First Principle Model Simulation Study

Contents

0.1 Quadratic Model

0.1.1 Intake Equation

$$E(t) = \beta_\theta + \beta_1 t + \beta_2 t^2$$

0.1.2 Time equation

$$t = min(\frac{-\beta_1 \pm \left(\beta_1^2 - 4(\beta_\theta - E(t))\beta_2\right)^{1/2}}{2\beta 2}$$

0.2 Thompson et al., 2017 First-Principles Dynamic Model

0.2.1 Orinqinal Equation in paper

$$E(t) = \frac{E_{max}\theta\left(e^{\frac{t(E_{max}r+\theta)}{E_{max}}} - 1\right)}{\theta\left(e^{\frac{t(E_{max}r+\theta)}{E_{max}}} + E_{max}r\right)}$$

0.2.2 Correct intake equation - took the integral of the derivative/eating rate equation

$$\frac{dE}{dt} = (rE(t) = \theta)\left(1 - \frac{E(t)}{E_{max}}\right)$$

$$\int \frac{dE}{dt} = \int (rE(t) = \theta)\left(1 - \frac{E(t)}{E_{max}}\right)$$

$$\vdots$$

$$E(t) = \frac{E_{max}\theta\left(e^{\frac{t(E_{max}r+\theta)}{E_{max}}} - 1\right)}{\theta\left(e^{\frac{t(E_{max}r+\theta)}{E_{max}}} + \frac{E_{max}r}{\theta}\right)}$$

$$= \frac{E_{max}\left(e^{\frac{t(E_{max}r+\theta)}{E_{max}}} - 1\right)}{e^{\frac{t(E_{max}r+\theta)}{E_{max}}} + \frac{E_{max}r}{\theta}}$$

(1)

$\theta \neq 0;\ integral\ constant\ c \neq 1;\ \theta \neq +E_{max}r$

0.2.3 Correct time equation

$$E(t) = \frac{E_{max}\left(e^{\frac{t(E_{max}r+\theta)}{E_{max}}} - 1\right)}{e^{\frac{t(E_{max}r+\theta)}{E_{max}}} + \frac{E_{max}r}{\theta}}$$

$$E(t)\left(e^{\frac{t(E_{max}r+\theta)}{E_{max}}} + \frac{E_{max}r}{\theta}\right) = E_{max}\left(e^{\frac{t(E_{max}r+\theta)}{E_{max}}} - 1\right)$$

$$E(t)\left(e^{\frac{t(E_{max}r+\theta)}{E_{max}}}\right) + E(t)\left(\frac{E_{max}r}{\theta}\right) = E_{max}\left(e^{\frac{t(E_{max}r+\theta)}{E_{max}}}\right) - E_{max}$$

$$E(t)\left(\frac{E_{max}r}{\theta}\right) + E_{max} = E_{max}\left(e^{\frac{t(E_{max}r+\theta)}{E_{max}}}\right) - E(t)\left(e^{\frac{t(E_{max}r+\theta)}{E_{max}}}\right)$$

$$E_{max}\left(\frac{E(t)r}{\theta} + 1\right) = e^{\frac{t(E_{max}r+\theta)}{E_{max}}}\left(E_{max} - E(t)\right)$$

$$\frac{E_{max}\left(\frac{E(t)r}{\theta} + 1\right)}{E_{max} - E(t)} = e^{\frac{t(E_{max}r+\theta)}{E_{max}}}$$

$$ln\left(\frac{E_{max}\left(\frac{E(t)r}{\theta} + 1\right)}{E_{max} - E(t)}\right) = \frac{t(E_{max}r + \theta)}{E_{max}}$$

$$\frac{E_{max}}{E_{max}r + \theta}ln\left(\frac{E_{max}\left(\frac{E(t)r}{\theta} + 1\right)}{E_{max} - E(t)}\right) = t$$

