Sapienza University of Rome

Master in Artificial Intelligence and Robotics

Machine Learning

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Prof. Luca Iocchi

Sapienza University of Rome, Italy - Machine Learning (2024/2025)

6. Probabilistic models for classification

Luca Iocchi

Overview

- Probabilistic generative models
- Probabilistic discriminative models
- Logistic regression

References

C. Bishop. Pattern Recognition and Machine Learning. Sect. 4.2, 4.3

Probabilistic Models for Classification

Given $f : \mathbf{X} \rightarrow C$ $(\mathbf{X} \subseteq \Re^d)$, $D = \{(\mathbf{x}_n, c_n)_{n=1}^{n}\}$ and $\mathbf{x} \notin D$, estimate

$$P(C_i|\mathbf{x}, D)$$

Simplified notation without D in the formulas.

$P(C_i|\mathbf{x})$: posterior, $P(\mathbf{x}|C_i)$: class-conditional densities

Two families of models:

- Generative: estimate $P(\mathbf{x}|C_i)$ and then compute $P(C_i|\mathbf{x})$ with Bayes
- Discriminative: estimate $P(C_i|\mathbf{x})$ directly

Probabilistic Generative Models

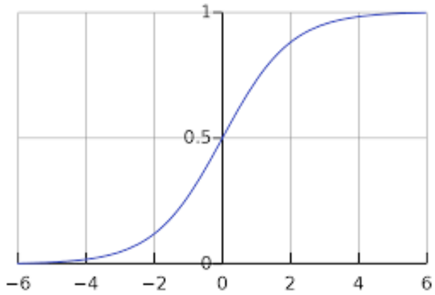
Consider two classes. Find the conditional probability:

$$P(C_1|\mathbf{x}) = \frac{P(\mathbf{x}|C_1)P(C_1)}{P(\mathbf{x})} = \frac{P(\mathbf{x}|C_1)P(C_1)}{P(\mathbf{x}|C_1)P(C_1) + P(\mathbf{x}|C_2)P(C_2)}$$
$$= \frac{1}{1+\exp(-a)} = \sigma(a)$$

with:

$$a = \ln \frac{P(\mathbf{x}|C_1)P(C_1)}{P(\mathbf{x}|C_2)P(C_2)}$$

$\sigma(a) = \frac{1}{1+\exp(-a)}$ *sigmoid function*



Probabilistic Generative Models

Consider parametric model $P(\mathbf{x}|C_i) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_i, \boldsymbol{\Sigma})$
same covariance matrix for all classes

$$a = \ln \frac{P(\mathbf{x}|C_1)P(C_1)}{P(\mathbf{x}|C_2)P(C_2)} = \ln \frac{\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_1, \boldsymbol{\Sigma})P(C_1)}{\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_2, \boldsymbol{\Sigma})P(C_2)} = \ldots = \mathbf{w}^T\mathbf{x} + w_0$$

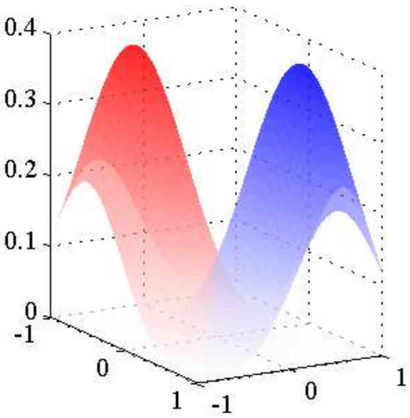
with:

$$\mathbf{w} = \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2),$$
$$w_0 = -\frac{1}{2}\boldsymbol{\mu}_1^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1 + \frac{1}{2}\boldsymbol{\mu}_2^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_2 + \ln\frac{P(C_1)}{P(C_2)}.$$

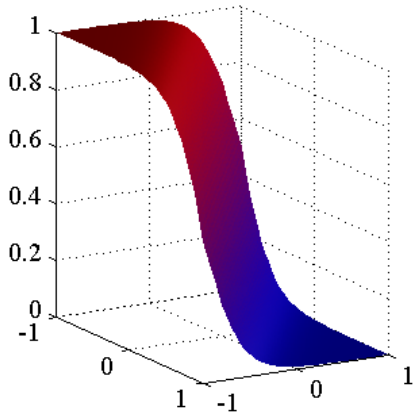
Thus

$$P(C_1|\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x} + w_0),$$

Probabilistic Generative Models



$P(\mathbf{x}|C_1), P(\mathbf{x}|C_2)$



$P(C_1|\mathbf{x})$

Decision rule: $c = C_1 \iff P(c = C_1|\mathbf{x}) > 0.5$

Probabilistic Generative Models

Summary

$$P(C_1|\mathbf{x}) = \sigma(a), \qquad a = \ln \frac{P(\mathbf{x}|C_1)P(C_1)}{P(\mathbf{x}|C_2)P(C_2)}$$

