Classification

Numerical Methods for Deep Learning

Logistic Regression

Assume our data falls into two classes. Denote by $\mathbf{c}_{\mathrm{obs}}(\mathbf{y})$ the probability that example $\mathbf{y} \in \mathbb{R}^{n_f}$ belongs to first category.

Since output of our classifier $f(\mathbf{y}, \boldsymbol{\theta})$ is supposed to be probability, use logistic sigmoid

$$\mathbf{c}(\mathbf{y}, \boldsymbol{\theta}) = \frac{1}{1 + \exp\left(-f(\mathbf{y}, \boldsymbol{\theta})\right)}.$$

Example (Linear Classification): If $f(\mathbf{y}, \boldsymbol{\theta})$ is a linear function (adding bias is easy), $\boldsymbol{\theta} = \mathbf{w} \in \mathbb{R}^{n_f}$ and

$$\mathbf{c}(\mathbf{y}, \mathbf{w}) = \frac{1}{1 + \exp(-\mathbf{w}^\top \mathbf{y})}.$$

for now: consider linear models for simplicity

Multinomial Logistic Regression

Suppose data falls into $n_c \geq 2$ categories and the components of $\mathbf{c}_{\mathrm{obs}}(\mathbf{y}) \in [0,1]^{n_c}$ contain probabilities for each class.

Applying the logistic sigmoid to each component of $f(\mathbf{y}, \mathbf{W})$ not enough (probabilities must sum to one). Use

$$\mathbf{c}(\mathbf{y}, \mathbf{W}) = \left(\frac{1}{\mathbf{e}_{n_c}^\top \exp(\mathbf{W}\mathbf{y})} \right) \exp(\mathbf{W}\mathbf{y}).$$

Note: Division and exp are applied element-wise!

Logistic Regression - Loss Function

How similar are $\mathbf{c}(\cdot, \mathbf{W})$ and $\mathbf{c}_{\text{obs}}(\cdot)$?

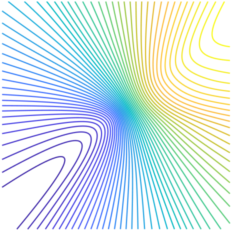
Naive idea: Let $\mathbf{Y} \in \mathbb{R}^{n_f \times n}$ be examples with class probabilities $\mathbf{C}_{\text{obs}} \in [0,1]^{n_c \times n}$, use

$$\phi(\mathbf{W}) = \frac{1}{2n} \sum_{j=1}^{n} \|\mathbf{c}(\mathbf{y}_j, \mathbf{W}) - \mathbf{c}_{j,\text{obs}}\|_F^2$$

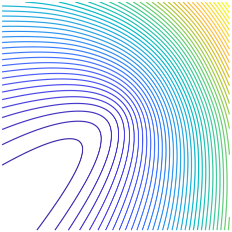
Problems

- ignores that $\mathbf{c}(\cdot, \mathbf{W})$ and $\mathbf{c}_{\text{obs}}(\cdot)$ are distributions.
- leads to non-convex objective function

Frobenius



Cross Entropy



Example: Designing a Code

Goal: Communicate using minimal number of bits.

Example: Bob talks $\mathbf{c} = [1/2, 1/4, 1/8, 1/8]$ of the time about dogs, cats, fish, and birds, respectively.
How many bits need to be transferred on average?

word	naive code	better code
dog	00	0
cat	01	10
fish	10	110
bird	11	111

Idea: Quantify information content in probability distribution using average length.

Entropy

Note: Length of word depends on its probability being used. How long should a word be?

Optimal choice for information for any category

$$I = \log_2(\mathbf{c}_j^{-1}) = -\log_2(\mathbf{c}_j)$$

The larger $\mathbf{c}_j$, the more common we use it, the shorter the word should be.

The entropy is the average (expectation) of information over all classes.

$$E(\mathbf{c}) = -\sum \mathbf{c}_j \log_2(\mathbf{c}_j) = -\mathbf{c}^\top \log_2(\mathbf{c})$$

Example: Designing a Code - 2

Entropy for Bob's code is

$$\frac{1}{2}\log(2) + \frac{1}{4}\log(4) + 2\frac{1}{8}\log(8) = 1.75$$

average length of word is 1.75 bits $<$ 2 bits for naive code!

