Recognition of Properties by Probabilistic Neural Networks

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Outline

Bayes Decision Scheme

$\mathbf{x} = (x_1, \ldots, x_N) \in \mathcal{X}$: N-dimensional binary data vectors, $\mathcal{N} = \{1, \ldots, N\}$

$\Omega = \{\omega_1, \omega_2, \ldots, \omega_J\}$: finite number of classes, probability $p(\omega), \omega \in \Omega$

$P(\mathbf{x}|\omega)p(\omega), \quad \omega \in \Omega$: conditional distributions of classes

full statistical decision information: *a posteriori* probabilities

$$p(\omega|\mathbf{x}) = \frac{P(\mathbf{x}|\omega)p(\omega)}{P(\mathbf{x})}, \quad \mathbf{x} \in \mathcal{X}, \quad \omega \in \Omega,$$

Bayes decision function: minimum-error classification

$$d : \mathcal{X} \to \Omega, \qquad d(\mathbf{x}) = \arg\max_{\omega \in \Omega}\{p(\omega|\mathbf{x})\} = \arg\max_{\omega \in \Omega}\{P(\mathbf{x}|\omega)p(\omega)\}, \qquad \mathbf{x} \in \mathcal{X}$$

formula of complete probability implies mutually exclusive classes

$$P(\mathbf{x}) = \sum_{\omega \in \Omega} P(\mathbf{x}|\omega)p(\omega), \quad \mathbf{x} \in \mathcal{X}$$

real life categories are usually non-exclusive

$\Rightarrow$ **we propose: identification of non-exclusive properties by using statistical one-class classifiers**

Binary Recognition of Non-exclusive Properties

finite set of non-exclusive properties: $\Omega = \{\omega_1, \ldots, \omega_K\}$

two alternatives for each property $\omega \in \Omega$:

ω: the property has been identified (positive decision)
$\bar{\omega}$: the property has not been identified (negative decision)

$\Rightarrow$ **finite number of binary classification problems:** $\{\omega, \bar{\omega}\}, \quad (\omega \in \Omega)$

two training data sets: $\mathcal{S}_\omega = \{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(K_\omega)}\}, \ \mathcal{S}_{\bar{\omega}} = \{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(K_{\bar{\omega}})}\}$

probabilistic description: $P(\mathbf{x}|\omega)p(\omega), \quad P(\mathbf{x}|\bar{\omega})p(\bar{\omega})$

$\Rightarrow$ **Bayesian decision-making:**

$$p(\omega|\mathbf{x}) = \frac{P(\mathbf{x}|\omega)p(\omega)}{P(\mathbf{x})}, \qquad p(\bar{\omega}|\mathbf{x}) = \frac{P(\mathbf{x}|\bar{\omega})p(\bar{\omega})}{P(\mathbf{x})}$$

$$d_\omega : \mathcal{X} \to \{\omega, \bar{\omega}\}, \quad d_\omega(\mathbf{x}) = \begin{cases} \omega, & p(\omega|\mathbf{x}) \geq p(\bar{\omega}|\mathbf{x}), \\ \bar{\omega}, & p(\omega|\mathbf{x}) < p(\bar{\omega}|\mathbf{x}), \end{cases} \qquad \mathbf{x} \in \mathcal{X}$$

PROBLEM: "negative" training data sets $\mathcal{S}_{\bar{\omega}}$ are rarely available

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Identification of Properties by One-Class-Classifiers

one-class classifier: only one training set for each property $\omega \in \Omega$:
$\mathcal{S}_\omega = \{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(K_\omega)}\}$, (*a priori* probability $p(\omega)$ unknown)

$\Rightarrow$ class-conditional distribution $P(\mathbf{x}|\omega)$ for the "target" class only
$\Rightarrow$ Bayes rule not applicable
$\Rightarrow$ **classification of properties by thresholding** $P(\mathbf{x}|\omega)$

we propose: thresholding of the log-likelihood ratio:

$$\Delta_\omega(\mathbf{x}) = \log \frac{P(\mathbf{x}|\omega)}{\prod_{n\in\mathcal{N}} f_n(x_n|0)} \geq \epsilon_\omega, \quad \mathbf{x} \in \mathcal{X}$$

