Least Squares Classification

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Outline

Classification

Least squares classification

Multi-class classifiers

Classification

- data fitting with outcome that takes on (non-numerical) values like
  - TRUE or FALSE
  - SPAM or NOT SPAM
  - DOG, HORSE, or MOUSE
- outcome values are called *labels* or *categories*
- data fitting is called *classification*

- we start with case when there are two possible outcomes
- called *Boolean* or *2-way* classification
- we encode outcomes as $+1$ (TRUE) and -1 (FALSE)
- classifier has form $\hat{y} = \hat{f}(x)$, $f : \mathbf{R}^n \to \{-1, +1\}$

Applications

- email spam detection
  - x contains features of an email message (word counts, ...)
- financial transaction fraud detection
  - x contains features of proposed transaction, initiator
- document classification (say, politics or not)
  - x is word count histogram of document
- disease detection
  - x contains patient features, results of medical tests
- digital communications receiver
  - y is transmitted bit; x contain n measurements of received signal

Prediction errors

- data point (x, y), predicted outcome $\hat{y} = \hat{f}(x)$
- only four possibilities:
  - *True positive.* $y = +1$ and $\hat{y} = +1$.
  - *True negative.* $y = -1$ and $\hat{y} = -1$.

  (in these two cases, the prediction is *correct*)
  - *False positive.* $y = -1$ and $\hat{y} = +1$.
  - *False negative.* $y = +1$ and $\hat{y} = -1$.

  (in these two cases, the prediction is *wrong*)
- the errors have many other names, like Type I and Type II

Confusion matrix

- given data set $x^{(1)}, \dots, x^{(N)}, \quad y^{(1)}, \dots, y^{(N)}$ and classifier $\hat{f}$
- count each four outcomes

	$\hat{y} = +1$	$\hat{y} = -1$	total
$y = +1$	N_{tp}	N_{fn}	N_{p}
$y = -1$	N_{fp}	N_{tn}	N_{n}
total	$N_{\mathrm{tp}} + N_{\mathrm{fp}}$	$N_{\mathrm{fn}} + N_{\mathrm{tn}}$	N

- off-diagonal terms are prediction errors
- many error rates and accuracy measures are used
  - *error rate* is $(N_{\mathrm{fp}} + N_{\mathrm{fn}})/N$
  - *true positive* (or *recall*) rate is $N_{\mathrm{tp}}/N_{\mathrm{p}}$
  - *false positive rate* (or *false alarm rate*) is $N_{\mathrm{fp}}/N_{\mathrm{n}}$
- a proposed classifier is judged by its error rate(s) on a test set

Example

- spam filter performance on a test set (say)

	$\hat{y} = +1$	$\hat{y} = -1$	total
$y = +1$	95	32	127
$y = -1$	19	1120	1139
total	114	1152	1266

- error rate is $(19 + 32)/1266 = 4.03\%$
- false positive rate is $19/1139 = 1.67\%$

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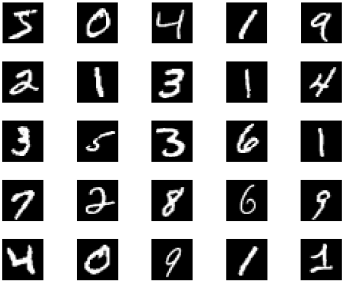
Least squares classification

- fit model $\tilde{f}$ to encoded (± 1) $y^{(i)}$ values *using standard least squares data fitting*
- $\tilde{f}(x)$ should be near $+1$ when $y = +1$, and near -1 when $y = -1$
- $\tilde{f}(x)$ is a *number*
- use model $\hat{f}(x) = \mathbf{sign}(\tilde{f}(x))$
- (size of $\tilde{f}(x)$ is related to the 'confidence' in the prediction)

Handwritten digits example

- MNIST data set of 70000 28×28 images of digits 0, . . . , 9
- divided into training set (60000) and test set (10000)
- x is 494-vector, constant 1 plus the 493 pixel values with at least one nonzero value in data
- $y = +1$ if digit is 0; -1 otherwise



