Multi-Layer Perceptrons and Deep Learning

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Outline

Features and layers

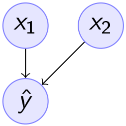
Algorithms

- Random projection
- Back propagation
- Derivatives
- Cost functions

Python libraries

- sklearn
- PyTorch
- TensorFlow

Perceptron vs linear regression



- Network output

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

- Chain rule

$$\nabla_\beta L = \nabla_{\hat{y}} L \nabla_\beta \hat{y}$$

- Network gradient

$$\nabla_\beta \hat{y} = (x_1, x_2)$$

Cost functions

The only difference are the cost functions

- Perceptron

$$L = -\mathbb{I}\{y \neq \hat{y}\}\, \hat{y}$$

with

$$\nabla L = -\mathbb{I}\{y \neq \hat{y}\}\, yx$$

- Linear regression

$$L = (\hat{y} - y)^2,$$

with

$$\nabla_{\hat{y}} L = 2(\hat{y} - y).$$

Layering and features

Fixed layers

- Input to layer $x \in R^n$
- Output from layer $\hat{\boldsymbol{y}} \in R^m$.

Intermediate layers

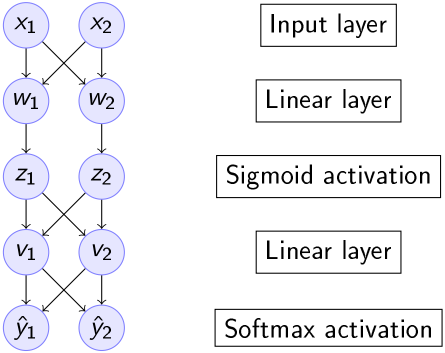
- Linear layer
- Non-linear activation function.

Linear layers types

- Dense
- Sparse
- Convolutional

Activation funnction

- Sigmoid
- Softmax



Linear layers

Example: Linear regression with n inputs, m outputs.

- Input: Features $\boldsymbol{x} \in \mathbb{R}^n$
- Dense linear layer with $\boldsymbol{B} \in \mathbb{R}^{m \times n}$
- Output: $\hat{\boldsymbol{y}} \in \mathbb{R}^m$

Dense linear layer

- Parameters $\boldsymbol{B} = \begin{pmatrix} \boldsymbol{\beta}_1 \\ \vdots \\ \boldsymbol{\beta}_m \end{pmatrix}$,
- $\boldsymbol{\beta}_i = [\beta_{i,1}, \ldots, \beta_{i,n}]$, $\boldsymbol{\beta}_i$ connects the i-th output y_i to the features $\boldsymbol{x}$:
$$y_i = \boldsymbol{\beta}_i \boldsymbol{x}$$
- In compact form:
$$\boldsymbol{y} = \boldsymbol{B}\boldsymbol{x}$$

ReLU layers

- Typically used in the hidden layers of neural networks

$$f(x) = \max(0, x)$$

Derivative

$$df/dxf(x) = \mathbb{I}\{x > 0\}$$

Sigmoid activation

Example: Logistic regression

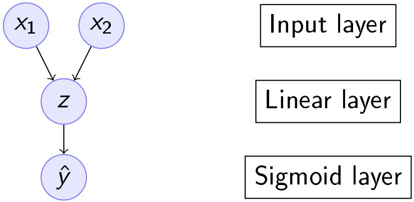
- Input $\boldsymbol{x} \in \mathbb{R}^n$
- Intermediate output: $z \in \mathbb{R}$,

$$z = \sum_{i=1}^{n} \beta_i x_i.$$

- Output: sigmoid activation $\hat{y} \in [0, 1]$.

$$f(z) = 1/[1 + \exp(-z)].$$

Now we can interpret $\hat{y} = P_\beta(y = 1|x)$.



