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Artificial neural network and multiple regression analysis models to predict essential oil content of ajowan (*Carum copticum* L.)

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ABSTRACT

Ajowan is an important medicinal plant that grows in arid and semi-arid regions of central Europe, India, Egypt, Iran, Iraq, Afghanistan, and Pakistan. Essential oil is the most consumable product of ajowan in pharmaceutical and food industrials, and correct predict of oil content is one of the main goals in breeding programs of ajowan. Two methods namely artificial neural network (ANN) and multiple regression model (MLR) were conducted to predict the oil content of ajowan from readily measurable plant characters. According to simple correlation analysis, four characters (number of rays, number of pedicels, number of flowers per umbellet, and number of umbellets in an umbel) were selected as input variables in both artificial neural network and multiple linear regressions models. The essential oil content of ajowan was well predicted using SigmoidAxon transfer function and two hidden layers of artificial neural network with a root mean square error (RMSE) of 0.192%, a mean absolute error (MAE) of 0.112% and a determination coefficient (R^2) of 0.901. The performance of ANN was better than MLR with a RMSE of 0.262 and a R^2 of 0.748. Based on stepwise regression and ANN analyses the most important characters for oil content of ajowan were number of umbellets in an umbel and number of flowers per umbellet and these traits can be assigned as selection criteria for essential oil content of ajowan.

1. Introduction

Ajowan (*Carum copticum* L.) is one the important industrial medicinal plants belong to *Apiaceae* family that can used in raw or processed forms in traditional medicine or modern pharmaceutical industry (Niazian et al., 2017a). This plant is mainly grows in arid and semi-arid regions of the east of India, northwest, central and eastern parts of Iran, central Europe, Iraq, Afghanistan, and Pakistan and also in Egypt (Ashraf and Orooj, 2006; Boskabady et al., 2014; Joshi, 2000; Moosavi et al., 2015). Ajowan seeds contain an essential oil with about 50% content of thymol, which has a strong germicide, anti-spasmodic and fungicidal effect (Ashraf and Orooj, 2006). Many of the medicinal and aromatic plants do not have stable production in their growing areas and usually are wild harvested to meet demands (Dalkani et al., 2012; Niazian et al., 2017b). Hence, attention to stable quality and quantity production of medicinal plants is important to respond to growing demands of pharmaceutical needs. Seed is the most important part of ajowan. Positive correlation of seed yield and essential oil content have been reported in ajowan (Fadaei Heidari et al., 2016), so seed yield and essential oil content are the most important breeding objectives in this plant. Seed yield and oil content are quantitative and complicate traits that are controlled with many genes and mainly affected by environmental conditions (Dalkani et al., 2011), that lead to low heritability of this traits. For such traits with low heritability, indirect selection through yield components and their association is the first choice of plant breeders, which help them to indirectly increase their desired traits (Dalkani et al., 2011). There are several methods for analysis of yield components that according to the objectives of the project can be chosen. Techniques such as analysis of variance, simple correlation coefficient, multiple regression and path analysis usually used to analyze yield component (Fraser and Eaton, 1983). One of the simplest methods that can help to better understand of yield component and

Abbreviations: ANN, artificial neural network; BY, biological yield; IL, average internodal length; LL, leaf length; MAE, mean absolute error; MLP, multi layered perception; MLR, multiple linear regressions; MSE, mean square error; NFU, number of flower per umbellet; NP, number of pedicels; NR, number of rays; NU, number of umbels; NUU, number of umbellets in an umbel; OC, oil content; PH, plant height; RMSE, root mean square error; SPSY, single plant seed yield

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Table 1
Means of all recorded characteristics of ajowan in 2014 and 2015 growing seasons.

