Class 9: Neural Networks & Deep Learning

MSA 8150: Machine Learning for Analytics

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Introduction

Topics that Will be Covered Today

- Brief overview of linear algebra and matrix notation
- Matrix notation for linear models, especially multi-output models
- Structure of the brain
- Neural network models in matrix form
- Gradient descent technique for minimization
- NN fitting objetive and (stochastic) gradient descent
- Introduction to signal processing and linear filtering
- Equipping NNs with convolutional layers
- Other variants of NNs, Recurrent NNs, Generative Adversarial Networks

Vectors and Matrices

- A vector is often referred to a 1-D array of numbers

$$\boldsymbol{a} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{bmatrix} \in \mathbb{R}^m, \qquad \text{Ex}: \quad \boldsymbol{a} = \begin{bmatrix} 1.2 \\ -3 \\ 2 \end{bmatrix} \in \mathbb{R}^3.$$

- A matrix is often referred to a 2-D array of numbers

$$\boldsymbol{A}_{m\times n} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}, \quad \text{Ex: } \boldsymbol{A} = \begin{bmatrix} 4 & -7 & 5 & 0 \\ -2 & 0 & 11 & 8 \\ 19 & 1 & -3 & 12 \end{bmatrix}.$$

Matrix Notation

m-by-n matrix

$a_{i,j}$ $\quad$ n columns $\quad$ j changes

m rows

i changes

$$\begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots \\ a_{2,1} & a_{2,2} & a_{2,3} & \cdots \\ a_{3,1} & a_{3,2} & a_{3,3} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

More on Matrices

- Transpose of a matrix:

$$\boldsymbol{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} \in \mathbb{R}^{m \times n}, \;\; \boldsymbol{A}^\top = \begin{bmatrix} a_{11} & a_{21} & \cdots & a_{m1} \\ a_{12} & a_{22} & \cdots & a_{m2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1n} & a_{2n} & \cdots & a_{mn} \end{bmatrix} \in \mathbb{R}^{n \times m}$$

- Example:

$$\boldsymbol{A} = \begin{bmatrix} 4 & -7 & 5 & 0 \\ -2 & 0 & 11 & 8 \\ 19 & 1 & -3 & 12 \end{bmatrix}, \;\; \boldsymbol{A}^\top = \begin{bmatrix} 4 & -2 & 19 \\ -7 & 0 & 1 \\ 5 & 11 & -3 \\ 0 & 8 & 12 \end{bmatrix}.$$

Matrix Product

- The product of two matrices $\boldsymbol{A}, \boldsymbol{B}$ with compatible sizes $n \times m$, $m \times p$ is denoted by $\boldsymbol{AB}$ and is of size $n \times p$:

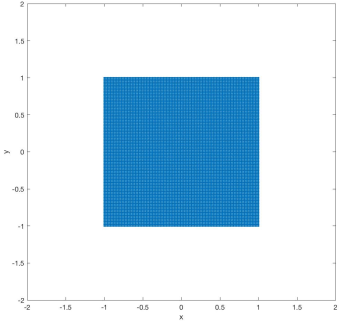
$$\begin{pmatrix} a_{11} & \cdots & a_{1m} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nm} \end{pmatrix} \begin{pmatrix} b_{11} & \cdots & b_{1p} \\ \vdots & \ddots & \vdots \\ b_{m1} & \cdots & b_{mp} \end{pmatrix} = \begin{pmatrix} \sum_{k=1}^{m} a_{1k} b_{k1} & \cdots & \sum_{k=1}^{m} a_{1k} b_{kp} \\ \vdots & \ddots & \vdots \\ \sum_{k=1}^{m} a_{nk} b_{k1} & \cdots & \sum_{k=1}^{m} a_{nk} b_{kp} \end{pmatrix}$$

- Example:

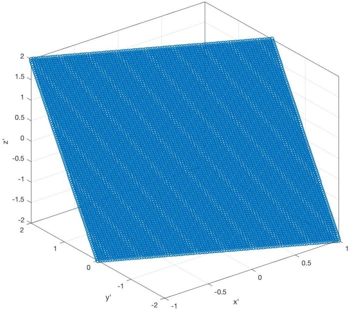
$$\begin{pmatrix} 1 & 0 \\ -1 & 1 \\ 0 & 2 \end{pmatrix} \begin{pmatrix} -2 & 0 \\ 1 & 2 \end{pmatrix} = \begin{pmatrix} -2 & 0 \\ 3 & 2 \\ 2 & 4 \end{pmatrix}$$

Matrices as a Way of Linear Transformation

$$\begin{pmatrix} x_1' & x_2' & \cdots & x_n' \\ y_1' & y_2' & \cdots & y_n' \\ z_1' & z_2' & \cdots & z_n' \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -1 & 1 \\ 0 & 2 \end{pmatrix} \begin{pmatrix} x_1 & x_2 & \cdots & x_n \\ y_1 & y_2 & \cdots & y_n \end{pmatrix}$$



$\Rightarrow$



Matrix Representation for the Linear Models

- For a linear model we had

$$y = b_0 + w_1 x_1 + \cdots + w_p x_p = w_0 + \boldsymbol{w}^\top \boldsymbol{x},$$

where

$$\boldsymbol{w} = \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_p \end{pmatrix}, \quad \boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{pmatrix}.$$

- So when we fit the model and want to evaluate it for a number of test points $\boldsymbol{x}^{t_1}, \boldsymbol{x}^{t_2}, \cdots, \boldsymbol{x}^{t_n}$ all we need to do is the following

$$\boldsymbol{y}^t = [y^{t_1}, \cdots, y^{t_n}] = [b_0, b_0, \cdots, b_0] + \boldsymbol{w}^\top \begin{pmatrix} x_1^{t_1} & x_1^{t_2} & \cdots & x_1^{t_n} \\ x_2^{t_1} & x_2^{t_2} & \cdots & x_2^{t_n} \\ \vdots & & & \vdots \\ x_p^{t_1} & x_p^{t_2} & \cdots & x_p^{t_n} \end{pmatrix}$$

Matrix Representation for the Linear Models (Multi Response)

- For a linear model with m responses

$$
\begin{aligned}
y_1 &= b_1 + w_{1,1}x_1 + \cdots + w_{1,p}x_p \\
y_2 &= b_2 + w_{2,1}x_1 + \cdots + w_{2,p}x_p \\
&\vdots \\
y_m &= b_m + w_{m,1}x_1 + \cdots + w_{m,p}x_p
\end{aligned}
$$

which can be written in the matrix form as

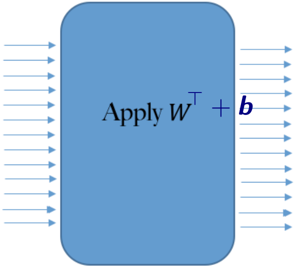
$$\boldsymbol{y} = \boldsymbol{b} + \boldsymbol{W}^\top \boldsymbol{x},$$

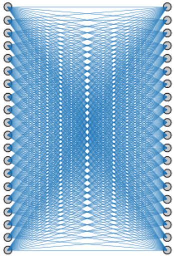
where

$$\boldsymbol{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{pmatrix}, \quad \boldsymbol{W} = \begin{pmatrix} w_{1,1} & w_{2,1} & \cdots & w_{m,1} \\ w_{1,2} & w_{2,2} & \cdots & w_{m,2} \\ \vdots & \vdots & \vdots & \vdots \\ w_{1,p} & w_{2,p} & \cdots & w_{m,p} \end{pmatrix}, \quad \boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{pmatrix}.$$