0.3   Log likelihood
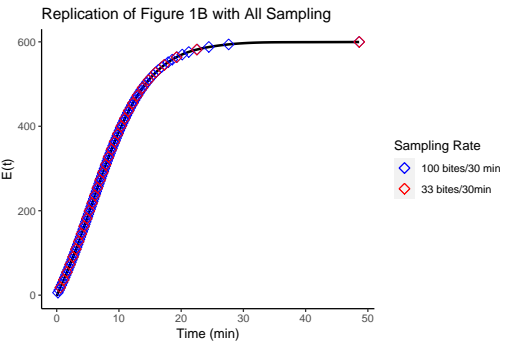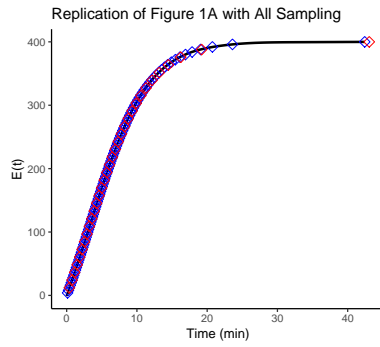
$$L(\hat{E(t)} + \epsilon, \sigma^2 | t, \theta, r, E_{max}) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(E_i - E(t_i))^2}{2\sigma^2}}$$

$$= \prod_{i=1}^{n} (2\pi\sigma^2)^{\frac{-1}{2}} e^{-\frac{1}{2\sigma^2}(E_i - E(t_i))^2}$$

$$= (2\pi\sigma^2)^{\frac{-n}{2}} \prod_{i=1}^{n} e^{-\frac{1}{2\sigma^2}(E_i - E(t_i))^2}$$

$$\ln\left(L(\hat{E(t)} + \epsilon, \sigma^2 | t, \theta, r, E_{max})\right) = \ln\left((2\pi\sigma^2)^{\frac{-n}{2}} \prod_{i=1}^{n} e^{-\frac{1}{2\sigma^2}(E_i - E(t_i))^2}\right)$$

$$= \ln\left((2\pi\sigma^2)^{\frac{-n}{2}}\right) + ln\left(\prod_{i=1}^{n} e^{-\frac{1}{2\sigma^2}(E_i - E(t_i))^2}\right) \tag{2}$$

$$= \ln\left((2\pi\sigma^2)^{\frac{-n}{2}}\right) + ln\left(e^{-\frac{1}{2\sigma^2}\sum_{i}^{n}(E_i - E(t_i))^2}\right)$$

$$= \frac{-n}{2} \ln\left(2\pi\sigma^2\right) + -\frac{1}{2\sigma^2} \sum_{i}^{n}(E_i - E(t_i))^2$$
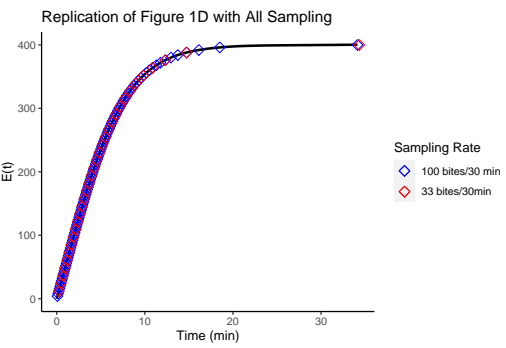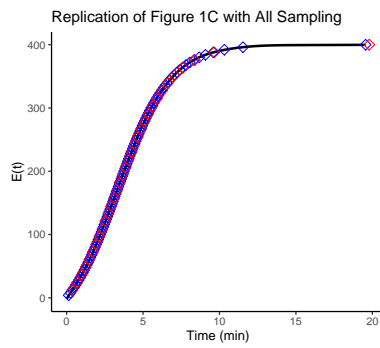
$$\sigma^2 = \frac{\sum_{i}^{n}(E_i - E(t_i))^2}{n}$$

$$\ln\left(L(\hat{E(t)} + \epsilon, \sigma^2 | t, \theta, r, E_{max})\right) = \frac{-n}{2} \ln\left(2\pi\left(\frac{\sum_{i}^{n}(E_i - E(t_i))^2}{n}\right)^2\right) + -\frac{1}{2\left(\frac{\sum_{i}^{n}(E_i - E(t_i))^2}{n}\right)^2} \sum_{i}^{n}(E_i - E(t_i))^2$$

