

Regional patterns and drivers of nitrogen trends in a human-impacted watershed and management implications

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November 21, 2022

Abstract

Nutrient enrichment is a major issue to many inland and coastal waterbodies worldwide, including Chesapeake Bay. River water quality integrates the spatial and temporal changes of watersheds and forms the foundation for disentangling the effects of anthropogenic inputs. However, many water-quality studies are focused on limited portions of the watershed or a subset of potential drivers. We demonstrate with the Chesapeake Bay Nontidal Monitoring Network (84 stations) that advanced machine learning approaches – i.e., hierarchical clustering and random forest – can be combined to better understand the regional patterns and drivers of total nitrogen (TN) trends in large monitoring networks. Cluster analysis revealed the regional patterns of short-term TN trends (2007–2018) and categorized the stations to three distinct clusters, namely, V-shape ($n = 25$), monotonic decline ($n = 35$), and monotonic increase ($n = 26$). Random forest models were developed to predict the clusters using watershed characteristics and major N sources, which provided information on regional drivers of TN trends. We show encouraging evidence that improved nutrient management has resulted in declines in agricultural nonpoint sources, which in turn contributed to water quality improvement. Additionally, water-quality improvements are more likely in watersheds underlain by carbonate rocks, reflecting the relatively quick groundwater transport of this terrain. However, TN trends are degrading in forested watersheds, suggesting new sources of N in forests. Finally, TN trends were predicted for the entire Chesapeake Bay watershed at the scale of 979 river segments, providing fine-level information that can facilitate targeted watershed management, especially in unmonitored areas. More generally, this combined use of clustering and classification approaches can be applied to other monitoring networks to address similar questions.

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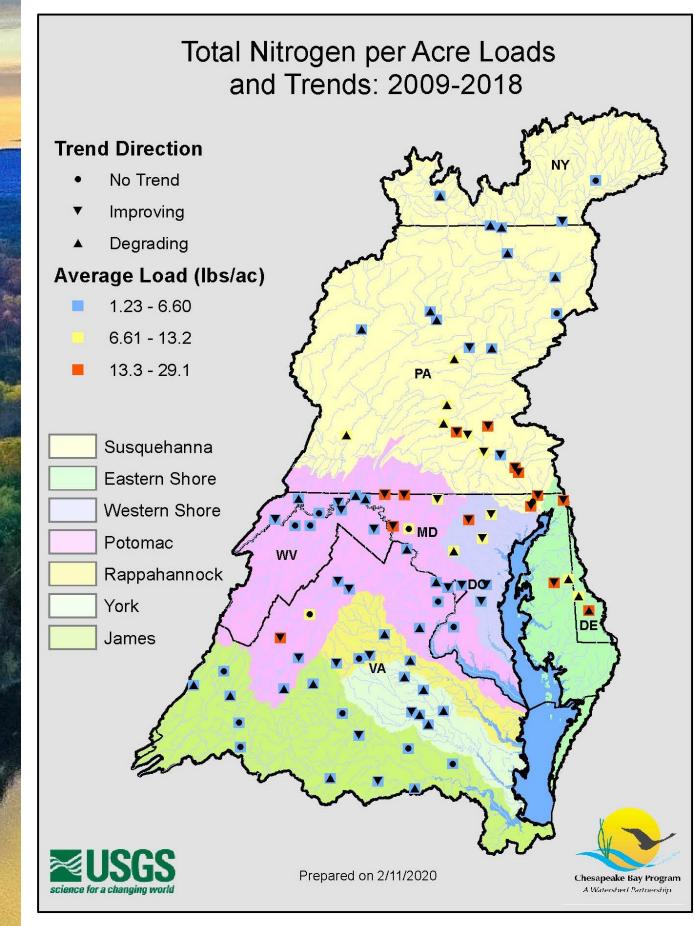
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Motivations

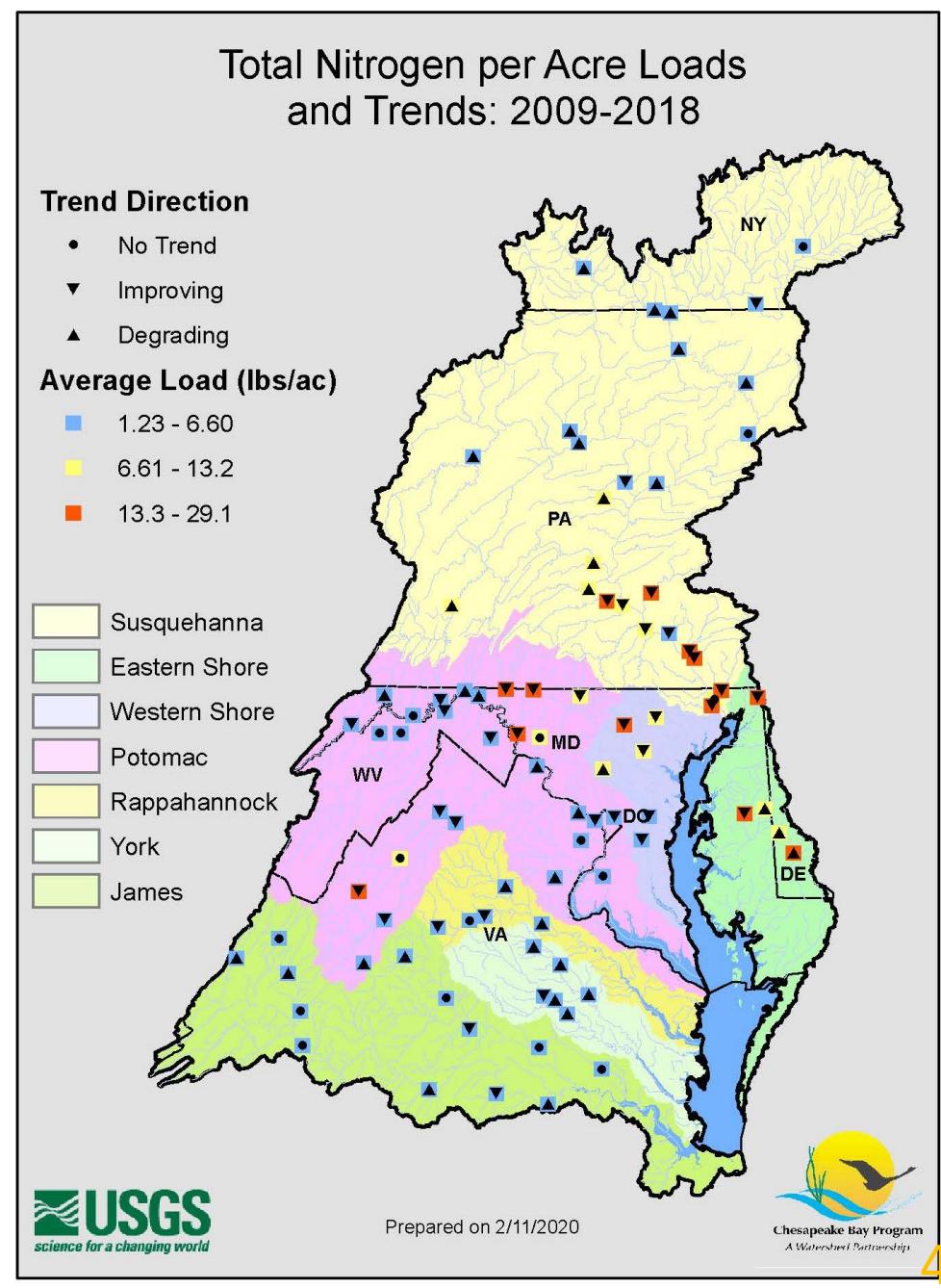
- River water-quality (WQ) trend studies often focus on one or a few monitoring locations, making conclusions difficult to generalize.
- Much can be learned from the similarity in WQ signals and the similarity in WQ responses to natural and anthropogenic drivers, which is made possible by data from regional monitoring networks.
- While many studies are aimed at the long-term scale (~30 years), short-term analysis can leverage data from newly established stations and provide relatively current information.
- Monitoring networks (i.e., CBNTN) do not often cover the entire watershed, leading to missing information in certain regions.
- Prior analyses of drivers do not always evaluate all major input sources, leading to potentially inaccurate or even contradicting inferences.

