Deep learning

5.1. Cross-entropy loss

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The usual form of a classification training set is

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

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

$$N \updownarrow \begin{pmatrix} 2 \\ 1 \\ 1 \\ 3 \\ 2 \end{pmatrix} \xrightarrow{\text{One-hot encoding}} \underbrace{\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}}_{\longleftrightarrow \; C}$$

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This can be done with `F.one_hot`.

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

$$y \qquad\qquad \hat{y} \qquad\qquad \hat{y}'$$

$$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \qquad \begin{pmatrix} 2 & -1 & -1 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 1 \end{pmatrix}$$

Both $\hat{y}$ and $\hat{y}'$ have a MSE of 1, even though the $\hat{y}$ leads to a perfect prediction, and the $\hat{y}'$ 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**

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

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from which

$$\begin{aligned}
&\log \mu_W(w \mid \mathscr{D} = \mathbf{d}) \\
&\qquad = \log \frac{\mu_{\mathscr{D}}(\mathbf{d} \mid W = w)\, \mu_W(w)}{\mu_{\mathscr{D}}(\mathbf{d})} \\
&\qquad = \log \mu_{\mathscr{D}}(\mathbf{d} \mid W = w) + \log \mu_W(w) - \log Z \\
&\qquad = \sum_n \log \mu_{\mathscr{D}}(x_n, y_n \mid W = w) + \log \mu_W(w) - \log Z \\
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If we ignore the penalty on w, it makes sense to minimize the average

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

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

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

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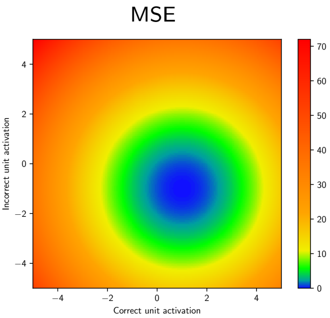
The range of values is 0 for perfectly classified samples, $\log(C)$ if the posterior is uniform, and up to $+\infty$ if the posterior distribution is "worse" than uniform.

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



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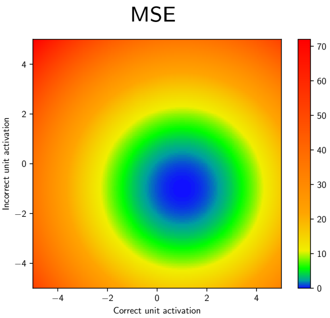

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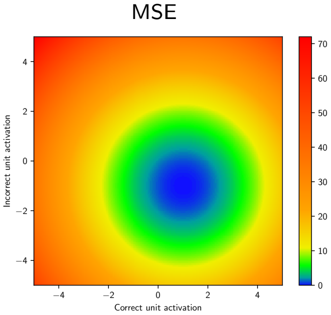

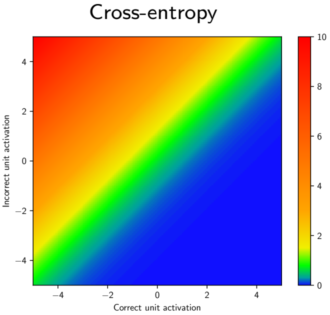

$$\mathscr{L} = (x-1)^2 + (y+1)^2$$

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

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

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

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>>> target = torch.tensor([0, 1])
>>> model = nn.LogSoftmax(dim = 1)
>>> criterion = torch.nn.NLLLoss()
>>> criterion(model(f), target)
tensor(2.5141)
```

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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is called soft-max since it computes a "soft arg-max Boolean label."

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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