Graphed-based Models for Data and Decision Making

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January 2014
Interim Report

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Graph-based Models for Data and Decision Making

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This effort is focused on developing and applying tools for modeling human information processing. Models include transformations of response time data from empirical studies, and complex network models for capturing broader dynamics of complex systems. Progress so far has resulted in some theoretical work in the area of response time modeling of workload capacity and dimer automata complex systems models of information transmission through a network. Additionally, new visual tools for pattern discovery and visual analytics are proposed based on topological data analysis theory. Several pieces of open source software have been developd for implementing these analyses and making them widely available.
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1. Summary

1.1 Systems Factorial Technology with R

A portion of the effort to date has been dedicated to the development of an open source implementation of systems factorial technology (SFT) measures and models within the R for statistical computing framework and language. SFT is one methodology utilized in this research for making inferences about human information processing mechanisms utilizing response time data. The first version of the package (sft 0.1) was released in 2012; we published a tutorial paper on utilizing SFT, its associated experimental methodology, the double factorial paradigm, and the basic functionality in the sft package (Houpt, J.W., Blaha, L.M., McIntire, J.P., Havig, P.R., & Townsend, J. T., 2013, Systems factorial technology with R. Behavior Research Methods [online publication doi 10.3758/s13428-013-0377-3]). Additional research efforts have both contributed new theory to the SFT framework, but have continued to increase the functionality of the sft toolbox to include new measures. The second major release of the sft package (version 1.0-1) was made in November 2012, accompanied by a presentation of the new functions at the 2013 Society for Computers in Psychology Meeting. A companion tutorial paper on the new functions is currently under review.


1.2 Models of Opinion Dynamics

Dimer automata models provide a framework for modeling information dynamics of complex systems represented as networks. Several simulation studies were run exploring the ability of two- and three-state dimer automata systems to capture opinion dynamics (also termed innovation diffusion) and influence maximization in different networks. Simulation experiments examined different networks structures, the influence of zealotry on the dynamics, and strategies for the placement of zealots in the network for maximum influence on the final opinion states. Initial experiments were presented at the 2013 Behavior Representation in Modeling and Simulation conference, and additional experiments were included in an article currently under review.


1.3 Generalized n-Channel Workload Capacity Space

Theoretical progress was made in the area of parallel models of response time by the formulation of generalized bounds on the capacity coefficient values predicted by standard parallel processes with \( n \geq 2 \) channels in the system. Previously, general n-channel bounds (upper and lower) on the range of cumulative distribution functions for standard parallel models had been defined for minimum time, single-target self-terminating maximum time stopping rules. Relatedly, capacity coefficient ratios had been defined for the same three stopping rules. Because the capacity coefficients are formulated by logarithmic transformations of the cumulative distribution functions, we can redefine the bounds to provide upper and lower limits on the capacity coefficient functions directly. These capacity space bounds were derived and proven in an article currently under review.


1.4 The Points to Pixels Pipeline (P2P²)

In order for patterns to be found in and for meaningful information to be extracted from high dimensional or complex network data, easy to use and manipulate visualization tools are needed for data exploration. We developed an open source framework for performing simplex clustering and visualizing data for visual analytics purposes. Data can be fed
into the pipeline framework as either the raw multivariate measures, a (dis)similarity matrix computed from that data, or as a graph of network-type data. From any of those formats, the appropriate transformations of the data are made and then a simplex is derived. The parameters governing the computations are easily manipulated by the user. And a set of easy visualizations are created by fitting a convex hull to each clique or cluster in the data and projecting that into lower dimensional space, augmented by color coding. By utilizing a set of free, open source (Python based) toolboxes, the P2P² framework is easily utilized by any researchers without need for specialized software or expensive licensing.


2. Manuscripts from the Current Effort

Included in the following pages are drafts of manuscripts based on the efforts described above. Each of these are embedded images from a pdf document that was typeset in LaTeX.
Latest Developments in Systems Factorial Technology with R

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Distribution A: Approved for public release; distribution unlimited.
88 ABW Cleared 02/13/2014; 88ABW-2014-0516.
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This work was supported by AFOSR grants FA9550-13-1-0087 to J.W.H. and LRIR 12RH14COR to L.M.B.

Distribution A: Approved for public release; distribution unlimited. 88ABW Cleared 01/17/2014; 88ABW-2014-0141.
Abstract

Systems factorial technology (SFT) is a powerful and mathematically rigorous framework for studying how cognitive systems make use of multiple sources of information. Articles about SFT tend to focus on the mathematics and development of the theory, making them inaccessible to many researchers. The sft package for R was recently introduced to facilitate the use of SFT by a wider range of researchers. The original package contained tools implementing only the basic theoretical tools. In the last few years, there have been a number of advances to SFT, which we will review, and we introduce their implementation in the sft package. In particular, we will demonstrate R functions for functional principal components analysis of the capacity coefficient (Burns, Houpt, Townsend, & Endres, 2013), calculating and plotting assessment functions (Townsend & Altieri, 2012), and calculating and plotting distributional bounds in a unified capacity space (Townsend & Eidels, 2011). Additionally, we expanded the package to include a function for the new capacity coefficient for single-target self-terminating (ST-ST) processing (Blaha, 2010), as well as functions supporting the plotting of cumulative distribution function bounds on the predictions of standard parallel processing models for minimum time, maximum time, and ST-ST decision rules.
Introduction

Systems Factorial Technology (SFT) is a framework for analyzing how multiple sources of information are used together in cognitive processing. Although the tools are quite powerful and broadly applicable, they can be inaccessible, or at least daunting, to psychology researchers. Houpt, Blaha, McIntire, Havig, and Townsend (2013) introduced an R (R Development Core Team, 2011) package to implement the basic measures and statistical analyses. However, SFT continues to advance and more tools continue to become available. In this article we give an overview of the new theoretical advancements in the SFT framework and describe their use and implementation in the sft R package. In particular we focus on four advances from the last few years: the single-target self-terminating (ST-ST) capacity coefficient (Blaha, 2010; Blaha & Townsend, under review), the unified workload capacity space measures (Townsend & Eidels, 2011), functional principal components analysis (fPCA) of the capacity coefficient (Burns et al., 2013), and the workload assessment functions (Townsend & Altieri, 2012).

We will begin with an overview of workload capacity in SFT to give readers who may be less familiar with the topic a foundation for the rest of the paper. This overview is brief and meant only to give readers the basic details needed to use these new analyses. We encourage readers wanting further details to read the SFT with R paper (Houpt et al., 2013) or some of the original papers on workload capacity in SFT and on the capacity coefficient (Townsend, 1974; Townsend & Ashby, 1983; Townsend & Nozawa, 1995; Townsend & Wenger, 2004; Wenger & Townsend, 2000).

First, a brief note on our notation. When we refer to the R package for the implementation of SFT theory, we will use sft. Any R code itself, like function names or input arguments, will be typeset as follows: function or input.arguument=value.
Workload Capacity and the Capacity Coefficient

Within SFT, workload capacity refers to a change in information processing performance as the number of information sources change. The original definitions focused on processing speed as measured by response times. Some of the recent generalizations discussed in this paper and implemented in the latest version of the R package include response accuracy as well. In this section we will focus on the response time only approach, then discuss the generalization in the Assessment Function section.

In most cases, a system takes longer to finish the more it has to do. However, just because a system takes longer to respond when it is required to process more sources of information, it does not mean that any of the individual information sources are processing at a slower speed. Likewise, when there is redundant information available, the overall processing speed being faster does not mean that the processing of any individual source is faster. For example, in parallel processes with redundant information, faster processing times may be due to statistical facilitation (Raab, 1962; Miller, 1982). Statistical facilitation refers to the fact that the minimum over a set of more than one random variable (i.e., source processing times) tends to be smaller than any of the individual random variables. Statistical inhibition refers to the analogous phenomenon when all processes must finish: the maximum of multiple random variables tends to be larger than any of the individual random variables. Thus, if all we can measure is a person’s response time with one or more sources of information present, and not the individual processing times of each source of information when multiple sources are available, it is important to compare the times against an appropriate baseline.

The baseline for the capacity coefficient in redundant target tasks is the unlimited-capacity, independent, parallel, first-terminating model (Townsend & Nozawa, 1995). We use the initialism UCIP for the first three assumptions and OR to refer to first-terminating (in reference to a logical OR decision rule). Because it is first-terminating, the model is finished as soon as any of the individual target processes have completed.
Equivalently, the model has not yet finished only if none of the individual target processes have finished,

\[ \Pr\{T_{UCIP-OR} > t\} = \Pr\{T_1 > t, \ldots, T_n > t\}. \]

We can use \( T_i \) to refer to the processing time for the \( i \)th target regardless of whether there are other sources present due to the unlimited capacity assumption. Using the independence assumption, we can split the right side into a product,

\[ \Pr\{T_1 > t, \ldots, T_n > t\} = \Pr\{T_1 > t\} \times \cdots \times \Pr\{T_n > t\}. \]

We can rewrite this equality more succinctly using survivor functions,

\[ S(t) = 1 - F(t) = \Pr\{T > t\}, \]

\[ S_{UCIP-OR}(t) = S_1(t) \times \cdots \times S_n(t) \]

where \( F(t) = \Pr\{T \leq t\} \) is the cumulative distribution function. Lower survivor functions correspond to faster processing times. To translate this identity to cumulative hazard functions we use \( H(t) = -\log S(t) \), so we see that larger cumulative hazard functions correspond to faster processing times.

The cumulative of the hazard function is convenient for statistical purposes and has the nice interpretation as the amount of work completed by the cognitive processing system in \( t \) amount of time. We take the natural logarithm of both sides of the previous equation to arrive at the baseline prediction of the UCIP-OR model in terms of cumulative hazard functions,

\[ H_{UCIP-OR}(t) = H_1(t) + \cdots + H_n(t). \]

The capacity coefficient is a ratio function comparing this UCIP model baseline to observed performance. Let \( C = \{1, \ldots, n\} \) denote the set of \( n \) active channels in an experiment. Using this set notation, we denote the empirical response time cumulative distribution function (CDF) on an OR task as \( F_C(t) = P[\min_C(T_c) \leq t] \), for all real \( t \geq 0 \) and \( c \in C \). The corresponding empirical cumulative hazard function is denoted \( H_C(t) \). The
capacity coefficient for tasks in which a first-terminating decision rule is expected is given by the ratio of cumulative hazard functions of response times when all $n$ targets are present to the sum of cumulative hazard functions of response times for cases when each of the $n$ targets is present in isolation,

$$C_{\text{OR}}(t) = \frac{H_C(t)}{H_{\text{UCIP-OR}}(t)} = \frac{H_C(t)}{H_1(t) + \cdots + H_n(t)}. \quad (1)$$

The baseline of UCIP-OR processing is estimated in the denominator, so if the performance measured when all targets sources are present is better than the estimated baseline, then $C_{\text{OR}}(t) > 1$. Likewise, worse than baseline performance would be indicated by $C_{\text{OR}}(t) < 1$.

The same logic can be used to derive the baseline for tasks in which the participant can only respond when all sources of information have been processed, i.e. exhaustive or AND tasks. For the UCIP-AND model to finish, it must finish processing all sources of information,

$$\Pr\{T_{\text{UCIP-AND}} \leq t\} = \Pr\{T_1 \leq t, \ldots, T_n \leq t\}$$

$$F_{\text{UCIP-AND}}(t) = F_1(t) \times \cdots \times F_n(t).$$

In terms of the cumulative reverse hazard function, $K(t) = \log F(t)$,

$$K_{\text{UCIP-AND}}(t) = K_1(t) + \cdots + K_n(t).$$

Lower CDFs correspond to slower processing, so lower cumulative reverse hazard functions correspond to worse performance. Because $F(t)$ is between 0 and 1, the logarithm of $F(t)$ is always negative, so lower values correspond to larger magnitudes. Hence, to keep the interpretation of $C(t) > 1$ corresponding to better than baseline, the AND capacity coefficient is flipped,

$$C_{\text{AND}}(t) = \frac{K_1(t) + \cdots + K_n(t)}{K_C(t)}. \quad (2)$$

Note that for the observed performance in an AND task, we use the response time CDF $F_C(t) = P[\max_{c} (T_c) \leq t]$, for all real $t \geq 0$ and $c \in C$, and we denote the cumulative
reverse hazard function $K_C(t)$. The baseline is now represented in the numerator, so larger magnitude cumulative reverse hazard functions for response times to all sources of information (the denominator) indicates worse than baseline performance and leads to $C_{\text{AND}}(t) < 1$. Likewise, better performance than the baseline leads to $C_{\text{AND}}(t) > 1$.

Experimentally, workload capacity analysis can be used on any tasks that require an AND or OR type of decision (and now single-target self-terminating, as we will explain below) and that utilize a manipulation that involves judgments on different numbers of information sources. There are two specific workload manipulations needed to utilize Equations 1 and 2. The first is a set of single information source trials that allow the estimation of the individual channel response time distributions. This is required for the UCIP baseline model estimates. The second necessary condition is one in which all the sources of information are presented together, to estimate the actual cognitive processing of $n$ active channels. For more on the experimental manipulations for capacity analysis, particularly in the context of the double factorial paradigm, see Houpt et al. (2013).

To make this concrete, imagine a visual or memory search task. In order to estimate the UCIP baseline model, participants must complete a series of single-target trials (i.e., one item in the search array) with one type of trial for each individual different source of information. Participants must also complete trials for $n$ items in the search array. If this array was all targets, then participants would be completing an OR redundant-targets task, and the experimenter would use Equation 1 for his analysis. If this array was all distractors, and all must be searched to determine the target was not present, then participants would be completing an AND task, and the experiment would use Equation 2 for the analysis for those response times.

Functions for calculating the traditional capacity coefficients and the associated test statistics from (Houp & Townsend, 2012) are available in the sft package and described in Houpt et al. (2013). With the basics of workload capacity analysis in SFT established, we can now summarize the latest developments and their corresponding functions in the sft.
package.

**Single-Target Self-Terminating Capacity**

Single-target self-terminating (ST-ST) processing refers to a response rule that sits between OR and AND processing. This is the condition where there is a single target of interest for the response. When this target is presented among other non-target information sources in a task, it may be the first or last item processed or somewhere in between. However, as soon as the target is identified, the observer can make a response (hence, the nomenclature 'self-terminating'). For example, ST-ST processing is often the stopping rule demanded in a visual or memory search task when a single target of interest is embedded in a search array of distractors.

