Point and list classifiers

Point classifiers

- a classifier predicts *one* value $\hat{v}$, given u
- sometimes called a *point classifier* or *point predictor*, since it makes just one guess

- in this lecture we'll study classifiers that produce more than just a single guess, given u
  - an ordered list of guesses, $e.g.$, $\hat{v}^{\mathsf{top}}, \hat{v}^{\mathsf{2nd}}, \hat{v}^{\mathsf{3rd}}$ (first, second, third guesses)
  - a probability distribution on $\mathcal{V}$, $e.g.$, 15% rain, 85% shine

List classifiers

- a *list classifier* produces an ordered list, such as $\hat{v}^{\text{top}}, \hat{v}^{\text{2nd}}, \hat{v}^{\text{3rd}}$
- we interpret as our top, second, and third guesses
- (we show three here, but any number, or a variable number, is possible)
- we're happiest when $v = \hat{v}^{\text{top}}$, *i.e.*, our top guess is correct, a bit less happy when $v = \hat{v}^{\text{2nd}}$, *etc.*

- common application: recommendation system
  - $u \in \mathcal{U}$ is a user query, $v \in \mathcal{V}$ is the item a user wants
  - list classifier gives our top 10 (ordered) guesses

Nearest-neighbor un-embedding for a list classifier

- we can generalize nearest-neighbor un-embedding to give a list classifier
- start with embedding $\psi_i = \psi(v_i) \in \mathbb{R}^m$
- a predictor guesses $\hat{y} \in \mathbb{R}^m$
- $\hat{v}^{\text{top}}$ is the closest representative ψ_i to $\hat{y}$
- $\hat{v}^{\text{2nd}}$ is the second closest representative ψ_i to $\hat{y}$, *etc.*

Probabilistic classifiers

Probability distribution on $\mathcal{V}$

- a *probability distribution* on $\mathcal{V}$ is a function $p : \mathcal{V} \to \mathbb{R}$
- $p(v)$ is the probability of the value v
- we have $p(v) \geq 0$ for all $v \in \mathcal{V}$ and $\sum_{v \in \mathcal{V}} p(v) = 1$
- example: with $\mathcal{V} = \{\text{RAIN}, \text{SHINE}\}$, $\quad p(\text{RAIN}) = 0.15$, $p(\text{SHINE}) = 0.85$

- can also represent distribution p as a K-vector, with $p_i = p(v_i)$, $i = 1, \ldots, K$
- in vector notation, $p \geq 0$ (elementwise) and $\mathbf{1}^T p = 1$

Probabilistic classifiers

- a *probabilistic classifier* produces a probability distribution $\hat{p}$ on $\mathcal{V}$, given u
- we write this as $\hat{p} = G(u)$
- this notation means
  - G is a function that takes $u \in \mathcal{U}$ and returns a distribution (which is itself a function)
  - if $\hat{p} = G(u)$ then $\hat{p}$ is a function
  - we can call the function; $\hat{p}(v_i)$ is the probability that $v = v_i$, when the independent variable is u
  - we can also write this as $G(u)(v_i)$
- at any point $u \in \mathcal{U}$, calling the predictor G returns the *probability distribution* $\hat{p}$
- we can evaluate $\hat{p}$ at any $v_i \in \mathcal{V}$

Point classifier as a probabilistic classifier

- a point classifier can be considered a special case of a probabilistic classifier
- if point classifier predicts $\hat{v} \in \mathcal{V}$, associated probabilistic classifier returns $\hat{p}$, with

$$\hat{p}(v) = \begin{cases} 1 & \text{if } v = \hat{v} \\ 0 & \text{otherwise} \end{cases}$$

- $i.e.$, we return a distribution that has 100% probability on our point guess $\hat{v}$, and 0% on others
- we'll see this is likely a poor probabilistic classifier

