Prior distribution choices for a mixture of experts *

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Abstract: The paper investigates a mixture of expert models. The mixture of experts is a set of experts and the gate function which weighs these experts. Each expert is a linear model. The gate function is a neural network with softmax on the last layer. The paper analyzes different prior distributions for each expert. The authors propose a method that takes into account the relationship between the prior distributions of different experts. The paper uses the EM algorithm for solving the optimization problem. This paper proposes to use the mixture of experts for the problem of circles parameters estimation. Each expert fits one circle in the image. The experiment uses synthetic and real data to test the proposed method. The real data is a human eye image from the iris detection problem.

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

1 Introduction

The paper studies the problem of a mixture of experts constructing. A mixture of experts is multimodel, which are weighed local models that approximate the dataset. The weighting coefficients depend on datum from the dataset.

Examples of multimodel are bagging, gradient boosting [1] and random forest [2]. There are approaches to multimodeling [3] suggests that the contribution of each expert to the answer depends on the object from the dataset. A mixture of experts uses a gate function that weights the prediction of each expert.

The main problem of multimodal is a convergence dependence on the initial point. We are using the probability approach for finding optimal mixture parameters and local

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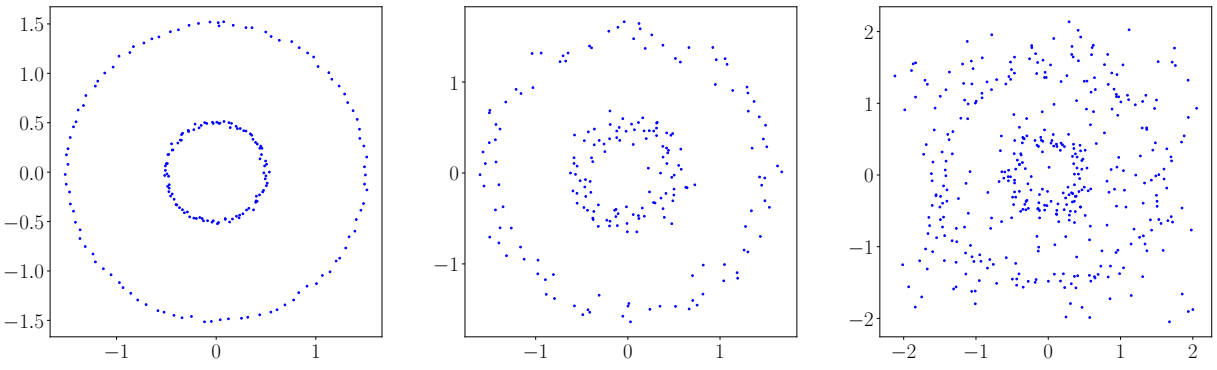
expert parameters. The paper proposes to use different prior distribution on parameters to improve convergence. The paper introduces the method which is using a dependence between prior distribution to improve multimodel quality.



(a) Without noise (b) Noise near circle (c) Uniform noise

Figure 1: An example of circles with different noise levels: (a) circle without noise; (b) noisy radius circle; (c) noisy radius circle, and uniform noisy on image

The paper analysis multimodel quality depending on the prior distribution of the expert's parameters. There solves a problem of finding circles on a binarized image. Examples of images are shown in fig. 1. In this paper, each expert is a linear model. A gate function is a two-layer fully connected neural network.

2 Related work

Many papers on a mixture of experts are devoted to the choice of a gateway function: softmax, the Dirichlet process [5], a neural network [4] with softmax function on the last layer. Some papers are devoted to the choice of expert type. Papers [6, 10] analyze linear models as experts. Papers [7, 8] analyze SVMs as experts. The paper [3] contains an overview of different methods for choosing a gate function and expert type.

A mixture of experts has many applications. Papers [11, 12, 13] use a mixture of experts in the task of forecasting time series. The paper [14] uses a mixture of experts in the task of recognizing handwritten numbers. Papers [15, 16, 17, 18] are devoted to methods of text and speech recognition by using a mixture of experts. The paper [19] analyzes a mixture of experts in the task of recognizing three-dimensional human movements.