As with AND processing, the ST-ST capacity coefficient compares performance on a task to a UCIP model using cumulative reverse hazard functions (Blaha, 2010; Blaha & Townsend, under review). The UCIP model prediction is the cumulative reverse hazard function for response times to the single target processed in isolation. Let $K_k(t)$ denote the response time cumulative reverse hazard function for single-target $k$ processed alone. Because the assumptions of the UCIP model are that the individual channel processing rates are independent of other channels and do not change as the total number of channels changes, then

$$K_{UCIP-STST} = K_k(t).$$

The cumulative reverse hazard function for processing of the same single target $k$ among $n$ total information sources ($n - 1$ distractors) is denoted $K_{k,C}(t)$, where again $C = \{1, \ldots, n\}$. The latter case is the higher workload condition of interest for workload capacity analysis. Taking a ratio of the UCIP model to the $n$-source processing performance gives the ST-ST capacity coefficient:

$$C_{STST}(t) = \frac{K_k(t)}{K_{k,C}(t)},$$

(3)
Similar to \( C_{\text{AND}}(t) \), the numerator is the baseline model, and a larger denominator indicates worse than baseline performance, giving \( C_{\text{STST}}(t) < 1 \), which is referred to as limited capacity processing. This indicates that either there are limited processing resources available, there is inhibition among the subprocesses, or the items are not processed in parallel (e.g., the items may be processed serially).

Likewise, better than baseline performance again leads to \( C_{\text{STST}}(t) > 1 \), which is referred to as super capacity processing. This indicates that either there are more processing resources available per process when there are more processes, that there is facilitation among the subprocesses, or the items are not processed in parallel (e.g., the items may be processed concurrently).

Additionally, Blaha and Townsend (under review) showed that a statistical test for \( C_{\text{STST}}(t) \) is a special case of the statistical test for AND capacity developed by Houpt and Townsend (2012). The estimator of the cumulative reverse hazard function is calculated with the `estimateHAK` function in the `sft` package, as covered in Houpt et al. (2013).

In the `sft` R package, the ST-ST capacity coefficient and corresponding statistical test (Blaha & Townsend, under review) are calculated by the `capacity.stst` function. It takes as its input a list containing two arrays of response time data. The first array in the list is assumed to be the response times from the single-target self-terminating condition with a total of \( n \) information sources, and the second array in the list is assumed to be the response times from the single target processed in isolation (the baseline estimate). The second input argument is an optional list of arrays of correct indicators; if the correct indicators are not provided (CR=\( \text{NULL} \)), the function assumes that all response times are from correct responses.

Finally, the `capacity.stst` function includes an indicator input `ratio`. If `ratio=\text{TRUE}`, then the ratio form of the capacity coefficient (Equation 3) is returned; examples of ratio \( C_{\text{STST}}(t) \) functions, simulated for super capacity, unlimited capacity, and limited capacity models, are shown in Figure 1. If `ratio=\text{FALSE}`, then the difference form
of the capacity coefficient is returned. The difference form of the ST-ST capacity coefficient is given by

$$C_{\text{STST}}(t) = K_{k,C}(t) - K_k(t).$$  \hspace{1cm} (4)

For the difference form of $C_{\text{STST}}(t)$, the reference value for unlimited capacity processing is 0 instead of 1. Negative values indicate worse than UCIP performance, and positive values indicate better than UCIP performance.

We can start with an simulated example data set to demonstrate the `capacity.stst` function. Recall that we need two sets of response times, the single target in isolation and the single target among other non-target processes. In this example, we simulate data from a limited-capacity condition, wherein the additional information sources slowed the processing rate of our target channel.

```r
rate1 <- .35
RT.pa <- rexp(100, rate1)
RT.pp.limited <- rexp(100, .5*rate1)
tvec <- sort(unique(c(RT.pa, RT.pp.limited)))
```

To evaluate $C_{\text{STST}}(t)$ and test the null hypothesis of UCIP-STST processing, we can use the function with a list of response time vectors.

```r
cap <- capacity.stst(RT=list(RT.pp.limited, RT.pa))
```

We use `print(cap$sctest)` to see the results of the statistical test.

**Houpt-Townsend UCIP test**

data:  RT and CR

$z = -3.4161$, $p$-value $= 0.0006353$

alternative hypothesis: response times are different than those predicted by the UCIP-AND model

The $z$-score is significantly negative, so we would reject the null hypothesis of UCIP-STST processing. Note that in this example, we used the default function calls of
CR=NULL (i.e., we assume all response times are from correct trials) and ratio=TRUE
(return the ratio version of the function). Also, note that the information about the
alternative hypothesis returned with the print command refers to the UCIP-AND model,
because the statistical test is a special case of the AND test with only a single channel in
the UCIP model (c.f. Blaha and Townsend (under review)). The data from this simulated
example are plotted as the solid red line in Figure 1.

The capacity.stat function returns an approxfun object representing the ST-ST
capacity ratio function (ratio=TRUE, which is the default) or the ST-ST capacity
difference function (ratio=FALSE), as well as the ucip.test for ST-ST processing. If
ratio=FALSE, capacity.stat also returns the variance estimate for the difference variant
for the capacity coefficient. If the reported p-value for the statistical test is less than the
user’s predetermined type I error α level, at least one of the UCIP assumptions has failed.

Unified Workload Capacity Space

Townsend and Eidels (2011) introduced unified capacity spaces, a set of inequalities
that enable both capacity coefficients and the parallel processing response time distribution
bounds to be plotted on the same coordinate system for direct visual comparison. In order
to do this, the bounds for standard parallel processing were transformed from standard
CDF values existing on the range [0,1] to inequalities of either cumulative hazard functions
or cumulative reverse hazard functions, depending on the stopping rule, for direct
comparison with the capacity coefficient values. Note that in this case, the capacity
coefficient assumes the ratio format which exists on the range [0, +∞]. Townsend and
Eidels (2011) derived the unified capacity space inequalities for AND and OR processing of
2-channel systems. (Blaha & Houpt, Under Review) extended this theory to general
n-channel models and derived the unified space inequalities for ST-ST processing.

In the sft package, we have developed a single function, estimate.bounds, that can
estimate both the traditional CDF versions of the bounds on parallel processing for all
stopping rules and the unified workload capacity space inequalities. First we review both versions of the inequalities, and then we explain the \texttt{estimate.bounds} function.

**Bounds on Standard Parallel Processing**

**OR.** Let \( F_C(t) = P\{ \min_{c \in C} (T_c) \leq t \} \), for all real \( t \geq 0 \) and \( c \in C \), denote the cumulative distribution of response times under a minimum time (logical OR) stopping rule. The general bounds for \( n \)-channel parallel processing under an OR stopping rule are (Colonius & Vorberg, 1994):

\[
\max_i \left[ F_{C \setminus \{i\}}(t) \right] \leq F_C(t) \leq \min_{i,j} \left[ F_{C \setminus \{i,j\}}(t) + F_{C \setminus \{j\}}(t) - F_{C \setminus \{i,j\}}(t) \right].
\]

(5)

Here, we have used the set notation \( C \setminus \{i\} \) to indicate response times with all sources present except \( i \) (i.e. \( n - 1 \) total processing channels). Under the assumption or conditions that the individual channels are identically distributed (IID), this inequality chain simplifies to

\[
F_{C \setminus \{i\}}(t) \leq F_C(t) \leq \left[ 2 \times F_{C \setminus \{1\}}(t) - F_{C \setminus \{1,2\}}(t) \right].
\]

(6)

When the model under scrutiny has only \( n = 2 \) channels, the inequality chain takes the form:

\[
\min \left| F_1(t), F_2(t) \right| \leq F_{\{1,2\}}(t) \leq \left[ F_1(t) + F_2(t) \right].
\]

(7)

The upper bound on this final inequality is often referred to as the ‘race-model inequality,’ which has long been used to test for evidence of cooperative processing architecture (Miller, 1982).

**AND.** Let \( G_C(t) = P\{ \max_{c \in C} (T_c) \leq t \} \), where again \( C = \{1, \ldots, n\} \) is the set of all \( n \) channels and \( c \in C \), denote the cumulative distribution of response times under a maximum time (logical AND, exhaustive) stopping rule. The general bounds for \( n \)-channel parallel processing under an AND stopping rule are (Colonius & Vorberg, 1994):

\[
\max_{i,j} \left[ G_{C \setminus \{i\}}(t) + G_{C \setminus \{j\}}(t) - G_{C \setminus \{i,j\}}(t) \right] \leq G_C(t) \leq \min_i \left[ G_{C \setminus \{i\}}(t) \right].
\]

(8)
Under the assumption or conditions that the individual channels are identically distributed, this inequality chain simplifies to
\[
\left[2 \ast G_{C \setminus [1]}(t) - G_{C \setminus [1,2]}(t)\right] \leq G_C(t) \leq G_{C \setminus [1]}(t). \tag{9}
\]

When the model under scrutiny has only \( n = 2 \) channels, the inequality chain takes the form:
\[
|G_1(t) + G_2(t) - 1| \leq G_{[1,2]}(t) \leq \min\left[G_1(t), G_2(t)\right]. \tag{10}
\]

**ST-ST.** Let \( F_{k,c}(t) = P[T_{k,c} \leq t] \) denote the CDF of response times under the ST-ST stopping rule, where the target of interest is on processing channel \( k \) among \( n \) active channels. The general bounds for \( n \)-channel parallel processing under an ST-ST stopping rule are (Blaha & Townsend, under review):
\[
\prod_{c=1}^{n} F_c(t) \leq F_{k,C}(t) \leq \sum_{c=1}^{n} F_c(t). \tag{11}
\]

Under the assumption or conditions that the individual channels are identically distributed, this inequality chain simplifies, for any channel \( c \in C \), to
\[
[F_c(t)]^n \leq F_{k,C}(t) \leq n \ast F_c(t). \tag{12}
\]

When the model under scrutiny has only \( n = 2 \) channels, the inequality chain takes the form:
\[
[F_1(t) + F_2(t)] \leq F_{k,[1,2]}(t) \leq |F_1(t) + F_2(t)|. \tag{13}
\]

Note that in this case, \( k = 1 \) or \( k = 2 \), but this may not be specifiable \textit{a priori} depending on experimental design.

Across all stopping rule conditions, violation of the upper bound indicates performance that is faster than can be predicted by an unlimited capacity parallel model. This may arise from positive (facilitatory) crosstalk between parallel channels, super capacity parallel processing, or some form of co-active architecture in the measured human response time data. Violation of the lower bound indicates performance that is slower than...
predicted by an unlimited capacity parallel model. This may arise from negative
(inhibitory) crosstalk between parallel channels, fixed or limited capacity processing, or
some form of serial architecture in the measured human response time data.

Bounds on Capacity Coefficient Space

The bounds on parallel processing defined above can be transformed from CDFs into
cumulative hazard and cumulative reverse hazard functions to form inequality chains with
the capacity coefficients. The bounds for all stopping rules and all models are summarized
in Table 1. For the derivation of these bounds, the reader is referred to Townsend and
Ekdels (2011) and Blaha and Houpt (Under Review).

The estimate.bounds function in the sft package can be flexibly used to compute
either the CDF or unified capacity space bounds on standard parallel processing. For its
first input argument, RT, it takes a list of numeric arrays of response times, each measured
from the individual channels to be modeled. The RT list can contain either one array for
each of the \( n \) channels to be estimated (so length(RT)=n), or it can have length(RT)=1
and the bounds can be found under an assumption that the \( n \) channels are identically
distributed. In the former case, the number of channels, \( n \), is estimated from the length of
the RT list, and so the user can keep the default input arguments assume.ID=FALSE and
numchannels=NULL. In the latter case, because the length of the RT list is only 1, the input
arguments assume.ID=TRUE and numchannels=n (where \( n \geq 2 \) ) must be specified by the
user.

The optional input argument CR is a list of correct indicators that should have the
same length as the input argument RT. If CR=\( \text{NULL} \) (default), then all the response times
are assumed to be from correct response trials.

Critically, the user must specify which stopping rule (OR, AND, ST-ST) should be
computed using the argument stopping.rule=("or", "and", "stst"). Finally, the
input argument unified.space indicates whether the bounds should be computed for
CDF space (unified.space=FALSE) or for the unified capacity coefficient space
(unified.space=TRUE).

Here, we demonstrate the use of the estimate.bounds function with data from the
dots dataset, which is included with the sft package. First, we load the data and extract
the necessary data to estimate the bounds for Participant S3 for the OR stopping rule
condition.

data(dots)
attach(dots)
sub <- 'S3'
cond <- 'OR'
chan1 <- RT[Subject==sub & Condition==cond & Correct & Channel1>0 & Channel2==0]
chan2 <- RT[Subject==sub & Condition==cond & Correct & Channel1==0 & Channel2>0]
redundant <- RT[Subject==sub & Condition==cond & Correct & Channel1>0 & Channel12>0]
rt <- list(redundant, chan1, chan2)

Next, we calculate the bounds using the estimate.bounds function.

cdf.bounds <- estimate.bounds(rt[2:3], corrects[2:3], stopping.rule='or')
capacity.bounds <- estimate.bounds(rt[2:3], corrects[2:3],
        stopping.rule='or', unified.space=TRUE)

We then calculate the redundant targets cdf to compare to bounds.

redundant.cdf <- ecdf(rts[[1]][corrects[1][1]>0])

And, we calculate the capacity coefficient.

or.cap <- capacity.or(rts, corrects)

Sample plots of parallel processing bounds computed with estimate.bounds are
shown in Figure 2. This figure shows both the AND and OR bounds, plotted in both CDF
and unified capacity space, for a single participant from the dots data set. In the CDF
space plots, the empirical CDF of the redundant target trials response time data for either
the AND and OR conditions is shown in the thick, solid black lines. The upper and lower bounds on those CDFs are plotted in the dashed and dotted (respectively) red lines. Note that in these traditional views, we would try to make inferences about capacity from the violations of the bounds.\footnote{For a full discussion of the inequality chains formed by the AND and OR processing bounds, as well as the inferences about capacity that are possible from these inequality chains, the reader is referred to Townsend and Wenger (2004).} For example, in the data shown in Figure 2 (lower half, OR task), there is a clear violation of the lower bound, roughly between 0 and 250 ms. Using the traditional CDF space plots, we would infer that Participant S3 is too slow to be performing like a race model with redundant targets. Now, using the unified capacity space plots, we can make more direct inferences about the relationships of the bounds and capacity coefficient. In the lower right plot of Figure 2, limited capacity $C_{DR}(t) < 1$ is observed for the whole range of response times, with violations of the lower bound obvious for the early response times.