Fitting Multi Response LMs

- An edge between two nodes is present when $W_{i,j} \neq 0$

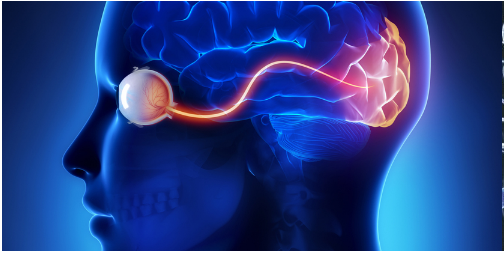


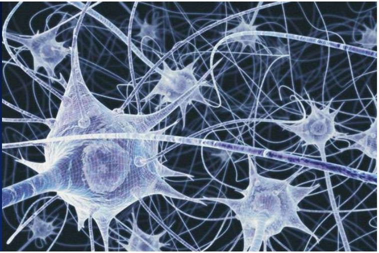


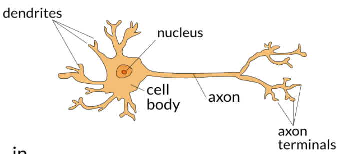
- Suppose we have the training samples $(\boldsymbol{x}_1, \boldsymbol{y}_1), \cdots, (\boldsymbol{x}_N, \boldsymbol{y}_N)$. To fit the model to the training data, we only need to minimize the following RSS:

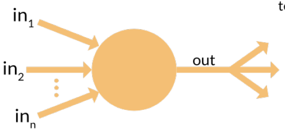
$$\min_{\boldsymbol{W}, \boldsymbol{b}} \sum_{i=1}^{N} \left\| \boldsymbol{y}_i - \boldsymbol{b} - \boldsymbol{W}^\top \boldsymbol{x}_i \right\|^2$$

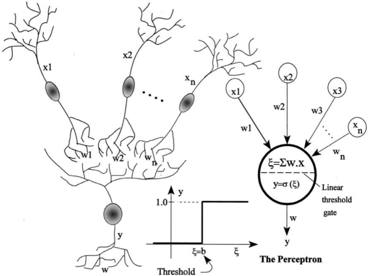
Structure of the Brain











Nonlinear Activation Applied to a Vector

- Sigmoid function:

$$\sigma(x) = \frac{e^x}{1 + e^x}$$

- When sigmoid is applied to a vector or a matrix, it applies to each component individually

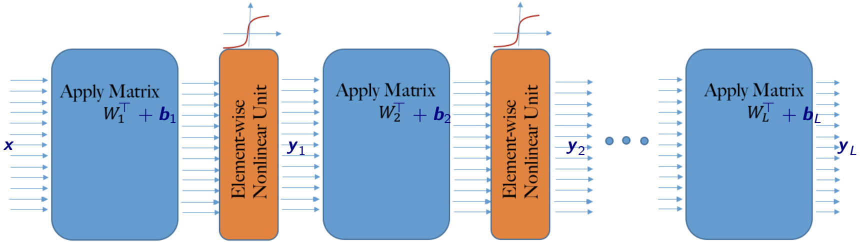
$$\sigma\left(\begin{bmatrix} 3 \\ -2 \\ -1 \end{bmatrix}\right) = \begin{bmatrix} \frac{e^3}{1+e^3} \\ \frac{e^{-2}}{1+e^{-2}} \\ \frac{e^{-1}}{1+e^{-1}} \end{bmatrix}$$

- Another widely used activation is the rectified linear unit:

$$\texttt{ReLU}(x) = \max(x, 0)$$

$$\texttt{ReLU}\left(\begin{bmatrix} 3 \\ -2 \\ -1 \end{bmatrix}\right) = \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix}$$

Standard Architecture of Neural Networks



- A neural network consists of a sequence of multi-output linear units followed by nonlinear activations

$$\boldsymbol{y}_1 = \sigma_1\left(\boldsymbol{W}_1^\top \boldsymbol{x} + \boldsymbol{b}_1\right)$$

$$\boldsymbol{y}_2 = \sigma_2\left(\boldsymbol{W}_2^\top \boldsymbol{y}_1 + \boldsymbol{b}_2\right)$$

$$\vdots$$

$$\boldsymbol{y}_L = \sigma_L\left(\boldsymbol{W}_L^\top \boldsymbol{y}_{L-1} + \boldsymbol{b}_L\right)$$