$f_n(x_n|0) = \theta_{0n}^{x_n}(1-\theta_{0n})^{1-x_n}, \; n \in \mathcal{N} \;\approx$ unconditional marginal probabilities

the threshold ϵ_ω can be related to the mean value of $\Delta_\omega(\mathbf{x})$:

$$\epsilon_\omega = \frac{1}{|\mathcal{S}_\omega|} \sum_{x\in\mathcal{S}_\omega} \log \frac{P(\mathbf{x}|\omega)}{\prod_{n\in\mathcal{N}} f_n(x_n|0)} \;\rightarrow\; \sum_{x\in\mathcal{X}} P^*(\mathbf{x}|\omega) \log \frac{P^*(\mathbf{x}|\omega)}{\prod_{n\in\mathcal{N}} f_n(x_n|0)}$$

ϵ_ω **converges to the Kullback-Leibler I-divergence**

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Structural Mixture Model

$\phi_{mn} \in \{0,1\}$ $\approx$ **binary structural parameters** (Grim et al. 1999, 2002)

$$P(\mathbf{x}|\omega) = \sum_{m \in \mathcal{M}_\omega} F(\mathbf{x}|m) f(m) = \sum_{m \in \mathcal{M}_\omega} f(m) \prod_{n \in \mathcal{N}} f_n(x_n|m)^{\phi_{mn}} f_n(x_n|0)^{1-\phi_{mn}}$$

$\phi_{mn} = 0$ $\Rightarrow$ distribution $f_n(x_n|m)$ is replaced by fixed "background" $f_n(x_n|0)$

$\mathcal{M}_\omega \approx$ component index set of the property $\omega \in \Omega$

$$P(\mathbf{x}|\omega) = F(\mathbf{x}|0) \sum_{m \in \mathcal{M}_\omega} G(\mathbf{x}|m, \phi_m) f(m), \qquad F(\mathbf{x}|0) = \prod_{n \in \mathcal{N}} f_n(x_n|0)$$

univariate distributions: $f_n(x_n|m) = \theta_{mn}^{x_n}(1-\theta_{mn})^{1-x_n}, \quad \theta_{mn} \in \langle 0,1 \rangle$

$$G(\mathbf{x}|m, \phi_m) = \prod_{n \in \mathcal{N}} \left[\frac{f_n(x_n|m)}{f_n(x_n|0)} \right]^{\phi_{mn}} = \prod_{n \in \mathcal{N}} \left[\left(\frac{\theta_{mn}}{\theta_{0n}} \right)^{x_n} \left(\frac{1-\theta_{mn}}{1-\theta_{0n}} \right)^{1-x_n} \right]^{\phi_{mn}}$$

$G(\mathbf{x}|m, \phi_m)$ $\approx$ may depend on different subsets of variables

structural model can be optimized in full generality ▸ EM algorithm

Identification of Non-exclusive Properties by PNN

mixture-based one-class classifier:

$$\Delta_\omega(\mathbf{x}) = \log \frac{P(\mathbf{x}|\omega)}{\prod_{n\in\mathcal{N}} f_n(x_n|0)} = \log \frac{P(\mathbf{x}|\omega)}{F(\mathbf{x}|0)} = \log \sum_{m\in\mathcal{M}_\omega} G(\mathbf{x}|m,\phi_m)f(m) \geq \epsilon_\omega$$

decision threshold ϵ_ω : related to the mean value of $\Delta_\omega(\mathbf{x})$