\textbf{iPCA for Capacity Coefficients}

Functional principal components analysis (fPCA) is an extension of standard principal components analysis to infinite dimensional (function) spaces (c.f. Ramsay & Silverman, 2005). Just as in standard principal components analysis, fPCA is a method for finding a basis set of lower dimensionality than the original space to represent the data. However, in place of basis vectors, fPCA has basis functions. Each function in the original dataset can then be represented by a linear combination of those bases, so that each datum is represented by a vector of coefficients (or scores) in that linear combination.

The capacity coefficient is a function across time, so the differences among capacity coefficients from different participants and/or conditions can rarely be characterized by simple greater than or less than relations. The nuances of variation in functions would be lost if one were to reduce the capacity estimates to a point by taking an average across time or the maximum/minimum of the function. By using fPCA we can maximize the
amount of variation we capture with a point estimate or small number of values: The factor scores can be used to examine differences among capacity coefficients, taking into account variation across the entire function.

The R function for fPCA implements the steps outlined in Burns et al. (2013). First, the data are shifted by subtracting the median response time within each condition for each participant, using the same shift for both single target and multiple target trials, so that the capacity curves will be registered. Second, each capacity coefficient is calculated with the shifted response times. Next, the mean capacity coefficient across participants and conditions is subtracted from each capacity coefficient, and the resulting capacity coefficients are represented using a b-spline basis. The fPCA procedure extracts the first basis function from the b-spline space that accounts for the largest variation across the capacity coefficients. The next basis function is chosen as that which explains the largest amount of remaining variation in the capacity coefficients, given the constraint that it must be orthogonal to the first. This process continues until the indicated number of bases have been extracted. Once the capacity functions are represented in the reduced space, a varimax rotation is applied to concentrate variability and increase interpretability.

The `fPCAcapacity` function can be called from the `sft` package using the following syntax:

```r
fPCAcapacity(sftData, dimensions, acc.cutoff = .75, OR = TRUE, ratio = TRUE, plotPCs = FALSE)
```

The data for fPCA analysis should be in the standard SFT data form, which is described thoroughly in Houpt et al. (2013): there should be a column for a participant identifier (`sftData$Subject`), a column for the condition (`sftData$Condition`), a column for the salience manipulation value of each source of information (`sftData$Channel`), a column for response times (`sftData$RT`), and finally a column indicating whether the participant was correct on each trial (`sftData$Correct`). The `fPCAcapacity` function also has a.

---

2The maximum possible number of basis functions is the number of input functions.
ratio flag to indicate whether to output capacity ratios (if ratio=TRUE) or differences, an OR flag indicating the version of the capacity coefficient (Equation 1 if OR=TRUE; Equation 2 if OR=FALSE), and an acc.cutoff input value to establish a minimum criterion for accuracy required for including data in the analysis. Two variables unique to the fPCA analysis are the dimensions value, which can be set by the experimenter to establish the number of basis functions used to represent the data, and the plotPCs indicator which will generate plots of the principal components if plotPCs=TRUE.

The output of the function is a list of length four. The first list entry is a data frame titled Scores, which contains the loading values (coefficients on the basis functions) for each participant and condition. MeanCT is the averaged capacity function across all participants and conditions, while PF is a list containing each of the principal functions, the number of which will have been specified by the dimensions argument in the call to the function. The last list entry is medianRT, which will keep track of the amount each capacity curve has been shifted during the registration step, measured in milliseconds of RT.

Figure 3 illustrates the output plots generated by the fPCAcApacity function when run on the dots data using the function call:

\[ \text{fPCAcApacity}(d\text{ots}, 2, \text{acc.cutoff} = .75, \text{OR} = \text{TRUE}, \text{ratio} = \text{TRUE}, \text{plotPCs} = \text{TRUE}). \]

Note that in the dots data, there are two conditions, OR and AND, referring to two task instructions given in the experiment; in the present analysis, we use Equation 1 in the fPCA analysis for all the data. In the above call, we asked for two dimensions, but again that choice is up to the experimenter. We can see that for the dots data, the first two components can together account for 93% of the variance (summing the values noted on the y-axis labels). The first component function mainly inflates (or deflates, depending on the sign of the loading value) capacity values for early- to mid-range reaction times. The second PC captures variation in the capacity function at early and late times; when PC2 is

\[ ^3 \text{Note that the ST-ST capacity coefficient has not yet been implemented in fPCAcApacity.} \]
higher, both early and late values of C(t) are higher. The scores for each of the ten participants, in the two stopping rule conditions, are shown in the right panel of Figure 3. In this example, both of the components can easily separate differences in the two tasks and between the various subjects. Combining the information from the Component plots and the Score values, the OR condition data are consistently higher than the AND condition data for all times and all participants. Within participants between conditions, the largest differences in capacity coefficient functions occur in the middle range of response times. fPCA also highlights differences in capacity among participants. In particular, participant S5 shows much lower variability between the OR and AND conditions than the other participants, and so S5’s loading scores are higher and closer together in the right-hand plots.

Because the principal component functions are specifically chosen to describe the variability between the capacity functions for participants and conditions, this tool provides an excellent method for looking for influences of task and individual differences in capacity functions. Whereas most previous analyses of capacity data have restricted themselves to a gross comparison with the baseline model (i.e. observed value relative to 1), this analysis is more relative, highlighting differences between observed functions, and picking up dynamic patterns across various reaction times.

For more details on fPCA for the capacity coefficient, see Burns et al. (2013). For more general details on using fPCA in R, see Ramsay, Hooker, and Graves (2009).

Assessment Functions

The assessment functions are a generalization of the workload capacity functions that account for incorrect responses. The original capacity coefficient established a baseline that assumed perfect accuracy. While the standard capacity coefficient is robust to slightly less than perfect performance by a participant (the rule of thumb is that above roughly 90% accuracy should be fine), when accuracy is low, either the assessment functions or a
parametric measure such as the linear ballistic accumulator (LBA) capacity (Eidels, Donkin, Brown, & Heathcote, 2010) should be used.

Townsend and Altiери (2012) derived four different assessment functions each for AND and OR tasks to compare performance on two target information sources with the performance of an unlimited-capacity, independent, parallel (UCIP) model. The UCIP model is augmented with an error generating process for both sources of information. Each error process is assumed to be independent of, and parallel to, the processes for the other source of information, but there is no assumption of independence between the correct and error processes for the same source of information.

The correct assessment functions assess performance on correct trials and the incorrect assessment functions assess performance on the trials with incorrect responses. The fast assessment functions use the cumulative distribution functions, similar to the AND capacity coefficient, and the slow assessment functions use the survivor functions, similar to the OR capacity coefficient.

In an OR task, the detection model assumes that the response will be correct if it is correct on either source, i.e., if either source is detected. Hence, the first source (A) correct processing time must be faster than first source incorrect time, $T_{AC} < T_{AI}$ or the second source (B) correct must be faster than the second source incorrect, $T_{BC} < T_{BI}$. For the CDF (fast) version of the assessment function, we are interested in whether the response was at or before $t$, so either $T_{AC} \leq t$ and $T_{AC} < T_{AI}$ or $T_{BC} \leq t$ and $T_{BC} < T_{BI}$. Using $f_{AC}$ for the completion time density for the first source correct process, $F_{AI}$ for the distribution of first source, incorrect processes completion times, and likewise for the second source, this probability can be written out as,

$$\int_0^t f_{AC}(t) [1 - F_{AI}] + \int_0^t f_{BC}(t) [1 - F_{BI}]$$

$$- \int_0^t f_{AC}(t) [1 - F_{AI}] \int_0^t f_{BC}(t) [1 - F_{BI}].$$

The same pattern of logic can be used to determine the baseline of processing for each of
other cases, slow-correct, fast-incorrect and slow-incorrect. For a full explication of the 
analysis functions and the derivation of each case, see Townsend and Altiere (2012). The 
assessment function with the sft package can be used for detection tasks with the 
following syntax:

assessment(RT, CR, OR, correct, fast, detection=TRUE)

The RT and CR are lists of response times and correct indicators for each trial. As in the 
standard capacity R functions, the first element in the list contains the measurements from 
trials in which both sources of information were present and the second and third elements 
are for each of the single-source conditions. The OR input is a TRUE/FALSE indicator of 
whether to calculate the assessment function using an UCIP-OR baseline (OR=TRUE) or an 
UCIP-AND baseline (OR=FALSE). The correct and fast parameters are TRUE/FALSE 
indicators to specify which of the four types of assessment functions to use.

For example, to evaluate a participant (S7) from the OR-decision dot detection task, 
we first extract the necessary data,

sub <- 'S7' 
cond <- 'OR' 
#select single channel data 
chan1 <- dots[Subject==sub & Condition==cond & Channel1>0 & Channel2==0, 
c('RT', 'Correct')] 
chan2 <- dots[Subject==sub & Condition==cond & Channel1==0 & Channel2>0, 
c('RT', 'Correct')] 
#select redundant target (2-channel) data 
redundant <- dots[Subject==sub & Condition==cond & Channel1>0 & Channel2>0, 
c('RT', 'Correct')] 
rt <- list(redundant$RT, chan1$RT, chan2$RT) 
corrects <- list(redundant$Correct, chan1$Correct, chan2$Correct)
Next, we simply apply the function:

\[
a.\text{or.cf} <- \text{assessment(rts, corrects, OR=TRUE, correct=TRUE, fast=TRUE, detection=TRUE)}
\]

The output is a stepfun object, so it can be plotted using:

\[
\text{plot(a.\text{or.cf}, ylim=c(0,2))}
\]

Figure 4 shows each of the correct/incorrect and fast/slow assessment functions for Participant 7 in the OR condition. Note that UCIP performance would show a value of 1 for all times in all plots.

In discrimination OR tasks, a participant may respond based on whichever source finishes first. Hence, the response will be incorrect if the first to finish is incorrect even if the second source would have been correct. This results in a slightly different baseline for performance assessment. Now, for a correct response, either \(T_{AC}\) or \(T_{BC}\) must be faster than both \(T_{AI}\) and \(T_{BI}\). The UCIP baseline for correct-fast, OR, discrimination is:

\[
\int_0^T f_{AC}(t) \, [1 - F_{AI}] \, [1 - F_{BI}] + \int_0^T f_{BC}(t) \, [1 - F_{AI}] \, [1 - F_{BI}]
\]

\[
- \int_0^T f_{AC}(t) \, [1 - F_{AI}] \, [1 - F_{BI}] \int_0^T f_{BC}(t) \, [1 - F_{AI}] \, [1 - F_{BI}]
\]

See Donkin, Little, and Houpt (2013), particularly the appendix, for details of the discrimination assessment functions. The R syntax for discrimination tasks is the same as the syntax for the detection task, but with the \text{detection} parameter set to \text{FALSE}.

\textbf{Conclusion}

Workload capacity analysis entails a powerful set of tools within SFT for examining the effects on information processing of differing numbers of information sources (different numbers of stimulus inputs, different numbers of active processing channels). Several recent theoretical additions to capacity analyses have both expanded the applicability of
capacity to a new stopping rule (ST-ST processing) and broadened the available tools for
capacity analysis, especially to allow more nuanced comparisons across participants and
experimental conditions. Despite being a powerful framework based on minimal
assumptions (and often relying on non-parametric analyses), SFT is underutilized within
the psychological research community, partly because researchers previously needed to
develop their own computational codes. We hope that by making the tools accessible with
open source R functions and with the present paper together with Houpt et al. (2013),
researchers can easily use the SFT tools more frequently.

Here, we have described briefly the new theoretical advances and provided a detailed
account of the new functions for utilizing the new tools in the R statistical computing
framework. These new functions constitute the first major additions to the sft package
beyond the initial functionality described in Houpt et al. (2013). The advantage of this
paper is that it focuses on the computational implementation for using the new capacity
tools with detailed examples of the R code. Researchers seeking to try capacity analysis
now have a standardized implementation of these functions, together with the other SFT
tools for assessing processing architecture made available in the sft package. We encourage
researchers to use this standardized R package to reduce the chance of implementation
errors that inevitably arise when each user is left to themselves to translate from a
theoretical paper to usable code. And as additional theoretical advances are made in SFT,
we will continue to update the sft package as the state of the science for SFT modeling.
References


(Manuscript submitted for publication)


Table 1  
*Summary of all Bounds on the Capacity Coefficient (from Blaha & Houpf (under review))*

### LOWER BOUNDS

<table>
<thead>
<tr>
<th>Stopping Rule</th>
<th>( n )-channels</th>
<th>( n ) IID channels</th>
<th>2 channels</th>
</tr>
</thead>
<tbody>
<tr>
<td>OR</td>
<td>( \frac{\ln(\min{S_{C_1(0)}(0)})}{\ln(\prod_{i=1}^{n-1} S_i(0))} )</td>
<td>( \frac{\ln(S_{C_1(1)}(0))}{\ln(\prod_{i=1}^{n-1} S_i(0))} )</td>
<td>( \frac{\ln(\min{S_i(0), S_{C_1(0)}(0)})}{\ln(S_i(0) + S_{C_1(0)}(0))} )</td>
</tr>
<tr>
<td>STST</td>
<td>( \frac{\ln(F_i(0))}{\sum_{i=1}^{n} \ln(F_i(0))} )</td>
<td>( \frac{\ln(F_i(0))}{\ln(n \times \ln(F_i(0)))} )</td>
<td>( \frac{\ln(F_i(0))}{\ln(F_i(0) + 1)} )</td>
</tr>
<tr>
<td>AND</td>
<td>( \frac{\ln(\prod_{i=1}^{n-1} G_i(0))}{\ln(\max{\prod_{i=1}^{n-1} G_i(0), \prod_{i=1}^{n-1} G_i(0) - \prod_{i=1}^{n-1} G_i(0)})} )</td>
<td>( \frac{\ln(\prod_{i=1}^{n-1} G_i(0))}{\ln(2 \times \prod_{i=1}^{n-1} G_i(0) - \prod_{i=1}^{n-1} G_i(0))} )</td>
<td>( \frac{\ln(G_i(0) + G_i(0))}{\ln(G_i(0) + G_i(0) - 1)} )</td>
</tr>
</tbody>
</table>