1A - theta: 30 g/min, r: 0.17 1/min, Emax = 400g

1B - theta: 30 g/min, r: 0.17 1/min, Emax = 600g

Replication of Figure 1A with All Sampling

Replication of Figure 1B with All Sampling

1C - theta: 30 g/min, r: 0.5 1/min, Emax = 400g

1D - theta: 50 g/min, r: 0.17 1/min, Emax = 400g

Replication of Figure 1C with All Sampling

Replication of Figure 1D with All Sampling

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0.3.1 Compare Parameter Fits by Sampling Rate
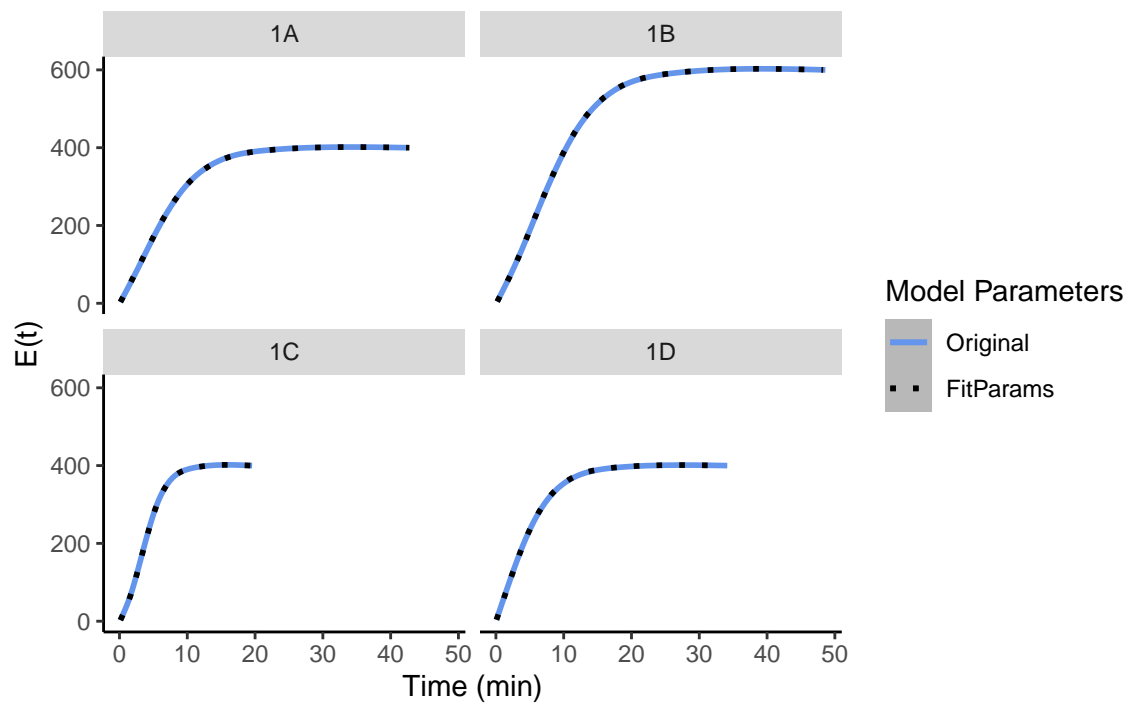
250 ms Sampling

Replication of Figure 1A with 250 ms sampling (for 30 min meal)
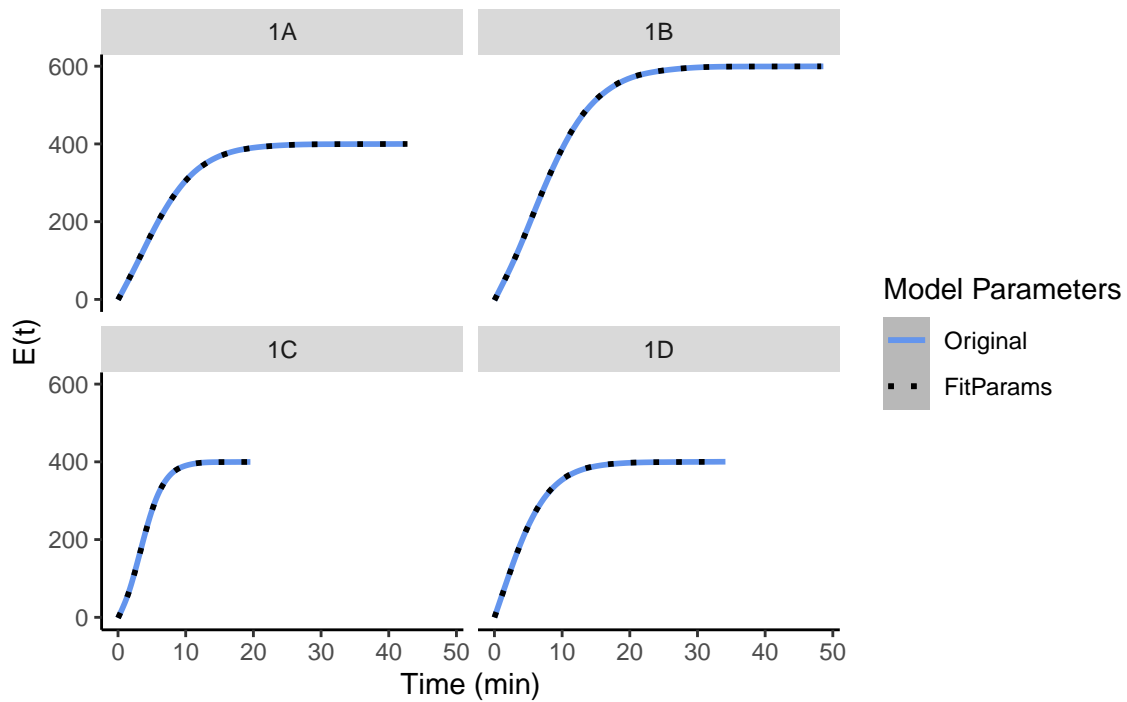
Replication of Figure 1 with 250 ms sampling (for 30 min meal)