Loss function: negative log likelihood

$$\ell(\hat{y}, y) = -[\mathbb{I}\{y = 1\} \ln(\hat{y}) + \mathbb{I}\{y = -1\} \ln(1 - \hat{y})]$$

Softmax layer

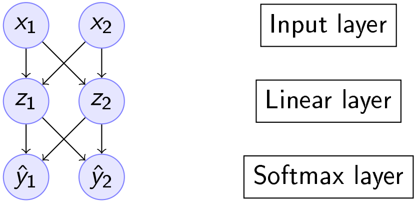
Example: Multivariate logistic regression with m classes.

- Input: Features $\boldsymbol{x} \in \mathbb{R}^n$
- Fully-connected linear activation layer

$$\boldsymbol{z} = \boldsymbol{B}\boldsymbol{x}, \qquad \boldsymbol{B} \in \mathbb{R}^{m \times n}.$$

- Softmax output

$$\hat{y}_i = \frac{\exp(z_i)}{\sum_{j=1^m} \exp(z_j)}$$



We can also interpret this as

$$\hat{y}_i \triangleq \mathbb{P}(y = i \mid \boldsymbol{x})$$

with usual loss $\ell(\hat{y}, y) = -\ln \hat{y}_y$

Features and layers

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Random projections

- Features x
- Hidden layer activation z
- Output y

Hidden layer: Random projection

Here we project the input into a high-dimensional space

$$z_i = \mathrm{sgn}(\boldsymbol{\beta}_i^\top x) = y_i$$

where $\boldsymbol{B} = [\boldsymbol{\beta}_i]_{i=1}^m$, $\beta_{i,j} \sim \mathrm{Normal}(0, 1)$

The reason for random projections

- The high dimension makes it easier to learn.
- The randomness ensures we are not learning something spurious.

Background on back-propagation

The problem

- We need to minimise a loss function L
- We need to calculate

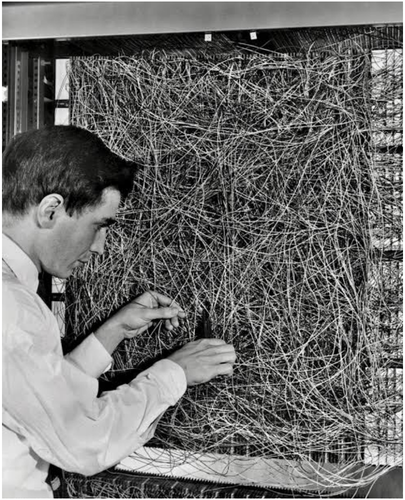
$$\nabla_{\boldsymbol{\beta}} \mathbb{E}_{\boldsymbol{\beta}}[L] \approx \frac{1}{T} \sum_{t=1}^{T} \nabla_{\boldsymbol{\beta}} \ell(x_t, y_t, \boldsymbol{\beta}).$$

- However $\ell(x_t, y_t, \boldsymbol{\beta})$ is a complex non-linear function of $\boldsymbol{\beta}$.
- We need many steps to calculate ℓ. How can we then do it?

The chain rule of differentiation

[1673] Liebniz

Chain rule applied to the perceptron



[1976] Rosenblat

Chain rule for deep neural netowrks

[1982] Werbos

Backpropagation given a name

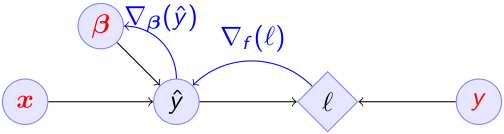
1986: Learning representations by back-propagating errors.

Rumelhart

Hinton

Williams

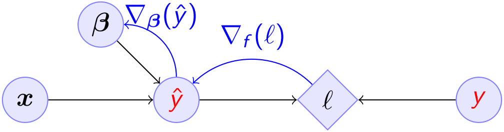
Elementary back-propagation: linear regression



- $f : X \to Y$, $\ell : Y \times Y \to \mathbb{R}$, chain rule: $\nabla_{\beta}\ell = \nabla_{\beta} f \nabla_{\hat{y}}\ell$
- Forward: follow the arrows to calculate variables

$$\hat{y} \triangleq f(\beta, x) = \sum_{i=1}^{n} \beta_i x_i, \qquad \ell(\hat{y}, y) = (\hat{y} - y)^2$$

