

Metamodeling for Bias Estimation of Biological Reference Points

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1 Introduction

set the context for my question

Data for a typical surplus-production model comes in the form of an index of abundance through time which is assumed to be proportional to the reproducing biomass for the population of interest. The index is often observed alongside a variety of other known quantities, but at a minimum, each observed index will be observed in the presence of some known catch for the period.

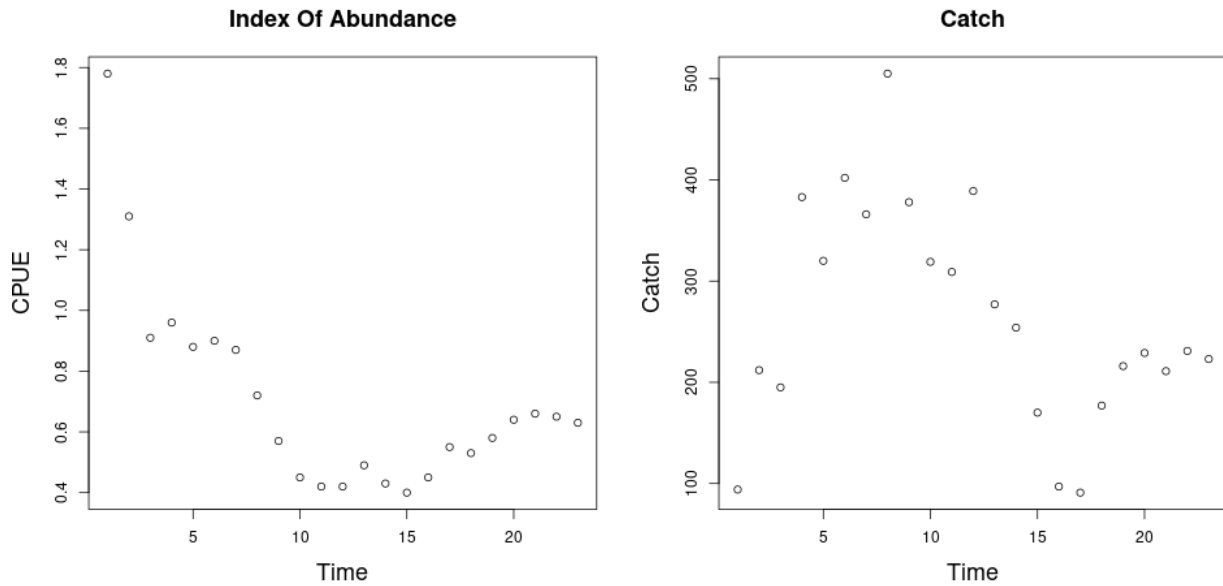


Figure 1: *left*: An observed series of index of abundance data for Namibian Hake from 1965 to 1987 (Hilborn & Mangel, 1997). *right*: The associated catch data for Namibian Hake over the same time period.

The observed indices are assumed to have multiplicative log-normal errors, and thus the following observation model arises naturally,

$$I_t = qB_te^\epsilon \quad \epsilon \sim N(0, \sigma^2). \quad (1)$$

Above q is often referred to as the “catchability parameter”; it serves as the proportionality constant mapping between the observed index of abundance and biomass. σ^2 models residual

variation. Biologically speaking q and σ^2 are often treated as nuisance parameters with the “biological parameters” entering the model through a process model on biomass.

Biomass is assumed to evolve as an ODE; in this case I focus on the following form,

$$\frac{dB}{dt} = P(B(t); \boldsymbol{\theta}) - Z(t)B(t). \quad (2)$$

Here biomass is assumed to change in time by two processes, net production of biomass into the population, $P(B)$, and various sources of biomass removal, Z , from the population.

Firstly, the population grows through a production function, $P(B)$. Production in this setting is defined as the net biomass increase due to all reproduction and maturation processes. The production function is assumed to be a parametric (generally non-linear) function relating the current biomass of the population to an aggregate production of biomass.

Secondly, the population decreases as biomass is removed by various sources that are assumed to remove biomass linearly with biomass. Above, $Z(t)$, is an aggregate rate of removal. When the fishing rate, $F(t)$, is the only source of removal $Z(t) = F(t)$, however often models will also included other linear terms in $Z(t)$. Commonly the rate of “natural mortality”, M , is also included as an additional term so that $Z(t) = M + F(t)$.

From a management perspective a major goal of modeling is to accurately infer a quantity known as *maximum sustainable yield* (MSY). One could maximize simple yield at a particular moment in time (and only for that moment) by fishing all available biomass in that moment. This strategy is penny-wise but pound-foolish (not to mention ecologically devastating) since it doesn’t leave biomass in the population to reproduce in the future. We seek to fish in a way that allows (or even encourages) future productivity in the population. This is accomplished by maximizing the equilibrium level of catch over time. Equilibrium yield is considered by replacing the steady state biomass (\bar{B}) in the assumed form for catch, so that $\bar{Y} = F\bar{B}(F)$, where $\bar{\cdot}$ indicates a value at steady state. MSY is found by maximizing $\bar{Y}(F)$ with respect to F , and F^* is the fishing rate at MSY. Going forward let $*$ decorate any value derived under the condition of MSY.

Fisheries are very often managed based upon reference points (RPs) which serve as simplified heuristic measures of population behavior. The mathematical form of RPs depends

upon the model assumptions through the production function. While a number of different RPs exist which describe the population in different (but related) ways, the most common RPs revolve around the concept of MSY (or robust ways of measuring MSY (Hilborn, 2010; Punt et al., 2016)). Here the focus is primarily on the RPs $\frac{B^*}{B(0)}$ and F^* ($\frac{F^*}{M}$ when appropriate) for their pervasive use in modern fisheries (Mangel et al., 2013; Punt & Cope, 2019).

F^* is the afore mentioned fishing rate which results in MSY. $\frac{B^*}{B(0)}$ is the depletion of the stock at MSY. That is to say $\frac{B^*}{B(0)}$ describes the fraction of the unfished population biomass that will remain in the equilibrium at MSY. In general $F^* \in \mathbb{R}^+$ and $\frac{B^*}{B(0)} \in (0, 1)$, however under the under the assumption of a two parameter production function production models will be structurally unable to capture the full theoretical range of RPs (Mangel et al., 2013).

Many of the most commonly used production functions depend only on two parameters. For example, the Schaefer model (cite) depends only on the biological parameters r and K , and limits RP inference so that under the Schaefer model $(F^*, \frac{B^*}{B(0)}) \in (\mathbb{R}^+, \frac{1}{2})$. Similarly the Beverton-Holt (Beverton & Holt, 1957, BH) and Ricker (Ricker, 1954) curves are also two parameter production functions that do not model the full theoretical space of RPs (Mangel et al., 2013).

The bias-variance trade-off (Ramasubramanian & Singh, 2017) makes it clear that the addition of a third parameter in the production function will necessarily reduce estimation bias. However the utility of this bias reduction is still under debate because the particular mechanisms and behavior (direction and magnitude) of these biases for key management quantities are not fully understood or described. Lee et al. (2012) provides some evidence that estimation of productivity parameters are dependent on biomass contrast as well as model specification. Conn et al. (2010) comes to similar conclusions via calibration modeling techniques. These studies indicate important factors that contribute to inferential failure, but they do not offer mechanisms of model failure, nor do they consider how different types of model misspecification interact with the information content of a given biomass series.

In this study I consider the behavior of inference when index data are simulated from three parameter PT and Schnute production models, but the simulated data are fit using intentionally misspecified two parameter logistic or BH production models. The work begins with a derivation of RPs under the three parameter models. The parametric forms of RPs

under the three parameter models are then inverted to develop a simulation setting for analyzing inference under the two parameter models. Finally a Gaussian Process (GP) metamodel (Gramacy, 2020) is constructed for exploration and analysis of RP biases.