randomly sampled number of bites: mean = 33, sd = 5

1A - theta: 30 g/min, r: 0.17 1/min, Emax = 400g

Replication of Figure 1A with 33 Bites
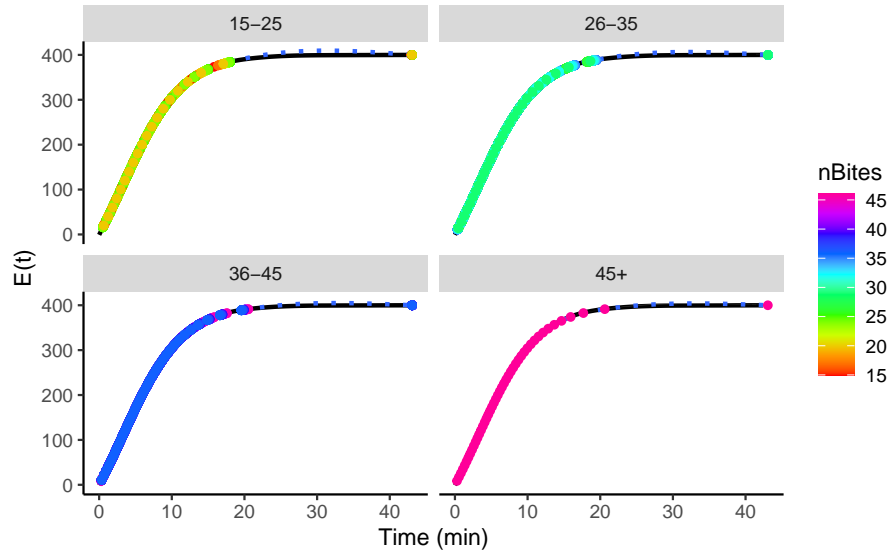
1B - theta: 30 g/min, r: 0.17 1/min, Emax = 600g

