Setting up ML application

Sidharth Baskaran

July 2021

Train/test/dev sets

- Divide original data into 3 different sets
- Use dev set to evaluate various models
- Use final model on test set for unbiased estimate
- For large m, dev and test sets become smaller
 - E.g. 0.98, 0.01, 0.01 distribution
- Mismatched train/test distribution
 - Source/quality of training set is different than dev/test sets
 - Ensure dev/test sets come from same distribution
- \bullet Can work without a test set \rightarrow unbiased estimate of chosen network

Bias/variance

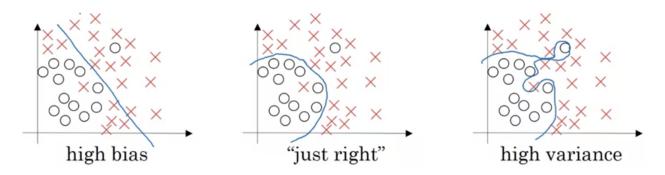


Figure 1: Cases

- High bias involves underfitting
 - Generalizes well but has high error
- High variance involves overfitting
 - Does not generalize well from train to dev set

Basic recipe for ML

- If high bias
 - Bigger network
 - Train longer
 - Try different NN architectures
- If high variance
 - More data

- Regularization
- NN architecture change
- Bias-variance tradeoff
 - Bigger network reduces bias without increasing variance, or more date \rightarrow less of tradeoff
 - Use regularization

Regularization

• Logistic regression \to find $\min_{w,b} J(w,b)$ with $w \in \mathbb{R}^{n_x}, b \in \mathbb{R}$

$$J(w,b) = \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2m} ||w||^2$$

where the L_2 (Euclidean) norm is $||w||_2^2 = \sum_{j=1}^{n_x} w_j^2 = w^T w$. Can omit reg. term for b.

 L_1 regularization: $\frac{\lambda}{2m}\sum_{i=1}^{n_x}|w|=\frac{\lambda}{2m}||w||_1$. w is sparse, i.e. has lots of zeros. Less often used.

• For multiple layers, use Frobenius norm

$$||w^{[l]}||_F^2 = \sum_{i=1}^{n^{[l]}} \sum_{j=1}^{n^{[l-1]}} (w_{i,j}^{[l]})^2$$

- Implementing gradient descent with regularization $dw^{[l]} = \text{backprop} + \frac{\lambda}{m}w^{[l]}$, then perform parameter update
- Called weight decay as this is equivalent to a coefficient $1 \frac{\alpha \lambda}{m}$

Why regularization reduces overfitting

- A high λ reduces weights so reduces impact of hidden units \rightarrow higher bias
- Leads to small range of z in tanh function, so approx. linear
 - So every layer ≈ linear

Dropout Regularization

- Give each node 0.5 chance of removal
 - Run simulation, and "kill" node connections from those chosen nodes → reduced network
- Inverted dropout
 - Check d3 = np.random.randn(*a3.shape) < keep_prob</pre>
 - Set a3 = np.multiply(a3,d3) to zero out nodes
 - Divide a3 by keep_prob to maintain expected value z
 - * a3 /= keep_prob
- Cannot rely on any one feature, so spread out weights
 - Shrinks the squared norm of weights
 - Varying keep_prob by layer
 - * Higher value for layers less prone to overfitting
 - * More hyperparameters
- Cost function J not well-defined anymore
 - Plot cost without dropout prior to usage

Other Regularization Methods

- Data augmentation
 - Use existing training examples and permute to create more
 - Rotation, flip, translation, etc.
 - Distortions and rotations on digits/characters

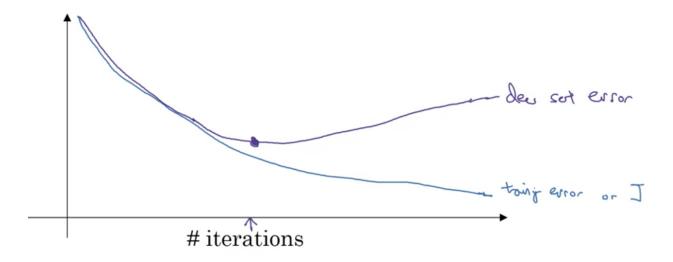


Figure 2: Early stopping

- Early stopping
 - Plot dev set error along with cost over iteratoins
 - Cut off training halfway so only a midsize $||w||_F^2$
 - However, stops optimization simulataneously with not overfitting

Normalizing Inputs

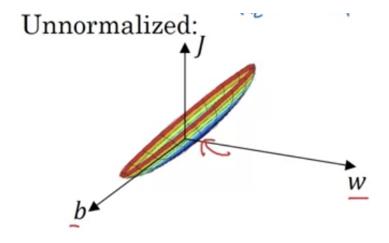


Figure 3: Unnormalized

- Subtract mean $\mu = \frac{1}{m} \sum_{i=1}^{m} x^{(i)}$ and divide by std. dev $\sigma^2 = \frac{1}{m} \sum_{i=1}^{m} x^{(i)2} * *2$ where both are vectors $-x := x \mu$ and $x/=\sigma$
- Normalize test and training data with μ and σ^2 from training data, not individually

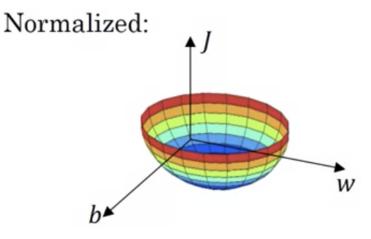


Figure 4: Normalized

Vanishing/exploding gradients

- If there is a deep network with L layers and all biases b=0
 - If weight matrix w values > 1, then \hat{y} exponentially increases, else if < 1 exponentially decreases
 - Thus gradients increase or decrease as well

Weight initialization for deep networks

- Can set $Var(w) = \frac{1}{n}$ where n is input feature number
- In practice, $W^{[L]}$ =np.random.randn(shape)*np.sqrt(2/n_prev) for ReLU or use $\sqrt{\frac{1}{n^{[l-1]}}}$ for tanh in place of np.sqrt
 - Can add hyperparameters

Numerical Approximation of Gradients

- Use the limit definition of the derivative If $f(\theta) = \theta^3$, then $\frac{d}{d\theta} f(\theta) \approx \frac{f(\theta+\epsilon) f(\theta-\epsilon)}{2\epsilon}$ Error is on order $O(\epsilon^2)$

Gradient Checking

- Reshape $W^{[1]}, b^{[1]}, \dots, W^{[L]}, b^{[L]}$ into large vector θ - Then, $J(\theta)$
- Reshape $dW^{[1]}, db^{[1]}, \dots, dW^{[L]}, db^{[L]}$ into $d\theta$
- Check if $d\theta$ is slope of θ
- Compute $d\theta_{\text{approx}}^{[i]}$ for each element in both matrices using $\frac{f(\theta+\epsilon)-f(\theta-\epsilon))}{2\epsilon}$ Use $\frac{||d\theta_{\text{approx}}-d\theta||}{||d\theta_{\text{approx}}||+||d\theta||}$
- - Accurate if $\epsilon \approx 10^{-7}$
- Only use in debugging
- Look at components of $d\theta$ to identify bug
- Must account for regularization term
- Does not work with dropout
- Run at random initialization and after some training
 - Could work initially and become inaccurate