

Deep learning

5.1. Cross-entropy loss

François Fleuret

<https://fleuret.org/dlc/>

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The usual form of a classification training set is

$$(x_n, y_n) \in \mathbb{R}^D \times \{1, \dots, C\}, \quad n = 1, \dots, N.$$

We can train on such a data-set with a regression loss such as the MSE using a “one-hot vector” encoding: that converts labels into a tensor $z \in \mathbb{R}^{N \times C}$, with

$$\forall n, z_{n,m} = \begin{cases} 1 & \text{if } m = y_n \\ 0 & \text{otherwise.} \end{cases}$$

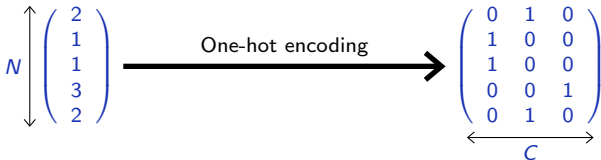
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For instance, with $N = 5$ and $C = 3$, we would have



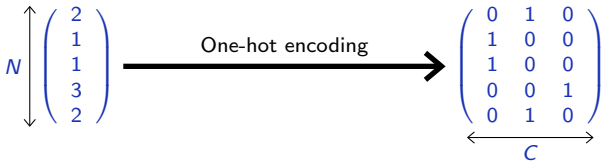
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Training matches the model's outputs with these binary values in a MSE sense.

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Consider this example with correct class 1, and two outputs \hat{y} and \hat{y}' .

$$\begin{array}{ccc} y & \hat{y} & \hat{y}' \\ (1 & 0 & 0) & (2 & -1 & -1) & (0 & 1 & 1) \end{array}$$

Both \hat{y} and \hat{y}' have a MSE of 1, even though the former leads to a perfect prediction and the latter to a perfectly wrong one.

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The criterion of choice for classification is the **cross-entropy**, which fixes these inconsistencies.

We can generalize the logistic regression to a multi-class setup with f_1, \dots, f_C functionals that we interpret as “logits”

$$P(Y = y | X = x, W = w) = \frac{1}{Z} \exp f_y(x; w) = \frac{\exp f_y(x; w)}{\sum_k \exp f_k(x; w)}$$

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from which

$$\begin{aligned} \log \mu_W(w | \mathcal{D} = \mathbf{d}) &= \log \frac{\mu_{\mathcal{D}}(\mathbf{d} | W = w) \mu_W(w)}{\mu_{\mathcal{D}}(\mathbf{d})} \\ &= \log \mu_{\mathcal{D}}(\mathbf{d} | W = w) + \log \mu_W(w) - \log Z \\ &= \sum_n \log \mu_{\mathcal{D}}(x_n, y_n | W = w) + \log \mu_W(w) - \log Z \\ &= \sum_n \log P(Y = y_n | X = x_n, W = w) + \log \mu_W(w) - \log Z' \\ &= \sum_n \log \left(\frac{\exp f_{y_n}(x; w)}{\sum_k \exp f_k(x; w)} \right) + \log \mu_W(w) - \log Z'. \end{aligned}$$

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If we ignore the penalty on w , it makes sense to minimize the average

$$\mathcal{L}(w) = -\frac{1}{N} \sum_{n=1}^N \log \left(\underbrace{\frac{\exp f_{y_n}(x_n; w)}{\sum_k \exp f_k(x_n; w)}}_{\hat{P}_w(Y=y_n|X=x_n)} \right).$$

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Given two distributions p and q , their **cross-entropy** is defined as

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So \mathcal{L} above is the average of the cross-entropy between the deterministic “true” posterior δ_{y_n} and the estimated $\hat{P}_w(Y = \cdot | X = x_n)$.