$$P(C_2|\mathbf{x}) = 1 - P(C_1|\mathbf{x})$$

Parametric model

$$P(C_1) = \pi \qquad P(C_2) = 1 - \pi$$

$$P(\mathbf{x}|C_1) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}) \qquad P(\mathbf{x}|C_2) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_2, \boldsymbol{\Sigma})$$

Unknown

$$\pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma}$$

this training phase

Maximum likelihood (2 classes)

Maximum likelihood solution for 2 classes

Assuming $P(C_1) = \pi$ (thus $P(C_2) = 1 - \pi$), $P(\mathbf{x}|C_i) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_i, \boldsymbol{\Sigma})$

Given data set $D = \{(\mathbf{x}_n, t_n)_{n=1}^N\}$, $t_n = 1$ if $\mathbf{x}_n$ belongs to class C_1, $t_n = 0$ if $\mathbf{x}_n$ belongs to class C_2

Let N_1 be the number of samples in D belonging to C_1 and N_2 be the number of samples in C_2 ($N_1 + N_2 = N$)

Likelihood function

given class C_1 given class C_2

$$P(\mathbf{t}|\pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma}, D) = \prod_{n=1}^{N} [\pi \mathcal{N}(\mathbf{x}_n; \boldsymbol{\mu}_1, \boldsymbol{\Sigma})]^{t_n} [(1-\pi)\mathcal{N}(\mathbf{x}_n; \boldsymbol{\mu}_2, \boldsymbol{\Sigma})]^{(1-t_n)}$$

ML solution: Estimate model parameters $\hat{\pi}$, $\hat{\boldsymbol{\mu}}_1$, $\hat{\boldsymbol{\mu}}_2$, $\hat{\boldsymbol{\Sigma}}$

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Maximum likelihood (2 classes)

Maximum likelihood solution for 2 classes
Maximizing log likelihood function, we obtain

$$\hat{\pi} = \frac{N_1}{N}$$

$$\hat{\boldsymbol{\mu}}_1 = \frac{1}{N_1}\sum_{n=1}^{N} t_n \mathbf{x}_n \qquad \hat{\boldsymbol{\mu}}_2 = \frac{1}{N_2}\sum_{n=1}^{N} (1-t_n)\mathbf{x}_n$$

$$\hat{\boldsymbol{\Sigma}} = \frac{N_1}{N} S_1 + \frac{N_2}{N} S_2$$

with $S_i = \frac{1}{N_i}\sum_{n \in C_i}(\mathbf{x}_n - \hat{\boldsymbol{\mu}}_i)(\mathbf{x}_n - \hat{\boldsymbol{\mu}}_i)^T$, $i = 1, 2$

Note: details in C. Bishop. PRML. Section 4.2.2

Maximum likelihood (2 classes)

Prediction of new sample $\mathbf{x}' \notin D$

$$P(C_1|\mathbf{x}') = \sigma(\mathbf{w}^T\mathbf{x}' + w_0) \begin{cases} > 0.5 \Rightarrow C_1 \\ \leq 0.5 \Rightarrow C_2 \end{cases}$$

with $\mathbf{w}$ and w_0 computed from $hat\pi, \hat{\boldsymbol{\mu}}_1, \hat{\boldsymbol{\mu}}_2, \hat{\boldsymbol{\Sigma}}$ (maximum likelihood solution)

Generative model

$\hat{P}(\mathbf{x}|C_i) = \mathcal{N}(\mathbf{x}; \hat{\boldsymbol{\mu}}_i, \hat{\boldsymbol{\Sigma}})$ can be used to generate new samples for C_i

Maximum likelihood (K classes)

Given

$f : \mathbf{X} \rightarrow \{C_1, \ldots, C_K\}, \; D = \{(\mathbf{x}_n, t_n)_{n=1}^N\}$

$t_n = (0, \ldots, 1, \ldots, 0)$: 1-of-K (one-hot) encoding ($t_{nk} = 1$ iff $f(\mathbf{x}_n) = C_k$)

estimate

$$P(C_k|\mathbf{x}) = \frac{P(\mathbf{x}|C_k)P(C_k)}{\sum_j P(\mathbf{x}|C_j)P(C_j)} = \frac{exp(a_k)}{\sum_j exp(a_j)}$$

