Multi-Class Classification

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Multi-class classification

Multi-class classification

- *classification* is *multi-class* when raw output variable v is a *categorical* $v \in \mathcal{V} = \{v_1, \ldots, v_K\}$ with $K > 2$
- v_i are called *classes* or *labels*
- we'll also denote them as $1, \ldots, K$
- examples:
  - $\mathcal{V} = \{\textsc{yes}, \textsc{maybe}, \textsc{no}\}$
  - $\mathcal{V} = \{\textsc{albania}, \textsc{azerbaijan}, \ldots\}$
  - $\mathcal{V} = \{\textsc{hindi}, \textsc{tamil}, \ldots\}$
  - $\mathcal{V} =$ set of English words in some dictionary
  - $\mathcal{V} =$ set of $m!$ possible orders of m horses in a race
- a *classifier* predicts label $\hat{v}$ given raw input u
- called a *K-class classifier*

Confusion matrix

Confusion matrix

- measure performance of a specific predictor on a data set with n records
- for each data record i, there are K^2 possible values of $(\hat{v}^i, v^i)$
- $K \times K$ *confusion matrix* is defined by

$$C_{ij} = \# \text{ records with } \hat{v} = v_i \text{ and } v = v_j$$

- entries in C add up to n
- column sums of C give number of records in each class in the data set
- C_{ii} is the number of times we predict v_i correctly
- C_{ij} for $i \neq j$ is the number of times we mistook v_j for v_i
- there are $K(K-1)$ different types of errors we can make
- there are $K(K-1)$ different *error rates*, C_{ij}/n, $i \neq j$

Neyman-Pearson error

- $E_j = \sum_{i \neq j} C_{ij}$ is number of times we mistook v_j for another class
- E_j/n is the error rate of mistaking v_j
- we will scalarize these K error rates using a weighted sum
- the *Neyman-Pearson error* is

$$\sum_{j=1}^{K} \kappa_j E_j = \sum_{i \neq j} \kappa_j C_{ij}$$

  where κ is a weight vector with nonnegative entries
- κ_j is how much we care about mistaking v_j
- for $\kappa_j = 1$ for all i, Neyman-Pearson error is the *error rate*

Embedding

Embedding v

- we embed raw output $v \in \mathcal{V}$ into $\mathbf{R}^m$ as $y = \psi(v) \in \mathbf{R}^m$ (*cf.* boolean classification, where we embed v into $\mathbf{R}$)
- we can describe ψ by the K vectors $\psi_1 = \psi(v_1), \ldots, \psi_K = \psi(v_K)$ (*i.e.*, just say what vector in $\mathbf{R}^m$ each $v \in \mathcal{V}$ maps to)
- we call the vector ψ_i the *representative* of v_i
- we call the set $\{\psi_1, \ldots, \psi_K\}$ the *constellation*
- examples:
  - $\text{TRUE} \mapsto 1$, $\text{FALSE} \mapsto -1$
  - $\text{YES} \mapsto 1$, $\text{MAYBE} \mapsto 0$ $\text{NO} \mapsto -1$
  - $\text{YES} \mapsto (1,0)$, $\text{MAYBE} \mapsto (0,0)$, $\text{NO} \mapsto (0,1)$
  - $\text{APPLE} \mapsto (1,0,0)$, $\text{ORANGE} \mapsto (0,1,0)$, $\text{BANANA} \mapsto (0,0,1)$
  - (Horse 3, Horse 1, Horse 2) $\mapsto (3,1,2)$
  - `word2vec` (maps 1M words to vectors in $\mathbf{R}^{300}$)

One-hot embedding

- a simple generic embedding of K classes into $\mathbf{R}^K$
- $\psi(v_i) = \psi_i = e_i$

- variation (embedding K classes into $\mathbf{R}^{K-1}$):
  - choose one of the classes as the *default*, and map it to $0 \in \mathbf{R}^{K-1}$
  - map the others to the unit vectors $e_1, \ldots, e_{K-1} \in \mathbf{R}^{K-1}$