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```
>>> f = torch.tensor([[ -1., -3., 4.], [-3., 3., -1.]])
>>> target = torch.tensor([0, 1])
>>> criterion = torch.nn.CrossEntropyLoss()
>>> criterion(f, target)
tensor(2.5141)
```

and indeed

$$-\frac{1}{2} \left(\log \frac{e^{-1}}{e^{-1} + e^{-3} + e^4} + \log \frac{e^3}{e^{-3} + e^3 + e^{-1}} \right) \simeq 2.5141.$$

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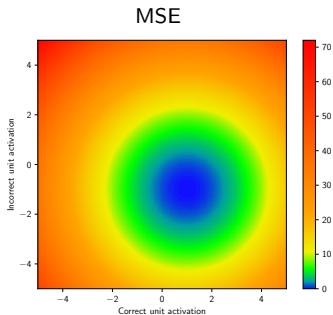
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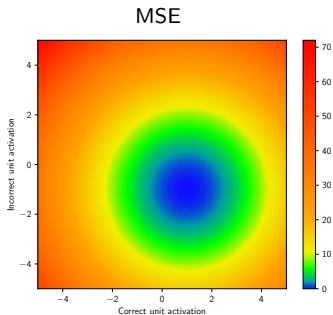
The range of values is 0 for perfectly classified samples, $\log(C)$ if the posterior is uniform, and up to $+\infty$ if the posterior distribution is “worse” than uniform.

Let's consider the loss for a single sample in a two-class problem, with a predictor with two output values.



$$\mathcal{L} = (x - 1)^2 + (y + 1)^2$$

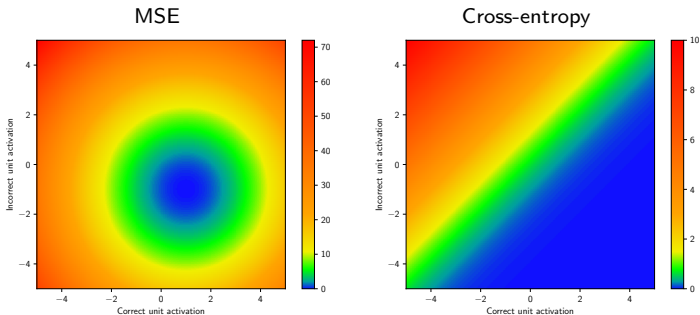
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$$\mathcal{L} = -\log\left(\frac{e^x}{e^x + e^y}\right)$$

MSE incorrectly penalizes outputs which are perfectly valid for prediction, contrary to cross-entropy.

The cross-entropy loss can be seen as the composition of a “log soft-max” to normalize the [logit] scores into logs of probabilities

$$(\alpha_1, \dots, \alpha_C) \mapsto \left(\log \frac{\exp \alpha_1}{\sum_k \exp \alpha_k}, \dots, \log \frac{\exp \alpha_C}{\sum_k \exp \alpha_k} \right),$$

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which can be done with the `torch.nn.LogSoftmax` module, and a read-out of the normalized score of the correct class

$$\mathcal{L}(w) = -\frac{1}{N} \sum_{n=1}^N f_{y_n}(x_n; w),$$

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>>> target = torch.tensor([0, 1])
>>> model = nn.LogSoftmax(dim = 1)
>>> criterion = torch.nn.NLLLoss()
>>> criterion(model(f), target)
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Hence, if a network should compute log-probabilities, it may have a `torch.nn.LogSoftmax` final layer, and be trained with `torch.nn.NLLLoss`.

The mapping

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```
>>> y = torch.tensor([[ -10., -10., 10., -5. ],
...                   [ 3., 0., 0., 0. ],
...                   [ 1., 2., 3., 4. ]])
>>> f = torch.nn.Softmax(1)
>>> f(y)
tensor([[ 2.0612e-09,  2.0612e-09,  1.0000e+00,  3.0590e-07],
        [ 8.7005e-01,  4.3317e-02,  4.3317e-02,  4.3317e-02],
        [ 3.2059e-02,  8.7144e-02,  2.3688e-01,  6.4391e-01]])
```

PyTorch provides many other criteria, among which

- `torch.nn.MSELoss`
- `torch.nn.CrossEntropyLoss`
- `torch.nn.NLLLoss`
- `torch.nn.L1Loss`
- `torch.nn.NLLLoss2d`
- `torch.nn.MultiMarginLoss`

The end