SOFTMAX function

(normalized exponential or softmax function)

with $a_k = \ln P(\mathbf{x}|C_k)P(C_k)$

Maximum likelihood (K classes)

Gaussian Naive Bayes

$P(C_k) = \pi_k, \; P(\mathbf{x}|C_k) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma})$

Training: Estimate from D

$$\hat{\pi}_k = \frac{N_k}{N}$$

$$\hat{\boldsymbol{\mu}}_k = \frac{1}{N_k} \sum_{n=1}^{N} t_{nk} \, \mathbf{x}_n$$

$$\hat{\boldsymbol{\Sigma}} = \sum_{k=1}^{K} \frac{N_k}{N} S_k \; , \qquad S_k = \frac{1}{N_k} \sum_{n=1}^{N} t_{nk} (\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^T$$

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Maximum likelihood (K classes)

Prediction of new sample $\mathbf{x}' \notin D$

$$\underset{C_k \in C}{\operatorname{argmax}} \hat{P}(C_k|\mathbf{x}') = \underset{k}{\operatorname{argmax}} \frac{exp(a_k)}{\sum_j exp(a_j)}$$

with $a_k = \ln \hat{P}(\mathbf{x}'|C_k)\hat{P}(C_k) = \ln \hat{\pi}_k \, \mathcal{N}(\mathbf{x}'; \hat{\boldsymbol{\mu}}_k, \hat{\boldsymbol{\Sigma}})$

Probabilistic Models

Represent posterior distributions with parametric models.

For two classes

$$P(C_1|\mathbf{x}) = \sigma(a)$$

For $k \geq 2$ classes

$$P(C_i|\mathbf{x}) = \frac{exp(a_k)}{\sum_j exp(a_j)}$$

$$a_k = \mathbf{w}^T \mathbf{x} + w_0$$

This is valid for all the class-conditional distributions in the exponential family (including Gaussians). [Bishop, Sect. 4.2.4]

Notation

Target function: $f : \Re^d \mapsto C$

Dataset $D = \{(\mathbf{x}_n, t_n)_{n=1}^N\} = \langle \mathbf{X}, \mathbf{t} \rangle$

$\mathbf{X}$: matrix $(N \times d)$ of input values

$\mathbf{t}$: vector (N) of output values

Compact notation

Model

$$\mathbf{w}^T \mathbf{x} + w_0 = (w_0 \ \mathbf{w}) \begin{pmatrix} 1 \\ \mathbf{x} \end{pmatrix}$$

$$\tilde{\mathbf{w}} = \begin{pmatrix} w_0 \\ \mathbf{w} \end{pmatrix}, \tilde{\mathbf{x}} = \begin{pmatrix} 1 \\ \mathbf{x} \end{pmatrix}$$

$$a_k = \mathbf{w}^T \mathbf{x} + w_0 = \tilde{\mathbf{w}}^T \tilde{\mathbf{x}}$$

Maximum Likelihood for parametric models

Likelihood for a parametric model $\mathcal{M}_\Theta$ of dataset $D = \langle \mathbf{X}, \mathbf{t} \rangle$: $P(\mathbf{t}|\Theta, \mathbf{X})$,

Maximum likelihood solution:

$$\Theta^* = \underset{\Theta}{\operatorname{argmax}} \ln P(\mathbf{t}|\Theta, \mathbf{X})$$

When $\mathcal{M}_\Theta$ belongs to the exponential family, likelihood $P(\mathbf{t}|\Theta, \mathbf{X})$ can be expressed in the form $P(\mathbf{t}|\tilde{\mathbf{w}}, \mathbf{X})$, with maximum likelihood

$$\tilde{\mathbf{w}}^* = \underset{\tilde{\mathbf{w}}}{\operatorname{argmax}} \ln P(\mathbf{t}|\tilde{\mathbf{w}}, \mathbf{X})$$

Probabilistic Discriminative Models

Estimate directly

$$P(C_k|\tilde{\mathbf{x}}, D) = \frac{exp(a_k)}{\sum_j exp(a_j)} \qquad a_k = \tilde{\mathbf{w}}^T \tilde{\mathbf{x}}$$

with maximum likelihood

$$\tilde{\mathbf{w}}^* = \underset{\tilde{\mathbf{w}}}{\operatorname{argmax}} \ln P(\mathbf{t}|\tilde{\mathbf{w}}, \mathbf{X})$$

without estimating the model parameters.