Replication of Figure 1B with 33 Bites

1C - theta: 30 g/min, r: 0.5 1/min, Emax = 400g

Replication of Figure 1C with 33 Bites

1D - theta: 50 g/min, r: 0.17 1/min, Emax = 400g

Replication of Figure 1D with 33 Bites

1 Simulations based on Fogel et al., 2017

1.1 Correlations between Microstructure Behaviors
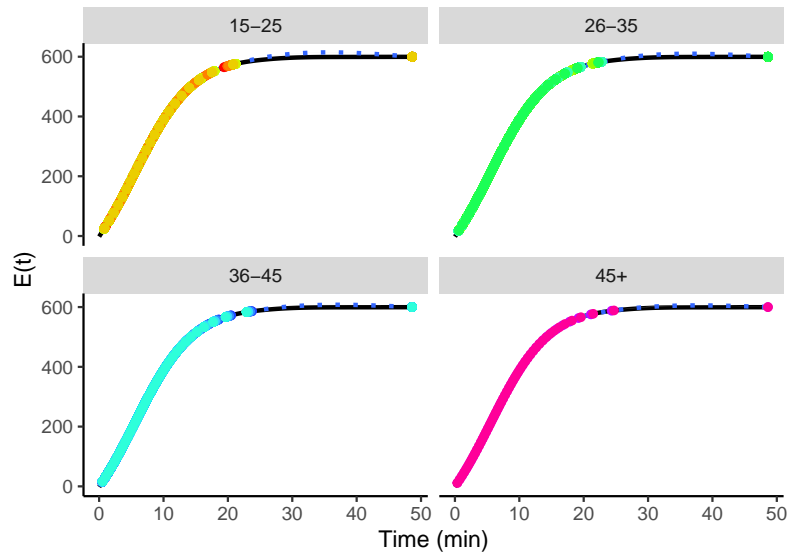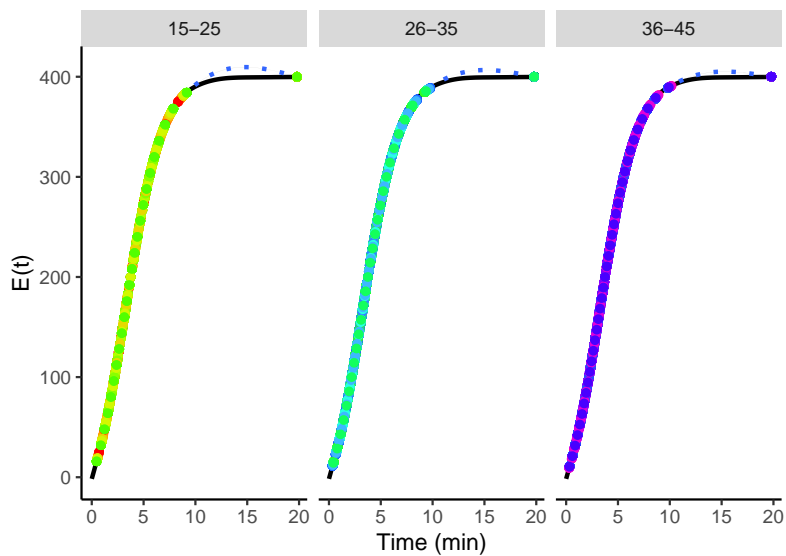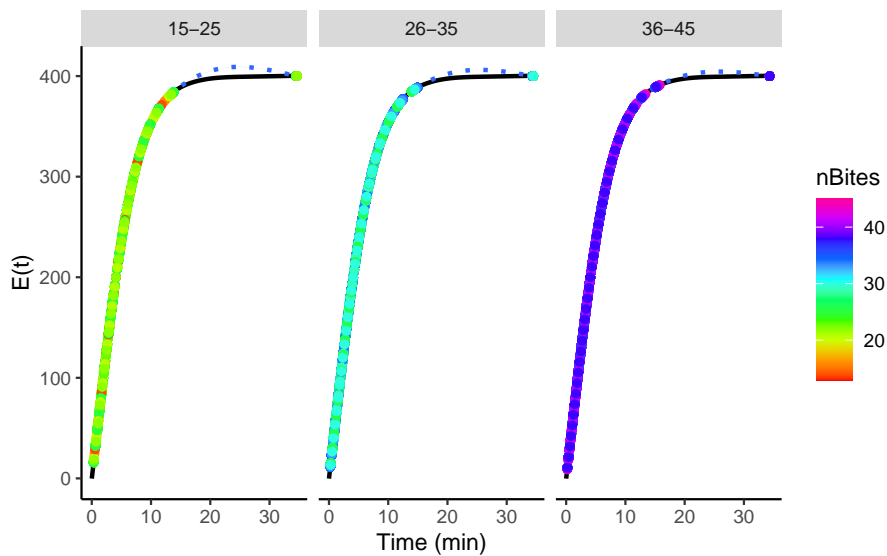
1.1.1 Corrleations Reported in Fogel et al., 2017 (Table 1)

Table 1: Correlations between Microstructure Behaviors - Simulated

nBites	BiteSize_g	BiteOralExposure_sec	ActiveMeal_pcent	TotalOralExposure_min	EatRate_g.min
NA	NA	NA	NA	NA	NA
-0.42*	NA	NA	NA	NA	NA
-0.58*	0.54*	NA	NA	NA	NA
0.11*	0.17*	0.16*	NA	NA	NA
0.54*	-0.01	0.02	0.33	NA	NA
0.15*	0.55*	-0.25*	-0.02	-0.05	NA

1.1.2 Corrleations Simulated

Table 2: Correlations between Microstructure Behaviors - Simulated

nBites	BiteSize_g	BiteOralExposure_sec	ActiveMeal_pcent	TotalOralExposure_min	EatRate_g.min	TotalIn
-0.42*						
-0.58*	0.54*					
0.11*	0.17*	0.16*				
0.44*	0.14*	0.48*	0.3*			
0.03	0.66*	-0.27*	0.05	-0.26*		
0.35*	0.7*	0.1*	0.26*	0.49*	0.71*	
0.05	0.41*	-0.17*	0.09*	-0.14*	0.63*	0.46*
0.42*	0.08	0.44*	-0.07	0.93*	-0.29*	0.41*

