Pakistan J. Zool., vol. 52(6), pp 2039-2045, 2020 DOI: https://dx.doi.org/10.17582/journal.pjz/20200129080117

Determination of Number and Position of Knots in Cubic Spline Regression for Modeling Individual Lactation Curves in Three Different Breed

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Article Information
Received 29 January 2020
Revised 01 March 2020
Accepted 04 March 2020
Available online 17 August 2020

Authors' Contribution
SHA, HO and MS designed and supervised the work. SHA and EY made statistical analysis. SHA, HO and MS wrote the article.

Key words
Cubic spline, Lactation curve, Jersey, Brown Swiss, Holstein Friesian.

ABSTRACT

Lactation curves are one of the basic tools in animal breeding. Therefore, modeling lactation curves with appropriate and precise equations are of great importance for obtaining estimates. Lactation curves have different tendencies in different breeds. To examine the tendencies and differences Jersey (J), Brown Swiss (BS) and Holstein Friesian (HF) breeds which are commonly raised in Turkey were used in this study. This study aimed to statistically determine the optimal position and number of knots in cubic spline regression used for modeling lactation curves. Knots were taken as 60, 90, 120 and 150 days and combinations of them for every breed. To compare the Mean Square Errors (MSE) of the models, the autocorrelation values of Durbin Watson (DW), the information criteria of Akaike (AIC) and the coefficient of determination (R^2) were used as comparison criteria. Kruskal Wallis H test was used to compare comparison criteria in different models. The Mann Whitney U test was used to compare the groups in pairs. Results showed that four knots was sufficient for J breed MSE: 0.640 ± 0.0652, DW: 2.272 ± 0.0232, AIC: 16.927 ± 1.0649, R^2: 0.982 ± 0.0020) and BS breed (MSE: 0.131 ± 0.0156, DW: 2.326 ± 0.1093, AIC: 3.567 ± 0.9193, R^2: 0,985 ± 0.0008), but three knot was sufficient for HF breed (MSE: 1.600 ± 0.132, DW: 2.114 ± 0.020, AIC: 22.596 ± 0.783, R^2: 0.972 ± 0.002). As a general result of the study show that four knots (60, 90, 120 and 150 days) for J and BS breeds and three knots (90, 120 and 150 days) for HF breed were sufficient to estimate lactation curve by cubic spline regression model.

INTRODUCTION

The lactation curve is a graphical presentation of the variations in milk production throughout the lactation period (Papajcsik and Bodero, 1988; White and Brotherstone, 1997; de Groot *et al*., 2003; Silvestre *et al*., 2006; Cunha *et al*., 2010). Lactation curves are one of the basic tools in animal breeding. Therefore, modeling the lactation curves with appropriate and precise equations is of great importance to estimate the milk yield of cows.

Some studies estimate lactation milk yield with different methods (Gantner *et al*., 2009). It has also been proposed different methods such as Ali Schaeffer, Random Regression, Wood and Wilmink to analyze the periods of lactation (Cankaya *et al*., 2014; Sahin *et al*., 2014; Harder *et al*., 2019; Younesi *et al*., 2019).

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0030-9923/2020/0006-2039 $ 9.00/0

In addition, splines are a useful type of function used in regression when the relationship between a response and a set of covariates is not known before (Vargas *et al*., 2000) to describe the lactation curve of dairy cows.

Splines are generally defined as piecewise polynomials of degree n with function values. Junction points are called knots. Cubic splines are smooth at knots (function, first and second derivatives of agreement). Cubic spline regression, knot points, usually from the internal or external convex near the start or end point are selected. On the other hand, in fitting the cubic spline regression model, the number of knots affects the fit rather than the position of the knots (Lopez-Villalobos *et al*., 2005; Cankaya *et al*., 2014). As the number of knots increases, the number of pieces increases. Therefore, increasing the number of knots generally increases the fit of the spline function for the data (White and Brotherstone, 1997; Walker *et al*., 2010; Cankaya *et al*., 2014).