A key insight of this approach is that bias is considered broadly across RP-space to uncover patterns and correlations between RPs. The GP metamodel is explicit about trade-offs between RPs so as to inform the full utility of reducing bias, as well as to suggest mechanisms for understanding what causes bias. Further, the effect of contrast on estimation is considered together with model misspecification.

2 Methods

2.1 PT Model

The three parameter PT family has a convenient form that includes, among others (Fox Jr., 1970; Rankin & Lemos, 2015), the logistic production function as a special case. Pella-Tomlinson production function is parameterized so that $\theta = [r, K, \gamma]$ and the family takes the following form,

$$P_p(B; [r, K, \gamma]) = \frac{rB}{\gamma - 1} \left(1 - \left(\frac{B}{K} \right)^{(\gamma-1)} \right). \quad (3)$$

γ is a parameter which breaks PT out of the restrictive symmetry of the logistic curve. In the special case of $\gamma = 2$ Eq (3) collapses back to the logistic curve, however in general $\gamma \in (1, \infty)$. The parameter r controls the maximum reproductive rate of the population in the absence of competition for resources (i.e. the slope of production function at the origin). K is the so called "carrying capacity" of the population. In this context the carrying capacity can be formally stated as steady state biomass in the

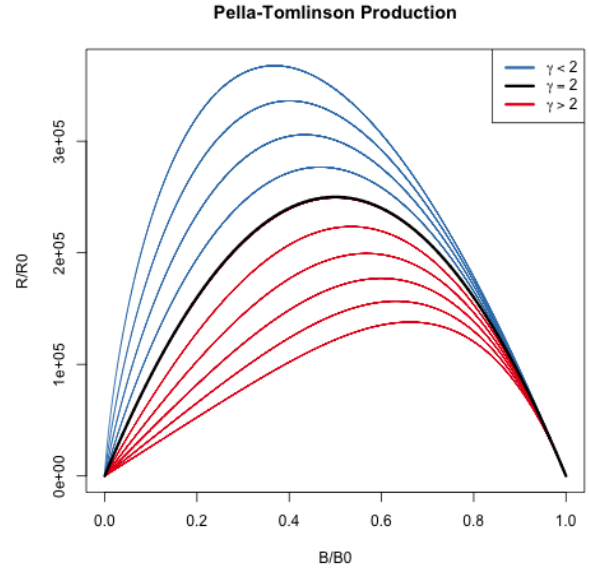


Figure 2: The PT production function plotted across a variety of parameter values. The special cases of Logistic production is shown in black, and the left-leaning and right-leaning regimes are shown in blue and red respectively.

90 absence of fishing (i.e. $\bar{B}(0) = K$). In Figure (2) PT recruitment is shown for a range of
 91 parameter values so as to demonstrate the various recruitment shapes that can be achieved
 92 by PT recruitment.

93 While the form of the PT curve produces some limitations ([cite](#)), importantly the intro-
 94 duction of a third parameter allows enough flexibility to fully describe the space of reference
 95 points used in management. To see this, the reference points are analytically derived for the
 96 PT model below.

97 **2 .1.1 PT Reference Points**

98 With $B(t)$ representing biomass at time t , under PT production, the dynamics of biomass
 99 are defined by the following ODE,

$$\frac{dB}{dt} = \frac{rB}{\gamma - 1} \left(1 - \left(\frac{B}{K} \right)^{\gamma-1} \right) - FB. \quad (4)$$

An expression for the equilibrium biomass is attained by setting Eq (4) equal to zero, and rearranging the resulting equation to solve for B . Thinking of the result as a function of F gives,

$$\bar{B}(F) = K \left(1 - \frac{F(\gamma - 1)}{r} \right)^{\frac{1}{\gamma-1}}. \quad (5)$$

100 At this point it is convenient to notice that $\bar{B}(0) = K$. The expression for B^* is given
 101 by evaluating Eq (5) at F^* . To get an expression for F^* , the equilibrium yield is maximized
 102 with respect to F ,

$$F^* = \operatorname{argmax}_F F \bar{B}(F). \quad (6)$$

In the case of PT production this maximization can be done analytically, by differentiating the equilibrium yield with respect to F as follows,

$$\frac{d\bar{Y}}{dF} = \bar{B}(F) + F \frac{d\bar{B}}{dF} \quad (7)$$

$$\frac{d\bar{B}}{dF} = -\frac{K}{r} \left(1 - \frac{F(\gamma - 1)}{r} \right)^{\frac{1}{\gamma-1}-1}. \quad (8)$$

Setting Eq (7) equal to 0, substituting $\bar{B}(F)$ and $\frac{d\bar{B}}{dF}$ by Equations (5) and (8) respectively, and solving for F produces the following expression for the fishing rate required to produce MSY,

$$F^* = \frac{r}{\gamma} \quad (9)$$

Plugging the above expression for F^* back into Eq (5) gives the following expression for biomass at MSY,

$$B^* = K \left(\frac{1}{\gamma} \right)^{\frac{1}{\gamma-1}}. \quad (10)$$

The above derived expressions for $\bar{B}(0)$, B^* , and F^* can then be used to build a specific analytical form for the biological reference points in terms of only productivity parameters.

$$F^* = \frac{r}{\gamma} \quad \frac{B^*}{\bar{B}(0)} = \left(\frac{1}{\gamma} \right)^{\frac{1}{\gamma-1}} \quad (11)$$

103 2.1.2 Simulation

Generating simulated indices of abundance from the PT model requires inverting the relationship between $\left(F^*, \frac{B^*}{\bar{B}(0)}\right)$, and (r, γ) . It is not generally possible to analytically invert this relationship for many three parameter production functions (Punt & Cope, 2019; J. T. Schnute & Richards, 1998). Most three parameter production functions lead to RPs that require expensive numerical methods to invert; more over the numerical inversion procedure can often be unstable. That said, for the case of PT this relationship is analytically invertible, and leads to the following relationship

$$r = \gamma F^* \quad \gamma = \frac{W \left(\frac{B^*}{\bar{B}(0)} \log \left(\frac{B^*}{\bar{B}(0)} \right) \right)}{\log \left(\frac{B^*}{\bar{B}(0)} \right)}. \quad (12)$$

104 Above W is the Lambert product logarithm function. More details about this derivation,
105 and the Lambert product logarithm, are given in Appendix (4).

106 Using Eq. (12) to obtain production parameters, a PT production model can be fully

defined for any combination of the RPs F^* and $\frac{B^*}{B(0)}$. Since K does not enter the RP calculation its value is fixed arbitrarily at 10000.

Indices of abundance are simulated from the three parameter PT production model broadly over the space of F^* and $\frac{B^*}{B(0)}$ via a space filling design as described in Section (2.3). A small amount of residual variation, $\sigma = 0.01$, is added to the simulated index, and these data are then fit with a Schaefer model, at various degrees of misspecification, so as to observe the effect of productivity model misspecification upon RP inference.

2.2 Schnute Model

The Schnute production function is a three parameter generalization of many of the most common two parameter production functions (Deriso, 1980; J. Schnute, 1985). It can be written in the following form, with parameters α , β , and γ ,

$$P_s(B; [\alpha, \beta, \gamma]) = \alpha B(1 - \beta\gamma B)^{\frac{1}{\gamma}}. \quad (13)$$

The BH and Logistic production functions arise when γ is fixed to -1 or 1 respectively, and the Ricker model is a limiting case as $\gamma \rightarrow 0$.

The behavior of RP inference under the BH model is of particular interest due to the overwhelming popularity of the BH assumption in fisheries models. Since Schnute production models can represent a quantifiably wide variety of possible productivity behaviors, they present an ideal simulation environment for inquiry of the reliability of inference under the BH assumption.

