CSED490F Lab: Autograd

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1 Automatic Differentiation

Reverse-mode automatic differentiation performs back-to-front accumulation of local gradients based on the chain rule. We omit the definitions and the local gradients of the `Add`, `Mul`, `Pow`, `Log`, and `Sum` operations as they are trivial, and show `ReLU` as an example.

$$\texttt{ReLU}(x) = \max(x, 0), \quad \frac{\partial \texttt{ReLU}(x)}{\partial x} = \begin{cases} 1 & x > 0, \\ 0 & x < 0 \end{cases}$$

1.1 Matrix Multiplication

Let $z = \texttt{MatMul}(x, y)$ for $x \in \mathbb{R}^{N \times D}$ and $y \in \mathbb{R}^{D \times M}$. Then, each element of $z \in \mathbb{R}^{N \times M}$ is computed as $z_{n,m} = \sum_d x_{n,d}\, y_{d,m}$. Any element $x_{n,m}$ of x only contributes to row n of z:

$$z_{n,*} = \begin{bmatrix} \sum_d x_{n,d}\, y_{d,1} & \sum_d x_{n,d}\, y_{d,2} & \cdots & \sum_d x_{n,d}\, y_{d,M-1} & \sum_d x_{n,d}\, y_{d,M} \end{bmatrix}$$

This gives $\partial \mathcal{L} / \partial x$ as the following:

$$\frac{\partial \mathcal{L}}{\partial x_{n,d}} = \sum_m \frac{\partial \mathcal{L}}{\partial z_{n,m}} \frac{\partial z_{n,m}}{\partial x_{n,d}} = \sum_m \frac{\partial \mathcal{L}}{\partial z_{n,m}} y_{d,m} = \frac{\partial \mathcal{L}}{\partial z_{n,*}} y_{d,*}^{\top}$$

Finally, we obtain the backpropagation rules for `MatMul`.

$$\frac{\partial \mathcal{L}}{\partial x} = \frac{\partial \mathcal{L}}{\partial \texttt{MatMul}(x, y)} y^{\top}, \quad \frac{\partial \mathcal{L}}{\partial y} = x^{\top} \frac{\partial \mathcal{L}}{\partial \texttt{MatMul}(x, y)}$$

1.2 Classification

Softmax. Following [1], we implement the softmax function with a shift for numerical stability. This shift has no impact on the output result or the gradient.

$$\texttt{Softmax}(x)_j = \frac{\exp\left(x_j - s\right)}{\sum_i \exp\left(x_i - s\right)}$$

By simple differentiation, we can obtain $\partial \texttt{Softmax}(x)_i / \partial x_j$ for $i = j$ and $i \neq j$ as the following:

$$\frac{\partial \texttt{Softmax}(x)_j}{\partial x_j} = \texttt{Softmax}(x)_j - \texttt{Softmax}(x)_j^2, \quad \frac{\partial \texttt{Softmax}(x)_i}{\partial x_j} = -\texttt{Softmax}(x)_i \texttt{Softmax}(x)_j$$

Using the above gradients, we can derive a backpropagation rule in matrix form:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial x_j} &= \sum_i \frac{\partial \mathcal{L}}{\partial \texttt{Softmax}(x)_i} \frac{\partial \texttt{Softmax}(x)_i}{\partial x_j} \\ &= \frac{\partial \mathcal{L}}{\partial \texttt{Softmax}(x)_j} \left(\texttt{Softmax}(x)_j - \texttt{Softmax}(x)_j^2\right) - \sum_{i \neq j} \frac{\partial \mathcal{L}}{\partial \texttt{Softmax}(x)_i} \texttt{Softmax}(x)_i \texttt{Softmax}(x)_j \\ &= \texttt{Softmax}(x)_j \left(\frac{\partial \mathcal{L}}{\partial \texttt{Softmax}(x)_j} - \sum_i \frac{\partial \mathcal{L}}{\partial \texttt{Softmax}(x)_i} \texttt{Softmax}(x)_i \right) \end{aligned}$$

