A priori distribution choices for a mixture of experts *

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Abstract: The paper investigates a mixture of expert models. A mixture of experts is a set of experts and gate function which weighs these experts. Each expert is a linear model. A gate function is a neural network with softmax on the last layer. In this article, we analyzed different a priori distributions for each expert. We proposed a method that takes into account the relationship between the a priori distributions of different experts. To solve the optimization problem, we used the EM algorithm. In this paper, the problem of circles parameters estimation is the task of a mixture of experts. Each circle in the image is one expert. For testing, we are using synthetic and real data. Real data is a human eye from the iris detection problem.

Keywords: mixture of Experts; bayesian model selection; prior distribution.

1 Introduction

2 Related work

3 Problem statement of circle parameters estimation

This data are binary image

$$\mathbf{M} \in \{0, 1\}^{m_1 \times m_2},$$

where 1 is a black pixel, an image, and 0 is a white pixel, the image background. The image $\mathbf{M}$ is mapped to the set of coordinates x_i, y_i $\mathbf{C}$. The coordinates x_i, y_i is a coordinates of black pixels in the image $\mathbf{M}$:

$$\mathbf{C} \in \mathbb{R}^{N \times 2},$$

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where N is the number of black pixels in the image $\mathbf{M}$.

Let a pair of coordinates x_0, y_0 is the center of the circle, and r is the radius of the circle in the image $\mathbf{M}$. The circle parameters x_0, y_0, r need to be found.

The points $(x_i, y_i) \in \mathbf{C}$ is geometric locus of circle points. The circle equation approximates this locus of points:

$$(x_i - x_0)^2 + (y_i - y_0)^2 = r^2.$$

Expand brackets:

$$(2x_0) \cdot x_i + (2y_0) \cdot y_i + (r^2 - x_0^2 - y_0^2) \cdot 1 = x_i^2 + y_i^2. \tag{1}$$

Equation (1) is a linear regression problem with following data:

$$\mathbf{X}\mathbf{w} \approx \mathbf{y}, \quad \mathbf{X} = [\mathbf{C}, \mathbf{1}], \quad \mathbf{y} = [x_1^2 + y_1^2, x_2^2 + y_2^2, \cdots, x_N^2 + y_N^2]^\mathsf{T}, \tag{2}$$

where the parameters $\mathbf{w} = \big[w_1, w_2, w_3\big]^\mathsf{T}$ reconstruct the circle parameters x_0, y_0, r:

$$x_0 = \frac{w_1}{2}, \quad y_0 = \frac{w_2}{2}, \quad r = \sqrt{w_3 + x_0^2 + y_0^2}.$$

The solution of the problem (2) reconstructs the circle parameters only if the number of circles in an image is equal to one. If the image consists of several circles, then the authors propose to use a multimodel. The multimodel is an ensemble of linear models. Each linear model approximates only one circle in the image. In this paper, multimodel is a mixture of experts.

4 Problem statement of building a mixture of experts

Generalize one circle approximation problem to the case of several circles. The data from equation (2) for several circles case, given by the following data:

$$\mathbf{X} \in \mathbb{R}^{N \times n},$$

where N is the number of datum and n is the number of features.

Definition 4.1. *A multimodel is mixture of experts if it has the following form*

$$\hat{\mathbf{f}} = \sum_{k=1}^{K} \pi_k \mathbf{f}_k, \qquad \pi_k(\mathbf{x}, \mathbf{V}) : \mathbb{R}^{n \times |\mathbf{V}|} \to [0, 1], \qquad \sum_{k=1}^{K} \pi_k(\mathbf{x}, \mathbf{V}) = 1,$$

where $\hat{\mathbf{f}}$ is the multimodel, $\mathbf{f}_k$ is the local models, π_k is the gate function, $\mathbf{w}_k$ is the parameters of local model and $\mathbf{V}$ is the parameters of gate function.

The linear models are considered as local models. A simple 2–layer fully connected neural network is considered as a gate function:

$$\mathbf{f}_k(\mathbf{x}) = \mathbf{w}_k^\mathsf{T}\mathbf{x}, \quad \boldsymbol{\pi}(\mathbf{x}, \mathbf{V}) = \text{softmax}\bigl(\mathbf{V}_1^\mathsf{T}\boldsymbol{\sigma}\left(\mathbf{V}_2^\mathsf{T}\mathbf{x}\right)\bigr),$$

where $\mathbf{V} = \bigl\{\mathbf{V}_1, \mathbf{V}_2\bigr\}$ — parameters of gate function.