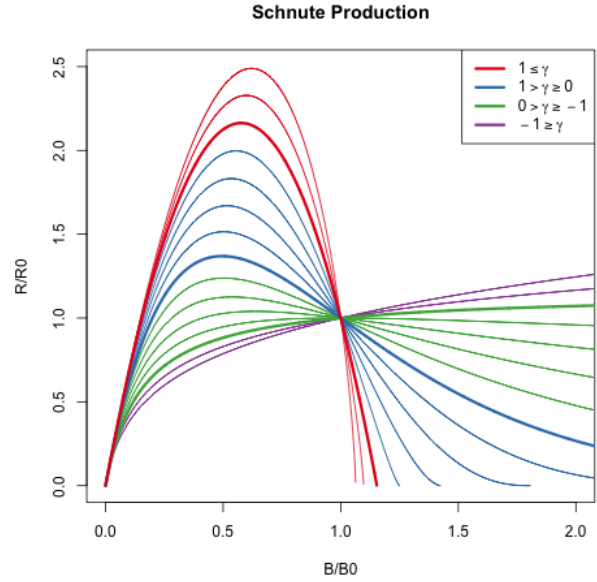


Figure 3: The Schnute production function plotted across a variety of parameter values. The special cases of BH, Ricker, and Logistic production are shown in green, blue, and red respectively.

Under Schnute production, biomass dynamics evolve according to the following ODE,

$$\frac{dB}{dt} = P_s(B; \theta) - (M + F)B. \quad (14)$$

125 This equation largely takes the same form as previously described, except that P_s is the
 126 Schnute production function and natural mortality, M , is modeled explicitly here. Natural
 127 mortality models the instantaneous rate of mortality from all causes outside of fishing. Ex-
 128 plicitly modeling natural mortality is not only a typical assumption of fisheries models, but
 129 is also key to the making RPs well defined over the relevant domain of γ .

The derivation of RPs under Eq. (14) follows a similar logic as under the PT model. An expression for equilibrium biomass is attained by setting $\frac{dB}{dt} = 0$ and rearranging the resulting expression to solve for B

$$\bar{B}(F) = \frac{1}{\gamma\beta} \left(1 - \left(\frac{M + F}{\alpha} \right)^\gamma \right). \quad (15)$$

The above expression quickly yields B_0 , B_{MSY} by evaluation at $F = 0$ and $F = F_{MSY}$ respectively,

$$B_0 = \frac{1}{\gamma\beta} \left(1 - \left(\frac{M}{\alpha} \right)^\gamma \right) \quad (16)$$

$$\frac{B_{MSY}}{B_0} = \frac{1 - \left(\frac{M + F_{MSY}}{\alpha} \right)^\gamma}{1 - \left(\frac{M}{\alpha} \right)^\gamma}. \quad (17)$$

Attaining an expression for F_{MSY} requires maximization of equilibrium yield, $\bar{Y} = F\bar{B}(F)$, with respect to F . Analytically maximizing proceeds by differentiating \bar{Y} to produce

$$\frac{d\bar{Y}}{dF} = \bar{B}(F) + F \frac{d\bar{B}}{dF} \quad (18)$$

$$\frac{d\bar{B}}{dF} = -\frac{1}{\beta} \left(\frac{\left(\frac{M+F}{\alpha} \right)^\gamma}{F + M} \right). \quad (19)$$

Setting $\frac{d\bar{Y}}{dF} = 0$, filling in the expressions for $\bar{B}(F)$ and $\frac{d\bar{B}}{dF}$, then rearranging to solve for F_{MSY} is less yielding here than it was in the case of the PT model. This procedure falls short of providing an analytical solution for F_{MSY} directly in terms of θ , but rather shows

that F_{MSY} must respect the following expression,

$$0 = \frac{1}{\gamma} - \left(\frac{1}{\gamma} + \frac{F_{MSY}}{F_{MSY} + M} \right) \left(\frac{F_{MSY} + M}{\alpha} \right)^\gamma. \quad (20)$$

The lack of an analytical solution here is understood. [J. T. Schnute and Richards \(1998, pg. 519\)](#) specifically points out that F_{MSY} cannot be expressed analytically in terms of productivity parameters, but rather gives a partial analytical expression for the inverse relationship. Although parameterized slightly differently, [J. T. Schnute and Richards \(1998\)](#) derives expressions for α and β as a function of RPs and γ .

Since RPs are left without a closed form expression, computing RPs from productivity parameters amounts to numerically solving the system formed by collecting the expressions (20), (16), and (17).

2.2.1 Simulation

For the purposed of simulation, it is not necessary to completely know the precise relationships mapping RPs $\mapsto \theta$ or $\theta \mapsto$ RPs. Simulation only requires enough knowledge of these mappings to gather a list of (α, β, γ) tuples, for data generation under the Schnute model, and the corresponding RPs in some reasonable space-filling design over RP space.

Similarly to [J. T. Schnute and Richards \(1998\)](#), expressions (20) and (16) are solved for α and β respectively. This leads to the partial mapping $(F_{MSY}, B_0) \mapsto (\alpha(\cdot, \gamma), \beta(\cdot, \cdot, \gamma))$ in terms of RPs and γ . By further working with Eq. (17), to identify γ , the following system is obtained,

$$\begin{aligned} \alpha &= (M + F_{MSY}) \left(1 + \frac{\gamma F_{MSY}}{M + F_{MSY}} \right)^{1/\gamma} \\ \beta &= \frac{1}{\gamma B_0} \left(1 - \left(\frac{M}{\alpha} \right)^\gamma \right) \\ \frac{B_{MSY}}{B_0} &= \frac{1 - \left(\frac{M + F_{MSY}}{\alpha} \right)^\gamma}{1 - \left(\frac{M}{\alpha} \right)^\gamma}. \end{aligned} \quad (21)$$

For a population experiencing natural mortality M , by fixing F_{MSY} , B_0 , and $\frac{B_{MSY}}{B_0}$ the above system can fully specify α and β for a given γ . Notice for a given γ a cascade of closed form solutions for α and β can be obtained. First $\alpha(\gamma)$ can be computed, and then

$\beta(\alpha(\gamma), \gamma)$ can be computed. If $\alpha(\gamma)$ is filled back into the expression for $\frac{B_{MSY}}{B_0}$, the system collapses into a single onerous expression for $\frac{B_{MSY}}{B_0}(\alpha(\gamma), \gamma)$. For brevity, define the function $\zeta(\gamma) = \frac{B_{MSY}}{B_0}(\alpha(\gamma), \gamma, F_{MSY}, M)$ based on Eq. (17).

Inverting $\zeta(\gamma)$ for γ , and computing the cascade of $\alpha(\gamma)$, and then $\beta(\alpha(\gamma), \gamma)$, fully defines the Schnute model for a given $(\frac{F_{MSY}}{M}, \frac{B_{MSY}}{B_0})$. However inverting ζ accurately is extremely difficult. Inverting ζ analytically is not feasible, and numerical methods for inverting ζ are unstable and can be computationally expensive. Rather than numerically invert precise values of $\zeta(\gamma)$, γ is sampled so that the overall simulation design is space filling as described in Section (2.3.2).

Each design location defines a complete Schnute production model with the given RP values. Indices of abundance are simulated from the Schnute model at each design location, a small amount of residual variation, $\sigma = 0.01$, is added to the simulated index, and the data are then fit with a misspecified BH production model. The design at large captures various degrees of model misspecification relative to the BH model, so as to observe the effect of productivity model misspecification upon RP inference.

2.3 Latin Hypercube Sampling

- a quick lit review of space filling designs

A Latin hypercube sample (LHS) of size n , in the 2 dimensional space defined by RPs, distributes samples so as to spread points across a design region in a broadly representative way. A LHS design extends the notion of a univariate random uniform sample across multiple dimensions so that each margin of the design space enjoys a uniform distribution.

