S&DS 365 / 565

Intermediate Machine Learning

Kernels and Neural Networks

September 18

Reminders

- Assignment 1 out; due September 27 (week from this Wed)
- Quiz 2 posted Wednesday, material up to today
- Check Canvas/EdD for office hours—please join us!

Today: Kernels and Neural nets

1. Recap/discussion of RKHS concepts
2. Basic architecture of feedforward neural nets
3. Backpropagation
4. Examples: TensorFlow
5. Next time: NTK and double descent

1: Mercer kernel recap

Summary from last time

- Smoothing methods compute local averages, weighting points by a kernel. The details of the kernel don't matter much
- Mercer kernels using penalization rather than smoothing
- Defining property: Matrix $\mathbb{K}$ is always positive semidefinite
- Equivalent to a type of ridge regression in function space
- The curse of dimensionality limits use of both approaches

Mercer Kernels: The big picture

Instead of using local smoothing, we can optimize the fit to the data subject to regularization (penalization). Choose $\widehat{m}$ to minimize

$$\sum_i (Y_i - \widehat{m}(X_i))^2 + \lambda \, \text{penalty}(\widehat{\text{m}})$$

where penalty($\widehat{\text{m}}$) is a *roughness penalty*.

λ is a parameter that controls the amount of smoothing.

How do we construct a penalty that measures roughness? One approach is: *Mercer Kernels* and *RKHS = Reproducing Kernel Hilbert Spaces.*

What is a Mercer Kernel?

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A Mercer kernel has a special property: For any set of points $x_1, \ldots, x_n$ the $n \times n$ matrix

$$\mathbb{K} = \left[K(x_i, x_j)\right]$$

is positive semidefinite (no negative eigenvalues)

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This property has many important (and beautiful!) mathematical consequences. It is a characterization of Mercer kernels.

Mercer Kernels: Key example

A Gaussian gives us a Mercer kernel:

$$K(x, x') = e^{-\frac{\|x-x'\|^2}{2h^2}}$$

Note: Here we fix the bandwidth *h*.

Basis functions

We can create a set of *basis functions* based on K.

Fix z and think of $K(z, x)$ as a function of x. That is,

$$K(z, x) = K_z(x)$$

is a function of the second argument, with the first argument fixed.

Defining an inner product (geometry)

Because of the positive semidefinite property, we can create an *inner product* and *norm* over the span of these functions

If $f(x) = \sum_r \alpha_r K_{z_r}(x)$, $g(x) = \sum_s \beta_s K_{y_s}(x)$, the inner product is

$$\begin{aligned}\langle f, g\rangle_K &= \sum_r \sum_s \alpha_r \beta_s K(z_r, y_s) \\ &= \alpha^T \mathbb{K} \beta\end{aligned}$$

where $\mathbb{K} = [K(z_r, y_s)]$

Defining an inner product (geometry)

Because of the positive semidefinite property, we can create an *inner product* and *norm* over the span of these functions

The norm is

$$\|f\|_K^2 = \langle f, f \rangle_K = \sum_r \sum_s \alpha_r \alpha_s K(z_r, z_s)$$
$$= \alpha^T \mathbb{K} \alpha \geq 0$$

In fact $\|f\|_K = 0$ *if and only if* $f = 0$ (see notes)

Assignment 1 will solidify your understanding of Mercer kernels and kernel ridge regression!

Reducing to finite dimensions

Representer Theorem

Let $\widehat{m}$ minimize

$$J(m) = \sum_{i=1}^{n} (Y_i - m(X_i))^2 + \lambda \|m\|_K^2.$$

Then

$$\widehat{m}(x) = \sum_{i=1}^{n} \alpha_i K(X_i, x)$$

for some $\alpha_1, \ldots, \alpha_n$.

So, we only need to find the coefficients

$$\alpha = (\alpha_1, \ldots, \alpha_n).$$

Gradient descent

The gradient descent updates to α are

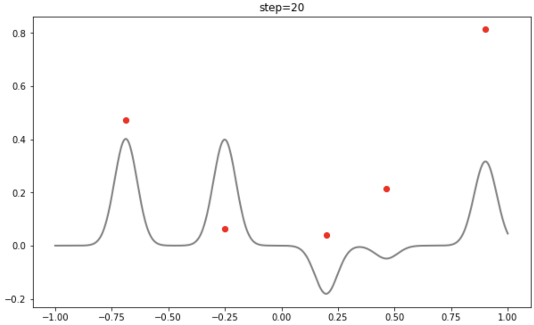
$$\alpha \longleftarrow \alpha + \eta \left(\mathbb{K}(y - \mathbb{K}\alpha) - \lambda \mathbb{K}\alpha \right)$$

where $\mathbb{K}$ is the $n \times n$ Gram matrix and $\eta > 0$ is a step size.