Objective

To reveal regional patterns and drivers of nitrogen trends using advanced machine learning approaches -- combined use of hierarchical clustering and random forest (RF).

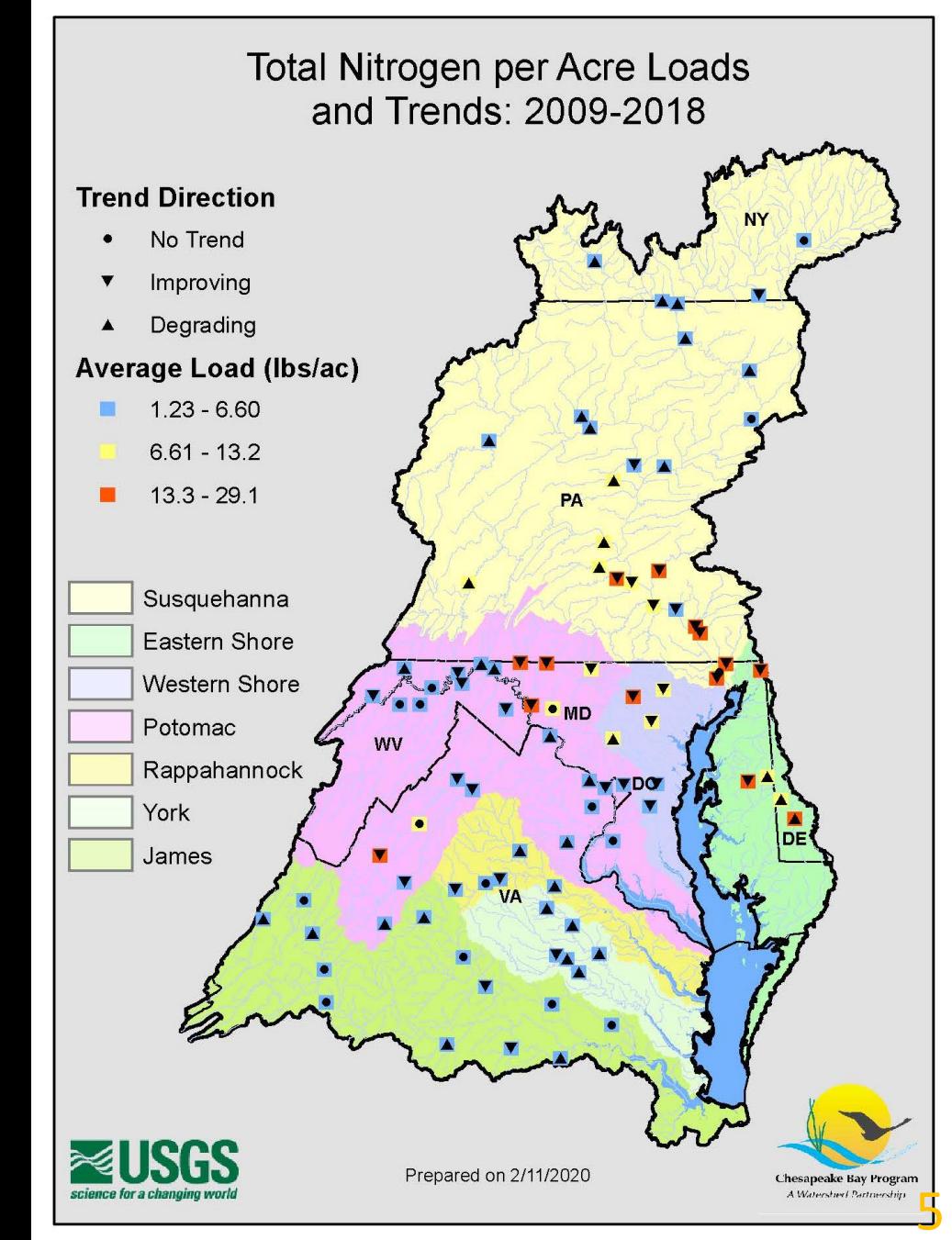
1. **Clustering**: Categorize the short-term (2007-2018) TN trends at the Chesapeake NTN stations (84) into distinct clusters,
2. **Classification**: Develop random forest (RF) models to identify the most influential drivers for the cluster assignment, and
3. **Prediction**: Use the RF model to predict short-term trend clusters for the entire watershed at a fine spatial resolution.

1. Regional patterns of nitrogen trends in the Bay watershed (Clustering)



CBNTN stations and TN data

- CBNTN watersheds ($n = 84$)
- 2007-2018 TN flow-normalized (FN) loads
- Standardized for each station (mean = 0, sd = 1)



Hierarchical cluster analysis

Dissimilarity method:

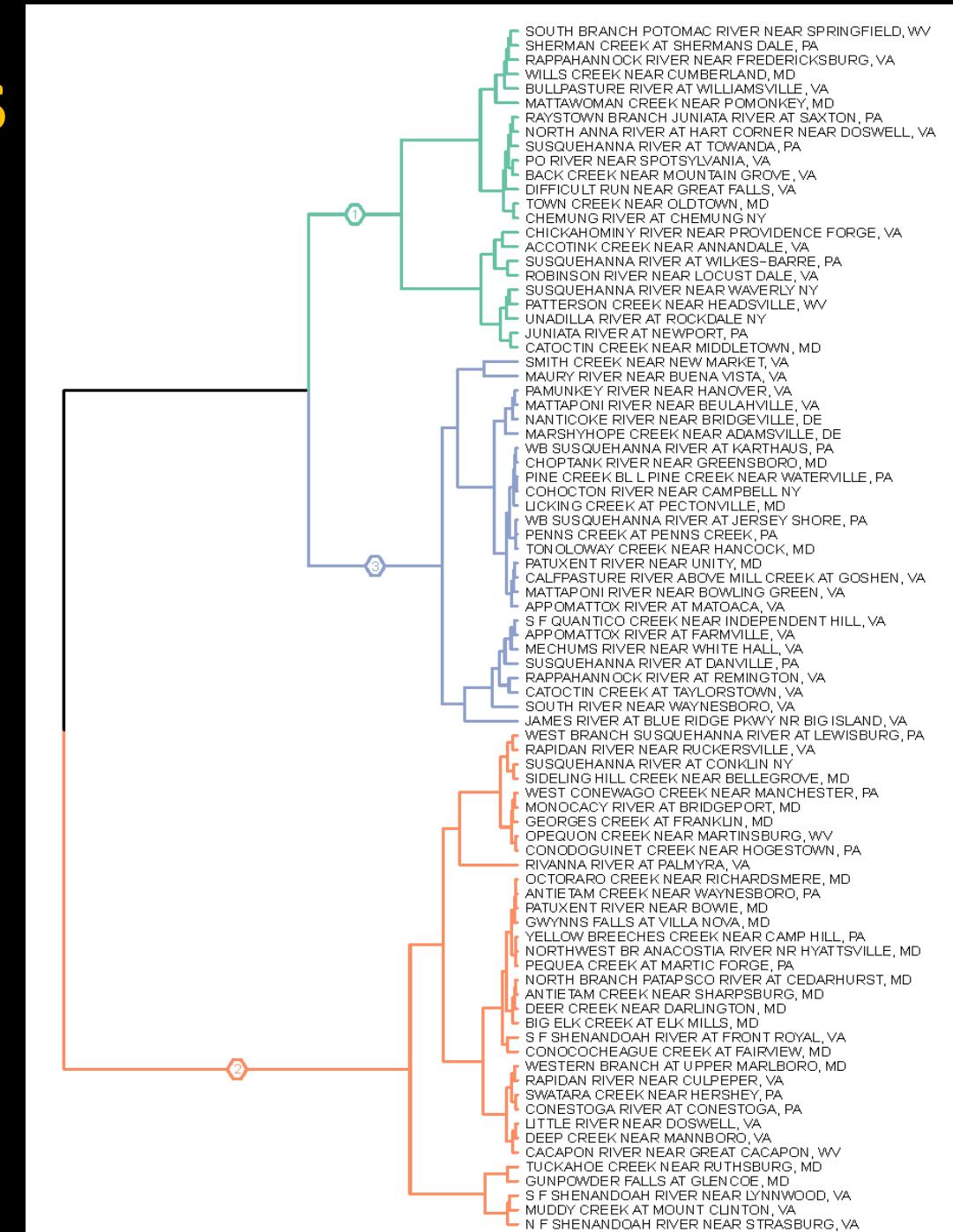
Euclidean distance

Linkage method:

Ward's minimum variance
method

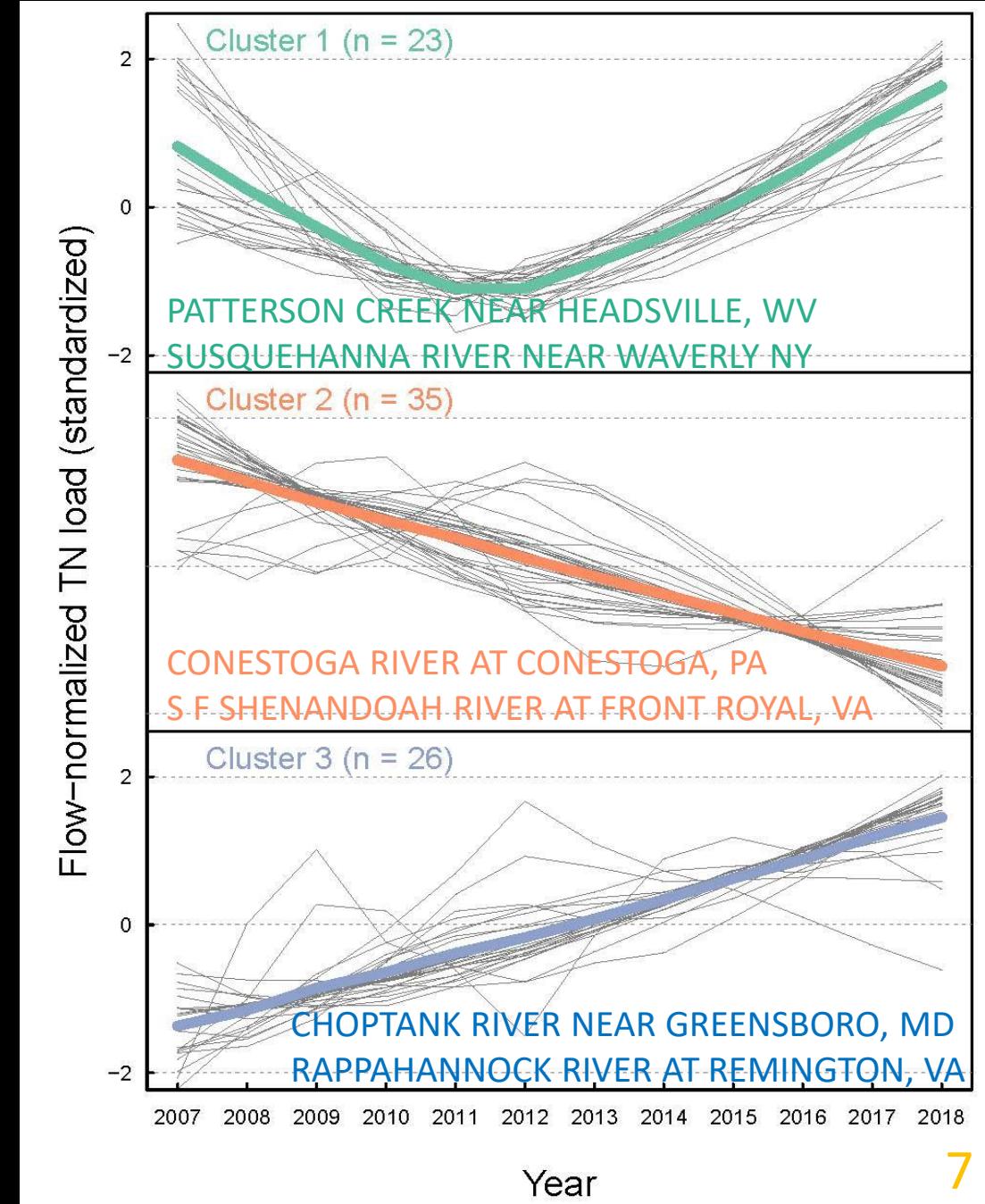
Optimal cluster number:

Total Within Sum of Square



Hierarchical cluster analysis

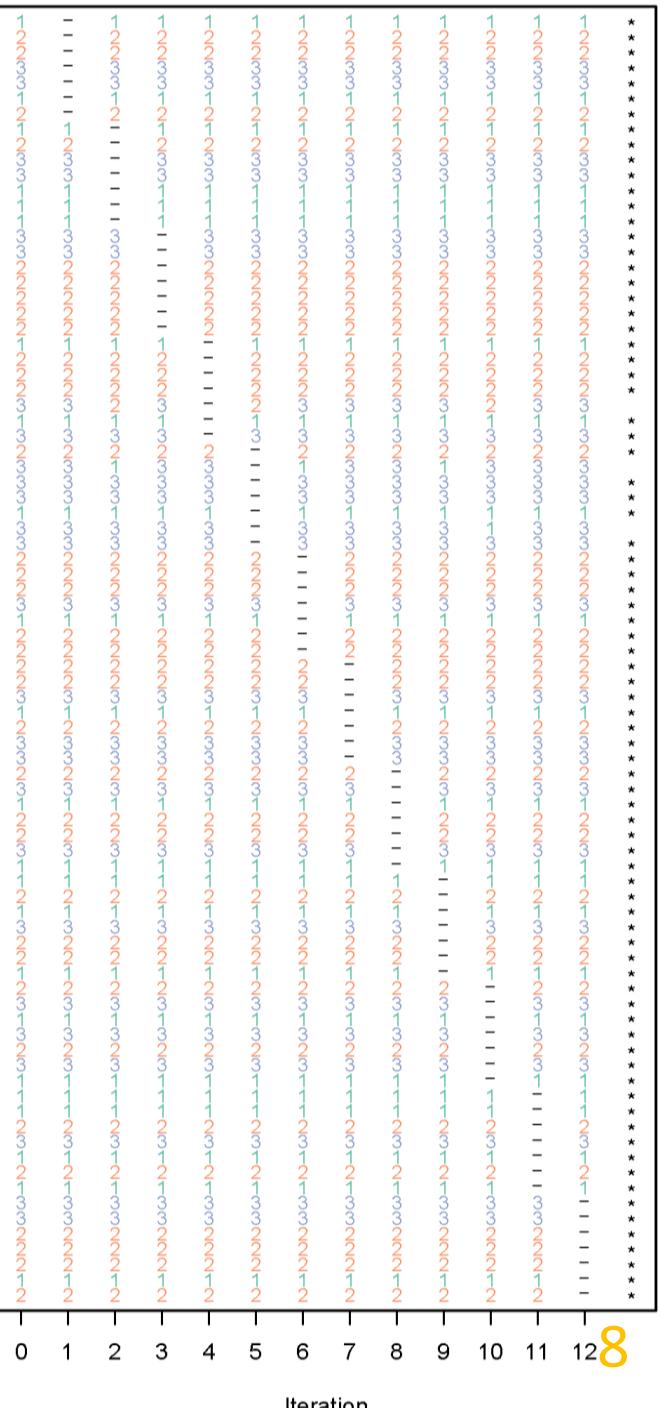
- Cluster 1 ($n = 23$):
a V-shape trajectory.
- Cluster 2 ($n = 35$):
a monotonic decline.
- Cluster 3 ($n = 26$):
a monotonic increase.



