First Principle Model Simulation Study

Contents

	0.1	•	
	0.2	Thompson et al., 2017 First-Principles Dynamic Model	2
	0.3	Log likelihood	4
1	Rep	plication of Figure 1 from Thompson et al 2017	5
	1.1	Compare by Sampling Rate	5
		Paremeter Recovery by Sampling Rate	
2	Sim	aulations based on Fogel et al., 2017	10
	2.1	Simulated Microbehaivor	10
	2.2	Correlations between Microstructure Behaviors	
	2.3	Fast vs Slow Eaters Microstructure Characteristics	
	2.4	Correlations Between Microstructure Behaviors	
	2.5	Eating Rate Distribution	
	2.6	Kissileff's Quadratic Model	
	2.7	First Principles Model	
	2.8	Correlations Between Parameters	
3	Cur	nulative Intake Curves Accross Parameter Distributions	18
	3.1		18
		First Principles Model	

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

$$t=min\big(\frac{-\beta_1\pm\left(\beta_1^2-4(\beta_\theta-E(t))\beta_2\right)^{1/2}}{2\beta2}$$

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

0.2.1 Oringinal 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

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

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

$$\vdots$$

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

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

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

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

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

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

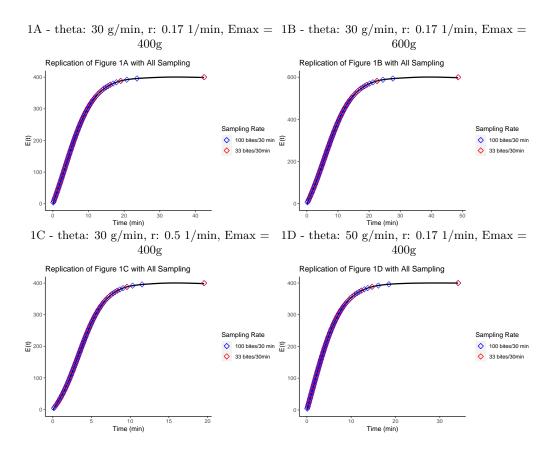
$$= \frac{-n}{2}\ln\left(2\pi\sigma^{2}\right) + -\frac{1}{2\sigma^{2}} \sum_{i}^{n} (E_{i} - E(t_{i}))^{2}$$
(2)

