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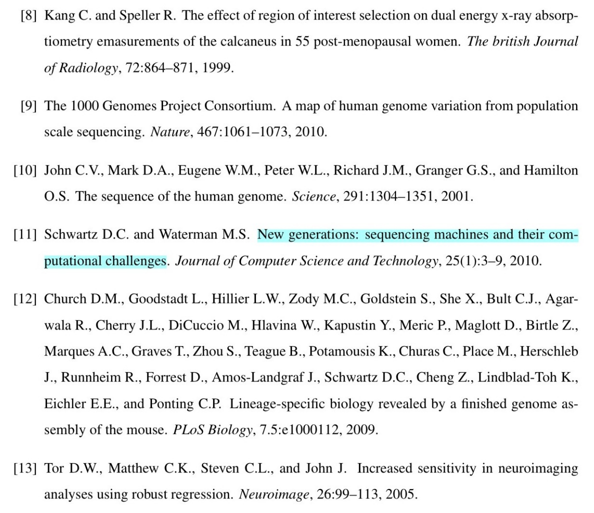

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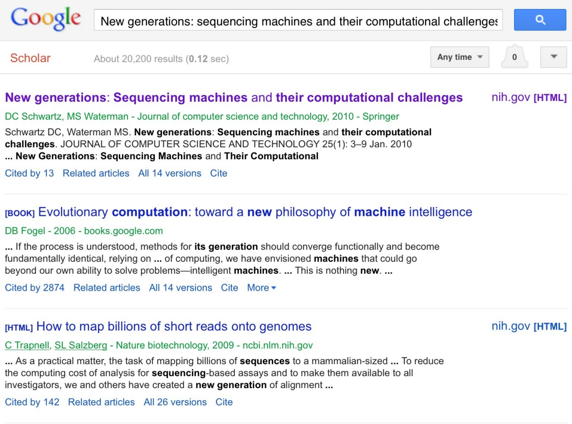

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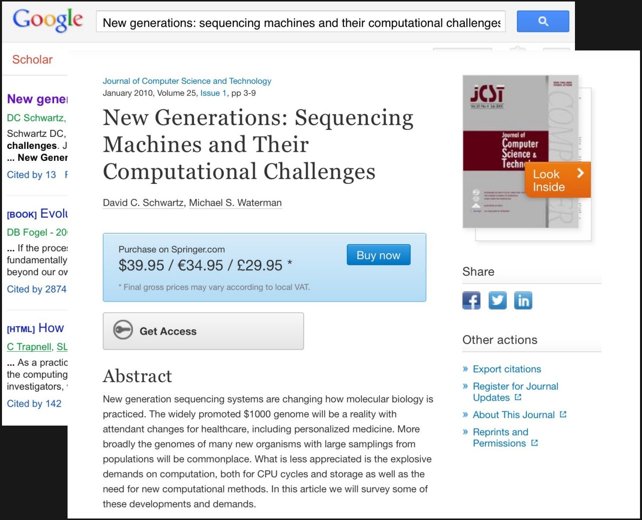

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David C. Schwartz, Michael S. Waterman

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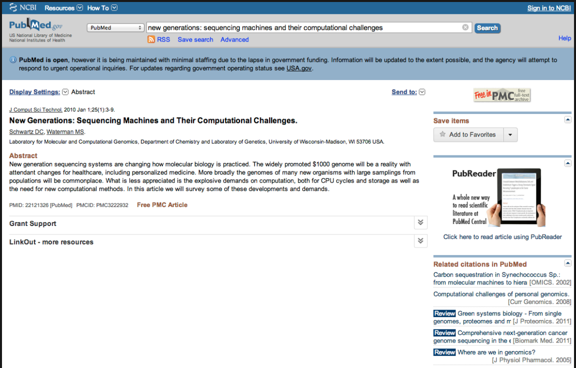

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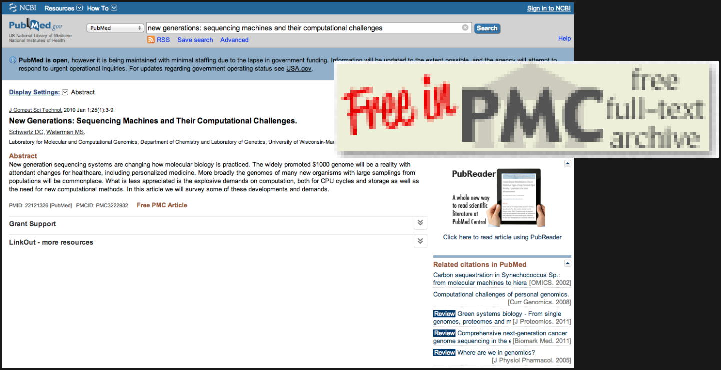

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J Dent Res. 2013 Jan;92(1):32-7. doi: 10.1177/0022034512463241. Epub 2012 Oct 11.