Point classifier from a probabilistic classifier

- conversely, we can construct a point classifier from a probabilistic classifier
- if probabilistic classifier gives $\hat{p}$, our point classifier guesses

$$\hat{v} = \underset{v \in \mathcal{V}}{\operatorname{argmax}}\, \hat{p}(v)$$

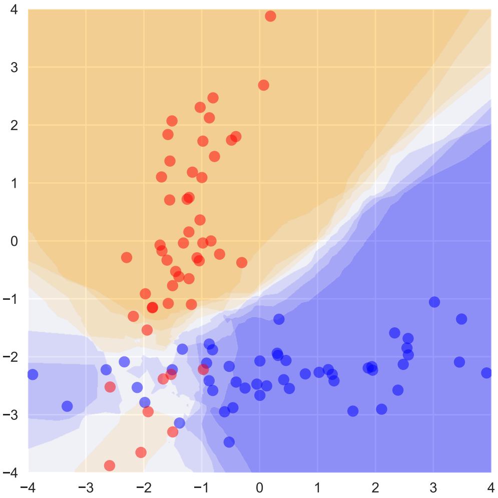
  $i.e.$, the value in $\mathcal{V}$ that has highest probability
- called a *maximum likelihood classifier*
- extends to a list classifier, by giving values sorted by probability, largest to smallest

Types of probabilistic classifiers

- tree-based probabilistic classifiers
  - decision tree with nodes labeled as feature and threshold
  - leaves contain distributions $\hat{p}$
- nearest-neighbor probabilistic classifiers
  - find k nearest neighbors of x to x^i
  - use empirical distribution of v^i among these as $\hat{p}$
- later we'll see probabilistic classifiers based on linear or neural network predictors

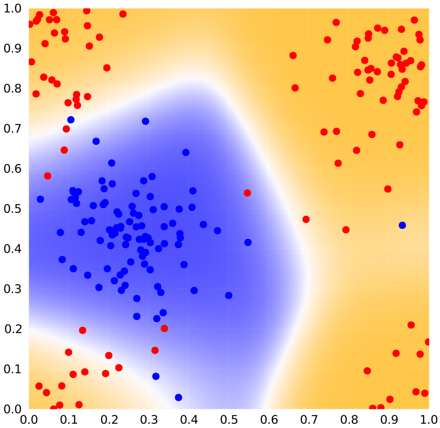
k-nearest neighbors based probabilistic classifier

- embed u^i as $x^i = \phi(u^i)$
- given u, find k nearest neighbors of $x = \phi(u)$
- guess $\hat{p}$ as the empirical distribution of v for these neighbors
- here $k = 8$



soft k-nearest neighbors based probabilistic classifier

- embed u^i as $x^i = \phi(u^i)$
- let w be the softargmax of the squared distances between x and the x^i
- w^i is the probability of record i
- let $\hat{p}$ be the distribution of y



Performance metrics

Judging list classifiers

- error rates versus list rank, $e.g.$, on a test data set
  - $v = \hat{v}^{\text{top}}$ ($i.e.$, our top guess is correct) for 68% of samples
  - $v \in \{\hat{v}^{\text{top}}, \hat{v}^{\text{2nd}}\}$ ($i.e.$, true value is among our top two guesses) for 79% of samples
  - $v \in \{\hat{v}^{\text{top}}, \hat{v}^{\text{2nd}}, \hat{v}^{\text{3rd}}\}$ ($i.e.$, the true value is one of our top three guesses) for 85% of samples

- average score on a test data set
  - three points for $v = \hat{v}^{\text{top}}$ (top guess correct)
  - two points if $v = \hat{v}^{\text{2nd}}$ (second guess correct)
  - one point if $v = \hat{v}^{\text{3rd}}$ (third guess correct)
  - zero points if v is not in your list (no guesses correct)

Judging a probabilistic classifier

- consider a data pair u, v with prediction $\hat{p} = G(u)$
- we'd like to have $\hat{p}(v) = G(u)(v)$ large, $i.e.$, *we assign high probability to the actual value*
- for rain / shine prediction example:
  - we want $\hat{p}(\text{RAIN})$ large when $v = \text{RAIN}$
  - we want $\hat{p}(\text{RAIN})$ small when $v = \text{SHINE}$
- there are several ways to formalize this
- we'll focus on most common formalization, based on *log-likelihood*

