Hyperparameter Tuning, Regularization, Optimization

Sidharth Baskaran

July 2021

Tuning Process

- Choose parameter combinations (points) at random in a space
- 2 parameters - grid
- 3 parameters - cube
- Coarse to fine sampling
  - Sample densely within a region with better parameter combinations
  - Coarse sample of all combinations

Scale to pick hyperparameters

- Use a log scale to range α for example
  - Set $r \in [a.b]$
  - Then $\alpha \in [10^a, 10^b]$ satisfying the range
- Hyperparameters for exponentially weighted averages
  - Set $r \in [a, b]$
  - $1 - \beta = 10^r$
  - $\beta = 1 - 10^r$
  - Sampling regime important, as small changes change the values in Adam optimization largely

Pandas vs. Caviar

- Babysitting one model
  - Adjust hyperparameters one day at a time while observing performance
  - Can't train many models at once
  - Panda approach
- Train many models in parameter with different hyperparameter settings
  - Caviar approach

Normalizing Activations

- $\mu = \frac{1}{M} \sum_i x^{(i)}$
- $x = x - \mu$
- $\sigma^2 = \frac{1}{m} \sum_i x^{2(i)}$
- $x = x/\sigma$
- Makes contours more circular, beneficial for gradient descent
- Batch normalization $\rightarrow$ normalize $a^{[2]}$ to train $w^{[3]}, b^{[3]}$ faster
- Normalize the values of $z^{[2]}$ instead of $a^{[2]}$
- Implementing Batch Norm
  - Given intermediate NN values $z^{(1)}, \ldots, z^{(i)}$

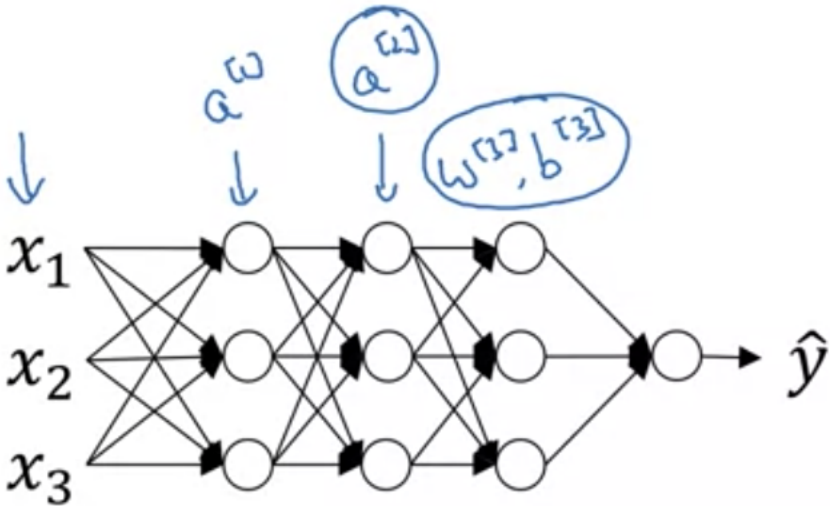

Figure 1: Batch norm

    - $\mu = \frac{1}{M}\sum_i x^{(i)}$
    - $\sigma^2 = \frac{1}{m}\sum_i (z_i - \mu)^2$
    - $z^{(i)}_{\text{norm}} = \frac{z^{(i)} - \mu}{\sqrt{\sigma^2 + \epsilon}}$
  - $\bar{z}^{(i)} = \gamma z^{(i)}_{\text{norm}} + \beta$
    - These are hyperparameters which allow for adjustment of $z^{(i)}_{\text{norm}}$
  - Use $\bar{z}^{[l](i)}$ instead of $z^{[l](i)}$

Fitting Batch Norm into network

- Example computation for first layer

$$x \overset{w^{[1]}, b^{[1]}}{\rightarrow} z^{[1]} \overset{\beta^{[1]}, \gamma^{[1]}}{\rightarrow} \bar{z}^{[1]} \rightarrow a^{[1]} = g^{[1]}(\bar{z}^{[1]})$$

- Repeat for each layer
- Parameters are $W^{[k]}, b^{[k]}, \beta^{[k]}, \gamma^{[k]}$ for $k \in [1, L]$ are the parameters
- Working with mini-batches
  - Conduct batch norm for each minibatch (i.e. starting with $X^{\{1\}}$)
  - Batch norm only uses examples from the current minibatch
- $b^{[l]}$ gets subtracted out in the mean subtraction step, so **eliminate this parameter, is redundant**
  - Simply remove from the subtraction
- Implementing gradient descent
  - For $t \in [1, \text{numMiniBatch}]$
    - Compute forward prop on $X^{\{t\}}$
      - In each hidden layer, use batch norm
    - Use backprop to calculate $dw^{[l]}, d\beta^{[l]}, d\gamma^{[l]}$ and update parameters

Batch norm reasoning

- Conducts input normalization but for hidden units
- Makes deeper weights robust to changes in weights of earlier layers
- Learning on shifting input distribution $\rightarrow$ covariant shift