Least squares classifier results

- training set results (error rate 1.6%)

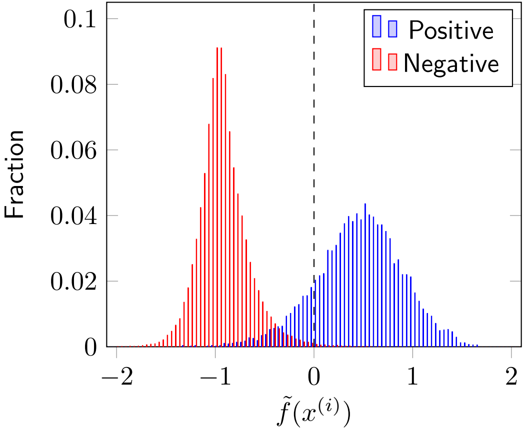
	$\hat{y}=+1$	$\hat{y}=-1$	total
$y=+1$	5165	758	5923
$y=-1$	179	53898	54077
total	5344	54656	60000

- test set results (error rate 1.6%)

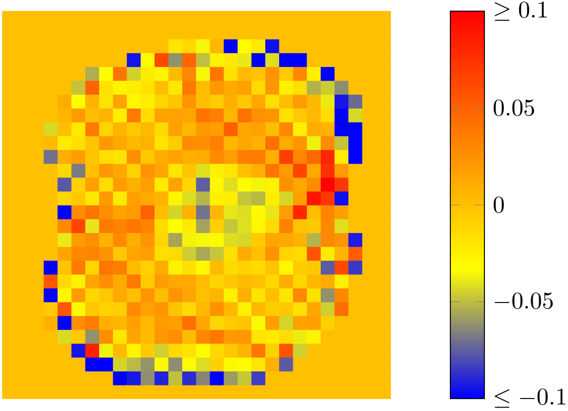
	$\hat{y}=+1$	$\hat{y}=-1$	total
$y=+1$	864	116	980
$y=-1$	42	8978	9020
total	906	9094	10000

- we can likely achieve 1.6% error rate on unseen images

- distribution of values of $\tilde{f}(x^{(i)})$ over training set



Coefficients in least squares classifier



Skewed decision threshold

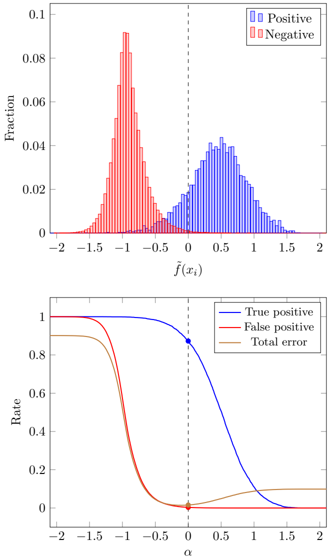
- use predictor $\hat{f}(x) = \mathbf{sign}(\tilde{f}(x) - \alpha)$, *i.e.*,

$$\hat{f}(x) = \begin{cases} +1 & \tilde{f}(x) \geq \alpha \\ -1 & \tilde{f}(x) < \alpha \end{cases}$$

- α is the *decision threshold*
- for positive α, false positive rate is lower but so is true positive rate
- for negative α, false positive rate is higher but so is true positive rate

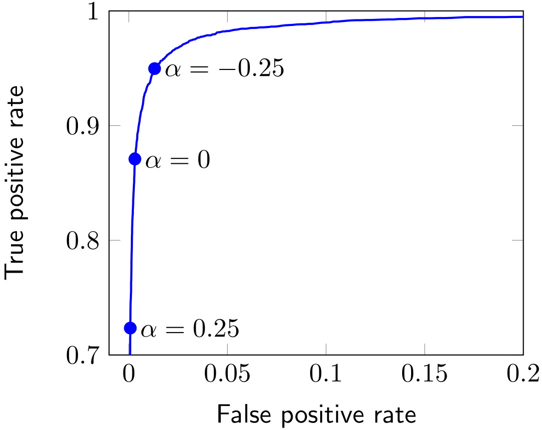
- trade off curve of true positive versus false positive rates is called *receiver operating characteristic* (ROC)