Cubic spline regression models have been used to model the lactation period using milk production per test day instead of the others. Because the cubic spline regression models have excellent consistency in modeling the lactation curves. At the same time, Sahin and Efe (2010) reported that more flexible curves can be obtained with an increase in the number of knots.

Superiority of cubic spline regression model can be obtained only if determination of sufficient number of knots and position of them were successful. On the other hand, lactation curves obtained from flock mean can give only a guideline. Individual lactation curves are needed to evaluate individual performance of animals and use of them in selection (Cankaya *et al*., 2014; Adediran *et al*, 2008).

In this study, it was aimed to determine the sufficient number of knots and their position for milk yield of three different cattle breeds.

MATERIALS AND METHODS

Lactation curves have different tendencies in different breeds. To examine the tendencies and differences Jersey (J), Brown Swiss (BS) and Holstein Friesian (HF) breeds which are commonly raised in Turkey were used in this study. The data consisted of total 3480 test day record of 348 cattle in J breed obtained from Karaköy Agricultural State Farm in Samsun-Turkey, 3500 test day records of 350 cattle in BS breed obtained from Sultansuyu Agricultural State Farm in Malatya-Turkey and HF breed obtained from Ceylanpınar Agricultural State Farm in Şanlıurfa-Turkey. Only animals had 10 test days record in second and third lactation were included in analysis. Totally 10480 test day records for 1048 animal were used.

In three different cattle breeds, lactation milk yield measurements were analyzed by regressions of cubic splines with different knots for the estimation of the lactation curve using the SAS package (SAS, 1999; Sherchand *et al*., 1995). The methods used for estimation parameters and comparison criteria in this study were introduced as follows. In this study, the methods and comparison criteria used for parameter estimations are introduced as follows.

Cubic spline regression

Cubic spline regression, with no endpoint requirement, the number of parameters required, except β_0, "k + 3" is the number (Stone and Koo, 1985). In this case, one (a) knots cubic spline function regression occurs as follows:

$$Y(t) = \beta_0 + \beta_1 t + \beta_2 t^2 + \beta_3 t^3 + \beta_4 (t-a)^3$$

A cubic spline regression model:

$$y = \beta_0 + \beta_1 t + \beta_2 t^2 + \beta_3 t^3 + \sum_{i=1}^{k} k(t-t_i)^3$$

Where, t refers to days in milk yield at the test; β_0, β_1, β_2, β_3 and β_4 are parameters to be estimated, and k is the number of knots in the splines.

Comparison criteria of the models

The goodness of the fit of the models was assessed according to the criteria Mean Square Error (MSE), the autocorrelation values of Durbin Watson (DW), Akaike Information Criteria (AIC), Coefficient of Determination (R^2) (Vargas *et al*., 2000; Burnham and Anderson, 2002; White *et al*., 1999). According to the results of Kolmogorov Smirnov test, MSE, AIC and R^2 values were not distributed normally (P<0.05). So, Kruskal Wallis H test was used for comparison of models with MSE, AIC and R^2. Mann Whitney U test was used to separate the groups (Onder, 2018).

RESULTS

In this study, which was carried out to statistically determine the most suitable knots in the cubic spline regression used to model lactation curves, lactation curves were estimated using 10 different knots combinations in the second and third lactation of J, BS and HF breeds. Determined knots and their positions were given in Table I.

The MSE, the autocorrelation values of DW, the information criteria of Akaike and the coefficient of determination estimated for three different cattle breeds for the knots and the combinations were given in Table II. As easily seen in Table II, increasing number of knots caused an observable increase on R^2 values and decrease on MSE and AIC values.

Table I.- Position and code of the knots for ten different cubic spline models.

