Advancing river corridor science beyond disciplinary boundaries with an inductive approach to hypothesis generation

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Plain Language Summary

Most studies of rivers begin with a hypothesis that is carefully built upon existing ideas and concepts. These ideas usually come from past work within a discipline and ask increasingly specific questions. It is harder to generate creative new ideas that span disciplinary boundaries. As a result, we have a lot of facts about rivers and their functions that are organized by discipline, but little ability to put these facts together into a complete, predictive understanding of rivers. So, we shook things up. Instead of starting with a hypothesis and testing it with some experimental data, we started with the most comprehensive data set we could find and generated hypotheses to explain it. We used machine learning tools to generate relationships that explain patterns in the data, even if these explanations did not fit with any pre-existing concepts of how and why rivers function. The approach generated some relationships that are consistent with things we expect to find, building confidence that at least some of the relationships we found are meaningful. Better yet, 84% of the relationships we generated have not been previously studied, suggesting that our approach was successful in generating new ideas that might spur creative thinking.

Key Points:

- Inductive approaches to science are useful complements to traditional, deductive approaches and may catalyze new ideas
- We identified 564 relationships between variables in the river corridor that have not been previously studied in the literature
- Empirical studies should characterize rivers with data beyond their discipline to maximize the value of their effort to synthesis efforts

Abstract

Traditional, deductive approaches have generated a large body of site-, scale-, process-, or method-specific understanding of the physical, chemical, and biological processes that occur within river corridors. However, this body of facts does not until itself constitute a predictive understanding of river corridors in their full complexity. We contend a new paradigm is required to synthesize existing knowledge with the goal of linking internal dynamics, external forcing, and historical contingencies to the emergent spatial structure, temporal dynamics, and ecosystem services that are derived from river corridors. Here, we prototype an inductive approach to synthesis, using machine learning as a hypothesis generator to identify potential couplings or feedbacks that would not necessarily arise from classical, deductive, disciplinary approaches. This approach generated a network of 672 relationships linking a suite of 157 variables each collected at 62 locations in a 5th order river network, 84% of which have not been previously co-investigated in the literature. We document the critically important role of collecting data beyond disciplinary norms (89% of predictive models required out-of-group data for optimal prediction), and both the emergence and shredding of spatial structure as variables combine to explain observed patters in the network. This study demonstrates the value of a hypothesis generation approach that is agnostic to disciplinary boundaries and pre-existing conceptual models as a compliment to traditional, deductive models of inquiry. Ultimately, the network of multi-scale, cross-disciplinary relationships generated here may catalyze new ideas and conceptualizations that would not be obvious starting from pre-existing conceptual models and approaches.

1. Introduction

A paradigm change is required to advance our conceptualization of the river corridor beyond site-, scale-, and mechanism-specific findings towards an integrative view of river corridors as complex, dynamic systems responding to external forcing (Turnbull et al., 2018). While decades of study have yielded a wealth of descriptions of many processes, we lack the ability to connect process dynamics across space and time in order to create a comprehensive understanding of the structure and function of river corridors. Most river corridors studies focus on a specific location, scale, or disciplinary perspective, and consequently investigate a limited set of ecosystem functions and process interactions (Turnbull et al., 2018; Ward, 2015; Ward & Packman, 2019). Consequently, we have accumulated a substantial body of observations and process-specific interpretations, but we are lacking a comprehensive model to distill this knowledge into general and transferable concepts. At present, few - if any - conceptual models account for the hierarchical, multi-scale, coupled physical-chemical-biological process dynamics that give rise to the observed spatio-temporal patterns of river corridor services and functions. A new approach is needed for conceptualizing the multi-scale, multi-discipline, multi-rate process dynamics that govern river corridors and determine the structural and functional attributes that can be observed at any specific place and time.

River corridors have classically been studied by a host of disciplines, each with primary interest in individual processes or functions (Ward, 2015). Consequently, techniques for river research are not standardized, relevant metadata have not been specified, and common variables needed to synthesize findings across sites are not defined (Ward, 2015; Ward & Packman, 2019). Thus, the core challenges facing river corridor scientists today are (a) developing theory to overcome our limited ability to observe the full spatio-temporal complexity of river corridors (Li et al., 2021), and (b) organizing river corridor science in a way that is explicitly integrative as opposed to disciplinary. One way to address these needs is to expand beyond the traditional, deductive approach to science, which bases measurements on a highly targeted set of causal mechanisms to be tested at a limited range of scales and locations. With the emergence of new experimental and data science techniques, the time has come to expand existing conceptual models for rivers to incorporate our new understanding of river corridors as complex dynamic systems. We posit that unified understanding must combine *deductive* science with *inductive* approaches that identify process interactions and couplings that emerge from the data themselves. We suggest that river corridor science can benefit from Complex Systems and Grounded Theory approaches that have proven useful in understanding many other problems that involve complex multiscale dynamics (Martin & Turner, 1986; Strauss & Corbin, 1994; e.g., Turnbull et al., 2018).

A unifying framework is required to organize and synthesize our understanding of river corridors and advance scientific understanding of the drivers and controls of their functioning. Stegen et al. (2018) propose one such model for microbial ecology, where the resultant ecosystem functions and services are explained by the relationships linking internal dynamics, external forcing, and historical contingencies. The principles of Stegen et al.'s conceptual framework are parallel to existing conceptualization that have been applied to river corridors. First, external forcing describes the role of factors extrinsic to the river corridor that shape its structure and function. For river corridors, this primarily means the larger spatial scale and longer temporal scale elements that are functionally decoupled (e.g., static or slowly-varying) relative to a process of interest. Studies with data collection spanning gradients in land use, geologic setting, climate, network position, or other factors that are considered to be extrinsic typically use geospatial and statistical approaches to describe patterns and trends (e.g., McGuire et al., 2014), while variation around spatially structured trends is often interpreted as random noise attributable to structural heterogeneity and/or unstudied, smaller-scale processes (Abbott et al., 2018). Next, internal dynamics are considered to be the interacting processes within the river corridor that give rise to the observed functions at a given location. Conceptual models based on this approach to river corridor science include hot spots and hot moments (Krause et al., 2011, 2017; Wallis et al., 2020), control points (Bernhardt et al., 2017), and patch dynamics (Pringle et al., 1988). River corridor dynamics are commonly studied through detailed observations at a relatively limited spatial scale, that allows sufficiently complete characterization to assess localized feedbacks between mechanisms. These approaches often lack sufficient sampling resolution to enable confident application of geostatistical approaches, and may not reliably support assessments of system dynamics (e.g., Lee-Cullin et al., 2018). Finally, historical contingencies are the biotic and abiotic histories or antecedent conditions that lead to the present characteristics of the river corridor and affect its response to future perturbations. Examples of river corridor studies include perturbation-response dynamics, commonly associated with floods (Czuba et al., 2019; Wu et al., 2018), droughts (Boulton et al., 2004; Wood et al., 2010), or restoration activities (Rana et al., 2017; Smidt et al., 2015), and large-scale historical perturbations such as land development (Liébault & Piégay, 2002; Walling & Fang, 2003; Wohl, 2005), river regulation (Gregory, 2006), and contamination (Byrne et al., 2012; Santschi et al., 2001). Such studies often involve little to no replication and may be biased towards response variables that are relatively rapid in timescale in comparison to processes that are functionally static for purposes of a given experiment.