$$\sigma^2 = \frac{\sum_{i}^{n} (E_i - E(t_i))^2}{n}$$

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

1 Replication of Figure 1 from Thompson et al 2017

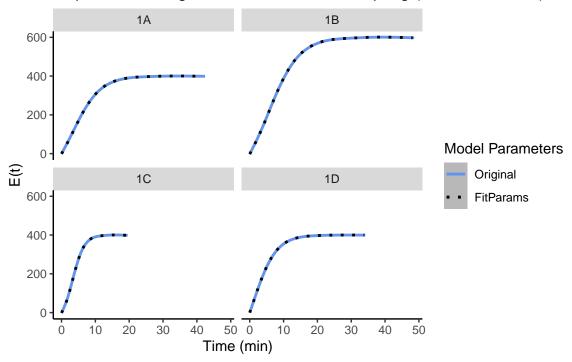
1.1 Compare by Sampling Rate



1.2 Paremeter Recovery by Sampling Rate

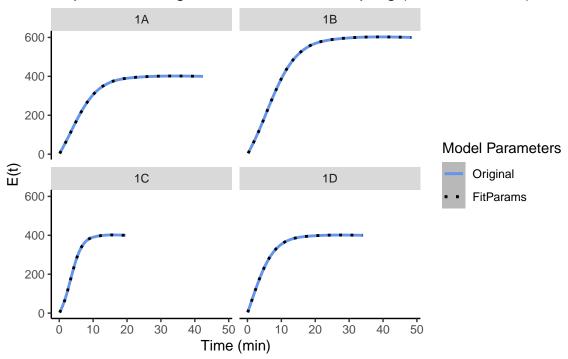
250 ms Sampling

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



100 bite Sampling

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

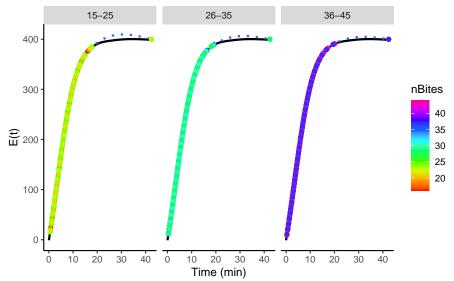


1.2.1 Parameter Recovery with Infrequent Bites (500 sims)

Randomly Sampled Number of Bites: mean = 33, sd = 5

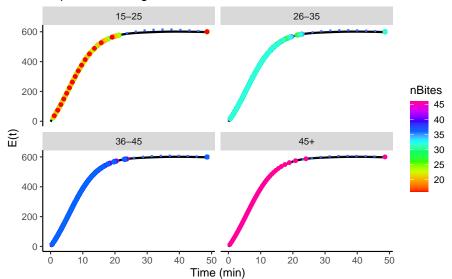
1A - theta: 30 g/min, r: 0.17 1/min, Emax = $400\mathrm{g}$

Replication of Figure 1A with 33 Bites



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

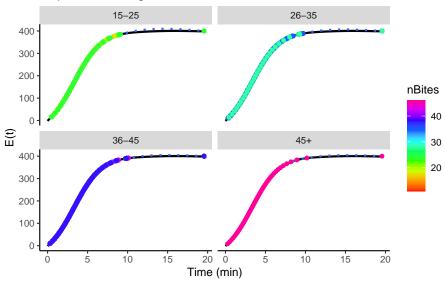
Replication of Figure 1B with 33 Bites



Randomly Sampled Number of Bites: mean = 33, sd = 5

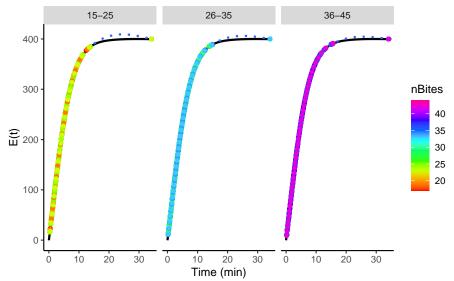
 $1\mathrm{C}$ - theta: 30 g/min, r
:0.51/min, Emax = $400\mathrm{g}$

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



2 Simulations based on Fogel et al., 2017

2.1 Simulated Microbehaivor

Data were simulated from a multivariate normal distribution for the following microbehaviors:

- •: Number of Bites rounded to whole number
- $\bullet \text{:}\ \text{Bite Size (g)} \text{restricted to be} > 0$
- •: Percent of Time Active (ie. eating) restricted be $\leq 100\%$
- •: Oral Exposure per Bite (sec)

2.1.1 Computed Microbehavior

The following microbehavior characteristics were calculated based on simulated data:

- \bullet : Total Oral Exposure (min); (Oral Exposure per Bite * Number of Bites)/60 restricted to be > 2 min to fit range reported in Fogel et. al., 2017
- •: Total Intake (g); Bite Size (g) * Number of Bites
- \bullet : Eating Rate (g/min); Total Intake (g)/Total Oral Exposure (min) restricted be >0 and <25 to approximate range depicted in Figure 1 in Fogel et al., 2017
- •: Meal Duration (min); Total Oral Exposure/(Percent of Time Active/100) restricted to be \leq 30 min as that was the longest duration the meal could go in the Fogel et al., 2017 paper

2.2 Correlations between Microstructure Behaviors

Table 1: Correlations between Microstructure Behaviors - Simulated

	nBites	EatRate	TotalOE_min	ActiveMeal_pcent	BiteOE_sec
nBites	NA	NA	NA	NA	NA
EatRate	0.15**	NA	NA	NA	NA
$TotalOE_min$	0.54*	-0.05	NA	NA	NA
$ActiveMeal_pcent$	0.11*	-0.02	0.33***	NA	NA
$BiteOE_sec$	-0.58****	-0.25***	0.02	0.16**	NA
TotalIntake_g BiteSize_g	NA -0.42***	NA 0.55*	NA -0.01	NA 0.17**	NA 0.54***

2.2.2 Corrleations Simulated

Table 2: Correlations between Microstructure Behaviors - Simulated

	nBites	EatRate	TotalOE_min	ActiveMeal_pcent	BiteOE_sec	TotalIntake_g
nBites						
EatRate	0.28*					
$TotalOE_min$	0.4*	-0.2*				
$ActiveMeal_pcent$	0.17*	0	0.38*			
$BiteOE_sec$	-0.68*	-0.4*	0.23*	0.14*		
$TotalIntake_g$	0.47*	0.67*	0.5*	0.22*	-0.14*	
BiteSize_g	-0.37*	0.44*	0.09*	0.14*	0.53*	0.53*