$$\epsilon_\omega = \frac{c_0}{|\mathcal{S}_\omega|}\sum_{x\in\mathcal{S}_\omega}\Delta_\omega(\mathbf{x}) = \frac{c_0}{|\mathcal{S}_\omega|}\sum_{x\in\mathcal{S}_\omega}\log\sum_{m\in\mathcal{M}_\omega} G(\mathbf{x}|m,\phi_m)f(m)$$

c_0 $\approx$ a constant to balance false positive and false negative decisions (to be optimized by validation set)

mean value of $\Delta_\omega(\mathbf{x})$ $\approx$ maximum-likelihood criterion

$$L_\omega = \frac{1}{|\mathcal{S}_\omega|}\sum_{x\in\mathcal{S}_\omega}\log P(\mathbf{x}|\omega)$$

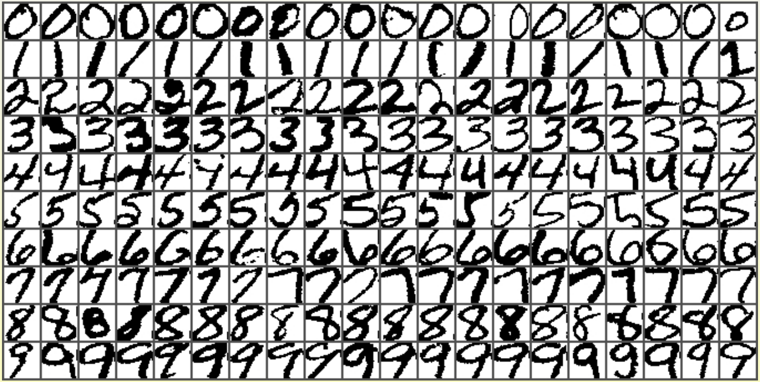
$$L_\omega = \frac{1}{|\mathcal{S}_\omega|}\sum_{x\in\mathcal{S}_\omega}\log F(\mathbf{x}|0) + \frac{1}{|\mathcal{S}_\omega|}\sum_{x\in\mathcal{S}_\omega}\log\left[\sum_{m\in\mathcal{M}_\omega} G(\mathbf{x}|m,\phi_m)f(m)\right]$$

▸ probabilistic neuron

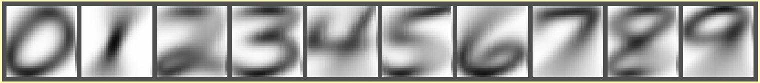
NIST SD19 Database of Hand-Written Numerals

NIST Special Database SD19: about 400000 **handwritten numerals**

examples of numerals normalized to 32x32 binary raster



class-means ("mean images") of training numerals



Computational Experiment

DATA

- **odd data vectors for training ($\sum |\mathcal{S}_\omega| = 201485$ numerals)**
- **even data vectors for testing ($\sum |\mathcal{S}_\omega^T| = 201479$ numerals)**
- all numerals normalized to 32x32 binary raster
- database extend by three differently rotated variants of each pattern (by -10,-5,+5 degrees)

estimation of class-conditional structural mixtures:

- conditional distributions $P(\mathbf{x}|\omega)$ estimated from $\mathcal{S}_\omega$ for all $\omega \in \Omega$
- initial number of components chosen identically in all classes: $M_\omega = 200$
- randomly initialized mixture parameters
- stopping rule: relative increment threshold

GOAL: to compare one-class classifiers with the mutually exclusive Bayesian decision-making - using the same distributions $P(\mathbf{x}|\omega)$

Bayesian Recognition of Mutually Exclusive Numerals

in rows: frequencies of decisions for test data from the respective classes
last column: percentage of false negative decisions in the class
last row: total false positive frequencies (in % of all test patterns)

