Softmax regression

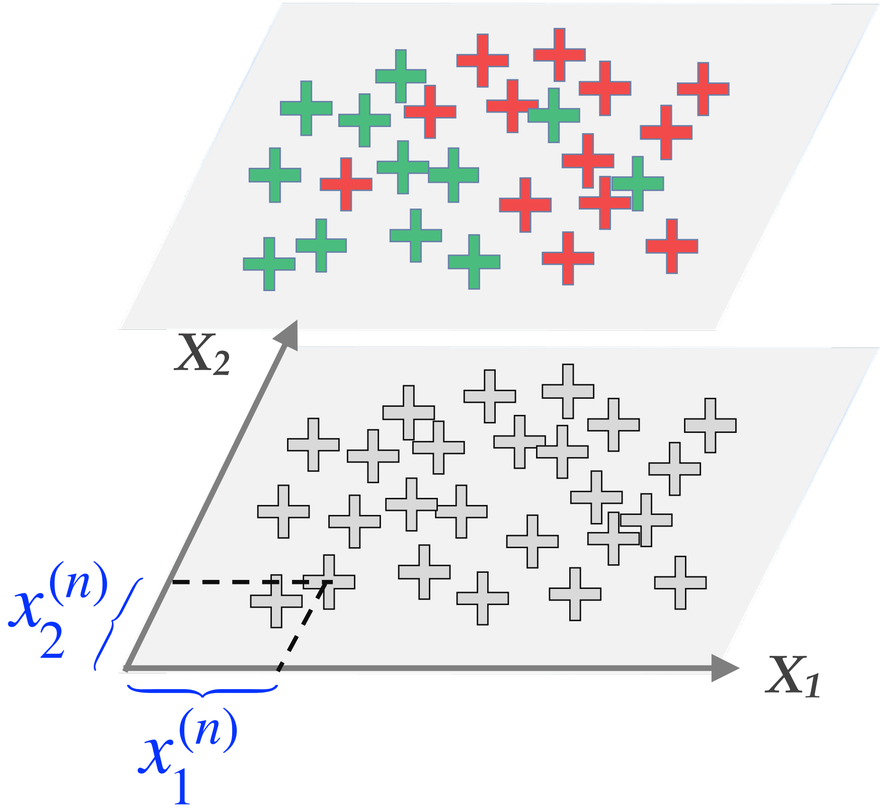
Classification by minimising cross-entropy loss

Srinandan Dasmahapatra

Classification: discrete output

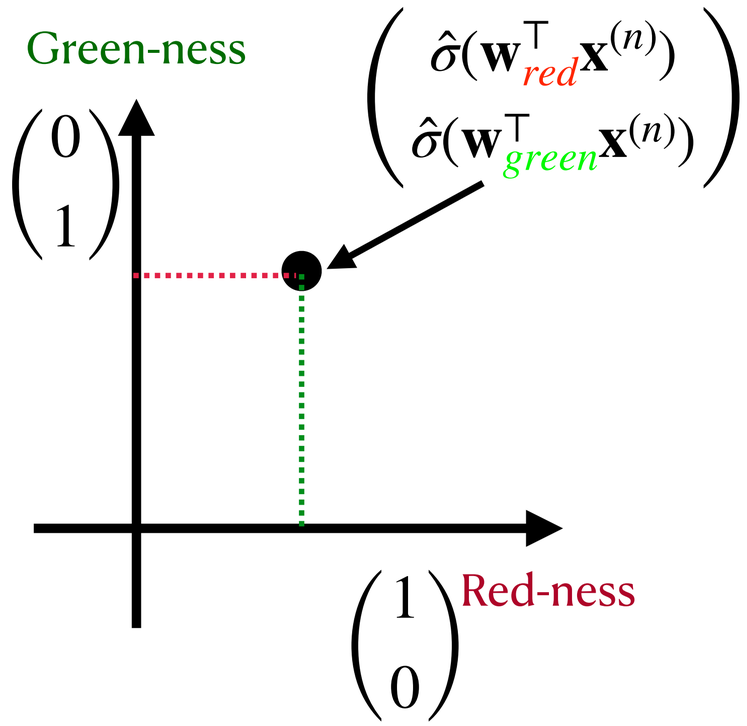
Minimise deviation of prediction from annotation