LHS designs achieve this notion of uniformity by first partitioning each dimension of the design space into regular grids of size

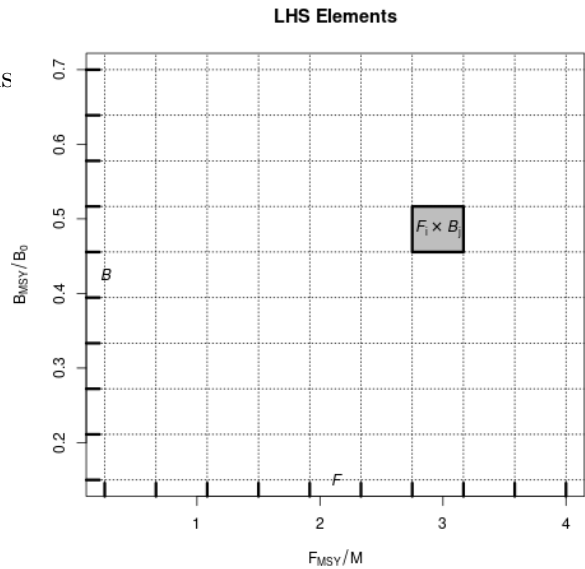


Figure 4: LHS grids. Intersecting \mathcal{F} and \mathcal{B} produces n^2 cells; a particular cell $\mathcal{F}_i \times \mathcal{B}_j$ is shown in grey. *Maybe just show points.*

n . By intersecting the grids of each dimension, cells are produced that evenly partition the design space. In two dimensions n^2 cells are produced, from which a total of n samples are taken. Crucially only one sample is taken from a given element of each grid in each dimension so as to reduce clumping of the n samples across the design space.

2.3.1 PT Design

Letting \mathcal{F} and \mathcal{B} be regular grids, of size $n = 100$, on $F_{MSY} \in (0.1, 0.7)$ and $\frac{B_{MSY}}{B_0} \in (0.2, 0.6)$ respectively, a LHS design of size 100 is collected among the cells produced by $\mathcal{F} \times \mathcal{B}$.

Each of the sampled LHS design locations represent a unique PT model with the sampled RP values. Since the relationship mapping RPs analytically to productivity parameters can be found for the PT model, LHS designs the the PT model are computed directly in RP space and Eq. (12) is used to map the sampled RP design locations to PT productivity parameters.

2.3.2 Schnute Design

Due to the lack of an analytical relationship mapping RPs $\mapsto \theta$, analogous to the PT model's Eq. (12), producing a LHS design over Schnute RPs requires a more tactful approach. The structured relationship between the RPs and productivity parameters, described in Section (2.2.1), allows an approximate LHS to be obtained by a careful navigation of the system of equations seen in Eq. (21).

Under the Schnute model, let \mathcal{F} and \mathcal{B} represent regular grids on $\frac{F_{MSY}}{M} \in (0.25, 4)$ and $\frac{B_{MSY}}{B_0} \in (0.15, 0.7)$ respectively which can serve as the scaffolding for computing an approximate LHS

Given B_0 , M , and F_{MSY} :

- 1) Draw $\gamma^* \sim \gamma | F_{MSY}, M$.
- 2) Compute $\frac{B_{MSY}}{B_0} = \zeta(\gamma^*)$
- 3) Compute $\alpha^* = \alpha(\gamma^*, F_{MSY}, M)$
- 4) Compute $\beta^* = \beta(\alpha^*, \gamma^*, M, B_0)$

Since it is not practical to invert $\zeta(\gamma)$, a uniform sample in $\frac{B_{MSY}}{B_0}$ can be obtained by modeling γ as a random variable, with realization γ^* , and thinking of $\zeta(\gamma)$ as its cumulative distribution function (CDF). The aim is to model γ as an easily sampled random

Figure 5: An outline of the sampling procedure for γ given B_0 , M , and F_{MSY} .

variable with a CDF that closely approximates ζ , so that $\zeta(\gamma^*) \sim U(\zeta_{min}, 1)$ as closely as possible. There may be many good models for the distribution of γ , but in this setting the following distribution is very effective,

$$\gamma \sim \zeta_{min} \delta(\gamma_{min}) + t(\mu, \sigma, \nu) \mathbf{1}_{\gamma > \gamma_{min}}. \quad (22)$$

Above, t is the density of the three parameter location-scale family Student's t distribution with location μ , scale σ , and degrees of freedom ν . $\mathbf{1}_{\gamma > \gamma_{min}}$ is an indicator function that serves to truncate Student's t distribution at the lower bound γ_{min} . $\delta(\gamma_{min})$ is the Dirac delta function evaluated at γ_{min} , which is scaled by the known value ζ_{min} ; this places probability mass ζ_{min} at the point γ_{min} . Since sampling from Student's t distribution is readily doable, sampling from a truncated Student's t mixture only requires slight modification.

Let T be the CDF of the modeled distribution of γ . Since the point $(\gamma_{min}, \zeta_{min})$ is known from the dynamics of the Schnute model at a given RP, full specification of Eq. (22) only requires determining the values for μ , σ , and ν which make T best approximate $\zeta(\gamma)$. Thus, the values of μ , σ , and ν are chosen by minimizing the L^2 distance between $T(\gamma)$ and $\zeta(\gamma)$.

$$[\hat{\mu}, \hat{\sigma}, \hat{\nu}] = \arg \min_{[\mu, \sigma, \nu]} \int_{\Gamma} (T(\gamma; \mu, \sigma, \nu) - \zeta(\gamma))^2 d\gamma \quad (23)$$

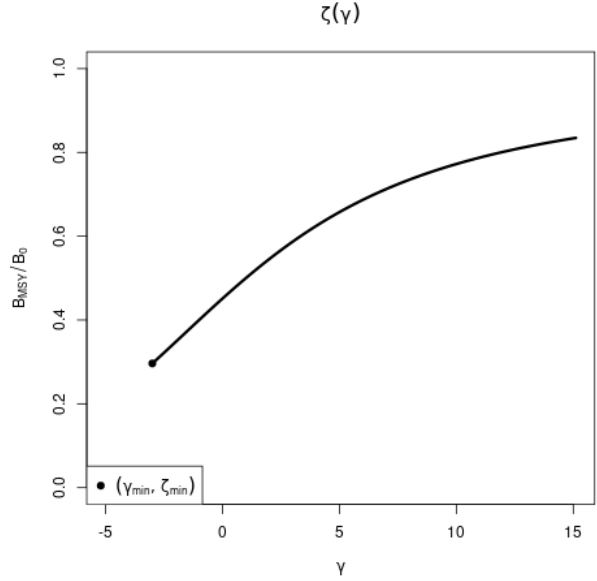


Figure 6: $\zeta(\gamma)$ Plotted for $F_{MSY} = 0.1$ and $M = 0.2$. The point $(\gamma_{min}, \zeta_{min})$ shows the lowest biologically meaningful value of γ ; below which productivity is negative.

211 Fitting the distribution $T(\gamma|\hat{\mu}, \hat{\sigma}, \hat{\nu})$ for
 212 use generating γ^* values at a specific F_{MSY}
 213 and M releases the need to invert ζ .
 214 $T(\gamma|\hat{\mu}, \hat{\sigma}, \hat{\nu})$, together with the structure in
 215 Eq. (21), allows for the collection of an
 216 approximate LHS sample via the algorithm
 217 seen in Algorithm (1).
 218 $\frac{F_{MSY}}{M}$ is drawn uniformly from \mathcal{F}_i . Con-
 219 ditioning on the sample of F_{MSY} , and M ,
 220 $T(\gamma|\hat{\mu}, \hat{\sigma}, \hat{\nu})$ is fit and γ^* is sampled. ζ^* is
 221 then computed and placed into the appropri-
 222 ate grid element \mathcal{B}_j . Given γ^* , the cascade
 223 $\alpha(\gamma^*)$, and $\beta(\alpha(\gamma^*), \gamma^*)$, can be computed.
 224 The algorithm continues until all of the de-
 225 sign elements, $(\frac{F_{MSY}}{M}, \zeta^*) \Leftrightarrow (\alpha^*, \beta^*, \gamma^*)$,
 226 have been computed for all $i \in [1, \dots, n]$.

