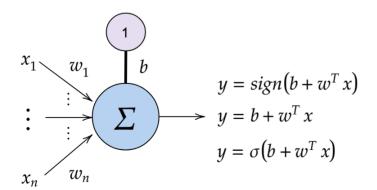


Class 6

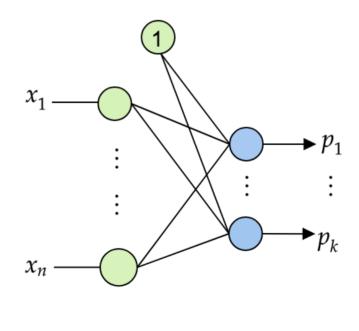
So far we've considered 3 networks and 3 cost functions

- **Perceptron** with error correcting algorithm
- **Linear regression** with squared error cost
- **Binary classification** with negative log likelihood cost

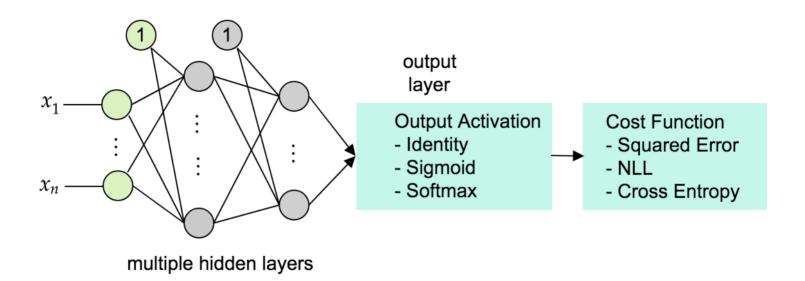


Softmax Regression

Multi-category classification (Softmax) with cross entropy cost



Network Models



Softmax

- Introduces 3^{rd} cost function: Cross-Entropy
- Will need to cover some information theory
- Cross-Entropy is
 - Differentiable in adjustable parameters
 - A minimum when performance is optimal
 - Convex if no hidden layers
- Starting next week will write code that supports all 3 cost functions
 - Squared Error
 - Negative Log-Likelihood
 - Cross-Entropy

Compare:

- Outcomes of a fair coin toss
- Outcomes of a fair 6-sided die toss

In each case the outcome removes all uncertainty

 More was learned from the roll of the die:

$$egin{aligned} P_t(toss) &= rac{1}{2} \ P_r(roll) &= rac{1}{6} \end{aligned}$$

Want information

What about using surprise

$$I(event) = \frac{1}{p}$$
?

Not additive for independent events:

$$egin{aligned} I(toss,roll) &= rac{1}{P(toss,roll)} \ &= rac{1}{P(toss)} \cdot rac{1}{P(roll)} = 12 \ &
eq I(toss) + I(roll) = 8 \end{aligned}$$

Taking log gives desired additivity:

$$I(event) = \log(\frac{1}{P(event)}) = \log(\text{surprise})$$

Since log is monotone increasing, $\log(1/p)$ increases with decreasing p.

• Now:

$$egin{aligned} I(toss, roll) &= \log rac{1}{P(toss, roll)} \ &= \log rac{1}{P(toss) \cdot P(roll)} \ &= \log (rac{1}{P(toss)}) + \log (rac{1}{P(roll)}) \ &= I(toss) + I(roll) \end{aligned}$$

An event E that has probability P(E) of occurrence has information content

$$I(E) = \log(\frac{1}{P(E)}) = -\log(P(E))$$

- If \log is \log_2 , information is in bits.
- If log is natural log, information is in nits.

Examples

- Fair coin toss, $I = \log_2(\frac{1}{1/2}) = 1$
- Fair die roll, $I = \log_2(\frac{1}{1/6}) \approx 2.6$
- Sequence of k fair coin tosses has $P = (\frac{1}{2})^k$, $I = \log(\frac{1}{1/2^k}) = k$

Entropy

Entropy is a measure of the average information of a distribution

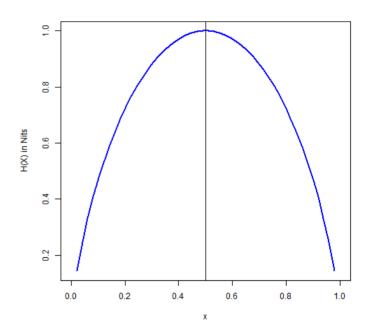
$$egin{aligned} H(\mathbf{x}) &= E[I(\mathbf{x}))] \ &= E[\log(rac{1}{P})] \ &= -E[\log P] \ &= -\sum_{\mathbf{x}_i} P(\mathbf{x}_i) \log P(\mathbf{x}_i) \end{aligned}$$