While external forcing, internal dynamics, and historical contingencies have each been studied in their own right, studies are beginning to relate these concepts into integrated understanding of river corridors. For example, Wisnoski and Lennon (2021) explicitly linked localized heterogeneity to systematic spatial patterns along the network, revealing that the local microbial assemblage in the headwaters of the H.J. Andrews Experimental Forest (Oregon, USA) was controlled by local physical and chemical conditions, but these local controls gave way to systemic organization from headwaters to larger downstream rivers. This explicit consideration of local and network scales is rare. We advocate that this approach be adopted more generally because it allows assessment of the transition in dominant controls from local heterogeneity to larger-scale spatial organization, the specific mechanisms of this transition, and the scale at which the transition occurs. Studies that have sought to explicitly link local spatiotemporal dynamics with long-term system-wide functions have found strong relationships between large-scale system structure, internal dynamics, and long-term emergent outcomes in flow, sediment transport, and biogeochemistry (Fisher et al., 1998; Harvey & Gooseff, 2015; Krause et al., 2017; Pinay et al., 2015). The success of these studies demonstrates our ability to identify a core set of transferable and scalable processes that govern river system dynamics, and unify seemingly-disparate observations into holistic understanding of river corridor structure and dynamics.

Thus, we confront the challenge of how a discipline classically organized around the deductive model of systematically collecting of site-, scale-, and mechanism-specific observations begins the process of synthesis that requires spanning these barriers? Put another way, how can we identify couplings that span scales and disciplinary expertise in absence of pre-existing conceptual models that would traditionally serve as the source of hypotheses for deductive testing? We propose an inductive approach to data synthesis, serving as a basis for the unconstrained generation of new and potentially unexpected hypotheses. To this end, we analyze a novel large data set for a 5th order river basin (Ward, Zarnetske, et al., 2019) using inductive approaches to generate novel hypotheses that span traditional disciplinary boundaries. We pilot a machine learning approach to synthesize complex, multi-scale observations independent of any pre-conceived conceptual models. This approach yields a set of relationships describing the structure and function of river corridors, which we critically evaluate relative to existing knowledge.

2. Methods

2.1 Data description and organization

2.1.1 Field site and synoptic campaign

The HJ Andrews Experimental forest (Western Cascades, Oregon, USA) is a 6,400 ha basin that is primarily covered in old-growth and second growth forest and drained by a 5th order river. The physical characteristics of the basin are well-described elsewhere (Deligne et al., 2017; Dyrness, 1969; Jefferson et al., 2004; Swanson & James, 1975; Swanson & Jones, 2002). A synoptic sampling campaign including detailed characterization of physical, chemical, and biological characteristics and processes in the river corridor at 62 sites across stream orders 1-5 was conducted by Ward et al. (2019), which forms the basis of our study data set. These data are the most uniform, comprehensive, and multi-scale available – to our knowledge – and, as such, are optimal for hypothesis generation.

2.1.2 Data reduction

Starting from this data set, we reduced the full suite of variables from Ward et al. (2019) to a subset we considered to be most representative summary of the data set. For example, we omitted identification of individual species and life-stages from macroinvertebrate data in favor of summary indices, and similarly reduced metabolomics data to a series of indices rather than attempting to explicitly analyze the 10,000+ individual organic molecules identified in the data set. In this process, we discussed traditional disciplinary approaches to the study of river corridors, and ultimately organized the variables into 7 subgroups representing distinct study domains that jointly characterize the structure, function, and dynamics of the river corridor and consistent with the design of the field campaign. These subgroups were: geologic setting (GEO), physical chemistry (PCHEM), bulk DOM characterization (DOM), dissolved nutrients (NUTS), solute tracers (TRACER), metabolomics (ICR), and macroinvertebrates (MACRO). A complete list of variables, subgroups, and summary findings for each variable is presented in Table S1). The reduced data set totaled 157 unique variables across the seven disciplinary subgroups and is the basis for all subsequent analysis in this study.

2.2 Principal components analysis

To identify major axes of (co)variation among measured variables, we performed a series of principal component analyses (PCAs) using the rotated PCA approach. Independent PCAs were performed first on the entire data set (all 157 variables) and subsequently on variables within each subgroup. For each PCA, we focused on results from the first two components (PC1 and PC2). We identified the most influential variables from each principal component as those with loadings greater than 0.6 or less than -0.6 (hereafter 'influential variables') and interpreted the variables aligned with each PC to describe the major axes of variation when possible.

2.3 Spatial structure of individual variables

For each variable, we tested for spatial structure throughout the network by assessing the change in variance as a function of distance between flow connected points (Ver Hoef et al., 2006; Isaak et al., 2014; McGuire et al., 2014). This analysis identifies variables for which variance is spatially uniform (i.e., no change in variance as a function of distance), increasing linearly (i.e., variance grows with distance), or variance that plateaus at a known distance (i.e., a semivariogram). A uniform relationship indicates no structure, while both linear relationships and semivariograms demonstrate spatial structure. The linear models were only considered significant if the estimate of the slope was significantly different from zero based on the 95% confidence interval for a linear model fit. The squared differences were normalized (squared difference subtracted from the mean, followed by division of the difference by the standard deviation) and binned (bin size of 30) before fitted to the semivariogram function:

$$\boxed{y = a + be^{\left(\frac{-x}{c}\right)}}$$

with the nls() function in R Studio. The nugget, sill and range are given by a, $a+b$ and $3\times c$, respectively. Semivariogram models were only considered significant, if the estimates of the parameters b and c were significantly different from zero, based on zero not being within the 95% confidence interval for the parameters.

2.4 Support vector machine regression

To derive a network of relationships among pairs of variables in the data set, and ultimately identify the interactions within the network, we constructed two sets of support vector machine regression (SVMR) models. Each model predicted an individual dependent variable using a suite of independent variables. The model used forward feature selection with leave-one-out cross-validation. Forward selection stopped adding additional independent variables when the coefficient of determination failed to improve when an additional variable was included. Gaussian kernels were used for all variables. For each SVRM we recorded the order in which features were selected and their contributions to model goodness of fit as measured by the improvement in the coefficient of determination. After each model was constructed, we tabulated the subgroup and spatial structure of each explanatory variable selected to assess whether the variables selected within these analyses (Section 2.2-2.3) also improved the predictive power of the variable choices selected within the SVMR models. The first set of SVMRs used all variables other than dependent variable as possible inputs, with the goal of identifying relationships between individual variables. The second set used PC1 and PC2 from each disciplinary subgroup as possible inputs with the goal of identifying more generalizable flows of information from the major axes of variation within and between subgroups.

2.5 Literature analysis

To assess the presence and relative frequency of studies jointly considering two of the variables in our data set, we conducted a series of searches using the Scopus database in October 2020, following methods from similar studies (Ward, 2015; Yoder et al., 2020). Each variable in our data set was assigned one or more keywords that would be used to conduct a relevant search of the literature (Ward, 2021). Literature was searched for every pairwise combination of variables (12,246 unique searches) for studies containing both keywords and a required term to indicate a study was likely relevant to our study of river corridors (one of: river, stream, water, aquatic).

We tabulated the total number of studies returned from each search to assess the interactions between variables that are more or less frequently studied jointly and compared these to the interactions found to be significant within the SVMR analysis. We also assessed if the interactions identified in the SVMRs were present in our literature analysis.