Algorithm 1 LHS of size n on rectangle R .

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1: procedure  $LHS_n(R)$ 
2:   Define  $n$ -grids  $\mathcal{F}, \mathcal{B} \in R$ 
3:   for each grid element  $i$  do
4:     Draw  $\frac{F_{MSY}}{M} \sim Unif(\mathcal{F}_i)$ 
5:     Compute  $[\hat{\mu}, \hat{\sigma}, \hat{\nu}]$  given  $F_{MSY}$  &  $M$ 
6:     while  $\mathcal{B}_j$  not sampled do
7:       Draw  $\gamma^* \sim T(\gamma|\hat{\mu}, \hat{\sigma}, \hat{\nu})$ 
8:       Compute  $\zeta^* = \zeta(\gamma^*)$ 
9:       Compute  $j$  such that  $\zeta^* \in \mathcal{B}_j$ 
10:    end while
11:    Compute  $\alpha^* = \alpha(\gamma^*, F_{MSY}, M)$ 
12:    Compute  $\beta^* = \beta(\alpha^*, \gamma^*, M, B_0)$ 
13:    Save  $(\frac{F_{MSY}}{M}, \zeta^*) \Leftrightarrow (\alpha^*, \beta^*, \gamma^*)$  in  $\mathcal{F}_i \times \mathcal{B}_j$ 
14:  end for
15: end procedure

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227 2.3.3 Design Refinement

228 Since the behavior of RP inference, under misspecified models, will vary in yet-unknown
 229 ways, the exact sampling design density may be hard to know a priori. Several factors,
 230 including the particular level of observation uncertainty, high variance (i.e. hard to resolve)
 231 features of the response surface, or simply "gappy" instantiations of the initial LHS design
 232 may necessitate adaptive design refinement, to accurately describe RP biases. Given the
 233 temperamental relationship between RPs and productivity parameters in the Schnute model,
 234 a recursive refinement algorithm, that makes use of the previously described LHS routine, is
 235 developed.

Holes in the existing design are identified based on maximin design principles. New design
 points are collected based on areas of the RP design space which maximizes the minimum dis-

tance between all pairs of points in the current design, based on the following distance function

$$d(\mathbf{x}, \mathbf{x}') = \sqrt{(\mathbf{x} - \mathbf{x}')^T \mathbf{D}^{-1} (\mathbf{x} - \mathbf{x}')} \quad (24)$$

$$\mathbf{D} = \mathbf{diag} \left[\left(\max(\mathcal{F}) - \min(\mathcal{F}) \right)^2, \left(\max(\mathcal{B}) - \min(\mathcal{B}) \right)^2 \right].$$

Above, d is a scaled distance function that defines the distance between points in the differing scales of $\frac{B_{MSY}}{B_0}$ and $\frac{F_{MSY}}{M}$. \mathbf{D} is a diagonal matrix that measures the squared size of the domain in each axis of so as to normalize distances to a common scale.

If \mathbf{X}_n is the initial design, computed on R_{full} , let \mathbf{x}_a be the augmenting point which maximizes the minimum distance between all of the existing design points,

$$\mathbf{x}_a = \underset{\mathbf{x}'}{\operatorname{argmax}} \min \{ d(\mathbf{x}_i, \mathbf{x}') : i = 1, \dots, n \}. \quad (25)$$

The point \mathbf{x}_a is used as an anchor for augmenting \mathbf{X}_n . An additional $LHS_{n'}$ (via Algorithm (1)) is collected, adding n' design points, centered around \mathbf{x}_a , to the overall design. The augmenting region, $R_{(x_a, d_a)}$, for collecting $LHS_{n'}$ is defined based on the square centered at \mathbf{x}_a with side length $2d_a$, where $d_a = \min \{ d(\mathbf{x}_i, \mathbf{x}_a) : i = 1, \dots, n \}$, in the space defined by the metric d .

Due to the tendency of maximin sampling to cluster augmenting points on the edges of the design space, $R_{(x_a, d_a)}$ is truncated by the outer most limits of R_{full} so as to focus design augmentation within the specified domain of the simulation. Furthermore, since the design space has a nonlinear constraint at low values of $\frac{B_{MSY}}{B_0}$, the calculation of x_a is further truncated based on a convex hull defined by the existing samples in the overall design.

Design refinement then proceeds as follows. An initial design is computed, $X_n = LHS_n(R_{full})$, based on an overall simulated region of RPs R_{full} . The maximin augmenting point, x_a , is computed at a maximin distance of d_a from the existing samples. An augmenting design $X_{n'} = LHS_{n'}(R_{(x_a, d_a)})$ is collected and added to X_n . Design refinement carries on recursively collecting augmenting designs in this way until the desired maximin distance falls below the desired level.

START HERE

2.4 Gaussian Process Metamodel

Each design location of the simulation results in an MLE of each of the productivity parameters under the restricted two parameter production model (i.e. Schaefer: $[\log(r), \log(K)]$, BH: $[\log(\alpha), \log(\beta)]$). Letting \mathbf{y} be a vector collecting the fitted log productivity parameter MLEs under the restricted model, and further letting $\boldsymbol{\omega}$ be a vector of the MLE standard error estimates, on the variance scale (via the inverted Fisher information of the production model log likelihood). The simulation produces the following mapping of

$$\mathbf{X} \mapsto \mathbf{y} \pm \boldsymbol{\omega} \quad (26)$$

For assessing the productivity parameters over the full region of simulated RPs a GP model is used as a flexible metamodel for describing the overall behavior of inference under misspecified two parameter productivity models.

A GP is a stochastic process generalizing the multivariate normal distribution to an infinite dimensional analog. GPs are often specified primarily through the choice of a covariance (or correlation) function which defines the relationship between locations in an index set. Typically the index set is spatial for GPs, with points closely related in the index set resulting in correlated effects in the model. In this setting the model is over the space of reference points. A GP model implies an n dimensional multivariate normal distribution on the observations of the model with a correlated error structure defined by the modeled covariance function.

For assessing the productivity parameters over the full region of simulated RPs a GP model is used as a flexible metamodel for describing the overall behavior of inference under misspecified two parameter productivity models. Each design location of the simulation produces an estimate of each of the productivity parameters under the restricted two parameter production model (i.e. Schaefer: $(\log(r), \log(K))$, BH: $(\log(\alpha), \log(\beta))$).

$$\mathbf{X} \mapsto \mathbf{y} \pm \boldsymbol{\omega} \quad (27)$$

Each of the fitted productivity parameter estimates are then modeled using independent

instances of the following model in Eq (28).

Let \mathbf{y} be a vector collecting the fitted log productivity parameter MLEs under the restricted two parameter production models. Furthermore, let $\boldsymbol{\omega}$ be a vector of the MLE standard error estimates, on the variance scale (via the inverted Fisher information of the production model log likelihood). \mathbf{X} is the $n \times 2$ LHS design matrix of RPs derived above for each respective three parameter data generating model.

$$\begin{aligned}\mathbf{y} &= \beta_0 + \mathbf{X}\boldsymbol{\beta} + \mathbf{v} + \boldsymbol{\epsilon} \\ \mathbf{v} &\sim N_n(\mathbf{0}, \tau^2 \mathbf{R}_\ell) \\ \boldsymbol{\epsilon} &\sim N_n(\mathbf{0}, \boldsymbol{\omega}' \mathbf{I})\end{aligned}\tag{28}$$

ϵ models independent normally distributed error, which provides an ideal mechanism for propagating uncertainty from inference in the simulation step into the metamodel. By matching each y_i with an observed ω_i variance term, ϵ serves to down weight the influence of each y_i in proportion to the inferred production model sampling distribution uncertainty. This has the effect of smoothing the GP model in a way similar to the nugget effect (Gramacy & Lee, 2012), although the application here models this effect heterogeneously.