For the complete tutorial on entropy, read
`http://colah.github.io/posts/2015-09-Visual-Information/`

Properties of Entropy

- recall $\lim_{x \to 0} x \log x = 0$
- prefer sparse distributions (why?)
- has been used in compressed sensing type methods

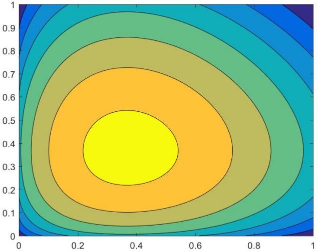


Figure: The entropy of a vector $\mathbf{c} = (c_1, c_2)^\top$

Cross Entropy

Measure the average word length when using code designed for $\mathbf{c}$ for sending information with probability $\widehat{\mathbf{c}}$

$$E(\widehat{\mathbf{c}}, \mathbf{c}) = -\widehat{\mathbf{c}}^\top \log(\mathbf{c}).$$

Clearly

$$E(\widehat{\mathbf{c}}, \mathbf{c}) \geq E(\mathbf{c}, \mathbf{c})$$

Example: Alice talks $\mathbf{c} = [1/8, 1/2, 1/4, 1/8]$ of the time about dogs, cats, fish, and birds, respectively. If she used Bob's code, the average word length would be

$$\frac{1}{8}\log(2) + \frac{1}{2}\log(4) + \frac{1}{4}\log(8) + \frac{1}{8}\log(8) = 2.25 > 1.75$$

E measures how similar the distributions $\mathbf{c}$ and $\widehat{\mathbf{c}}$ are.

One flaw: $E(\mathbf{c}, \widehat{\mathbf{c}}) \neq E(\widehat{\mathbf{c}}, \mathbf{c})$ (verify for our example!)

Cross Entropy for Logistic Regression - 1

Recall: For a single example and two classes we have

$$\mathbf{c}(\mathbf{y}, \mathbf{w}) = \begin{pmatrix} \frac{1}{1+\exp(-\mathbf{w}^\top \mathbf{y})} \\ 1 - \frac{1}{1+\exp(-\mathbf{w}^\top \mathbf{y})} \end{pmatrix} \stackrel{\text{def}}{=} \begin{pmatrix} h(\mathbf{w}^\top \mathbf{y}) \\ 1 - h(\mathbf{w}^\top \mathbf{y}) \end{pmatrix}$$

Assume we have the observation $\mathbf{c}_{\text{obs}} = \begin{pmatrix} \mathbf{c}_{\text{obs}} \\ 1 - \mathbf{c}_{\text{obs}} \end{pmatrix}$ then

$$\begin{aligned} E(\mathbf{c}_{\text{obs}}, \mathbf{c}) &= -\mathbf{c}_{\text{obs}}^\top \log(\mathbf{c}(\mathbf{y}, \mathbf{w})) \\ &= -\mathbf{c}_{\text{obs}} \log(h(\mathbf{w}^\top \mathbf{y})) - (1 - \mathbf{c}_{\text{obs}}) \log(1 - h(\mathbf{w}^\top \mathbf{y})). \end{aligned}$$

where

$$h(z) = \frac{1}{1 + \exp(-z)}$$

Cross Entropy for Logistic Regression - 2

In the case we have many examples need to sum over the data

$$\mathbf{C}(\mathbf{Y}, \mathbf{w}) = \begin{pmatrix} \frac{1}{1+\exp(-\mathbf{w}^\top \mathbf{Y})} \\ 1 - \frac{1}{1+\exp(\mathbf{w}^\top \mathbf{Y})} \end{pmatrix} \stackrel{def}{=} \begin{pmatrix} h(\mathbf{w}^\top \mathbf{Y}) \\ 1 - h(\mathbf{w}^\top \mathbf{Y}) \end{pmatrix} \in \mathbb{R}^{2\times n}$$

Assume we have the observation $\mathbf{c}_{\mathrm{obs}} \in \mathbb{R}^n$. Define

$$\mathbf{C}_{\mathrm{obs}} = \begin{pmatrix} \mathbf{c}_{\mathrm{obs}}^\top \\ 1 - \mathbf{c}_{\mathrm{obs}}^\top \end{pmatrix} \in \mathbb{R}^{2\times n}.$$