Simplified notation (dataset omitted): $P(\mathbf{t}|\tilde{\mathbf{w}})$

Logistic regression

Probabilistic discriminative model based on maximum likelihood.

Two classes

Given data set $D = \{(\tilde{\mathbf{x}}_n, t_n)_{n=1}^N\}$, with $t_n \in \{0, 1\}$

Likelihood function:

$$p(\mathbf{t}|\tilde{\mathbf{w}}) = \prod_{n=1}^{N} y_n^{t_n}(1 - y_n)^{1-t_n}$$

with $y_n = p(C_1|\tilde{\mathbf{x}}_n) = \sigma(\tilde{\mathbf{w}}^T \tilde{\mathbf{x}}_n)$

Note: t_n: value in the data set corresponding to $\mathbf{x}_n$,
y_n: posterior prediction of the current model $\tilde{\mathbf{w}}$ for $\mathbf{x}_n$.

Logistic regression

Cross-entropy error function (negative log likelihood)

$$E(\tilde{\mathbf{w}}) \equiv -\ln p(\mathbf{t}|\tilde{\mathbf{w}}) = -\sum_{n=1}^{N}[t_n \ln y_n + (1-t_n)\ln(1-y_n)]$$

Solution concept: solve the optimization problem

$$\tilde{\mathbf{w}}^* = \operatorname*{argmin}_{\tilde{\mathbf{w}}} E(\tilde{\mathbf{w}})$$

Many solvers available.

Iterative reweighted least squares

Apply *Newton-Raphson* iterative optimization for minimizing $E(\tilde{\mathbf{w}})$.

Gradient of the error with respect to $\tilde{\mathbf{w}}$

$$\nabla E(\tilde{\mathbf{w}}) = \sum_{n=1}^{N}(y_n - t_n)\tilde{\mathbf{x}}_n$$

Gradient descent step

$$\tilde{\mathbf{w}} \leftarrow \tilde{\mathbf{w}} - \boldsymbol{H}(\tilde{\mathbf{w}})^{-1}\nabla E(\tilde{\mathbf{w}})$$

$\boldsymbol{H}(\tilde{\mathbf{w}}) = \nabla\nabla E(\tilde{\mathbf{w}})$ is the Hessian matrix of $E(\tilde{\mathbf{w}})$ (second derivatives with respect to $\tilde{\mathbf{w}}$).

Iterative reweighted least squares

Given

$$\tilde{\mathbf{X}} = \begin{pmatrix} \tilde{\mathbf{x}}_1^T \\ \dots \\ \tilde{\mathbf{x}}_N^T \end{pmatrix} \quad \mathbf{t} = \begin{pmatrix} t_1 \\ \dots \\ t_N \end{pmatrix},$$

$\mathbf{y}(\tilde{\mathbf{w}}) = (y_1, \dots, y_n)^T$ posterior predictions of model $\tilde{\mathbf{w}}$

$\boldsymbol{R}(\tilde{\mathbf{w}})$: diagonal matrix with $R_{nn} = y_n(1 - y_n)$

we have

$$\nabla E(\tilde{\mathbf{w}}) = \tilde{\mathbf{X}}^T(\mathbf{y}(\tilde{\mathbf{w}}) - \mathbf{t})$$

$$\boldsymbol{H}(\tilde{\mathbf{w}}) = \nabla\nabla E(\tilde{\mathbf{w}}) = \sum_{n=1}^{N} y_n(1 - y_n)\tilde{\mathbf{x}}_n\tilde{\mathbf{x}}_n^T = \tilde{\mathbf{X}}^T\boldsymbol{R}(\tilde{\mathbf{w}})\tilde{\mathbf{X}}$$

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Iterative reweighted least squares

Iterative method:

1. Initialize $\tilde{\mathbf{w}}$
2. Repeat until termination condition

$$\tilde{\mathbf{w}} \leftarrow \tilde{\mathbf{w}} - (\tilde{\mathbf{X}}^T\,\boldsymbol{R}(\tilde{\mathbf{w}})\,\tilde{\mathbf{X}})^{-1}\tilde{\mathbf{X}}^T(\mathbf{y}(\tilde{\mathbf{w}}) - \mathbf{t})$$

Multiclass logistic regression

K **classes**

$$P(C_k|\tilde{\mathbf{x}}) = \frac{exp(a_k)}{\sum_j exp(a_j)} \qquad a_k = \tilde{\mathbf{w}}_k^T \tilde{\mathbf{x}} \qquad k = 1, \dots, K$$

$$\tilde{\mathbf{X}} = \begin{pmatrix} \tilde{\mathbf{x}}_1^T \\ \dots \\ \tilde{\mathbf{x}}_N^T \end{pmatrix} \qquad \mathbf{T} = \begin{pmatrix} t_1^T \\ \dots \\ t_N^T \end{pmatrix}$$ 1-of-K encoding of labels