Clustering tooth surfaces into biologically informative caries outcomes.

Shaffer JR, Feingold E, Wang X, Weeks DE, Weyant RJ, Crout R, McNeil DW, Marazita ML.

Department of Human Genetics, Graduate School of Public Health, University of Pittsburgh, Pittsburgh, PA 15261, USA. jr8@pitt.edu

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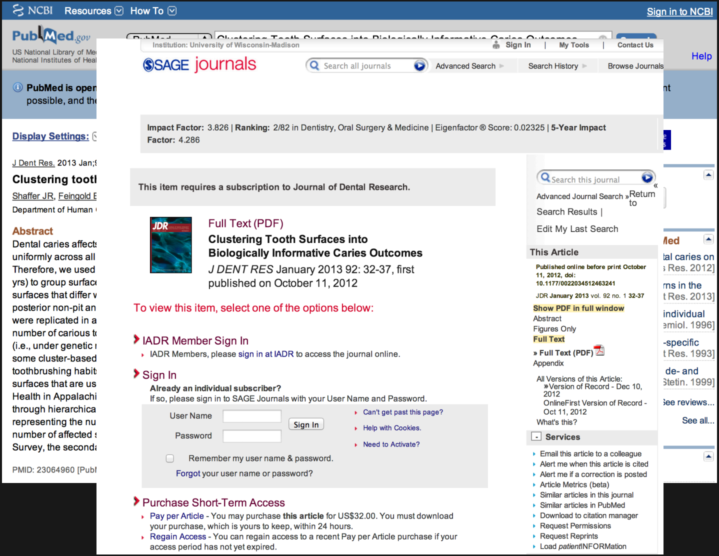

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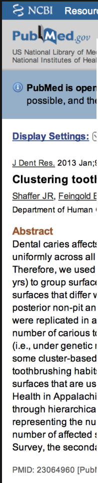

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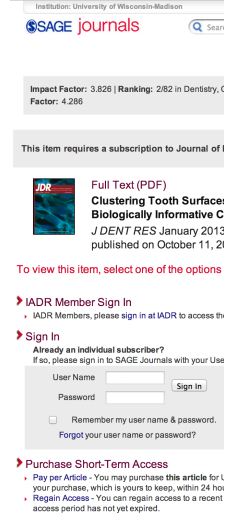

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R.J. Weyant[2,6], R. Crout[2,7],
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J Dent Res 92(1):32-37, 2013

Clustering Tooth Surfaces into Biologically Informative Caries Outcomes

ABSTRACT

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KEY WORDS: dental caries, permanent dentition, white spots, hierarchical clustering, cluster analysis, heritability.

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INTRODUCTION

Dental caries, which affects the great majority of adolescents and adults throughout the world, is a multi-factorial disease caused by the effects of numerous environmental, behavioral, and genetic factors. Many risk factors have been identified, such as: host genetics (Horowitz *et al.*, 1958); environmental exposures, including fluoride, cariogenic bacteria, and pH-altering agents; behavioral factors, including diet and oral hygiene; characteristics of the dentition, including enamel composition and positions and morphology of teeth; characteristics of the oral environment, including saliva composition, flow rate, and pH buffering capacity; and demographic factors, including age, sex, race, ethnicity, socio-economic status, and access to oral health care (Hunter, 1988). This complexity is further compounded by the disease phenotype, which may manifest as innumerable combinations of caries lesions across tooth surfaces of the full dentition. Because caries risk factors may exert differential effects across tooth surfaces of the permanent dentition, measurable caries experience may be modeled as the cumulative result of multiple superimposed patterns of decay due to the various risk factors (Batchelor and Sheiham, 2004; Shaffer *et al.*, 2012a).

In epidemiological studies, however, caries experience is typically reduced to a single measure of decay, such as the widely used DMFT/S index (calculated as the sum of decayed, missing due to decay, or filled/restored teeth/surfaces). Such global measures of caries experience ignore the fact that categories of tooth surfaces exhibit differences in susceptibility to decay and are differentially affected by risk factors. Because they ignore the patterns of dental caries across the dentition, global measures of decay such as DMFT/S index may be limited in their ability to identify caries risk factors that exert their effects on specific categories of tooth surfaces. Indeed, previous studies have demonstrated that modeling the patterns of tooth decay is beneficial for epidemiological (Psoter *et al.*, 2003, 2009) and genetic studies (Shaffer *et al.*, 2012a, 2012b). We used hierarchical clustering analysis to group tooth surfaces into categories based on co-occurrence of caries lesions. We then generated novel caries outcomes reflecting these tooth-surface categories, and explored their utility for studying caries etiology.

