S&DS 365 / 565
Intermediate Machine Learning

Neural Networks for Classification

February 9 and 14

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Reminders

- Assignment 1 will be posted later today
- Quiz 1 will be Wednesday, Feb 16; material up to Feb 14
- Check Canvas/EdD for office hours

Today: RKHS and overview of neural nets

- Discussion of RKHS concepts
- Basic architecture of feedforward neural nets
- Backpropagation
- Examples from TensorFlow
- We’ll assume some familiarity with these ideas

Recall: Logistic Regression

Form of conditional probability model:

$$\log\left(\frac{P(y=1\,|\,x)}{P(y=0\,|\,x)}\right) = \beta^T x + \beta_0$$

Equivalently:

$$P(Y=1\,|\,x) \propto e^{\beta^T x + \beta_0}$$

Recall: Logistic Regression

In the multi-class case we have

$$P(Y = k \mid x) \propto e^{\beta_k^T x + \beta_{k0}}, \quad k = 1, \ldots, K-1$$

We can write this in ML terminology as

$$\text{Softmax}\left(\left\{\beta_k^T x + \beta_{k0}\right\}\right)$$

Note: Can also use β_k for $k = \underline{0}, \ldots, K-1$. This will be "overparameterized"

Logistic Regression

What if x is an image, represented as pixels? It might be hard to get an accurate classifier.

Want to learn *feature representation* $\phi(x)$.

The model becomes

$$P(Y = k \mid x) \propto e^{\beta_k^T \phi(x) + \beta_{k0}}, \quad k = 0, 1, \ldots, K - 1$$

The parameters of ϕ and the parameters β need to be learned/trained.

Starting with regression

For linear regression, our loss function for an example (x, y) is

$$\begin{aligned}\mathcal{L} &= \frac{1}{2}(y - \beta^T x - \beta_0)^2 \\ &= \frac{1}{2}(y - f)^2\end{aligned}$$

where $f = \beta^T x + \beta_0$.

Adding a layer

Loss is

$$\mathcal{L} = \frac{1}{2}(y - f)^2$$

where now $f = \beta^T h + \beta_0$ where $h = Wx + b$.

This can be viewed graphically.

Equivalent to linear model

But this is just a linear model

$$f = \widetilde{\beta}^T x + \widetilde{\beta}_0$$

We get a reparameterization of a linear model; nothing new.

Need to add *nonlinearities*

Nonlinearities

Add nonlinearity

$$h = \phi(Wx + b)$$

applied component-wise.

For regression, the last layer is just linear:

$$f = \beta^T h + \beta_0$$

Nonlinearities

Commonly used nonlinearities:

$$\phi(u) = \tanh(u) = \frac{e^u - e^{-u}}{e^u + e^{-u}}$$

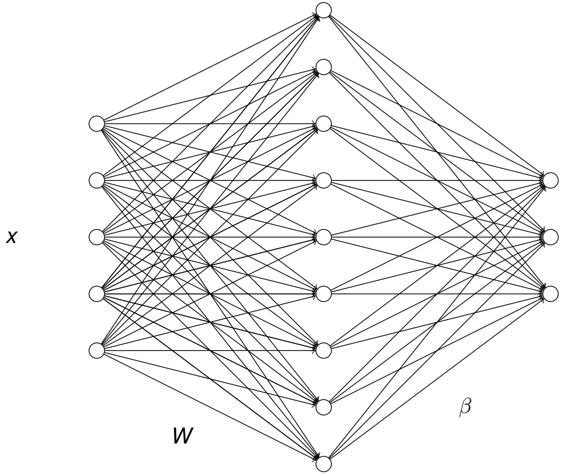
$$\phi(u) = \text{sigmoid}(u) = \frac{e^u}{1 + e^u}$$

$$\phi(u) = \text{relu}(u) = \max(u, 0)$$

Nonlinearities

So, a neural network is nothing more than a parametric regression model with a restricted type of nonlinearity

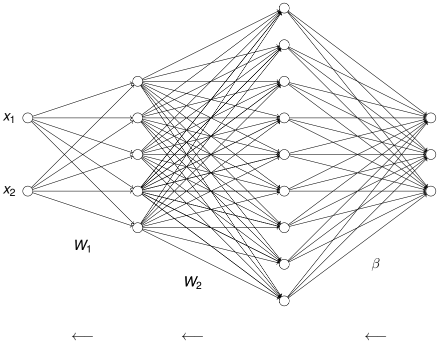
Two-layer dense network



Training

- The parameters are trained by stochastic gradient descent.
- To calculate derivatives we just use the chain rule, working our way backwards from the last layer to the first.