All parameters optimises according to the maximum likelihood principle:

$$p\bigl(\mathbf{y}, \mathbf{W}|\mathbf{X}, \mathbf{V}\bigr) = \prod_{k=1}^{K} p^k\bigl(\mathbf{w}_k\bigr)\prod_{i=1}^{N}\left(\sum_{k=1}^{K}\pi_k p_k\bigl(y_i|\mathbf{w}_k, \mathbf{x}_i\bigr)\right), \tag{3}$$

where $\mathbf{W} = \bigl[\mathbf{w}_1, \mathbf{w}_2, \cdots, \mathbf{w}_K\bigr]^\mathsf{T}$.

The optimisation problem for finding optimal parameters of local models and optimal mixture parameters:

$$\hat{\mathbf{W}}, \hat{\mathbf{V}} = \arg\max_{\mathbf{W},\mathbf{V}} p\bigl(\mathbf{y}, \mathbf{W}|\mathbf{X}, \mathbf{V}\bigr). \tag{4}$$

5 EM–algorithm as a solver of optimisation problem

To build a mixture of experts, consider the following probabilistic statement of the problem:

1) a likelihood $p_k\left(y_i|\mathbf{w}_k, \mathbf{x}_i\right) = \mathcal{N}\left(y_i|\mathbf{w}_k^\mathsf{T}\mathbf{x}_i, \beta^{-1}\right)$, where β is a noise parameter,

2) a priori distribution of parameters $p^k\left(\mathbf{w}_k\right) = \mathcal{N}\left(\mathbf{w}_k|\mathbf{w}_k^0, \mathbf{A}_k\right)$, where $\mathbf{w}_k^0$ — a vector of size $n \times 1$, $\mathbf{A}_k$ — covariance matrix of parameters,

3) a priori regularisation $p\left(\boldsymbol{\varepsilon}_{k,k'}|\boldsymbol{\Xi}\right) = \mathcal{N}\left(\boldsymbol{\varepsilon}_{k,k'}|\mathbf{0}, \boldsymbol{\Xi}\right)$, where $\boldsymbol{\Xi}$ — covariance matrix $\boldsymbol{\varepsilon}_{k,k'} = \mathbf{w}_k^0 - \mathbf{w}_{k'}^0$.

Under the previous assumption, the likelihood (3) is rewritten to:

$$\begin{aligned} p\bigl(\mathbf{y}, \mathbf{W}|\mathbf{X}, \mathbf{V}, \mathbf{A}, \mathbf{W}^0, \boldsymbol{\Xi}, \beta\bigr) = &\prod_{k,k'=1}^{K}\mathcal{N}\left(\boldsymbol{\varepsilon}_{k,k'}|\mathbf{0}, \boldsymbol{\Xi}\right)\cdot \\ &\cdot\prod_{k=1}^{K}\mathcal{N}\left(\mathbf{w}_k|\mathbf{w}_k^0, \mathbf{A}_k\right)\prod_{i=1}^{N}\left(\sum_{k=1}^{K}\pi_k\mathcal{N}\left(y_i|\mathbf{w}_k^\mathsf{T}\mathbf{x}_i, \beta^{-1}\right)\right), \end{aligned} \tag{5}$$

where $\mathbf{A} = \bigl\{\mathbf{A}_1, \cdots, \mathbf{A}_K\bigr\}$.

Consider the matrix of hidden variables $\mathbf{Z}$ for solving problem (4) under assumption (5). In matrix $\mathbf{Z}$ all $z_{ik} = 1$ if and only if object i related to local model k and $z_{ik} = 0$ otherwise.

Logarithm of likelihood (5) rewrites to following view by using matrix $\mathbf{Z}$:

$$\begin{aligned}\log p\bigl(\mathbf{y}, \mathbf{Z}, \mathbf{W} | \mathbf{X}, \mathbf{V}, \mathbf{A}, \mathbf{W}^0, \boldsymbol{\Xi}, \beta\bigr) = \\ = \sum_{i=1}^{N}\sum_{k=1}^{K} z_{ik}\left[\log \pi_k\left(\mathbf{x}_i, \mathbf{V}\right) - \frac{\beta}{2}\left(y_i - \mathbf{w}_k^{\mathsf{T}}\mathbf{x}_i\right)^2 + \frac{1}{2}\log\frac{\beta}{2\pi}\right] + \\ + \sum_{k=1}^{K}\left[-\frac{1}{2}\left(\mathbf{w}_k - \mathbf{w}_k^0\right)^{\mathsf{T}}\mathbf{A}_k^{-1}\left(\mathbf{w}_k - \mathbf{w}_k^0\right) + \frac{1}{2}\log\det\mathbf{A}_k^{-1} - \frac{n}{2}\log 2\pi\right] + \\ + \sum_{k=1}^{K}\sum_{k'=1}^{K}\left[-\frac{1}{2}\left(\mathbf{w}_k^0 - \mathbf{w}_{k'}^0\right)^{\mathsf{T}}\boldsymbol{\Xi}^{-1}\left(\mathbf{w}_k^0 - \mathbf{w}_{k'}^0\right) + \frac{1}{2}\log\det\boldsymbol{\Xi} - \frac{n}{2}\log 2\pi\right].\end{aligned} \tag{6}$$

The optimisation problem (4) for log–likelihood (6) rewrites as follows

$$\mathbf{W}, \mathbf{Z}, \mathbf{V}, \mathbf{W}^0, \mathbf{A}, \beta = \arg\max_{\mathbf{W},\mathbf{Z},\mathbf{V},\mathbf{W}^0,\mathbf{A},\beta} \log p\bigl(\mathbf{y}, \mathbf{Z}, \mathbf{W} | \mathbf{X}, \mathbf{V}, \mathbf{A}, \mathbf{W}^0, \boldsymbol{\Xi}, \beta\bigr). \tag{7}$$

To find a local minimum in the optimization problem (7), we use the variational EM–algorithm [23].

E–step. Let the variational distribution $q\left(\mathbf{Z}, \mathbf{W}\right)$ satisfy the assumption [23] of mean field approximation $q\left(\mathbf{Z}, \mathbf{W}\right) = q\left(\mathbf{Z}\right)q\left(\mathbf{W}\right)$. Find the variational distribution $q\left(\mathbf{Z}, \mathbf{W}\right)$ closest to $p\bigl(\mathbf{Z}, \mathbf{W} | \mathbf{y}, \mathbf{X}, \mathbf{V}, \mathbf{A}, \mathbf{W}^0, \boldsymbol{\Xi}, \beta\bigr)$. In the text below, the symbol $\propto$ means equality up to an additive constant. First, find the distribution of the hidden variable $q\left(\mathbf{Z}\right)$:

$$\begin{aligned}\log q\left(\mathbf{Z}\right) = \mathsf{E}_{q/\mathbf{Z}}\log p\bigl(\mathbf{y}, \mathbf{Z}, \mathbf{W} | \mathbf{X}, \mathbf{V}, \mathbf{A}, \mathbf{W}^0, \boldsymbol{\Xi}, \beta\bigr) \propto \\ \propto \sum_{i+1}^{N}\sum_{k=1}^{K} z_{ik}\left[\log \pi_k\left(\mathbf{x}_i, \mathbf{V}\right) - \frac{\beta}{2}\left(y_i^2 - \mathbf{x}_i^{\mathsf{T}}\mathsf{E}\mathbf{w}_k + \mathbf{x}_i^{\mathsf{T}}\mathsf{E}\mathbf{w}_k\mathbf{w}_k^{\mathsf{T}}\mathbf{x}_i\right) + \frac{1}{2}\log\frac{\beta}{2\pi}\right] \\ p\left(z_{ik} = 1\right) = \frac{\exp\left(\log \pi_k\left(\mathbf{x}_i, \mathbf{V}\right) - \frac{\beta}{2}\left(\mathbf{x}_i^{\mathsf{T}}\mathsf{E}\mathbf{w}_k\mathbf{w}_k^{\mathsf{T}}\mathbf{x}_i - \mathbf{x}_i^{\mathsf{T}}\mathsf{E}\mathbf{w}_k\right)\right)}{\sum_{k'=1}^{K}\exp\left(\log \pi_{k'}\left(\mathbf{x}_i, \mathbf{V}\right) - \frac{\beta}{2}\left(\mathbf{x}_i^{\mathsf{T}}\mathsf{E}\mathbf{w}_{k'}\mathbf{w}_{k'}^{\mathsf{T}}\mathbf{x}_i - \mathbf{x}_i^{\mathsf{T}}\mathsf{E}\mathbf{w}_{k'}\right)\right)}.\end{aligned} \tag{8}$$