### UPPER BOUNDS

<table>
<thead>
<tr>
<th>Stopping Rule</th>
<th>( n )-channels</th>
<th>( n ) IID channels</th>
<th>2 channels</th>
</tr>
</thead>
<tbody>
<tr>
<td>OR</td>
<td>( \frac{\ln(\max{S_{C_1(0)}(0) + S_{C_1(1)}(0) - S_{C_1(2)}(0)})}{\ln(\prod_{i=1}^{n-1} S_i(0))} )</td>
<td>( \frac{\ln(2 \times S_{C_1(1)}(0) - S_{C_1(2)}(0))}{\ln(\prod_{i=1}^{n-1} S_i(0))} )</td>
<td>( \frac{\ln(S_i(0) + S_{C_1(2)}(0) - 1)}{\ln(S_i(0) + S_{C_1(1)}(0))} )</td>
</tr>
<tr>
<td>STST</td>
<td>( \frac{\ln(F_i(0))}{\ln(\sum_{i=1}^{n} F_i(0))} )</td>
<td>( \frac{\ln(F_i(0))}{\ln(n \times \ln(F_i(0)))} )</td>
<td>( \frac{\ln(F_i(0))}{\ln(F_i(0) + 1)} )</td>
</tr>
<tr>
<td>AND</td>
<td>( \frac{\ln(\prod_{i=1}^{n-1} G_i(0))}{\ln(\min{\prod_{i=1}^{n-1} G_i(0), \prod_{i=1}^{n-1} G_i(0) - \prod_{i=1}^{n-1} G_i(0)})} )</td>
<td>( \frac{\ln(\prod_{i=1}^{n-1} G_i(0))}{\ln(\min{G_i(0), G_i(0)})} )</td>
<td>( \frac{\ln(G_i(0) + G_i(0))}{\ln(\min{G_i(0), G_i(0)})} )</td>
</tr>
</tbody>
</table>
Figure 1. Plots of ST-ST processing capacity coefficients, in ratio=TRUE form. The data were simulated from ST-ST processing, including a model exhibiting limited, unlimited, and super capacity processing rates, and the corresponding Carst estimates are plotted in red, green, and blue (respectively). The baseline reference model, giving Carst = 1 is plotted in the thin, black line.
Figure 2. Example bounds on standard parallel processing from one participant (S2) in the dots data included in the sfit package. The top row shows the bounds for AND processing, and the lower row illustrates the bounds for OR processing. The left hand plots give the traditional CDF space plots, with the bounds on the CDF for the redundant signals response times. The right hand plots show the newer unified capacity space version of the same bounds, plotted against the empirical capacity coefficient function.
Figure 3. Sample fPCA plots computed on the dots data included in the sft package. The far left plots show the component functions together with the mean capacity function; the center plots show the difference between the component and the mean capacity functions. The right-hand plots show the loading scores for each participant (x-axis) and for each experimental condition (here, termed OR and AND).
Figure 4. Sample assessment function plots computed on one participant (S7) in the the system data included in the sft package.
Opinions, Influence, and Zealotry

Author Name Omitted

the date of receipt and acceptance should be inserted later

Abstract A novel dinier automaton model for innovation diffusion based on a simplification of the AB model and zealot model is proposed. The model assumes that two opposing opinions are competing to be the dominant opinion among individuals in a network. Zealots are stubborn individuals whose opinion is not susceptible to influence by others. The amount of zealots required for consensus is measured experimentally in a number of different situations. The threshold density of zealots is far lower than the control experiment, suggesting that zealots have a much larger influence than normal individuals in the model. This threshold can be further reduced by placing zealots at critical nodes in the network, determined by standard social network measures or by using a greedy algorithm. Other experiments show that when both opinions have zealots, the outcome depends on the total number of zealots in addition to the ratio of zealots of opposite opinion, and often results in an “underdized” outcome.

Address(es) of author(s) should be given
1 Introduction

Innovation diffusion addresses the adoption of new technologies throughout society [20]. Since its introduction, the concept has been applied to a number of different domains not originally envisioned, and innovation diffusion is often used as a metaphor to describe any number of things (technologies, opinions, attitudes, decisions) that spread through a population. The innovation rate (i.e., the number of individuals who adopted the new technology) over time typically follows logistic-like growth (i.e., growing exponentially, and then slowing as the innovation nears full adoption). Ideally, from a marketing standpoint, understanding innovation diffusion helps answer the question “how do I ensure my product takes off?” Many studies have looked at this problem in hindsight, but general purpose, accurate, and reliable predictors are not currently available.

This paper introduces a new individual modeling and simulation approach for innovation diffusion that is predictive for a certain class of idealized, but realistic scenarios. The proposed model, which is certainly a gross oversimplification of human behavior, allows an individual to have a state taken from a small finite set of possible states. Individuals change their states over time by interacting with other individuals in a pairwise fashion according to a deterministic rule (however the order of interactions is random). Interactions are assumed to occur only between adjacent individuals in the user-defined network. Despite the limitations of this oversimplified individual model, there are several advantages worth highlighting.

First, and from a practical standpoint, the simplicity allows for a very efficient computer implementation. For example, a million simulations, each with ten thousand individuals, were completed in a few minutes using the proposed model on
a single workstation with an adequate CPU. Second, models designed to be “realistic” often become so complex that it is difficult or impossible to reason about which components are most directly influencing the observed behavior, or are even important to the model. Simple models are more easily communicated between researchers in disparate areas, and can be implemented and modified with little effort to produce new results. Furthermore, the fine details of individual complexity tend to “wash out” when one considers the collective behavior of populations. Use of a simpler model can help circumvent these issues. Finally, a simpler model is more amenable to future rigorous analytical treatment, especially if it can be shown that the model elegantly captures some interesting behavior. Thus, these advantages make simple individual models attractive for use in large scale simulations, which are necessary to understand and predict the collective behavior of individuals.

1.1 Related Work

Threshold models were one of the earliest attempts to understand how individual variations throughout a population affected the innovation diffusion curve [17]. These models assume that each individual has complete information about all other individuals and has some threshold for taking action based on this information. However, the assumption for individuals to have complete information may not always be appropriate, so relaxation of this assumption led to models such as the Linear Threshold Model [24]. In this model, a individual has a state encoding whether they have or have not adopted. Once adopted, the individual cannot un-adopt, so the diffusion is progressive. With the Linear Threshold Model, individuals adopt if the fraction of neighbors having adopted is larger than their
given threshold. The threshold can be randomly assigned, or fixed (e.g., to 1/2).
Models like this strive to represent the behavior of an individual in a way that allows
the collective behavior of the population to be an emergent property of the
system. The power of individual models is that, when successful, they illuminate
the relationship between individual actions and collective outcomes.

There are many other individual models of social dynamics including broad ac-
cess such as opinions, cultures, languages, and crowds [5]. Another adoption model,
The Independent Cascade Model, assumes a stochastic law, giving each newly
adopting individual one opportunity to influence each of its neighbors according
to some probability [10]. The voter model is a simple and popular model for opin-
ion dynamics [12]. In this model, one picks a vertex at random and the state of
that vertex is then changed to take on the state of a randomly chosen neighbor,
which performs coarsening via interface noise. There have been many variants and
explorations into this simple model. The ideas presented in this paper are based on
the zealot variant [21, 22] and the centrist/AB variant [26, 4]. In the zealot variant,
some vertices are "zealots" and have a bias towards one opinion over the other.
The existence of a few zealots can significantly affect the long term outcome of
the system. In the centrist/AB variant, an additional intermediate state is intro-
duced, and it is assumed that states cannot change without first passing through
the intermediate state (i.e., in order to change from A (left) to B (right) one must
first become AB). In the AB model, the probability that A → AB, AB → B, etc.,
is based on the neighborhood density of A, B, and AB.

It is known that models with intermediate states like the AB model accomplish
coarsening by reducing the surface tension along the boundary between opposing
domains. Such models are sometimes referred to as "curvature driven" models.
as opposed to interface noise models. Furthermore, the models discussed above are different from rumor and epidemic models, since the opinions compete for territory versus quickly spreading within vulnerable regions as epidemic models do. The model presented in this paper is a combination of the zealot and the AB model, and a simplification of both.

Given a model of influence and opinion or adoption like those discussed above, is it possible to determine a small set of individuals that, when influenced, can catalyze change throughout the entire network? This question is at the heart of the research area of Influence Maximization [8]. A solution close to optimal is very valuable in a marketing context, for example, as it could lead to an effective allocation of advertising resources. The current basis for influence maximization techniques is to assume an adoption model like the Linear Threshold Model [24] or the Independent Cascade Model [16] and compute the smallest set of seeds that will cause adoption to spread throughout the entire network.

The greedy algorithm by Domingos et al., works by computing the spread of influence throughout the network for a given set (which is initially empty), and finding the individual (who is not in that set) that increases the spread of influence the most [8]. That individual is chosen and added to the set, and the algorithm repeats until the influence has covered the entire network, with the solution being the set after termination of the algorithm. Kempe et al. later proved that the greedy algorithm will reach within 63% of optimal for these models [15]. Because the greedy algorithm is effective, but computationally expensive, researchers have developed techniques that improve the efficiency of influence maximization techniques [27, 8, 11, 19].
1.2 Proposed Model

The model to be proposed here is a dimer automaton model of opinion dynamics involving zealots and curvature-driven coarsening via an intermediate state. Dimer automata are similar to voter models; however, instead of updating one vertex at a time, one edge is chosen per asynchronous update step. For this reason a dimer automaton can be thought of as a pattern matching and substitution system. Both endpoints of that edge may be simultaneously changed, avoiding the asymmetry problem with the voter model [3]. Formally, we assume some graph $G = (V, E)$ where $V$ and $E$ can be interpreted as the individuals and their relationships in the model, respectively. Let $x_j^t$ be the state of vertex (individual) $i$ at time $t$. To perform an update, an edge $(i, j) \in E$ is chosen at random, and the endpoints of the edge are updated symmetrically such that

$$x_i^{t+1} = R(x_i^{t}, x_j^{t}), \quad x_j^{t+1} = R(x_i^{t}, x_j^{t}).$$

(1)

The application of the rule to $x_i^{t}$ and $x_j^{t}$ can be thought of abstractly as $i$ and $j$ interacting at time $t$. Also, $t$ is simply a counter of the number of edges updated so far, and only one edge is updated at a time (but edges can be updated many times over the course of the simulation). The extremely large space of rules for a given set of states is gives dimer automata the potential to model a wide range of phenomena. The rule behaves as a finite state automaton from the viewpoint of each $x_i$. For the opinion dynamics model for this paper, let the rule be defined as

$$R(\sigma, \tau) = \begin{cases} 
|\tau| & \text{if } \sigma = 0 \\
0 & \text{if } \sigma > 0 \text{ and } \sigma \neq |\tau| \text{ and } \tau \neq 0, \\
\sigma & \text{else}
\end{cases}$$

(2)
which is based on earlier 3-state dimer automaton rule for domains concerning [1]. This logic encoded in this rule is “generalized,” meaning the rule can support an arbitrary number of possible opinions without any modification.

It is important to differentiate between the opinion of an individual and the state of that individual. An individual with state $s$ has opinion $[s]$. Thus, the sign of the state designates whether that individual is a zealot or not (zealots are negative). State $0$ acts as the intermediate (i.e., centrist/AB) state that positive states must pass through to change from one opinion to another. Since dimer automaton rules are deterministic, the proposed model is a simplification of the centrist/AB model. The allowable transitions are equivalent, but it is not necessary to know the how many neighbors have a particular state, which simplifies the model and improves the computational efficiency. Finally, it is worth noting that the meaning of “zealot” in a dimer automaton is slightly different than in the previous literature. Voter model zealots have a bias towards a particular opinion, which is implemented as an increased probability that the zealot will take on that state. However, a zealot in the dimer automaton model can be thought of having maximal bias towards a particular opinion (i.e., the probability the zealot takes on its favored opinion is 1). This is a result of dimer automaton rules being deterministic, as opposed to voter model rules which are probabilistic.

For clarity, consider the following example. Suppose there are two political parties referred to as “red” and “blue,” which are equivalent to opinion 1 and opinion 2 respectively. Suppose Alice and Bob are friends (i.e., the edge $(Alice, Bob) \in E$ so the dimer automaton can randomly choose the edge connecting Alice and Bob and update their states). Let $x_A$ and $x_B$ refer to the state of Alice and Bob, respectively. If Alice and Bob are both red or both blue (i.e., $x_A = x_B$), then no
change occurs when they interact since $R(1, 1) = 1$ and $R(2, 2) = 2$. However, suppose Alice is red and Bob is blue (i.e., $x^0_A = 1$ and $x^0_B = 2$); after they interact, both Alice and Bob would become undecided and susceptible to influence (i.e., $x_B^{t+1} = x_B^{t+1} = 0$ since $R(1, 2) = R(2, 1) = 0$). It would then fall to another friend of Alice and/or Bob to reorient their affiliations. For example, suppose Eve is friends with Alice, and Eve is blue. Then, when Eve interacts with the undecided Alice, Eve persuades Alice to become blue (i.e., $x_A^{t+2} = 2$ since $R(0, 2) = 2$). Thus, Alice has switched from red to blue through the influence of both Bob and Eve. This mechanism is what drives the curvature based dynamics since, on average, Alice will adopt the opinion of the majority of her neighbors.

The zealot is a simple mechanism intended to account for stubborn individuals, since a zealot never changes their opinion. In the political debate, it is generally accepted that a certain percentage of individuals will never change their political affiliation; in fact people may change their friends to suit their affiliations [5]. So, suppose this time that Alice is a red zealot, and Bob is still just blue (i.e., $x_A' = 1$ and $x_B' = 2$). When Alice and Bob interact, Alice remains a red zealot, but Bob becomes undecided (i.e., $x_A^{t+1} = -1$ and $x_B^{t+1} = 0$ since $R(-1, 2) = -1$ and $R(2, -1) = 0$). The same effect happens when Alice and Eve interact. If Alice and Bob interact again (with Bob now undecided), Bob will be recruited over to red from undecided, however Bob never becomes a zealot (i.e., $x_A^{t+2} = -1$ and $x_B^{t+2} = 1$ since $R(1, -1) = -1$ and $R(0, -1) = 1$). The rule is designed such that non-zealots never become zealots, and zealots never become non-zealots.
2 Experiments

2.1 Control

We are interested in understanding how opinions collectively change over time, and how this change depends on the initial configuration of the system (i.e., $a_i^0$ for each $i \in V$). For this section we consider a simple case where the system is almost entirely non-neutral blue, aside for a handful of red nodes. Each node is assigned to a randomly chosen vertex in the graph. Does the system reach a consensus after a reasonable amount of time? An example of this is shown in Fig. 1. The four snapshots show the configuration of the system after the application of Eqn. 2 millions of times. Initially the system consists only of blue states (shown as white) and a few red states (shown as black), but the red states are able to quickly spread their influence and dominate the entire system.