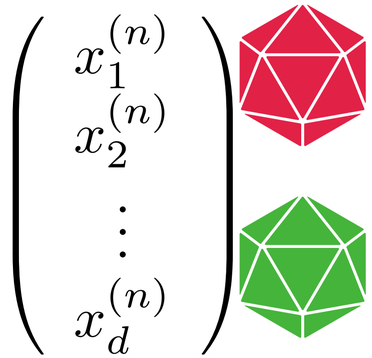
- Given training set represented by points labelled green and red, variable Y ...
- ... where each point has two featu
  $\mathscr{D} := \{((x_1{}^{(n)}, x_2{}^{(n)}), y^{(n)}) \mid n = 1,$
- Task: find function $f(x_1{}^{(n)}, x_2{}^{(n)}) = \hat{y}^{(n)}$ that reproduces given labels



Analogy with seeing in colour

Opsins (photopigments) in cones respond to colour preferentially



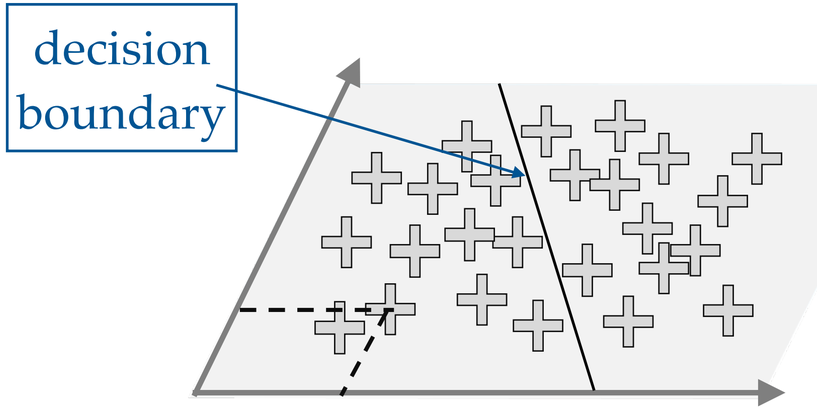


$\mathbf{w}_{red} := (w_{red,1}, w_{red,2}, \ldots, w_{red,d})$

$\mathbf{w}_{green} := (w_{green,1}, w_{green,2}, \ldots, w_{green,d})$

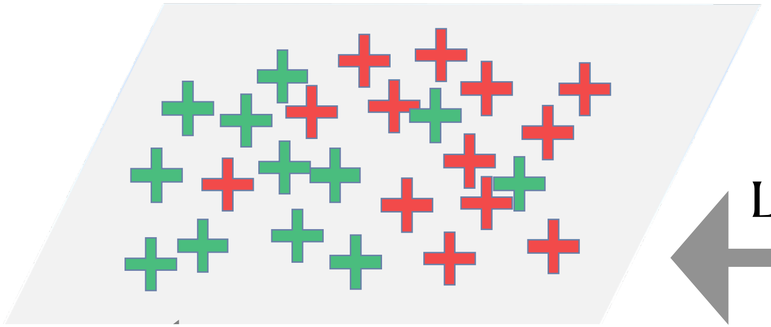
Find equation for decision boundary

Assign probability for each point being green/red



$$f(x_1, x_2; \mathbf{w}) = w_0 + w_1 x_1 + w_2 x_2$$

$$\sigma(f) = \frac{1}{1 + \exp(-f)}$$



Learning = adjusting weights until agreement with data

Constructing scale for comparing predictions with training labels

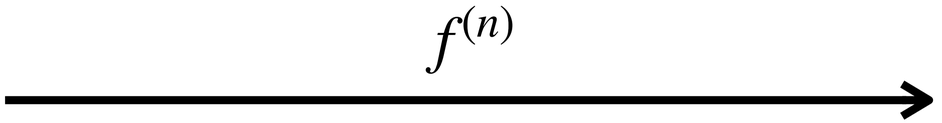
- Output $f(\mathbf{x}^{(n)}; \mathbf{w}^i) \triangleq f_i^{(n)}$, $i =$ red/green, $C = 2$,
- $0 \leq \sigma(f_i^{(n)}) \leq 1$ probability, with $\sum_{i=1}^{C} \sigma(f_i^{(n)}) = 1$
- Let $\hat{y}_i^{(n)} = \sigma(f_i^{(n)})$
- $y^{(n)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ or $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ for red/green
- Evaluation of classification: cost($y^{(n)}, \hat{y}^{(n)}$)
- Compare two different costs — quadratic and logarithmic
- Logarithm penalises mistakes more, also has a sharper drop (large gradient to guide weights to lower loss)