2.3 Fast vs Slow Eaters Microstructure Characteristics

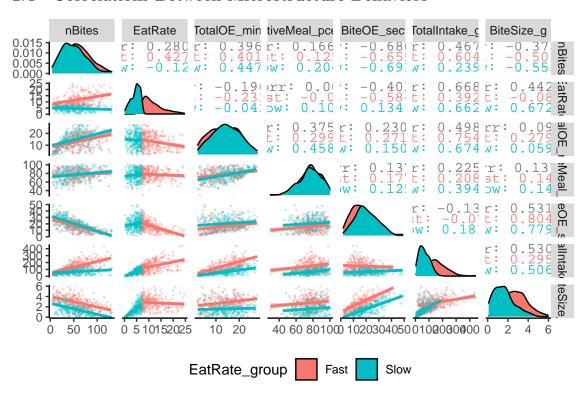
2.3.1 $\,$ Means (SEM): Reported in Fogel et al., 2017 (Table 2)

	Slow	Fast	t p
Bites(#)	57.7 (2.5)	$\overline{68.4\ (2.5)}$	$\overline{3.04}$ 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

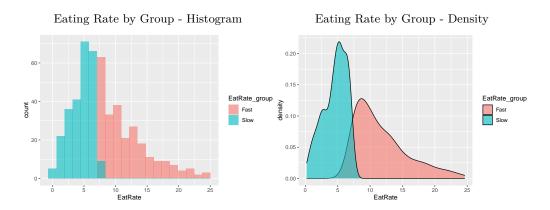
${\bf 2.3.2}$ Means (SEM): From Simulated and Calculated Data

	Slow		Fast			
	Mean (SE)	Range	Mean (SE)	Range	t	p
Bites(#)	50.28 (1.6)	4 - 131	58.74 (1.7)	5 - 130	15.53	< 0.001
Bite Size (grams/bite)	1.6(0.1)	0.1 - 4.6	2.8(0.1)	0.5 - 6.0	12.56	< 0.001
Oral Exposure per Bite (sec)	20.5(0.6)	2.0 - 48.8	15.7(0.5)	2.0 - 41.4	-6.14	< 0.001
Active Mealtime (%)	76.8(0.8)	44.7 - 100	73.6(0.7)	29.7 - 98.6	0.553	0.581
Total Oral Exposure (min)	14.5(0.4)	2.2 - 27.0	13.1 (0.34	2.2 - 27.7	-2.66	0.008
Total Intake (grams)	66.2(2.4)	3.7 - 188.5	149.0(4.8)	16.3 - 441.3	15.53	< 0.001

