LOGISTIC REGRESSION IN PYTHON

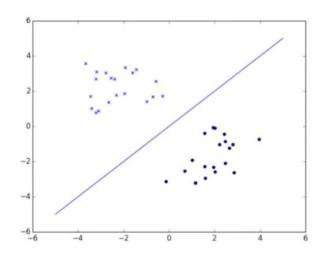
2-dimensional classification

y = mx + b

or

$$0 = ax + by + c$$

$$a = 1, b = -1, c = 0$$



Machine learning lingo

We call $(x,y) \Rightarrow (x_1, x_2) = x$

We rename the constants to w

We call the bias term / intercept ${\rm w}_{\rm o}$

$$h(\mathbf{x}) = W_0 + W_1 X_1 + W_2 X_2$$

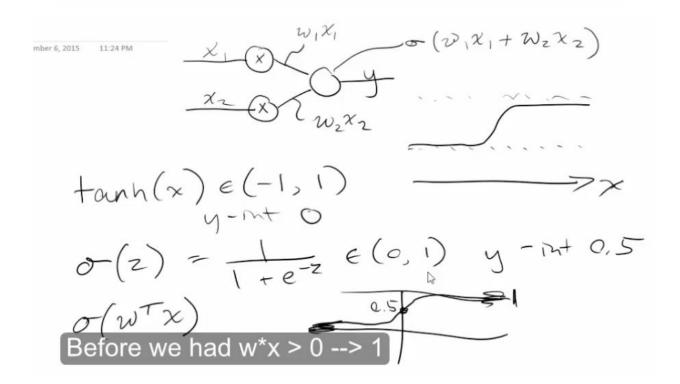
We say h() is a linear combination of the components of x

In vector form: $h(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$

In 3-dimensions: line → plane, In > 3 dimensions: hyperplane

Neuron Analogies

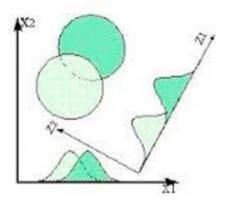
- Many inputs → One output
- Spike or no spike → 0/1 output
- Synapse strengths → linear weights



Problem Description

- 2 Gaussian Clouds
- Both have the same covariance
- Multivariate Gaussian PDF:

$$p(x) = \frac{1}{\sqrt{(2\pi)^D |\Sigma|}} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)}$$



Bayes' Rule

 $p(Y \mid X) = p(X \mid Y)p(Y) / p(X)$

I.e.:

$$p(Y=1 \mid X) = p(X \mid Y=1)p(Y=1) / p(X)$$

 $p(Y=0 \mid X) = p(X \mid Y=0)p(Y=0) / p(X)$

- \bullet p(X | Y) is the Gaussian we calculate it over all the data that belongs to class Y
- p(Y) is just the frequency estimate of Y →
 e.g. p(Y=1) = #times class 1 appeared / # total

Put it into the logistic regression framework

Manipulate Bayes' Rule

$$p(y = 1 \mid x) = \frac{p(x \mid y=1)p(y=1)}{p(x)} = \frac{p(x \mid y=1)p(y=1)}{p(x \mid y=1)p(y=1) + p(x \mid y=0)p(y=0)}$$

Divide top and bottom by $p(x \mid y=1)p(y=1)$

$$p(y = 1 \mid x) = \frac{1}{1 + \frac{p(x \mid y=0)p(y=0)}{p(x \mid y=1)p(y=1)}}$$

Looks a lot like Logistic Regression!

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Divide top and bottom by p(x | y=1)p(y=1)

$$p(y = 1 \mid x) = \frac{1}{1 + \frac{p(x \mid y = 0)p(y = 0)}{p(x \mid y = 1)p(y = 1)}}$$

Looks a lot like Logistic Regression!