CLASS	0	1	2	3	4	5	6	7	8	9	False n.
♯ Test s.	20182	22352	20038	20556	19577	18303	19969	20947	19790	19767	
0	19950	8	43	19	39	32	36	0	38	17	1.1%
1	2	22162	30	4	35	7	18	56	32	6	0.9%
2	32	37	19742	43	30	9	8	29	90	16	1.5%
3	20	17	62	20021	4	137	2	28	210	55	2.6%
4	11	6	19	1	19170	11	31	51	30	247	2.1%
5	25	11	9	154	4	17925	39	6	96	34	2.1%
6	63	10	17	6	23	140	19652	1	54	3	1.6%
7	7	12	73	10	73	4	0	20497	22	249	2.1%
8	22	25	53	97	30	100	11	11	19369	72	2.1%
9	15	13	25	62	114	22	3	146	93	19274	2.5%
♯ False p.	197	139	537	396	352	462	148	328	665	699	
False p.	0.09%	0.07%	0.27%	0.20%	0.17%	0.23%	0.07%	0.16%	0.33%	0.35%	**1.84%**

Remark: **one decision for each data vector**
mean false negative: **1.84%**

Recognition of Numerals by Using One-Class Classifiers

in columns: frequencies of positive decisions for the respective classifiers

CLASS	0	1	2	3	4	5	6	7	8	9
♯ Test s.	20182	22352	20038	20556	19577	18303	19969	20947	19790	19767
0	18815	2	954	23	30	292	76	0	406	103
1	6	21857	55	46	2756	111	52	4436	5039	410
2	4	9	18660	105	5	2	6	6	207	3
3	6	2	43	18971	1	1733	0	12	3177	373
4	1	0	6	1	18494	5	5	83	265	3229
5	7	2	4	918	0	17211	35	0	1246	282
6	50	10	30	0	60	888	18833	0	360	1
7	1	5	601	324	209	4	0	19817	242	6735
8	9	13	22	620	19	289	6	5	18201	154
9	3	4	6	70	1722	90	2	1060	1266	18667
♯ False neg.	1367	495	1378	1585	1083	1092	1136	1130	1599	1100
False neg.	6.8%	2.2%	6.9%	7.7%	5.5%	6.0%	5.7%	5.4%	8.0%	5.6%
♯ False pos.	87	47	1721	2107	4802	3414	182	5602	12208	11290
False pos.	0.00%	0.00%	0.01%	0.01%	0.02%	0.02%	0.00%	0.03%	0.06%	0.06%

Remark: **ten(!) independent decisions for each data vector**
mean false negative: **5.98%**

Concluding Remarks

Bayes Decision Function

- minimizes the classification error in case of mutually exclusive classes
- fails completely in case of non-exclusive properties

One-Class Classifier

- less precise in case of mutually exclusive classes
- clearly preferable in case of non-exclusive properties
- applicable both to the non-exclusive and exclusive properties
- can be transformed to Bayes decision function by norming in case of equiprobable mutually exclusive classes
- provides a unified approach to recognition of properties and feature extraction

$\Rightarrow$ **assumption of mutually exclusive classes is not suitable to model biological neural networks**

References

EM Algorithm for Structural Mixture Model

structural optimization can be included into EM algorithm

$$L = \frac{1}{|\mathcal{S}_\omega|} \sum_{x \in \mathcal{S}_\omega} \log \Big[\sum_{m \in \mathcal{M}_\omega} F(\mathbf{x}|0) G(\mathbf{x}|m, \phi_m) f(m) \Big], \qquad F(\mathbf{x}|0) = \prod_{n \in \mathcal{N}} f_n(x_n|0)$$

EM Algorithm: $(m \in \mathcal{M}_\omega, n \in \mathcal{N}, \mathbf{x} \in \mathcal{S}_\omega)$

$$q(m|\mathbf{x}) = \frac{G(\mathbf{x}|m, \phi_m) f(m)}{\sum_{j \in \mathcal{M}_\omega} G(\mathbf{x}|j, \phi_j) f(j)},$$

$$f^{'}(m) = \frac{1}{|\mathcal{S}_\omega|} \sum_{\mathbf{x} \in \mathcal{S}_\omega} q(m|\mathbf{x}), \qquad \theta^{'}_{mn} = \frac{1}{\sum_{\mathbf{x} \in \mathcal{S}_\omega} q(m|\mathbf{x})} \sum_{\mathbf{x} \in \mathcal{S}_\omega} x_n q(m|\mathbf{x})$$

