# Application of Bayesian Multivariate Method to Time Dependent Data

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*Abbstract*– Time dependent data have widespread scientific applications. A very interesting area of its applications is growth curve models. Researchers have considered these models under different real-world scenarios, including complicated variancecovariance structures with autocorrelations. In this paper, the goal is to incorporate these types of structures into the models for multivariate random variables under Bayesian formality. Due to the complexity of the models many other models in literature have to make compromising assumptions. However, this paper will make Bayesian estimates of parameters for these highly complicated models with greater similarity to real world situations. Through judicial choices of priors, we obtain highly informative posteriors in the estimation procedures. The models presented in this paper are useful and competitive alternatives to frequentist's approach.

*Keywords*- Multivariate, Growth curve, Bayesian analysis, Autocorrelation

#### 1. Introduction

Time dependent data, such as growth curve models, are useful especially for studying growth behavior of time series in economics, biology, medical research and epidemiological problems [1], [2], have a long history. Their initiation may be attributed to Potthoff and Roy [3], who introduced their formulation and then studied the growth curve problems. Then subsequently, Rao [4], Khatri [5], Geisser [6] and von Rosen [7]-[9] became the primary researchers in analyzing the growth curve models. However, it took nearly a decade before the Bayesian approach (including predictive problem from a Bayesian perspective) was applied to the analysis of growth curve models and different assumptions about covariance matrices were also made accordingly. Lindley and Smith [10] and Geisser [11] assumed that covariance matrices were known, Fearn [12] assumed that they were identity matrices with unknown variances. Barry [13] gave a different treatment of the problem under Bayesian approach but also assumed identity matrix for covariances. The motivation for building multivariate models in this research is that we can study the effect of several variables acting simultaneously. This gives a closer resemblance to our intuition as well as better understanding about the relationship between the variables. When more variables are analyzed simultaneously, greater statistical power will be obtained and we gain easier visualization and interpretation of the data through graphical measures, such as scatter plots or higher dimensional plots (e.g. 3D plots). So our focus is also spontaneously shifted from individual or isolated factors to the relationships among several variables of interest in a data set.

In this research, similar general multivariate growth problems are studied by assuming that the multivariate dependent variables (such as weight, height, etc.) can be described by some commonly used nonlinear growth curves in terms of the independent variable (time) with a certain correlation (dependence) relationship in the covariance matrix. So the multivariate growth curve models proposed in this paper will include nonlinear growth curves with autocorrelated errors in their covariance structures. The classical analysis for these types of realistic models becomes either too complicated to obtain analytical solutions or may require a lot of simplifying assumptions, thus becoming unrealistic. Bayesian analysis, including experts' opinions, can help us computationally to get to the estimates of the parameters for growth curve models and thus become more appealing, as well as important to researchers. No similar models which consider such complex scenarios are available in the literature. The model formulation will be presented in the following first two section with the Gompertz growth curve as an example. Then in the last two sections, the applications of the models using a bivariate growth data set will be demonstrated. The simulation results will be discussed in the conclusion.

#### 2. Models

Let's consider a single subject of *n* observations.  $Y_j$ , for j = 1, ..., n, is a vector of *p*-variate correlated dependent variables. If we let  $W = (w_1, ..., w_n)$  be a vector of the independent variable time and  $\bigoplus_{\substack{q \neq p \\ q \neq 1 \\ q$ 

$$\begin{split} Y_{(p\times n)} &= \begin{pmatrix} y'_1 \\ \vdots \\ y'_p \end{pmatrix}_{(p\times n)}, \text{ where } y_k = \begin{pmatrix} y_{1k} \\ \vdots \\ y_{nk} \end{pmatrix} \text{ for } k = 1, ..., p \text{ , and } \underset{(p\times n)}{M} = \\ \begin{pmatrix} \mu'_1 \\ \vdots \\ \mu'_p \end{pmatrix}_{(p\times n)} &= \left[ f(W|\Theta)_{n\times p} \right]', \text{ where } \mu_k = \begin{pmatrix} \mu_{1k} \\ \vdots \\ \mu_{nk} \end{pmatrix} = f(W|\Theta_k) \text{ for } k = 1, ..., p \text{ .} \end{split}$$