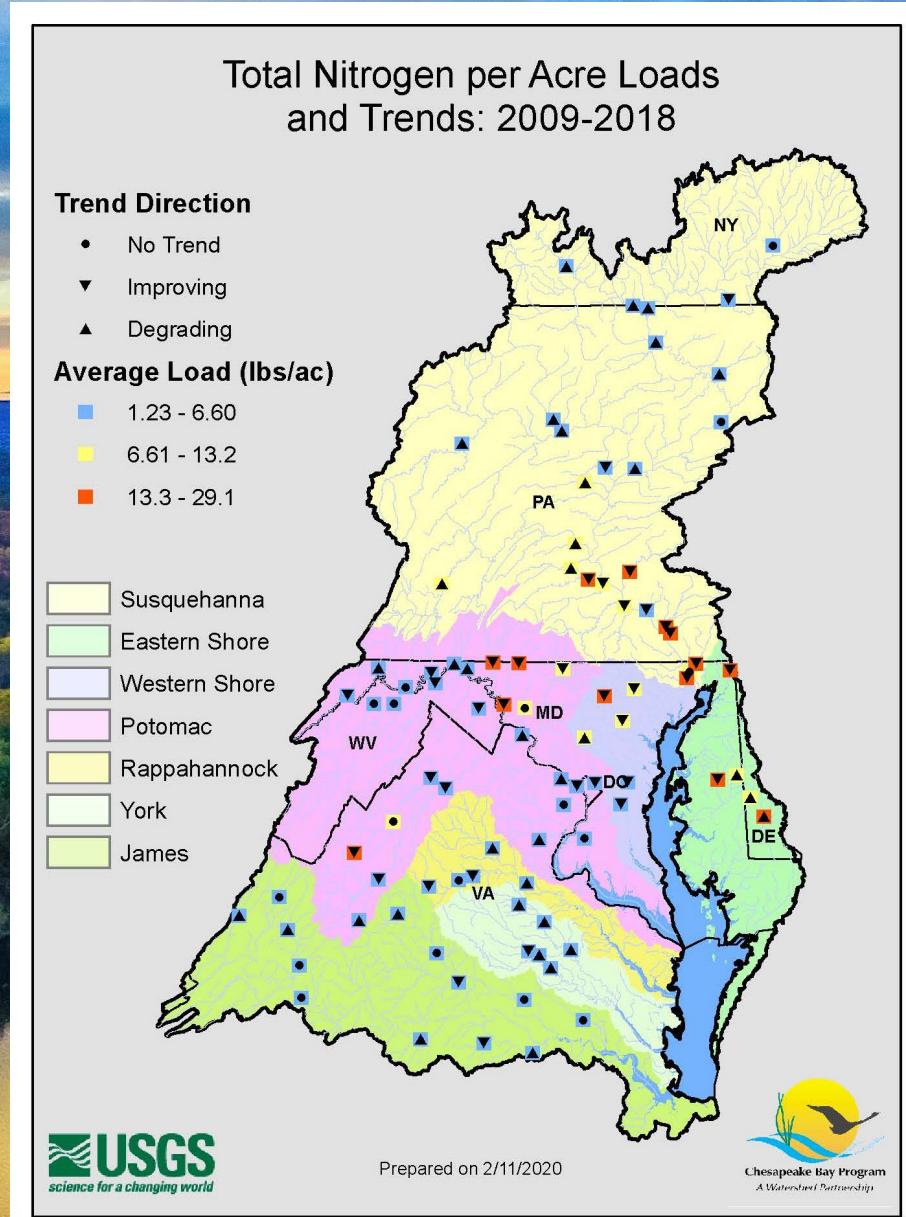
Sensitivity Analysis

- 1/12 of the stations ($n = 7$) were removed without replacement.
- The remaining stations ($n = 77$) were reanalyzed using the same procedure.
- The number of clusters was set at three to be consistent.
- Cluster assignments are almost always consistent among the iterations.

ACCOTINK CREEK NEAR ANNANDALE, VA
ANTIETAM CREEK NEAR SHARPSBURG, MD
ANTIETAM CREEK NEAR WAYNESBORO, PA
APPOMATTOX RIVER AT FARMVILLE, VA
APPOMATTOX RIVER AT MATOACA, VA
BACK CREEK NEAR MOUNTAIN GROVE, VA
BIG ELK CREEK AT ELK MILLS, MD
BULL PASTURE RIVER AT WILLIAMSVILLE, VA
CACAPON RIVER NEAR GREAT CACAPON, WV
CALFPASTURE RIVER ABOVE MILL CREEK AT GOSHEN, VA
CATOCTIN CREEK AT TAYLORTOWN, VA
CATOCTIN CREEK NEAR MIDDLETOWN, MD
CHEMUNG RIVER AT CHEMUNG NY
CHICKAHOMINY RIVER NEAR PROVIDENCE FORGE, VA
CHOPTANK RIVER NEAR GREENSBORO, MD
COHOCOTON RIVER NEAR CAMPBELL NY
CONESTOGA RIVER AT CONESTOGA, PA
CONOCOQUEAGUE CREEK AT FAIRVIEW, MD
CONODOGUINET CREEK NEAR HOGESTOWN, PA
DEEP CREEK NEAR MANNBORO, VA
DEER CREEK NEAR DARLINGTON, MD
DIFFICULT RUN NEAR GREAT FALLS, VA
GEORGES CREEK AT FRANKLIN, MD
GUNPOWDER FALLS AT GLENCOE, MD
GWYNNS FALLS AT VILLA NOVA, MD
JAMES RIVER AT BLUE RIDGE PKWY NR BIG ISLAND, VA
JUNIATA RIVER AT NEWPORT, PA
LICKING CREEK AT PEC TONVILLE, MD
LITTLE RIVER NEAR DOSWELL, VA
MARSHYHOPE CREEK NEAR ADAMSVILLE, DE
MATTAPONI RIVER NEAR BEULAHVILLE, VA
MATTAWOMAN CREEK NEAR POMONKEY, MD
MAURY RIVER NEAR BUENA VISTA, VA
MECHUMS RIVER NEAR WHITE HALL, VA
MONOCACY RIVER AT BRIDGEPORT, MD
MUDDY CREEK AT MOUNT CLINTON, VA
N F SHENANDOAH RIVER NEAR STRASBURG, VA
NANTICOKE RIVER NEAR BRIDGEVILLE, DE
NORTH ANNA RIVER AT HART CORNER NEAR DOSWELL, VA
NORTH BRANCH PATAPSCO RIVER AT CEDARHURST, MD
NORTHWEST BR ANACOSTIA RIVER NR HYATTSVILLE, MD
OCTORARO CREEK NEAR RICHARDSMERE, MD
OPEQUON CREEK NEAR MARTINSBURG, WV
PAMUNKEY RIVER NEAR HANOVER, VA
PATTERSON CREEK NEAR HEADSVILLE, WV
PATUXENT RIVER NEAR BOWIE, MD
PATUXENT RIVER NEAR UNITY, MD
PENNS CREEK AT PENNS CREEK, PA
PEQUEA CREEK AT MARTIC FORGE, PA
PINE CREEK BL L PINE CREEK NEAR WATERVILLE, PA
PO RIVER NEAR SPOTSYLVANIA, VA
RAPIDAN RIVER NEAR CULPEPER, VA
RAPIDAN RIVER NEAR RUCKERSVILLE, VA
RAPPAHANNOCK RIVER AT REMINGTON, VA
RAYSTOWN BRANCH JUNIATA RIVER AT SAXTON, PA
RIVANNA RIVER AT PALMYRA, VA
ROBINSON RIVER NEAR LOCUST DALE, VA
S F QUANTICO CREEK NEAR INDEPENDENT HILL, VA
S F SHENANDOAH RIVER AT FRONT ROYAL, VA
S F SHENANDOAH RIVER NEAR LYNNWOOD, VA
SHERMAN CREEK AT SHERMANS DALE, PA
SIDELING HILL CREEK NEAR BELLEGROVE, MD
SMITH CREEK NEAR NEW MARKET, VA
SOUTH BRANCH POTOMAC RIVER NEAR SPRINGFIELD, WV
SOUTH RIVER NEAR WAYNESBORO, VA
SUSQUEHANNA RIVER AT CONKLIN NY
SUSQUEHANNA RIVER AT DANVILLE, PA
SUSQUEHANNA RIVER AT TOWANDA, PA
SUSQUEHANNA RIVER AT WILKES-BARRE, PA
SUSQUEHANNA RIVER NEAR WAVERLY NY
SWATARA CREEK NEAR HERSHLEY, PA
TONOLAWAY CREEK NEAR HANCOCK, MD
TOWN CREEK NEAR OLDTOWN, MD
TUCKAHOE CREEK NEAR RUTHSBURG, MD
UNADILLA RIVER AT ROCKDALE NY
WB SUSQUEHANNA RIVER AT JERSEY SHORE, PA
WB SUSQUEHANNA RIVER AT KARTHaus, PA
WEST BRANCH SUSQUEHANNA RIVER AT LEWISBURG, PA
WEST CONEWAGO CREEK NEAR MANCHESTER, MD
WESTERN BRANCH AT UPPER MARLBOROUGH, MD
WILLS CREEK NEAR CUMBERLAND, MD
YELLOW BREECHES CREEK NEAR CAMP HILL, PA



