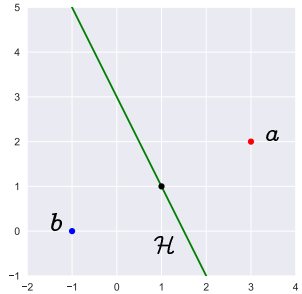
Multi-class classification

- multi-class classification with $\mathcal{V} = \{1, \ldots, K\}$
- embed the K classes as $\psi_1, \ldots, \psi_K \in \mathbf{R}^m$
- use nearest-neighbor un-embedding, $\hat{v} = \mathrm{argmin}_i \, ||\hat{y} - \psi_i||_2$
- use RERM to fit predictor
- validate using Neyman-Pearson metric on test data
  - Neyman-Pearson metric is $\sum_j \kappa_j E_j$
  - E_j is rate of mistaking $v = j$
  - κ_j is our relative distaste for mistaking $v = j$
  - with $\kappa_1 = \cdots = \kappa_K = 1$, reduces to error rate

Signed distances

When is a vector closer to one given vector than another?



- when is $\hat{y} \in \mathbf{R}^m$ closer to a than b, where $a \neq b$?
- square both sides of $||\hat{y} - a||_2 < ||\hat{y} - b||_2$ to get

$$2(b-a)^\top \hat{y} - ||b||_2^2 + ||a||_2^2 < 0$$

- the *decision boundary* is given by $||\hat{y} - a||_2 = ||\hat{y} - b||_2$, *i.e.*,

$$2(b-a)^\top \hat{y} - ||b||_2^2 + ||a||_2^2 = 0$$

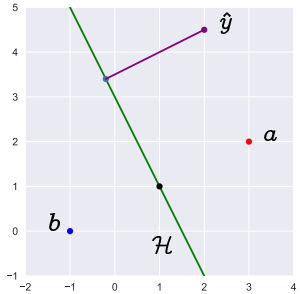
- this defines a *hyperplane* $\mathcal{H}$ in $\mathbf{R}^m$, with *normal vector* $b - a$, passing through the midpoint $(a+b)/2$

Signed distance to the decision boundary

- the *signed distance* of $\hat{y}$ to $\mathcal{H}$ is

$$D(\hat{y}, a, b) = \frac{2(b-a)^{\mathsf{T}}\hat{y} - ||a||_2^2 + ||b||_2^2}{2||b-a||_2}$$

- $D(\hat{y}, a, b) < 0$ when $\hat{y}$ is closer to a than b
- $|D(\hat{y}, a, b)|$ is the distance of $\hat{y}$ to $\mathcal{H}$
- $D(\hat{y}, a, b) = 0$ gives the decision boundary
- $D(\hat{y}, a, b)$ is an affine function of $\hat{y}$



Signed distances

- now consider un-embedding the prediction $\hat{y} \in \mathbf{R}^m$, *i.e.*, finding which ψ_i is closest
- define signed distance functions D_{ij}, for $i \neq j$, as

$$D_{ij}(\hat{y}) = D(\hat{y}, \psi_i, \psi_j) = \frac{2(\psi_j - \psi_i)^T \hat{y} - ||\psi_i||_2^2 + ||\psi_j||_2^2}{2||\psi_j - \psi_i||_2}$$

- $D_{ij}(\hat{y}) < 0$ means $\hat{y}$ is closer to ψ_i than ψ_j
- $\hat{y}$ is closest to ψ_i when $D_{ij} < 0$ for $j \neq i$, or

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

- loss function should encourage this, when $y = \psi_i$

Examples

- Boolean, with $\psi_1 = -1$ and $\psi_2 = 1$

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

  so, when $y = -1$, we'd like $\hat{y} < 0$; when $y = +1$, we'd like $\hat{y} > 0$