Nearest neighbor un-embedding

- given prediction $\hat{y} \in \mathbf{R}^m$, we *un-embed* to get $\hat{v}$
- we denote our un-emdedding using the symbol $\psi^\dagger : \mathbf{R}^m \to \mathcal{V}$
- we *define* the un-embedding function $\psi^\dagger$ as

$$\psi^\dagger(\hat{y}) = \underset{v \in \mathcal{V}}{\operatorname{argmin}} \, ||\hat{y} - \psi(v)||$$

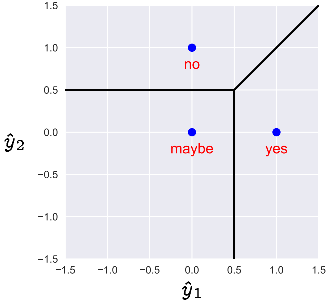
  (we can break ties any way we like)
- *i.e.*, we choose the raw value associated with the nearest representative
- called *nearest neighbor un-embedding*

Un-embedding boolean

- embed $\textsc{true} \mapsto 1 = \psi_1$ and $\textsc{false} \mapsto -1 = \psi_2$
- un-embed via

$$\psi^\dagger(\hat{y}) = \begin{cases} \textsc{true} & \hat{y} \geq 0 \\ \textsc{false} & \hat{y} < 0 \end{cases}$$

Un-embedding yes, maybe, no



- embed YES $\mapsto (1, 0)$, MAYBE $\mapsto (0, 0)$, NO $\mapsto (0, 1)$
- un-embed via

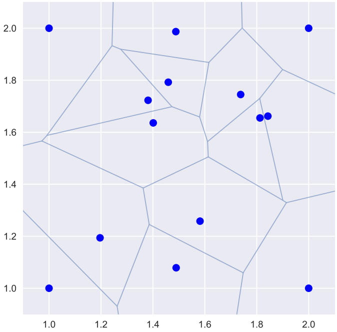
$$\psi^\dagger(\hat{y}) = \begin{cases} \text{YES} & \hat{y}_1 > 1/2,\ \hat{y}_1 > \hat{y}_2 \\ \text{MAYBE} & \hat{y}_1 < 1/2,\ \hat{y}_2 < 1/2 \\ \text{NO} & \hat{y}_2 > 1/2,\ \hat{y}_1 < \hat{y}_2 \end{cases}$$

(can choose any value on boundaries)

Un-embedding one-hot

- one-hot embedding: $\psi_i = e_i$, $i = 1, \ldots, K$
- un-embed via $\psi^\dagger(y) = \mathtt{argmin}_i \, \|y - e_i\|_2 = \mathtt{argmax}_i \, y_i$
- intuition:
  - you can subtract one from one component of a vector
  - to get the smallest norm
  - best choice is the largest entry of the vector

Voronoi diagram



- $\psi^\dagger$ *partitions* $\mathbf{R}^m$ into the K regions $\{y \mid \psi^\dagger(y) = v_i\}$, for $i = 1, \ldots, K$
- regions are *polyhedra*
- called *Voronoi diagram*
- boundaries between regions are perpendicular bisectors between pairs of representatives ψ_i, ψ_j

Margins

Margins and decision boundaries

- given prediction $\hat{y} \in \mathbf{R}^m$, we un-embed via $\hat{v} = \psi^\dagger(\hat{y})$
- $\psi^\dagger(\hat{y}) = v_j$ when $\hat{y}$ is closer to ψ_j than the other representatives, *i.e.*,

$$\|\hat{y} - \psi_j\| < \|\hat{y} - \psi_i\| \text{ for } i \neq j$$

- define the *negative margin* function M_{ij} by

$$\begin{aligned} M_{ij}(\hat{y}) &= \left(\|\hat{y} - \psi_j\|^2 - \|\hat{y} - \psi_i\|^2\right) / \left(2\|\psi_i - \psi_j\|\right) \\ &= \frac{2(\psi_i - \psi_j)^\mathsf{T}\hat{y} + \|\psi_j\|^2 - \|\psi_i\|^2}{2\|\psi_i - \psi_j\|} \end{aligned}$$