3. Results

3.1 Principal component analysis

3.1.1 Principal component analysis on all variables

The PCA on all variables identified major axes of co-variation without regard to disciplinary grouping. PC1 explained 20% of the total variance (Table 2A), and contained mainly variables from the metabolomics subgroup, generally representing a gradient moving from terrestrially-derived aromatic compounds that are more thermodynamically favorable for microbial respiration to more microbially-derived compounds that are less thermodynamically favorable. PC2 explained 17% of the total variance and contained variables from the geologic setting subgroup, such as valley width and stream slope, showing marked gradients from headwaters to downstream reaches. Taken together PC1 and PC2 suggest that sampling sites within the river network are organized by organic matter chemistry and geology.

3.1.2 Principal component analysis on disciplinary subgroups

PCAs were conducted on each subgroup to identify major axes of variation within individual disciplinary perspectives. The first two PCs within each subgroup explain an average of 52% of the within group variance (median 46%, range 33-76%; Fig. 2A; Table 1). For physical chemistry, we interpret PC1 as representing weathering rate (from high to low) and PC2 as representing age of water (from high to low). For the geophysical setting, we interpret PC1 as representing network position (from headwaters to larger rivers) and PC2 as representing surficial geology. For nutrients we interpret PC1 as representing enzymatic activity (low to high) which is itself the inverse of nutrient availability, and PC2 represents the accumulated organic matter in the shallow streambed. For metabolomics, we interpret PC1 as reflecting gradients from terrestrially-derived aromatic compounds that are more thermodynamically favorable for microbial respiration to more microbially-derived compounds that are less thermodynamically favorable. The metabolomics PC2 is interpreted as a gradient being dominated by products from organic matter degradation at one end and less-processed terrestrially-derived organic matter at the other end. For bulk DOM, we interpret PC1 as representing DOM quality from less to more humic or terrestrial in origin, and PC2 as representing microbial and proteic DOM (from more to less). For macroinvertebrates, we interpret PC1 as representing richness (high to low) and PC2 as representing abundance (high to low). For stream solute tracers, we interpret PC1 as representing short-term storage of tracers (low to high) and PC2 as representing the importance of advection and longitudinal dispersion to tracer transport (low to high).

Table 1. Result of principal components analyses conducted on all variables in a single analysis (top) and on each expert subgroup (bottom).

PCA on all variables

	PC1			*PC2*		
	Variance explained (%)	**Positive loadings**	**Negative loading**	**Variance explained (%)**	**Positive loadings**	**Negative loading**
All variables	20	Nominal oxidation state of Carbon, % tannin, % condensed hydrocarbons, Modified aromiticity inded, % lignin	Gibbs free enerbgy, % lipids, double-bond equivalency minus Oxygen, % protein	17	stream valley width, stream order, alluvium, valley width, discharge upstream, discharge downstream, advection-dispersion: MAD and D, segment sinuosity	valley segment slope, stream segment slope

PCA on subgroups

	PC1			*PC2*		
	Variance explained (%)	**Positive loadings**	**Negative loading**	**Variance explained (%)**	**Positive loadings**	**Negative loading**
Physical Chemistry (PCHEM)	40 *	—	Mg, Ca	26 *	18O, 2H	—
Geologic Setting (GEO)	17 *	stream order, channel width, channel depth, segment sinuosity, alluvium, segment valley width, cobbly-sandy-loam	segment stream slope, segment valley slope, valley slope, stream slope	16	soil depth < 3 ft, % clastic flows, gravelly-clay-loam, greenish breccia residuum/colluvium, soi erosion severity, poor water yield	travel time to outlet, glacial drift, soil gravelly sandy loam, % soil depth 3-to-10ft, % ridge-capping lava flow, moderate water yield, live biomass
Nutrients and enzimatic activity (NUTS)	29 *	beta-D-glucosidase (C-acquiring), Leucine aminopeptidase (C-acquiring)	—	14	% Organic Matter in sediment	—
Metabolomics (ICR)	48	Nominal oxidation state of carbon, % tannin, % Condensed Hydrocarbons, Modified Aromiticity Index	Gibbs free energy, % lipids, Double bond equivalency minus Oxygen, % protein	28	% AminoSugars, % Carbohydrates	Aromiticity index, Double-bond equivalence
Dissolved Organic Matter (DOM)	47	peak A (humic-like), peak C (humic-like), total fluorescence	—	20	peak T (protein-like)	fluorescence index
Macroinvertebrates (MACRO)	30	—	Richness, Shannon, index, Richness of collector-gatherers, Richness of predators	16	Abundance of collector-gatherers	Abundance of shredders, Abudnacne of small body size
Stream Solute Tracer (TRACER)	19 *	—	short term storage (holdback, skewness, CV)	16	Dispersion, Fraction of mass in A/D, velocity, upstream and downstream discharge	—

*** Indicates the PC is spatially structured***

3.2 Spatial structure

Next, we assessed the degree to which variance in each variable can be explained by spatial structure. Of the 157 variables considered, we identified 56 variables (about 36%) as having spatial structure, compared to 101 variables (about 64%) of variables without spatial structure. All structured variables were identified based on a linear semivariogram, with none exhibiting a spatial scale at which variation stopped increasing with spacing between sample locations. This indicates variance in these spatially structured variables either (a) increases without bound or (b) only plateaus at scales that are larger than were included in the 5th order river basin we studied.

The largest proportion of spatially structured variables were in the nutrient subgroup (69%), and the least were in the macroinvertebrates subgroup (9.5%; Fig. 1C). We did not find that the variables included in the individual PCs separated into two distinct groups, structured vs. unstructured variables. Instead, we found 44% of influential variables were spatially structured (23% in PC1 and 21% in PC2) compared to an overall representation of 36%. Similarly, the fraction of influential variables with spatial structure was consistent across subgroups (Fig. 1B, 1C), and 6 of 14 subgroup of PCs contained both structured and unstructured variables.

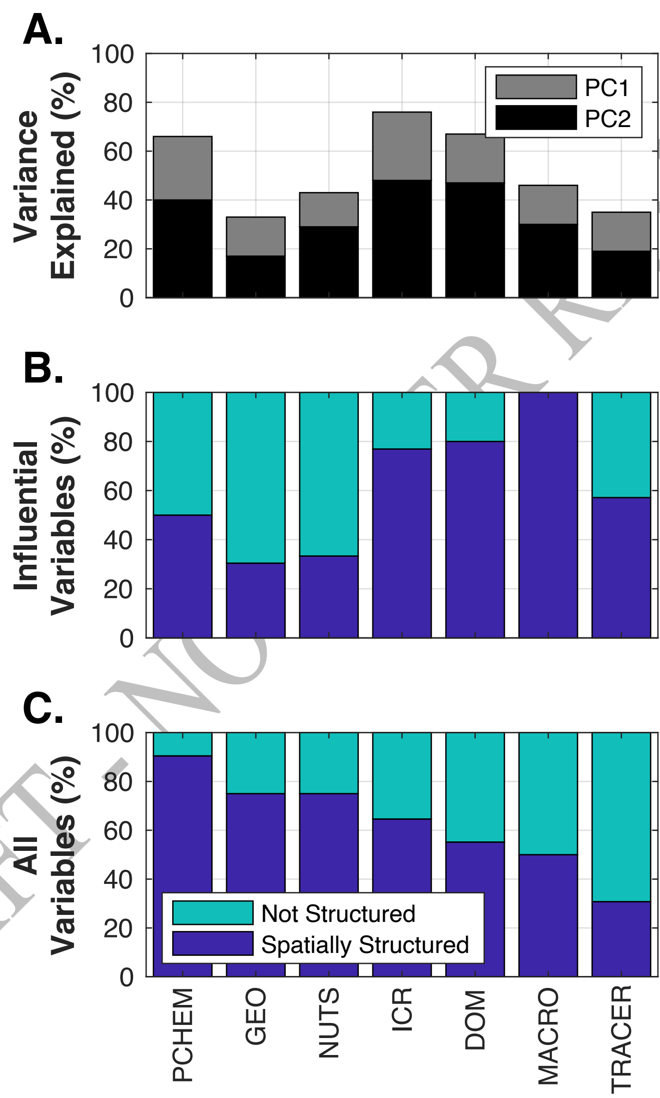

Fig. 1. (A) Variance in the data set explained by PC1 and PC2 for each expert subgroup. (B) Percentage of influential variables (i.e., the variables included in the PCs) that do and do not have spatial structure. (C) Percentage of all variables within each subgroup that do and do not have spatial structure.