High level idea



Start at last layer, send error information back to previous layers

Start simple

Loss is

$$\mathcal{L} = \frac{1}{2}(y - f)^2$$

The change in loss due to making a small change in output f is

$$\frac{\partial \mathcal{L}}{\partial f} = (f - y)$$

We now send this backward through the network

Example

So if $f = Wx + b$ then

$$\frac{\partial \mathcal{L}}{\partial W} = \frac{\partial \mathcal{L}}{\partial f}\, x^T$$

$$= (f - y)\, x^T$$

Example

So if $f = Wx + b$ then

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial f}$$
$$= (f - y)$$

Two layers

Now add a layer:

$$f = W_2 h + b_2$$
$$h = W_1 x + b_1$$

Then we have

$$\frac{\partial \mathcal{L}}{\partial W_2} = \frac{\partial \mathcal{L}}{\partial f}\; h^T$$
$$= (f - y)\; h^T$$

$$\frac{\partial \mathcal{L}}{\partial h} = W_2^T\; \frac{\partial \mathcal{L}}{\partial f}$$
$$= W_2^T\; (f - y)$$

Two layers

Now send this back (backpropagate) to the first layer:

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial W_1} &= \frac{\partial \mathcal{L}}{\partial h}\, x^T \\
&= W_2^T\, \frac{\partial \mathcal{L}}{\partial f}\, x^T \\
&= W_2^T\, (f - y)\, x^T
\end{aligned}
$$

Adding a nonlinearity

Remember, this just gives a linear model! Need a nonlinearity:

$$h = \varphi(W_1 x + b_1)$$

$$f = W_1 h + b_2$$

Adding a nonlinearity

If $\varphi(u) = ReLU(u) = \max(u, 0)$ then this just becomes

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial W_1} &= \mathbb{1}(h > 0)\, \frac{\partial \mathcal{L}}{\partial h}\, x^T \\ &= \mathbb{1}(h > 0)\, W_2^T\, \frac{\partial \mathcal{L}}{\partial f}\, x^T \\ &= \mathbb{1}(h > 0)\, W_2^T\, (f - y)\, x^T\end{aligned}$$

where

$$\mathbb{1}(u) = \begin{cases} 1 & u > 0 \\ 0 & \text{otherwise} \end{cases}$$

See notes on backpropagation for details

Classification

For classification we use softmax to compute probabilities

$$(p_1, p_2, p_3) = \frac{1}{e^{f_1} + e^{f_2} + e^{f_3}} \left(e^{f_1}, e^{f_2}, e^{f_3} \right)$$

The loss function is

$$\mathcal{L} = -\log P(y \mid x) = \log \left(e^{f_1} + e^{f_2} + e^{f_3} \right) - f_y$$

So, we have

$$\frac{\partial \mathcal{L}}{\partial f_k} = p_k - \mathbb{1}(y = k)$$

Interactive examples

`https://playground.tensorflow.org/`

Neural tangent kernel

There is a kernel view of neural networks that has been useful in understanding the dynamics of stochastic gradient descent for neural networks.

This is based on something called the *neural tangent kernel (NTK)*

Parameterized functions

Suppose we have a parameterized function $f_\theta(x) \equiv f(x;\theta)$

Almost all machine learning takes this form — for classification and regression, these give us estimates of the regression function

For neural nets, the parameters θ are all of the weight matrices and bias (intercept) vectors across the layers.

Feature maps

Suppose we have a parameterized function $f_\theta(x) \equiv f(x;\theta)$

We then define a *feature map*

$$x \mapsto \varphi(x) = \nabla_\theta f(x;\theta) = \begin{pmatrix} \frac{\partial f(x;\theta)}{\partial \theta_1} \\ \frac{\partial f(x;\theta)}{\partial \theta_2} \\ \vdots \\ \frac{\partial f(x;\theta)}{\partial \theta_p} \end{pmatrix}$$

This defines a Mercer kernel

$$K(x,x') = \varphi(x)^T \varphi(x') = \nabla_\theta f(x;\theta)^T \nabla_\theta f(x';\theta)$$

NTK and SGD

- The NTK has been used to study the dynamics of stochastic gradient descent
- Upshot: As the number of neurons in the layers grows, the parameters in the network barely change during training, even though the training error quickly decreases to zero
- We'll discuss this further next week

Summary

- Neural nets are trained using stochastic gradient descent
- Implemented using backpropagation
- Can be automated to train complex networks (with no math!)