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:

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

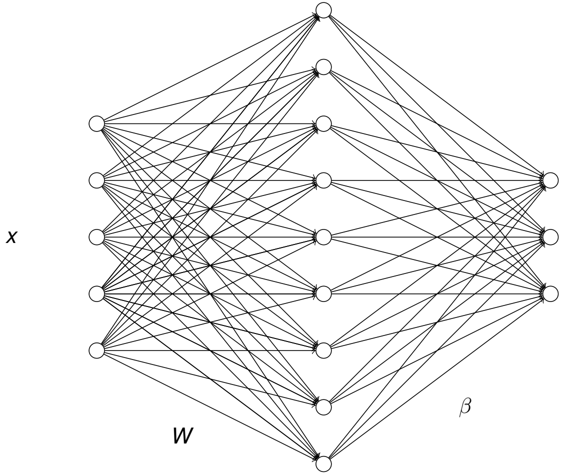
$$\phi(u) = \text{sigmoid}(u) = \frac{e^u}{1 + e^u}$$

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

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.

Training

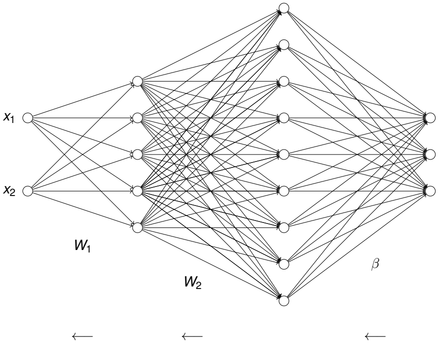
- For the last layer, $\mathcal{L} = \frac{1}{2}(y - f)^2$ and

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

- Next, we compute

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \beta} &= \frac{\partial \mathcal{L}}{\partial f}\frac{\partial f}{\partial \beta} \\
&= -(y - f)\frac{\partial f}{\partial \beta} \\
&= -(y - f)h
\end{aligned}$$

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

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial W} &= \frac{\partial \mathcal{L}}{\partial f}\; x^T \\ &= (f - y)\; x^T \end{aligned}$$

Example

So if $f = Wx + b$ then

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial b} &= \frac{\partial \mathcal{L}}{\partial f} \\ &= (f - y)\end{aligned}$$

Two layers

Now add a layer:

$$
\begin{aligned}
f &= W_2 h + b_2 \\
h &= W_1 x + b_1
\end{aligned}
$$

Then we have

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

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

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!)