The distribution $q\bigl(z_{ik}\bigr)$ is a Bernoulli distribution with probability z_{ik} from the equation (8). Second, find the distribution of parameters $q\left(\mathbf{W}\right)$

$$\begin{aligned}\log q\left(\mathbf{W}\right) = \mathsf{E}_{q/\mathbf{W}}\log p\bigl(\mathbf{y}, \mathbf{Z}, \mathbf{W} | \mathbf{X}, \mathbf{V}, \mathbf{A}, \mathbf{W}^0, \boldsymbol{\Xi}, \beta\bigr) \propto \\ \propto \sum_{i=1}^{N}\sum_{k=1}^{K} \mathsf{E}z_{ik}\left[\log \pi_k\left(\mathbf{x}_{i,\mathbf{V}}\right) - \frac{\beta}{2}\left(y_i - \mathbf{w}_k^{\mathsf{T}}\mathbf{x}_i\right)^2 + \frac{1}{2}\log\frac{\beta}{2\pi}\right] + \\ + \sum_{k=1}^{K}\left[-\frac{1}{2}\left(\mathbf{w}_k - \mathbf{w}_k^0\right)^{\mathsf{T}}\mathbf{A}_k^{-1}\left(\mathbf{w}_k - \mathbf{w}_k^0\right) + \frac{1}{2}\log\det\mathbf{A}_k^{-1} - \frac{n}{2}\log 2\pi\right] \\ \propto \sum_{k=1}^{K}\left[\mathbf{w}_k^{\mathsf{T}}\left(\mathbf{A}_k^{-1}\mathbf{w}_k^0 + \beta\sum_{i=1}^{N}\mathbf{x}_i y_i \mathsf{E}z_{ik}\right) - \frac{1}{2}\mathbf{w}_k^{\mathsf{T}}\left(\mathbf{A}_k^{-1} + \beta\sum_{i=1}^{N}\mathbf{x}_i\mathbf{x}_i^{\mathsf{T}}\right)\mathbf{w}_k\right].\end{aligned}$$

The distribution $q(\mathbf{w}_k)$ is a normal distribution with mean $\mathbf{m}_k$ and covariance matrix $\mathbf{B}_k$. The distribution parameters $\mathbf{m}_k, \mathbf{B}_k$ are calculated as follows:

$$\mathbf{m}_k = \mathbf{B}_k \left(\mathbf{A}_k^{-1} \mathbf{w}_k^0 + \beta \sum_{i=1}^{N} \mathbf{x}_i y_i \mathsf{E} z_{ik} \right), \qquad \mathbf{B}_k = \left(\mathbf{A}_k^{-1} + \beta \sum_{i=1}^{N} \mathbf{x}_i \mathbf{x}_i^{\mathsf{T}} \mathsf{E} z_{ik} \right)^{-1}.$$

M–step. Find hyperparameters $\mathbf{V}, \mathbf{W}^0, \mathbf{A}, \beta$ from maximisation expected value of log-likelihood under the condition of a variational distribution $q\left(\mathbf{Z}, \mathbf{W}\right)$.

$$\begin{aligned}\mathcal{F}\left(\mathbf{V}, \mathbf{W}^0, \mathbf{A}, \beta\right) &= \mathsf{E}_q \log p\big(\mathbf{y}, \mathbf{Z}, \mathbf{W} | \mathbf{X}, \mathbf{V}, \mathbf{A}, \mathbf{W}^0, \Xi, \beta\big) = \\ &= \sum_{i=1}^{N}\sum_{k=1}^{K} \mathsf{E} z_{ik} \left[\log \pi_k\left(\mathbf{x}_i, \mathbf{V}\right) - \frac{\beta}{2} \mathsf{E}\left(y_i - \mathbf{w}_k^{\mathsf{T}}\mathbf{x}_i\right)^2 + \frac{1}{2}\log\frac{\beta}{2\pi} \right] + \\ &+ \sum_{k=1}^{K} \left[-\frac{1}{2} \mathsf{E}\left(\mathbf{w}_k - \mathbf{w}_k^0\right)^{\mathsf{T}} \mathbf{A}_k^{-1} \left(\mathbf{w}_k - \mathbf{w}_k^0\right) + \frac{1}{2}\log\det \mathbf{A}_k^{-1} - \frac{n}{2}\log 2\pi \right] + \\ &+ \sum_{k=1}^{K}\sum_{k'=1}^{K} \left[-\frac{1}{2} \left(\mathbf{w}_k^0 - \mathbf{w}_{k'}^0\right)^{\mathsf{T}} \Xi^{-1} \left(\mathbf{w}_k^0 - \mathbf{w}_{k'}^0\right) + \frac{1}{2}\log\det \Xi - \frac{n}{2}\log 2\pi \right].\end{aligned} \tag{9}$$

