S&DS 365 / 565

**Intermediate Machine Learning**

# Kernels and Neural Networks

September 16

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# Reminders

- Assignment 1 out; due September 25 (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*.

$\lambda$ 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?

A kernel is a bivariate function $K(x, x')$. We think of this as a measure of "similarity" between points $x$ and $x'$.

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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 $f(x) = \sum_i \alpha_i K_{x_i}(x)$, $g(x) = \sum_i \beta_i K_{x_i}(x)$, the inner product is

$$\begin{aligned} \langle f, g \rangle_K &= \sum_i \sum_j \alpha_i \beta_j K(x_i, x_j) \\ &= \alpha^T \mathbb{K} \beta \end{aligned}$$

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

# 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

$$\|f\|_K^2 = \langle f, f \rangle_K = \sum_i \sum_j \alpha_i \alpha_j K(x_i, x_j)$$
$$= \alpha^T \mathbb{K} \alpha \geq 0$$

*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 $\alpha$ are

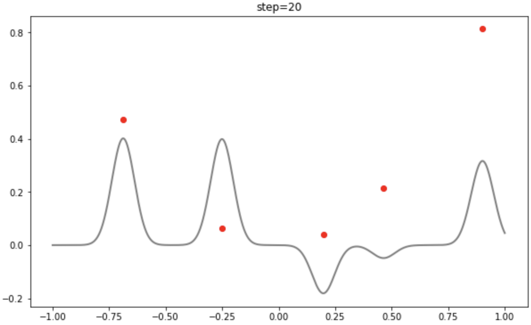
$$\alpha \longleftarrow \alpha + \eta\,(\mathbb{K}(y - \mathbb{K}\alpha) - \lambda\mathbb{K}\alpha)$$

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...

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

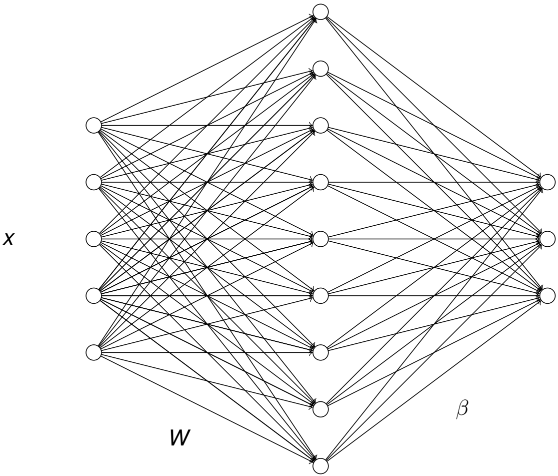
# Adding a layer

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:

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

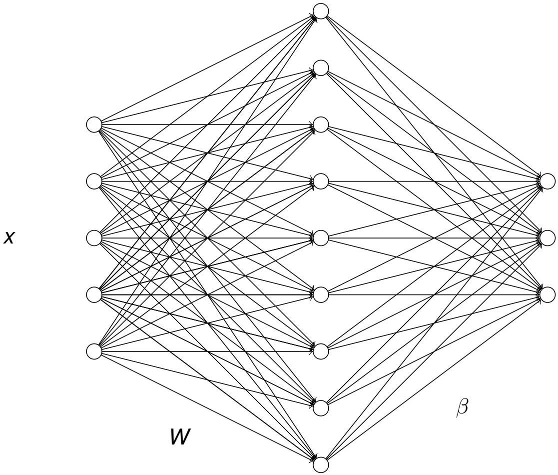
$$\varphi(u) = \text{sigmoid}(u) = \frac{e^u}{1 + e^u}$$

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

# 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)

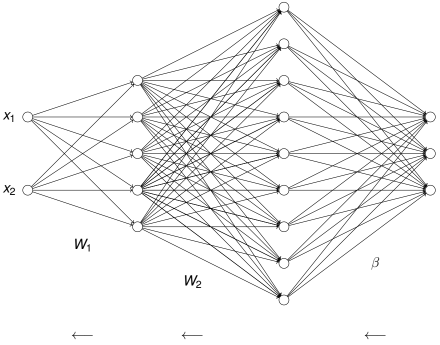


# 3: Backprop

# 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

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

# 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:

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

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

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

# 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!)