Code of knots	Position of knots (day)	Code of knots	Position of knots (day)
1	60	6	90, 120
2	90	7	120, 150
3	120	8	60, 90, 120
4	150	9	90, 120, 150
5	60,90	10	60, 90, 120, 150

As seen in Table II, in every cattle breeds, by means of MSE, AIC and R^2 values differences among knots were found statistically significant (P<0.05) according to Kruskal Wallis H test results. In point of MSE the best position of knots were obtained from code of knots 10 for J and BS breeds. For HF breed the best position of knots were obtained from code of knots 3, 6, 8, 9 and 10. In point of AIC the best groups was code of knots 10 for J and BS breeds as MSE, for HF breed the best position of knots were obtained from code of knots 9 and 10. On the other hands, in point of R^2 the best knot combination were 5, 8 and 10 for J breed, 5, 8, 9 and 10 for BS breed, and 9 and 10 for HF breed according to Table II.

When the autocorrelations examined it was understood that there was no autocorrelation (Uysal and Gunay, 2001) in code of knots 10 in J and BS breeds and code of knots 9 and 10 for HF breed.

As seen Table II, when the breeds evaluated together according to MSE, AIC, DW and R^2; in J breed (MSE: $0.640^{c} \pm 0.065$, DW: 2.272 ± 0.023, AIC: $16.927^{c} \pm 1.065$, R^2: $0.982^{a} \pm 0.002$) and BS breed (MSE: $0.131^{e} \pm 0.016$, DW: 2.326 ± 0.109, AIC: $3.567^{d} \pm 0.919$, R^2: $0.985^{a} \pm 0.001$) for code of knots 10, in HF breed for code of knots 9 and 10 (code of knots 9: MSE: $1.600^{b} \pm$ 0,132, DW: 2.114 ± 0.020, AIC: $22.596^{c} \pm 0.783$, R^2: $0.972^{a} \pm 0.002$, code of knots 10: MSE: $1.585^{b} \pm 0.207$, DW: 2.244 ± 0,026, AIC: $21.120^{c} \pm 1.004$, R^2: $0.976^{a} \pm 0.003$) were yield best results.

The estimation values for the parameters of three different breeds, different knot points and combinations are given in Table III. Cubic splines regression curves for individual lactation generated using the control days were presented in Figure 1. An increase in the number of nodes, in the dispersion of the points, is caused to obtain a more flexible curve and can express the best of the distribution shown in Figure 1.

As shown in Figure 1, the closest estimates to the actual milk yields were observed at code of knots 10 for J and BS breeds, respectively. Figure 1 also shows that code of knots 9 shows the estimate closest to the actual milk yields. Also, Figure 1 shows that the closest estimate of code of knots 9 to actual milk yields was obtained.

Table II.- Comparison results of MSE, DW, AIC and R^2 values for different breeds according to each code of knots position.