To find the parameters $\mathbf{V}$, which maximising the function (9), we use the gradient optimization method. This method guarantees convergence to local extrema. Let find the parameters $\mathbf{A}_k$, which maximising the function (9):

$$\begin{aligned}\frac{\partial \mathcal{F}\left(\mathbf{V}, \mathbf{W}^0, \mathbf{A}, \beta\right)}{\partial \mathbf{A}_k^{-1}} &= \frac{1}{2}\mathbf{A}_k - \frac{1}{2}\mathsf{E}\left(\mathbf{w}_k - \mathbf{w}_k^0\right)\left(\mathbf{w}_k - \mathbf{w}_k^0\right)^{\mathsf{T}} = 0, \\ \mathbf{A}_k &= \mathsf{E}\mathbf{w}_k\mathbf{w}_k^{\mathsf{T}} - \mathbf{w}_k^0 \mathsf{E}\mathbf{w}_k^{\mathsf{T}} - \mathsf{E}\mathbf{w}_k \mathbf{w}_k^{0\mathsf{T}} + \mathbf{w}_k^0\mathbf{w}_k^{0\mathsf{T}}.\end{aligned}$$

Similarly, we find optimal value of β and $\mathbf{w}_0^k$.

$$\begin{aligned}\frac{\partial \mathcal{F}\left(\mathbf{V}, \mathbf{W}^0, \mathbf{A}, \beta\right)}{\partial \beta} &= \sum_{k=1}^{K}\sum_{i=1}^{N}\left(\frac{1}{\beta}\mathsf{E}z_{ik} - \frac{1}{2}\mathsf{E}z_{ik}\left[y_i^2 - 2y_i\mathbf{x}_i^{\mathsf{T}}\mathsf{E}\mathbf{w}_k + \mathbf{x}_i^{\mathsf{T}}\mathbf{w}_k\mathbf{w}_k^{\mathsf{T}}\mathbf{x}_i\right]\right) = 0, \\ \frac{1}{\beta} &= \frac{1}{N}\sum_{i=1}^{N}\sum_{k=1}^{K}\left[y_i^2 - 2y_i\mathbf{x}_i^{\mathsf{T}}\mathsf{E}\mathbf{w}_k + \mathbf{x}_i^{\mathsf{T}}\mathsf{E}\mathbf{w}_k\mathbf{w}_k^{\mathsf{T}}\mathbf{x}_i\right]\mathsf{E}z_{ik}.\end{aligned}$$

$$\begin{aligned}\frac{\partial \mathcal{F}\left(\mathbf{V}, \mathbf{W}^0, \mathbf{A}, \beta\right)}{\partial \mathbf{w}_k^0} &= \mathbf{A}_k^{-1}\big(\mathsf{E}\mathbf{w}_k - \mathbf{w}_k^0\big) + \Xi\sum_{k'=1}^{K}\big[\mathbf{w}_{k'}^0 - \mathbf{w}_k^0\big] = 0, \\ \mathbf{w}_k^0 &= \left[\mathbf{A}_k^{-1} + (K-1)\,\Xi\right]^{-1}\left(\mathbf{A}_k^{-1}\mathsf{E}\mathbf{w}_k + \Xi\sum_{k'=1,\ k'\neq k}^{K}\mathbf{w}_{k'}^0\right).\end{aligned} \tag{10}$$

The formulas (8–10) are an iterative procedure which convergence to local maximum of optimisation problem (7). If in the list of probabilistic statements we consider only the statement 1) then find solution the optimisation problem (5) without any priori distribution. If in the list of probabilistic statements we considers statements 1) and 2) then find solution the optimisation problem with a priori distribution on the local models parameters. If in the list of probabilistic statements we considers all statements 1), 2) and 3) then find solution the optimisation problem (7) with a priori distributions and relationships between a priori distributions of different local models.

6 Computational experiment

7 Conclusion

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