Example:

Let X model the outcome of a coin toss with probability of success (head) *p*.

$$egin{aligned} H(X) &= -\sum_{\mathbf{x}_i} P(\mathbf{x}_i) \log P(\mathbf{x}_i) \ &= -p \log p - (1-p) \log (1-p) \end{aligned}$$

- Entropy is maximized when $p = \frac{1}{2}$ • (Set H' = 0 and solve)
- Entropy is zero when outcome is a certain value

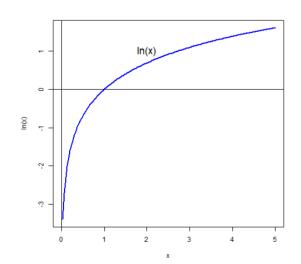


• ln(x) is monotone increasing

$$\frac{d}{dx}\ln(x) = \frac{1}{x} > 0$$

• ln(x) is concave

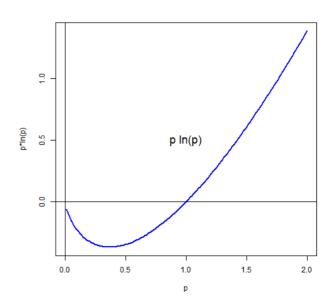
$$rac{d^2}{dx^2}{
m ln}(x)=-rac{1}{x^2}$$



$$\lim_{p o 0} p \cdot \log p = 0$$

Plot shows $\lim_{\mathbf{x}\downarrow 0} \mathbf{x} \log \mathbf{x} = 0$.

The missing point at the origin is due to R returning NaN at for ln(0)



Properties of Entropy

Entropy is completely defined given a set of probabilities

$$H(p_1,\cdots,p_k) = \sum_i p_i \log rac{1}{p_i} \ \sum p_i = 1$$

Entropy is non-negative

$$H(X) \geq 0$$
 because $p \in [0,1], rac{1}{p} \geq 1$ $\log rac{1}{p} \geq 0$

- **(1) Entropy** H(p) is maximized when $p_i = \frac{1}{k}; \ i = 1, \dots, k$
- (2) For any distribution $q_i = P(Y = x_i), q_i \neq p_i$ for some i

$$H(X) = \sum p_i \log rac{1}{p_i} < \sum_i p_i \log rac{1}{q_i}$$

- **(3)** $H(X) \leq \log k$, with equality if $p_i = \frac{1}{k}$ for all i
- **(4)** H(X) decreases as X becomes less uniform

Jensen's Inequality

Convexity

A function *f* is convex provided

$$f(tx_1+(1-t)x_2) \leq tf(x_1)+(1-t)f(x_2)$$

Jensen's Inequality (finite)

Generalizes the statement of convexity to n terms. If $p_i \in [0,1]$ and $\sum_i p_i = 1$ then Jensen's inequality states that for convex f

$$f(\sum_i p_i x_i) \leq \sum_i p_i f(x_i)$$

The definition of convexity shows relation is true fo n = 2.

Induction

Assume result true for n and show true for n + 1

$$egin{align} f(\sum_{i=1}^{n+1}p_ix_i) &= f(p_1x_1 + (1-p_1)\sum_{i=2}^{n+1}rac{p_i}{1-p_1}x_i) \ &\leq p_1f(x_1) + (1-p_1)f(\sum_{i=2}^{n+1}rac{p_i}{1-p_1}x_i) \end{aligned}$$

The result follows because the term on the right is a sum of n terms with coefficients summing to 1

$$\sum_{i=1}^{n+1} p_i = 1 \qquad \implies \qquad \sum_{i=2}^{n+1} p_i = 1-p_1$$

Properties of Entropy

If X is a random variable that takes on k values, then

$$H(X) \le \ln k$$

The result follows from Jensen's inequality for concave functions. \ln is concave, so

