S&DS 365 / 565

Intermediate Machine Learning

Kernels and Neural Networks

September 19

Yale

Reminders

- Assignment 1 out; due September 28 (week from this Wed)
- Quiz 2 posted Wednesday, material up to today
- Check Canvas/EdD for office hours—please join us!

Today: Neural nets

1. Recap/discussion of RKHS concepts
2. Basic architecture of feedforward neural nets
3. Backpropagation
4. Examples: np-complete and TensorFlow
5. 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?

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 a norm from the kernel

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 a norm from the kernel

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

The norm is

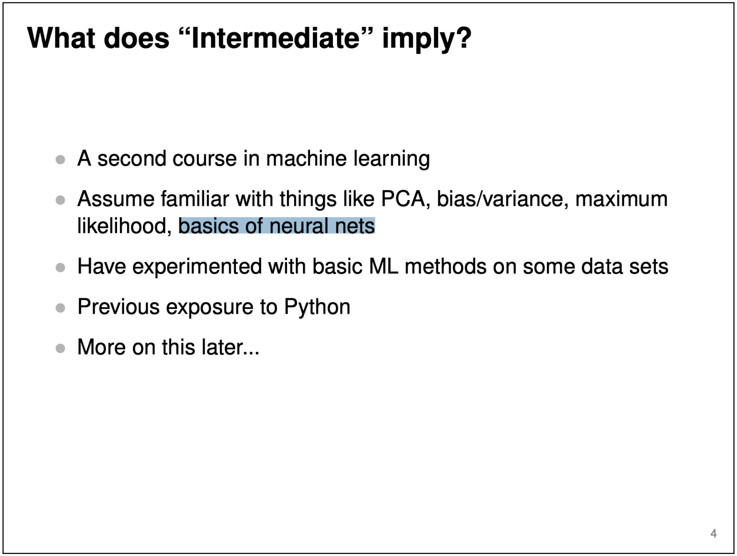
$$\begin{aligned}\|f\|_K^2 = \langle f, f\rangle_K &= \sum_r \sum_s \alpha_r \alpha_s K(z_r, z_s) \\ &= \alpha^T \mathbb{K} \alpha \geq 0\end{aligned}$$

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!

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

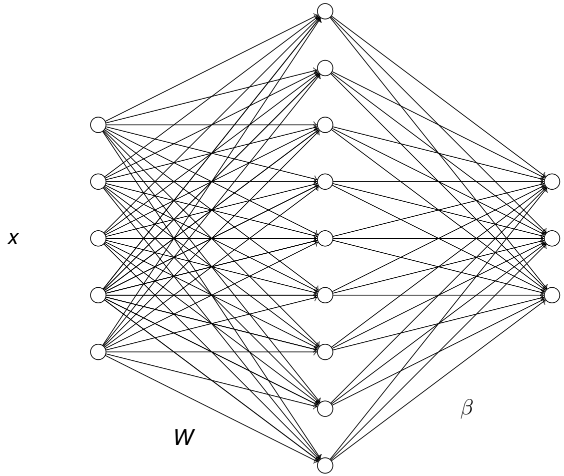
Adding a layer

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:

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

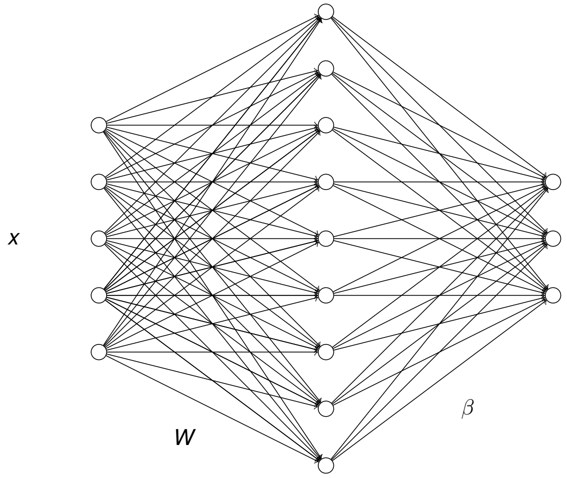
$$\varphi(u) = \text{sigmoid}(u) = \frac{e^u}{1 + e^u}$$