3.3 Support Vector Machine Regression (SVMR)

3.3.1 Prediction of each variable using all other variables

We identified 672 relationships in the SVMR analysis that, taken together, demonstrate a complex network of interactions among variables of different research domains measured in the river network (Fig. 2) and each of which represents a potential coupling of variables or processes. The SVMRs were able to explain much of the variance in the underlying data, with an overall mean r^2 of 0.83 (median 0.94, range 0.00 - 1.00). SVMRs for individual variables selected an average of 4.4 variables as predictors (median 4, range 1 to 10), indicating reasonably parsimonious models were formulated. Overall, the models built for 141 variables had r^2>0.50. The models built for spatially structured variables had an overall mean r^2 of 0.91 (median 0.97, range 0.08 - 1.00) compared to a mean r^2 of 0.78 for unstructured variables (median 0.90, range 0.00 - 1.00). Goodness of fit was statistically better for the spatially structured variables (p = 0.008; one-way ANOVA), indicating that spatially structured variables were more accurately predicted (i.e., higher r^2) compared to unstructured variables.

Of the 157 variables predicted, 22% (34 variables) are informed by only out-of-group variables (i.e., variables from a different subgroup), and 11% (17 variables) are informed by only within-group variables (i.e., variables in the same subgroup). Thus, 67% of variables (106 out of 157) required both in-group and out-of-group information for optimal prediction by the SVMRs. Moreover, we find out-of-group information dominates predictor selection, representing an average of 59% of variables selected (median 66%, range 0-100%; Fig. 2, Table S1). Spatially structured variables represent an average of 27.3% of variables selected for individual SVMRs (Fig. S3). Across the 157 SVMRs constructed, 30% (47 variables) did not select any spatially structured features. We found 3% of models (5 variables) selected only spatially structured features, and the remaining 67% (105 variables) selected a combination of structured and unstructured variables.

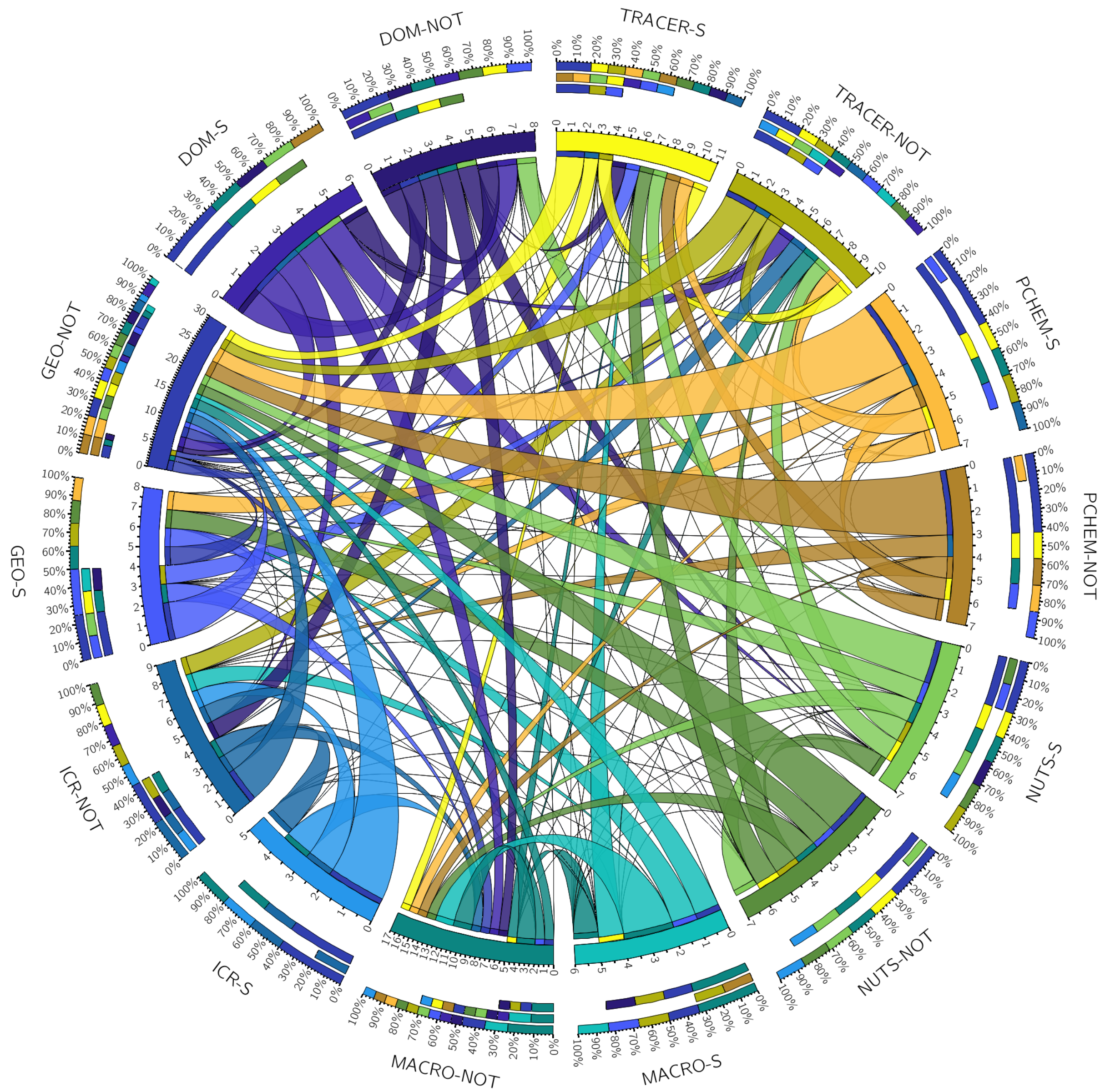

Fig. 2. Information flow within and among subgroups of variables commonly used as descriptive of river corridor dynamics based on the suite of SVMRs constructed for each variable (Section 3.3.1). The variables included in the 7 subgroups are further organized by those with spatial structure ("-S") and without spatial structure ("-NOT").

The width of each 'ribbon' denotes the frequency of interaction between variable groups. The three 'rings' represented around the outside of the plot represent information flow as: Inner Ring: the source of information (i.e., which groups contributed information to make predictions for a given group). Middle Ring: destination of information from each subgroup goes (i.e., which groups needed information from a given group for their predictions). Outer Ring: Total interactions with other groups (i.e., the sum of the inner and middle rings).