Demo

```
    if step % 10 == 0:
        plot_function_and_data(x, f, X, y, t=step, sleeptime=.5)
    alpha = alpha + stepsize * (K.T @ (y - K @ alpha) - lam * K
```

[6] 6.4s



2: Neural net basics

Recall :-)

What does “Intermediate” imply?

- A second course in machine learning
- Assume familiar with things like PCA, bias/variance, maximum likelihood, basics of neural nets
- Have experimented with basic ML methods on some data sets
- Previous exposure to Python
- More on this later...

4

Starting with regression

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

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

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

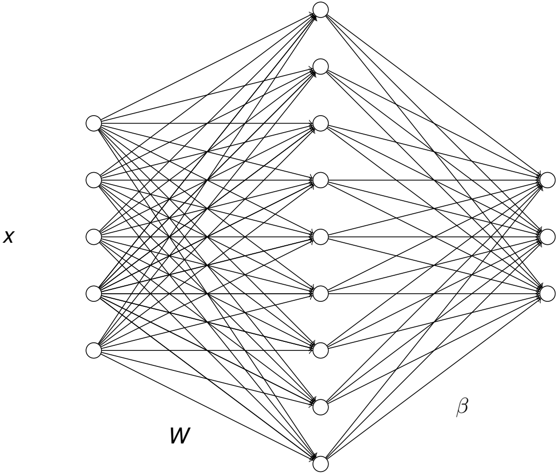
Adding a layer

Loss is

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

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

This can be viewed graphically.


x
W
β

Equivalent to linear model

But this is just another linear model

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

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

Need to add *nonlinearities*

Nonlinearities

Add nonlinearity

$$h(x) = \varphi(Wx + b)$$

applied component-wise.

For regression, the last layer is just linear:

$$f(x) = \beta^T h(x) + \beta_0$$

Nonlinearities

Commonly used nonlinearities:

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

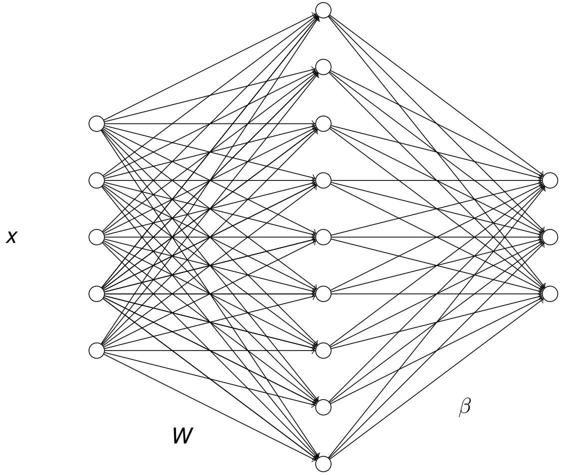
$$\varphi(u) = \text{sigmoid}(u) = \frac{e^u}{1 + e^u}$$

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

Nonlinearities

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

Two-layer dense network (multi-layer perceptron)

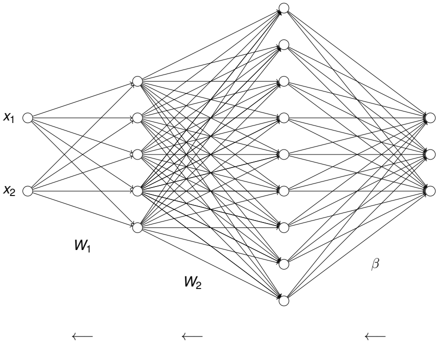


3: Backprop

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

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

Example

So if $f = Wx + b$ then

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

Two layers

Now add a layer:

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

Then we have

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

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

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

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

4: Demos

Interactive examples

https://playground.tensorflow.org/

What's going on?

- These models are curiously robust to overfitting
- Why is this?
- Some insight: Kernels and double descent

Next time!

Summary

- Neural nets are layered linear models with nonlinearities added
- Trained using stochastic gradient descent with backprop
- Can be automated to train complex networks (with no math!)