Standard Architecture of Neural Networks

- Normally all activations are taken to be identical except the last layer
- If we have regression problem, often no activation is used at the output, i.e.,

$$\boldsymbol{y}_L = \boldsymbol{W}_L^\top \boldsymbol{y}_{L-1} + \boldsymbol{b}_L$$

- For classification problems, often a soft-max unit is used at the output, i.e., for $\boldsymbol{y} = [y_1, \cdots, y_m]^\top$

$$\sigma_L(y_i) = \frac{e^{y_i}}{\sum_{j=1}^m e^{y_j}}, \quad i = 1, \cdots, L.$$

- Example:

$$\begin{pmatrix} 0.5 \\ 1.8 \\ -2.3 \\ 0.9 \\ 0.3 \end{pmatrix} \overset{\texttt{soft-max}}{\Rightarrow} \begin{pmatrix} 0.14 \\ 0.52 \\ 0.01 \\ 0.21 \\ 0.12 \end{pmatrix}$$

How to Fit (Train) Neural Networks

- For the proposed architecture, we need to learn $\boldsymbol{W}_1, \cdots, \boldsymbol{W}_L$ and $\boldsymbol{b}_1, \cdots, \boldsymbol{b}_L$
- Let's first derive the function that relates $\boldsymbol{x}$ to $\boldsymbol{y}_L$. Lets define

$$f_\ell(\boldsymbol{z}) = \sigma_\ell\left(\boldsymbol{W}_\ell^\top \boldsymbol{z} + \boldsymbol{b}_\ell\right),$$

then we have

$$\begin{aligned}\boldsymbol{y}_L &= f_L(\boldsymbol{y}_{L-1}) \\ &= f_L(f_{L-1}(\boldsymbol{y}_{L-2})) \\ &\vdots \\ &= f_L(f_{L-1}(f_{L-2}(\cdots f_1(\boldsymbol{x})\cdots)))\end{aligned}$$

- Basically

$$\boldsymbol{y}_L = \mathcal{M}(\boldsymbol{x}), \quad \text{where} \quad \mathcal{M}(\boldsymbol{x}) = f_L(f_{L-1}(f_{L-2}(\cdots f_1(\boldsymbol{x})\cdots)))$$

How to Fit (Train) Neural Networks

- Suppose we have the training samples $(\boldsymbol{x}^{(1)}, \boldsymbol{y}^{(1)}), \cdots, (\boldsymbol{x}^{(N)}, \boldsymbol{y}^{(N)})$
- For **regression** problems we normally skip an activation in the last layer and try to solve the following minimization

$$\min_{\boldsymbol{W}_1, \cdots, \boldsymbol{W}_L, \boldsymbol{b}_1, \cdots \boldsymbol{b}_L} \frac{1}{N} \sum_{n=1}^{N} \left\| \boldsymbol{y}^{(n)} - \mathcal{M}\left(\boldsymbol{x}^{(n)}\right) \right\|^2$$

- For **classification** problems we use a soft-max in the last layer. Suppose having K classes, then $\boldsymbol{y}^{(n)}$ are vectors of length K, where for each sample the corresponding index is active

$$\min_{\boldsymbol{W}_1, \cdots, \boldsymbol{W}_L, \boldsymbol{b}_1, \cdots \boldsymbol{b}_L} \frac{1}{N} \sum_{n=1}^{N} \mathcal{H}\left(\boldsymbol{y}^{n}, \mathcal{M}\left(\boldsymbol{x}^{(n)}\right)\right)$$