  - If X distribution changes, must retrain for $X \to Y$ mapping, so values input to a hidden layer change
  - Batch norm reduces this effect, layers are more independent
- Batch norm as regularization
  - Each minibatch scaled by mean/variance of the examples in it
  - Adds noise to $z^{[l]}$, so adds noise to hidden layer activations similar to dropout
  - Has slight regularization effect, but with a larger minibatch size this is reduced

Batch Norm at Test Time

- Need to estimate μ, σ^2 at test time using weighted average across minibatches
- Calculate $\mu^{\{1\}l}, \ldots, \mu^{\{n\}l}$, using a moving average, same for σ^2

Softmax regression

- If there are multiple classes (e.g. Chick, Dog, Cat with classes 3, 2, 1, and 0 if none)
  - Indexes are $i \in [0, C-1]$ with C classes

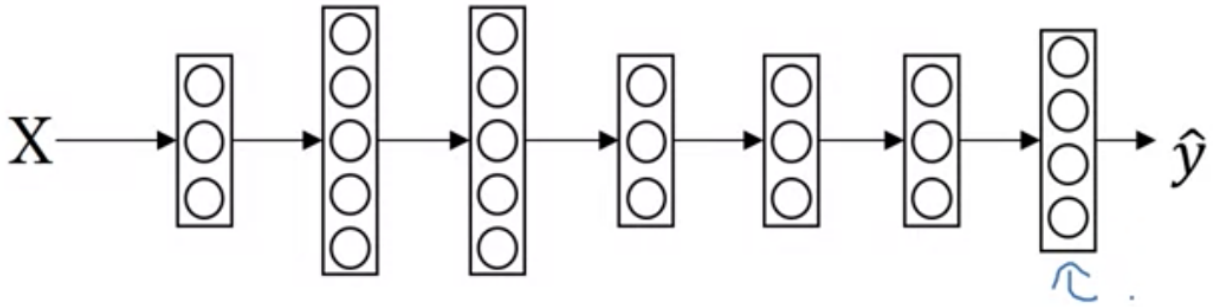

Figure 2: Softmax NN

- Output is a 4-dim layer, each node contains probability $P(\text{class}|x)$
  - Sum must be 1
- Softmax output layer generates these outputs
  - Is an activation function
- Compute a temp. var $t = e^{z^{[L]}}$ elementwise of dim (4,1)
  - $a^{[L]} = \frac{e^{z^{[L]}}}{\sum_{i=1}^{4} t_i}$ such that $a_i^{[L]} = \frac{t_i}{\sum_{i=1}^{4} t_i}$
- Resulting probabilities are the desired classifications
- Unusual as it takes in vectorial input, not some $\mathbb{R}$f
- Softmax can represent linear decision boundaries between multiple classes (without hidden layers to learn nonlinear ones)

Training a Softmax Classifier

- A hardmax would map the vector $z^{[L]}$ to either 0 or 1, whereas softmax is a gentle, more precise mapping
- Is a generalization of logistic regression to C classes
- Loss function
  - Makes corresponding probability of the ground truth class as high as possible $\to$ minimizes the loss

$$a^{[L]} = g^{[L]}(z^{[L]}) = \begin{bmatrix} e^5/(e^5+e^2+e^{-1}+e^3) \\ e^2/(e^5+e^2+e^{-1}+e^3) \\ e^{-1}/(e^5+e^2+e^{-1}+e^3) \\ e^3/(e^5+e^2+e^{-1}+e^3) \end{bmatrix} = \begin{bmatrix} 0.842 \\ 0.042 \\ 0.002 \\ 0.114 \end{bmatrix}$$

Figure 3: Example

$$\mathcal{L}(\hat{y}, y) = -\sum_{j=1}^{4} y_j \log \hat{y}_j$$

- Cost J on entire training set

$$J = \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)})$$

- Gradient descent with softmax
  - Key equation is $dz^{[L]} = \hat{y} - y$ which are all (4,1) vectors

Deep learning frameworks

- Ease of programming
- Running speed
- Open source

TensorFlow

- Motivating problem
  - Want to minimize $J(w) = w^2 - 10w + 25 = (w-5)^2$

```
import numpy as np
import tensorflow as tf

# initialize to 0 float32
w = tf.Variable(0, dtype=tf.float32)
# alpha=0.1
optimizer = tf.keras.optimizers.Adam(0.1)

# one training step iteration
def train_step():
  with tf.GradientTape() as tape:
    cost = w**2 - 10*w + 25
  trainable_variables = w
  grads = tape.gradient(cost, trainable_variables)
  optimizer.apply_gradients(zip(grads, trainable_variables))
```

- Gradient tape records order of operations, thus only need to implement forward prop step
- Can also implement this using optimization

```
w = tf.Variable(0, dtype=tf.float32)
x = np.array([1.0,-10.0,25.0], dtype=np.float32)
optimizer = tf.keras.optimizers.Adam(0.1)

def training(x,w,optimizer):
    def cost_fn():
      return x[0]*w**2 + x[1]*w + x[2]
    for i in range(1000):
      optimizer.minimize(cost_fn, [w])
    return w

w = training(x,w,optimizer)
```