No.	Ecotype	PH (cm)		NR		NP		NFU		NU		NUU		LL (cm)		IL (cm)		BY (g)		SPSY (g)		OC (%)	
		2014	2015	2014	2015	2014	2015	2014	2015	2014	2015	2014	2015	2014	2015	2014	2015	2014	2015	2014	2015	2014	2015
1	Karaj	86.66	90.66	10.66	8.33	5.00	5.00	14.33	14.32	21.00	22.00	7.66	7.33	3.66	4.00	7.66	7.166	206.96	197.67	100.33	102.97	4.33	4.35
2	Esfahan	93.33	106.33	9.33	6.33	6.00	6.00	13.00	13.33	17.00	17.00	5.66	4.00	4.66	4.00	9.33	9.33	147.80	135.87	41.46	50.33	3.76	3.20
3	Ardabil1	105.33	109.00	6.33	6.33	6.00	6.00	11.33	10.66	17.33	17.00	5.00	5.00	5.66	4.66	6.66	10.66	99.60	99.10	36.10	35.20	2.17	2.23
4	Flavarjan	80.00	77.33	7.33	8.00	6.00	5.00	11.66	11.33	18.33	18.41	5.66	5.30	5.66	6.00	5.60	6.50	78.10	87.33	39.76	45.83	2.41	2.52
5	Ardabail2	51.00	47.00	6.66	6.33	3.66	4.00	12.00	12.66	15.66	17.66	3.00	4.00	4.00	4.66	5.00	5.63	118.26	110.8	51.66	44.77	2.66	2.56
6	Hamadan	50.66	46.667	5.33	6.00	4.33	5.00	9.00	9.00	18.33	17.00	5.66	4.33	5.66	6.00	7.66	6.66	16.90	23.00	14.63	17.73	1.60	1.23
7	Shahedye	99.00	78.33	8.33	6.66	4.33	5.00	14.60	14.10	21.00	20.66	7.66	6.66	4.33	4.33	5.60	7.33	183.80	181.33	85.00	76.40	3.46	3.07
8	Sadogh	83.33	83.33	5.66	4.66	5.00	6.00	11.00	12.00	19.00	19.00	5.00	4.00	3.66	3.66	6.60	5.33	184.10	162.33	71.93	65.00	2.25	1.83
9	Ghazvin	62.66	71.33	7.33	7.66	4.66	5.00	13.00	14.66	21.66	22.66	5.00	4.33	4.33	4.00	7.00	6.83	34.80	65.00	15.66	24.37	1.40	1.20
10	Yazd	76.66	92.66	7.33	6.66	6.00	5.00	13.66	12.30	19.33	16.66	5.66	5.66	4.33	4.66	5.60	6.00	167.16	158.6	38.23	54.07	2.78	2.50
11	Rafsanjan1	45.00	57.00	5.66	6.66	5.30	6.00	9.00	8.33	14.00	14.66	3.33	2.20	4.66	6.00	7.66	4.00	40.10	36.67	16.80	15.30	1.56	1.43
12	Rafsanjan2	80.00	85.33	6.00	7.66	5.30	4.66	14.00	14.00	19.66	19.33	4.10	4.00	4.00	4.33	7.33	7.50	166.60	158.07	46.90	52.27	2.61	2.51
13	Yazd2	82.33	93.33	6.66	6.66	7.00	4.66	12.30	12.00	19.33	20.33	5.00	4.66	7.33	7.00	8.66	7.33	145.60	137.03	52.40	56.93	2.56	2.68
14	Sarbisheh	39.00	52.00	8.33	8.33	5.30	6.00	12.33	13.00	21.00	21.33	5.00	5.00	3.33	3.50	7.33	8.66	46.26	43.33	20.76	23.20	1.39	1.10
15	Birjand1	53.33	58.66	8.33	7.33	5.00	5.33	8.33	10.00	18.00	20.00	4.33	5.00	5.66	4.50	4.50	7.16	49.23	54.27	10.53	30.90	2.16	2.16
16	Birjand2	57.66	71.33	6.33	5.33	5.00	4.30	11.00	11.66	17.66	17.33	4.33	5.66	3.66	3.83	5.00	5.00	131.79	146.93	48.46	45.83	2.66	2.58
17	Ghaen	40.00	50.00	10.66	8.00	5.00	6.66	11.33	14.66	23.33	23.33	7.33	7.90	4.00	4.33	7.66	6.00	261.56	277.77	111.06	78.96	3.81	3.68
18	Boshroye	61.00	56.66	10.66	7.00	5.00	5.33	11.66	14.20	21.66	21.66	5.00	5.00	3.83	4.50	9.33	6.50	187.43	166.77	80.80	84.07	3.53	3.74
19	Sarbishe2	95.00	81.00	8.33	7.00	5.00	5.66	13.00	8.33	19.66	19.00	3.00	4.66	3.66	5.00	6.66	8.66	108.83	110.93	35.70	37.10	1.9	1.51
20	Ghoom	70.00	63.00	5.33	6.33	4.66	4.66	12.66	13.33	20.00	16.33	5.33	5.00	5.00	4.33	6.66	8.00	91.56	95.33	40.70	40.15	2.16	2.16
21	Shiraz	59.00	58.33	10.66	7.00	5.00	5.00	14.20	14.00	21.66	23.45	7.33	7.00	3.33	4.66	4.66	6.33	177.00	165.43	162.93	143.47	4.13	3.47
22	Arak	30.33	28.33	8.66	6.33	4.00	4.00	9.33	8.33	17.66	16.66	3.00	4.00	1.33	2.66	7.00	4.83	32.23	49.00	10.33	13.80	1.55	1.23
23	Marvdasht	66.33	77.33	5.66	6.00	5.00	5.00	7.32	9.33	16.20	16.33	4.66	4.33	4.83	5.33	7.66	8.00	77.43	78.07	15.00	16.23	1.19	1.04

PH: plant height, NR: number of rays, NP: number of pedicels, NFU: number of flowers per umbellet, NU: number of umbels, NUU: number of umbellets in an umbel, LL: leaf length, IL: average internodal length, BY: biological yield, SPSY: single plant seed yield, OC: oil content.