Logistic Regression

$$p(y = 1 \mid x) = \frac{1}{1 + \frac{p(x \mid y = 0)p(y = 0)}{p(x \mid y = 1)p(y = 1)}} = \frac{1}{1 + exp(-w^T x)}$$

$$-w^T x = ln\left(\frac{p(x \mid y=0)p(y=0)}{p(x \mid y=1)p(y=1)}\right)$$

Let's just manipulate the right side and remember that it equals to the left

Logistic Regression

Let:
$$p(y = 1) = 1 - \alpha, p(y = 0) = \alpha$$

$$ln\left(\frac{p(x\mid y=0)p(y=0)}{p(x\mid y=1)p(y=1)}\right) = ln\;p(x\mid y=0) \; + ln\alpha - ln\;p(x\mid y=1) - ln(1-\alpha)$$

$$= \ln \frac{1}{\sqrt{(2\pi)^{D}|\Sigma|}} e^{-\frac{1}{2}(x-\mu_{0})^{T} \Sigma^{-1}(x-\mu_{0})} - \ln \frac{1}{\sqrt{(2\pi)^{D}|\Sigma|}} e^{-\frac{1}{2}(x-\mu_{1})^{T} \Sigma^{-1}(x-\mu_{1})} + \ln \frac{\alpha}{1-\alpha}$$

Logistic Regression

$$= \ln \frac{1}{\sqrt{(2\pi)^D |\Sigma|}} e^{-\frac{1}{2}(x-\mu_0)^T \Sigma^{-1}(x-\mu_0)} - \ln \frac{1}{\sqrt{(2\pi)^D |\Sigma|}} e^{-\frac{1}{2}(x-\mu_1)^T \Sigma^{-1}(x-\mu_1)} + \ln \frac{\alpha}{1-\alpha}$$

1 / sqrt(...) cancels out

$$= -\frac{1}{2}(x^{T}\Sigma^{-1}x - x^{T}\Sigma^{-1}\mu_{0} - \mu_{0}^{T}\Sigma^{-1}x + \mu_{0}^{T}\Sigma^{-1}\mu_{0}) + \frac{1}{2}(x^{T}\Sigma^{-1}x - x^{T}\Sigma^{-1}\mu_{1} - \mu_{1}^{T}\Sigma^{-1}x + \mu_{1}^{T}\Sigma^{-1}\mu_{1}) + ln\frac{\alpha}{1-\alpha}$$

Logistic Regression

$$= -\frac{1}{2}(x^{T}\Sigma^{-1}x - x^{T}\Sigma^{-1}\mu_{0} - \mu_{0}^{T}\Sigma^{-1}x + \mu_{0}^{T}\Sigma^{-1}\mu_{0}) + \frac{1}{2}(x^{T}\Sigma^{-1}x - x^{T}\Sigma^{-1}\mu_{1} - \mu_{1}^{T}\Sigma^{-1}x + \mu_{1}^{T}\Sigma^{-1}\mu_{1}) + ln\frac{\alpha}{1-\alpha}$$

- Quadratic term cancels out
- Is $x^T \Sigma^{-1} \mu = \mu^T \Sigma^{-1} x$? Yes! Try it on paper to prove to yourself. Remember the covariance, and hence its inverse, is symmetric

Logistic Regression

$$= \mu_0^T \Sigma^{-1} x - \mu_1^T \Sigma^{-1} x - \frac{1}{2} \mu_0^T \Sigma^{-1} \mu_0 + \frac{1}{2} \mu_1^T \Sigma^{-1} \mu_1 + \ln \frac{\alpha}{1-\alpha}$$

$$= (\mu_0^T - \mu_1^T) \Sigma^{-1} x - \frac{1}{2} \mu_0^T \Sigma^{-1} \mu_0 + \frac{1}{2} \mu_1^T \Sigma^{-1} \mu_1 + \ln \frac{\alpha}{1-\alpha}$$

$$= -(w^T x + b)$$

Finally!