Elementary back-propagation: linear regression



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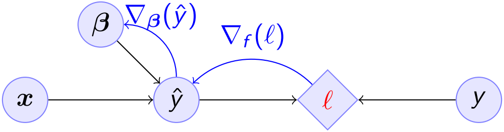

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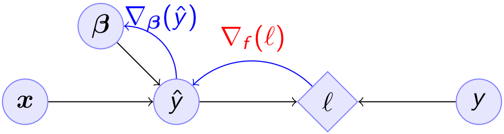

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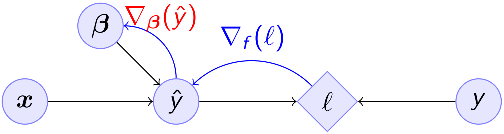
- Backward: return to calculate the gradients

$$\begin{aligned} \nabla_{\boldsymbol{\beta}} \ell(\hat{y}, y) &= \nabla_{\boldsymbol{\beta}} f(\boldsymbol{\beta}, \boldsymbol{x}) \times \nabla_{\hat{y}} \ell(\hat{y}, y) && (1) \\ &= \nabla_{\boldsymbol{\beta}} f(\boldsymbol{\beta}, \boldsymbol{x}) \times 2[\hat{y} - y] && (2) \end{aligned}$$

Elementary back-propagation: linear regression



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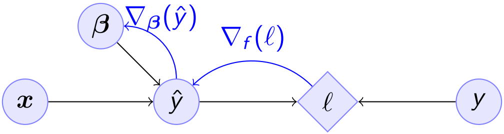
Elementary back-propagation: linear regression



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$$= \nabla_{\beta} f(\beta, x) \times 2[\hat{y} - y] \tag{2}$$

- Update:

$$\beta_{t+1} = \beta_t - \alpha_t \times \nabla_{\beta} \ell(\hat{y}_t, y_t)$$

Gradient descent with *back-propagation*

- Dataset D, cost function $L = \sum_t \ell_t$
- Parameters $\boldsymbol{B}_1, \ldots, \boldsymbol{B}_k$ with k layers
- Intermediate variables: $\boldsymbol{z}_j = h_j(\boldsymbol{z}_{j-1}, \boldsymbol{B}_j)$, $\boldsymbol{z}_0 = \boldsymbol{x}$, $\boldsymbol{z}_k = \hat{\boldsymbol{y}}$.

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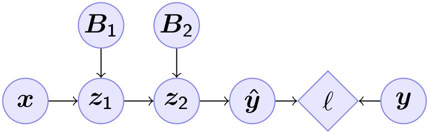
Dependency graph



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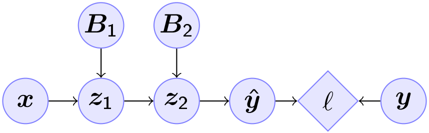


Backpropagation with steepest stochastic gradient descent

- Forward step: For $j = 1, \ldots, k$, calculate $\boldsymbol{z}_j = h_j(k)$ and $\ell(\hat{\boldsymbol{y}}, \boldsymbol{y})$
- Backward step: Calculate $\nabla_{\hat{\boldsymbol{y}}} \ell$ and $d_j \triangleq \nabla_{\boldsymbol{B}_j} \ell = \nabla_{\boldsymbol{B}_j} z_j d_{j+1}$ for $j = k \ldots, 1$
- Apply gradient: $\boldsymbol{B}_j -= \alpha d_j$.

Other algorithms and gradients

Natural gradient

Defined for probabilistic models

ADAM

Exponential moving average of gradient and square gradients

BFGS: Broyden–Fletcher–Goldfarb–Shanno algorithm

Newton-like method

Linear layer

Definition

This is a linear combination of inputs $x \in \mathbb{R}^n$ and parameter matrix $\boldsymbol{B} \in \mathbb{R}^{m \times n}$