Code of knots		Jersey				Brown Swiss				Holstein			
		MSE	DW	AIC	R^2	MSE	DW	AIC	R^2	MSE	DW	AIC	R^2
		$\bar{X}$ $(S_{\bar{X}})$	$\bar{X}$ $(S_{\bar{X}})$	$\bar{X}$ $(S_{\bar{X}})$	$\bar{X}$ $(S_{\bar{X}})$	$\bar{X}$ $(S_{\bar{X}})$	$\bar{X}$ $(S_{\bar{X}})$	$\bar{X}$ $(S_{\bar{X}})$	$\bar{X}$ $(S_{\bar{X}})$	$\bar{X}$ $(S_{\bar{X}})$	$\bar{X}$ $(S_{\bar{X}})$	$\bar{X}$ $(S_{\bar{X}})$	$\bar{X}$ $(S_{\bar{X}})$
1		1.062^{a} (0.088)	2.677 (0.035)	28.100^{a} (0.741)	0.928^{c} (0.006)	0.316^{a} (0.024)	2.511 (0.025)	16.205^{a} (0.620)	0.965^{c} (0.002)	1.778^{ab} (0.129)	2.599 (0.025)	30.196^{a} (0.773)	0.945^{bc} (0.003)
2		1.089^{a} (0.088)	2.738 (0.035)	28.441^{a} (0.738)	0.926^{c} (0.006)	0.293^{ab} (0.022)	2.580 (0.026)	15.682^{a} (0.622)	0.967^{c} (0.002)	1.805^{ab} (0.131)	2.665 (0.024)	30.525^{a} (0.774)	0.945^{bc} (0.003)
3		0.800^{ab} (0.065)	2.858 (0.0348)	24.617^{ab} (0.802)	0.934^{c} (0.006)	0.245^{b} (0.020)	2.720 (0.024)	13.253^{ab} (0.561)	0.976^{b} (0.002)	1.571^{b} (0.118)	2.811 (0.024)	27.595^{ab} (0.851)	0.948^{bc} (0.003)
4		1.182^{a} (0.087)	2.820 (0.034)	29.345^{a} (0.740)	0.918^{cd} (0.006)	0.267^{b} (0.020)	2.677 (0.026)	14.778^{a} (0.539)	0.971^{ab} (0.002)	1.966^{ab} (0.142)	2.769 (0.023)	32.286^{a} (1.228)	0.939^{c} (0.003)
5		0.690^{c} (0.063)	3.070 (0.030)	21.184^{bc} (0.906)	0.972^{a} (0.003)	0.193^{d} (0.015)	2.958 (0.022)	9.630^{c} (0.662)	0.982^{a} (0.001)	1.733^{ab} (0.133)	2.867 (0.024)	28.946^{ab} (0.906)	0.952^{ab} (0.003)
6		0.825^{ab} (0.072)	2.957 (0.035)	24.469^{ab} (0.836)	0.956^{b} (0.004)	0.228^{c} (0.019)	2.819 (0.023)	12.640^{ab} (0.557)	0.970^{b} (0.001)	1.535^{b} (0.118)	2.916 (0.023)	27.190^{ab} (0.847)	0.962^{ab} (0.002)
7		1.392^{a} (0.121)	2.826 (0.033)	30.354^{a} (0.780)	0.908^{d} (0.007)	0.258^{c} (0.020)	2.721 (0.025)	14.639^{a} (0.529)	0.971^{ab} (0.002)	2.158^{a} (0.158	2.800 (0.021)	31.969^{a} (0.756)	0.936 (0.004)
8		0.674^{c} (0.062)	3.175 (0.029)	21.057^{bc} (0.892)	0.972^{a} (0.003)	0.253^{c} (0.013)	3.088 (0.019)	8.897^{c} (0.619)	0.983^{a} (0.001)	1.548^{b} (0.124)	3.102 (0.019)	24.722^{b} (0.906)	0.952^{ab} (0.001)
9		0.994^{ab} (0.091)	3.171 (0.029)	26.434^{ab} (0.812)	0.947^{b} (0.005)	0.195^{d} (0.014)	3.066 (0.020)	11.464^{bc} (0.564)	0.979^{a} (0.001)	1.600^{b} (0.132)	2.114 (0.020)	22.596^{c} (0.783)	0.972^{a} (0.002)
10		0.640^{c} (0.065)	2.272 (0.023)	16.927^{c} (1.065)	0.982^{a} (0.002)	0.131^{e} (0.016)	2.326 (0.109)	3.567^{d} (0.919)	0.985^{a} (0.001)	1.585^{b} (0.207)	2.244 (0.026)	21.120^{c} (1.004)	0.976^{a} (0.003)
Kruskal-Wallis H	χ^2	345.00	-	27.02	69.74	133.35	-	59.13	280.55	47.60	-	145.12	282.43
	P	<0001	-	<0001	<0001	<0001	-	<0001	<0001	<0001	-	<0001	<0001

[a,b,c,] There is a difference between the values indicated by different letters in the same column (P<0.05). ($\bar{X}$: Mean $S_{\bar{X}}$: Standard Error).

Table III.- Predicted parameter values for three different cattle breeds and code of knot positions.