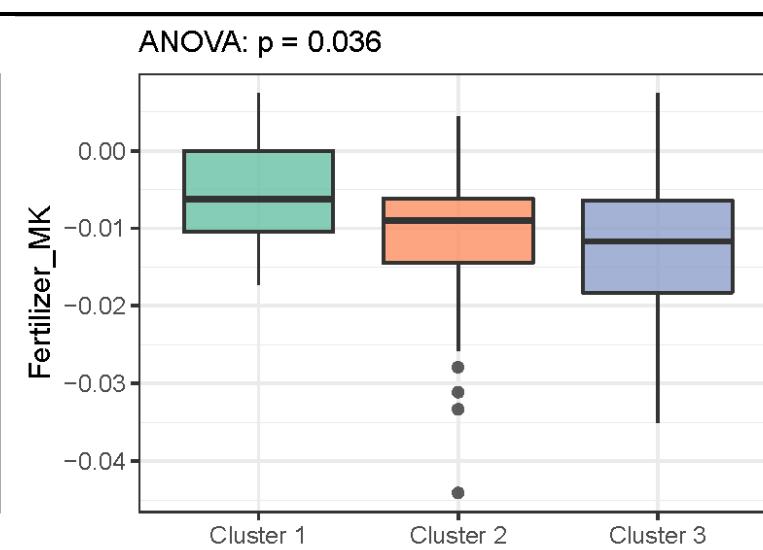
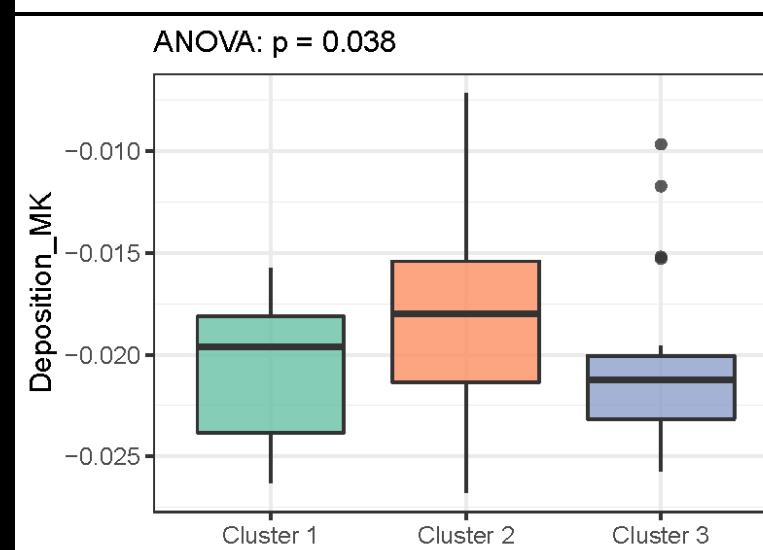
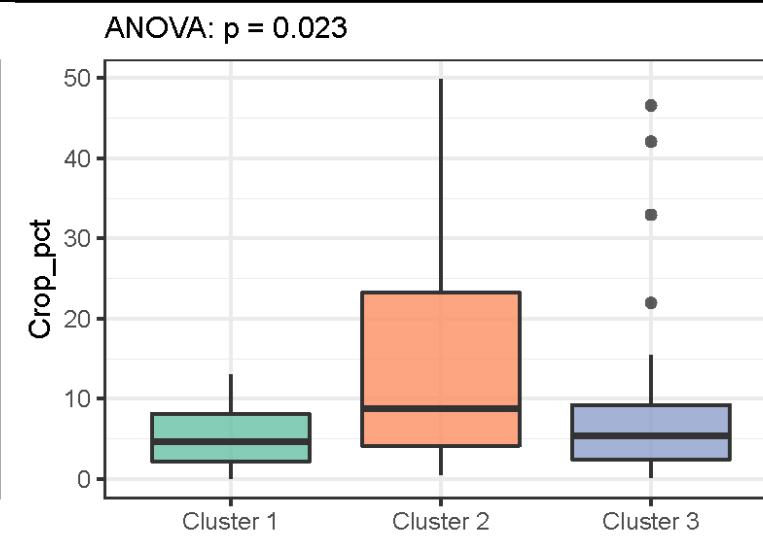
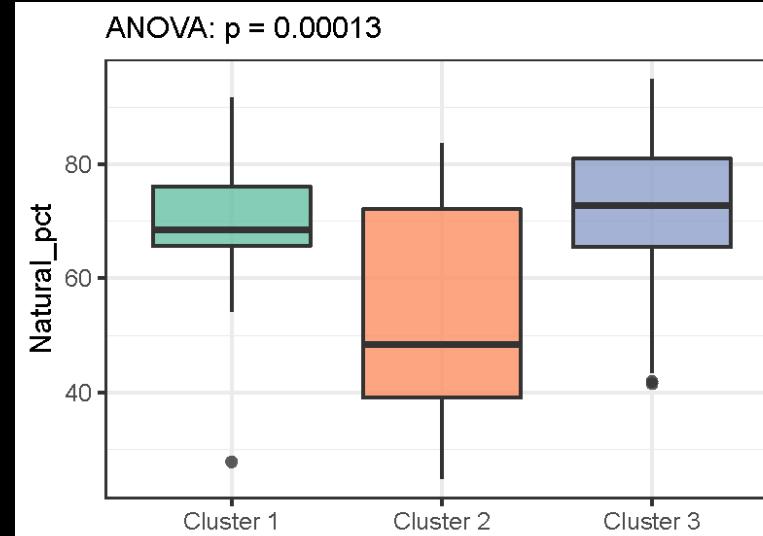
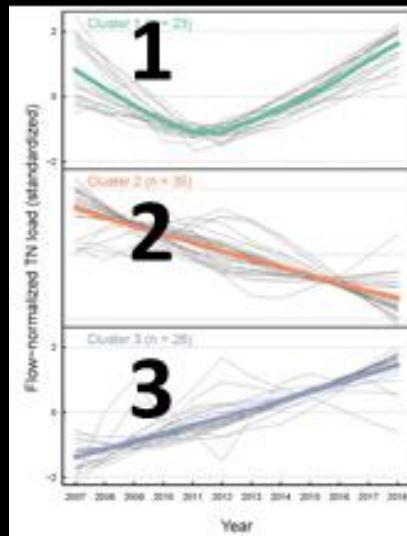
2. Regional drivers of nitrogen trend clusters (Classification)