$\hat{y}^{(n)} = \sigma(f^{(n)})$

0.5

$-y^{(n)} \ln \hat{y}^{(n)}$

$y^{(n)} - \hat{y}^{(n)})^2$



For a one component (scalar) output

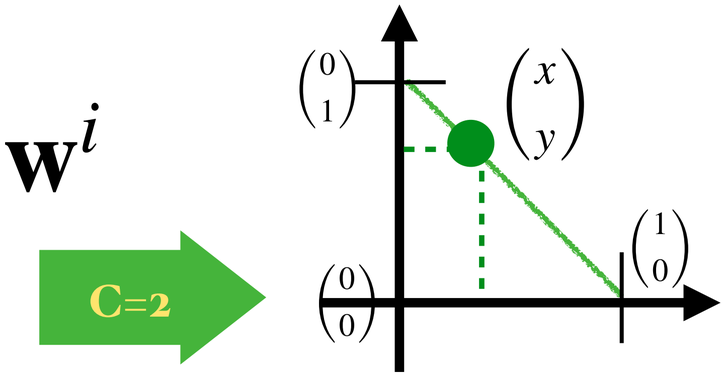
Multiclass classification

Input: images 32 x 32 x 3 dimensions, Output: one-hot encodings: 10 dimensions

CIFAR-10: Example dataset for multi class classification

$$\text{CAT} \mapsto \mathbf{e}_4 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad \text{SHIP} \mapsto \mathbf{e}_9 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

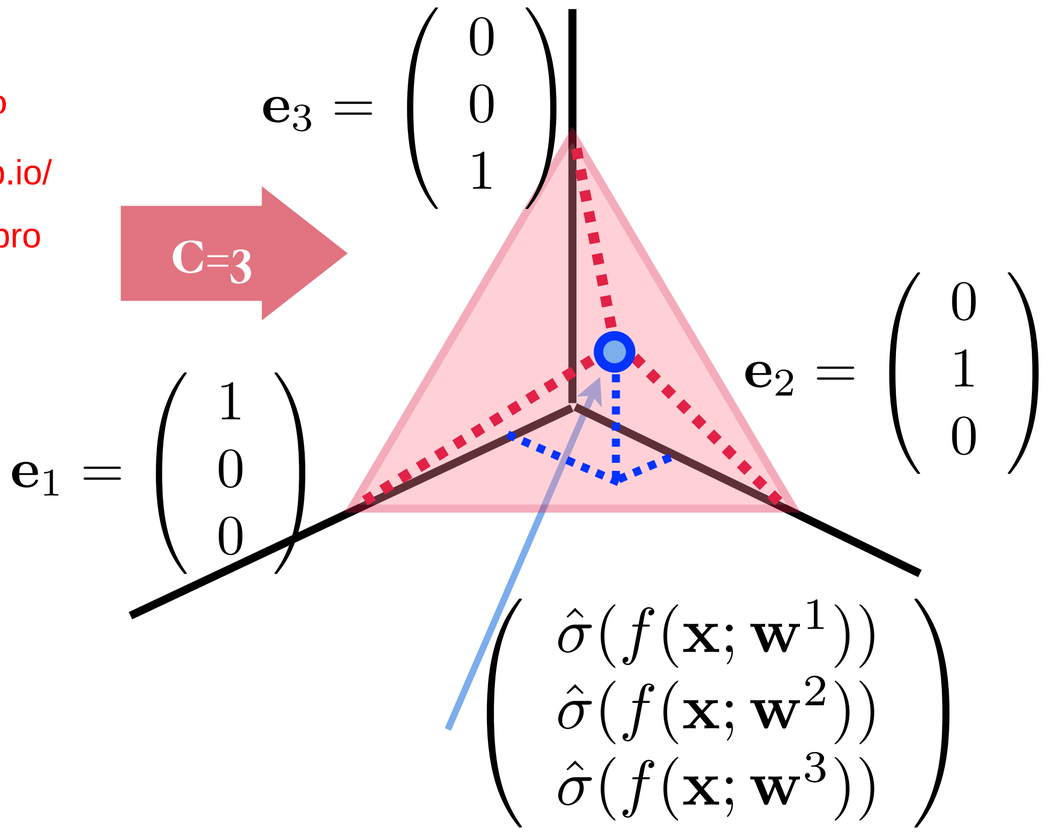
C-classes C different weight vectors $\mathbf{w}^i$



- For each input vector (say a representation of an image or sound file), produce an output on the (C-1)-dimensional surface embedded in C-dimensional Euclidean space

- Cost for input $\mathbf{x}^{(n)}$ = measure of mismatch between C-dimensional prediction $\hat{\sigma}(f(\mathbf{x}^{(n)}; \mathbf{w}^i))$ and true label $\mathbf{e}_i$