Breeds	β_i	Code of knots									
		1	2	3	4	5	6	7	8	9	10
Jersey	β_0	-1.4E+01± 1.9E+00	3.7E+00± 6.6E-01	-1.5E+01± 8.4E+00	7.6E+00± 4.8E-01	5.0E+00± 2.6E+01	1.7E+00± 1.0E+00	9.5E+00± 4.3E-01	1.7E+00± 1.1E+00	5.5E+00± 6.1E-01	2.9E+01± 8.6E+01
	β_1	1.6E+00± 1.1E-01	4.9E-01± 3.1E-02	1.7E+00± 5.3E-01	2.8E-01± 1.8E-02	-1.0E+00± 2.7E+00	6.3E-01± 7.2E-02	2.4E-01± 8.4E-02	6.0E-01± 6.2E-02	4.4E-01± 9.2E-02	1.5E+00± 6.9E+00
	β_2	-2.8E-02± 2.0E-03	-6.2E-03± 4.1E-04	-3.0E-02± 1.0E-02	-3.0E-03± 2.0E-04	9.1E-02± 1.5E-01	-6.5E-03± 2.4E-03	-1.7E-03± 2.6E-04	-4.8E-03± 4.9E-03	-4.4E-03± 3.5E-04	-1.4E-01± 2.8E-01
	β_3	1.6E-04± 1.1E-05	2.4E-05± 1.7E-06	1.7E-04± 6.2E-05	9.2E-06± 6.4E-07	-1.8E-03± 2.8E-03	1.0E-05± 3.3E-05	3.0E-06± 3.0E-06	-1.9E-05± 7.8E-05	1.5E-05± 1.4E-06	3.1E-03± 5.1E-03
	β_4	-1.6E-04± 1.1E-05	-2.4E-05± 1.8E-06	-1.7E-04± 7.3E-05	-1.0E-05± 7.8E-07	4.4E-05± 2.5E-04	-3.9E-05± 6.5E-06	-6.4E-06± 5.2E-07	-3.8E-05± 9.6E-06	-2.5E-05± 3.0E-06	2.5E-04± 8.5E-04
	β_5	-	-	1.9E-06± 1.2E-05	-	-6.1E-05± 6.4E-05	6.6E-06± 2.9E-06	-	5.7E-06± 7.7E-06	1.1E-05± 2.0E-06	-6.6E-05± 2.3E-04
	β_6	-	-	-	-	1.1E-05± 1.1E-05	-	-	6.8E-07± 2.9E-06	-	2.7E-05± 5.6E-05
	β_7	-	-	-	-	-	-	-	-	-	-4.8E-07± 1.0E-05
Brown Swiss	β_0	1.7E+01± 8.0E-01	1.8E+01± 3.8E-01	1.4E+01± 2.8E+00	1.8E+01± 4.5E-01	9.6E+00± 1.0E+01	1.8E+01± 3.9E-01	1.8E+01± 3.1E-01	1.7E+01± 3.9E-01	1.8E+01± 3.3E-01	6.9E+01± 3.2E+01
	β_1	2.4E-02± 4.5E-02	-4.7E-03± 1.3E-02	2.1E-01± 1.7E-01	-8.5E-03± 7.9E-03	5.1E-01± 6.5E-01	1.0E-02± 1.4E-02	-1.1E-02± 6.2E-03	2.2E-02± 1.5E-02	-5.2E-03± 8.0E-03	-3.3E+00± 2.1E+00
	β_2	-5.9E-04± 7.0E-04	-1.3E-04± 1.9E-04	-2.8E-03± 2.9E-03	-7.6E-05± 8.7E-05	-7.8E-03± 1.1E-02	-5.4E-04± 2.5E-04	-7.4E-05± 6.4E-05	-5.9E-04± 2.3E-04	-1.3E-04± 1.0E-04	1.3E-01± 8.3E-02