- The central objective is the cross-entropy, for $\boldsymbol{y}$ and $\boldsymbol{y}'$ of length K:

$$\mathcal{H}\left(\boldsymbol{y}, \boldsymbol{y}'\right) = -\sum_{k=1}^{K} y_k \log y'_k$$

Gradient Descent for Minimization

- We saw that our fitting problem boils down to a minimization problem

$$\min_{\boldsymbol{p}} \ \mathcal{C}(\boldsymbol{p})$$

in our case $\boldsymbol{p}$ includes all the unknowns $\boldsymbol{W}_1, \cdots, \boldsymbol{W}_L, \boldsymbol{b}_1, \cdots \boldsymbol{b}_L$ and $\mathcal{C}$ is either one of the objectives in the previous slide

- Assuming $\boldsymbol{p} \in \mathbb{R}^L$, a numerical way of minimization is to start from a point $\boldsymbol{p}^{(0)}$ and iteratively perform the following steps

$$\boldsymbol{p}^{k+1} = \boldsymbol{p}^{(k)} - \eta \nabla \mathcal{C}\Big|_{\boldsymbol{p}=\boldsymbol{p}^{(k)}} \quad \text{where} \quad \nabla \mathcal{C} = \begin{pmatrix} \partial \mathcal{C}/\partial p_1 \\ \partial \mathcal{C}/\partial p_2 \\ \vdots \\ \partial \mathcal{C}/\partial p_L \end{pmatrix}$$

parameter η is called the **learning rate**

- Let's go through a simple example to see how gradient descent works (see the MATLAB code and the next slide)

Gradient Descent for Minimization

- Please refer to the MATLAB `gradientDescent.m` script
- Lets consider the very simple objective

$$\mathcal{C}(p_1, p_2) = (1 - p_1)^2 + (1 - p_2)^2 - 2\exp(-3p_1^2 - 3p_2^2)$$

  The gradient can be calculated as

$$\nabla\mathcal{C} = \begin{pmatrix} 2(p_1 - 1) + 12p_1 \exp(-3p_1^2 - 3p_2^2) \\ 2(p_2 - 1) + 12p_2 \exp(-3p_1^2 - 3p_2^2) \end{pmatrix}$$

- We can see that this objective has multiple local minimizers (two)
- Depending on where we start from we may land in either one
- A too small LR (learning rate) can make the minimization slow
- A too large LR can also make it slow or never converging!
- LR can affect which minimizer we converge to, but this is beyond our control

What is Stochastic Gradient Descent?

- Recall when we had N training samples $(\boldsymbol{x}^{(1)}, \boldsymbol{y}^{(1)}), \cdots, (\boldsymbol{x}^{(N)}, \boldsymbol{y}^{(N)})$ our fitting objective was in one of the forms:

$$\min_{\boldsymbol{p}} \; \frac{1}{N}\sum_{n=1}^{N} \left\| \boldsymbol{y}^{(n)} - \mathcal{M}_{\boldsymbol{p}}\left(\boldsymbol{x}^{(n)}\right) \right\|^2 \qquad \min_{\boldsymbol{p}} \; \frac{1}{N}\sum_{n=1}^{N} \mathcal{H}\left(\boldsymbol{y}^{n}, \mathcal{M}_{\boldsymbol{p}}\left(\boldsymbol{x}^{(n)}\right)\right)$$

  Here $\boldsymbol{p}$ is a hyper parameter representing all our unknowns $\boldsymbol{W}_1, \cdots, \boldsymbol{W}_L, \boldsymbol{b}_1, \cdots \boldsymbol{b}_L$.
- In other words, we are interested in objectives of the form

$$\mathcal{C}(\boldsymbol{p}) = \frac{1}{N}\sum_{n=1}^{N} \mathcal{C}_n(\boldsymbol{p}),$$

  where $\mathcal{C}_n$ only depends on the sample $(\boldsymbol{x}^{(n)}, \boldsymbol{y}^{(n)})$.
- Notice that to calculate $\nabla \mathcal{C}$ we need to calculate N gradients

$$\nabla \mathcal{C}(\boldsymbol{p}) = \frac{1}{N}\sum_{n=1}^{N} \nabla \mathcal{C}_n(\boldsymbol{p})$$