This model considers a covariance structure between weight and length in that, under normal conditions, the lengthier the subject grows, the weightier it becomes and vice versa. Assume that *Y* follows a  $p \times n$  matrix normal distribution, which is actually a special case of the *pn*-variate multivariate normal distribution when the covariate matrix is separable. Then denote a *pn*-variate normal distribution with *pn*-dimensional mean  $\mu$  and  $pn \times pn$  covariance matrix  $\Omega$ , the p.d.f. function will be as follows:

$$g(y|\mu, \Omega) = (2\pi)^{-\frac{np}{2}} |\Omega|^{-\frac{1}{2}} \exp\left\{-\frac{1}{2}(y-\mu)'\Omega^{-1}(y-\mu)\right\}$$
(1),  
where  $y = vect(Y') = (y'_1, ..., y'_p)'$ ,  $\mu = vect(M') = (\mu'_1, ..., \mu'_p)'$ ,

in which the operator  $vect(\cdot)$  stacks the columns of its matrix argument from left to right in a single vector. The separable matrix  $\Omega = \Sigma \otimes \Phi$ , where  $\otimes$  is the Kronecker product which multiplies every entry of its first matrix argument by its entire second matrix argument, can be written as:

$$\Sigma \otimes \Phi = \begin{pmatrix} \sigma_{11} \Phi_{\dots} \sigma_{1p} \Phi \\ \vdots & \vdots \\ \sigma_{p1} \Phi^{\dots} \sigma_{pp} \Phi \end{pmatrix}.$$

Also we know that  $\Omega^{-1} = (\Sigma \otimes \Phi)^{-1} = \Sigma^{-1} \otimes \Phi^{-1}$  and  $|\Sigma \otimes \Phi|^{-\frac{1}{2}} = |\Sigma|^{-\frac{n}{2}} |\Phi|^{-\frac{p}{2}}$ . Then we have

$$g(y|\mu, \Sigma, \Phi) = (2\pi)^{-\frac{n\nu}{2}} |\Sigma|^{-\frac{n}{2}} |\Phi|^{-\frac{\nu}{2}}$$

$$\exp\left\{-\frac{1}{2}(y-\mu)'(\Sigma\otimes\Phi)^{-1}(y-\mu)\right\}.$$

Note that also with the matrix identity, we have

$$(y-\mu)'_{1\times np}(\Sigma\otimes\Phi)^{-1}_{np\times np}(y-\mu)_{np\times 1} = tr\Sigma^{-1}_{p\times p}(Y-M)_{p\times n}\Phi^{-1}_{n\times n}(Y-M)'_{n\times p},$$

$$g(Y|M, \Sigma, \Phi) = (2\pi)^{-\frac{np}{2}} |\Sigma|^{-\frac{n}{2}} |\Phi|^{-\frac{p}{2}}.$$
  

$$\exp\left\{-\frac{1}{2}tr\Sigma_{p\times p}^{-1}(Y-M)_{p\times n}\Phi_{n\times n}^{-1}(Y-M)'_{n\times p}\right\}$$
(2).

So *Y* is a random variable that follows a  $p \times n$  matrix normal distribution and can be denoted as:

$$Y|(M, \Sigma, \Phi) \sim N_{p \times n}(M, \Sigma \otimes \Phi),$$

where  $(M, \Sigma, \Phi)$  parameterize the above distribution with  $Y \in \mathbb{R}^{p \times n}$ ,  $M \in \mathbb{R}^{p \times n}$  and  $\Sigma, \Phi > 0$  ( $\Sigma$  and  $\Phi$  are commonly referred to as the within and between covariance matrices). Recall that M is a function of  $\Theta$  and assume that  $\Phi$  is a function of correlation coefficient  $\rho$  and that, for simplicity,  $\Theta$ ,  $\Sigma$  and  $\Phi$  are independent and adopt vague prior distributions for  $(\Theta, \Phi, \Sigma)$ . Then we have  $h(\Theta, \Phi, \Sigma) = h(\Theta)h(\Phi)h(\Sigma)$  and because  $\Phi$  is a function of  $\rho$ , their prior distribution assumptions are as follows:  $h(\Theta) \propto constant$ ,  $\rho \propto (1 + \rho)^{\tilde{\alpha} - 1}(1 - \rho)^{\tilde{\beta} - 1}$  for  $-1 < \rho < 1$  (i.e.,  $(1 + \rho)/2$   $Beta(\tilde{\alpha}, \tilde{\beta})$ , where  $\tilde{\alpha}$  and  $\tilde{\beta}$  can be chosen such that the mean  $\tilde{\alpha}/(\tilde{\alpha} + \tilde{\beta})$  is consistent with the empirical value for  $\rho$ ) and  $h(\Sigma) \propto \frac{1}{|\Sigma|^{(\rho+1)/2}}$ . So the prior distribution is  $h(\Theta, \rho, \Sigma) \propto \frac{(1 + \rho)^{\tilde{\alpha} - 1}(1 - \rho)^{\tilde{\beta} - 1}}{|\Sigma|^{(\rho+1)/2}}$ , and the joint posterior distribution of the parameters follows:

$$\pi(\Sigma, \Phi(\rho), \Theta | W, Y) = (2\pi)^{-\frac{np}{2}} |\Sigma|^{-\frac{n+p+1}{2}} |\Phi|^{-\frac{p}{2}} (1+\rho)^{\tilde{\alpha}-1} \cdot (1-\rho)^{\tilde{\beta}-1} \exp\left\{-\frac{1}{2}tr\Sigma_{p\times p}^{-1}(Y-M)_{p\times n}\Phi_{n\times n}^{-1}(Y-M)'_{n\times p}\right\}$$
(3)  
Let  $G = (Y-M)\Phi^{-1}(Y-M)'$  then (3) becomes

$$\pi(\Sigma, \Phi(\rho), \Theta|W, Y) \propto \left[ |\Sigma|^{-\frac{n+p+1}{2}} \exp\left\{-\frac{1}{2}tr\Sigma^{-1}G\right\} \right] \cdot |\Phi|^{-\frac{p}{2}} (1 + \rho)^{\tilde{\alpha}-1} (1-\rho)^{\tilde{\beta}-1}.$$

This can be reduced to the joint distribution of  $\Phi$  and  $\Theta$  and become  $\pi(\Phi(\rho), \Theta | W, Y)$  if we integrate out  $\Sigma$ .

The integration can be worked out by recognizing that if  $\Sigma^{-1}$  follows a Wishart distribution [14] then it can be written as:

$$\pi(\Theta, \Phi(\rho)|W, Y) \propto \frac{|\Phi|^{-\frac{p}{2}} (1+\rho)^{\tilde{\sigma}-1} (1-\rho)^{\tilde{\beta}-1}}{|G|^{n/2}}$$
(4).

Assume an autocorrelation matrix for  $\Phi$  with correlation coefficient  $\rho$  as follows:

$$\Phi = \begin{pmatrix} 1 & \rho & \rho^2 \dots \rho^{n-1} \\ \rho & 1 & \rho \dots \rho^{n-2} \\ \vdots & \vdots & \vdots \\ \rho^{n-1} \rho^{n-2} \rho^{n-3} \dots & 1 \end{pmatrix}$$
(5),

where  $\rho$  is the correlation coefficient. Then we can substitute the results that

$$|\Phi| = (1 - \rho^2)^{n-1}$$
, into (4) and get the posterior function

$$\pi(\Theta, \Phi(\rho)|W, Y) \propto \frac{(1+\rho)^{(\tilde{\alpha}-1)-p(n-1)/2}(1-\rho)^{(\tilde{\beta}-1)-p(n-1)/2}}{|G|^{n/2}}$$
(6)

# 3. An Illustrative Example

If we take the Gompertz curve as an illustrative example in fitting a bivariate data set which has weight and length as the variables and the following priors for

$$\Theta = \{\theta_1 \ \theta_2\} = \begin{cases} a_1 & a_2 \\ b_1 & b_2 \\ c_1 & c_2 \end{cases}, \text{ where } a_1 \sim Expon(\frac{1}{\tilde{a}_1}), a_2 \sim Expon(\frac{1}{\tilde{a}_2}), \\ \begin{cases} b_1 \\ b_2 \end{cases} \sim N_2\left(\left\{\tilde{b}_1 \\ \tilde{b}_2\right\}, \tilde{\Sigma}_b\right), c_1 \sim Expon(\frac{1}{\tilde{c}_1}) \text{ and } c_2 \sim Expon(\frac{1}{\tilde{c}_2}). \end{cases}$$