The term, \mathbf{v} , contains spatially correlated GP effects. The correlation matrix, \mathbf{R}_ℓ describes how RPs closer in the simulation design are more correlated. This spatial effect is modeled with a squared exponential correlation function,

$$R(\mathbf{x}, \tilde{\mathbf{x}}) = \exp \left(\sum_{i=1}^2 \frac{-(x_i - \tilde{x}_i)^2}{2\ell_j^2} \right).\tag{29}$$

R has an anisotropic separable form which allows for differing length scales, ℓ_1 and ℓ_2 , in the different RP axes. The flexibility to model correlations separately in the different RP axes is key due to the differences in the extent of the RP domains marginally. The metamodel parameters β_0 , $\boldsymbol{\beta}$, τ^2 , ℓ_1 and ℓ_2 are fit via MLE against the observations \mathbf{y} , \mathbf{X} , and $\boldsymbol{\omega}$ from simulation fits.

Predictive estimates are obtained via kriging (cite).

$$\hat{y}(\mathbf{x}) = \beta_0 + \mathbf{x}\boldsymbol{\beta} + \mathbf{r}(\mathbf{x})'\mathbf{R}_\ell^{-1}\left(\mathbf{y} - (\beta_0 + \mathbf{X}\boldsymbol{\beta})\right) \quad (30)$$

$\hat{y}(\mathbf{x})$ is a predicted value of the metamodel at the RP location \mathbf{x} . $\mathbf{r}(\mathbf{x})$ is defined as the vector of correlation function evaluations for the predictive location \mathbf{x} against all observations in \mathbf{X} (i.e. $\mathbf{r}(\mathbf{x}) = \mathbf{R}(\mathbf{x}, \mathbf{x}_i) \forall \mathbf{x}_i \in \mathbf{X}$).

Maybe a bit of hinting at uses.

2.5 Catch

It is known that the behavior of catch can effect inference on the productivity parameters (Hilborn & Walters, 1992). In this setting contrast refers to changes in the long term trends of index data. Figure (7, right) demonstrates an example of biomass that includes contrast induced by catch. It is not well understood how contrast may factor into inferential failure induced by model misspecification. A variety of catches are investigated.

Catch is parameterized so that $F(t)$ can be controlled with respect to F^* . Recall that catch is assumed to be proportional to biomass, so that $C(t) = F(t)B(t)$. To control $F(t)$ with respect to F^* , $C(t)$ is specified by defining the quantity $\frac{F(t)}{F^*}$ as the relative fishing rate. $B(t)$ is defined by the solution of the ODE, and F^* is defined by the biological parameters of the model, see Eq (??). By defining $\frac{F(t)}{F^*}$, catch can then be written as $C(t) = F^* \left(\frac{F(t)}{F^*} \right) B(t)$.

Intuitively $\frac{F(t)}{F^*}$ describes the fraction of F^* that $F(t)$ is specified to for the current $B(t)$. When $\frac{F(t)}{F^*} = 1$, $F(t)$ will be held at F^* , and the solution of the ODE brings $B(t)$ into equilibrium at B^* . For constant $\frac{F(t)}{F^*}$ biomass comes to equilibrium as an exponential decay from K approaching B^* . When $\frac{F(t)}{F^*} < 1$, $F(t)$ is lower than F^* and $B(t)$ is pushed toward $\bar{B} > B^*$. Contrarily, when $\frac{F(t)}{F^*} > 1$, $F(t)$ is higher than F^* and $B(t)$ is pushed toward $\bar{B} < B^*$; the precise values of \bar{B} can be calculated from Eq (15).

In practice, catch is determined by a series of observed, assumed known, catches. Catch observations are typically observed on a quarterly (or yearly) basis, so that the ODE may be discretized via Euler's method with integration step sizes to match the observation frequency of the modeled data. In this case, catch is sampled as would be done in practice however,

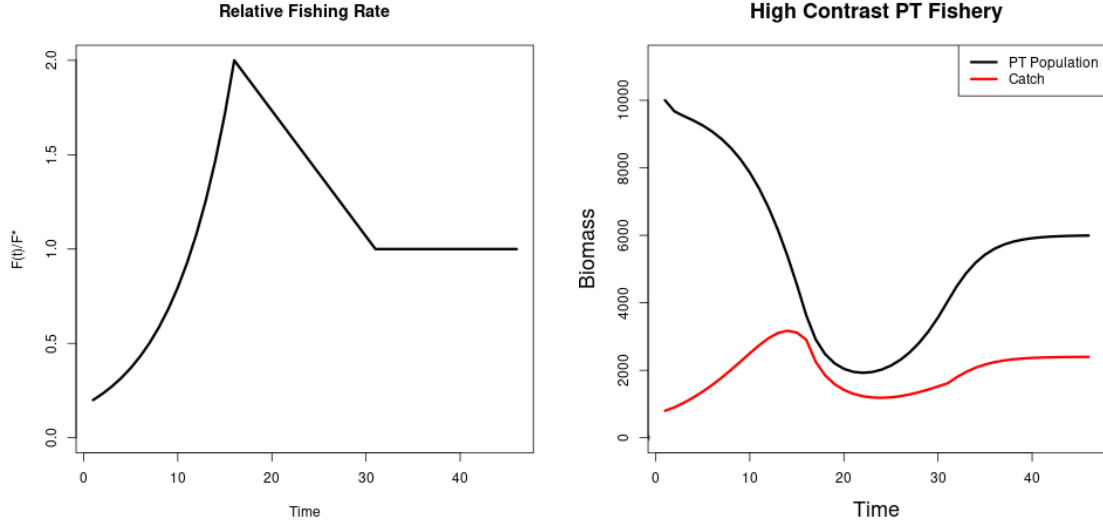


Figure 7: (left) Relative fishing specified so as to induce contrast. (right) Population biomass and catch demonstrating contrast in a **PT population** with $F^* = 0.4$ and $\frac{B^*}{B(0)} = 0.6$.

the simulation can encounter a variety of issues working with the naively discretized ODE. As a result the ODE is integrated implicitly via the Livermore Solver (Radhakrishnan, 1993, lsode), and catch is linearly interpolated between sampled epochs.

- ?quantification of degrees of information? (avg curvature?)
- remake picture w/o PT references

2.6 Continuous model formulation

a preface to regularity issues: identifiability, stiffness, and continuity.

An important (and often overlooked) implementation detail is the solution to the ODE which defines the progression of biomass through time (See Eq(2)). As a statistical model it is of paramount importance that this ODE not only have a solution, but also that the solution be unique. Of primary concern, uniqueness of the ODE solution is necessary for the identifiability of the statistical model.

If the form of $\frac{dB}{dt}$ is at least Lipschitz continuous, then the Cauchy-Lipschitz-Picard theorem provides local existence and uniqueness of $B(t)$. Recall from Eq(2) that $\frac{dB}{dt}$ is separated into a term for recruitment into the population, $R(B)$, and a term for removals via catch, C .

For determining Lipschitz continuity of $\frac{dB}{dt}$, the smallest Lipschitz constant of $\frac{dB}{dt}$ will be the sum of the constants for each of the terms $R(B)$ and C separately. Typically any choice of $R(B)$ will be continuously differentiable, which implies Lipschitz continuity (since the set of continuous differentiable functions is a subset of the set of Lipschitz continuous functions). Thus, the assumed form of $R(B)$ does not typically introduce continuity concerns, unlike some potential assumptions for C .