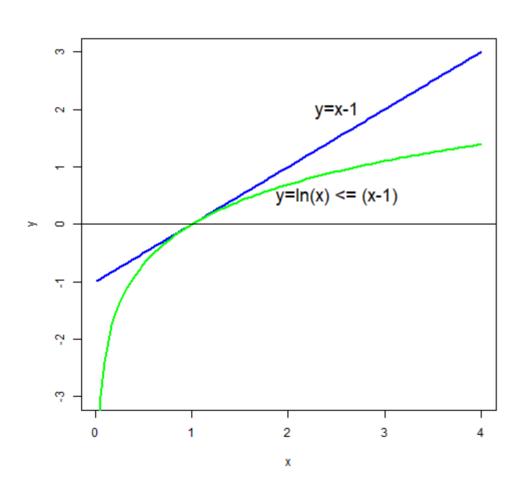
$$egin{aligned} H(X) &= \sum_{i=1}^k p_i \ln rac{1}{p_i} \ &\leq \ln (\sum_{i=1}^k p_i \cdot rac{1}{p_i}) \ &= \ln k \end{aligned}$$

When X is uniform, $p_i = k^{-1}, i = 1, \dots, k$

$$H(rac{1}{k},\ldots,rac{1}{k})=\sum_{i=1}^{k}rac{1}{k}{
m ln}\,k$$

It follows that entropy is maximized when *X* is uniform

Bound on In(x)



Kullback-Liebler Divergence

KL Divergence is used as measure of similarity between distributions. For $X \sim p(x_i)$

$$D_{KL}(p||q) = \sum_{x_i} p(x_i) \ln rac{p(x_i)}{q(x_i)} = -\sum_{x_i} p(x_i) \ln rac{q(x_i)}{p(x_i)}$$

Note that if $p(x_i) = q(x_i)$ for all i then $D_{KL}(p||q) = 0$. Using $-\ln x \ge -(x-1)$ gives

$$egin{aligned} D_{KL}(p||q) &\geq -\sum_i p_i (rac{q_i}{p_i} - 1) \ &= \sum_i p_i - \sum_i q_i \ &= 1 - \sum_i q_i \ &\geq 0 \end{aligned}$$

The lower bound will be 0 if q has the same support as p

Since KL Divergence is non-negative and equal to zero when the distributions match, it can function as a distance between distributions. It is not called a distance because in general

$$D_{KL}(p||q)
eq D_{KL}(q||p)$$

Cross Entropy

When training a model want the generated distribution to match the empirical data distribution. It makes sense to use the KL Divergence as a cost function.

If $X \sim p(x_i)$ is empirical data distribution and $Y \sim q(x_i)$ is generated by model training

$$egin{aligned} D_{KL}(p||q) &= \sum_{x_i} p(x_i) \ln rac{p(x_i)}{q(x_i)} \ &= \sum_{x_i} p(x_i) \ln p(x_i) \ &- \sum_{x_i} p(x_i) \ln q(x_i) \ &= H(p,q) - H(p) \end{aligned}$$

The new symbol H(p,q) is called the **cross-entropy**.

$$egin{aligned} H(p,q) &= H(p) + D_{KL}(p||q) \ & \ D_{KL}(p||q) \geq 0 \quad \Rightarrow \quad H(p) \leq H(p,q) \end{aligned}$$

Want to train the model to make $Y \sim X$. Because H(p) is not affected by changing model parameters, minimizing $D_{KL}(p||q)$ is equivalent to minimizing the cross-entropy H(p,q).

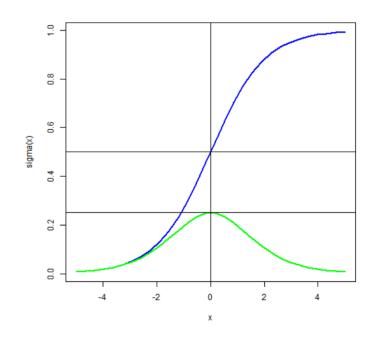
It is standard to use the crossentropy cost function for multicategory classification.