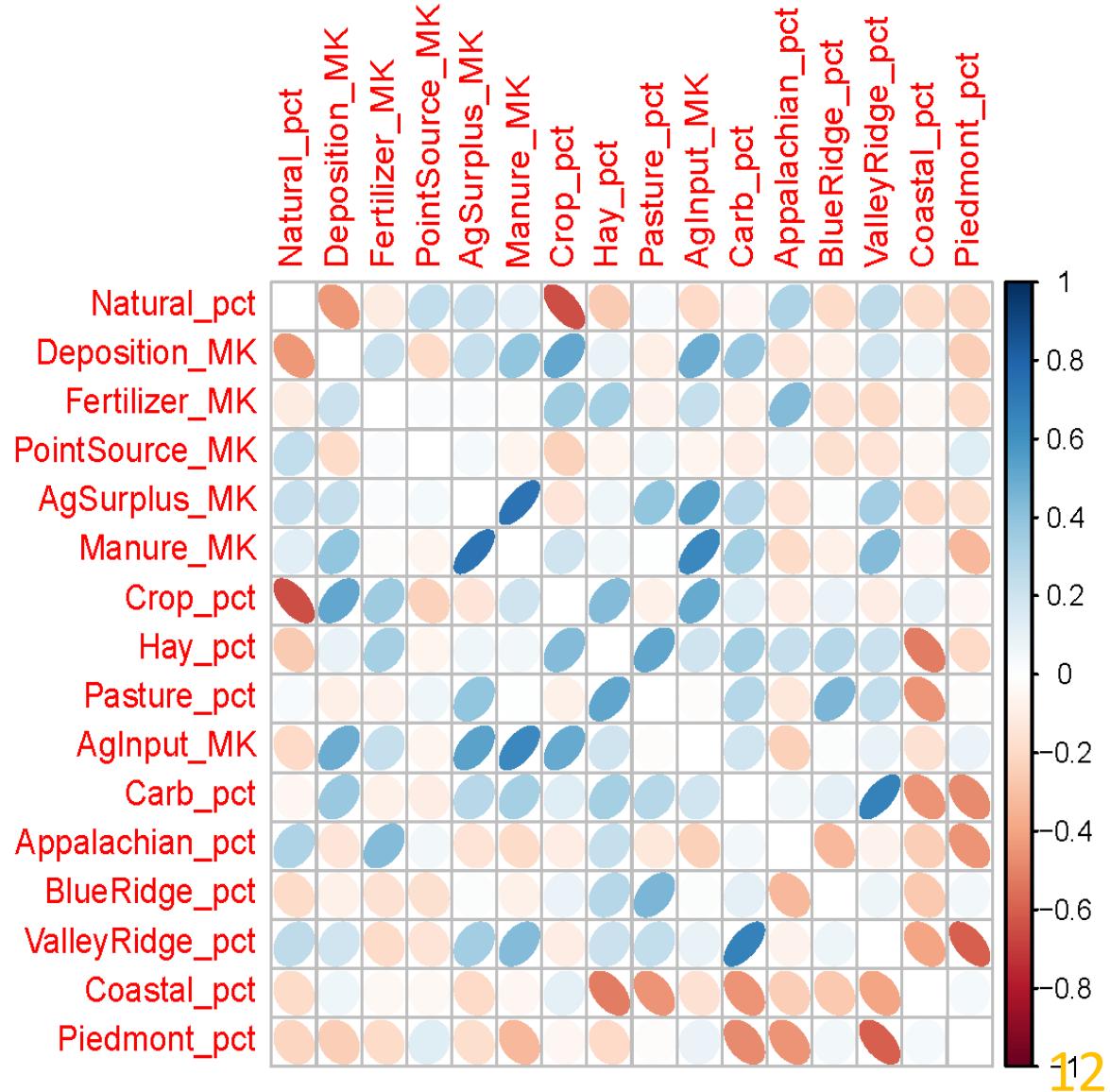
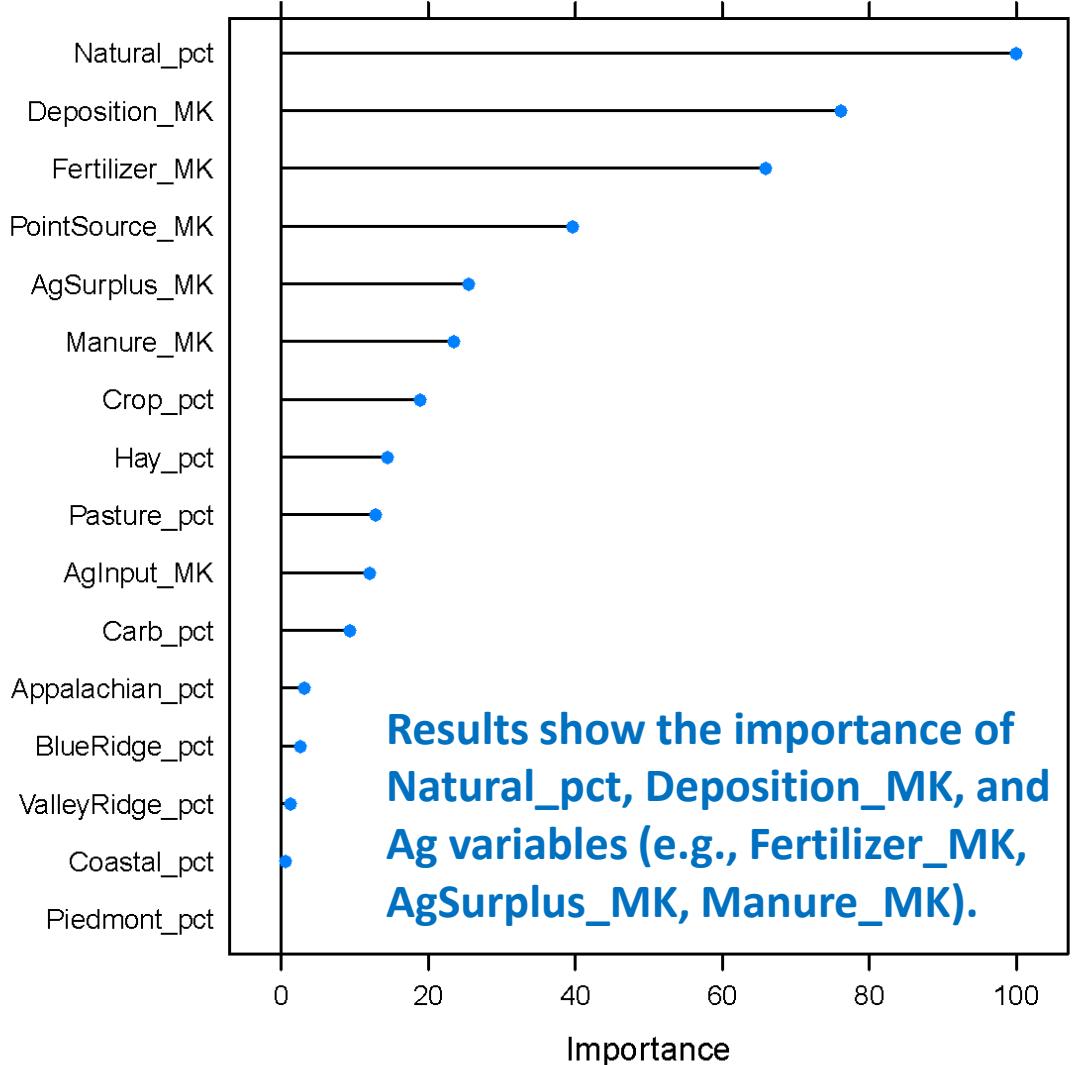
Explanatory Variables (Features)

- Watershed size (n = 1) - `Area_km2`
- Land uses, in % (n = 4) - `Natural_pct`, `Crop_pct`, `Pasture_pct`, `Hay_pct`
- Geology, in % (n = 1) - `Carb_pct`
- Physiography, in % (n = 5) - `Appalachian_pct`, `BlueRidge_pct`,
`ValleyRidge_pct`, `Piedmont_pct`, `Coastal_pct`
- N input source trends (n = 6) - `PointSource_MK`, `Deposition_MK`,
`Fertilizer_MK`, `Manure_MK`, `AgInput_MK`, `AgSurplus_MK`
 1. CAST data aggregated for each NTN watershed – 2007-2018 for point sources; 1997-2018 for nonpoint sources.
 2. Annual time series scaled by respective period-of-record medians.
 3. Mann-Kendall trend and Sen's slopes computed.

Explanatory Variables (Features)



Random Forest (Base Model)



Exhaustive Search for Optimal Models ($n \leq 6$)

Model	Model form	OOB accuracy, percent			
		Overall	Cluster1	Cluster2	Cluster3
A	Class ~ Natural_pct + Fertilizer_MK + ValleyRidge_pct + Deposition_MK + Carb_pct	70.5	66.7	68.8	76.0
B	Class ~ AgSurplus_MK + Fertilizer_MK + Deposition_MK + Natural_pct	70.5	66.7	75.0	68.0
C	Class ~ BlueRidge_pct + Deposition_MK + Coastal_pct + Crop_pct + Fertilizer_MK + Natural_pct	69.2	81.0	65.6	64.0

The selected models have varying accuracies for each cluster, indicating that each model settled on a specific set of features that are most useful to explain a specific cluster. To make predictions, an ensemble model approach was adopted to combine the strengths of these three models – i.e., choosing the prediction with the highest probability from the three models.

Regional Drivers

Message 1 (AgSurplus_MK, Fertilizer_MK):

- Agricultural nutrient management contributed to water quality improvement.

Message 2 (Carb_pct, Coastal_pct):

- Water-quality improvements are more likely in carbonate areas (relatively quick infiltration and faster groundwater transport) but less likely in Coastal Plain areas (accumulations of legacy N in the groundwater).