$$w^{T} = (\mu_{1}^{T} - \mu_{0}^{T}) \Sigma^{-1}$$

$$b = \frac{1}{2} \mu_{0}^{T} \Sigma^{-1} \mu_{0} - \frac{1}{2} \mu_{1}^{T} \Sigma^{-1} \mu_{1} - \ln \frac{\alpha}{1 - \alpha}$$

Our data

$$\mu_0 = (-2, -2)^T$$
, $\mu_1 = (+2, +2)^T$, $\sigma^2 = 1$

w = (4, 4), b = 0 (assume equal number of samples of each class)

- Exercise: Solve it yourself on paper!
- Exercise: Make sure you can do the derivation yourself without watching the lectures.
- Also called: Linear Discriminant Analysis (LDA)
- If covariance is a diagonal matrix: Naive Bayes (why?)
- If we have different covariances: Quadratic Discriminant Analysis (QDA)
 - o Exercise: Write your own code and compare the performance vs. LDA
- This solution is optimal provided assumptions about distributions are true

Input Size

- N = number of samples we've collected
 - o i.e. I measure the height of 10 students to find the average height. N=10
- D = number of dimensions or features per sample
 - o i.e I measure height, weight, and girth, to try and predict body fat %. D=3 (height, weight, girth)
- A matrix of data called X would be an NxD matrix
 - o Each row is a sample
 - o Each column is the value of one feature in each sample

Data and Targets

- Sometimes we say we train a model on inputs X and targets Y
- If we consider all Ys at the same time, then it is an Nx1 matrix (for binary classification, an Nx1 matrix of 0s and 1s)
- Sometimes we use T for the target instead
 - o i.e. The cross-entropy error function: $-[t \log(y) + (1 t) \log(1 y)]$
- Now Y is used for something else: output of logistic regression.
- Before the output was more precise, P(Y=1 | X)
- But that takes longer to write...

Cost function

- Cost function = error function = objective function
- We want to minimize cost and error easy to see semantically
- Objective function can mean something to maximize OR minimize
- Trivial sign flipping minimizing $x^2 = maximizing x^2$
- We will first maximize likelihood P(data | model)
- Same as maximizing log-likelihood L = log P(data | model)
 - o i.e. If A > B, then log(A) > log(B)
- Sometimes, we use the letter J
 - May be in the form J = L → Maximize it
 - Or J = -L → Minimize it

Logistic Regression Error

Linear Regression - Squared Error

$$J = \sum_{n} (t_{n} - y_{n})^{2}$$

Assumes Gaussian-distributed error, because log(Gaussian) = squared function

Logistic Regression Error can't be Gaussian distributed, because:

- Target is only 0/1
- Output is only a number between 0-1

We want: 0 if correct, > 0 if not correct, more wrong == bigger cost

Cross-Entropy Error

 $J = -\{ tlog(y) + (1-t)log(1-y) \} (t = target, y = output of logistic)$

If t = 1, only first term matters, if t = 0, only second term matters

 $log(y) \rightarrow number between 0 and -inf$

Ex:

- $t = 1, y = 1 \rightarrow 0$
- $t = 0, y = 0 \rightarrow 0$
- $t = 1, y = 0.9 \rightarrow 0.11$
- $t = 1, y = 0.5 \rightarrow 0.69$
- $t = 1, y = 0.1 \rightarrow 2.3$

Multiple Training Examples

$$J = -\sum_{n=1}^{N} t_n log(y_n) + (1 - t_n) log(1 - y_n)$$

Saturday, November 7, 2015 12:18 AM MAXIMUM LIKE LIHOD

CON P(H) = P
$$P(T) = 1 - P$$
 $N = 10$
 T_{R}^{H}
 $3T$
 $L = P^{7}(1-P)^{3}$
 $= log [P^{7}(1-P)^{3}]$
 $= log P^{7} + log(1-P)^{3}$
 $= 7log P + 31$