Let  $\tilde{\Theta} = (\tilde{a}_1, \tilde{a}_2, \tilde{b}_1, \tilde{b}_2, \tilde{c}_1, \tilde{c}_2, \tilde{\Sigma}_b)$  be a set of empirical Bayes estimates of the coefficients which can be estimated through nonlinear least square regression method. MATLAB *nlinfit* function can be used to fit *nonlinear* Jenss, Gompertz and Richards curves and *polyfit* function to fit *polynomial* curves (MATLAB Help and [15]). Depending on the data, although sometimes we could get estimates of  $\tilde{\Sigma}_b$ , most of the time we have to assume them to be equal to some proper value for our Bayesian analysis. So the prior distributions are:

$$h(\Theta|\Theta) \propto \frac{1}{\tilde{a}_1 \tilde{a}_2 \tilde{c}_1 \tilde{c}_2 |\tilde{\Sigma}_b|^{1/2}} \cdot \exp\left\{-\frac{1}{2} \binom{b_1 - \tilde{b}_1}{b_2 - \tilde{b}_2}' \tilde{\Sigma}_b^{-1} \binom{b_1 - \tilde{b}_1}{b_2 - \tilde{b}_2} - \left(\frac{a_1}{\tilde{a}_1} + \frac{a_2}{\tilde{a}_2} + \frac{c_1}{\tilde{c}_1} + \frac{c_2}{\tilde{c}_2}\right)\right\}$$
(7).

Let (7) be substituted into (6), then it becomes

$$\pi(\Theta, \Phi(\rho)|W, Y) \propto \frac{(1+\rho)^{(\tilde{\alpha}-1)-p(n-1)/2}(1-\rho)^{(\tilde{\beta}-1)-p(n-1)/2}}{\left|(Y-M)\Phi^{-1}(Y-M)'\right|^{n/2}}.$$

$$\exp\left\{-\left(\frac{a_{1}}{\tilde{a}_{1}}+\frac{c_{1}}{\tilde{c}_{1}}+\frac{a_{2}}{\tilde{a}_{2}}+\frac{c_{2}}{\tilde{c}_{2}}\right)-\frac{1}{2}\binom{b_{1}-\tilde{b}_{1}}{b_{2}-\tilde{b}_{2}}'\tilde{\Sigma}_{b}^{-1}\binom{b_{1}-\tilde{b}_{1}}{b_{2}-\tilde{b}_{2}}\right\}$$
(8).

Then we get the full conditionals of the parameters as follows:

$$\pi(\rho|\cdot) \propto \frac{(1+\rho)^{(\tilde{a}-1)-p(n-1)/2}(1-\rho)^{(\tilde{\beta}-1)-p(n-1)/2}}{|(Y-M)\Phi^{-1}(Y-M)'|^{n/2}}$$
(9),

$$\pi(a_1|\cdot) \propto \frac{\exp\{-a_1/\tilde{a}_1\}}{\left|(Y-M)\Phi^{-1}(Y-M)'\right|^{n/2}}$$
(10),

$$\exp\left\{-\frac{1}{2} \begin{pmatrix} b_1 - \tilde{b}_1 \\ b_2 - \tilde{b}_2 \end{pmatrix}' \tilde{\Sigma}_b^{-1} \begin{pmatrix} b_1 - \tilde{b}_1 \\ b_2 - \tilde{b}_2 \end{pmatrix}\right\}$$
(12),

$$\pi(b_2|\cdot) \propto \frac{1}{|(Y-M)\Phi^{-1}(Y-M)'|^{n/2}} \cdot \exp\left\{-\frac{1}{2} \binom{b_1 - \tilde{b}_1}{b_2 - \tilde{b}_2}' \tilde{\Sigma}_b^{-1} \binom{b_1 - \tilde{b}_1}{b_2 - \tilde{b}_2}\right\}$$
(13).

$$\pi(c_1|\cdot) \propto \frac{\exp\{-c_1/\tilde{c}_1\}}{\left|(Y-M)\Phi^{-1}(Y-M)'\right|^{n/2}}$$
(14),

$$\pi(c_2|\cdot) \propto \frac{\exp\{-c_2/\tilde{c}_2\}}{|(Y-M)\Phi^{-1}(Y-M)'|^{n/2}}$$
(15).