Then the cross entropy is

$$\begin{aligned} E(\mathbf{C}_{\mathrm{obs}}, \mathbf{C}) &= -\frac{1}{n}\mathrm{tr}(\mathbf{C}_{\mathrm{obs}}^\top \mathbf{C}) \\ &= -\frac{1}{n}\mathbf{c}_{\mathrm{obs}}^\top \log(h(\mathbf{w}^\top \mathbf{Y}) \\ &\quad -\frac{1}{n}(1 - \mathbf{c}_{\mathrm{obs}})^\top \log(1 - h(\mathbf{w}^\top \mathbf{Y}))) \end{aligned}$$

Cross Entropy for Multinomial Logistic Regression

Similarly, for general case ($n_c \geq 2$ classes, n examples).
Recall:

$$\mathbf{C}(\mathbf{Y}, \mathbf{W}) = \exp(\mathbf{W}\mathbf{Y}) \, \mathrm{diag}\left(\frac{1}{\mathbf{e}_{n_c}^{\top} \exp(\mathbf{W}\mathbf{Y})}\right)$$

Get cross entropy by summing over all examples

$$E(\mathbf{C}_{\mathrm{obs}}, \mathbf{C}(\mathbf{Y}, \mathbf{W})) = -\frac{1}{n} \mathrm{tr}(\mathbf{C}_{\mathrm{obs}}^{\top} \log(\mathbf{C}(\mathbf{Y}, \mathbf{W}))).$$

We will also call this the *softmax* (cross-entropy) function.

Simplifying the Softmax Function

Let $\mathbf{S} = \mathbf{W}\mathbf{Y}$, then

$$E(\mathbf{C}_{\mathrm{obs}}, \mathbf{S}) = -\frac{1}{n}\mathrm{tr}\left(\mathbf{C}_{\mathrm{obs}}^{\top} \log\left(\exp(\mathbf{S})\mathrm{diag}\left(\frac{1}{\mathbf{e}_{n_c}^{\top}\exp(\mathbf{S})}\right)\right)\right).$$

Verify that this is equal to

$$\begin{aligned} E(\mathbf{C}_{\mathrm{obs}}, \mathbf{S}) = &-\frac{1}{n}\mathbf{e}_{n_c}^{\top}\left(\mathbf{C}_{\mathrm{obs}} \odot \mathbf{S}\right)\mathbf{e}_n \\ &+ \frac{1}{n}\mathbf{e}_{n_c}^{\top}\mathbf{C}_{\mathrm{obs}} \log\left(\mathbf{e}_{n_c}^{\top}\exp(\mathbf{S})\right)^{\top} \end{aligned}$$

($\odot$ is Hadamard product, exp and log component-wise)

If $\mathbf{C}_{\mathrm{obs}}$ has a unit row sum (why?) then $\mathbf{e}_{n_c}^{\top}\mathbf{C}_{\mathrm{obs}}^{\top} = \mathbf{e}_n^{\top}$ and

$$E(\mathbf{C}_{\mathrm{obs}}, \mathbf{S}) = -\frac{1}{n}\mathbf{e}_{n_c}^{\top}\left(\mathbf{C}_{\mathrm{obs}} \odot \mathbf{S}\right)\mathbf{e}_n + \frac{1}{n}\log(\mathbf{e}_{n_c}^{\top}\exp(\mathbf{S}))\mathbf{e}_n$$

Numerical Considerations

Scale to prevent overflow. Note that for an arbitrary $s \in \mathbb{R}$ we have

$$E(\mathbf{C}_{\text{obs}}, \mathbf{WY} - s) = E(\mathbf{C}_{\text{obs}}, \mathbf{WY})$$

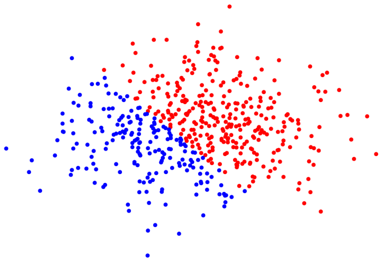
This prevents overflow, but may lead to underflow (and divisions by zero).

Note that s does not need to be the same in each row (example). Hence, we can choose $\mathbf{s} = \max(\mathbf{WY}, [], 1) \in \mathbb{R}^{1 \times n}$ to avoid underflow and overflow.

For stability use $E(\mathbf{C}_{\text{obs}}, \mathbf{S})$ where $\mathbf{S} = \mathbf{WY} - \mathbf{e}_{n_c}\mathbf{s}$.