Individual variables were selected an average of 4.3 times (median 3, range 0-26), where the most commonly selected variable was in-stream NH_3 concentration. However, this variable only contributed 0.046 improvement in r^2 summed across the 26 models where it was selected. In contrast, the largest improvements associated with r^2 were associated with the functional richness index for macroinvertebrate communities, which provided a total improvement in r^2 of 6.3 summed across the 20 models where it was selected (average improvement in r^2 was 0.315 when including this variable in a model).

Across all 157 SVMRs constructed with the entire variable set, out-of-group variables were selected more frequently than within-group variables and contributed more to the overall r^2 of the model. We found out-of-group variables represent about 30% of all selections within the SVMRs (Fig. S2c), but contribute more than 50% of the improvements in model performance (Fig. S2d). Spatially structured variables represent about 36% of all variables selected and contribute about 40% of the improvements in model performance (Fig. S3).

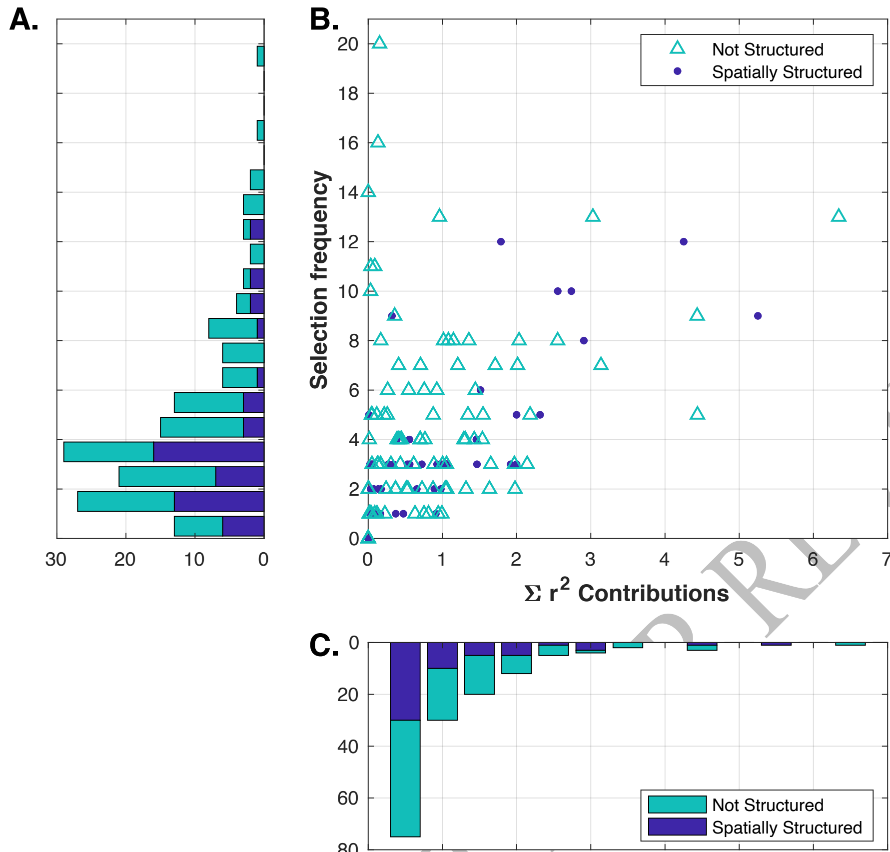

Fig. 3. For all 157 SVRMs constructed on all variables: (A) Histogram of the frequency with which individual variables were selected. (B) Variable selection frequency vs. total improvement. (C) Histogram of contributions of variables to r^2.

3.3.2 Prediction of each variable using principal components from each subgroup

PCs for each subgroup define major axes of variation in the river network, but still leave an average of 48% of variance unexplained within each subgroup. To relate major axes of variation between subgroups, we constructed SVRMs for each variable using the PCs from each subgroup as possible inputs. In-group PCs were always selected more frequently than PCs from any other subgroup (Table S2). In fact, about 25% of variables (39 of 157) were predicted solely from their in-group PCs. The explanatory power of PCs for in-group variance is unsurprising given that PC1 and PC2 were successful in explaining an average of 52% of variance within their group. However, we also found about 26% of variables (41 of 157) used only out-of-group PCs, and

118 variables selected at least one out-of-group PCs. Notably, variables in each subgroup drew information from nearly every other subgroup (see Table S1), These findings indicate that studies that are limited to one discipline are unlikely to explain as much variance as those that intentionally span disciplinary boundaries, even if they only characterize the major axes of variation from other subgroups.