What is Stochastic Gradient Descent?

$$\nabla \mathcal{C}(\boldsymbol{p}) = \frac{1}{N} \sum_{n=1}^{N} \nabla \mathcal{C}_n(\boldsymbol{p})$$

- Since gradient calculation can be computationally expensive, in stochastic GD, at each minimization iteration we pick a **random** subset of all the samples $B \subset \{1, 2, \cdots, N\}$ and use it as an approximation of the gradient

$$\nabla \mathcal{C}(\boldsymbol{p}) \approx \frac{1}{\text{size }(B)} \sum_{n \in B} \nabla \mathcal{C}_n(\boldsymbol{p})$$

- If B is too small our gradient approximation may be too off!
- On the other hand large B may require a lot of gradient calculations
- Usually, after selecting the batch size, N_B we split our N data samples into N/N_B batches and in each GD iteration use one batch
- Each SGD **iteration** goes through one batch. Each **epoch** indicates going through the whole training set

Back Propagation

- This is another terminology that you probably hear a lot in deep learning
- Recall that you had to calculate the derivative with respect to each sample and each sample function is a complicated nested function, e.g.,

$$C_n = \left\| \boldsymbol{y}^{(n)} - f_L(f_{L-1}(f_{L-2}(\cdots f_1(\boldsymbol{x}_n)\cdots))) \right\|^2, \quad f_\ell(\boldsymbol{z}) = \sigma_\ell \left(\boldsymbol{W}_\ell^\top \boldsymbol{z} + \boldsymbol{b}_\ell \right)$$

- Back propagation is simply the application of the chain rule to calculate the derivative of nested functions like C_n in terms of all the unknown parameters $\boldsymbol{W}_1, \cdots, \boldsymbol{W}_L, \boldsymbol{b}_1, \cdots \boldsymbol{b}_L$
- Since the actual story goes through a lot of indexing complications, let me explain things via a simple example

Back Propagation

- You can skip this example if don't have time
- Find the derivative of the following function at $w = 2$:

$$f(w) = \big(\sin\big(w^2 + 1\big)\big)^2$$

- **Method 1:** go through the pain of calculating the derivative and find

$$f'(w) = 4w\cos(w^2 + 1)\sin(w^2 + 1)$$

- Then plug in $w = 2$ to get

$$f'(2) = 8\cos(5)\sin(5)$$

Back Propagation

- Find the derivative of the following function at $w = 2$:

$$f(w) = \left(\sin\left(w^2 + 1\right)\right)^2$$

- **Method 2:** Notice that

$f = g_1(g_2(g_3(w)))$, where $g_1(g_2) = g_2^2,\ g_2(g_3) = sin(g_3),\ g_3(w) = w^2 + 1$

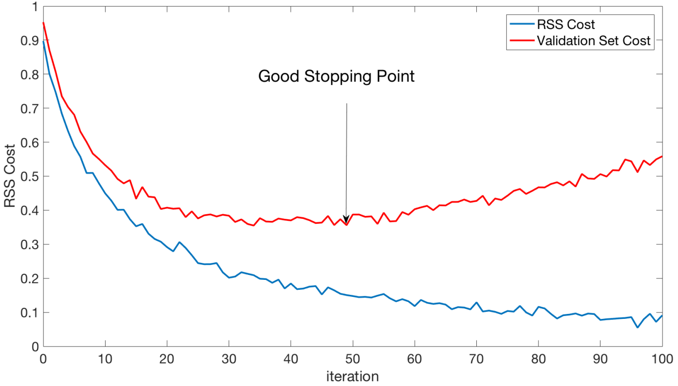
and use the chain rule

$$\frac{\partial f}{\partial w} = \frac{\partial g_1}{\partial w} = \frac{\partial g_1}{\partial g_2}\frac{\partial g_2}{\partial g_3}\frac{\partial g_3}{\partial w} = 2\sin(5) \times \cos(5) \times 4$$