Test Problem: Linear Classification

Generate data that is linearly separable:



```
a = 3; b = 2;

Y = randn(2,500);
C = a*Y(1,:) + b*Y(2,:) + 1;
C(C>0) = 1; C(C<0) = 0;
C = [C; 1-C]
```

Coding: Softmax Regression Objective Function

Write a function that computes the softmax function given a data matrix **Y**, its class **C**, and a matrix **W**.

```
function[E] = softmaxFun(W,Y,C)

% Your code here


end
```

Test your code using `testSoftmax.m`

Linear Classification

If $\mathbf{W}$ can separate the classes then the goal is to minimize the cross entropy (with some potential regularization)

$$\mathbf{W}^* = \arg\min_{\mathbf{W}} \quad -\frac{1}{n}\mathbf{e}_{n_c}^\top \left(\mathbf{C}_{\rm obs} \odot \mathbf{S}\right) \mathbf{e}_n + \frac{1}{n} \log(\mathbf{e}_{n_c}^\top \exp(\mathbf{S}))\mathbf{e}_n$$
$$\text{subject to } \mathbf{S} = \mathbf{W}\mathbf{Y} - \mathbf{e}_{n_c}\mathbf{s}$$

This is a smooth convex optimization problem
$\Rightarrow$ many existing optimization techniques will work

For large-scale problems, use derivative-based optimization algorithm. (Examples: Steepest Descent, Newton-like methods, Stochastic Gradient Descent, ADMM, ...)

Excellent references: [3, 2, 1**?**]

Differentiating the Softmax Function - 1

We need to compute the derivative of the cross entropy function with respect to $\mathbf{W}$. Three hints:

- $\sum \mathbf{w} \odot \mathbf{y} = \mathbf{w}^\top \mathbf{y}$
- $\nabla_{\mathbf{w}}(\mathbf{w}^\top \mathbf{y}) = \mathbf{y}$
- $\mathrm{vec}(\mathbf{WY}) = (\mathbf{Y}^\top \otimes \mathbf{I})\mathrm{vec}(\mathbf{W}) = (\mathbf{I} \otimes \mathbf{W})\mathrm{vec}(\mathbf{Y})$

where $\otimes$ is the Kronecker product.

We use the common notation:

- $\mathrm{vec}(\mathbf{A})$ reshapes matrix $\mathbf{A}$ (column-wise) into vector
- $\mathrm{mat}(\mathbf{a})$ reshapes vector $\mathbf{a}$ into matrix, $\mathrm{mat}(\mathrm{vec}(\mathbf{A})) = \mathbf{A}$.
- $\mathrm{diag}(\mathbf{A}) = \mathrm{diag}(\mathrm{vec}(\mathbf{A}))$ builds diagonal matrix with entries given by $\mathbf{A}$.

Differentiating the Softmax Function - 2

Do it in three steps:

1. $\nabla_{\mathbf{S}} E(\mathbf{S})$ with $\mathbf{S} = \mathbf{YW}$ (assume w.l.o.g. no shift)
2. $\nabla_{\mathbf{W}} \mathbf{S} = \nabla_{\mathbf{W}} (\mathbf{WY})$
3. use chain rule to get $\nabla_{\mathbf{W}} E(\mathbf{WY})$.

Break the first step down into two terms

$$E(\mathbf{S}) = \frac{1}{n} \overbrace{-\mathrm{tr}(\mathbf{C}_{\mathrm{obs}}^{\top} \mathbf{S})}^{E1} + \frac{1}{n} \overbrace{\log(\mathbf{e}_{n_c} \exp(\mathbf{S}))\mathbf{e}_n}^{E2},$$

First term is linear

$$\nabla_{\mathbf{S}} E_1 = \nabla_{\mathbf{S}} \mathrm{tr}(\mathbf{C}_{\mathrm{obs}}^{\top} \mathbf{S}) = \mathbf{C}_{\mathrm{obs}}.$$

Differentiating the Softmax Function - 3

$$E(\mathbf{S}) = \frac{1}{n}\overbrace{-\mathrm{tr}(\mathbf{C}_{\mathrm{obs}}^\top \mathbf{S})}^{E1} + \frac{1}{n}\overbrace{\log(\mathbf{e}_{n_c}^\top \exp(\mathbf{S}))\mathbf{e}_n}^{E2}$$