- one-hot, with $\psi_j = e_i$, $j = 1, \ldots, K$

$$D_{ij} = \frac{y_j - y_i}{\sqrt{2}}, \quad i \neq j$$

  so, when $y = e_i$, we want $\max_{j \neq i} D_{ij}(\hat{y}) < 0$, *i.e.*, $\operatorname{argmax}_j \hat{y}_j = i$

Multi-class loss functions

Loss function for multi-class classification

- we need to give the K functions of $\hat{y}$

$$\ell(\hat{y}, \psi_i), \quad i = 1, \ldots, K$$

- $\ell(\hat{y}, \psi_i)$ is how much we dislike predicting $\hat{y}$ when $y = \psi_i$
- loss function $\ell(\hat{y}, \psi_i)$ should be
  - small when $\max_{j \neq i} D_{ij}(\hat{y}) < 0$
  - larger when $\max_{j \neq i} D_{ij}(\hat{y}) \not< 0$

Neyman-Pearson loss

- Neyman-Pearson loss is

$$\ell(\hat{y}, \psi_i) = \begin{cases} 0 & \max_{j \neq i} D_{ij} < 0 \\ \kappa_i & \text{otherwise} \end{cases}$$

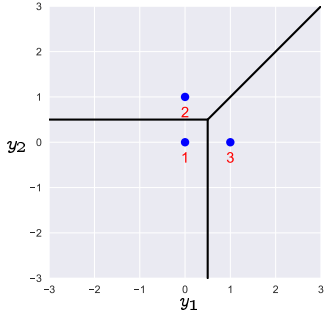
  i.e., zero when ψ_i is decoded correctly, κ_i otherwise

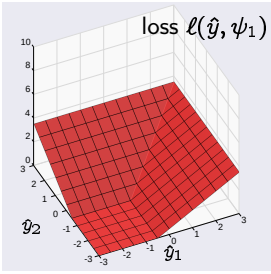
- it's hard to minimize $\mathcal{L}(\theta)$
- we do better with a *proxy loss* that
  - approximates, or at least captures the flavor of, the Neyman-Pearson loss
  - is more easily optimized (*e.g.*, is convex, differentiable)

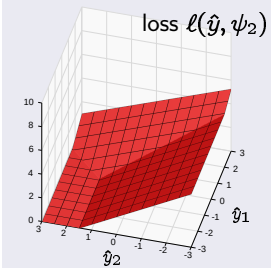
Multi-class hinge loss

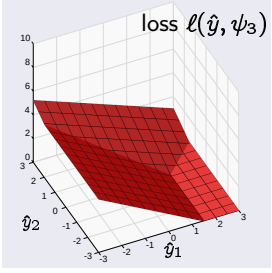
- *hinge loss* is
$$\ell(\hat{y}, \psi_i) = \kappa_i \max_{j \neq i} (1 + D_{ij}(\hat{y}))_+$$
- $\ell(\hat{y}, \psi_i)$ is zero when $\hat{y}$ is correctly un-embedded, with a margin at least one
- convex but not differentiable
- with quadratic regularization, called *multi-class SVM*
- for Boolean 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

$$\ell(\hat{y}, \psi_i) = \kappa_i \log \left(\sum_{j=1}^{K} \exp(D_{ij}(\hat{y})) \right)$$

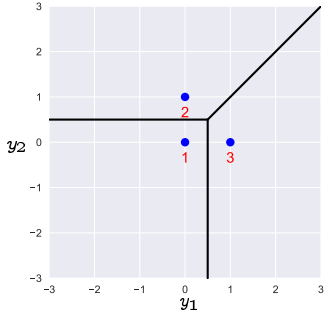
  (where we take $D_{jj} = 0$)

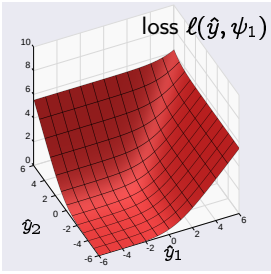
- convex and differentiable
- called *multi-class logistic regression*
- for Boolean embedding with $\psi_1 = -1$, $\psi_2 = 1$, reduces to