The paper [22] is devoted to a review of the study results on the iris detection in the image. The methods of highlighting the borders of the iris and pupil are described in papers [20, 21].

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 a set of coordinates $\mathbf{C} = \{x_i, y_i\}_{i=1}^{N}$. The pair of coordinates (x_i, y_i) is a black pixel in $\mathbf{M}$:

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

where N is the number of black pixels.

Let (x_0, y_0) be the center of the circle, and r is radius of the circle.

The coordinates $(x_i, y_i) \in \mathbf{C}$ is a circle locus of points defined by

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

Expand brackets:

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

Rewrite equation (1) to set the linear regressions problem for all points in the dataset:

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

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 problem (2) reconstructs the circle parameters only if the number of circles in an image is equal to one. The authors propose to use the multimodel for the image, which consists of several circles. The multimodel is an ensemble of the 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 for this case is

$$\mathbf{X} \in \mathbb{R}^{N \times n}, \tag{3}$$

where N is a number of datum and n is a number of features. In this paper, n is equal to 3.

Definition 4.1. *Call the multimodel* $\hat{\mathbf{f}}$ *a mixture of experts if*

$$\hat{\mathbf{f}} = \sum_{k=1}^{K} \pi_k \mathbf{f}_k, \qquad \pi_k\left(\mathbf{x}, \mathbf{V}\right) : \mathbb{R}^{n \times |\mathbf{V}|} \to [0,1], \qquad \sum_{k=1}^{K} \pi_k\left(\mathbf{x}, \mathbf{V}\right) = 1, \tag{4}$$

where $\mathbf{f}_k$ *is a local model,* π_k *is a gate function, vector* $\mathbf{w}_k$ *is some parameters of the local model and* $\mathbf{V}$ *is some parameters of the gate function.*

This paper asserts the local model a linear model. The gate function is the two–layer fully connected neural network

$$\mathbf{f}_k\left(\mathbf{x}\right) = \mathbf{w}_k^{\mathsf{T}}\mathbf{x}, \quad \boldsymbol{\pi}\left(\mathbf{x}, \mathbf{V}\right) = \operatorname{softmax}\big(\mathbf{V}_1^{\mathsf{T}}\boldsymbol{\sigma}\left(\mathbf{V}_2^{\mathsf{T}}\mathbf{x}\right)\big), \tag{5}$$

where $\mathbf{V} = \big\{\mathbf{V}_1, \mathbf{V}_2\big\}$ is a set of the gate function parameters.

Combining (4) and (5), obtain the likelihood solution:

$$p\big(\mathbf{y}, \mathbf{W}|\mathbf{X}, \mathbf{V}\big) = \prod_{k=1}^{K} p^k\big(\mathbf{w}_k\big) \prod_{i=1}^{N} \left(\sum_{k=1}^{K} \pi_k p_k\big(y_i|\mathbf{w}_k, \mathbf{x}_i\big) \right), \tag{6}$$

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

The optimal parameters is delivered by the maximum likelihood solution:

$$\hat{\mathbf{W}}, \hat{\mathbf{V}} = \arg\max_{\mathbf{W},\mathbf{V}} p\big(\mathbf{y}, \mathbf{W}|\mathbf{X}, \mathbf{V}\big). \tag{7}$$

5 EM–algorithm as a solver of optimisation problem

To build a mixture of experts, set the following probabilistic statement for the problem (3):

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

2) a prior 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 $\mathbf{w}_k^0$ is a vector of size $n \times 1$ and $\mathbf{A}_k$ is a covariance matrix,