- so $\psi^\dagger(\hat{y}) = v_j$ when $M_{ij}(\hat{y}) < 0$ for all $i \neq j$

Margins and decision boundaries

- linear equation

$$M_{ij}(\hat{y}) = 0$$

  defines a *hyperplane* called the *perpendicular bisector* between ψ_i and ψ_j

- it is the *decision boundary* between ψ_i and ψ_j
- $\hat{y}$ is the correct prediction, when $v = v_j$, if

$$\max_{i \neq j} M_{ij}(\hat{y}) < 0$$

Margins and decision boundaries

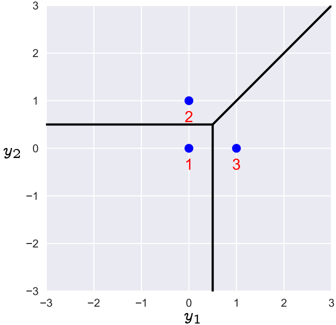
- boolean: $\psi_1 = -1$ and $\psi_2 = 1$ and

$$M_{21}(\hat{y}) = \hat{y} \qquad M_{12}(\hat{y}) = -\hat{y}$$

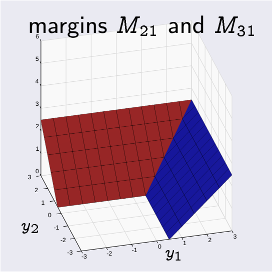
- one-hot: $\psi_j = e_j$ for all j, so

$$M_{ij} = \frac{y_i - y_j}{\sqrt{2}}$$

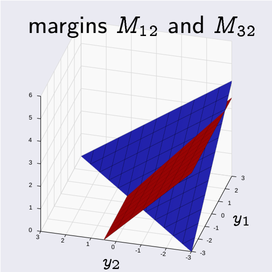
Margins



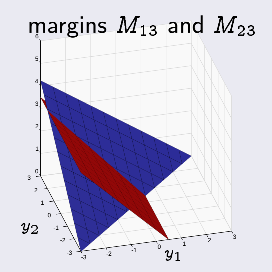
2
1
3
y_2
y_1



margins M_{21} and M_{31}
y_2
y_1



margins M_{12} and M_{32}
y_1
y_2



margins M_{13} and M_{23}
y_2
y_1

Vector ERM

Vector prediction

- after embedding raw data u and v we have data pair (x, y)
- the target y is a *vector* (which takes only the values $\psi_1, \ldots, \psi_K$)
- predictor is a function $g : \mathbf{R}^d \to \mathbf{R}^m$
- our final (raw) prediction is $\hat{v} = \psi^\dagger(\hat{y})$

Vector linear predictor

- *vector linear predictor* has form $\hat{y} = g(x) = \theta^{\mathsf{T}} x$
- same form as when y is a scalar, but here θ is a $d \times m$ *parameter matrix*
- θ_{23} is how much x_2 affects $\hat{y}_3$
- reduces to the usual parameter vector when $m = 1$ (*i.e.*, y is scalar)

Vector ERM

- linear model $\hat{y} = \theta^T x$, $\theta \in \mathbf{R}^{d \times m}$
- choose parameter matrix θ to minimize $\mathcal{L}(\theta) + \lambda r(\theta)$
- $\mathcal{L}(\theta)$ is the empirical risk

$$\mathcal{L}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(\hat{y}^i, y^i) = \frac{1}{n} \sum_{i=1}^{n} \ell(\theta^T x^i, y^i)$$

  with loss function $\ell : \mathbf{R}^m \times \mathbf{R}^m \to \mathbf{R}$ (*i.e.*, ℓ takes two arguments, each in $\mathbf{R}^m$)