Second term requires a bit more care

$$\mathbf{J_S} E_2 = \mathbf{J_S}\mathbf{e}_n^\top \log(\mathbf{e}_{n_c}^\top \exp(\mathbf{S})) = \mathbf{e}_n^\top \mathbf{J_S} \log(\mathbf{e}_{n_c}^\top \exp(\mathbf{S}))$$

and

$$\mathbf{J_S} \log(\mathbf{e}_{n_c}^\top \exp(\mathbf{S})) = \mathrm{diag}\left(\frac{1}{\mathbf{e}_{n_c}^\top \exp(\mathbf{S})}\right) \mathbf{J_S}\left(\mathbf{e}_{n_c}^\top \exp(\mathbf{S})\right)$$

Differentiating the Softmax Function - 4

Recall:

$$\mathbf{J_S} E_2 = \mathbf{e}_n^\top \mathrm{diag}\left(\frac{1}{\mathbf{e}_{n_c}^\top \exp(\mathbf{S})}\right) \mathbf{J_S}\left(\mathbf{e}_{n_c}^\top \exp(\mathbf{S})\right)$$

Focus on last term:

$$\begin{aligned}\mathbf{J_S}(\mathbf{e}_{n_c}^\top \exp(\mathbf{S})) &= \mathbf{J_S}\left(\left(\mathbf{I} \otimes \mathbf{e}_{n_c}^\top\right) \mathrm{vec}(\exp(\mathbf{S}))\right) \\ &= (\mathbf{I} \otimes \mathbf{e}_{n_c}^\top)\mathrm{diag}(\mathrm{vec}(\exp(\mathbf{S})))\end{aligned}$$

Putting it together

$$\mathbf{J_S} E_2 = \mathbf{e}_n^\top \ \mathrm{diag}\left(\frac{1}{\mathbf{e}_{n_c}^\top \exp(\mathbf{S})}\right) \ (\mathbf{I} \otimes \mathbf{e}_{n_c}^\top)\mathrm{diag}(\mathrm{vec}(\exp(\mathbf{S})))$$

Left to do: Take transpose

Differentiating the Softmax Function - 5

$$\nabla_{\mathbf{S}} E_2 = \mathrm{diag}(\mathrm{vec}(\exp(\mathbf{S})))(\mathbf{I} \otimes \mathbf{e}_{n_c})\mathrm{diag}\left(\frac{1}{\mathbf{e}_{n_c}^\top \exp(\mathbf{S})}\right)\mathbf{e}_n$$

simplifying

$$\nabla_{\mathbf{S}} E_2 = \mathrm{diag}(\mathrm{vec}(\exp(\mathbf{S})))(\mathbf{I} \otimes \mathbf{e}_{n_c})\left(\frac{1}{\mathbf{e}_{n_c}^\top \exp(\mathbf{S})}\right)$$

Avoid diag and simplify using matrix representation

$$\nabla_{\mathbf{S}} E_2 = \exp(\mathbf{S}) \odot \left(\mathbf{e}_{n_c}\left(\frac{1}{\mathbf{e}_{n_c}^\top \exp(\mathbf{S})}\right)\right)$$

Finally combine gradients of E_1 and E_2

$$\nabla_{\mathbf{S}} E = -\frac{1}{n}\mathbf{C}_{\mathrm{obs}} + \frac{1}{n}\exp(\mathbf{S}) \odot \left(\mathbf{e}_{n_c}\left(\frac{1}{\mathbf{e}_{n_c}^\top \exp(\mathbf{S})}\right)\right).$$

Differentiating the Softmax Function - 6

$$E(\mathbf{W}) = -\frac{1}{n}\overbrace{\mathrm{tr}(\mathbf{C}_{\mathrm{obs}}^\top(\mathbf{W}\mathbf{Y}))}^{E1} + \frac{1}{n}\overbrace{\mathbf{e}_n^\top \log(\mathbf{e}_{n_c}^\top \exp(\mathbf{W}\mathbf{Y}))}^{E2}$$

Note that

$$\nabla_{\mathbf{W}}\mathbf{S} = \nabla_{\mathbf{W}}(\mathbf{W}\mathbf{Y}) = \nabla_{\mathbf{W}}\left((\mathbf{Y}^\top \otimes \mathbf{I})\mathrm{vec}(\mathbf{W})\right) = \mathbf{Y} \otimes \mathbf{I}.$$

Hence, applying the chain rule gives

$$\nabla_{\mathbf{W}} E = \frac{1}{n}\left(-\mathbf{C}_{\mathrm{obs}} + \exp(\mathbf{S}) \odot \left(\mathbf{e}_{n_c}\left(\frac{1}{\mathbf{e}_{n_c}^\top \exp(\mathbf{S})}\right)\right)\right)\mathbf{Y}^\top.$$

Coding: Differentiating the Softmax Function

Extend your softmax function, so that it returns the gradient if needed.

```
function[E,dE] = softmaxFun(W,Y,C)

% Your code from before

if nargout > 1

% Your code for gradient here
end

end
```

Testing your Derivatives

Your derivatives are assumed to be wrong unless you prove otherwise.