Message 3 (Natural_pct, Deposition_MK):

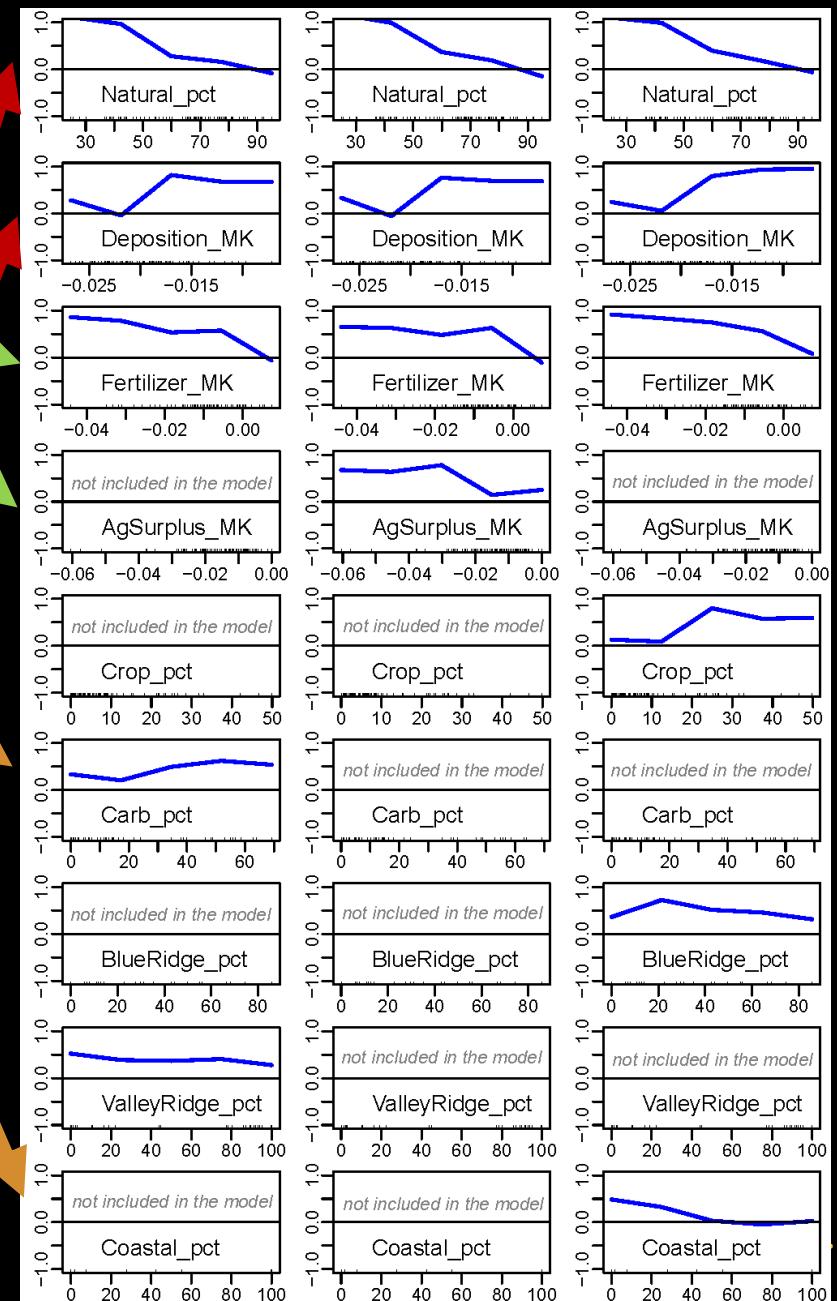
- We speculate that recent trends of increased TN in forested watersheds are attributed to: (1) increasing N inputs to non-forest regions and (2) mobilization of N from internal pools possibly due to deacidification and/or warming of forest soils.