#### Regarding the MH Algorithm:

Let's take the sampling of  $a_2$  in Gompertz curve as an example. To define the algorithm, let  $\varphi(a_2^{(old)}, a_2^{(new)})$  denote a source density for a candidate draw  $a_2^{(new)}$  given the current value  $a_2^{(old)}$  in the sampled sequence. The density  $\varphi(a_2^{(old)}, a_2^{(new)})$  is referred to as the proposal or candidate generating density. Then, the MH algorithm is defined by two steps: a first step in which a proposal value is drawn from the candidate generating density and a second step in which the proposal value is accepted as the next iterate in the Markov chain according to the probability:

$$\alpha \left( a_{2}^{(old)}, a_{2}^{(new)} \right) = \min \left\{ \frac{\pi_{2}(a_{2}^{(new)})\varphi(a_{2}^{(new)}, a_{2}^{(old)})}{\pi_{2}(a_{2}^{(old)})\varphi(a_{2}^{(old)}, a_{2}^{(new)})}, 1 \right\},$$
  
if  $\pi_{2}(a_{2}^{(old)})\varphi\left( a_{2}^{(old)}, a_{2}^{(new)} \right) > 0$  (otherwise  $\alpha \left( a_{2}^{(old)}, a_{2}^{(new)} \right) = 1$ ).

If the proposal value is rejected, then the next sampled value is taken to be the current value. Let's follow this Metropolis-Hastings Algorithm:

- 1)
- Specify an initial value  $a_2^{(0)}$ . Repeat for j = 1, 2, ..., M: 2)
  - a) Propose  $a_2^{(new)} \sim \varphi(a_2^{(j)}, \cdot)$ , and b) Let  $a_2^{(j+1)} = a_2^{(new)}$  if  $U(0, 1) \leq \alpha(a_2^{(j)}, a_2^{(new)})$ otherwise  $a_2^{(j+1)} = a_2^{(j)}$ .
- Return the values  $a_2^{(1)}, a_2^{(2)}, ..., a_2^{(M)}$ . 3)

Then follow the above algorithm in taking samples of  $\Theta$  and  $\rho$ by using (9)-(15) through the following steps:

- Set j = 0 and select a set of initial parameter values for 1)  $\Theta^{(0)}$ ,  $B^{(0)}$  and  $\rho^{(0)}$ .
- Sample  $\rho^{(j+1)}$  from (9) (using MH algorithm). 2)
- Sample  $\Theta^{(j+1)}$  from (10)-(15) (using MH algorithm). 3)
- Replace  $\rho^{(j)}$  by  $\rho^{(j+1)}$ ,  $\Theta^{(j)}$  by  $\Theta^{(j+1)}$  and  $B^{(j)}$  by  $B^{(j+1)}$ . 4)
- 5) Set j = j + 1 and repeat steps 2 through 4.

Drop the initial burn-in sets and retain the rest of the data for marginal distribution analysis. This analysis includes highest density regions for the estimated parameters. In addition to this analysis of parameters, we can also generate 90% Credible Intervals (CIs or HDR's, Highest Density Regions) for the bestfit growth curve under this Bayesian formulation by using the 5% and 95% percentiles of y calculated by substituting the Msamples of  $\Theta$  at a given  $w_i$ .

#### 4. Real-world Data as Example

An intrauterine growth retarded rats data set [16] in this section as an example to demonstrate how to apply our approach to Bayesian analysis of multivariate growth curve model in a bivariate data setting (weight and length). In their experiment, in [16], they chose fifty female rats that were mated overnight with ten adult males and then divided the pregnant female rats into three groups: control group, intrauterine growth control group and sham-operated group. They then measured body weight, body length, and other facial characteristics of the rats that were in those three groups, respectively, every four days for twenty days. For illustrative purposes and for simplifying our analysis, the control group has been chosen and only use the bivariates body weight and body length in our growth curve model. The data set for rats growth is in Table 1. Four classic growth curve models explicitly for this specific example includes Jenss curve:  $f(w) = a + bw - \exp(c + dw);$ Gompertz curve:  $f(w) = a \exp[-\exp(b + cw)]$ ; Richards curve:  $f(w) = a\{1 + b \exp[c(d - w)]\}^{-1/b}$ ; Polynomial curve: f(w) = $a + bw + cw^2 + dw^3$ .