- Hat $\hat{\cdot}$ on $\hat{\sigma}$ indicates normalisation: entries add up to one: $\hat{\sigma}(f(\mathbf{x}; \mathbf{w}^1)) + \hat{\sigma}(f(\mathbf{x}; \mathbf{w}^2)) + \hat{\sigma}(f(\mathbf{x}; \mathbf{w}^3)) = 1$



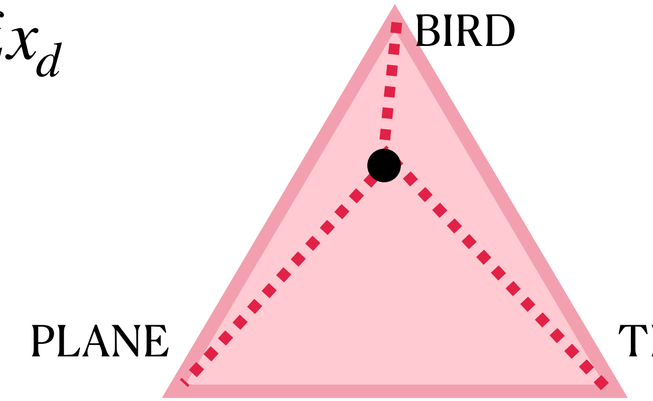
Multiclass classification

Weight vectors for each class

- $\mathbf{w}^c = (w_0^c, w_1^c, \ldots, w_d^c), c = 1,\ldots, C$.
- C - number of classes, 10 for CIFAR-10
- d - dimensionality of data, $\mathbf{x} = (x_1, x_2, \ldots, x_d)$
- $f(\mathbf{x}; \mathbf{w}^c) = w_0^c \cdot 1 + w_1^c x_1 + \cdot + w_d^c x_d$
  : for each input data point, compute output for all classes

$$\begin{pmatrix} w_0^{\text{PLANE}} & w_1^{\text{PLANE}} & \cdots & w_d^{\text{PLANE}} \\ \vdots & \vdots & \ddots & \vdots \\ w_0^{\text{BIRD}} & w_1^{\text{BIRD}} & \cdots & w_d^{\text{BIRD}} \\ \vdots & \vdots & \ddots & \vdots \\ w_0^{\text{TRUCK}} & w_1^{\text{TRUCK}} & \cdots & w_d^{\text{TRUCK}} \end{pmatrix} \begin{pmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ \vdots \\ x_{d-1} \\ x_d \end{pmatrix}$$

$d+1$ (over the matrix), C (left of the matrix), $d+1$ (right of the vector)



$$\begin{pmatrix} \hat{\sigma}(f(\mathbf{x}; \mathbf{w}^{\text{PLANE}})) \\ \hat{\sigma}(f(\mathbf{x}; \mathbf{w}^{\text{BIRD}})) \\ \hat{\sigma}(f(\mathbf{x}; \mathbf{w}^{\text{TRUCK}})) \end{pmatrix}$$

Set up gradient descent of loss for classification

Re-phrasing what has been done

- For each class each data point $\mathbf{x}^{(n)}$ is assigned a score $s_c^{(n)} = f(\mathbf{x}^{(n)}; \mathbf{w}^c), c = 1, \ldots, C$
- Choose the largest of the C scores as the predicted class for $\mathbf{x}^{(n)}$
  - $c^* = \arg \max_{c \in \{1,\ldots,C\}} s_c^{(n)}$

- Replace max by softmax: $\max(s_1, s_2, s_3) \longrightarrow \text{softmax}(s_1, s_2, s_3) = \ln(e^{s_1} + e^{s_2} + e^{s_3})$
- Exponential function: monotonic in argument ($x \nearrow \implies e^x \nearrow$)
- Normalise exponential scores: $s_c^{(n)} \mapsto \dfrac{e^{s_c^{(n)}}}{e^{s_1^{(n)}} + e^{s_2^{(n)}} + \cdots + e^{s_C^{(n)}}} =: \hat{\sigma}(s_c^{(n)}) = [\hat{y}^{(n)}]_c$
- Treat component c of $[\hat{y}^{(n)}]_c = \hat{\sigma}(s_c^{(n)})$ as probability that $\mathbf{x}^{(n)}$ belongs to class c : $P(c \mid \mathbf{x}^{(n)})$