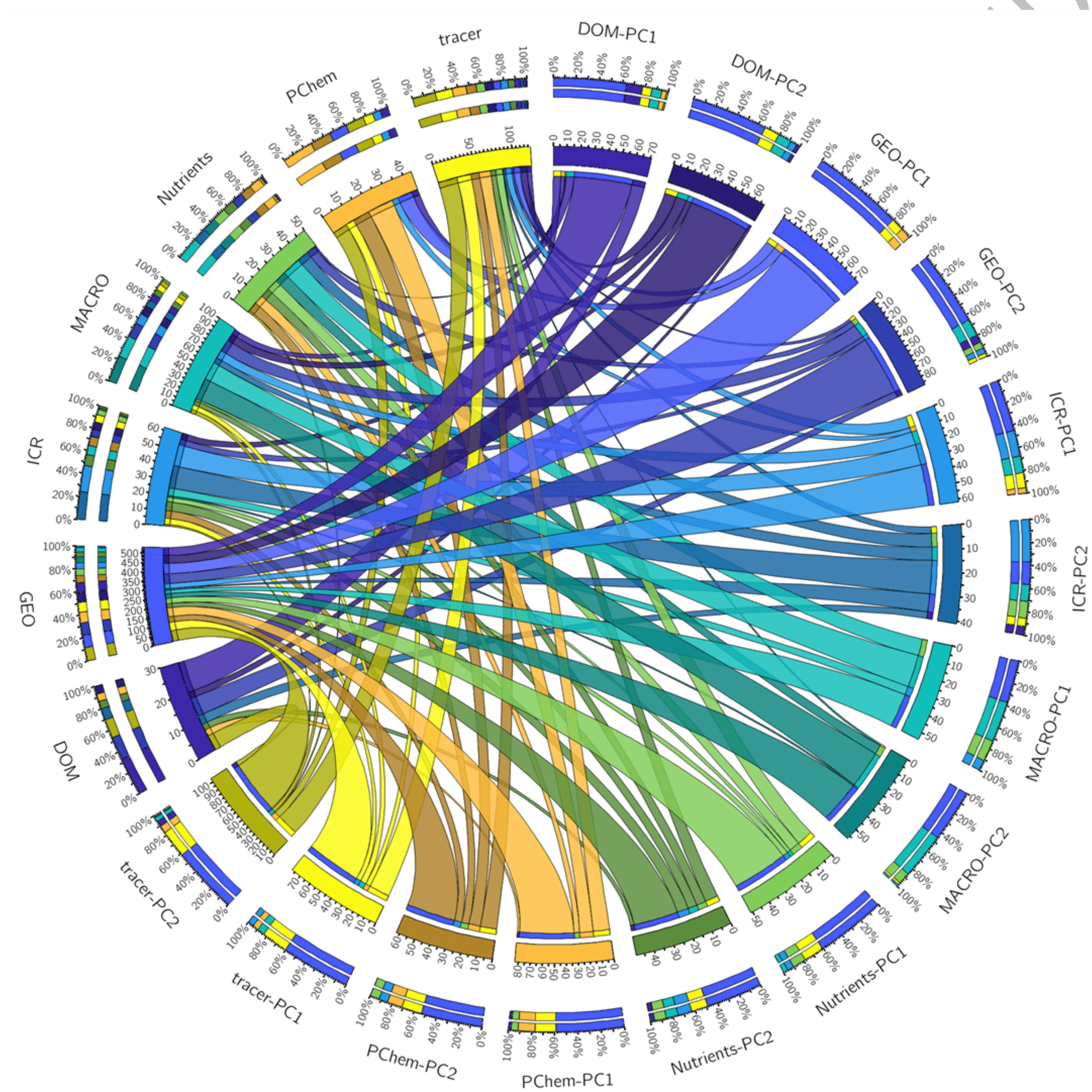

Fig. 4. Circos plot showing the one-way flow of information from the subgroup PCs (Table 1; labeled "XXX-PCY" where XXX is the subgroup and Y in the PC number) to variables predicted by the suite of SVMRs described in Section 3.3.2.

3.4 Frequency of existing studies in the literature

Our literature search identified 4,075 combinations of variables that have been studied pairwise in the literature (of 12,246 possible combinations). The pairwise literature search returned a total of 2,731,694 results. The number of studies identified for any given pair of variables was highly skewed, with pairwise frequency ranging from 1 to 270,015 studies of any given pair of variables (mean 670, median 14). For example, 50% of the studies identified included the 18 most commonly studied pairs of variables, indicating a bias toward the co-observation and reporting of a limited number of pairwise studies, consistent with a past study that manually reviewed search results (Ward, 2015). We also found the existing literature is more focused on in-group relationships (57.2% of pairwise results) compared to between-group relationships (42.8% of pairwise results). In contrast, our SVMR approach identified a total of 672 pairwise relationships. Notably, about 84% or 564 variable pairs do not appear to have been studied previously because our literature search did not return any manuscripts sharing the key search terms. The remaining 28.2% (108 relationships) have been previously studied in the literature (Fig. 5; Fig. S5; Table S4). The 108 relationships found in both the literature and in our study represent about 2.6% of all relationships in the literature, but include more than 16% of all studies identified indicating a large focus on a small number of relationships. Moreover, 68.8% of SVMR-derived relationships are between-group, compared to only 42.8% of literature-derived relationships.

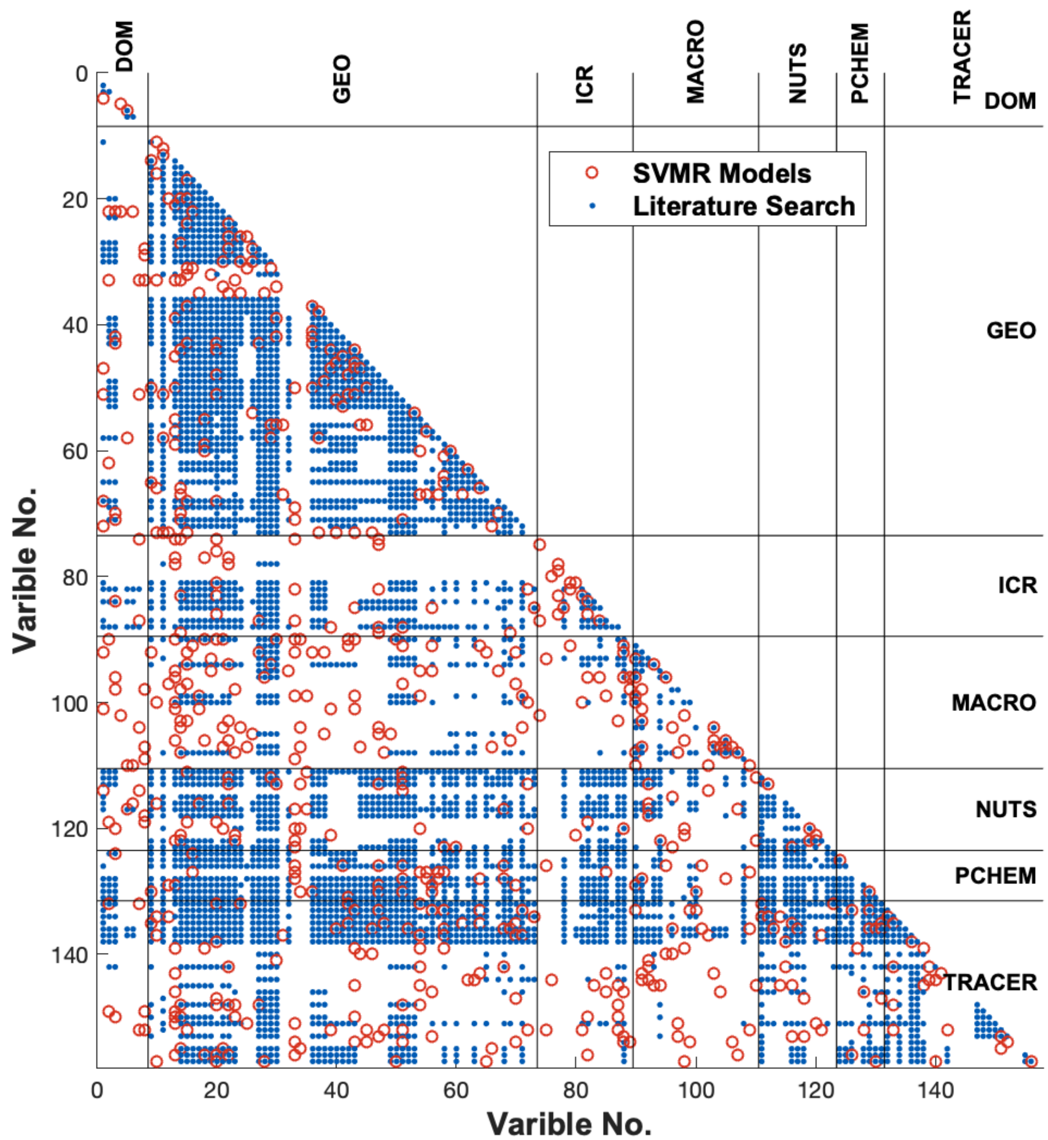

Fig. 5. Scatterplot showing evidence of pairwise study in the literature (blue dots) and identification of a relationship in our SVMR approach (red circles). Variable numbers correspond to the order variables are summarized in Table S1.

4. Discussion

4.1 Relating large-scale spatial patterns and localized heterogeneity in the river corridor

We found that spatially structured variables were selected less frequently than would be expected by random chance (i.e., structures variables are 27% of the variables included by SVMRs although they make up 36% of the total variable set). This means the predictions of spatially structured variables were not dominated by structure from a small number of structured variables, suggesting spatial structure alone is not sufficient to explain the patterns we observed in the river corridor.

A majority of variables observed (about 64%) were not themselves spatially structured, and five subgroups (PCHEM, GEO, NUTS, ICR, TRACER) result in at least one PC that is not spatially structured. These results indicate that spatial structure is not ubiquitous in the river corridor. Instead, some variables represent 'noise' on the network-scale 'signal' described by Vannote et al. (1980). This heterogeneity is either independent from large-scale system structure (i.e., controlled by local process interactions and does not influence larger scale pattern) or simply sufficiently high to obscure larger-scale trends.