Likelihood

- we have a probabilistic classifier $\hat{p} = G(u)$, and data set $u^1, \ldots, u^n$, $v^1, \ldots, v^n$
- at the ith data point, the predicted probability distribution is $\hat{p}^i = G(u^i)$
- assuming outcomes v^i are independent with distributions $\hat{p}^i$, probability of observing these outcomes is

$$\mathbf{prob}(v^1, v^2, \ldots, v^n) = \prod_{i=1}^{n} \hat{p}^i(v^i)$$

- this probability is called the *likelihood* of $\hat{p}^1, \ldots, \hat{p}^n$; we'd like it to be high
- a fundamental measure of how well the predicted distribution matches the data
- we can compare two probabilistic classifiers G and $\tilde{G}$ by their associated likelihood on test data

Negative log likelihood

- it's more convenient to work with log probabilities, since the likelihood is a product
- the *negative log likelihood* of a probabilistic classifier on a data set is

$$-\log \mathsf{prob}(v^1, v^2, \ldots, v^n) = -\log \prod_{i=1}^{n} \hat{p}^i(v^i) = -\sum_{i=1}^{n} \log \hat{p}^i(v^i)$$

- the negative log likelihood is nonnegative; we'd like it to be small
- to compare likelihood on different size data sets ($e.g.$, train and test) we use the *average negative log likelihood*

$$\mathcal{L} = -\frac{1}{n} \sum_{i=1}^{n} \log \hat{p}^i(v^i)$$

Constant probabilistic classifier

Constant probabilistic classifier

- consider a constant probabilistic classifier
- $i.e.$, distribution $\hat{p}$ does does not depend on u (which need not even exist)
- given data set $v^1, \ldots, v^n$, guess distribution $\hat{p}$ on $\mathcal{V}$
- suppose we choose $\hat{p}$ to minimize average negative log likelihood

$$-\frac{1}{n}\sum_{i=1}^{n} \log \hat{p}(v^i)$$

(subject to $\hat{p}(v) \geq 0$ for all $v \in \mathcal{V}$ and $\sum_{v\in\mathcal{V}} \hat{p}(v) = 1$)

- the *empirical distribution* of the data is

$$q(v) = \text{fraction of } v^j \text{ that have value } v$$

- we'll see: *the optimal constant probabilistic classifier is* $\hat{p} = q$
- . . . a very sensible prediction of $\hat{p}$

Cross entropy

- we can express average negative log likelihood as

$$-\frac{1}{n}\sum_{i=1}^{n}\log\hat{p}(v^i) = -\sum_{j=1}^{K} q(v_j)\log\hat{p}(v_j)$$

- the quantity $H(q,\hat{p}) = -\sum_{j=1}^{K} q(v_j)\log\hat{p}(v_j)$ is called the *cross entropy* of $\hat{p}$ relative to q

- compare with the entropy $H(p) = -\sum_{k=1}^{K} p(v_k)\log p(v_k)$

Kullback-Leibler divergence

For p, q two probability distributions, the *Kullback-Leibler divergence* is

$$d_{kl}(q, p) = H(q, p) - H(q)$$

- *$d_{kl}(q, p) \geq 0$ for all distributions p, q*, because

$$\begin{aligned} d_{kl}(q, p) &= -\sum_{j=1}^{K} q_j \log(p_j / q_j) \\ &\geq -\sum_{j=1}^{K} q_j (p_j / q_j - 1) = 0 \qquad \text{because } \log x \leq x - 1 \text{ for all } x > 0 \end{aligned}$$

- can be shown even if some $q_j = 0$

Constant predictor

- the optimal constant probabistic classifier is the $\hat{p}$ that minimizes $H(q, \hat{p})$, which is

$$H(q, \hat{p}) = d_{kl}(q, \hat{p}) + H(q)$$

- optimal choice is $\hat{p} = q$, then $H(q, \hat{p}) = H(q)$

Summary

Summary

- a point classifier makes a single guess of v, given u
- a probabilistic classifier guesses a probability distribution on $\mathcal{V}$, given u
- we judge a probabilistic classifier by its average log likelihood on test data