- Still want to learn more about back propagation? Try these videos:
  - `https://www.youtube.com/watch?v=Ilg3gGewQ5U`
  - `https://www.youtube.com/watch?v=tIeHLnjs5U8`

Using a Validation Set to Control the Minimization

- As you observed in the previous slides gradient descent gradually decreases the RSS (or cross entropy cost) to find a minimizer
- One way to avoid overfitting, is to use a "**validation set**", independent of the training set and stop the gradient descent iterations when the validation error starts to increase

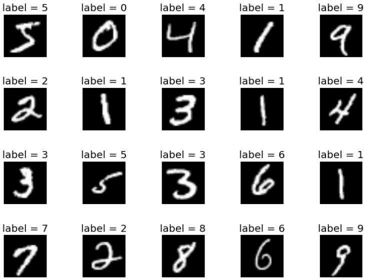


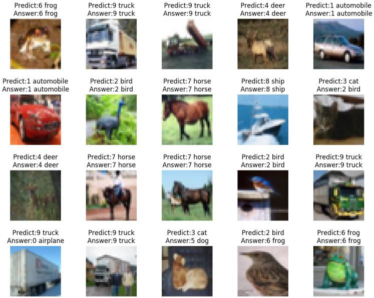
Regularization of Neural Networks to Avoid Overfitting

- Similar to linear models there are variety of techniques to avoid overfitting in neural networks
    - L_2 regularizers (similar to Ridge)
    - L_1 regularizers (Similar to LASSO)
    - Dropout and DropConnect (which drops some of the updates in the gradient descent)
        - See video: `https://www.youtube.com/watch?v=ARq74QuavAo`
        - See papers: Paper 1, Paper 2
    - Net-Trim and compression algorithms
        - See video: `https://www.youtube.com/watch?v=WxU8dp7iYg0&t`
        - See papers and code: Here
- See one implementation of NNs **in R using the H2O package**

Convolutional Neural Networks

- Deep learning has shown a lot of promise in classifying images

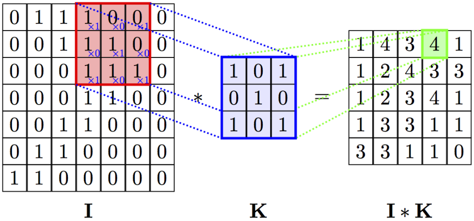




- One immediate candidate for the features is the image pixels. But if the images are too large, this would make our problem unnecessarily large
- Convolutional neural nets are a solution to this problem

Linear Filtering and Images

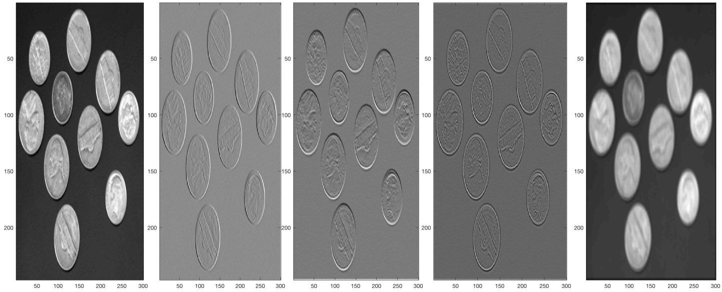
- Convolution is a linear operator widely used in image and signal processing



$$\boldsymbol{I} \star \boldsymbol{K}(m,n) = \sum_{i=1}^{M} \sum_{j=1}^{N} \boldsymbol{I}(m-i, n-j)\boldsymbol{K}(i,j)$$