Fig. 1: The configuration of the system over time (moving from left to right) shows the consensus transforming from opinion 1 (white) to opinion 2 (black).

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1 Consensus is measured as the ratio of the number of opinion 2 non-neutral to total non-neutral. Red dots are left out of this ratio since the population is known at the start of the simulation and does not change.

2 The graph used is a 100 x 100 square lattice with von Neumann neighborhoods and periodic boundary conditions, since this has a straightforward visualization.
For subsequent experiments in this section we use a Watts-Strogatz small world network [29] with rewire probability 0.1 and size 100 × 100. Fig. 2 shows how the consensus changes over time. The dynamics are more complicated than classical population-based models of innovation diffusion, which often follow a logistic curve. The system goes through a period of slowing growth, then quickening growth, and again slowing as consensus is nearly reached. This curve exhibits two inflection points, as opposed to the logistic curve which has only one.

![Diffusion of Innovation](image)

**Fig. 2** The average consensus over time has two inflection points, a more complex and realistic behavior than the typical logistic curve associated with innovation diffusion.

2.2 A Simple Experiment with Zealots

What effect, if any, do zealots have on the system, and how do we measure this? To begin, we must first run a control experiment with no zealots present, and observe the outcomes of different ratios of initial opinions. In other words, what is the
outcome starting with mostly red versus mostly blue? Fig. 3 shows the outcome of 9246 experiments with varying opinion densities in the initial configuration. There is only a small window centered around 0.5 (i.e., equal quantities of opinion 1 and 2) where the density of the final configuration is between 0 or 1 (i.e., the outcome is uncertain). So, 0.5 appears to be a critical point for the system with any density slightly above or below moving quickly to 1 or 0. Based on this, we can set 0.5 be a reasonable threshold to determine whether or not the zealots have taken over the system. In other words, once an opinion is held by more than half the population, that opinion tends to quickly take over the rest of the network.

Fig. 3: Control experiment varying the initial density of opinion 1 and 2 (no zealots) for a small world network (Watts-Strogatz, d = 2, p = 0.5).

Now we can determine what initial density of zealots is necessary to shift the consensus from the prevailing opinion to the opinion of the zealots. If zealots only exert short range influence, then the control suggests the threshold for consensus

---

3 Experiments were efficiently conducted in parallel on the GPU using the technique described in [2].
would remain close to 0.5. Repeating and averaging a number of independent trials for a range of zealot densities tests this hypothesis. For each experiment and once the number of zealots are determined, each zealot is assigned to random vertex in the network. We define the “critical zealot density” \( Z_* \) as the initial zealot density that produces a consensus above \( \epsilon \), and for this experiment let \( \epsilon = 0.5 \).

This quantity is computed in a straightforward manner according to Algorithm 1. An example of this measurement is shown in Fig. 4, where the order provided to the algorithm was a random permutation of the nodes in the network. Surprisingly, we can see that \( Z_* \) (approximately 0.074, shown by the dotted line) is nearly an order of magnitude lower than the density observed in the control. Zealots have a much higher influence on the outcome than expected.

Algorithm 1 Compute \( Z_* \) for a given order.

1. Let \((v_1, v_2, ..., v_{|V|})\) be an ordering of the vertices in the network
2. \( i \leftarrow 1 \)
3. \( Z_* = \epsilon / |V| \)
4. procedure consensus()
5. \( X \leftarrow \{1, 1, ..., 1\} \quad \triangleright \text{has length } |V| \)
6. \( X(v_1) = -2 \quad \triangleright \text{assign zealots based on order} \)
7. run an experiment with \( X_0 \) as the initial configuration
8. measure the consensus at the end of the experiment
9. return \( \frac{1}{|Y|} \sum_{i \in Y} \epsilon_i \)
10. end procedure
2.3 Varying Network Structure

The previous experiment is repeated with different graphs to determine the effect of the network used on the critical zealot density. The Watts-Strogatz small world network [29] is a common way to explore how a model or phenomenon is affected by network structure. This model defines a rewire probability $p$, which generates networks that transition between uniformity (e.g., a square lattice) and randomness. From Fig. 5 we can see that the graph has an interesting effect on the critical zealot threshold. As the rewire probability is increased (and the network becomes more disorganized) $Z_c$ increases quickly. However, this threshold appears to level out and does not surpass 0.1, even for a fully disorganized network. From this we can conclude that the network structure has a significant effect on $Z_c$, so subsequent experiments consider a variety of networks.
2.4 Influence Maximization

Influence maximization is a useful application for models of opinion dynamics such as the one proposed in this paper. Given a model and network, influence maximization helps us find a small set of individuals that can precipitate a change throughout the entire network [8]. For the zealot dimer automaton model proposed in this paper, the problem of influence maximization translates into finding the optimal set of nodes in the network that should start as zealots in the initial configuration. Past research in influence maximization has shown that the greedy algorithm outperforms random selection as well as other heuristics based on social network analysis measures such as closeness, betweenness, and degree. The purpose of the following experiment is to determine whether this result also holds for the zealot dimer automaton model.

Based on the experiment in the previous section, we know that the structure of the network can have a significant effect on the consensus threshold $\xi_c$, even if

Fig. 5: As the network transitions from order to disorder, the critical zealot density increases.
Table 1: Networks for Influence Maximization Experiment

| name         | |V|   | |E|   | details                                                                 | ref(s) |
|--------------|---|----|---|----|-------------------------------------------------------------------------|-------|
| wiki-Vote    | 7110 | 100699 | who votes on whom for Wikipedia ad- | [17,18] |
|              |     |     |   |    | membership elections                                                   |       |
| ca-HepTh     | 9877 | 25598 | High Energy Physics-Theory arXiv  | [18]  |
|              |     |     |   |    | collaboration network                                                  |       |
| ca-GrQc      | 5242 | 14496 | General Relativity and Quantum Cos- | [18]  |
|              |     |     |   |    | mology arXiv collaboration network                                      |       |
| Power Law Cluster | 10600 | 20699 | random scale free network with m = | [14]  |
|              |     |     |   |    | 3, p = 0.1                                                             |       |
| Erdos-Renyi  | 10000 | 50008 | random graph with $p = 1.24 \times 10^{-3}$ | [3] | |
| Watts-Strogatz| 10600 | 20600 | random small world network with k = | [25]  |
|              |     |     |   |    | 9, p = 0.2                                                             |       |

Zealots are chosen randomly. Therefore, the following experiment considers several types of networks (see Table 1) as well as several different heuristics for influence maximization. Heuristics are based on centrality metrics from social network analysis centrality: degree, closeness, and betweenness [28]. Degree centrality simply measures the number of neighbors adjacent to a given node. Closeness centrality is the inverse of the average distance for a given node to all other nodes. Betweenness centrality considers the fraction of all shortest paths that pass through a given node. Each of these metrics are measured for all nodes in the network to determine a ranking. These metrics determine an ordering of the nodes in the network, which are used by Algorithm 1 to compute the critical zealot density resulting from that particular ordering.

These heuristics are compared against a variation of the classical greedy algorithm for influence maximization [8], adapted for use with the zealot dimer automa-
Table 2: Summary of Results for Influence Maximization Experiment

<table>
<thead>
<tr>
<th>Graph Model</th>
<th>betweenness</th>
<th>random</th>
<th>degree</th>
<th>greedy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Erdős-Rényi</td>
<td>$6.89 \times 10^{-2}$</td>
<td>$7.44 \times 10^{-2}$</td>
<td>$6.43 \times 10^{-2}$</td>
<td>$8.44 \times 10^{-2}$</td>
</tr>
<tr>
<td>Watts-Strogatz</td>
<td>$6.00 \times 10^{-2}$</td>
<td>$6.93 \times 10^{-2}$</td>
<td>$6.90 \times 10^{-2}$</td>
<td>$6.50 \times 10^{-2}$</td>
</tr>
<tr>
<td>Power Law Cluster</td>
<td>$9.13 \times 10^{-5}$</td>
<td>$2.20 \times 10^{-5}$</td>
<td>$9.00 \times 10^{-5}$</td>
<td>$9.60 \times 10^{-5}$</td>
</tr>
<tr>
<td>ca-GrQc</td>
<td>$1.81 \times 10^{-2}$</td>
<td>$1.34 \times 10^{-2}$</td>
<td>$1.37 \times 10^{-2}$</td>
<td>$1.37 \times 10^{-2}$</td>
</tr>
<tr>
<td>ca-HepTh</td>
<td>$1.94 \times 10^{-2}$</td>
<td>$2.22 \times 10^{-2}$</td>
<td>$8.00 \times 10^{-3}$</td>
<td>$1.49 \times 10^{-2}$</td>
</tr>
<tr>
<td>wiki-Vote</td>
<td>$9.70 \times 10^{-3}$</td>
<td>$1.21 \times 10^{-2}$</td>
<td>$8.15 \times 10^{-3}$</td>
<td>$1.14 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

The model, which is outlined in Algorithm 2, this algorithm starts with an initial configuration $X_0$ and a set of allowable moves encoded in $M = \{(v_1, \sigma_1), (v_2, \sigma_2), \ldots\}$, where the $k$th move changes the state of node $v_k$ to $\sigma_k$ in the initial configuration. In the simplest case where we start with all opinion $1$ and want to see how many opinion-2 residents are needed to reach the critical threshold, we would let $X_0 = (1, 1, \ldots, 1)$ and $M = \{(i, -2) : i \in V\}$. Algorithm 2 also requires an objective function $\phi$ to minimize. In this case $\phi$ measures the consensus by counting the nodes in the network not having opinion 2, thus

$$\phi = \frac{1}{|V|} \sum_{i \in V} \delta(2, |x_i|). \quad (3)$$

The results of the comparison for each graph and heuristic are shown in Figure 6, and a summary of the critical node densities is provided in Table 2. Surprisingly, no single heuristic nor the greedy algorithm is a clear winner, though, the random heuristic usually results the worst critical density. Another interesting feature seen in Figure 6 is that the greedy algorithm tends to dominate the other heuristics early in the simulation, but may not be the first to reach criticality.
Algorithm 2 Greedy algorithm for influence maximization for the zealot model
1. $X_0$ is the initial configuration of the network
2. $\phi$ is an objective function that scores the configuration of the network
3. $M$ is the list allowable moves
4. $M$ = current random number generator state
5. while convergence criteria not met do
6. $h_i = \arg\max_{h} \phi(X_i, h)$
7. $(i, \sigma) = M(h)$
8. $X_{i+1}(i) = \sigma$
9. end while
10. procedure score($X, h$)
11. set random number generator state to $M$
12. $(i, \sigma) = M(h)$
13. $X(i) = \sigma$
14. $X^\prime = \text{result of experiment with initial input of } X$
15. return $\phi(X^\prime)$
16. end procedure

2.5 Competitive Zealotry and Political Polarization

Realistically, we can expect to encounter both individuals who advocate for change, and those who resist it. In other words, we should investigate scenarios where zealots are present for both opinions. Clearly the outcome will depend on the ratio of these two types of zealots, but it may also depend on the total quantity of both types of zealots as well. Fig. 7] measures the consensus of the system for $95^2$ different pairs of zealot densities in the range from 0 to 0.5. For each pair, the experiment is run 100 times for a reasonable sample size. In this figure, a line is drawn showing when the consensus crosses 35% and 65%, which separates the diagram into three distinct regions.
Fig. 6 The greedy algorithm for influence maximization is compared against rankings based on social network analysis metrics for several different graphs.

Fig. 7 Phase diagram for multi zealot experiment on Barabási-Albert network
If the consensus was solely dependent on the ratio of competing zealots, we
would expect the transition between opinion 1 and 2 to follow a straight line whose
slope was equal to the critical ratio. However, this transition follows a curved line.
Furthermore, when the quantity of both zealots passes a certain threshold, the
outcome becomes meta-stable (i.e., a stable combination of both opinions), which
we refer to this as the "undecided" phase. When the density of opinion 1 zealots
is low (e.g., < 0.1), the system chooses only between red and blue. However, with
high enough densities of red and blue zealots, the system tends to remain in an
undecided state, with significant amounts of both opinions present. This suggests
that this model may be applicable to phenomena like political polarization where
opposing opinions are held by significant fractions of the population.

To test this, we apply the influence maximization algorithm for the zealot
model to a dataset consisting of politically charged communications between users
of social media [7]. In addition to containing a social network, each node in the
dataset is labeled as either left or right leaning, providing ground truth about
opinions that can be leveraged. Applying influence maximization to this dataset
requires some modifications since we are now maximizing influence for more than
one target opinion. First, we assume that the initial configuration consists entire
of some arbitrary third opinion, thus $X_0 = (3, 3, ..., 3)$. Now, assuming that $X_T$
is the target configuration of opinions in the network (i.e., the ground truth), the
objective function becomes

$$\phi = \sum_{i \in V} 1 - \mathbb{I}(x_i \neq x_T(i))$$  \hspace{1cm} (4)

and the set of allowable moves are $M = \{(i, -X_T(i)) : i \in V\}$. 

Distribution A: Approved for public release; distribution unlimited.
88 ABW Cleared 02/13/2014; 88ABW-2014-0516.
3 Discussion

4 Conclusions & Future Work

The dimer automaton model presented combines and simplifies two variants models of opinion dynamics: the zealot model and the AB model. The resulting coarsening phenomena is curvature driven, and is used to investigate innovation diffusion. Using this model, we investigated some basic questions, namely, how many zealots are needed to reach consensus? The critical threshold of zealots required was significantly lower than 0.5, meaning only a few zealots in random locations in the network can significantly influence the entire system. This threshold depends on the network structure and the initial placement of the zealots in the network.