	β_3	6.6E-06± 5.4E-06	2.3E-07± 6.9E-07	3.0E-05± 1.9E-05	2.6E-07± 2.8E-07	4.0E-05± 6.5E-05	1.1E-06± 1.1E-06	1.5E-07± 1.7E-07	2.3E-06± 1.1E-06	3.6E-07± 4.4E-07	2.5E-03± 3.0E-03
	β_4	-6.4E-06± 4.2E-06	-7.5E-07± 7.6E-07	-2.9E-05± 2.2E-05	-5.1E-07± 4.5E-07	-9.3E-05± 8.5E-05	-2.8E-06± 1.8E-06	-8.6E-08± 2.4E-07	-5.2E-06± 2.5E-06	-5.3E-07± 9.8E-07	3.7E-04± 2.8E-04
	β_5	-	-	3.0E-06± 3.8E-06	-	1.3E-05± 2.1E-05	1.1E-06± 9.3E-07	-	4.4E-06± 2.4E-06	3.1E-07± 7.0E-07	-1.6E-04± 9.8E-05
	β_6	-	-	-	-	-3.0E-07± 3.9E-06	-	-	-5.1E-07± 1.4E-06	-	2.8E-05± 2.0E-05
	β_7	-	-	-	-	-	-	-	-	-	-5.1E-06± 3.9E-06
Holstein Friesian	β_0	-5.1E+00± 2.7E+00	1.2E+01± 1.1E+00	-1.7E-01± 6.9E+00	1.5E+01± 8.9E-01	1.1E+01± 8.9E+00	1.0E+01± 1.3E+00	1.7E+01± 9.3E-01	1.1E+01± 1.4E+00	1.4E+01± 9.8E-01	-5.4E+00± 7.9E+01
	β_1	1.7E+00± 1.2E-01	5.1E-01± 3.2E-02	1.2E+00± 4.4E-01	3.0E-01± 1.9E-02	5.6E-01± 5.6E-01	5.7E-01± 5.2E-02	2.1E-01± 1.4E-02	5.6E-01± 5.7E-02	3.9E-01± 2.7E-02	1.3E+01± 5.1E+00
	β_2	-2.8E-02± 1.9E-03	-6.4E-03± 4.2E-04	-2.0E-02± 8.0E-03	-3.2E-03± 2.0E-04	-8.3E-03± 1.1E-02	-7.2E-03± 7.7E-04	-2.0E-03± 1.3E-04	-7.2E-03± 8.5E-04	-4.4E-03± 3.3E-04	-2.5E-01± 9.9E-02
	β_3	1.5E-04± 1.1E-05	-7.5E-06± 3.2E-05	1.0E-04± 5.0E-05	-1.5E-06± 1.1E-05	4.6E-05± 8.0E-05	2.0E-05± 9.6E-06	1.2E-04± 1.2E-04	2.7E-05± 4.0E-06	9.2E-06± 4.8E-06	1.6E-03± 6.1E-04
	β_4	-1.5E-04± 1.1E-05	-2.4E-05± 1.7E-06	-9.4E-05± 5.7E-05	1.6E-04± 1.7E-04	6.7E-06± 1.2E-04	-3.6E-05± 6.5E-06	1.1E-04± 1.3E-04	-3.2E-05± 7.5E-06	-2.3E-05± 2.7E-06	-2.0E-03± 7.6E-04
	β_5	-	-	-9.6E-06± 8.7E-06	-	7.5E-05± 1.2E-04	1.9E-04± 1.9E-04	-	2.5E-04± 2.5E-04	1.4E-04± 1.3E-04	4.6E-04± 2.0E-04
	β_6	-	-	-	-	2.6E-07± 8.5E-06	-	-	1.6E-04± 1.3E-04	-	-1.2E-04± 5.0E-05
	β_7	-	-	-	-	-	-	-	-	-	2.1E-05± 8.6E-06