- $\lambda \geq 0$ is regularization parameter
- $r(\theta)$ is the regularizer

Derivative of the empirical risk

- loss $\mathcal{L}(\theta) = \frac{1}{n}\sum_{i=1}^{n} \ell(\theta^{\mathsf{T}} x^{i}, y^{i})$
- we'd like to apply the gradient method
- $D\mathcal{L}(\theta)$ is the derivative of $\mathcal{L}$ with respect to θ (a matrix)
- we have

$$\big(D\mathcal{L}(\theta)\big)_{ij} = \frac{\partial \mathcal{L}(\theta)}{\partial \theta_{ij}}$$

- then the first-order Taylor approximation is

$$\mathcal{L}(\theta + \delta\theta) \approx \mathcal{L}(\theta) + \mathrm{trace}(D\mathcal{L}(\theta)^{\mathsf{T}} \delta\theta)$$

- we have

$$D\mathcal{L}(\theta) = \frac{1}{n}\sum_{i=1}^{n} x^{i} \big(\nabla_1 \ell(\theta^{\mathsf{T}} x^{i}, y^{i})\big)^{\mathsf{T}}$$

  where ∇_1 means the gradient with respect to the first argument

Matrix regularizers

Matrix regularizers

- general penalty regularizer: $r(\theta) = \sum_{i=1}^{d} \sum_{j=1}^{m} q(\theta_{ij})$
- sum square regularizer: $r(\theta) = ||\theta||_F^2 = \sum_{i=1}^{d} \sum_{j=1}^{m} \theta_{ij}^2$
- the *Frobenius norm* of a matrix θ is $\left(\sum_{i,j} \theta_{ij}^2\right)^{1/2}$
- sum absolute or ℓ_1 regularizer: $r(\theta) = ||\theta||_1 = \sum_{i=1}^{d} \sum_{j=1}^{m} |\theta_{ij}|$

Multi-class loss functions

Multi-class loss functions

- $\ell(\hat{y}, y)$ is how much prediction $\hat{y}$ bothers us when observed value is y
- but the only possible values of y are $\psi_1, \ldots, \psi_K$
- so we can simply give the K functions of $\hat{y}$

$$\ell(\hat{y}, \psi_j), \quad j = 1, \ldots, K$$

- $\ell(\hat{y}, \psi_j)$ is how much we dislike predicting $\hat{y}$ when $y = \psi_j$

Neyman-Pearson loss

- Neyman-Pearson loss is

$$\ell^{\mathrm{NP}}(\hat{y}, \psi_j) = \begin{cases} 0 & \text{if } \max_{i \neq j} M_{ij} < 0 \\ \kappa_j & \text{otherwise} \end{cases}$$

- Neyman-Pearson risk $\mathcal{L}^{\mathrm{NP}}(\theta)$ is the Neyman-Pearson error
- but $\nabla \mathcal{L}^{\mathrm{NP}}(\theta)$ is either zero or undefined
- so there's no gradient to tell us which way to change θ to reduce $\mathcal{L}(\theta)$

Proxy loss

- we will use a *proxy loss* that
  - approximates, or at least captures the flavor of, the Neyman-Pearson loss
  - is more easily optimized (*e.g.*, is convex or has nonzero derivative)

- we want a proxy loss function
  - with $\ell(\hat{y}, \psi_j)$ small whenever $M_{ij} < 0$ for $i \neq j$
  - and not small otherwise
  - which has other nice characteristics, *e.g.*, differentiable or convex