Sigmoid (Logistic) Function

Recall that the Sigmoid function maps (squashes) any set of real numbers to the interval [0,1]

Standard Sigmoid Function

$$egin{aligned} \sigma(x) &= rac{1}{1+e^{-x}}, \quad \sigma(0) = rac{1}{2} \ & \sigma' = \sigma(1-\sigma), \quad \sigma'(0) = rac{1}{4} \ & \lim_{x \uparrow + \infty} \sigma(x) = 1, \lim_{x \downarrow - \infty} \sigma(x) = 0 \ & \lim_{x \uparrow + \infty} \sigma'(x) = 0, \lim_{x \downarrow - \infty} \sigma'(x) = 0 \end{aligned}$$



The sigmoid function is the *CDF* of the logistic distribution

Softmax Function

The softmax function is a vector valued generalization of $\sigma(x)$. Given a vector $\mathbf{x} \in \mathbb{R}^k$, the softmax of \mathbf{x} is

$$S(\mathbf{x}) = rac{1}{\sum_{i=1}^k e^{\mathbf{x}_i}} egin{bmatrix} e^{\mathbf{x}_1} \ dots \ e^{\mathbf{x}_k} \end{bmatrix} = egin{bmatrix} S_1 \ dots \ S_k \end{bmatrix}$$

Two properties are obvious:

$$rac{e^{\mathbf{x}_i}}{\sum_j e^{\mathbf{x}_j}} > 0$$

$$rac{e^{\mathbf{x}_i}}{\sum_j e^{\mathbf{x}_j}} > 0$$
 $\sum_{i=1}^k S_i(\mathbf{x}) = 1$

So the components of S satisfy conditions for a probability distribution

Softmax Function

The sigmoid function resulted naturally from inverting the logit.

$$\operatorname{logit}(p_i) = \ln(p_i/(1-p_i) = w_0 + \mathbf{w}_1 \cdot \mathbf{x}$$

Gave:

$$egin{aligned} p_i &= \operatorname{logit}^{-1}(w_0 + \mathbf{w}_1 \cdot \mathbf{x}) \ &= \sigma(w_0 + \mathbf{w}_1 \cdot \mathbf{x}) \ &= rac{1}{1 + e^{-(w_0 + \mathbf{w}_1 \cdot \mathbf{x})}} \end{aligned}$$

For K classes, assume each class probability can be linearly related to the data. $\ln z$ will serve as a normalizing factor

$$\ln P(y^{(i)}=1) = \mathbf{w}_1^T \mathbf{x}^{(i)} - \ln z$$

$$\ln P(y^{(i)} = K) = \mathbf{w}_K^T \mathbf{x}^{(i)} - \ln z$$

Softmax Function

Using the constraint:

$$egin{aligned} \sum_{k=1}^K P(y^{(i)} = k) &= 1 \ \sum_{k=1}^K e^{\mathbf{w}_k^T \mathbf{x}^{(i)} - \ln z} &= 1 \end{aligned}$$

Implies

$$z = \sum_{k=1}^K e^{\mathbf{w}_k^T \mathbf{x}^{(i)}}$$

$$P(y^{(j)} = i) = rac{e^{\mathbf{w}_i^T\mathbf{x}^{(j)}}}{\sum_{k=1}^K e^{\mathbf{w}_k^T\mathbf{x}^{(j)}}}$$

Softmax Numerical Stability

Numerical Stability

Double precision floating point numbers use an 11-bit exponent giving a maximum value around $2^{1023}\sim 10^{308}$. It is relatively easy for the exponentials in the softmax to exceed this. R will produce a non-numeric "Inf" result on overflow.

Normalizing Softmax

$$egin{align} S_j &= rac{e^{\mathbf{x}_j}}{\sum_{k=1}^K e^{\mathbf{x}_k}} = rac{Ce^{\mathbf{x}_j}}{C\sum_{k=1}^K e^{\mathbf{x}_k}} \ &= rac{e^{\mathbf{x}_j + \ln C}}{\sum_{k=1}^K e^{\mathbf{x}_k + \ln C}} \ &= rac{e^{\mathbf{x}_j + b}}{\sum_{k=1}^K e^{\mathbf{x}_k + b}} \end{aligned}$$

Where $b = \ln C$

Softmax Numerical Stability

Taking

$$b = -\max_k(\mathbf{x}_k)$$

shifts all exponents to be ≤ 0 . Large negative exponents will generate 0, so they don't cause a problem.