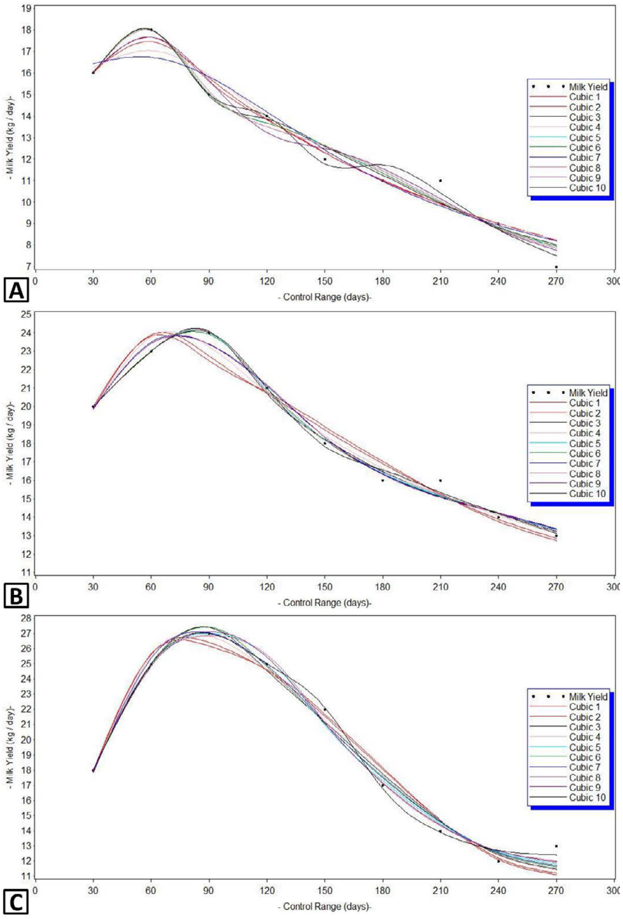

Fig. 1. Individual lactation curves with different knots for J (A), BS (B) and HF (C) breeds.

DISCUSSION

MSE, DW, AIC, and R^2 estimates results showed that the best knots were a position of knots 10 (60, 90, 120 and 150 days) for J and BS breeds, for HF breed the best knots were a position of 9 (90, 120 and 150 days) and 10 (60, 90, 120 and 150 days).

Makram *et al.* (2011) compare linear regression, quadratic regression, cubic regression and fixed factor models with cubic-spline interpolation models in first lactation Holstein cows for estimating the effects of inbreeding on milk yield. They found that the cubic-spline interpolation model with seven knots had the lowest AIC values. Bohmanova *et al.* (2008) compared a random regression model with both random and fixed regressions fitted by Legendre polynomials of order 4 with 3 alternative models fitting linear splines with 4, 5 and 6 knots at Canadian Holstein cows. As a result, they stated that the 6-knot spline model showed the best performance considering the model comparison criteria. Jamrozik *et al.* (2010) examined splines with a number of knots between 4 and 7 at random regression test-day models for different breeds. The results indicated that the optimal knot position for the linear splines differed between genetic and permanent environmental effects, as well as between traits and lactations. Cankaya *et al.* (2014) have compared wood lactation curve model and one and two knots cubic spline regression models at Jersey cows. They reported that the two-knot cubic spline regression model gave the best results. Similar results have obtained with the results of Bohmanova *et al.* (2007), Quinn *et al.* (2006), Gipson *et al.* (2010) and Koncagul and Yazgan (2011). Use of cubic spline regression to estimate lactation curves should be evaluated for other cattle breeds and milking animals such as goats and sheep.

CONCLUSION

It can be concluded that cubic spline regression models' that four knots (60, 90, 120 and 150 days) for J and BS breeds and three knots (90, 120 and 150 days) for HF breed can be used for the modeling of individual lactation curves. Therefore, the use of cubic spline regression models would provide useful information on the herd management decision for milk production.

ACKNOWLEDGEMENTS

This research was presented as an oral presentation at the International Congress on Domestic Animal Breeding Genetics and Husbandry (ICABGEH-2018) held on 26-28 September 2018 in Antalya.

Statement of conflict of interest

The authors have no conflict of interest.

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