Individual variables also reflect complex interactions that can lead to either the emergence of spatial structure or overwhelming of underlying spatial structure. We found six variables that were spatially structured for which the SVMRs only included unstructured variables. In these cases, spatial structure emerged or was generated by the interaction of variables that did not themselves, have spatial structure. Conversely, 60 of the SVMRs for unstructured variables included at least one spatially structured variable as an input (38 selected 1, 14 selected 2, and 8 selected 3 spatially structured variables). This pattern suggests that spatial structure does not necessarily propagate from one variable to another. Put another way, we observe "signal shredding" (Jerolmack & Paola, 2010), where information is erased by the interaction of variables. In the river corridor, this may indicate that localized feedbacks can overwhelm underlying spatial structure.

4.2 Benchmarking inductive relationships to established, deductive science

A majority of the relationships identified in the SVMR are novel compared to the literature. However, some relationships identified in the inductive approach are consistent with pre-existing conceptual models and published at the H.J. Andrews Experimental Forest. The inductive identification of patterns and couplings that are consistent with deductive work is important, as it builds confidence in the approach. Below we detail three examples of consistency between inductive and deductive science in the basin, including relationships that are generally viewed as important in the river corridor: hydrologic exchange processes, microbial ecology, and the River Continuum Concept (Vannote et al., 1980). Taken together, these examples demonstrate the potential value in the novel hypotheses generated in our study.

4.2.1 River Corridor Exchange

In prior analysis, we focused on spatial patterns in reach-scale solute transport and identified substantial, unexplained heterogeneity in univariate regressions (Ward, Wondzell, et al., 2019). The SVMRs in this study included 35 unique variables to predict the 11 variables common to our analysis and the prior work. These variables primarily fall within the geologic setting (n = 10), tracer (8), and macroinvertebrate (7) groups. Of those variables, the abundance of the oldest exposed lava flows was included most commonly (5 times), followed by slope stability and forest cover (3 times each). Five additional variables were selected twice (two associated with geological setting, two with tracer, and one with macroinvertebrates), while 26 variables were selected by only one SVMR. Taken together, these results indicate that geologic setting, and the resultant land cover and soils, are important controls on solute transport patterns in the river network. Notably, geologic setting is selected more frequently than other descriptors of tracer transport, suggesting autocorrelation amongst metrics describing tracers is not sufficiently strong to overcome the heterogeneity imparted by the landscape on these experiments. This finding is in good agreement with several past studies from other field sites that have identified geologic setting as a high-level control in both field studies (Payn et al., 2009; e.g., Valett et al., 1996) (e.g., Valet, Payn) and conceptual models (Cardenas, 2008; e.g., Frissell et al., 1986; Wondzell & Gooseff, 2014; Wörman et al., 2007).

Ward et al.'s (2019) observation of monotonic trends between most exchange metrics and discharge - which they describe as a proxy for network position - agree with our finding of spatial structure in several variables describing geomorphic setting (including hydraulic conductivity, valley slope, valley width, sinuosity), river flow (velocity, discharge), and several solute transport metrics (e.g., median travel time, skewness). We did not find spatial structure for other metrics of exchange where Ward et al. did, including the coefficient of variation, holdback, channel water balance. Further, many of the relationships identified by Ward et al. have low explanatory power as evidenced by low r^2 values, indicating the system cannot be described by a single explanatory variable. Indeed, Ward et al. explicitly call for multivariate and nonlinear responses to better explain the observed patterns in river corridor exchange which we have implemented in this study.

4.2.2 Microbial Community Assembly

Interactions along river corridor can not only 'shred' or erase information (sensu Jerolmack & Paola, 2010), but can also generate new information and patterns. For example, Wisnoski and Lennon (2021) studied microbial community assemblages in the H.J. Andrews from data collected in 2015 whereas the data set analyzed here was collected in 2016. In their study, microbial assemblages in headwater streams were habitat-dependent, while the microbial community became more homogeneous with distance downstream. Additionally, Wisnoski and Lennon found that taxonomic β-diversity was explained by an axis with positive loadings for elevation and dissolved organic carbon, and negative loadings for fluid electrical conductivity, pH, total nitrogen, and total phosphorus. Microbial assemblages are known to arise in response to local heterogeneity in the landscape, integrating inputs and environmental variables in space and time. While we did not analyze microbial assemblages explicitly, here we compare underlying geomorphic and water quality variables with prior observations of the microbial community assemblage. Our results show spatial structure in fluid conductivity and several geomorphic variables that are known to vary with elevation, but no spatial structure in total dissolved phosphorus, DOC, nor total dissolved nitrogen. Thus, we interpret the spatial organization of the microbial assemblage as the emergence of structure from a suite of largely unstructured variables in the river corridor. Consequently, studies focused at single locations along a stream may be missing information from the catchment headwaters, or interpreting signals that were generated along the river corridor and misinterpreting their origin as being on the landscape.

4.2.3 River Continuum Concept

The River Continuum Concept (Vannote et al., 1980) -- perhaps the most widely cited conceptual model of river corridors -- argues that Leopold's conceptual model that geomorphology reflects energy equilibrium can be extended into ecosystem functions (Langbein & Leopold, 1966; L B Leopold et al., 1964; Luna B. Leopold & Langbein, 1962). Vannote et al.

(1980) specifically proposed: (a) biological communities and their functions should achieve an equilibrium to optimize the use of available energy (i.e., organic matter); and (b) energy availability will vary systematically from headwaters to large downstream rivers. Our PCA on all variables is consistent with these assertions. We found organic matter chemistry and geological setting explained 37% of the variance across the entire data set. We also found spatial structure in about 36% of all variables across all disciplinary subgroups, consistent with the idea that large-scale gradients will drive systematic trends across physical and biogeochemical processes. Six of the fourteen subgroup PCs were spatially structured (Table 1), reflecting broad spatial structure in this study catchment. Our findings of broad patterns along the river network, as evidenced by spatial structure, is broadly consistent with the River Continuum Concept, which was based on a much more limited set of measurements. Our findings on the importance of organic carbon chemistry also support Vannote et al.'s expectation of the importance of energy availability on structuring ecosystems along the river corridor.

4.3 On the interpretation of inductive hypotheses and future directions

The suite of models we constructed include 672 relationships, 84% of which have not been previously studied based on our literature search. We identify four possibilities to explain the absence of these couplings in prior studies, relate each to existing science, and reflect on how these hypotheses can be used to advance our goal of synthetic science and comprehensive descriptions of the structure and function of river corridors.

4.3.1 Spurious correlation and autocorrelation may exist

The relationships identified in our study may represent spurious correlation of disparate data. In this case, the inductive approach is identifying mathematical artifacts rather than actual process interactions. These relationships may also reflect redundant information (i.e., several different variables may reflect similar features on the landscape, and the autocorrelation amongst independently-measured variables may obscure underlying relationships). For example, if geology, land cover, and soils all systematically vary with increasing elevation, then these variables will all show consistent relationships that may confound interpretation. We emphasize here the relationships identified by SVMR and other machine learning methods only provide a starting point for generation of hypotheses. The next step for investigation of such putative relationships would be to hypothesize a causal mechanism and design a study to collect the specific data needed to test it.