Negative log-likelihood. The negative log-likelihood loss (with log-probability input) is defined as the following, with trivial local gradients:

$$\texttt{NLLLoss}(\log \hat{p}, p) = -\sum_i p_i \log \hat{p}_i, \quad \frac{\partial \texttt{NLLLoss}(\log \hat{p}, p)}{\partial p} = -\log \hat{p}, \quad \frac{\partial \texttt{NLLLoss}(\log \hat{p}, p)}{\partial \log \hat{p}} = -p$$

Cross-entropy. The cross-entropy loss (with logit inputs) can be seen as a composition of `Softmax` and `NLLLoss`.

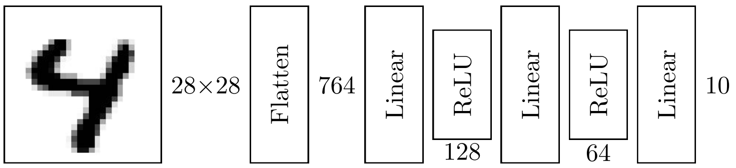
$$\texttt{CrossEntropyLoss}(\hat{x}, p) = \texttt{NLLLoss}\Big(\log\big(\texttt{Softmax}(\hat{x})\big), p\Big) = -\sum_i p_i \log\big(\texttt{Softmax}(\hat{x}_i)\big)$$

The local gradients can be found accordingly by the chain rule on `Log`, `Softmax`, and `NLLLoss`.

$$\frac{\partial \texttt{CrossEntropyLoss}(\hat{x}, p)}{\partial \hat{x}_j} = \texttt{Softmax}(\hat{x})_j - p_j, \quad \frac{\partial \texttt{CrossEntropyLoss}(\hat{x}, p)}{\partial p_j} = -\log\big(\texttt{Softmax}(\hat{x})\big)_j$$

2 MNIST Classification

Utilizing the operators described in section 1, we train an MLP f_θ to perform classification on the MNIST dataset [2]. The MLP architecture used is shown below.



The cross-entropy loss is used with L2 regularization. We found that using `NLLLoss`, `Log`, and `Softmax` separately resulted in numerical instability and NaN values during training, so the fused `CrossEntropyLoss` operator was used directly.

$$\begin{aligned}
\mathcal{L}(\theta; I, p) &= \mathcal{L}_{\text{class}}(\theta; I, p) + \lambda_{\text{L2}} \mathcal{L}_{\text{L2}}(\theta) \\
\mathcal{L}_{\text{class}}(\theta; I, p) &= \texttt{CrossEntropy}\big(f_\theta(I_i), p_i\big) = -\sum p_i \log\Big(\texttt{Softmax}\big(f_\theta(I_i)\big)\Big) \\
\mathcal{L}_{\text{L2}}(\theta) &= \sum_{W \in \theta} \|W\|_2^2
\end{aligned}$$

The model is trained for 10 epochs with a batch size of 100 and a learning rate of 0.1 via SGD. We report our results on varying λ_{L2} values below, taking the mean of 50 runs for each setting.

λ_{L2}	0	10^{-7}	10^{-6}	10^{-5}	10^{-4}	10^{-3}	10^{-2}
Acc. % (↑)	97.23	97.17	97.26	97.24	97.21	96.74	90.81

We conclude that L2 regularization is not necessary in this problem. While $\lambda_{\text{L2}} = 10^{-6}$ did give the best results, the improvements were marginal and could be attributed to stochasticity. Large λ_{L2} values were significantly detrimental to training. We attribute this to the low parameter count and the short training duration.

References

[1] Pierre Blanchard, Desmond J Higham, and Nicholas J Higham. "Accurately computing the log-sum-exp and softmax functions". In: *IMA Journal of Numerical Analysis* 41.4 (Aug. 2020), pp. 2311–2330.
[2] Yann LeCun. *The MNIST database of handwritten digits*. 1998.