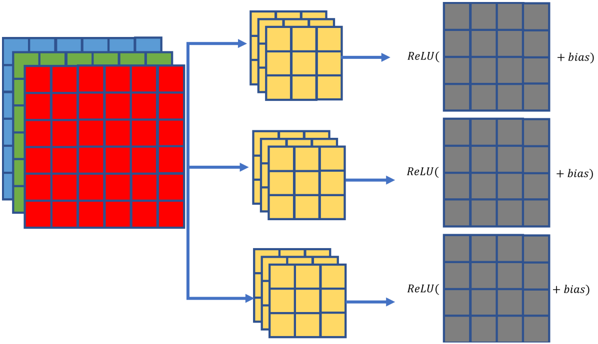
- Depending on the type of filter we pick for $\boldsymbol{K}$ the output image can have different properties (blurred, sharpened, edges detected, etc)
- See the MATLAB code `convExample.m`

Example of Image Convolution with Different Kernels



- If the filters are selected wisely, their output can be considered as alternative features to pixels
- In a CNN, we let the neural network learn these filters! In other words, CNN wisely chooses the right features that are the best for prediction
- For color images (RGB) we can have 3D filters each filter applicable to one channel

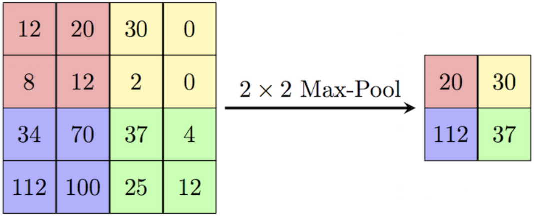
Convolutional Layers



- We can define as many 2D or 3D convolutional filters (here 3 3D filters of size $3 \times 3 \times 3$)
- The total number of parameters that need to be learnt for this layer is going to be $3 \times (27 + 1)$
- An input image of $6 \times 6 \times 3$ is mapped to a tensor of size $4 \times 4 \times 3$

Max Pooling

- Is another operation that allows us to reduce the input size by taking a max operation over smaller windows across the image



- To help you better understand the topic, we will consider an implementation of the CNN that learns to read handwritten digits (MNIST data set) — see the Python code

Recurrent Neural Networks

- While CNNs work quite promising for images, they may not be the best modeling tools for other data sets such as time series data
- For time series data and stream inputs (e.g., text analytics), **recurrent neural networks (RNNs)** are of major attention
- Remember in standard neural network the output of the hidden layer was in the form

$$\boldsymbol{h} = \sigma\left(\boldsymbol{W}_x^\top \boldsymbol{x} + \boldsymbol{b}\right)$$

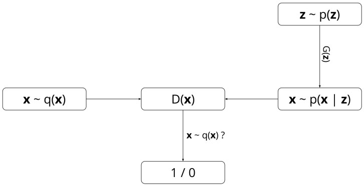
- In RNNs the input is stream $\boldsymbol{x}_t$ and we have another coefficient matrix that makes the current hidden output dependent on the previous one:

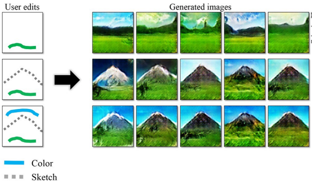
$$\boldsymbol{h}_t = \sigma\left(\boldsymbol{W}_x^\top \boldsymbol{x}_t + \boldsymbol{W}_h^\top \boldsymbol{h}_{t-1} + \boldsymbol{b}\right)$$

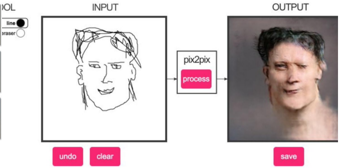
- To learn more and see some cool applications see: `https://www.youtube.com/watch?v=6niqTuYFZLQ&t=1850s`

Generative Adversarial Networks

- Is the most recent breakthrough in machine learning started in 2015
- Basically once we pass enough samples to a GAN network, it starts to learn how to generate similar samples







- To learn more and see some interesting applications see: This Video ; or This Video

Questions?

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