$$L = log \left[p^{7} (1-p)^{3} \right]$$

$$= log p^{7} + log(1-p)^{3}$$

$$= 7 log p + 3 log(1-p)$$

$$= 7 + 3 log(1-p)$$

$$=$$

L = 10g [p7 (1-p)3] = logp7 + log(1-p)3 = 710gp + 3 log(1-p) 3P = 7 + 3- (-1) = 0 $\frac{7}{P} = \frac{3}{1-P}$ 1-P = 3 p-1 = 3

$$P = \frac{1}{7}$$

$$P = \frac{1}{7}$$

$$P = \frac{1}{7} = P(H)$$

How to optimize the weights

- IF we assume data is Gaussian-distributed with equal covariance, we can use the Bayes method
- But we want something that will work in general
- Linear regression:
- Take derivative, set to 0, solve for weights
- Can't do this with logistic regression / cross-entropy (but you're encouraged to try)

Gradient Descent

Idea: take small steps in direction of derivative

Step size == learning rate (1 for this example)

Ex:

w = -2

$$w = -2 - 1*(-1) = -1$$

Now we're closer to the optimal point! (w=0)

Note: slope is 0 at the bottom, so no more changes will occur



Bias Term

$$\frac{\partial J}{\partial w_0} = \sum_{n=1}^{N} (y_n - t_n) x_{n0} = \sum_{n=1}^{N} (y_n - t_n)$$

Gradient Descent for Logistic Regression

$$J = -\sum_{n=1}^{N} t_n log(y_n) + (1 - t_n) log(1 - y_n)$$

Split into 3 derivatives:

$$\frac{\partial J}{\partial w_i} = \sum_{n=1}^{N} \frac{\partial J}{\partial y_n} \frac{\partial y_n}{\partial a_n} \frac{\partial a_n}{\partial w_i}$$
$$a_n = w^T x_n$$

Derivatives

$$J = -\sum_{n=1}^{N} t_n log(y_n) + (1 - t_n) log(1 - y_n)$$

$$\frac{\partial J}{\partial y_n} = -t_n \frac{1}{y_n} + (1 - t_n) \frac{1}{1 - y_n} (-1)$$

Derivatives

$$y_n = \sigma(a_n) = \frac{1}{1 + e^{-a_n}}$$

$$\frac{\partial y_n}{\partial a_n} = \frac{-1}{(1+e^{-a_n})^2} (e^{-a_n})(-1)$$

$$\frac{\partial y_n}{\partial a_n} = \frac{e^{-a_n}}{(1+e^{-a_n})^2} = \frac{1}{1+e^{-a_n}} \frac{e^{-a_n}}{1+e^{-a_n}} = y_n (1-y_n)$$

Derivatives

$$a_n = w^T x_n$$

$$a_n = w_0 x_{n0} + w_1 x_{n1} + w_2 x_{n2} + \dots$$

$$\frac{\partial a_n}{\partial w_i} = x_{ni}$$

Putting them all together

$$\frac{\partial J}{\partial w_i} = -\sum_{n=1}^{N} \frac{t_n}{y_n} y_n (1 - y_n) x_{ni} - \frac{1 - t_n}{1 - y_n} y_n (1 - y_n) x_{ni}$$

$$\frac{\partial J}{\partial w_i} = -\sum_{n=1}^{N} t_n (1 - y_n) x_{ni} - (1 - t_n) y_n x_{ni}$$

$$\frac{\partial J}{\partial w_i} = -\sum_{n=1}^{N} [t_n - t_n y_n - y_n + t_n y_n] x_{ni}$$

$$\frac{\partial J}{\partial w_i} = \sum_{n=1}^{N} (y_n - t_n) x_{ni}$$

Vectorize

$$\frac{\partial J}{\partial w} = \sum_{n=1}^{N} (y_n - t_n) x_n$$

Vectorize More

Dot product is a sum over some index

X is N x D Y, T are N x 1

Multiply $X^T(Y - T)$:

Shape is $(D \times N)(N \times 1) \rightarrow (D \times 1)$

Which is the correct shape for w

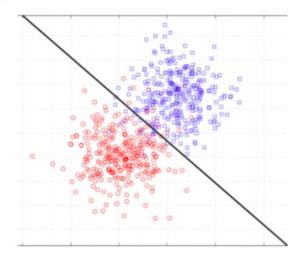
N gets summed over

$$a^T b = \sum_{n=1}^N a_n b_n$$

$$\frac{\partial J}{\partial w} = X^T (Y - T)$$

Generalization and Overfitting

- Recall our "Gaussian cloud" problem
- 2 clouds
- One centered at (2,2)
- Other centered at (-2,-2)
- Exact Bayesian solution was:
- W = [0, 4, 4]
- Represent as y = mx + b
- High school math!
- 0 + 4x + 4y = 0
- y = -x



$$y = -x$$

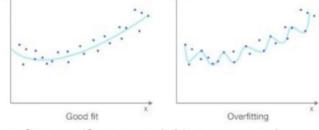
- Slope: -1, y-intercept: 0
- Why is the Bayesian solution (4, 4)?
- Why not (1, 1)? Why not (10, 10)?
- These all would represent the same line
- First hint at why we might need regularization

Objective function

- J = tlog(y) + (1-t)log(1-y)
- This y is the output of logistic regression
- Take a test point $(x_4, x_2) = (1, 1)$ and existing weights (0, 4, 4)
- Should be classified as 1
- $\sigma(0+4+4)=\sigma(8)=0.99966$
- What would be better? Exactly 1!
- With $y = \sigma(8)$, J = -0.00033540637289566265
- What if my weights are (0, 1, 1)? \rightarrow J = -0.12692801104297263
- Not as good
- What if my weights are (0, 10, 10)? $\rightarrow J = -2.0611536942919273e-09$
- The "best" weights are thus (0, infinity, infinity)
- In the computer, that's an error

Regularization

- People usually explain regularization in terms of overfitting (image on the right)
- But this is regression so it's not exactly applicable
- If your data fills up the space of
 all possible inputs, you shouldn't overfit even if your model is very complex



- That's why we want to have lots of data
- Your model overfits when it has to "guess" what the output should be in a space it's never seen
- But if the train set entirely covers all future test sets, then it's fine

Regularization

- This scenario is different we could have a perfectly split up dataset that covers the entire possible input space
- Logistic regression would still try to go to w = (0, infinity, infinity)
- Solution: regularization
- Penalizes very large weights
- Existing cost function: J = -[tlog(y) + (1 t)log(1 y)]
- Add a penalty for big weights:
- $J_{reg} = J + (\lambda/2)||w||^2 = J + (\lambda/2)w^Tw$
- Now we won't try to go to (0, 10, 10)
- λ = smoothing parameter (usually ~0.1, 1) but depends on your data
- No universal formula to choose (maybe, but too advanced for this class)

Regularization

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 Good fit
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Solving for w

- Still do gradient descent
- Now we want dJ_{reg} / dw instead of dJ / dw
- Addition doesn't affect other terms in derivative
- reg_cost = $(\lambda/2)(w_0^2 + w_1^2 + w_2^2 + ...)$
- d(reg_cost)/dw_i = λw_i
- In vector form: d(reg_cost)/dw = λw
- $dJ_{reg} / dw = X^{T}(Y T) + \lambda w$

Probabilistic Perspective

- Cross-entropy maximizes the likelihood, since J = -log(likelihood)
- Let's make J something we want to maximize:
- $J = +[t \log y + (1 t) \log(1 y)] (\lambda/2)||w||^2$
- $\exp(J) = y^{t}(1-y)^{(1-t)} \exp(-\lambda ||w||^{2}/2)$
- Exponentiate the first part: Bernoulli (the likelihood)
- Exponentiate -ve squared term: Gaussian (the prior)
- t ~ Bernoulli(y)
- $w \sim N(0, 1/\lambda)$