We also considered the case where both opinions have zealots, and some combination of zealots of both opinions leaves the system in an undecided state. Thus, the presence of individuals who refuse to change (e.g., opinion 1 zealots) could be an explanation of why some innovations fail to take hold.
A further challenge is to then verify these results against actual data such as marketing trials or elections. Real-world data is often incomplete or contains uncertainty, so an additional path for future work is to incorporate this into the model, perhaps by biasing how edges are randomly chosen by the dimer automaton according to a given probability distribution. Additionally it may be reasonable to upgrade the model so an individual’s state lies on some spectrum between the two extremes instead of being a sharp choice between two opposing opinions. Hopefully this can be done in a manner that preserves the simplicity and elegance of the original model. This approach may be necessary if the simple model presented in this paper is not sufficiently predictive for real-world data and scenarios.

References


Generalized Capacity Space

Running head: GENERALIZED CAPACITY SPACE

Generalized n-Channel Workload Capacity Space

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Draft: January 30, 2014
Please do not circulate or cite without authors' permission.

Keywords: workload, capacity, human information processing, race model
Abstract

We provide the n-channel extension of the unified workload capacity space bounds for standard parallel processing models with minimum-time, maximum-time, and single-target self-terminating stopping rules. This extension enables powerful generalizations of this approach to multiple stopping rules and any number of channels of interest. Mapping the bounds onto the unified capacity space enables a single plot to be used to compare the capacity coefficient values to the upper and lower bounds on standard parallel processing in order to make direct inferences about extreme workload capacity.
Generalized \( n \)-Channel Workload Capacity Space

The study of the combination of multiple sources of information is ubiquitous in cognitive psychology. Examples include visual and memory search tasks, in which the multiple sources are the array items through which a participant must search, and complex decision making tasks in which multiple types of information must be combined to make a good decision. One question that often arises is the extent to which adding more sources of information affects the processing of each individual source. For example, one might inquire whether it takes longer to determine the presence of a particular object in a stimulus when there are more total objects in the stimulus. In this paper, we refer to a cognitive system's response to variations in the number of information sources as its workload capacity.

One of the most commonly used measures of workload capacity is the Race Model Inequality (Miller, 1982), which gives an upper bound on the response speed of a parallel processing model with context invariance (defined below) for testing one versus two sources of information using cumulative distribution functions (CDFs) in the context of minimum-time, redundant target decisions. Subsequent to Miller's paper, the basic logic of the Race Model Inequality has been extended to develop a lower bound on minimum-time models as well as upper and lower CDF bounds for other stopping criteria (e.g., all information must be processed rather than any one source) and more sources of information (Grice et al., 1984; Colonius & Vorberg, 1994). Using a stronger set of assumptions, together with a well-defined baseline model, Townsend and colleagues derived an equality to test workload capacity, termed the capacity coefficient (Townsend & Nozawa, 1995; Townsend & Wenger, 2004; Blaha & Townsend, under review).

Recently, Townsend & Kedel (2011) introduced the notion of a unified workload capacity space for plotting both the capacity coefficient and the CDF bounds on standard parallel processing on the same plot space. This work served to transform the upper and
lower bounds on parallel processing from probability space (ordinate values bounded on $(0, 1]$) into the same unit-less axis as the capacity coefficient, with ordinate values bounded on $[0, +\infty)$. Practically, this unified space allows investigators to directly compare the same plot capacity coefficient values with the bounds on standard parallel processing, which enables some estimation of possible extreme capacity values (very high super capacity, very low limited capacity), as well as some inferences about possible model architectures (e.g., violation of the race model with super capacity implies a possible reactive model architecture). Unfortunately, Townsend & Eidelš (2011) limited their derivations to models with only two possible operating channels. The capacity coefficients are defined for $n \geq 2$ channels (Townsend & Wenger, 2004), as are the CDF bounds on standard parallel processing (Colonius & Vorberg, 1994), so the restriction to $n = 2$ channels is an unnecessary limitation of the applicability for the new unified space.

Herein, we complete the derivation of the unified workload capacity space by extending the transformations of the parallel model bounds to the general case of $n$ channels, where $n \geq 2$. We also provide the alternative versions for the unified space when the marginal distributions of the channels are assumed to be independent and identically distributed (IID), which serves to simplify the computations. Finally, in addition to the AND and OR cases derived in previous work, we add the bounds for single-target self-terminating processing, recently introduced in Blaha (2010) and Blaha & Townsend (under review).

We use the following notation throughout the paper. Let $F_{\mathcal{C}}(t) = P[T_{\mathcal{C}} \leq t]$ be the CDF of response times for a system with the set of $n$ active channels, $\mathcal{C} = \{1, \ldots, n\}$. To denote the CDF of a single channel $c$ among the $\mathcal{C}$ channels, we use $F_{c, \mathcal{C}}(t)$, and to denote the processing of a single channel $c$ alone (i.e., no other active channels in the model or $n = 1$), we use $F_{c}(t)$. We use set minus notation $\mathcal{C} \setminus \{c\}$ to indicate the full set of channels $\mathcal{C}$ except $c$. 
In this work, standard parallel processing is used to refer to a processing system that exhibits independent channel distributions (no cross-talk, no statistical facilitation/degradation). This means that for any number of active channels, the CDF for all channels active simultaneously is the product of the marginal distributions,

\[ F_C(t) = \prod_{c=1}^{n} F_{cC}(t). \]

Additionally, standard parallel processing exhibits context independence, or context invariance. This means that the marginal distribution of any given channel \( c \) is identically distributed when any number of additional channels are also operating. We denote this by \( F_c(t) = F_{cC}(t) \). Functionally, this allows the individual channels to be estimated by single-target or single-feature conditions in an experiment, which often greatly simplifies the number of conditions the experimenter needs to test in order to use these models.

Additionally, we note that standard parallel processing is often referred to as the parallel race model, the parallel horse-race model, or simply the race model (see, for example, Miller, 1982). This analogy specifically refers to the case when the first channel to finish processing is enough to make a response. This is the case of minimum time processing, also termed first-terminating stopping or an OR (logical OR-gate) stopping rule. This would be the stopping rule engaged in tasks like visual search among redundant targets (no distractors) where the identification of the first target to be searched is enough to complete the task. The standard parallel model architecture is engaged under other stopping rules, as well, including exhaustive stopping (last-terminating or logical AND stopping), and the in-between case of single-target self-terminating (ST-ST) stopping. In the former case, all channels must complete processing before a response is made. In the latter case, the completion of a specific single target channel is enough to terminate the processing, but the target channel may be any of the \( n \) possible channels - first, last, or somewhere in between. Each of these stopping rules changes the form of the capacity coefficient and the predictions of the race model bounds, so we will present the derivation
of the bounds in unified workload capacity space for each model in turn.

Before we get into the derivation of the unified response time bounds, we want to remind readers that all CDFs and survivor functions exist on the range $[0, 1]$, so the natural logarithm of those functions produce negative values. Thus, cumulative reverse hazard functions (natural log of the CDF) exist on the range $(-\infty, 0]$, as do the natural logarithms of any bounds formed by a single CDF or products of CDFs (sums of CDFs can range above 1, and so the natural log can exist on $(-\infty, +\infty)$). These negative values will influence the derivation of inequality chains throughout this paper. Note also that the cumulative hazard function used in the minimum time bounds, is found as the negative natural log of the survivor function, and so it exists on the range $[0, +\infty)$, leaving fewer negative signs to track in these proofs.

**Minimum Time Bounds**

Let $F_c(t) = P_{\min_{c'}(T_{c'}) \leq t}$, for all real $t \geq 0$ and $c \subseteq c'$, be the CDF for an $n$-channel system operating under a minimum time stopping rule, where $c' = \{1, \ldots, n\}$ is the set of all possible channels. Define $F_{c \setminus i}(t) = P_{\min_{c \setminus i}(T_{c \setminus i}) \leq t}$ as the CDF if all channels except $i$ are running, and define $F_{c \setminus i, j}(t) = P_{\min_{c \setminus i,j}(T_{c \setminus i,j}) \leq t}$, $i \neq j$, for the CDF of all channels but $i$ and $j$. Further, define the survivor function as $S_c(t) = 1 - F_c(t)$.

We measure the amount of work completed in each channel $c$ with the cumulative hazard function, defined as:

$$H_c(t) = \int_{s=0}^{t} \frac{f_c(\tau)}{S_c(\tau)} d\tau = -\ln(S_c(t))$$

which can easily be estimated directly from the empirical response time survivor function for any experimental condition.

The capacity coefficient for minimum time (first-terminating, OR) processing for an $n$-channel model is defined as a ratio of cumulative hazard functions (Townsend &
Nozawa, 1995; Townsend & Wenger, 2004):\[ C_{OR}(t) = \frac{H_c(t)}{\sum_{c=1}^{m} H_c(t)} \] (1)

The numerator in Equation 1 is the observed processing of \( n \) active channels, while the denominator is the prediction of a benchmark standard parallel processing model, exhibiting independence and, in this terminology, unlimited capacity. Thus, capacity is qualitatively inferred relative to a ratio equal to 1, which is where observed processing is equal to the benchmark model prediction and unlimited capacity is concluded. If \( C_{OR}(t) > 1 \), then super capacity, or better-than-benchmark, performance is inferred. And if \( C_{OR}(t) < 1 \), then limited capacity, worse-than-benchmark performance, is inferred.\footnoteref{fn:1}

The original race model CDF bound by Miller (1982) provided an upper bound on the CDF from the parallel, minimum-time model with \( n = 2 \) channels given by \( F_{A,B}(t) \leq F_A(t) + F_B(t) \), where \( A, B \) denote the two parallel channels. Grice et al. (1984) introduced the concept of a lower bound for the same processing model, which is defined as \( F_{A,B}(t) \geq \min \{ F_A(t), F_B(t) \} \).

Colonius & Vorberg (1994) provided the \( n \)-channel generalization of both CDF bounds on parallel minimum-time processing in the inequality chain
\[ \max_i \left[ F_{C_i}(t) \right] \leq C(t) \leq \min_{i,j} \left[ F_{C_{ij}}(t) + F_{C_{ij}}(t) - F_{C_{ij}}(t) \right] \] (2)

**Theorem 1.** The unified workload capacity space inequality chain for the capacity of an \( n \)-channel, minimum-time system is, for \( i \neq j \),
\[ \ln \left( \min \left\{ \frac{C(t)}{\prod_{s=1}^{n} S_s(t)} \right\} \right) \leq \ln \left( \max_{i,j} \left[ S_{C_{ij}}(t) + S_{C_{ij}}(t) - S_{C_{ij}}(t) \right] \right) \] (3)

**Proof.** From Equation 1, \( C_{OR}(t) \) \( = \min(\prod_{s=1}^{n} S_s(t)) = \ln(\sum_{s=1}^{n} S_s(t)) \). Rewrite the upper bound from Equation 2 in terms of the survivor functions to get
\[ S_{C}(t) \geq \min_{i,j} \left[ S_{C_{ij}}(t) - S_{C_{ij}}(t) - S_{C_{ij}}(t) \right] \]
It follows that

\[ C_{GR}(t) + \ln \left( \prod_{i=1}^{n} S_i(t) \right) \geq \ln \left\{ \max_{i,j} \left[ S_{C\setminus\{i\}}(t) + S_{C\setminus\{j\}}(t) - S_{C\setminus\{i,j\}}(t) \right] \right\} \]

\[ \Rightarrow C_{GR}(t) \leq \frac{\ln \left\{ \max_{i,j} \left[ S_{C\setminus\{i\}}(t) + S_{C\setminus\{j\}}(t) - S_{C\setminus\{i,j\}}(t) \right] \right\}}{\ln \left( \prod_{i=1}^{n} S_i(t) \right)} . \]

Similarly, rewrite the lower bound of Equation 2 as

\[ \min_{i} \left[ S_{C\setminus\{i\}}(t) \right] > S_C(t) \]

and it follows that

\[ C_{GR}(t) = \ln \left( \prod_{i=1}^{n} S_i(t) \right) \leq \ln \left\{ \min_{i} \left[ S_{C\setminus\{i\}}(t) \right] \right\} \]

\[ \Rightarrow C_{GR}(t) \geq \frac{\ln \left\{ \min_{i} \left[ S_{C\setminus\{i\}}(t) \right] \right\}}{\ln \left( \prod_{i=1}^{n} S_i(t) \right)} . \]

\[ \Box \]

Under the assumption that the marginal distributions for each channel are IID, then all \( F_{C\setminus\{i\}}(t) \) are the same for any choice of \( i \in C \) and we can write this as \( F_{C\setminus\{1\}}(t) \) to denote the CDF for a \( \alpha = 1 \) active channels. Similarly, the IID assumption means the \( F_{C\setminus\{i,j\}}(t) \) are the same for any choice of \( i,j \in C \), and we write this as \( F_{C\setminus\{2\}}(t) \) for the CDF with \( n - 2 \) active channels. Consequently, Equation 2 simplifies to (Colonius & Vorberg, 1994)

\[ F_{C\setminus\{1\}}(t) \leq F_C(t) \leq \left[ 2 \times F_{C\setminus\{2\}}(t) - F_{C\setminus\{1,2\},(t)} \right] . \]

**Lemma 1.** When the marginal distributions of the parallel model are IID, the unified workload capacity space inequality chain for the capacity of an \( n \)-channel, minimum-time system is defined by

\[ \frac{\ln \left\{ \min_{i} \left[ S_{C\setminus\{i\}}(t) \right] \right\}}{\ln \left( \prod_{i=1}^{n} S_i(t) \right)} \leq C_{GR}(t) \leq \frac{\ln \left\{ 2 \times \left[ S_{C\setminus\{1\}}(t) - S_{C\setminus\{2\}}(t) \right] \right\}}{\ln \left( \prod_{i=1}^{n} S_i(t) \right)} \]

\[ (5) \]

The proof of Lemma 1 is similar to the proof of Theorem 1 and is left to the reader.
Maximum Time Bounds

Let $G_C(t) = P[\max_{c \in C}(T_c) \leq t]$, where again $C = \{1, \ldots, n\}$ is the set of all $n$ channels and $c \in C$, be the cumulative distribution function of response times for an $n$-channel system under a maximum time (logical AND, exhaustive) stopping rule.\footnote{\cite{Townsend2004}}

In order for the capacity coefficient inferences to be consistent with those for Equation 1, we utilize the cumulative reverse hazard function to measure the work throughput for each channel under the maximum-time stopping rule (for a full discussion of the reasoning, see Townsend & Wenger, 2004; Townsend & Fadel, 2011).