Test based on Taylor theorem. Let $\mathbf{W}$ be fixed and $\mathbf{D}$ be a random direction (same size as $\mathbf{W}$):

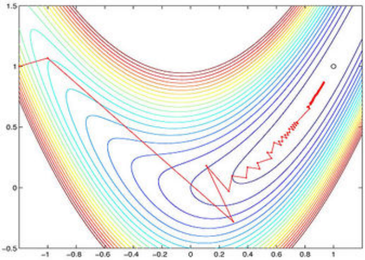
h	$E(\mathbf{W} + h\mathbf{D}) - E(\mathbf{W})$	$E(\mathbf{W} + h\mathbf{D}) - E(\mathbf{W}) - h\,\mathrm{tr}(\mathbf{D}^\top \nabla E(\mathbf{W}))$
1		
2^{-1}		
2^{-2}		
2^{-3}		
2^{-4}		
2^{-5}		

First column should decay as $\mathcal{O}(h)$

Second column should decay as $\mathcal{O}(h^2)$

Derivative-Based Optimization: Steepest Descent

To minimize the energy go “down-hill”



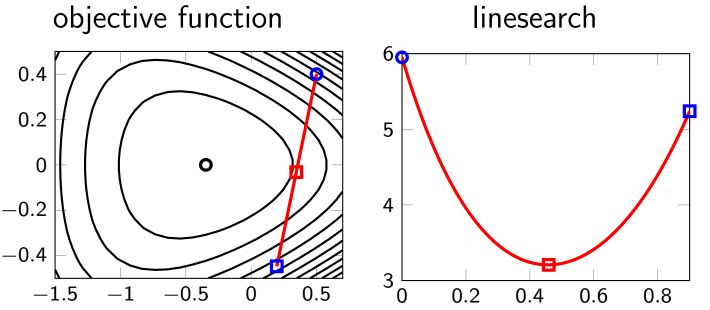
Iterate:

$$\mathbf{W}_{k+1} = \mathbf{W}_k + \alpha \mathbf{D}, \quad \mathbf{D} = -\nabla E(\mathbf{W}_k).$$

Guaranteed to be a descent direction but need to make sure that

$$E(\mathbf{W}_k + \alpha \mathbf{D}) < E(\mathbf{W}_k)$$

Line Search Problem



Let E be the cross entropy, $\mathbf{W}_k$ the current weights, and $\mathbf{D}$ the search direction. The line search problem is:

$$\min_{\alpha > 0} \phi(\alpha) \quad \text{where} \quad \phi(\alpha) = E(\mathbf{W}_k + \alpha \mathbf{D}).$$

Armijo Line Search

A method for inexact line search

- Start with $\alpha = \alpha_0$
- Test $E(\mathbf{W} + \alpha\mathbf{D}) < E(\mathbf{W})$
- If fail $\alpha \leftarrow \frac{1}{2}\alpha$

A few (small) but helpful tricks

- Choose your α_0 based on the problem
- If line search is needed $(\alpha \neq \alpha_0)$ at iteration k set $\alpha_0 = \alpha_k$ in next iteration.
- If no line search is needed $(\alpha = \alpha_0)$ at iteration k set $\alpha_0 = \gamma\alpha_k$, $\gamma > 1$ in next iteration.

Coding: Steepest Descent

Write a code for steepest descent with Armijo linesearch.

```
function W = steepestDescent(E,W,param)
% Inputs:
%     E  - function that provides value and gradient
%     W  - starting guess
%  param - struct with parameters

alpha     = param.maxStep; % max step size
maxIter   = param.maxIter; % max number of iterations

for i=1:maxIter

% Your code here
end
```

Newton-like Methods

Goal: Solve $\min_{\mathbf{W}} E(\mathbf{W})$. Consider kth iteration. Assume E convex.