structural criterion: Kullback-Leibler I-divergence

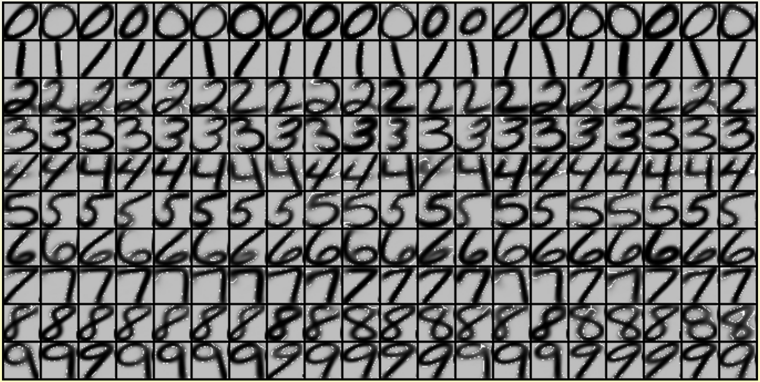
$$\gamma^{'}_{mn} = f^{'}(m) \left[\theta^{'}_{mn} \log \frac{\theta^{'}_{mn}}{\theta_{0n}} + (1 - \theta^{'}_{mn}) \log \frac{(1 - \theta^{'}_{mn})}{(1 - \theta_{0n})} \right]$$

structural parameter optimization: $\phi^{'}_{mn} = 1$ for the r highest values $\gamma^{'}_{mn}$

Remark. The “structural” EM algorithm converges monotonically. Back

Component Means of the Estimated Mixtures $P(\mathbf{x}|\omega)$

examples of component parameters $\theta_{mn} \in \langle 0, 1 \rangle$ displayed in raster arrangement (the white fields denote unused variables with $\phi_{mn} = 0$)



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Probabilistic Neuron for Identification of Properties

output layer neuron for the property ω **:**

$$\Delta_\omega(\mathbf{x}) = \sum_{m \in \mathcal{M}_\omega} q(m|\mathbf{x}) \log \left[G(\mathbf{x}|m, \phi_m) f(m) \right] + \sum_{m \in \mathcal{M}_\omega} -q(m|\mathbf{x}) \log q(m|\mathbf{x})$$

$$q(m|\mathbf{x}) = \frac{G(\mathbf{x}|m, \phi_m) f(m)}{\sum_{j \in \mathcal{M}_\omega} G(\mathbf{x}|j, \phi_j) f(j)}, \qquad H(q(\cdot|\mathbf{x})) = \sum_{m \in \mathcal{M}_\omega} -q(m|\mathbf{x}) \log q(m|\mathbf{x})$$

$$\Delta_\omega(\mathbf{x}) = H(q(\cdot|\mathbf{x})) + \sum_{m \in \mathcal{M}_\omega} q(m|\mathbf{x}) \left[\log f(m) + \sum_{n \in \mathcal{N}} \phi_{mn} \log \left(\frac{f_n(x_n|m)}{f_n(x_n|0)} \right) \right]$$

hidden layer neuron: $(m \in \mathcal{M}_\omega)$

$$y_m(\mathbf{x}) = \left[\log f(m) + \sum_{n \in \mathcal{N}} \phi_{mn} \log \left(\frac{1 - \theta_{mn}}{1 - \theta_{0n}} \right) + x_n \log \left(\frac{\theta_{mn}(1 - \theta_{0n})}{\theta_{0n}(1 - \theta_{mn})} \right) \right]$$

$$\Delta_\omega(\mathbf{x}) = H(q(\cdot|\mathbf{x})) + \sum_{m \in \mathcal{M}_\omega} q(m|\mathbf{x}) y_m(\mathbf{x})$$

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