Numerically Stable Softmax

$$egin{align} b = -\max_k(\mathbf{x}_k) \ & \mathbf{ ilde{x}} = \mathbf{x} + b \ & (S(\mathbf{x}))_i = (S(\mathbf{ ilde{x}}))_i = rac{e^{\mathbf{ ilde{x}}_i}}{\sum_{k=1}^K e^{\mathbf{ ilde{x}}_k}} \end{split}$$

Encoding

For many modeling algorithms, data must be converted to numeric values

- Images are arrays of pixel values, so already numeric
- Text data must be encoded -In cases where data has a natural order, simple integer encoding can be used
 - sometimes called label encoding

• For text(or other non-numeric data) which are unordered, use one-hot encoding.

text	code	
"small"	1	
"medium"	2	
"large"	3	

Label

encoding for data with natural order

Encoding

There are 3 common ways to encode text for ML:

One-hot encoding

sparse encoding of text

TF-IDF: Term frequency-Inverse Document Frequency

• many variants

$$\operatorname{tf}(w,d) \cdot \log rac{N}{|\{d \in D : w \in d\}|}$$

` Word Embedding

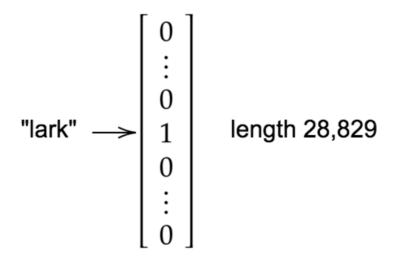
• technique to generate dense encodings from one-hot encoding

One-Hot Encoding

The Shakespeare corpus contains 28,829 unique words, 884,421 total words.

Example:

One-hot encoding of text data from Shakespeare corpus



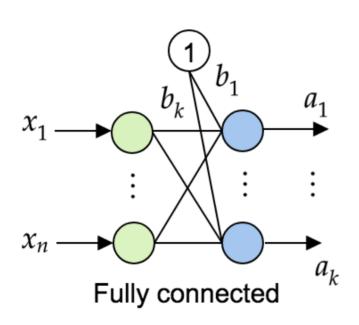
One-Hot Encoding

Equivalent to using the dummy variables:

	is.dog	is.cat	is.bird	is.other
"dog"	1	0	0	0
"cat"	0	1	0	0
"bird"	0	0	1	0
"other"	0	0	0	1

Special techniques are needed for NLP when the number of words is large (over 50,000)

- Hierarchical softmax regression
 - Output layer is structured as a binary tree



Softmax regression has K output activations generated by the softmax function. Let X be the full data matrix with m data samples $\mathbf{x}^{(i)}, i = 1, \dots, m$ arranged by column.

$$X = egin{bmatrix} \mathbf{x}_1^{(1)} & \cdots & \mathbf{x}_1^{(m)} \ dots & & dots \ \mathbf{x}_n^{(1)} & \cdots & \mathbf{x}_n^{(m)} \ \end{bmatrix}$$

The weight matrix W maps n-dimensional input vectors to K-dimensional outputs $W:\mathbb{R}^n \to \mathbb{R}^K$

So W is a $K \times n$ matrix. To simplify, let Z be the input to the softmax function:

$$Z = \mathbf{b} egin{bmatrix} 1 \ dots \ 1 \end{bmatrix}^T + WX$$

There is a bias for each output node, so $\mathbf{b} \in \mathbb{R}^K$.

$$Z = \mathbf{b}[\underbrace{1,\cdots,1}_{m}] + \underbrace{W}_{k \ge n} \underbrace{X}_{n \ge m}$$

The result Z is $K \times m$ and the softmax function computes probabilities from each column $\mathbf{z^{(i)}}$ of Z

The predicted responses are $H(X; \mathbf{b}, W) = S(Z)$

Both Z and H(X) are $K \times m$.

$$H(X) = egin{bmatrix} rac{\vdots}{e^{z_i^{(1)}}} & \cdots & rac{e^{z_i^{(m)}}}{\sum_j e^{z_j^{(m)}}} \ dots & dots \ \end{bmatrix} \ = egin{bmatrix} dots & & dots \ p_i^{(1)} & \cdots & p_i^{(m)} \ dots & & dots \ \end{bmatrix}$$

Let $\mathbf{y} \in \mathbb{R}^m$ where each $y_i \in \{1, 2, \cdots, K\}$ be the training data class labels

One-hot encode y to get m length K one-hot vectors

$$T = egin{bmatrix} dots & & dots \ t_i^{(1)} & \cdots & t_i^{(m)} \ dots & & dots \end{bmatrix} igg\} \quad K imes m \ dots & dots \ dots & dots \ dots \end{pmatrix}$$

Where each $t^{(i)}$ has a single element 1, and all other elements 0.

