ML & Neural Network Tutorial

ANAIS 2023

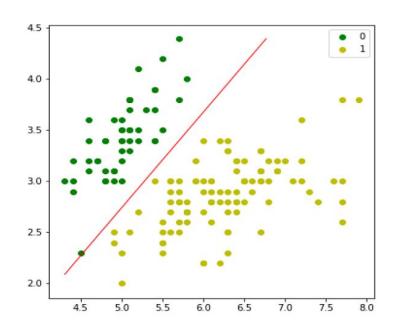
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Different types of ML algorithms

- KNNs
- Logistic regression
- Support vector machines (SVC / SVR)
- Random Forest
- Boosted trees
- Neural networks / Deep Learning

Linear model: Logistic regression

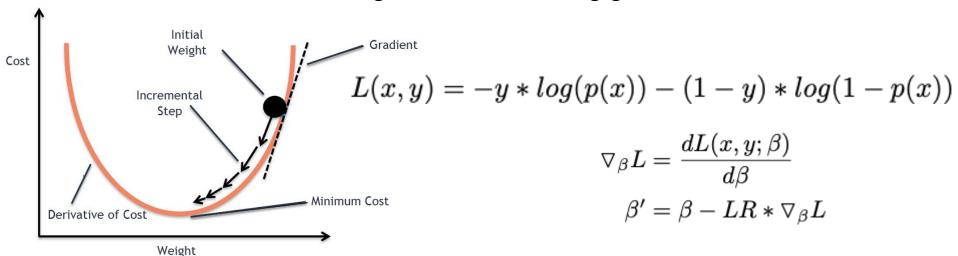
$$p(x) = \frac{1}{1 + e^{-\beta x}}$$



A line (in 2D) separates the 2 sets of points in a binary classification problem.

Finding the optimal parameters

- How to find the optimal beta?
- For 1-2 dimensions, we can do trial and error, but not scalable.
- We minimize the following loss function using gradient descent:



Gradient computation*

$$\begin{split} p(x) &= \frac{1}{1 + e^{-\beta x}} \\ L(x, y; \beta) &= -y ln(p(x)) - (1 - y) * ln(1 - p(x)) \\ \frac{dL(x, y; \beta)}{d\beta} &= \frac{dL(x, y; \beta)}{dp(x)} * \frac{dp(x)}{d\beta} \\ \frac{dL(x, y; \beta)}{dp(x)} &= -\frac{d}{dp(x)} (y ln(p(x)) - (1 - y) * ln(1 - p(x))) \\ &= -\frac{y}{p(x)} + \frac{1 - y}{1 - p(x)} \\ &= -\frac{y(1 - p(x)) + (y - 1)p(x)}{p(x)(1 - p(x))} \\ &= -\frac{y - p(x)}{p(x)(1 - p(x))} \end{split}$$

$$\frac{dp(x)}{d\beta} = \frac{d}{d(1 + e^{-\beta x})} (1 + e^{-\beta x})^{-1} * \frac{d(1 + e^{-\beta x})}{d\beta}$$

$$= -\frac{1}{(1 + e^{-\beta x})^2} (-xe^{-\beta x})$$

$$= p(x)^2 * \frac{x(1 - p(x))}{p(x)} = p(x)x(1 - p(x))$$

$$\frac{dL(x, y; \beta)}{d\beta} = p(x)x(1 - p(x)) * -\frac{(y - p(x))}{p(x)(1 - p(x))}$$

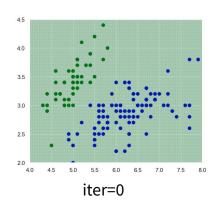
$$= -x(y - p(x))$$

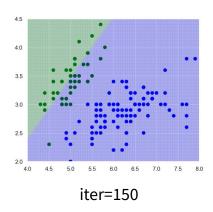
$$= x(p(x) - y)$$

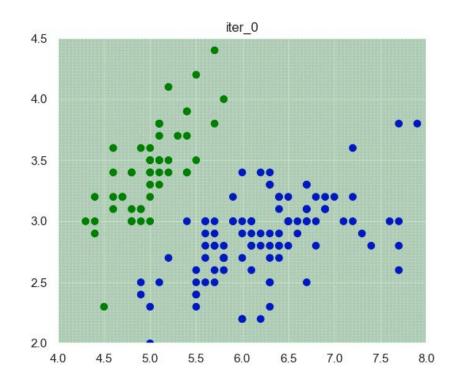
Gradient descent

- Initialize **beta** with some random values or **zero**.
- For each step:
 - Compute the gradient of the loss function at that value of beta, call it **grad**.
 - Update beta = beta LR * grad. Where LR is the learning.
 - Terminate if the magnitude of the change (grad) is too small or after **T** number of iterations.
- Learning rate (LR) can be adapted as steps progress. Higher in the beginning and slower later.
- Talso needs to be adapted depending on the problem.
- Gradient can be computed directly (exactly) or analytically using a small perturbation around the variable.

