , then

$$\frac{\partial \mathcal{L}}{\partial B} = \frac{\partial \mathcal{L}}{\partial A} C^T \quad (1)$$

$$\frac{\partial \mathcal{L}}{\partial C} = B^T \frac{\partial \mathcal{L}}{\partial A}. \quad (2)$$

This can be shown directly using the “usual” chain rule. You should check that the dimensions match up!

The function  $\mathcal{L}$  is our loss function. The use of this is called “backpropagation” because we start with the derivatives in the last layer of the network, and recursively send these “back” to compute the derivatives in the earlier part of the network.

So, if  $f = Wx + b$  then

$$\frac{\partial \mathcal{L}}{\partial W} = \frac{\partial \mathcal{L}}{\partial f} x^T. \quad (3)$$

If the loss  $\mathcal{L}$  is squared error  $\mathcal{L} = \frac{1}{2}(y - f)^2$  then

$$\frac{\partial \mathcal{L}}{\partial f} = (f - y). \quad (4)$$

Now, if

$$f = W_2 h + b_2 \quad (5)$$

$$h = W_1 x + b_1 \quad (6)$$



then

$$\frac{\partial \mathcal{L}}{\partial W_2} = \frac{\partial \mathcal{L}}{\partial f} h^T = (f - y) h^T \quad (7)$$

$$\frac{\partial \mathcal{L}}{\partial h} = W_2^T \frac{\partial \mathcal{L}}{\partial f} = W_2^T (f - y) \quad (8)$$

$$\frac{\partial \mathcal{L}}{\partial b_2} = \frac{\partial \mathcal{L}}{\partial f} = (f - y). \quad (9)$$

Then, we have that

$$\frac{\partial \mathcal{L}}{\partial W_1} = \frac{\partial \mathcal{L}}{\partial h} x^T = W_2^T \frac{\partial \mathcal{L}}{\partial f} x^T = W_2^T (f - y) x^T \quad (10)$$

$$\frac{\partial \mathcal{L}}{\partial b_1} = \frac{\partial \mathcal{L}}{\partial h} = W_2^T (f - y). \quad (11)$$

This is just another linear model, so it will train to be equivalent to least squares regression. But if we add a ReLU nonlinearity, we get the two-layer neural network

$$h = \text{ReLU}(W_1 x + b_1) \quad (12)$$

$$f = W_2 h + b_2. \quad (13)$$

Let the loss for an example  $(x, y)$  be  $\mathcal{L} = \frac{1}{2}(y - f(x))^2$ . From the above calculations we then have for the second layer

$$\frac{\partial \mathcal{L}}{\partial W_2} = \frac{\partial \mathcal{L}}{\partial f} h^T \quad (14)$$

$$\frac{\partial \mathcal{L}}{\partial h} = W_2^T \frac{\partial \mathcal{L}}{\partial f} \quad (15)$$

$$\frac{\partial \mathcal{L}}{\partial b_2} = \frac{\partial \mathcal{L}}{\partial f}. \quad (16)$$

For the hidden layer we have

$$\frac{\partial \mathcal{L}}{\partial W_1} = \mathbb{1}(h > 0) \frac{\partial \mathcal{L}}{\partial h} x^T \quad (17)$$

$$= \mathbb{1}(h > 0) W_2^T \frac{\partial \mathcal{L}}{\partial f} x^T \quad (18)$$

$$\frac{\partial \mathcal{L}}{\partial b_2} = \mathbb{1}(h > 0) \frac{\partial \mathcal{L}}{\partial h} \quad (19)$$

$$= \mathbb{1}(h > 0) W_2^T \frac{\partial \mathcal{L}}{\partial f}. \quad (20)$$

For a two-layer network *for classification* we have

$$h = \text{ReLU}(W_1 x + b_1) \quad (21)$$

$$f = W_2 h_1 + b_2 \quad (22)$$

$$p = \text{Softmax}(f) \quad (23)$$

where again  $W_j$  and  $b_j$  are matrices or vectors of the appropriate dimensions. Let the loss for an example  $(x, y)$  be the log-loss  $\mathcal{L} = -\log p(y | x)$ . Then

$$\frac{\partial \mathcal{L}}{\partial f} = \begin{pmatrix} p_1 - \mathbb{1}(y = 1) \\ p_2 - \mathbb{1}(y = 2) \\ p_3 - \mathbb{1}(y = 3) \end{pmatrix} \in \mathbb{R}^3 \quad (24)$$

Backpropagating to the second layer we have

$$\frac{\partial \mathcal{L}}{\partial W_2} = \frac{\partial \mathcal{L}}{\partial f} h_1^T \quad (25)$$

$$\frac{\partial \mathcal{L}}{\partial h} = W_2^T \frac{\partial \mathcal{L}}{\partial f} \quad (26)$$

$$\frac{\partial \mathcal{L}}{\partial b_2} = \frac{\partial \mathcal{L}}{\partial f} \quad (27)$$

Then backpropagating to the first layer

$$\frac{\partial \mathcal{L}}{\partial W_1} = \mathbb{1}(h > 0) \frac{\partial \mathcal{L}}{\partial h} x^T \quad (28)$$

$$= \mathbb{1}(h > 0) W_2^T \frac{\partial \mathcal{L}}{\partial f} x^T \quad (29)$$

$$\frac{\partial \mathcal{L}}{\partial b_1} = \mathbb{1}(h > 0) \frac{\partial \mathcal{L}}{\partial h} \quad (30)$$

$$= \mathbb{1}(h > 0) W_2^T \frac{\partial \mathcal{L}}{\partial f}. \quad (31)$$

We'll leave it to you to extend the calculations (and implementation!) to a three-layer network, if you are so-inclined.