2.4 Correlations Between Microstructure Behaviors

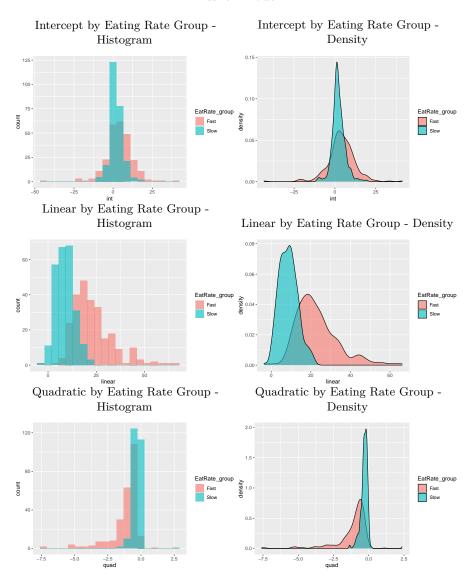


2.5 Eating Rate Distribution



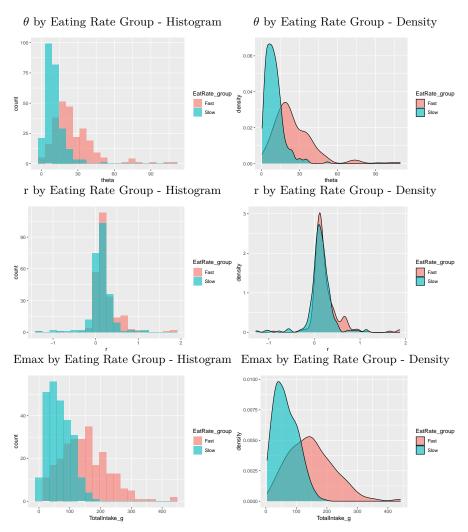
2.6 Kissileff's Quadratic Model

Kissileff Model

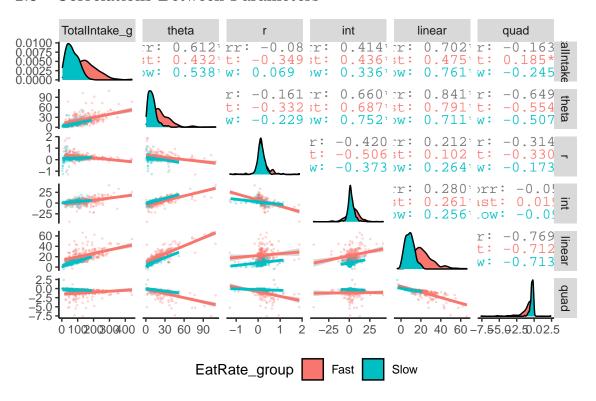


2.7 First Principles Model

First Principles Model



2.8 Correlations Between Parameters

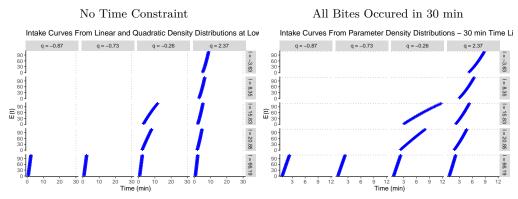


3 Cumulative Intake Curves Accross Parameter Distributions

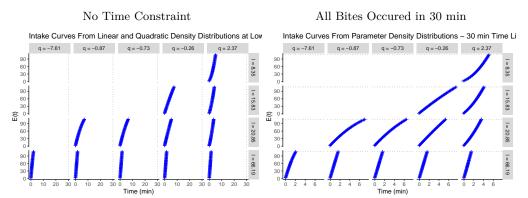
Set Emax and number of bites to the average of the distributions

3.1 Kissileff Quadratic Model

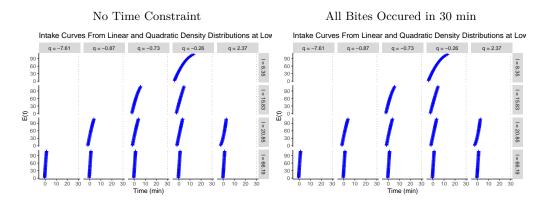
Kissileff Cumulative Intake Curves: Lowest Intercept (-43.43)



Kissileff Cumulative Intake Curves: Mean Intercept (3.13)



Kissileff Cumulative Intake Curves: Highest Intercept (41.2)

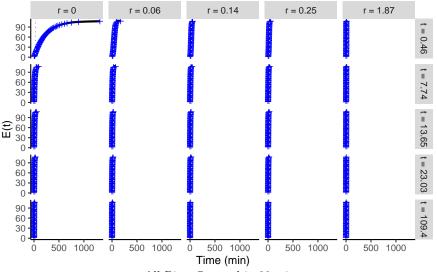


3.2 First Principles Model

First Prinicples Model Cumulative Intake Curves

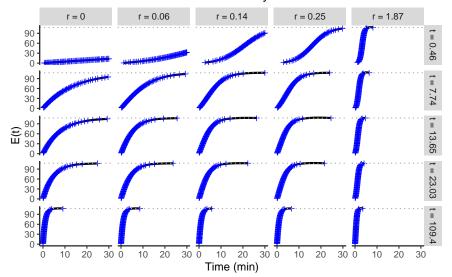
No Time Constraints

Intake Curves From Parameter Density Distributions (55 bites, Emax :



All Bites Occured in 30 min

Intake Curves From Parameter Density Distributions - 30 min Time Li

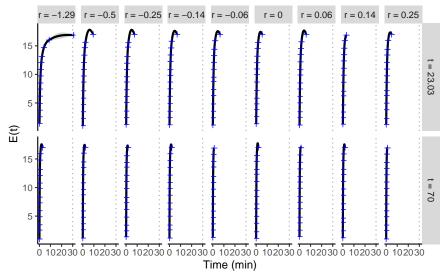


3.2.1 Zoom in on r - negative and small values

First Prinicples Model Cumulative Intake Curves

No Time Constraints

Emax calculated to work at lowest r and Bites Size set to 25th percen-



All Bites Occured in 30 min

Emax calculated to work at lowest r and Bites Size set to 25th percen-