Gradient descent



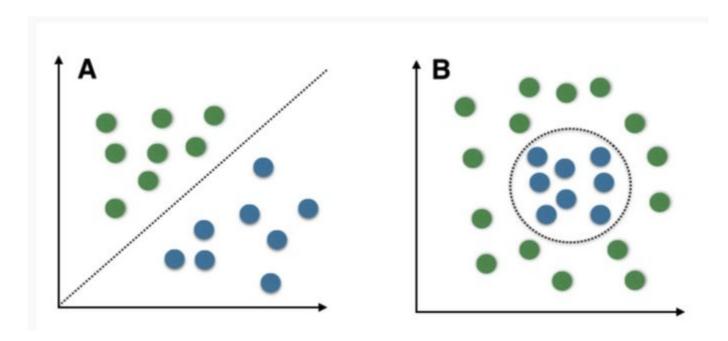




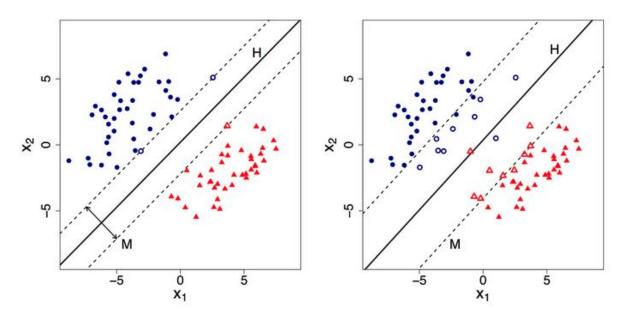
Exercise: implementing logistic

regression w gradient descent

Importance of non-linearity

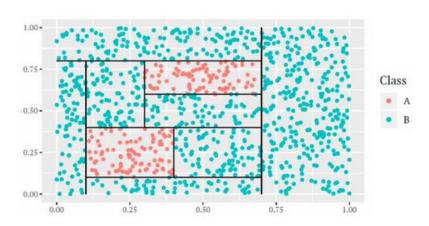


Support vector machines



Hard margin (left) and soft margin (right) SVMs.

Tree based methods



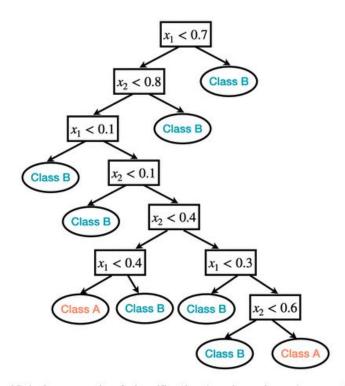


Figure 13.1: An example of classification tree based one two predictors.

Neural network: backpropagation

- Gradient descent is used to optimize the parameters for neural networks as well.
- More specifically, **stochastic gradient descent**, is used:
 - This just means gradient descent is done in a 'random' portion of the data called the batch.
- Backpropagation is used to propagate the gradient back to the layers and update weights.

Summary: the equations of backpropagation

$$\delta^L = \nabla_a C \odot \sigma'(z^L) \tag{BP1}$$

$$\delta^l = ((w^{l+1})^T \delta^{l+1}) \odot \sigma'(z^l)$$
 (BP2)

$$\frac{\partial C}{\partial b_j^l} = \delta_j^l$$
 (BP3)

$$\frac{\partial C}{\partial w_{jk}^{l}} = a_k^{l-1} \delta_j^{l} \tag{BP4}$$

Neural network: backpropagation

Feedforward part:

for i in range(len(layers)):

$$a(i) = o(i-1).w[i]$$

$$o(i) = \frac{1}{1 + e^{-a(i)}}$$

$$= sigmoid(a(i))$$

Backpropagate part:

```
for the output layer:
error[L] = o[L] - y
grad[L] = error * sigmoid_deriv(o[L])
for other layers:
error[i] = grad[i+1].W[i]
grad[i] = error[i] * sigmoid_deriv(o[i])
```

algorithm.

components of the backpropagation

Exercise: looking at different