Probabilistic Perspective

- We have one probability distribution x another probability distribution
- Your first baby steps toward a Bayesian perspective of ML
- posterior ∝ likelihood x prior
- t ~ Bernoulli(y) → (likelihood)
- $w \sim N(0, 1/\lambda) \rightarrow (prior)$
- Our "prior belief" about w is that it's Gaussian distributed with variance 1/λ

Bayes rule

- $P(w|X, Y) \propto P(X, Y|w) P(w)$
- Just a consequence of:
- P(B|A) = P(A|B)P(B) / P(A) = P(A,B) / P(A)
- Bottom part is just $\Sigma_B P(A,B) = \Sigma_B P(A|B)P(B)$
- Without regularization, we maximize the likelihood
- With regularization, we maximize the posterior
- This is called "maximum a posteriori" or MAP estimation

Previously: you saw that even adding a column of <u>completely random noise</u> can improve R² In general, we want D << N (# features << # samples)

Skinny (D << N) (ideal)

Fat (D > N) (not ideal)

L1 Regularization

- L2 regularization used L2 norm for penalty term
- As you might guess, L1 regularization uses L1 norm for penalty term

$$J_{RIDGE} = -\sum_{n=1}^{N} (t_n log y_n + (1 - t_n) log (1 - y_n)) + \lambda ||w||_2^2$$

$$J_{LASSO} = -\sum_{n=1}^{N} (t_n log y_n + (1 - t_n) log (1 - y_n)) + \lambda ||w||_1$$

L1 Regularization

- This also puts a prior on w, so it's also a MAP estimation of w
- We can determine the distribution by taking the negative exponential of the penalty
- Laplace distribution

$$p(w) = \frac{\lambda}{2} exp\left(-\left.\lambda \middle| w \middle|\right)$$

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L1 Regularization

$$J = -\sum_{n=1}^{N} t_n log(y_n) + (1-t_n)log(1-y_n) + \lambda |w|$$

$$\partial J/\partial w = X^{T}(Y-T) + \lambda sign(w)$$

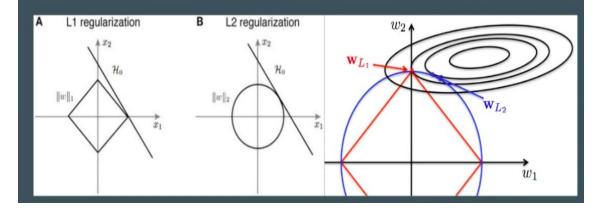
- sign(x) = 1 if x > 0, -1 if x < 0, 0 if x = 0
- Use the same gradient descent algorithm we've already been using

L1 vs L2 Regularization

- What's the difference?
- We'll look at the result first, then at how they emerge from the math
- L1: encourages a sparse solution (few w's non-zero, many equal to 0)
- L2: encourages small weights (all w's close to 0, but not exactly 0)
- Both help you prevent overfitting, by not fitting to noise
- L1 accomplishes this by choosing the most important features
- L2 accomplishes this by making the assertion that none of the weights are extremely large

L1 vs L2 Regularization

- I find this visualization awful, yet it's very commonly taught
- Contour plot of negative log-priors
- Ugh!

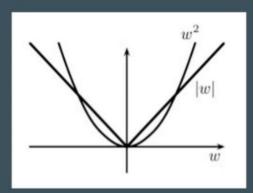


L1 vs L2 Regularization

Think of a 1-dimensional weight:

L2 penalty is quadratic, L1 is absolute function Key is the derivative (since the solution uses gradient descent)

Quadratic: as $w \to 0$, derivative $\to 0$ If w is already small, further gradient descent won't change it much



Absolute: derivative is always +/-1 (0 at w=0)

Doesn't matter where w is, it will fall at a constant rate

When it reaches 0, it stays there forever!