Softmax regression commonly uses the cross-entropy cost function. For a single data sample:

$$C^{(i)} = -\sum_{k=1}^K t_k^{(i)} \ln p_k^{(i)}$$

If sample (i) is class k^* , then $C^{(i)} = -\ln p_{k^*}^{(i)}$

For the full data set:

$$C = rac{1}{m} \sum_{i=1}^m C^{(i)} = -rac{1}{m} \sum_{i=1}^m \sum_{k=1}^K t_k^{(i)} \ln p_k^{(i)}$$

Now need to compute the gradient of C w.r.t the vector \mathbf{b} and the matrix W.

Since

$$abla C = rac{1}{m} \sum_i
abla C^{(i)}$$

will focus just on one data vector at a time and drop the superscript (i):

$$egin{aligned} rac{\partial C}{\partial z_i} &= -\sum_{k=1}^K rac{t_k}{p_k} rac{\partial p_k}{\partial z_i} \ p_k &= rac{e^{z_k}}{\sum_{j=1}^K e^{z_j}} \end{aligned}$$

As homework show that

$$rac{1}{p_k}rac{\partial p_k}{\partial z_i}=\delta_{ik}-p_i$$

$$rac{\partial C}{\partial z_i} = -\sum_{k=1}^K t_k (\delta_{ik} - p_i)$$

$$rac{\partial C}{\partial z_i} = -\sum_{k=1}^K t_k (\delta_{ik} - p_i)$$

Every term in this summation is zero unless k is this sample's label class. There are two possibilities. Let k^* be the sample's class. The sum reduces to

$$rac{\partial C}{\partial z_i} = -t_{k^*}(\delta_{i,k^*} - p_i) = p_i - \delta_{i,k^*}$$

$$ullet \ i=k^*, (t_i=1)\,, rac{\partial C}{\partial z_i}=(p_i-1)=p_i-t_i$$

$$ullet \ i
eq k^*, (t_i=0)\,, rac{\partial C}{\partial z_i} = p_i = p_i - 0 = p_i - t_i$$

As before, the Z-gradient is the error:

$$\frac{\partial C}{\partial z} = (\mathbf{p} - \mathbf{t})$$

Just like logistic regression but now the gradient is a vector for each sample.

To implement gradient descent will need gradient w.r.t the adjustable parameters \mathbf{b} and \mathbf{W} . For softmax the bias \mathbf{b} is a vector with an element for each of the K class output probabilities. Applying the chain rule gives

$$egin{aligned} rac{\partial C}{\partial b_i} &= \sum_j rac{\partial C}{\partial z_j} rac{\partial z_j}{\partial b_i} \ &= \sum_j rac{\partial C}{\partial z_j} \delta_{ij} \ &= rac{\partial C}{\partial z_i} \end{aligned}$$

So, for a single sample vector, the length *K* b partial of *C* is

$$\frac{\partial C}{\partial \mathbf{b}} = \frac{\partial C}{\partial \mathbf{z}}$$

Two steps left:

- Compute $\frac{\partial C}{\partial W}$
- Write equations for full batch X, not just a single sample $\mathbf{x}^{(i)}$

$$egin{aligned} rac{\partial C}{\partial W_{ij}} &= \sum_k rac{\partial C}{\partial z_k} rac{\partial z_k}{\partial W_{ij}} \ z_k &= b_k + \sum_p W_{kp} \mathbf{x}_p \qquad ext{for one } \mathbf{x}^{(i)} \end{aligned}$$

 $\frac{\partial z_k}{\partial W_{ij}}$ looks like a 3-dimensional tensor. Fortunately, since z_k only depends on row k of W, all $\frac{\partial z_k}{\partial W_{ij}}$ for $i \neq k$ are zero and can be ignored (they contribute nothing to \sum above.)

$$egin{aligned} rac{\partial z_k}{\partial W_{kj}} &= rac{\partial}{\partial W_{kj}} (b_k + W_{k1} \mathbf{x}_1 + \dots + W_{kn} \mathbf{x}_n) = \mathbf{x}_j \ & rac{\partial z_k}{\partial W_{i,j}} &= \left\{egin{aligned} 0 & ext{if } k
eq i \ x_j & ext{o.w.} \end{aligned}
ight. \end{aligned}$$