The cumulative reverse hazard function for processing channel $c$ is given by

$$K_c(t) = \int_{t=0}^{t} \frac{g_c(\tau)}{G_C(\tau)} d\tau = \ln(G_C(t))$$

which, again, can easily be estimated directly from the empirical response time CDF for any experimental condition.

The capacity coefficient for maximum time processing is defined as (Townsend & Wenger, 2004)

$$C_{\text{AND}}(t) = \frac{\sum_{c=1}^{n} K_c(t)}{K_C(t)} \tag{6}$$

The numerator in the AND case is the prediction of the benchmark unlimited capacity, independent parallel model, while the denominator is the observed processing of $n$ channels under the maximum-time stopping rule. Capacity inferences, again, are relative to the value $C_{\text{AND}}(t) = 1$, which indicates unlimited capacity. $C_{\text{AND}}(t) > 1$ indicates super capacity processing, and $C_{\text{AND}}(t) < 1$ indicates limited capacity processing.

Derived by Colonius & Verberg (1994), the general bounds for $n$ exhaustively processed channels are

$$\max_{i,j} [G_{C_i}(t) + G_{C_j}(t) - G_{\min}(t)] \leq G_C(t) \leq \min_{i,j} [G_{C_i}(t)]. \tag{7}$$
Theorem 2. The unified workload capacity space inequality chain for the capacity of an n-channel, maximum-time system is, for \( i \neq j \),

\[
\ln \left( \prod_{j=1}^{n} G_{j}(t) \right) \leq \ln \left( \max_{i,j} \left[ G_{i\setminus j}(t) + G_{j\setminus i}(t) - G_{C_{i\setminus j}}(t) \right] \right) \leq C_{\text{AND}}(t) \leq \ln \left( \prod_{j=1}^{n} G_{j}(t) \right) \leq \ln \left( \min_{i,j} \left[ G_{C_{i\setminus j}}(t) \right] \right). \tag{8}
\]

Proof. From Equation 6, \( C_{\text{AND}}(t) = \ln \left( \prod_{j=1}^{n} G_{j}(t) \right) \). Utilizing Equation 7, it follows that, for the upper bound,

\[
\ln \left( \prod_{j=1}^{n} G_{j}(t) \right) \leq \ln \left( \min_{i,j} \left[ G_{C_{i\setminus j}}(t) \right] \right) \leq C_{\text{AND}}(t) \approx \ln \left( \prod_{j=1}^{n} G_{j}(t) \right) \geq C_{\text{AND}}(t).
\]

Similarly, for the lower bound,

\[
\ln \left( \prod_{j=1}^{n} G_{j}(t) \right) \geq \ln \left( \max_{i,j} \left[ G_{i\setminus j}(t) + G_{j\setminus i}(t) - G_{C_{i\setminus j}}(t) \right] \right) \geq C_{\text{AND}}(t) \approx \ln \left( \prod_{j=1}^{n} G_{j}(t) \right) \geq C_{\text{AND}}(t).
\]

\[\square\]

Under the assumption that the marginal distributions for each channel are IID, for any choice of \( i \in \mathcal{C} \), all \( G_{C_{i\setminus j}}(t) \) are the same and for any choice of \( i, j \in \mathcal{C} \), all \( G_{C_{i\setminus j}}(t) \) are the same. We write these as \( G_{C_{i\setminus j}}(t) \) and \( G_{C_{i\setminus j}}(t) \), for \( n - 1 \) and \( n - 2 \) active processing channel systems, respectively. It follows that Equation 7 simplifies to (Colonius & Vorberg, 1994):

\[
2 \cdot G_{C_{i\setminus j}}(t) - G_{C_{i\setminus j}}(t) \leq G_{C_{i\setminus j}}(t) \leq G_{C_{i\setminus j}}(t). \tag{9}
\]
**Lemma 2.** When the marginal distributions of the parallel model are IID, the unified workload capacity space inequality chain for the capacity of an n-channel, maximum-time system is defined by

\[
\frac{\ln\left(\prod_{k=1}^{n-1} G_k(t)\right)}{\ln\left(2 + \frac{G_{\text{AND}}(t)}{G_{\text{AND}}(t) - G_{\text{AND}}(t)}\right)} < C_{\text{AND}}(t) < \frac{\ln\left(\prod_{k=1}^{n-1} G_k(t)\right)}{\ln\left(G_{\text{AND}}(t)\right)}. \tag{10}
\]

The proof of Lemma 2 is similar to the proof of Theorem 2 and is left to the reader.

**Single-Target Self-Terminating Bounds**

Blaha (2010) recently introduced a new capacity coefficient for ST-ST processing, with full details explicated in Blaha & Townsend (under review). For completeness with respect to the results in Townsend & Eldees (2011), we here give the ST-ST parallel processing CDF bounds for both \(n = 2\)-channel models and \(n \geq 2\)-channel models.

Let \(F_{k,C}(t) = P[T_{k,C} < t]\) denote the CDF of response times for target channel \(k \in \mathcal{C}\). Let \(K_{k,C}(t) = \int_0^t \frac{f_{k,C}(r)}{F_{k,C}(r)} dr = \ln(F_{k,C}(t))\) be the cumulative reverse hazard function for target channel \(k \in \mathcal{C}\).

The capacity coefficient for ST-ST processing is defined as (Blaha, 2010; Blaha & Townsend, under review)

\[
C_{\text{ST-ST}}(t) = \frac{K_k(t)}{K_{k,C}(t)}. \tag{11}
\]

The benchmark parallel model is in the numerator of \(C_{\text{ST-ST}}(t)\), and the observed processing of target channel \(k\) among \(n\) active channels is in the denominator. The inferences about unlimited, limited, and super capacity are the same as the OR and AND models.

The bounds on ST-ST processing are

\[
\prod_{c=1}^{n} F_c(t) < F_{k,C}(t) < \sum_{c=1}^{n} F_c(t). \tag{12}
\]
For $n = 2$ channels, with the two channels denoted $\mathcal{C} = \{1, 2\}$, the bounds simplify to

\[ F_1(t) \cdot F_2(t) \leq F_{k,c}(t) \leq F_1(t) - F_2(t). \]

**Theorem 3.** The unified workload capacity space inequality chain for the capacity of an $n$-channel, single-target self-terminating system is,

\[
\frac{\ln \{ F_k(t) \}}{\sum_{c=1}^{n} \ln \{ F_c(t) \}} \leq C_{ST-ST}(t) \leq \frac{\ln \{ F_k(t) \}}{\ln \{ \sum_{c=1}^{n} F_c(t) \}},
\]

(13)

The proof of Theorem 3 is nearly identical to the proof of Theorem 2, substituting the capacity coefficient and bounds for ST-ST capacity in for those of maximum-time processing.

Under the assumption that the marginal distributions for each channel are IID, we use the CDF of a single channel $c \in \mathcal{C}$, and rewrite Equation 12 as

\[
\{ F_c(t) \}^n \leq F_{k,c}(t) \leq n \cdot F_c(t).
\]

(14)

**Lemma 3.** When the marginal distributions are IID, the unified capacity space bounds for ST-ST processing are

\[
\frac{\ln \{ F_k(t) \}}{n \cdot \ln \{ F_c(t) \}} \leq C_{ST-ST}(t) \leq \frac{\ln \{ F_k(t) \}}{\ln \{ n \cdot F_c(t) \}}.
\]

(15)

The proof of this is trivial and left to the reader.

**Conclusion**

We have provided the straightforward extension of the unified workload capacity space bounds for standard parallel processing from the limited existing definitions for $n = 2$ channels given in Townsend & Elseds (2011) to the full $n \geq 2$-channel situation for
minimum-time, maximum-time, and single-target self-terminating stopping rules. The full set of bounds, including all special cases considered to date, are summarized in Table 1.

This extension enables powerful generalizations of this approach to multiple stopping rules and any number of channels of interest, in order to model the complete processing mechanisms for an experiment of interest. Mapping the bounds onto the unified capacity space for any number of channels enables a single plot to be used to compare the capacity coefficient values to the upper and lower bounds on standard parallel processing in order to make more direct inferences about extreme capacity values.

References


Author Note

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This research was supported by AFOSR grant 12RH14COR to L.M.B and AFOSR FA0001-13-1-0087 to J.W.H.

Distribution A: Approved for public release; distribution unlimited. 88ABW

Cleared 01/17/2014; 88ABW-2014-0140
Footnotes

1 We note that appropriate statistical tests for inferences about $C_{GR}(t)$ are available (Haupt & Townsend, 2012), but their details are beyond the scope of this paper.

2 Note that the change in notation here is to simply help the reader distinguish the CDFs for minimum- and maximum-time stopping rules.
### Table 1

*Summary of all Bounds on the Capacity Coefficient*

#### LOWER.getBounds

<table>
<thead>
<tr>
<th>Stopping Rule</th>
<th>( n )-channels</th>
<th>( n ) IID channels</th>
<th>2 channels</th>
</tr>
</thead>
<tbody>
<tr>
<td>OR</td>
<td>( \frac{\ln(\max_t</td>
<td>S_t</td>
<td>)}{\ln(\sum_{i=1}^{n} S_i)} )</td>
</tr>
<tr>
<td>STST</td>
<td>( \frac{\ln(F_{(t)} \cdot \sum_{i=1}^{n} \ln(F_{(i)})}{n} )</td>
<td>( \frac{\ln(F_{(t)} + \ln(F_{(t)})}{n} )</td>
<td>( \frac{\ln(F_{(t)} + \ln(F_{(t)})}{n} )</td>
</tr>
<tr>
<td>AND</td>
<td>( \frac{\ln(\prod_{i=1}^{n} G_{(i)}}{\ln(\max_{i=1}\prod_{i=1}^{n} G_{(i)}} )</td>
<td>( \frac{\ln(\prod_{i=1}^{n} G_{(i)}}{\ln(\max_{i=1}\prod_{i=1}^{n} G_{(i)}} )</td>
<td>( \frac{\ln(G_{(1)} + G_{(2)} + G_{(1)} + G_{(2)})}{\ln(\max_{i=1}\prod_{i=1}^{n} G_{(i)}} )</td>
</tr>
</tbody>
</table>

#### UPPER.getBounds

<table>
<thead>
<tr>
<th>Stopping Rule</th>
<th>( n )-channels</th>
<th>( n ) IID channels</th>
<th>2 channels</th>
</tr>
</thead>
<tbody>
<tr>
<td>OR</td>
<td>( \frac{\ln(\max_t</td>
<td>S_t</td>
<td>)}{\ln(\sum_{i=1}^{n} S_i)} )</td>
</tr>
<tr>
<td>STST</td>
<td>( \frac{\ln(F_{(t)} \cdot \sum_{i=1}^{n} \ln(F_{(i)})}{n} )</td>
<td>( \frac{\ln(F_{(t)} + \ln(F_{(t)})}{n} )</td>
<td>( \frac{\ln(F_{(t)} + \ln(F_{(t)})}{n} )</td>
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</tr>
</tbody>
</table>
The Points to Pixels Pipeline (P2P)\textsuperscript{1}: an Open Source Framework for Multivariate, Similarity, and Network Data Visualization

Dustin Arendt\textsuperscript{1,2}  Brett Jefferson  Simon Su
Air Force Research Laboratory  Indiana University  Air Force Research Laboratory

ABSTRACT
Principal Component Analysis, Multidimensional Scaling, and other advanced dimension reduction techniques are often used to help visualize complex multivariate datasets. However, these visualizations reduce observations to a cloud of points, which may stop short of conveying more interesting topological relationships present. Our contribution is P2P\textsuperscript{1}, a modular framework for transforming a set of points or observations into a visualization that conveys information about the simplicial complexes present in the dataset. The framework is abstracted in a manner that open source Python packages are leveraged to perform the computational “heavy lifting.” In addition to making this framework accessible to a much wider audience, this allows a more sophisticated component set to replace nearly any portion of the pipeline. An additional contribution of this work is a robust method for computing a global distance threshold that is grounded in information theory and complex network theory.

Index Terms: C.2.2 [Discrete Mathematics]: Graph Theory—Graph Algorithms; H.1.2 [Information Systems]: User/Machine Systems—Human information processing

1 INTRODUCTION

MANY problems in data analytics revolve around discovering useful insights from a set of observations. However, observations could take on many different forms given the context. For example, observations could consist of sets of points embedded in high dimensional space. Or, observations could be measured as a matrix of similarities between other observations. Furthermore, observations could be represented as a network of relationships between other observations. Additionally, each observation might also be labeled with some kind of descriptive attribute or class (e.g., man/woman, young/old, sick/healthy, etc.).

Given a set of observations, useful insights we may wish to gain can be answered to questions like:
- Which observations are “similar” and which are “outliers”?
- Do observations group together, and how are those groups related?
- What is the relationship between classes and observations?

There are many sophisticated techniques from machine learning, statistics, complex network analysis, and other fields that can be applied to help answer the above questions. However it is usually the case that specific criteria about the data and the answer being sought must be met before any technique can be effectively leveraged. For this reason, visual analytics can be employed to obtain an overview or basic intuition about the dataset before more sophisticated techniques are applied.

More of the popular tools for dimension reduction and embedding assume the problem is solved once the set of observations have been suitably mapped into the desired lower dimension. Furthermore, many algorithms (e.g., Isomap, Locally Linear Embedding, Spectral Embedding) rely on determining the nearest neighbors for observations, which induces a graph from the set of observations. However, this graph though it may contain useful information about the underlying topology of the dataset, is not often represented in the visualization. One contribution of P2P\textsuperscript{1} is that it goes beyond simply determining a good placement for each vertex; P2P\textsuperscript{1} also determines how to appropriately fill in the space in-between points based on the topology of the underlying observations.

Towards this end, this paper presents a general methodology for data visualization that can be applied broadly to many of the different types of observations described above. Recently there has been significant improvements in the availability, quality, and ease of use of open source tools for scientific computing and data analysis, especially for the Python scripting language. In this paper we also highlight how several open source packages can be combined to perform nearly all of the “heavy lifting” required to implement this pipeline. Aside from making the proposed visualization technique accessible to a wider audience, reliance on open source software in this manner abstracts the visualization pipeline in a way that is easily extensible. It is straightforward to plug in a different algorithm at the user’s discretion for any of the main steps in the pipeline.