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

Combining assumptions $1), 2), 3)$ and equation (6), obtain

$$\begin{aligned} p\big(\mathbf{y}, \mathbf{W}|\mathbf{X}, \mathbf{V}, \mathbf{A}, \mathbf{W}^0, \boldsymbol{\Xi}, \beta\big) = & \prod_{k,k'=1}^{K} \mathcal{N}\left(\boldsymbol{\varepsilon}_{k,k'}|\mathbf{0}, \boldsymbol{\Xi}\right) \cdot \\ & \cdot \prod_{k=1}^{K} \mathcal{N}\left(\mathbf{w}_k|\mathbf{w}_k^0, \mathbf{A}_k\right) \prod_{i=1}^{N} \left(\sum_{k=1}^{K} \pi_k \mathcal{N}\left(y_i|\mathbf{w}_k^{\mathsf{T}}\mathbf{x}_i, \beta^{-1}\right) \right), \end{aligned} \tag{8}$$

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

Introduce a binary matrix $\mathbf{Z}$. Its element z_{ik} is equal to 1 if and only if the object i is related to the local model k. Integrating the binary matrix $\mathbf{Z}$ in (8), obtain:

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

Obtain a new optimisation problem combining (7) and (9):

$$\mathbf{W}, \mathbf{Z}, \mathbf{V}, \mathbf{W}^0, \mathbf{A}, \beta = \arg\max_{\mathbf{W}, \mathbf{Z}, \mathbf{V}, \mathbf{W}^0, \mathbf{A}, \beta} \log p\big(\mathbf{y}, \mathbf{Z}, \mathbf{W}|\mathbf{X}, \mathbf{V}, \mathbf{A}, \mathbf{W}^0, \boldsymbol{\Xi}, \beta\big). \tag{10}$$

Use the expectation-maximization [23] algorithm to find the maximum likelihood solution (10) for the multimodel (8) with latent variable $\mathbf{Z}$.

E–step. Let a join distribution $q\left(\mathbf{Z}, \mathbf{W}\right)$ satisfies the following assumption $q\left(\mathbf{Z}, \mathbf{W}\right) = q\left(\mathbf{Z}\right)q\left(\mathbf{W}\right)$ [23]. The symbol $\propto$ means that both sides are equal to up to an additive constant. First, find the distribution $q\left(\mathbf{Z}\right)$:

$$\begin{aligned}\log q\left(\mathbf{Z}\right) = \mathsf{E}_{q/\mathbf{Z}}\log p\big(\mathbf{y}, \mathbf{Z}, \mathbf{W}|\mathbf{X}, \mathbf{V}, \mathbf{A}, \mathbf{W}^0, \boldsymbol{\Xi}, \beta\big) \propto \\ \propto \sum_{i+1}^{N}\sum_{k=1}^{K} z_{ik}\left[\log \pi_k\left(\mathbf{x}_i, \mathbf{V}\right) - \frac{\beta}{2}\left(y_i^2 - \mathbf{x}_i^{\mathsf{T}}\mathsf{E}\mathbf{w}_k + \mathbf{x}_i^{\mathsf{T}}\mathsf{E}\mathbf{w}_k\mathbf{w}_k^{\mathsf{T}}\mathbf{x}_i\right) + \frac{1}{2}\log\frac{\beta}{2\pi}\right] \\ p\left(z_{ik} = 1\right) = \frac{\exp\left(\log \pi_k\left(\mathbf{x}_i, \mathbf{V}\right) - \frac{\beta}{2}\left(\mathbf{x}_i^{\mathsf{T}}\mathsf{E}\mathbf{w}_k\mathbf{w}_k^{\mathsf{T}}\mathbf{x}_i - \mathbf{x}_i^{\mathsf{T}}\mathsf{E}\mathbf{w}_k\right)\right)}{\sum_{k'=1}^{K}\exp\left(\log \pi_{k'}\left(\mathbf{x}_i, \mathbf{V}\right) - \frac{\beta}{2}\left(\mathbf{x}_i^{\mathsf{T}}\mathsf{E}\mathbf{w}_{k'}\mathbf{w}_{k'}^{\mathsf{T}}\mathbf{x}_i - \mathbf{x}_i^{\mathsf{T}}\mathsf{E}\mathbf{w}_{k'}\right)\right)}.\end{aligned} \tag{11}$$