Multi-class hinge loss

- *hinge loss* is

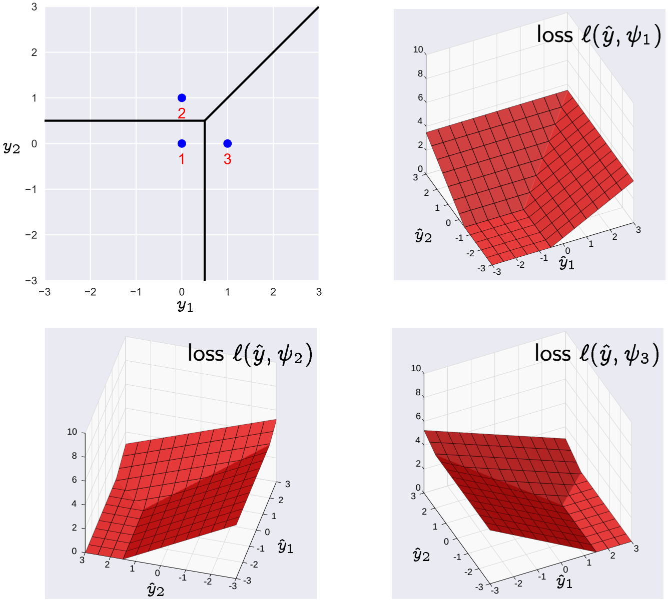
$$\ell(\hat{y}, \psi_j) = \kappa_j \max_{i \neq j} (1 + M_{ij}(\hat{y}))_+$$

- $\ell(\hat{y}, \psi_j)$ is zero when the correct prediction is made, with a margin at least one
- convex but not differentiable
- for boolean embedding with $\psi_1 = -1$, $\psi_2 = 1$, reduces to

$$\ell(\hat{y}, -1) = \kappa_1 (1 + \hat{y})_+, \qquad \ell(\hat{y}, 1) = \kappa_2 (1 - \hat{y})_+$$

  usual hinge loss when $\kappa_1 = 1$

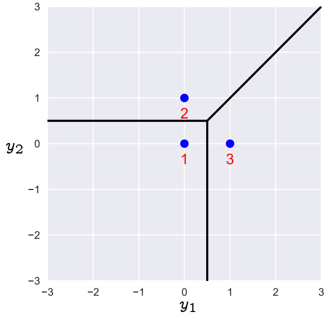
Multi-class hinge loss

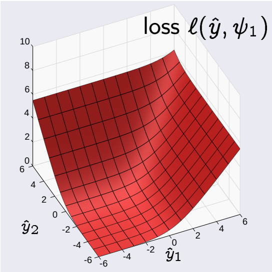


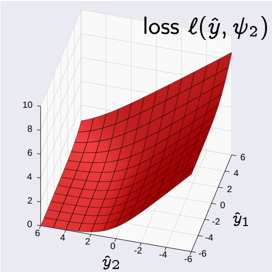
Multi-class logistic loss

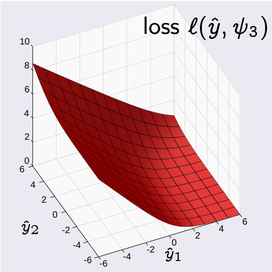
- *logistic loss* is
$$\ell(\hat{y}, \psi_j) = \kappa_j \log \left(\sum_{i=1}^{K} \exp(M_{ij}(\hat{y})) \right)$$
- recall that $M_{jj} = 0$
- convex and differentiable
- for boolean embedding with $\psi_1 = -1$, $\psi_2 = 1$, reduces to
$$\ell(\hat{y}, -1) = \kappa_1 \log(1 + e^{\hat{y}}), \qquad \ell(\hat{y}, 1) = \kappa_2 \log(1 + e^{-\hat{y}})$$
usual logistic loss when $\kappa_1 = 1$