2 BACKGROUND & RELATED WORK

The problem of how to best display a set of (possibly high dimensional) observations in a low dimensional space is so fundamental to understanding scientific datasets that the basic techniques have been used for decades. For this type of problem we have a dataset \( X \) consisting of \( n \) \( p \)-dimensional observations, where \( x_i \in \mathbb{R}^p \). One such technique is Principal Components Analysis (PCA), where a set of high dimensional points is rotated in a manner that gives the leading components the most amount of variance \([9]\). PCA can be used as a data visualization and exploratory tool; when the number of principal components is 2 or 3, the points can be rendered on the screen to reveal relationships within the data. PCA can also be used simply as a dimension reduction technique for preprocessing the data before it is tackled by other algorithms. Multidimensional scaling (MDS) addresses a problem similar to PCA, but assumes that only the distances between points are known \([2]\).

In other words, the dataset \( D \) consists of \( n \) observations of \( n \) dimensions where \( d_{ij} \) is the observed distance between observation \( i \) and \( j \). Such data could arise from preference questionnaires, for example. Essentially, MDS algorithms attempt to minimize the discrepancy between the distances separating the embedded points and the distances given in the input.

Many other techniques exist that improve on PCA or MDS in some way, with one of the most popular techniques being Isomap \([1]\). This algorithm constructs a graph connecting the closest observations to each other, and then the geodesic distances between these neighboring observations is used to determine a suitable lower dimensional embedding. Other embedding techniques include Locally Linear Embedding \([14]\), Laplacian Eigenmaps \([2]\), and Spec-
Distilling Embedding [11]. All of the techniques discussed above are available in the Scikit-learn python package for machine learning [13].

Suppose that in addition to having a set of observations \( X \), that we also have a corresponding label for each observation \( X_i \), where \( y_i \in \mathbb{Z} \). Visual analytics can help us discover if there is any meaningful relationship between \( X \) and \( Y \). When we wish to learn a function \( f : X \to Y \) that accurately predicts \( y_i \) from \( x_i \), this is referred to as supervised learning (specifically classification when \( Y \) is discrete) [15]. Since this is such a common task, some researchers have developed algorithms that take into account both \( X \) and \( Y \) when determining the embedding, with one well known example being t-SNE [16].

3 METHODS & RESULTS

Given the following:
- \( X \) a set of multivariate observations, where \( x_i \in \mathbb{R}^p \).
- \( D \) a matrix of dissimilarities between observations, or
- \( G = (V, E) \) a graph representing the relationships between observations.

one of our goals is to determine an effective two-dimensional embedding of the observations \( P \), where \( p_{ij} \) is the \((x, y)\) coordinate of observation \( i \) in the visualization. Our approach, \( \text{P}^2\text{E} \), builds on the realization that several related modern algorithms compute the nearest neighbors of observations. Thus, there appears to be a very natural progression of \( X \to D \to G \to P \) that will yield an effective visualization. Furthermore, at this level of abstraction, one can see that the same algorithm can be used regardless whether we start with \( X \), \( D \), or \( G \) when we do not start with \( X \) we are simply short-cutting the pipeline. Furthermore, each mapping in the pipeline is easily implemented with an open source Python package function call, making the mappings interchangeable with other algorithms according to one’s preference.

However, we do not stop once \( P \) is computed, noting that \( G \) may have additional structure that can be conveyed effectively in a visualization. Specifically, \( G \) may contain a number of cliques (i.e., complete subgraphs), and we believe that rendering cliques as filled-in polygons instead of as the traditional node-link style improves the usability of the visualization. One reason for this belief is that a significant number of edges can be replaced with a single uniform polygon, a clique of size \( k \) would have to be drawn as \( k(k-1)/2 \) edges, but would be replaced with a polygon having at most \( k - 1 \) edges. The color of the polygon can encode the size of the clique so that density information can be gleaned from the visualization at a glance.

Given the set of maximal cliques \( C \) and an embedding of the observations \( P \), it is necessary to compute the convex hull of each clique in order to render each clique as a polygon. This is because \( P \) actually defines a projection of the simplex corresponding to that clique into a lower dimensional space. As a result of this projection, some of the vertices in the simplex may end up as interior points. Computing the convex hull of the clique given \( P \) will identify which vertices are on the true boundary of the projected polygon.

The entire \( \text{P}^2\text{E} \) procedure is described in Algorithm 1, and a description of open source function calls made by \( \text{P}^2\text{E} \) is shown in Table 1. The results of applying \( \text{P}^2\text{E} \) to are shown in Figures 1, 2, and 3. Figure 1 illustrates how computing the convex hulls of cliques might improve the usability of the visualization by reducing the number of edges drawn, and filling in some of the negative space.

Figure 2 shows how choosing the distance threshold \( \varepsilon \) affects the visualization. When \( \varepsilon \) is trivially small, no observations are considered neighbors, which results in a completely disconnected graph. As \( \varepsilon \) increases more of the underlying structure becomes evident, until eventually \( \varepsilon \) is large enough that all observations are considered neighbors and belong to a single clique. Clearly a value for \( \varepsilon \) that is “just right” must lie somewhere between these two extremes, which have little utility. We provide a way to compute a solution to this “Goldilocks” problem, which is detailed in Section 4.2.

Figure 3 shows \( \text{P}^2\text{E} \) applied to a larger multivariate dataset representing over 1000 hand drawn digits.

Algorithm 1 Basic outline of the \( \text{P}^2\text{E} \) abstraction

1. start with \( X, n \times m \) matrix of points
2. find (or start with) \( D, a n \times n \) matrix of distances between points
3. find \( \varepsilon \), a global distance threshold
4. find (or start with) \( G \), a graph induced from \( D \) and \( \varepsilon \)
5. find \( P \), an embedding of \( G, D \), or \( X \) in \( \mathbb{R}^2 \)
6. find \( C \), the set of maximal cliques in \( G \)
7. find \( H \), the convex hulls of each clique in \( G \) given \( P \)
8. draw each hull in \( H \) as a 2-D polygon

Figure 1: Comparison of a typical node-link rendering of a network (left) versus the \( \text{P}^2\text{E} \) embellishment (right). The graph data is from the Zachary’s karate club network [19] which can be accessed with networkx/karate club graph.

4 DISCUSSION

4.1 Considerations for Large Datasets

The \( X \to D \) mapping will create scalability issues when \( |X| \) is large; when the number of observations is becomes much greater than \( 10^4 \), the average machine will not have sufficient memory to store \( D \), which grows as \( O(|X|^2) \). To address this issue, one can instead map \( X \) directly to \( G \) by leveraging sophisticated data structures like the KDTree. For example, SciPy’s KDTree allows for the efficient computation of \( k \)-nearest neighbors (the \( k \) nearest neighbors with a distance less than \( \varepsilon \)) given a set of points \( X \). However, the KDTree can become inefficient when the number of dimensions are high (e.g., \( \varepsilon > 15 \) for this case). So when the dataset is both large and high dimensional, a reasonable solution to this problem is to use a fast dimension reduction technique like PCA to reduce the number of dimensions in \( X \), down to a tractable number, hopefully without much loss in accuracy.

4.2 Choosing \( \varepsilon \)

\( \text{P}^2\text{E} \) maps an \( X \) or \( D \) to a graph through the application of an arbitrary distance threshold. Clearly this threshold can have a significant detrimental effect to the usability of the visualization if chosen poorly, as demonstrated with Figure 2. So we outline her a method for determining a good choice for \( \varepsilon \) with a solid basis from information theory and complex network theory. First, we assume that we have a set of class labels \( Y \) corresponding to each observation in \( X \) or \( D \). The intuition for choosing a good value of \( \varepsilon \) then that the edges in the graph induced by \( \varepsilon \) should have edges that are likely to connect observations with the same label). This is often referred to...
<table>
<thead>
<tr>
<th>step</th>
<th>function call</th>
<th>description</th>
<th>ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,5</td>
<td>sklearn.decomposition.PCA</td>
<td>dimension reduction (use for large, high dimensional datasets) or as a vertex encoder</td>
<td>[9, 13]</td>
</tr>
<tr>
<td>2</td>
<td>scipy.spatial.distance.pdist</td>
<td>compute the distance between all pairs of points (many distance norms available to choose from)</td>
<td>[10]</td>
</tr>
<tr>
<td>3</td>
<td>scipy.optimize.minimize_scalar</td>
<td>scalar minimization of objective (use bounded=True with bounds=(0, 10^6)) (see Eqn. 7)</td>
<td>[4, 10]</td>
</tr>
<tr>
<td>4</td>
<td>networks.Graph</td>
<td>efficient computation of k-ϵ neighbors (use for large datasets, but only implemented for L2 norms)</td>
<td>[10]</td>
</tr>
<tr>
<td>4</td>
<td>networks.draw.graphviz</td>
<td>create a graph data structure a list of edges (from nearest neighbors) or an adjacency matrix (from thresholded distance matrix)</td>
<td>[7]</td>
</tr>
<tr>
<td>5</td>
<td>sklearn.manifold.MDS</td>
<td>compute 2-d spatial embedding for graph vertices (use &quot;n睂&quot; option for very large graphs)</td>
<td>[6]</td>
</tr>
<tr>
<td>5</td>
<td>networks.find_cliques</td>
<td>embed vertices into R^2 directly from D</td>
<td>[3, 13]</td>
</tr>
<tr>
<td>6</td>
<td>networks.find_cliques</td>
<td>find maximally connected components (e.g., complete subgraphs)</td>
<td>[5, 7]</td>
</tr>
<tr>
<td>7</td>
<td>scipy.spatial.ConvexHull</td>
<td>&quot;rubber band&quot; fit to a set of points in order to count interior points from the projection of the simplex</td>
<td>[1, 10]</td>
</tr>
<tr>
<td>8</td>
<td>matplotlib.collections.PolyCollection</td>
<td>render polygons</td>
<td>[8]</td>
</tr>
</tbody>
</table>

Figure 2: P2P^2 visualization of the Iris classification dataset with $k$ varying linearly from the minimum to maximum euclidean distance between observations. The data can be accessed with sklearn.datasets.load_iris.

Figure 3: P2P^2 visualization of the Digits classification dataset. The Digits dataset can be accessed with sklearn.datasets.load_digits.

found as "assortative mixing," or the tendency for adjacent nodes in a network to have the same properties [12], and a number of techniques exist to measure it.

Classically, assortative mixing is measured with statistical correlation techniques, which has several known issues. Recently information theory, specifically mutual information has proven to be a useful tool for understanding complex networks, including the phenomenon of assortative mixing [16]. Thus, our measure for assortative mixing is based on the mutual information $I(E;A)$, where $E$ and $A$ are Boolean random variables corresponding to two nodes having equal state, and two nodes being adjacent, respectively. $I(E;A)$ is found as follows:

$$I(E;A) = H(E) - H(E|A),$$  \hspace{1cm} (1)

and

$$H(E|A) = P(A = 1) \cdot H(E|A = 1) + P(A = 0) \cdot H(E|A = 0).$$  \hspace{1cm} (2)

where $H$ is the entropy of an arbitrary probability distribution $X$. The following probabilities are directly measured given $G = (V,E)$ and $X$, the network and the state of the nodes on the network, re-
\[ P(E = 1) = \frac{1}{n} \sum_{\alpha \in E} \alpha (\alpha - 1), \]
\[ P(A = 1) = \frac{2m}{n(n+1)}, \]
\[ P(E = 1|A = 1) = \frac{\sum_{e \in E} \delta(y_e - y_x)}{\alpha_{\alpha} - m}. \]

where \( n \) is the size of the dataset, \( m \) is the number of edges, \( \alpha \) is the density of the graph, and \( \delta \) is the Dirac delta function. The remaining quantity that is not immediately found due to the law of total probability is
\[ P(E = 1|A = 0) = \frac{\sum_{e \in E} \delta(y_e - y_x)}{\alpha_{\alpha} - m}. \]

Note that computing \( P(E|A) \) scales effectively with the size of the dataset since, the most expensive computation loops over the edge set, requiring only \( O(m) \) time to complete.

The ideal threshold is
\[ \varepsilon_0 = \min_{\varepsilon} \mathcal{J}(G(X, \varepsilon), Y), \]

where \( \mathcal{J}(X, \varepsilon) \) induces a graph from the set of observations and a given \( \varepsilon \), and \( \mathcal{J}(G, Y) \) computes the assortative mixing of the graph \( G \) with corresponding labels \( Y \). The optimization program can be bounded to \( (\varepsilon_{\text{max}}, \varepsilon_{\text{min}}) \) where
\[ \varepsilon_{\text{min}} = \min_{\varepsilon} \mathcal{J}(G(X, \varepsilon), Y), \]

\[ \varepsilon_{\text{max}} = \max_{\varepsilon} \mathcal{J}(G(X, \varepsilon), Y). \]

If \( X \) is large (e.g., \( |X| > 10^3 \)) then a smaller random subset of \( X \) should be a sufficient replacement for \( X \) to compute \( \varepsilon_{\text{max}} \).

One subtle issue is that because mutual information must be positive, then both \( I(A) \) and \( I(E) \) are upper bounds of \( I(E|A) \). As we vary \( \varepsilon \), we can expect \( I(E) \) to remain constant; however, as we increase \( \varepsilon \), the density of the graph also increases, causing \( I(A) \) to increase until the density of the graph reaches 1/2. Therefore, a fairer way to compare the mixing of two graphs that have different densities would be to normalize the mutual information by \( I(A) \). Figure 4 shows the beneficial effect this normalization has on the mixing scores for the digit dataset. When \( I(E|A) \) is normalized by \( I(A) \), the optimal value of \( \varepsilon \) decreases.

5 Conclusions & Future Work

Conclusion

For future work, we intend to implement FC2 in an immersive 3-D virtual environment. From an algorithmic standpoint, making this jump is readily trivial due to the modular nature of FC2. One must simply exchange the current graph drawing algorithm with one that embeds vertices into 3-D (or, alternatively, use MDS or PCA to project X onto D instead of 2 dimensions). Furthermore, the convex hull algorithm also generalizes to 3 dimensions, where polygons are simply sets of triangles instead of line segments. The main effort in the implementation in the virtual environment will be in an effective interface for exploratory visual analytics, as well as effective volume rendering of the 3-D convex hulls.

Acknowledgements

This work was supported by the National Science Foundation under Grant No. 0725450.

References


