Homework 03: Jacobians and the application of Chain Rule.

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This problem set is designed to practice the application of chain rule and the differentiations of various multivariate functions. This is what you need to do to write the `bprop` method of a module.

If you know how to compute the derivatives of simple functions, you have all the skills necessary to complete this problem set.

1 Exponential Module

The scalar exponential module maps a scalar variable $x$ to a scalar variable $y$ using the following formula:

$$y = \exp(-\beta x)$$

where $\beta$ is a parameter.

1.1 Question: jacobian with respect to $X$

Assuming that the partial derivatives of the energy with respect to $y$ is known, give the expression for the partial derivative of the energy with respect to $x$. To do so, calculate $\frac{\partial y}{\partial x}$, and apply Chain Rule:

$$\frac{\partial E}{\partial x} = \frac{\partial E}{\partial y} \frac{\partial y}{\partial x}$$

1.2 Question: jacobian with respect to $\beta$

Now calculate the derivative of the energy with respect to $\beta$:

$$\frac{\partial E}{\partial \beta} = \frac{\partial E}{\partial y} \frac{\partial y}{\partial \beta}$$

2 Component Scaling Module

The scaling module maps an $N$-dimensional column vector $X = [x_1, x_2, \ldots, x_n]'$ to an $N$-dimensional column vector $Y = [y_1, y_2, \ldots, y_n]'$ with the following formula:

$$y_i = k_i x_i \quad \forall i \in [1, N].$$

where the $k_i$'s are the components of a vector of parameters $K = [k_1, k_2, \ldots, k_n]$.

2.1 Question: jacobian with respect to $X$

Assuming that the partial derivatives of the energy with respect to all the $y_i$ are known, give the expression for the partial derivative of the energy with respect to the $x_j$. To do so, calculate $\frac{\partial y_i}{\partial x_j}$, and apply Chain Rule:

$$\frac{\partial E}{\partial x_j} = \sum_{i=1}^{N} \frac{\partial E}{\partial y_i} \frac{\partial y_i}{\partial x_j}$$

Hint: $\frac{\partial y_i}{\partial x_j}$ is equal to 0 for $j \neq i$. You can view the operation on each component $y_i = k_i x_i$ as a separate module operating on scalar values.
2.2 Question: jacobian with respect to $K$

Now calculate the derivative of the energy with respect to each of the $k_j$'s:

$$\frac{\partial E}{\partial k_j} = \sum_{i=1}^{N} \frac{\partial E}{\partial y_i} \frac{\partial y_i}{\partial k_j}$$

Hint: $\frac{\partial y_i}{\partial k_j}$ is equal to 0 for $j \neq i$.

3 Global Scaling Module

The global scaling is similar to the component scaling module, except that it uses a single coefficient to scale all the components of $X$. It maps an $N$-dimensional column vector $X = [x_1, x_2, \ldots, x_n]'$ to an $N$-dimensional column vector $Y = [y_1, y_2, \ldots, y_n]'$ with the following formula:

$$y_i = k x_i \quad \forall i \in [1, N].$$

where the $k$ is a scalar parameters.

3.1 Question: jacobian with respect to $X$

Assuming that the partial derivatives of the energy with respect to all the $y_i$ are known, give the expression for the partial derivative of the energy with respect to the $x_j$. To do so, calculate $\frac{\partial y_i}{\partial x_j}$, and apply Chain Rule:

$$\frac{\partial E}{\partial x_j} = \sum_{i=1}^{N} \frac{\partial E}{\partial y_i} \frac{\partial y_i}{\partial x_j}$$

3.2 Question: jacobian with respect to $K$

Now calculate the derivative of the energy with respect to $k$:

$$\frac{\partial E}{\partial k} = \sum_{i=1}^{N} \frac{\partial E}{\partial y_i} \frac{\partial y_i}{\partial k}$$

Note the difference with the component scaling module.

4 Softmax Module

The so-called softmax module maps an $N$-dimensional column vector $X = [x_1, x_2, \ldots, x_n]'$ to an $N$-dimensional column vector $Y = [y_1, y_2, \ldots, y_n]'$ with the following formula:

$$y_i = \frac{\exp(-\beta x_i)}{\sum_{j=1}^{N} \exp(-\beta x_j)} \quad \forall i \in [1, N].$$

where $\beta$ is a parameter. The softmax module can be used to transform a vector of real numbers into something that looks like a probability distribution: a vector of numbers that are all between 0 and 1 and whose sum is equal to 1.

4.1 Question: jacobian with respect to $X$

Assuming that the partial derivatives of the energy with respect to all the $y_i$ are known, give the expression for the partial derivative of the energy with respect to the $x_j$. To do so, calculate $\frac{\partial y_i}{\partial x_j}$, and apply Chain Rule:

$$\frac{\partial E}{\partial x_j} = \sum_{i=1}^{N} \frac{\partial E}{\partial y_i} \frac{\partial y_i}{\partial x_j}$$

4.2 Question: jacobian with respect to $\beta$

Now calculate the derivative of the energy with respect to $\beta$:

$$\frac{\partial E}{\partial \beta} = \sum_{i=1}^{N} \frac{\partial E}{\partial y_i} \frac{\partial y_i}{\partial \beta}$$
5 Logsum Module

The logsum module maps an \( N \)-dimensional vector \( X \) to a scalar \( y \) with the following formula:

\[
y = -\frac{1}{\beta} \log \left( \sum_{j=1}^{N} \exp(-\beta x_j) \right)
\]

5.1 Question: jacobian with respect to \( X \)

Assuming that the partial derivatives of the energy with respect to the \( y \) is known, give the expression for the partial derivative of the energy with respect to the \( x_j \). To do so, calculate \( \frac{\partial y}{\partial x_j} \), and apply Chain Rule:

\[
\frac{\partial E}{\partial x_j} = \frac{\partial E}{\partial y} \cdot \frac{\partial y}{\partial x_j}
\]

5.2 Question: jacobian with respect to \( \beta \)

Now calculate the derivative of the energy with respect to \( \beta \):

\[
\frac{\partial E}{\partial \beta} = \frac{\partial E}{\partial y} \cdot \frac{\partial y}{\partial \beta}
\]