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

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)

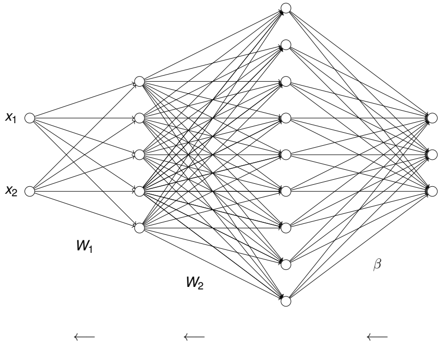


3: Backprop

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

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

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

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

4: Demos

Demos

https://colab.research.google.com/github/YData123/sds265-fa21/blob/master/demos/neural-nets/neural-nets-regress.ipynb

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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

5: Kernels and double descent

Double descent

We'll go over notes on the double descent phenomenon on the board, which will allow you to complete Problem 4 on the first assignment.

`https://github.com/YData123/sds365-fa22/raw/main/notes/double-descent.pdf`

OLS and minimal norm solution

OLS: $p < n$

$$\widehat{\beta} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T Y$$

Minimal norm solution: $p > n$:

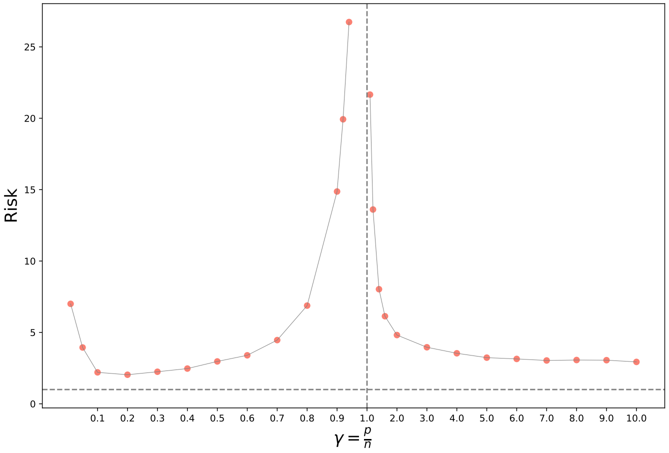
$$\widehat{\beta}_{\mathrm{mn}} = \mathbb{X}^T(\mathbb{X}\mathbb{X}^T)^{-1} Y$$

“Ridgeless regression”

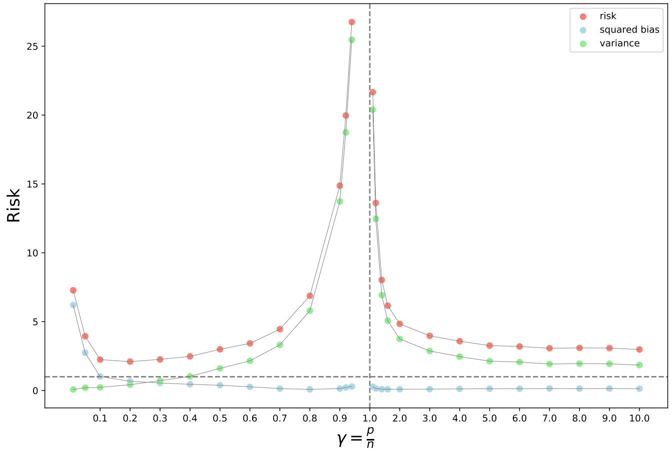
As λ decreases to zero, the ridge regression estimate:

- Converges to OLS in the “classical regime” $\gamma < 1$
- Converges to $\widehat{\beta}_{\text{mn}}$ in “overparameterized regime” $\gamma < 1$

Double descent



Double descent



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

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

Feature maps

This defines a Mercer kernel

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

What is the NTK for the random features model?

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

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!)
- Key to understanding risk properties: Double descent
- Kernel connection: NTK