Example



Positive
Negative
Fraction
0.1
0.08
0.06
0.04
0.02
0
−2 −1.5 −1 −0.5 0 0.5 1 1.5 2
$\tilde{f}(x_i)$
True positive
False positive
Total error
Rate
1
0.8
0.6
0.4
0.2
0
−2 −1.5 −1 −0.5 0 0.5 1 1.5 2
α

ROC curve



1
0.9
0.8
0.7
0
0.05
0.1
0.15
0.2
$\alpha = -0.25$
$\alpha = 0$
$\alpha = 0.25$
True positive rate
False positive rate

Outline

Multi-class classifiers

- we have $K > 2$ possible labels, with label set $\{1, \ldots, K\}$
- predictor is $\hat{f} : \mathbf{R}^n \to \{1, \ldots, K\}$
- for given predictor and data set, confusion matrix is $K \times K$
- some off-diagonal entries may be much worse than others

Examples

- handwritten digit classification
  - guess the digit written, from the pixel values
- marketing demographic classification
  - guess the demographic group, from purchase history
- disease diagnosis
  - guess diagnosis from among a set of candidates, from test results, patient features
- translation word choice
  - choose how to translate a word into several choices, given context features
- document topic prediction
  - guess topic from word count histogram

Least squares multi-class classifier

- create a least squares classifier for each label versus the others
- take as classifier

$$\hat{f}(x) = \underset{\ell \in \{1,\ldots,K\}}{\operatorname{argmax}} \tilde{f}_\ell(x)$$

  (*i.e.*, choose ℓ with largest value of $\tilde{f}_\ell(x)$)
- for example, with

$$\tilde{f}_1(x) = -0.7, \quad \tilde{f}_2(x) = +0.2, \quad \tilde{f}_3(x) = +0.8$$

  we choose $\hat{f}(x) = 3$

Handwritten digit classification

confusion matrix, test set

	Prediction										
Digit	0	1	2	3	4	5	6	7	8	9	Total
0	944	0	1	2	2	8	13	2	7	1	980
1	0	1107	2	2	3	1	5	1	14	0	1135
2	18	54	815	26	16	0	38	22	39	4	1032
3	4	18	22	884	5	16	10	22	20	9	1010
4	0	22	6	0	883	3	9	1	12	46	982
5	24	19	3	74	24	656	24	13	38	17	892
6	17	9	10	0	22	17	876	0	7	0	958
7	5	43	14	6	25	1	1	883	1	49	1028
8	14	48	11	31	26	40	17	13	756	18	974
9	16	10	3	17	80	0	1	75	4	803	1009
All	1042	1330	887	1042	1086	742	994	1032	898	947	10000

error rate is around 14% (same as for training set)

Adding new features

- let's add 5000 random features (!), $\max\{(Rx)_j, 0\}$
  - R is 5000×494 matrix with entries ± 1, chosen randomly
- now use least squares classification with 5494 feature vector

- results: training set error 1.5%, test set error 2.6%
- can do better with a little more thought in generating new features
- indeed, even better than humans can do (!!)

Results with new features

confusion matrix, test set

	Prediction										
Digit	0	1	2	3	4	5	6	7	8	9	Total
0	972	0	0	2	0	1	1	1	3	0	980
1	0	1126	3	1	1	0	3	0	1	0	1135
2	6	0	998	3	2	0	4	7	11	1	1032
3	0	0	3	977	0	13	0	5	8	4	1010
4	2	1	3	0	953	0	6	3	1	13	982
5	2	0	1	5	0	875	5	0	3	1	892
6	8	3	0	0	4	6	933	0	4	0	958
7	0	8	12	0	2	0	1	992	3	10	1028
8	3	1	3	6	4	3	2	2	946	4	974
9	4	3	1	12	11	7	1	3	3	964	1009
All	997	1142	1024	1006	977	905	956	1013	983	997	10000