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J.R. Shaffer[1,2]
X. Wang[2,4,5],
R.J. Weyant[2],
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ABSTRACT

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Clustering Tooth Surfaces into Biologically Informative Caries Outcomes

APPENDIX

COHRA Population Characteristics

Descriptive characteristics of the COHRA sample are shown in the Appendix Table. Compared with the general US population, this Appalachian sample from rural West Virginia and Pennsylvania is poorer, less educated, and underserved with respect to oral health care.

Cross-validation and Defining Separate Clusters

Determining the number of separate clusters is the principal challenge in the field of cluster analysis, and there is currently very little statistical theory in this area. Defining *a priori* minimum distances between clusters is arbitrary and may lead to over-fitting. Therefore, we instead performed two-fold cross-validation (*e.g.,* Salvador and Chan, 2004), a commonly used approach for determining the number of clusters. Cross-validation allows us to determine the sensitivity of our clusters to perturbations of the input data and to identify what level of within-cluster similarity and between-cluster dissimilarity defines stable clusters. We randomly divided our sample into two halves and performed hierarchical clustering on each half. This process was repeated for 10 random halves. By comparing dendrograms, we determined the maximum number of separate clusters that were consistently observed across all random halves. Overall, tooth surfaces were distributed across 5 very stable clusters. Example cluster results for two complementary halves (which total to the full sample) are shown in Appendix Fig. 1. Similarly, to assess any effects of the inclusion of biological relatives in our sample, we repeated hierarchical clustering in the maximal subset of unrelated individuals (see Appendix Fig. 2), which were nearly identical to the total COHRA and NHANES 1999-2000 samples.

In both the total COHRA sample and in the NHANES 1999-2000 sample, the fifth cluster was subdivided into maxillary and mandibular components (indicating possibly 6 instead of 5 clusters). However, these subdivisions were not consistently observed *via* cross-validation of the COHRA sample. That is, in some randomly chosen halves of the COHRA sample, the sixth cluster did not distinguish maxillary and mandibular components of the fifth cluster. Therefore, we have conservatively shown results for the 5 stable clusters, as well as the maxillary and mandibular subdivisions of the fifth cluster.

Overwhelmingly, the cluster results were stable within the COHRA sample, and consistent between the COHRA sample and NHANES 1999-2000 sample. That being stated, there were subtle differences observed among cluster results. For example, left-right asymmetry was observed, albeit rarely, in the random halves (*e.g.,* Appendix Fig. 1A, tooth #20 and tooth #29). Likewise, some tooth surfaces physically positioned on the border between two adjacent clusters shifted membership (*e.g.,* Appendix Figs. 1A and 2, tooth #21 and tooth #28). In many cases, the result of such shifts in cluster membership echoed the subtle differences between COHRA and NHANES 1999-2000. We speculate that the all-or-nothing nature of our clustering approach represents an oversimplification of the relationships among tooth surfaces with respect to dental caries risk factors

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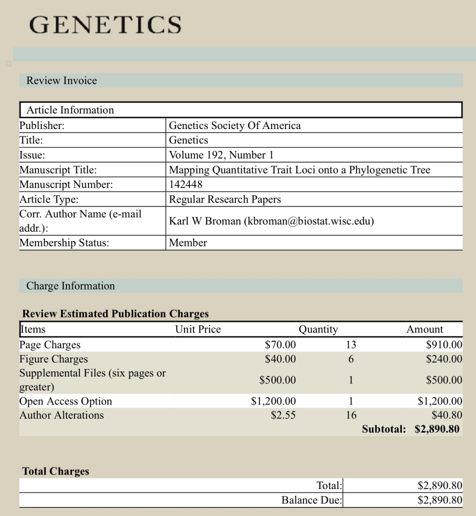

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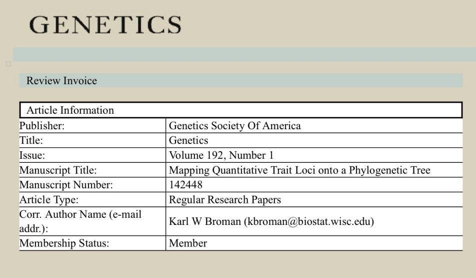

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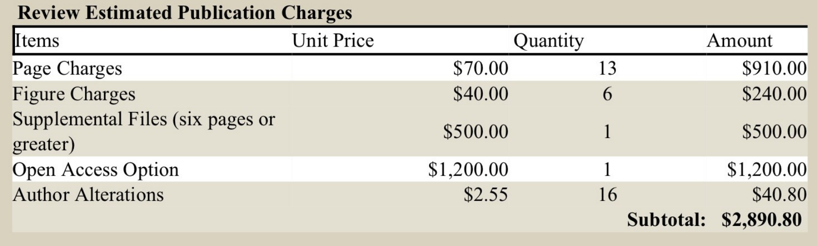

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