$$\text{where } \boldsymbol{B} = \begin{bmatrix} \boldsymbol{\beta}_1 \\ \vdots \\ \boldsymbol{\beta}_i \\ \vdots \\ \boldsymbol{\beta}_m \end{bmatrix} = \begin{bmatrix} \beta_{1,1} & \cdots & \beta_{1,j} & \cdots & \beta_{1,m} \\ \vdots & \ddots & \vdots & \ddots & \cdots \\ \beta_{i,1} & \cdots & \beta_{i,j} & \cdots & \beta_{i,m} \\ \vdots & \ddots & \ddots & \ddots & \cdots \\ \beta_{n,1} & \cdots & \beta_{i,j} & \cdots & \beta_{n,m} \end{bmatrix}$$

$$f(\boldsymbol{B}, \boldsymbol{x}) = \boldsymbol{B}\boldsymbol{x} \qquad f_i(\boldsymbol{B}, \boldsymbol{x}) = \boldsymbol{\beta}_i \cdot \boldsymbol{x} = \sum_{j=1}^{n} \beta_{i,j} x_j,$$

Gradient

Each partial derivative is simple:

$$\frac{\partial}{\partial \beta_{i,j}} f_k(\boldsymbol{B}, \boldsymbol{x}) = \sum_{k=1}^{n} \frac{\partial}{\partial \beta_{i,j}} \beta_{i,k} x_k = x_j$$

Sigmoid layer

- This layer is used for binary classification.
- It is used in the logistic regression model to obtain label probabilities.

$$f(z) = 1/(1 + \exp(-z))$$

Derivative

So let us ignore the other inputs for simplicity:

$$\frac{d}{dz} f(z) = \exp(-z)/[1 + \exp(-z)]^2$$

Softmax layer

- This layer is used for multi-class classification

$$y_i(\boldsymbol{z}) = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

Derivative

$$\frac{\partial}{\partial z_i} y_i(\boldsymbol{z}) = \frac{e^{z_i} e^{\sum_{j \neq i} z_j}}{\left(\sum_j e^{z_j}\right)^2}$$

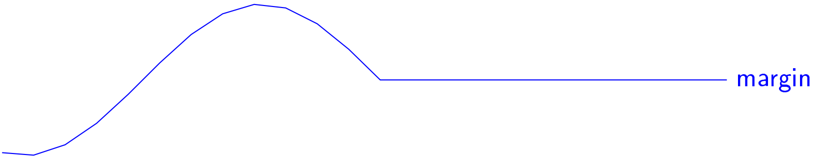
$$\frac{\partial}{\partial z_i} y_k(\boldsymbol{z}) = \frac{e^{z_i + z_k}}{\left(\sum_j e^{z_j}\right)^2}$$

Classification cost functions

Error margin

If z is a confidence level for the positive class then

$$\ell(z, y) = -\mathbb{I}\left\{zy < 0\right\} zy$$



Negative log likelihood (aka cross-entropy)

If z are label probabilities, then

$$\ell(z, y) = -\ln z_y.$$

Regression cost functions

Squared error

If z is a prediction for the dependent variable then

$$\ell(z, y) = (y - z)^2$$

This also corresponds to negative log likelihood under a Gaussianity assumption.

Huber loss

If z is a prediction, then

$$\ell(z, y) = \begin{cases} \frac{1}{2}(z - y)^2 & |z - y| \leq \delta \\ \delta(|z - y| - \frac{1}{2}\delta) & \text{otherwise.} \end{cases} \tag{3}$$

sklearn neural networks

Classification

Uses the cross entropy cost

```
from sklearn.neural_network import MLPClassifier
clf = MLPClassifier(hidden_layer_sizes=(5, 2))
clf.fit(X, y)
clf.predict(X_test)
```

- Main condition is layer sizes.

Regression

```
from sklearn.neural_network import MLPRegressor
model = MLPRegressor(hidden_layer_sizes=(5, 2))
```

Datasets

```
X_train = torch.tensor(X_train, dtype=torch.float32)
train_dataset = TensorDataset(X_train, y_train)
train_loader = DataLoader(train_dataset, batch_size=16, shuffle=True
mlp = nn.Sequential(nn.Linear(input_size , 50), nn.ReLU())
```

TensorFlow

This is another library, no need to use this for this course