Multi-class loss function: cross entropy

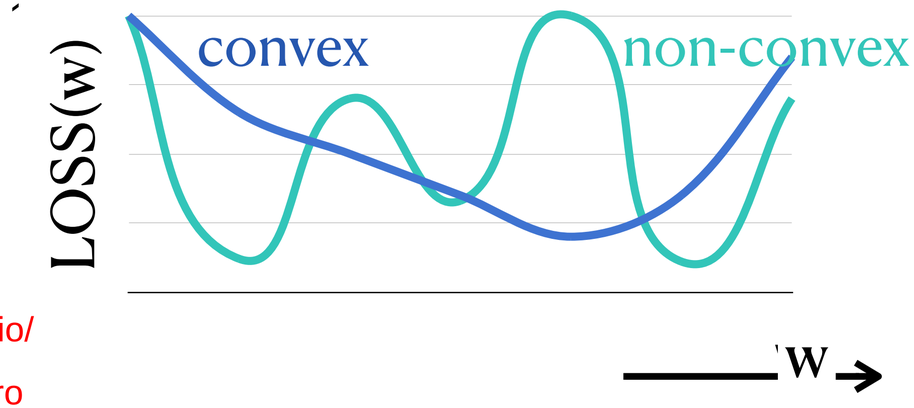
Measures information about label distribution from input data and choice of weights

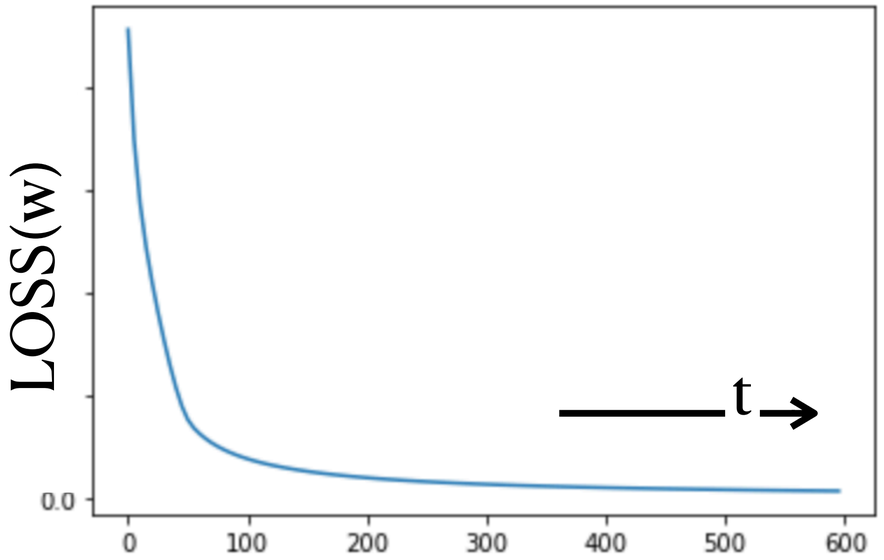
- For each data point $\mathbf{x}^{(n)}$ sum over costs $-\sum_{c=1}^{C} y_c^{(n)} \ln \hat{y}_c^{(n)}$ for all classes
- Sum costs over all data points $L(\mathbf{W}) := L(\{\mathbf{w}_c\}) = \sum_{n=1}^{N} \sum_{c=1}^{C} y_c^{(n)} \ln \hat{y}_c^{(n)}$, called cross-entropy.
- **Eg**: target $y^{(n)} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$ prediction $\hat{y}^{(n)} = \begin{pmatrix} \hat{y}_1^{(n)} \\ \hat{y}_2^{(n)} \\ \hat{y}_3^{(n)} \\ \hat{y}_4^{(n)} \end{pmatrix} : -(0 \cdot \ln \hat{y}_1^{(n)} + 1 \cdot \ln \hat{y}_2^{(n)} + 0 \cdot \ln \hat{y}_3^{(n)} + 0 \cdot \ln \hat{y}_4^{(n)}) = -\ln \hat{y}_2^{(n)}$
- $L(\mathbf{W}) = -\ln \left(\hat{y}_{c_1}^{(1)} \cdot \hat{y}_{c_2}^{(2)} \cdots \hat{y}_{c_N}^{(N)} \right) = -\sum_{n=1}^{N} \ln \hat{y}_{c_n}^{(n)}$: reduce negative of log(predicted probabilities)

Gradient descent on cross-entropy finds optimal weights

For linear maps *f*, cross-entropy is convex

- Learning: Reduce $L(\mathbf{W})$ by changing weights
- $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla_{\mathbf{w}} L(\mathbf{W})$
- **All** weights are contained in $\mathbf{w}$
- Jupyter notebook





Example: data x; 2-class problem

Compare probability assignment for arg max with arg softmax

$$\frac{f[0,(s-5)]}{f[0,(s-5)]+f[0,-(s-5)]}$$

- f=Max
- f=Softmax