$\mathbf{y}_n^T = (y_{n1} \dots y_{nK})^T$ posterior prediction of $\tilde{\mathbf{x}}_n$ for model $\tilde{\mathbf{w}}_1, \dots, \tilde{\mathbf{w}}_K$

$$\mathbf{Y}(\tilde{\mathbf{w}}_1, \dots, \tilde{\mathbf{w}}_K) = \begin{pmatrix} \mathbf{y}_1^T \\ \dots \\ \mathbf{y}_N^T \end{pmatrix}$$ posterior predictions of model $\tilde{\mathbf{w}}_1, \dots, \tilde{\mathbf{w}}_K$

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Multiclass logistic regression

Discriminative model

$$P(\mathbf{T}|\tilde{\mathbf{w}}_1, \dots, \tilde{\mathbf{w}}_K) = \prod_{n=1}^{N} \prod_{k=1}^{K} P(C_k|\tilde{\mathbf{x}}_n)^{t_{nk}} = \prod_{n=1}^{N} \prod_{k=1}^{K} y_{nk}^{t_{nk}}$$

with $y_{nk} = \mathbf{Y}[n, k]$ and $t_{nk} = \mathbf{T}[n, k]$.

Multiclass logistic regression

Cross-entropy error function

$$E(\tilde{\mathbf{w}}_1, \dots \tilde{\mathbf{w}}_K) = -\ln P(\mathbf{T}|\tilde{\mathbf{w}}_1, \dots \tilde{\mathbf{w}}_K) = -\sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \ln y_{nk}$$

Iterative algorithm

gradient $\nabla_{\tilde{\mathbf{w}}_j} E(\tilde{\mathbf{w}}_1, \dots \tilde{\mathbf{w}}_K) = \dots$

Hessian matrix $\nabla_{\tilde{\mathbf{w}}_k} \nabla_{\tilde{\mathbf{w}}_j} E(\tilde{\mathbf{w}}_1, \dots \tilde{\mathbf{w}}_K) = \dots$

Summary

Given a target function $f : \mathbf{X} \to C$, and data set D

assume a parametric model for the posterior probability $P(C_k|\tilde{\mathbf{x}}, \tilde{\mathbf{w}})$
sigmoid $\sigma(\tilde{\mathbf{w}}^T \tilde{\mathbf{x}})$ (2 classes) or softmax $\frac{exp(\tilde{\mathbf{w}}_k^T \tilde{\mathbf{x}})}{\sum_{j=1}^{K} exp(\tilde{\mathbf{w}}_j^T \tilde{\mathbf{x}})}$ (K classes)

Define an error function $E(\tilde{\mathbf{w}})$ (negative log likelihood)

Solve the optimization problem

$$\tilde{\mathbf{w}}^* = \operatorname*{argmin}_{\tilde{\mathbf{w}}} E(\tilde{\mathbf{w}})$$

Classify new sample $\tilde{\mathbf{x}}'$ as C_{k^*} where $k^* = \mathrm{argmax}_{k=1,\dots,K} P(C_k|\tilde{\mathbf{x}}', \tilde{\mathbf{w}}^*)$

Generalization

Given a target function $f : \mathbf{X} \rightarrow C$, and data set D

assume a prediction parametric model $y(\mathbf{x}; \theta)$, $\quad y(\mathbf{x}; \theta) \approx f(\mathbf{x})$

Define an error function $E(\theta)$

Solve the optimization problem

$$\theta^* = \operatorname*{argmin}_{\theta} E(\theta)$$

Classify new sample $\mathbf{x}'$ as $y(\mathbf{x}'; \theta^*)$

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Learning in feature space

All methods described above can be applied in a transformed space of the input (*feature space*).

Given a function $\phi : \tilde{\mathbf{X}} \mapsto \mathbf{\Phi}$ ($\mathbf{\Phi}$ is the *feature space*)
each sample $\tilde{\mathbf{x}}_n$ can be mapped to a feature vector $\boldsymbol{\phi}_n = \phi(\tilde{\mathbf{x}}_n)$

Replacing $\tilde{\mathbf{x}}_n$ with $\boldsymbol{\phi}_n$ in all the equations above, makes the learning system to work in the feature space instead of the input space.

We will see in the next lectures why this trick is useful.