So:

$$egin{aligned} rac{\partial C}{\partial W_{i,j}} &= \sum_k rac{\partial C}{\partial z_k} rac{\partial z_k}{\partial W_{i,j}} \ &= \sum_k rac{\partial C}{\partial z_k} \delta_{i,k} x_j \ &= rac{\partial C}{\partial z_i} \mathbf{x}_j \end{aligned}$$

This can be written in vector notation as

$$egin{aligned} rac{\partial C}{\partial W} &= rac{\partial C}{\partial \mathbf{z}} \mathbf{x}^T \ &= egin{bmatrix} rac{\partial C}{\partial z_1} \ dots \ rac{\partial C}{\partial z_k} \end{bmatrix} egin{bmatrix} x_1 & \dots & x_n \end{bmatrix} \end{aligned}$$

Giving $\frac{\partial C}{\partial W}$ as a $k \times n$ matrix.

For the full data set, each data point $\mathbf{x}^{(i)}$ contributes to the gradient. A good approach is to compute the gradient for all m data points using matrix operations, and then average.

The $m \frac{\partial C}{\partial \mathbf{b}}$ gradients are

$$egin{bmatrix} dots \ rac{\partial C(x^{(i)})}{\partial \mathbf{b}} & \cdots & rac{\partial C(x^{(m)})}{\partial \mathbf{b}} \ dots & dots \ \end{bmatrix} \ = rac{\partial C}{\partial Z} \ = S(Z) - T$$

Where $S(Z) = S(\mathbf{b} + WX)$ is the softmax on the entire input data matrix.

For homework, show that sum of the $\frac{\partial C}{\partial W}$ matrices is as shown:

$$egin{aligned} \sum_{i=1}^{m} rac{\partial C^{(i)}}{\partial W} &= \sum_{i=1}^{m} rac{\partial C^{(i)}}{\partial \mathbf{z}^{(i)}} (\mathbf{x}^{(i)})^{T} \ &= rac{\partial C}{\partial Z} X^{T} \ &= (S(Z) - T) X^{T} \end{aligned}$$

Now compute averages over all samples

$$\langle rac{\partial C}{\partial b}
angle = rac{1}{m} (S(Z) - T) egin{bmatrix} 1 \ dots \ 1 \end{bmatrix}$$

$$\langle rac{\partial C}{\partial W}
angle = rac{1}{m} (S(Z) - T) X^T$$

Check dimensions: S(Z) - T is $K \times m$, so the row sums of S(Z) - T form a length K vector matching the length of **b**

Check dimensions: S(Z) - T is $K \times m$, X is $n \times m$ so $(S(Z) - T)X^T$ is $K \times n$ matching the dimension of W

Softmax Regression

Softmax Algorithm

```
Select a learning rate parameter lpha Initialize \mathbf{b} \in \mathbb{R}^k and W \in \mathbb{R}^{k \times n} for i=1,\cdots,\max iterations do Compute error E=S(Z)-T update parameters b=b-\alpha<\frac{\partial C}{\partial \mathbf{b}}> W=W-\alpha<\frac{\partial C}{\partial W}>  save relevant information end
```

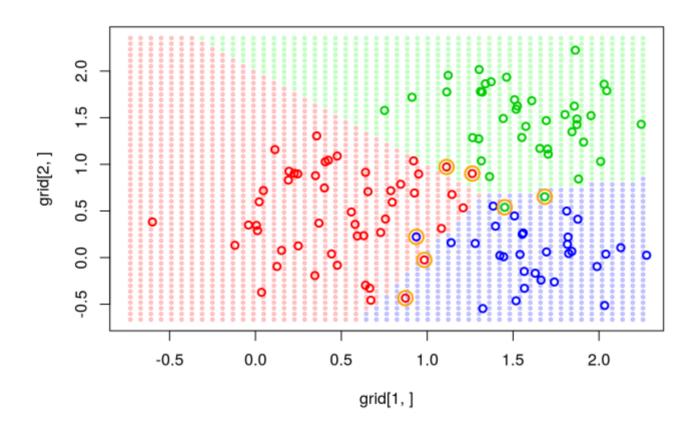
Where $<\cdot>$ means averaged over entire dataset

Binary or Softmax?

Softmax vs. K Binary Classifiers

- If only 1 class possible
 - use Softmax
- If more than one class (characteristic) possible
 - use K binary classifiers and select highest probabilities

Softmax Decision Boundary



MNIST Digits