In practice C is determined by a series of observed, assumed known, catches. Catch observations are typically observed on a quarterly basis, but in practice may not be complete for every quarter of the modeled period. It is overwhelmingly common to discretize the ODE via Euler's method with integration step sizes to match the observation frequency of the modeled data. This is often convenient but can present several issues. This strategy often pushes the assumption of catch continuity under the rug, but for identifiability of the statistical model an implicit assumption of continuity of the catches is required. While mechanistically at the finest scale fishers must only catch discrete packets of biomass (i.e. individual fish), it is sensible to consider catches at the quarterly (or yearly) scale as accruing in a continuous way. Furthermore any assumption of continuity will be required to be at least Lipschitz continuous for the required regularity of the model.

Here I assume catches accrue linearly between observed catches. This assumption defines the catch function as a piecewise linear function of time, with the smallest Lipschitz constant for the catch term defined by the steepest segment of the catch function. This assumption represents one of the simplest ways of handling catch, while retaining Lipschitz continuity overall. Furthermore linearly interpolated catch is adequately parsimonious for the typical handling of catches.

2 .6.1 Integration and Stiffness

As previously mentioned, the overwhelming majority of implementations of population dynamics models discretize the ODE using Euler's method with the integration step sized fixed so as to match the observation frequency. In this setting we explore model parameterizations that explore the full extent of biologically relevant reference points. This exercise produces some combinations of parameters that result in numerically stiff ODEs.

The concept of stiffness in ODEs is hard to precisely characterize (cite). Hairer and Wanner [5, p. 2] describe stiffness in the following pragmatic sense, "Stiff equations are problems for which explicit methods don't work". It is hard to make this definition more mathematically precise, but this is without a doubt a consistent issue for models parameterized so that ζ is greater than about $\frac{1}{2}$. Euler's method, as often implemented, is particularly poorly suited for these stiff regions of parameter space. In these stiff regions it is necessary to integrate the ODE with an implicate integration method.

Several of the most common implicate methods were tried including the Livermore Solver for ODEs (lsode), and the Variable Coefficient ODE Solver (vode) as implemented in the deSolve package of R (cite). The difference between implicate solvers is negligible, while most explicit methods result in wildly varying solutions to the ODE, and in still regions of parameter space explicate methods completely fail to represent the model as stated in the stiff regions of parameter space. Results shown here are computed using the lsode integration method since it runs relatively quickly and has a relatively smaller footprint in system memory.

3 Results

While metamodeling occurs on the inferred productivity parameters of the restricted production model, the metamodel can also be used to build metamodeled estimates of major biological RPs. The relevant transformations are given Eqs. (11, 17, 20) with γ fixed to the restricting case.

Applying the metamodel predictive surfaces to the RP estimate allows for the quantification of RP bias induced by model misspecification of two parameter production functions. Below RP bias is quantified by the following relative measure of bias, similar to a percent error calculation.

$$\text{Relative Bias} = \frac{\hat{RP} - RP}{RP} \quad (31)$$

Above RP is a stand in for the the true value of any of the biological reference points under the three parameter data generating production model, and \hat{RP} refers to the metamodel

estimate of each RP quantity under the two parameter restricted cases.

3.1 PT/Schaefer

region of chaotic fits due to model misspecification

- RP break out plots with mechanism of failure

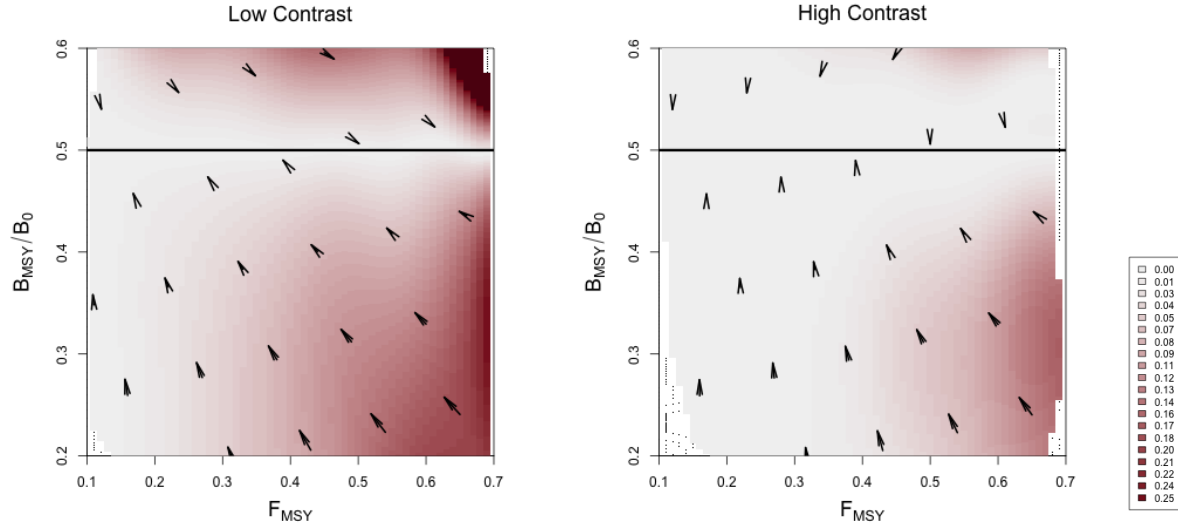


Figure 8: Joint bias direction for $(F_{MSY}, \frac{B_{MSY}}{B_0})$ estimates under the misspecified Schaefer Model. The intensity of color represents the excess bias relative to the shortest possible mapping.

- Mechanism plot on SRR LHS Grid plot
- some detail views in B_{MSY} , B_0 , F_{MSY} , $?F_{SPR?}$, MSY

Figure (9) shows four of the most misspecified example production function fits as compared to the true data generating PT production functions. In the rug plots below each set of curves the observed biomasses demonstrate the exponential decay from K to B^* in each case. In particular, notice how only biomasses greater than the PT B^* are observed.

Due to the leaning of the true PT curves, and the symmetry of the logistic parabola, the logistic curve only observes information about its slope at the origin from data observed on the right portion of the PT curves. Above the Schaefer line PT is steeper on the right of B^* than it is on the left, and so the logistic curve over-estimates r , and thus F^* , for data generated above the Schaefer line. Below the Schaefer line the vice versa phenomena occurs. Below the Schaefer line PT is shallower to the right of B^* than it is on the left and so the logistic parabola estimate tends to under estimate F^* .

Figure (9) indicates that the individual biases of B^* and K may behave quite differently. B^* appears to be estimated fairly accurately while K does not.

Figure (??) also gives some examples of the relative behavior of B^* and K . In Figure (??) it is clear that the bias behavior of $\frac{B^*}{B(0)}$ is locked in a fixed pattern under the Schaefer model. Figure (??) indicates that the individual biases of B^* and K may behave quite differently. B^* appears to be estimated fairly accurately while K does not.

3.2 Schnute/BH

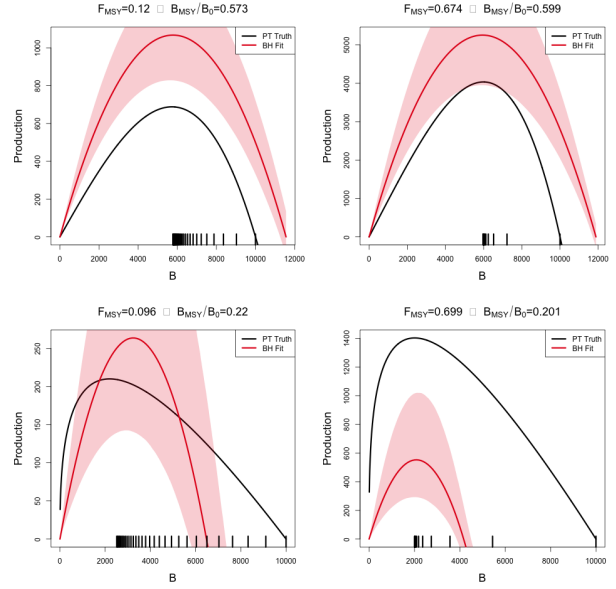


Figure 9: A comparison of the true PT production function (in black) and the estimated logistic curve (in red) with 95% CI shown. The examples shown represent the four corners of maximum model misspecification in the simulated RP-space. Observed biomasses are plotted in the rug plots below the curves.