Multi-class logistic loss









Soft-max function

- the function $f : \mathbf{R}^n \to \mathbf{R}$

$$f(x) = \log \sum_{i=1}^{n} \exp(x_i)$$

  is called the *log-sum-exp* function

- it is a convex differentiable approximation to the max function

- we have

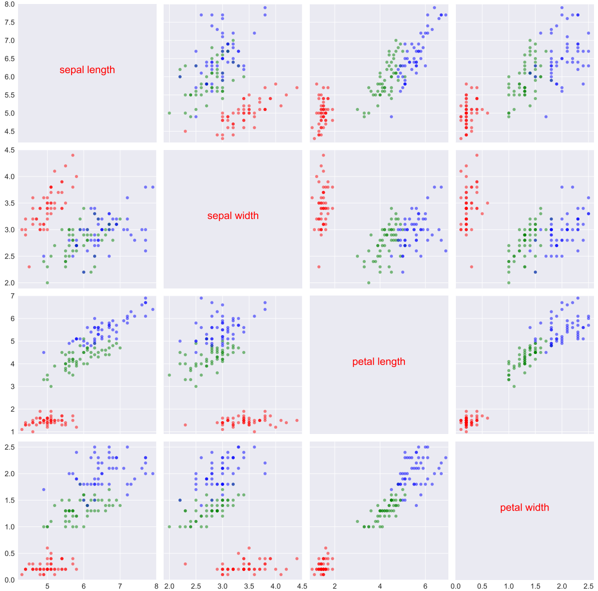
$$\max\{x_1, \ldots, x_n\} \leq f(x) \leq \max\{x_1, \ldots, x_n\} + \log(n)$$

Example: Iris

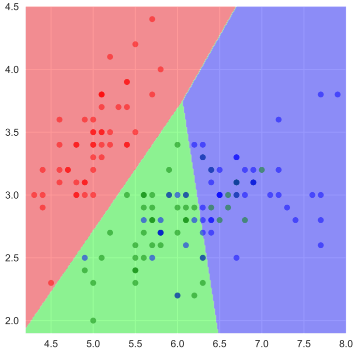
Example: Iris

- famous example dataset by Fisher, 1936
- measurements of 150 plants, 50 from each of 3 species
- iris setosa, iris versicolor, iris virginica
- four measurements: sepal length, sepal width, petal length, petal width

Example: Iris

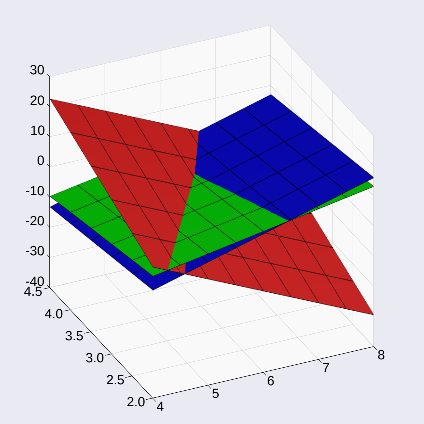


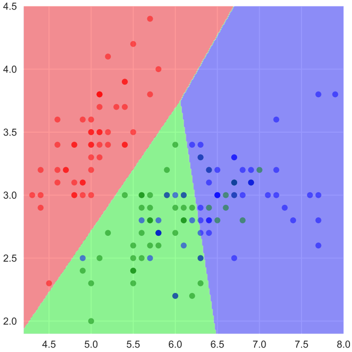
Classification with two features



- using only `sepal_length` and `sepal_width`
- one-hot embedding, multi-class logistic loss
- confusion matrix $C = \begin{bmatrix} 50 & 0 & 0 \\ 0 & 38 & 13 \\ 0 & 12 & 37 \end{bmatrix}$

Classification with two features





- let θ_i be the ith column of θ
- plot shows $\theta_i^\mathsf{T} \phi(u)$ as function of u
- one-hot embedding of v, so un-embedding is $\hat{v} = \arg\max_i \theta_i^\mathsf{T} x$

Example: Iris confusion matrix

- we train using multi-class logistic loss, with $\kappa_i =$ for all i
- for this example, train using all the data
- resulting confusion matrix is

$$C = \begin{bmatrix} 50 & 0 & 0 \\ 0 & 49 & 1 \\ 0 & 1 & 49 \end{bmatrix}$$