To find optimal step $\mathbf{D}$, use Taylor's theorem

$$E(\mathbf{W}_k + \mathbf{D}) = E(\mathbf{W}_k) + \nabla E(\mathbf{W}_k)^\top \mathbf{D} + \frac{1}{2}\mathbf{D}^\top \nabla^2 E(\mathbf{W}_k)\mathbf{D} + \mathcal{O}(\|\mathbf{D}\|^3)$$

and differentiate w.r.t $\mathbf{D}$ to obtain

$$\nabla^2 E(\mathbf{W}_k)\mathbf{D} = -\nabla E(\mathbf{W}_k).$$

Practical Newton methods (see, e.g., [3, Ch.7])

- do not compute $\mathbf{D}$ accurately (add line search for safety)
- use, e.g., Conjugate Gradient (CG) methods
- do not generate $\nabla^2 E$ since CG only needs mat-vecs
- give quadratic/superlinear/good linear convergence

Newton-like Methods for Softmax

Need to compute Hessian $\nabla^2 E$. Recall:

$$\begin{aligned}\nabla_{\mathbf{W}} E &= \frac{1}{n}\left(-\mathbf{C}_{\text{obs}} + \exp(\mathbf{S}) \odot \left(\mathbf{e}_{n_c}\left(\frac{1}{\mathbf{e}_{n_c}^\top \exp(\mathbf{S})}\right)\right)\right)\mathbf{Y}^\top \\ &= \nabla_{\mathbf{S}} E(\mathbf{S})\mathbf{Y}^\top,\end{aligned}$$

where $\mathbf{S} = \mathbf{WY}$. For Hessian we know

$$\nabla^2_{\mathbf{W}} E(\mathbf{W}) = \mathbf{Y} \nabla^2_S E(\mathbf{S}) \mathbf{Y}^\top$$

Remarks:

- size of $\nabla^2_{\mathbf{S}} E$ is $n_c n \times n_c n$, typically sparse
- size of $\nabla^2_{\mathbf{W}} E$ is $n_c n_f \times n_c n_f$, typically dense
- building Hessian can be costly (when n is large)
- Hessian is spd since E is convex in $\mathbf{S}$

Hessian of Softmax Function - 1

Recall

$$\nabla_{\mathbf{S}} E = \frac{1}{n}\left(-\mathbf{C} + \exp(\mathbf{S}) \odot \frac{1}{\mathbf{e}_{n_c}\mathbf{e}_{n_c}^\top \exp(\mathbf{S})}\right)$$

Let's first vectorize this $\mathbf{s} = \mathrm{vec}(\mathbf{S})$ and $\mathbf{c} = \mathrm{vec}(\mathbf{C})$

$$\nabla_{\mathbf{s}} E = \frac{1}{n}\left(-\mathbf{c} + \exp(\mathbf{s}) \odot \frac{1}{(\mathbf{I} \otimes (\mathbf{e}_{n_c}\mathbf{e}_{n_c}^\top))\exp(\mathbf{s})}\right)$$

Use product rule

$$\begin{aligned}
\nabla_{\mathbf{s}}^2 E &= \mathrm{diag}\left(\frac{1}{(\mathbf{I} \otimes (\mathbf{e}_{n_c}\mathbf{e}_{n_c}^\top))\exp(\mathbf{s})}\right)\mathbf{J}_{\mathbf{s}}\exp(\mathbf{s}) + \\
&\quad \mathrm{diag}(\exp(\mathbf{s}))\mathbf{J}_{\mathbf{s}}\left(\frac{1}{(\mathbf{I} \otimes (\mathbf{e}_{n_c}\mathbf{e}_{n_c}^\top))\exp(\mathbf{s})}\right) \\
&= \nabla_{\mathbf{s}}^2 E_1 + \nabla_{\mathbf{s}}^2 E_2
\end{aligned}$$

Hessian of Softmax Function - 2

First term is easy

$$\begin{aligned}\nabla^2_{\mathbf{s}} E_1 &= \mathrm{diag}\left(\frac{1}{(\mathbf{I} \otimes (\mathbf{e}_{n_c}\mathbf{e}_{n_c}^\top))\exp(\mathbf{s})}\right)\mathrm{diag}\left(\exp(\mathbf{s})\right)\\ &= \mathrm{diag}\left(\frac{\exp(\mathbf{s})}{(\mathbf{I} \otimes (\mathbf{e}_{n_c}\mathbf{e}_{n_c}^\top))\exp(\mathbf{s})}\right)\end{aligned}$$