In that data set, assume that  $\tilde{\Sigma}_b$  is equal to  $s^2 \begin{bmatrix} 1 & 0.1 \\ 0.1 & 1 \end{bmatrix}$  for Gompertz curve. Similar assumption has been made for the other growth curves for comparison.  $s^2$  can be quite small if prior knowledge is reliable. The value assumed here would allow some moderate correlation relationship between the covariates length and weight. The results of Bayesian estimates are displayed in Table 2. Using BIC, in conjunction with the graphs and CIs, it seems natural to say that the Cubic growth curve is the model of selection for this specific bivariate intrauterine growth retarded rats data.

Regarding diagnostic testing for the model, careful consideration has been given to the useful approach presented by Franses [17] for residual autocorrelation in growth curve models. However, it's natural to concurr with his own conlcusion that there are obvious drawbacks in applying his method to small sample sizes, other growth curve models and to various model selection criteria as well. Needless to mention that this research is dealing with a multivariate scenario.

#### 5. Discussion

The 90% Credible Intervals, the fitted curves, and the estimates of the model parameters for the four growth curves in Figures 1-4 and Table 1-2 have been presented in this paper. There, we can see that for weight versus time (Figure 1) and length vs. time (Figure 2), the 90% CI of Cubic curve is the narrowest among all four curves when time is small but diverges like a funnel shape as time increases to approximately more than 15 days; for weight vs. time in Figure 1, Jenss and Gompertz curves both have relatively narrow 90% CIs, whereas for length vs. time in Figure 2, Jenss curve has smaller 90% CI. In Figures 3-4, we observed that on the one hand, the data display a positive trend that as length increases, the rate of change in weight also increases; on the other hand, when weight increases, the rate of change in length decreases. Although all four curves fit the data reasonably well, the Cubic curve is apparently the best fit curve among them. In addition, as time increases approximately before the fifteenth day, the rate of change in length and in weight both increase as weight and length increase. It's obvious that Cubic curve appears to be the best fit curve for the given data. Besides, BIC is useful criteria in model selection because the smaller value it is, the better curve fitting it will be, and this is consistent with our observations in those Figures.

In summary, the Bayesian multivariate growth curve models in this study provide a formulation for generating Bayesian estimates as well as describing the dependence relationship between variables with a certain autocorrelation relationship under consideration. Further research topic may include better diagnostic testing methods for more growth curve models as well as smaller multivariate sample size data using various selection criteria.

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Age (Days)	Weight (g)	Length (mm)		
1	6.6 54.5			
5	10.4	65.6		
9	16.3	77.2		
13	23.2	87.5		
17	28.6	94.6		
21	38.4	110.4		
	TABLE 1			

Rats Growth Data

(Units for ages: Days; Weight: Grams and Length: mm)

	Je	Jenss Gompertz		Richards		Cubic Polynomial		
Estimates	Length vs. Time	Weight vs. Time						
a	52.299	21.536	275.231	146.321	966.688	747.626	50.226	5.325
ь	2.674	1.575	0.501	1.167	-0.744	-0.393	3.998	1.051
c	0.115	2.906	0.027	0.041	0.005	0.01	-0.162	0.012
d	-0.861	0	-	-	37.458	76.668	0.005	0.001
ρ	-0.336		-0.361		-0.36		-0.369	
BIC	7.73		5.74		5.59		5.57	



Note: Take the numbers in the two columns under Gompertz as example: they are the estimates of the parameters (coefficients) of the bivariate growth curves (for length and weight, respectively), where

 $Length(w) = 275.231 \exp \left[-\exp(0.501 + 0.027w)\right],$ Weight(w) = 146.321 exp [- exp(1.167 + 0.041w)].

90% Credible Interval for Jenss Growth Curve

-----Upper& LowerBound:

Bayesian Estimates

O rig in all C urve

80

60 - D



Figure 2 Length vs. Time Credible Intervals for the Four Different Growth Curves







Figure 4 Three Dimensional Plot (Time, Weight and Length)



80

60

90% Credible Interval for Gompertz Growth Curve

Figure 1 Weight vs. Time Credible Intervals for the Four Different Growth Curves

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