1.1.3 Corrleations Simulated - After Rounding Simulated Number of Bites

Table 3: Correlations between Microstructure Behaviors - Simulated, Rounded

nBites	BiteSize_g	BiteOralExposure_sec	ActiveMeal_pcent	TotalOralExposure_min	EatRate_g.min	TotalIn
-0.41*						
-0.58*	0.54*					
0.11*	0.17*	0.16*				
0.45*	0.15*	0.47*	0.29*			
0.04	0.66*	-0.27*	0.05	-0.25*		
0.36*	0.7*	0.1*	0.26*	0.5*	0.71*	
-0.03	0.42*	-0.16*	-0.01	-0.21*	0.61*	0.4*
0.43*	0.09*	0.43*	-0.07	0.93*	-0.28*	0.43*

1.2 Fast vs Slow Eaters Microstructure Characteristics

### 1.2.1 Means (SEM) Reported in Fogel et al., 2017 (Table 2)

	Slow	Fast	t	p
Bites(#)	57.7 (2.5)	68.4 (2.5)	3.04	0.003
Bite Size (grams/bite)	1.4 (0.1)	2.4 (0.1)	9.17	<0.001
Oral Exposure per Bite (sec)	20.1 (0.9)	15.6 (0.5)	4.11	<0.001
Active Mealtime (%)	75.0 (1.0)	76.0 (1.0)	0.56	0.570
Total Oral Exposure (min)	15.1 (0.4)	15.2 (0.4)	0.08	0.930
Total Intake (kCal)	175.3 (6.09)	306.7 (9.9)	11.28	<0.001

1.2.2 Means (SEM) After Rounding Simulated Number of Bites

1.3 Parameter Distributions - Quadratic

1.4 Parameter Distributions - First Principles Model

1.4.1 Histogram: Overall Distributions
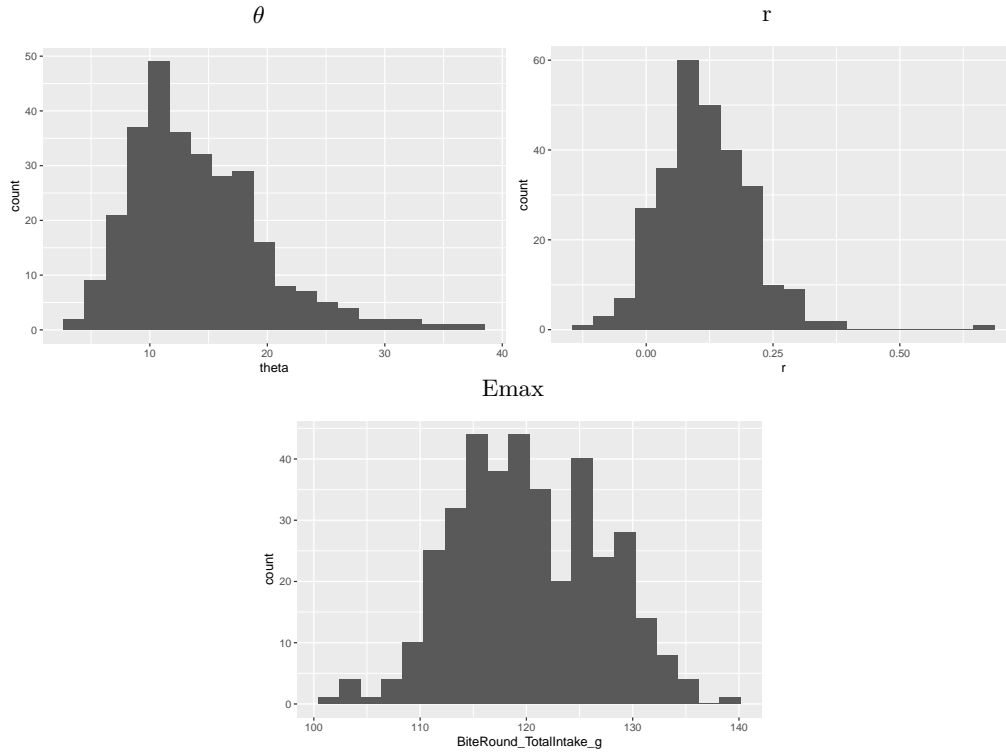
1.4.2 Histogram: Distributions by Eating Rate Group

1.4.3 Density: Distributions by Eating Rate Group

θ by Eating Rate Group

r by Group

Emax by Group

θ by Eating Rate Group

r by Group

Emax by Group