Reshaped back, a matrix-vector-product with $\mathbf{V} \in \mathbb{R}^{n_c \times n_f}$ is

$$\mathbf{H}_1\mathbf{V} = \left(\left(\frac{\exp(\mathbf{S})}{\mathbf{e}_{n_c}\mathbf{e}_{n_c}^\top \exp(\mathbf{S})}\right) \odot (\mathbf{V}\mathbf{Y})\right)\mathbf{Y}^\top$$

Hessian of Softmax Function - 3

$$E_2 = \mathrm{diag}(\exp(\mathbf{s}))\,\underbrace{\mathbf{J_s}\left(\frac{1}{(\mathbf{I}\otimes(\mathbf{e}_{n_c}\mathbf{e}_{n_c}^\top))\exp(\mathbf{s})}\right)}_{=:\mathbf{T}}.$$

Using chain rule, we get

$$\mathbf{T} = -\mathrm{diag}\left(\frac{1}{\left((\mathbf{I}\otimes(\mathbf{e}_{n_c}\mathbf{e}_{n_c}^\top))\exp(\mathbf{s})\right)^2}\right)(\mathbf{I}\otimes(\mathbf{e}_{n_c}\mathbf{e}_{n_c}^\top))\mathrm{diag}(\exp(s))$$

After reshape the matrix-vector-product with $\mathbf{V}\in\mathbb{R}^{n_f\times n_c}$ is

$$\mathbf{H}_2\mathbf{V} = -\left(\frac{(\exp(\mathbf{S}))}{\mathbf{e}_{n_c}(\mathbf{e}_{n_c}^\top\exp(\mathbf{S}))^2}\right)\odot(\mathbf{e}_{n_c}\mathbf{e}_{n_c}^\top(\exp(\mathbf{S})\odot(\mathbf{VY})))\mathbf{Y}^\top$$

Newton-CG for Softmax function

Mat-vecs with Hessian can be computed as

$$
\begin{aligned}
\nabla^2_{\mathbf{W}} E(\mathbf{W})\mathbf{V} = \quad & \frac{1}{n}\left(\left(\frac{\exp(\mathbf{S})}{\mathbf{e}_{n_c}\mathbf{e}_{n_c}^\top \exp(\mathbf{S})}\right) \odot (\mathbf{VY})\right)\mathbf{Y}^\top \\
- \quad & \frac{1}{n}\left(\frac{(\exp(\mathbf{S}))}{\mathbf{e}_{n_c}(\mathbf{e}_{n_c}^\top \exp(\mathbf{S}))^2}\right) \odot (\mathbf{e}_{n_c}\mathbf{e}_{n_c}^\top(\exp(\mathbf{S}) \odot (\mathbf{VY})))\mathbf{Y}^\top
\end{aligned}
$$

(possible to further simplify this to reduce operations)

Now, ready to use matrix-free Newton method with Armijo linesearch and CG solver that computes

$$
\nabla^2_{\mathbf{W}} E(\mathbf{W})\mathbf{D} \approx -\nabla_{\mathbf{W}} E(\mathbf{W}).
$$

Remarks:

- how well to solve? use large tolerance on relative residual
- can accelerate CG with preconditioning $\rightsquigarrow$ PCG
- possible to omit second term in Hessian?

Coding: Hessian of Softmax Function

Extend your softmax function, so that it returns a function handle computing mat-vecs with Hessian if needed.

```
function[E,dE,d2Emv] = softmaxFun(W,Y,C)

% Your code from before
if nargout > 1
% Your code from before
end

if nargout > 2

% Your new code here
d2Emv = @(V) ...;
end
end
```

Don't forget to check your derivatives!

Newton-like Methods - Derivatives

Consider the softmax function

$$E(\mathbf{W}) = -\sum \mathbf{Y} \odot (\mathbf{XW}) + \sum \log \left(\sum \exp(\mathbf{XW}) \right)$$

Class problems:

1. Compute the Hessian of the cross entropy function
2. Write code that constructs the matrix it and do a derivative check at a random point $\mathbf{W}_0$.
3. Write a code that performs matrix vector products with the Hessian (without constructing it). Test by comparing results with the matrix-based code for a random vector.

References

[1] A. Beck. *Introduction to Nonlinear Optimization*. Theory, Algorithms, and Applications with MATLAB. SIAM, Philadelphia, Oct. 2014.

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[3] J. Nocedal and S. Wright. *Numerical Optimization*. Springer Series in Operations Research and Financial Engineering. Springer Science & Business Media, New York, Dec. 2006.