ElasticNet

• It's possible to include both L1 and L2 simultaneously (fancy name is ElasticNet)

$$J_{RIDGE} = J + \lambda_2 |w|^2$$

$$J_{LASSO} = J + \lambda_1 |w|$$

$$J_{ELASTICNET} = J + \lambda_1 |w| + \lambda_2 |w|^2$$

Outline of our sentiment analyzer

- We'll just look at the electronics category, but you can try the same code on others
- We could use 5 star targets to do regression, but let's just do classification since they are already marked "positive" and "negative"
- XML parser (BeautifulSoup)
- Only look at key "review_text"
- We'll need 2 passes, one to determine vocabulary size and which index corresponds to which word, and one to create data vectors
- After that, we can just use any SKLearn classifier as we did previously
- But we'll use logistic regression so we can interpret the weights

Skipping implementation details..

2-class problem vs. 7-class problem

- When we switch to softmax (which we will in Deep Learning part 1), will the problem get easier or harder?
- 2 class:
 - o Guess at random expect 50% error
- 7 class:
 - Guess at random expect 6/7 = 86% error
- K class: 1/K chance of being correct

Kaggle top score: ~70% correct

Normalize the data

- Images have pixel intensities 0... 255 (8 bit integers have 2^8 = 256 different possible values)
- We want to normalize these to be from 0... 1
- (Another way to normalize is z = (x mean) / stddev)
- Reason: sigmoid / tanh are most active in the -1... +1 range

Sensitivity and Specificity

- Used in medical field
- Sensitivity:

True positive rate = TPR = TP / (TP + FN)

Specificity:

True negative rate = TNR = TN / (TN + FP)

Precision and Recall

- Used in information retrieval
- Precision

```
TP / (TP + FP)
```

Recall

$$TP/(TP + FN)$$

Note: recall = sensitivity

F1-score

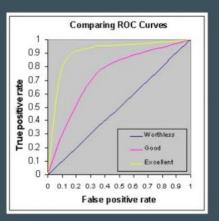
• Combines precision and recall into a balanced measure

```
F1 = 2 * (precision * recall) / (precision + recall)
```

Harmonic mean of precision and recall

ROC and AUC

- In logistic regression we use 0.5 as a threshold, makes sense because P(Y=1|X) > 0.5 → guess 1, P(Y=1|X) < 0.5 → guess 0
- But we can use any threshold
- Different thresholds → different TPR and FPR
- Receiver operating characteristic (ROC curve is a plot of these for every value of threshold between 0 and 1)
- Area under curve = AUC
 - 1 = perfect classifier, 0.5 = random guessing

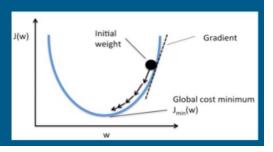


Unsupervised Machine Learning

Hidden Markov Models in Python LazyProgrammer

Gradient Descent Tutorial

- Optimization method
- Used extensively in deep learning, useful in a wide variety of situations
- Idea:
- You have a function you want to minimize, J(w) = cost or error
- Can maximize things too, just switch signs



Example

 $J = w^2$

(we know min is at w = 0, but let's pretend we don't)

dJ/dw = 2w, set initial w = 20, learning rate = 0.1

Iteration 1: $w \leftarrow 20 - 0.1*40 = 16$

Iteration 2: $w \leftarrow 16 - 0.1*2*16 = 12.8$

Iteration 3: $w \leftarrow 12.8 - 0.1*2*12.8 = 10.24$

Why is it so important?

- As we progress in deep learning / machine learning, functions will get more complicated
- Regular neural networks with softmax → might take you few hours or days to get derivatives the first time
 - Hopefully you did your homework!
- Convolutional and Recurrent Networks → possible, but don't want to
- Theano / TensorFlow can calculate gradients for us
- Understand how it works, so you can use it on anything

Exercise

Try to optimize: $J(w_1, w_2) = w_1^2 + w_2^4$

Maximizing the likelihood is the same as minimizing the cross-entropy function.