The distribution $q\big(z_{ik}\big)$ is the Bernoulli distribution with probability z_{ik} from equation (11). Second, find the distribution $q\left(\mathbf{W}\right)$:

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

The distribution $q\big(\mathbf{w}_k\big)$ is the normal distribution with mean $\mathbf{m}_k$ and covariance matrix $\mathbf{B}_k$:

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

M–step. The distribution $q\left(\mathbf{Z}, \mathbf{W}\right)$ is fixed, while the lower bound $\mathcal{L}\left(\mathbf{V}, \mathbf{W}^0, \mathbf{A}, \beta\right)$ is maximized with respect to the parameters $\mathbf{V}, \mathbf{W}^0, \mathbf{A}, \beta$:

$$\begin{aligned}
\mathcal{L}\left(\mathbf{V}, \mathbf{W}^0, \mathbf{A}, \beta\right) &= \mathsf{E}_q \log p\big(\mathbf{y}, \mathbf{Z}, \mathbf{W} | \mathbf{X}, \mathbf{V}, \mathbf{A}, \mathbf{W}^0, \boldsymbol{\Xi}, \beta\big) = \\
&= \sum_{i=1}^N \sum_{k=1}^K \mathsf{E} z_{ik} \left[\log \pi_k\left(\mathbf{x}_i, \mathbf{V}\right) - \frac{\beta}{2} \mathsf{E}\left(y_i - \mathbf{w}_k^{\mathsf{T}} \mathbf{x}_i\right)^2 + \frac{1}{2} \log \frac{\beta}{2\pi} \right] + \\
&+ \sum_{k=1}^K \left[-\frac{1}{2} \mathsf{E}\left(\mathbf{w}_k - \mathbf{w}_k^0\right)^{\mathsf{T}} \mathbf{A}_k^{-1} \left(\mathbf{w}_k - \mathbf{w}_k^0\right) + \frac{1}{2} \log \det \mathbf{A}_k^{-1} - \frac{n}{2} \log 2\pi \right] + \\
&+ \sum_{k=1}^K \sum_{k'=1}^K \left[-\frac{1}{2} \left(\mathbf{w}_k^0 - \mathbf{w}_{k'}^0\right)^{\mathsf{T}} \boldsymbol{\Xi}^{-1} \left(\mathbf{w}_k^0 - \mathbf{w}_{k'}^0\right) + \frac{1}{2} \log \det \boldsymbol{\Xi} - \frac{n}{2} \log 2\pi \right].
\end{aligned} \tag{12}$$

To find the optimal parameters $\mathbf{V}$, use the gradient optimization algorithm. It convergences to some local maximum. Using (12), we get

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

Similarly, we get

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

$$\begin{aligned}
\frac{\partial \mathcal{L}\left(\mathbf{V}, \mathbf{W}^0, \mathbf{A}, \beta\right)}{\partial \mathbf{w}_k^0} &= \mathbf{A}_k^{-1}\big(\mathsf{E}\mathbf{w}_k - \mathbf{w}_k^0\big) + \boldsymbol{\Xi} \sum_{k'=1}^K \big[\mathbf{w}_{k'}^0 - \mathbf{w}_k^0\big] = 0, \\
\mathbf{w}_k^0 &= \left[\mathbf{A}_k^{-1} + (K-1)\,\boldsymbol{\Xi}\right]^{-1} \left(\mathbf{A}_k^{-1} \mathsf{E}\mathbf{w}_k + \boldsymbol{\Xi} \sum_{k'=1,\ k' \neq k}^K \mathbf{w}_{k'}^0 \right).
\end{aligned} \tag{13}$$

Formulas (11–13) define an iterative procedure, which convergence to some local maximum of the optimization problem (10).

6 Computational experiment

7 Conclusion

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