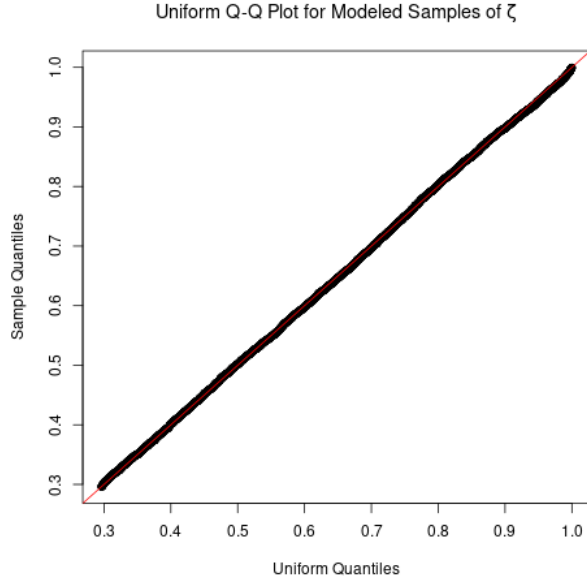


Figure 10: Uniform Q-Q plot for sampled ζ against theoretical uniform quantiles.

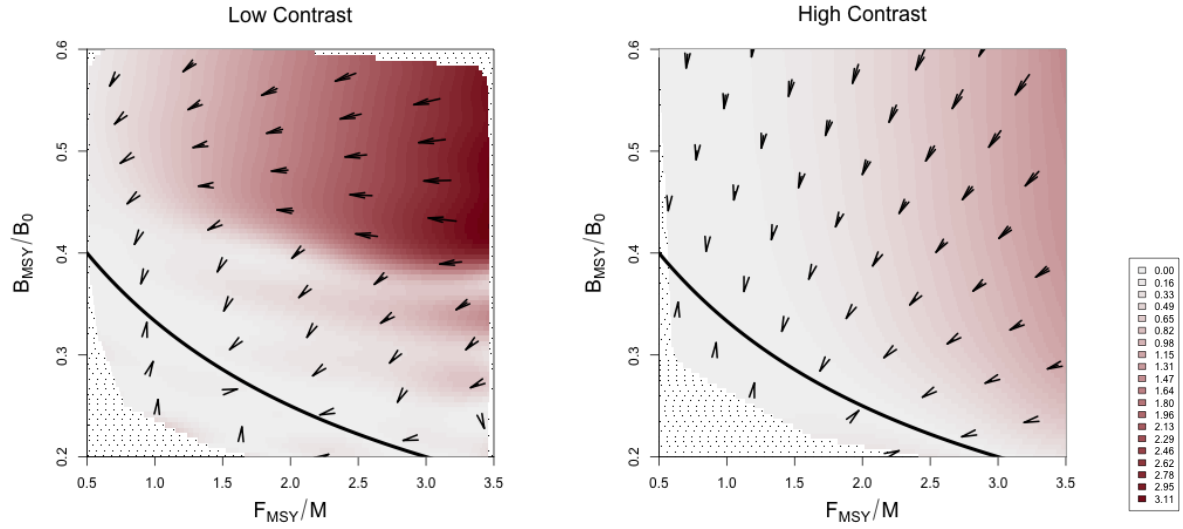


Figure 11: Joint bias direction for $(\frac{F_{MSY}}{M}, \frac{B_{MSY}}{B_0})$ estimates under the misspecified BH Model. The intensity of color represents the excess bias relative to the shortest possible mapping.

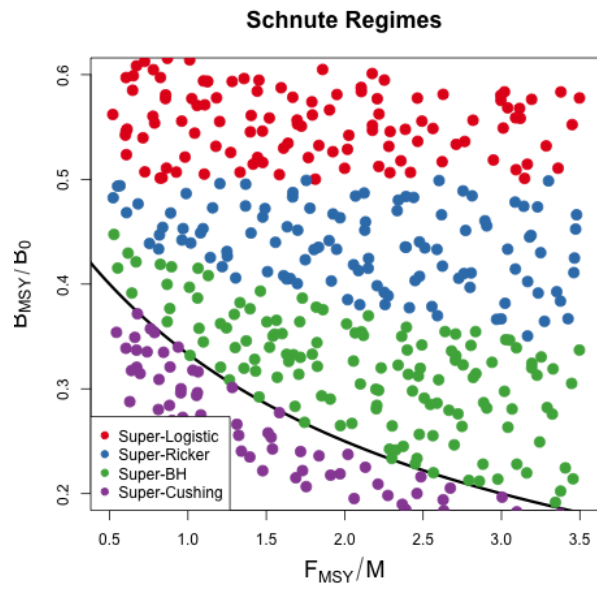


Figure 12: grid plot of production functions.)

4 Appendix: Inverting $\frac{B^*}{B(0)}$ and γ for the PT Model

For brevity let $\zeta = \frac{B^*}{B(0)}$.

$$\begin{aligned}\zeta &= \left(\frac{1}{\gamma}\right)^{\frac{1}{\gamma-1}} \\ \zeta &= \gamma \zeta^\gamma \\ \zeta &= \gamma e^{\gamma \log(\zeta)} \\ \zeta \log(\zeta) &= \gamma \log(\zeta) e^{\gamma \log(\zeta)}\end{aligned}$$

The Lambert product logarithm, W , is defined as the inverse function of $z = xe^x$ such that $x = W(z)$. Applying this definition allows for the isolation of γ .

$$\begin{aligned}\gamma \log(\zeta) &= W(\zeta \log(\zeta)) \\ \gamma &= \frac{W(\zeta \log(\zeta))}{\log(\zeta)}\end{aligned}\tag{32}$$

The Lambert product logarithm is a multivalued function with a branch point at $-\frac{1}{e}$. The principal branch, $W_0(z)$, is defined on $z \in (-\frac{1}{e}, \infty)$, and the lower branch, $W_{-1}(z)$, is defined on $z \in (-\frac{1}{e}, 0)$. Taken individually, each respective branch is analytic, but cannot be expressed in terms of elementary functions.

When $\zeta \in (0, \frac{1}{e})$ the solution of interest in Eq. (12) comes from W_0 . When $\zeta \rightarrow \frac{1}{e}$, the Fox Model emerges as $\gamma \rightarrow 1$. When $\zeta \in (\frac{1}{e}, 1)$ the solution of interest comes from W_{-1} . For the use case presented here, Eq. (12) is to be interpreted as,

$$\gamma = \begin{cases} \frac{W_0(\zeta \log(\zeta))}{\log(\zeta)} & \zeta \in (0, \frac{1}{e}) \\ \frac{W_{-1}(\zeta \log(\zeta))}{\log(\zeta)} & \zeta \in (\frac{1}{e}, 1) \end{cases}.\tag{33}$$

Prager 2002, Figure(2).

<https://math.stackexchange.com/questions/3004835/is-the-lambert-w-function-analytic-if-not-everywhere-then-on-what-set-is-it-analytic> <https://researchportal.bath.ac.uk/en/publications/algebraic-properties-of-the-lambert-w-function-from-a-result-of-r>

<https://cs.uwaterloo.ca/research/tr/1993/03/W.pdf>

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