4.3.2 Relationships may be scale dependent

Both the structure and function of river corridors are known to be scale-dependent (Frissell et al., 1986; McCluney et al., 2014). The network scale considered here is larger than many studies of river corridors (Tank et al., 2008; Ward, 2015). It is possible that the relationships identified between variables here by SVMR do not hold at all scales, or that the relationships are real but have not been tested over the range of scales we included in our analysis. Prior studies of river structure have found that self-similarities and scale dependencies generally only occur over a limited range of scales, and either average out at large scales or are limited by a physical constraint (such as water depth, channel width, or valley width) (Jerolmack & Paola, 2010; Nikora & Hicks, 1997; Rodríguez-Iturbe & Rinaldo, 1997). As with relationships between individual variables, scale dependencies and scaling limits identified from broad data analysis must be considered as hypotheses and tested using directed observations and/or model simulations with competing or alternative formulations.

4.3.3 Disciplinary, deductive science is the predominant mode of inquiry

The norms of classical research funding opportunities and publications require deductive approaches, where the limited resources of time and financial support are focused on testing hypotheses. Consequently, researchers tend to focus efforts and resources on a narrow suite of specific observations rather than collection of data that appear to be extraneous for hypothesis testing based on prior understanding in the field. However, this paradigm is shifting with emphasis on macrosystems research (Heffernan et al., 2014) and the explicit design of networks to facilitate synthesis (e.g., AmeriFlux, NEON, Critical Zone Collaborative Networks). Our results show that the inherent complexity of river corridors and networks means that experimental programs of limited scope will often miss important process controls. This finding provides further support for our past recommendation that all river corridor studies collect a standard set of observations for system characterization [cite], as this information is likely to be important to testing specific hypotheses in ways that may not be apparent in the initial study design.

4.3.4 Data limitations have restricted comparable analyses

Our analysis relies on the most comprehensive catchment-scale characterization of interacting physical, chemical, and biological processes in the river corridor to-date. The dataset we analyzed also builds upon extensive prior work and data from the H.J. Andrews Experimental Forest. Such comprehensive datasets have not previously been available, and require extensive interdisciplinary collaboration to obtain. One example is measurements of organic matter chemistry, which is only recently emerging as part of river corridor science (Graham et al., 2018; Stegen, Johnson, et al., 2018; Zhou et al., 2019). To make further progress in unraveling the complexity of river corridors, we recommend combining standardized system characterization across many streams and rivers with intensive study of select watersheds to generate the rich datasets needed to evaluate process interconnections and scale dependencies (Stegen & Goldman, 2018).

4.4 Toward a unified conceptual framework for river corridors

A unified conceptual framework for river corridors will require studies to move beyond the discipline-specific and site-specific studies that have dominated our field in the past decades [Ward, 2015]. Instead, we need to augment our existing body of knowledge with ‘connective tissue’ that allows integration of our findings across spatial scales, temporal scales, and processes. Here, we endorse the conceptual organization Stegen et al. (2018) posed for microbial ecology, where we can begin to arrange our past and future studies around external forcing, internal dynamics, and historical context to explain and predict both temporal-variability and resultant services and functions of river corridors. Indeed, the framework of separating external forcing from internal dynamics is consistent with emerging theories in catchment hydrology where the same language has been applied to river corridors (Harman et al., 2016). However, this organization ultimately requires consideration of our studies in a synthetic framework rather than from a disciplinary framework.

Our study suggests that one avenue toward progress in river corridor science is through the collection of uniform metadata and even out-of-group observations as part of disciplinary studies. We demonstrate here that, in the dataset we collected, out-of-group data were important to explaining many of the disciplinary (i.e., in-group) patterns that were observed. Thus, the out-of-group data not only enable synthesis, but may simultaneously improve disciplinary studies. While the concepts of uniform metadata and common observations have been previously called for (Ward, 2015; Ward & Packman, 2019), our study demonstrates the value of these data to improve prediction of individual variables or functions in the river corridor. One potentially valuable path forward would be to complete comprehensive characterization of several river corridors and at multiple times of year to help screen which of the relationships we identify may be spurious, time-variable, or organized by larger climactic or geologic patterns.

In this study, we have applied machine learning approaches to generate hypotheses that may ultimately serve as the 'connective tissue' that link our understanding across spatiotemporal scales and disciplines. Indeed, the step of organizing raw observations to spin hypotheses is at the core of the scientific method. Hypothesis generation is touted as one of the core values of field-based observation and monitoring (Burt & McDonnell, 2015; Lovett et al., 2007), where observations demand explanations. The inductive approach used here presents a body of potential couplings for subsequent study, at least some of which are consistent with existing conceptualization of river corridors (i.e., section 4.2). We do not propose that such approaches supplant deductive science, but rather that the two approaches are coupled in the scientific methods. Rather than rely upon individual scientists and our disciplinary training to spin hypotheses, the inductive approach can provide an unbiased or naive data synthesis, which has the potential to reveal patterns or relationships that would not be obvious from our present, disciplinary perspectives. This is consistent with iteration between hypotheses, empirical studies, and mechanistic models to screen potential hypotheses that are a hallmark of integrated model-experimental frameworks (US Department of Energy, 2021). We expect these relationships are one path toward the integrative studies required for advancing our predictive understanding of river corridors.

5. Conclusions

In this study, we have prototyped an inductive approach to complement the traditional deductive model of inquiry that is common to studies of river corridors. We used machine learning techniques to generate a series of relationships that may warrant further inquiry. Relationships identified in our approach do not rely on pre-existing conceptual models, allowing the potential for cross-scale and multidisciplinary interactions that might not be considered using a deductive approach, providing a complementary basis for data synthesis. Importantly, this approach and the hypotheses generated may be one way to advance toward a unified conceptual model, where findings are organized in a synthetic framework instead of discipline-, scale-, site-, or method-dependent bodies of knowledge.

While the study of river corridors has made great progress using deductive models of science, our analyses have identified 564 pairwise relationships that were not previously explored in the literature. Put another way, we have generated a web of 564 new hypotheses that may reveal new couplings in the river corridor. Moreover, the network of relationships we have identified is consistent with several past studies from the field site (Vannote et al., 1980; Ward, Wondzell, et al., 2019; Wisnoski & Lennon, 2021), providing confidence that at least some of these relationships are more than spurious correlations.

Most of the relationships we identified, including a majority of those not present in the literature, include between-group flows of information. Our results show that interactions between processes that are typically studied by different disciplines is critically important to explain structure and function in the river corridor. This conclusion is, perhaps, unsurprising as a macrosystems view would acknowledge and expect to find cross-scale and interdisciplinary relationships (Heffernan et al., 2014; McCluney et al., 2014). Still, this view is seldom fully captured in existing experimental designs and the resulting data sets and literature. Importantly, we also demonstrated that spatial structure can be both generated through the interaction of unstructured data as well as destroyed or overprinted along the network. Thus, consideration of how an observed pattern may emerge or not be visible along a spatial gradient is a critically important consideration prior to interpretation of data sets.

Building connections between existing studies requires explicitly planning for synthesis in future efforts. Here, we demonstrated the value of collecting data sets that enabled synthesis within and between locations, disciplines, and scales. This does not diminish the value of traditional, disciplinary hypothesis testing. Instead, common metadata and even a small number of out-of-group observations may enable synthesis efforts based on inductive approaches.

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