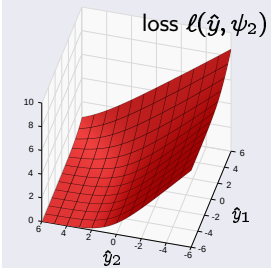
$$\ell(\hat{y}, -1) = \kappa_1 \log(1 + e^{\hat{y}}), \qquad \ell(\hat{y}, 1) = \kappa_2 \log(1 + e^{-\hat{y}})$$

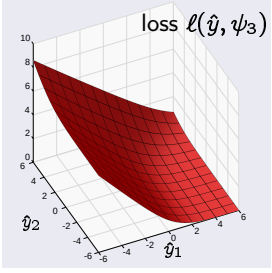
  usual logistic loss when $\kappa_1 = 1$

Multi-class logistic loss









Log-sum-exp 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
- sometimes called the *softmax* function; but that term is also used for other functions
- we have

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

Example: Iris

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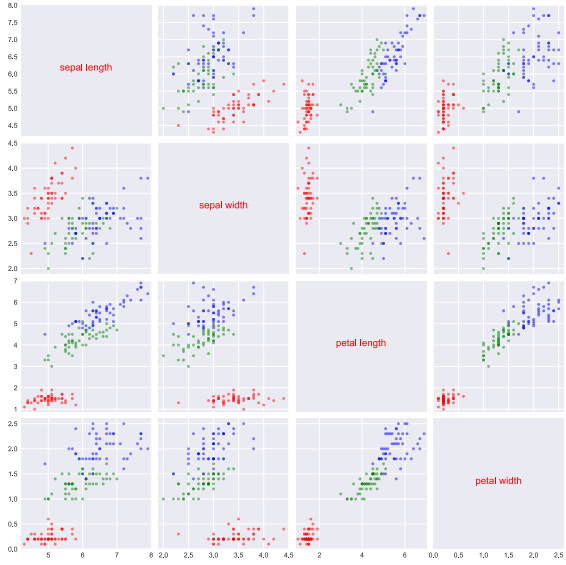
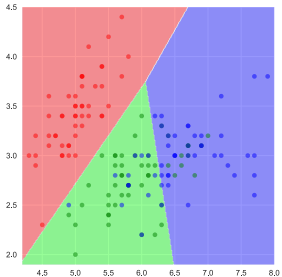
- famous example dataset by Fisher, 1936
- measurements of 150 plants, 50 from each of 3 species
- iris setosa, iris versicolor, iris virginica
- four measurements: sepal length, sepal width, petal length, petal width

Example: Iris



Classification with two features



- using only `sepal_length` and `sepal_width`
- one-hot embedding, multi-class logistic loss with $\kappa_i = 1$ for all i, trained on all data
- confusion matrix $C = \begin{bmatrix} 50 & 0 & 0 \\ 0 & 38 & 13 \\ 0 & 12 & 37 \end{bmatrix}$

Classification with all four features

- use all four features
- one-hot embedding, multi-class logistic loss with $\kappa_i =$ for all i, trained on all data
- confusion matrix $C = \begin{bmatrix} 50 & 0 & 0 \\ 0 & 49 & 1 \\ 0 & 1 & 49 \end{bmatrix}$

Summary

Summary

- loss functions for multi-class classification should encourage correct un-embedding, *i.e.*,
  - $\ell(\hat{y}, \psi_i)$ is small when $\hat{y}$ is closest to ψ_i
  - $\ell(\hat{y}, \psi_i)$ is not small when $\hat{y}$ is not closest to ψ_i
- most common losses are multi-class hinge loss and multi-class logistic
  - associated classifiers are called multi-class SVM and multi-class logistic
  - both losses are convex, so easy to solve ERM or RERM problems