Marginal Effects of Features on Cluster 2

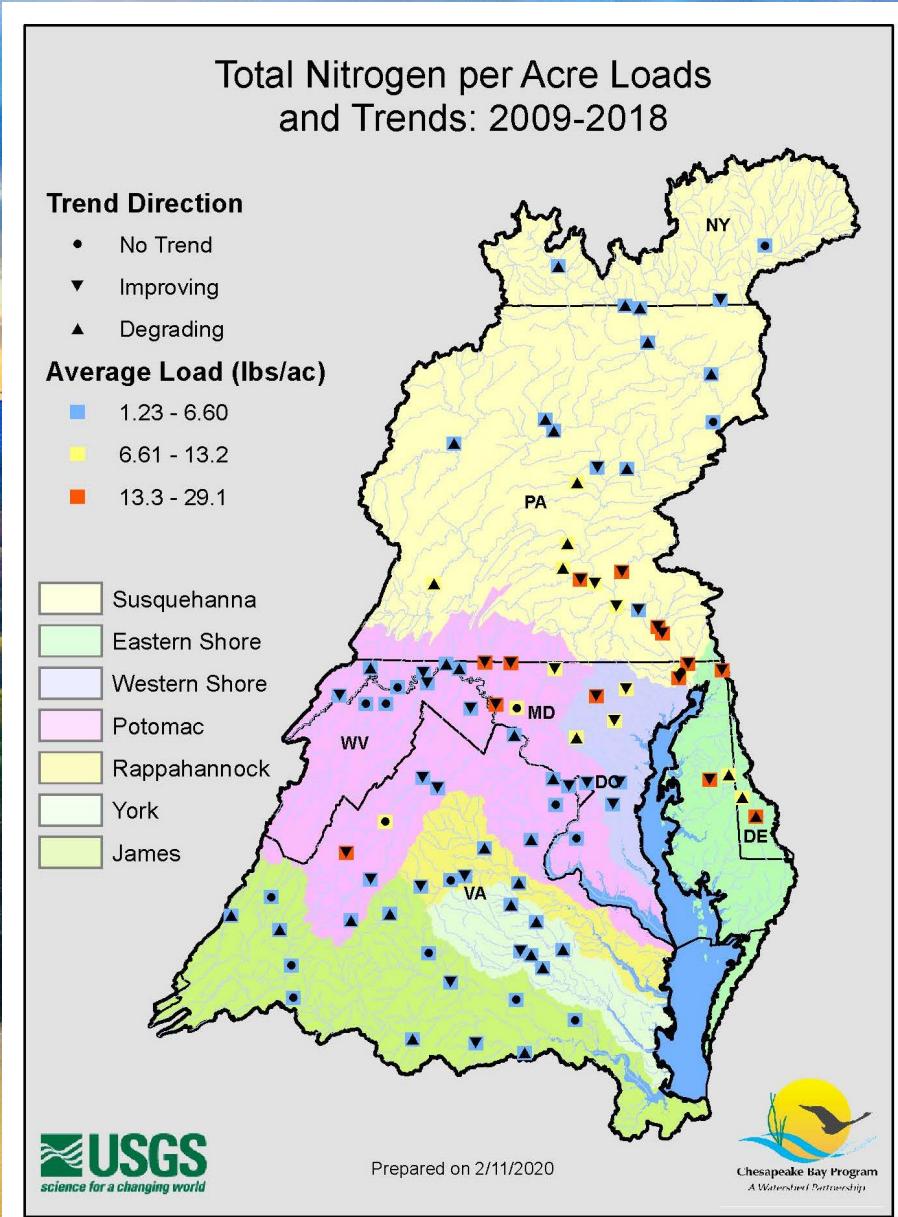
Model A

Model B

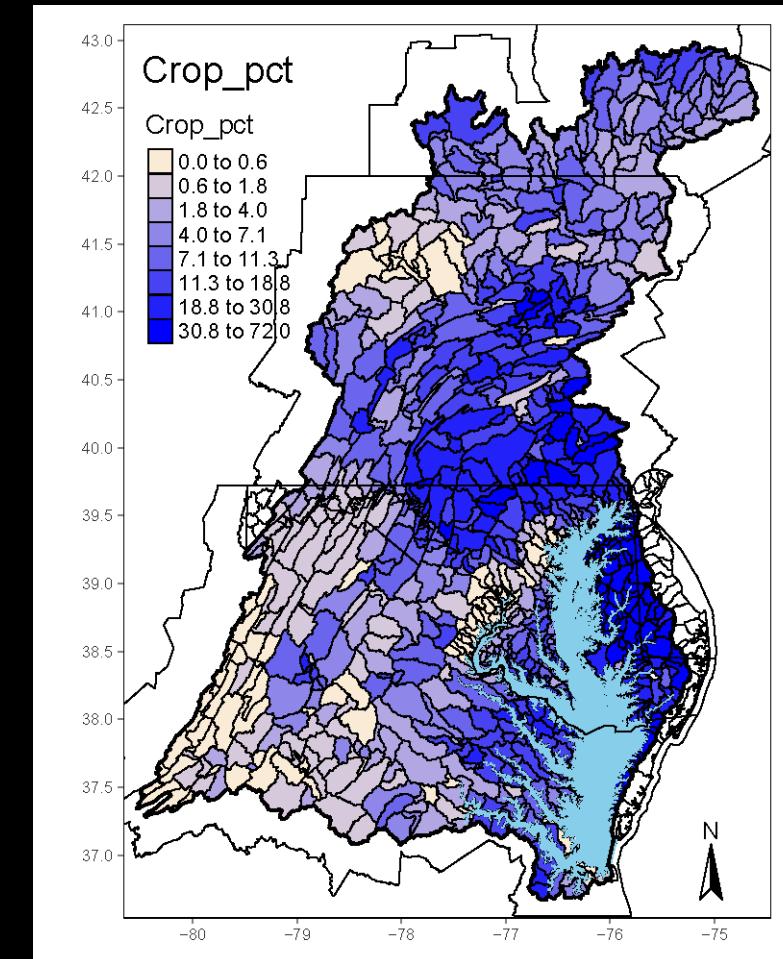
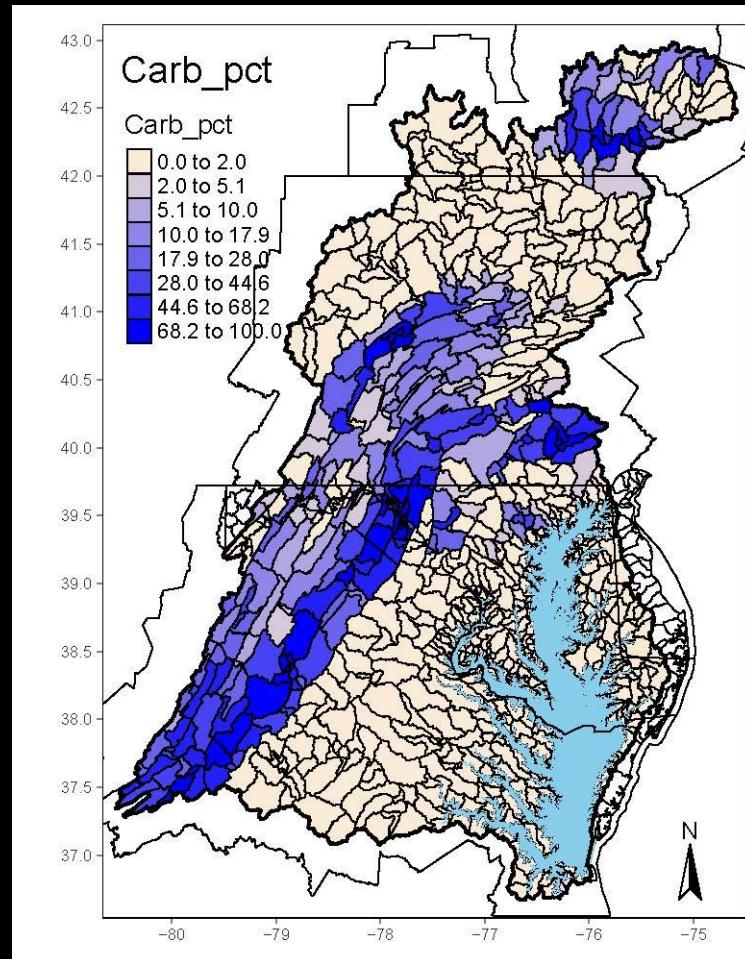
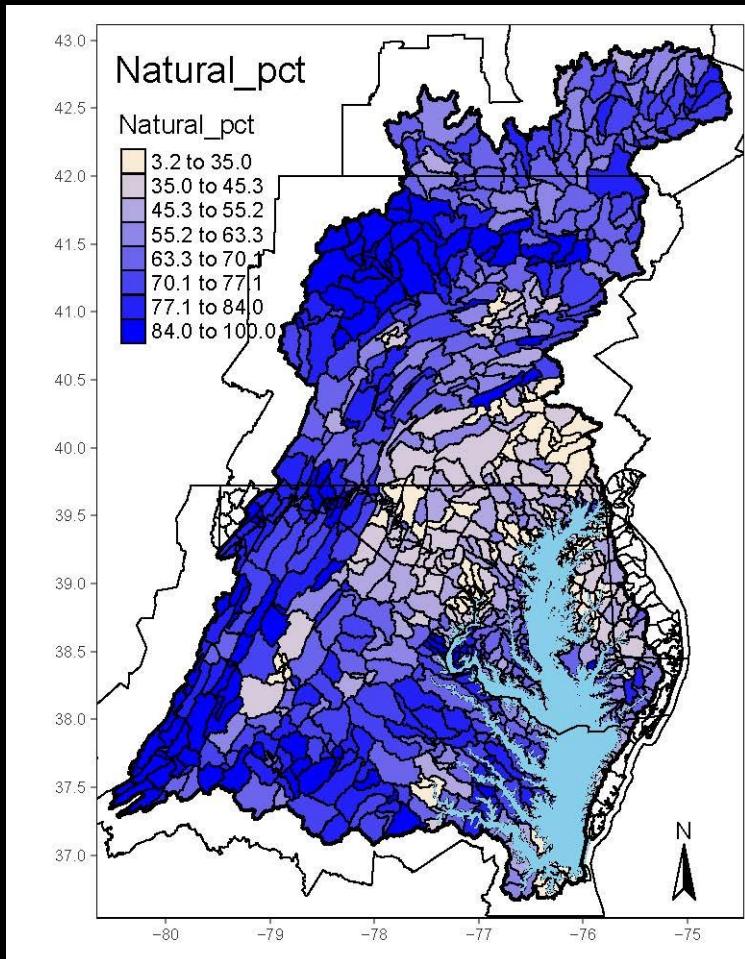
Model C



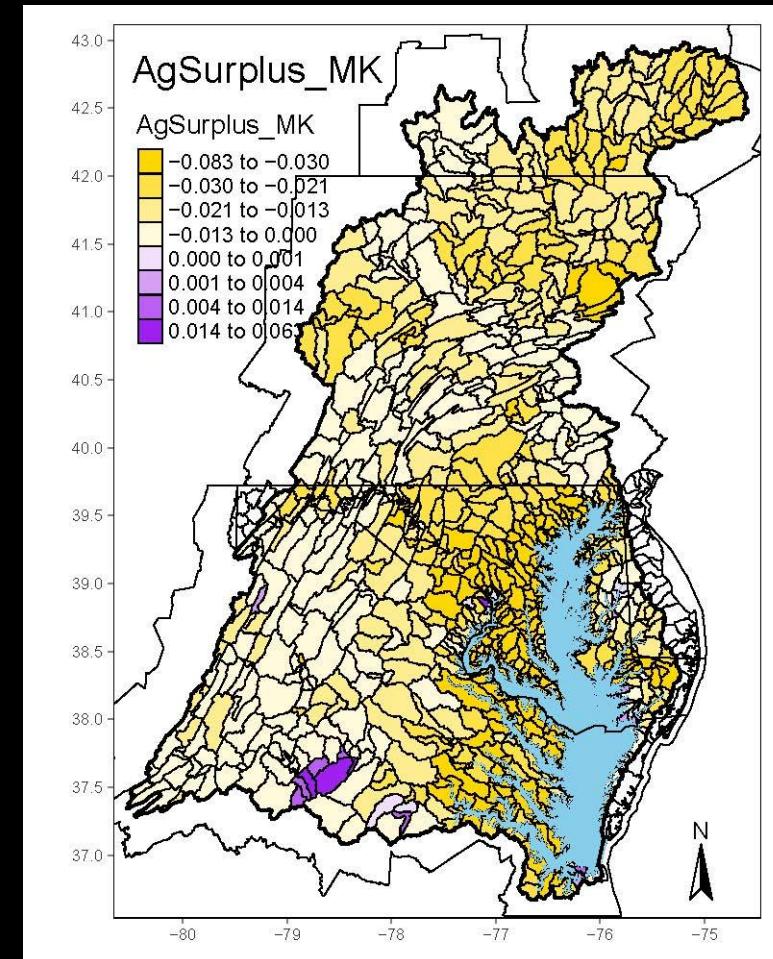
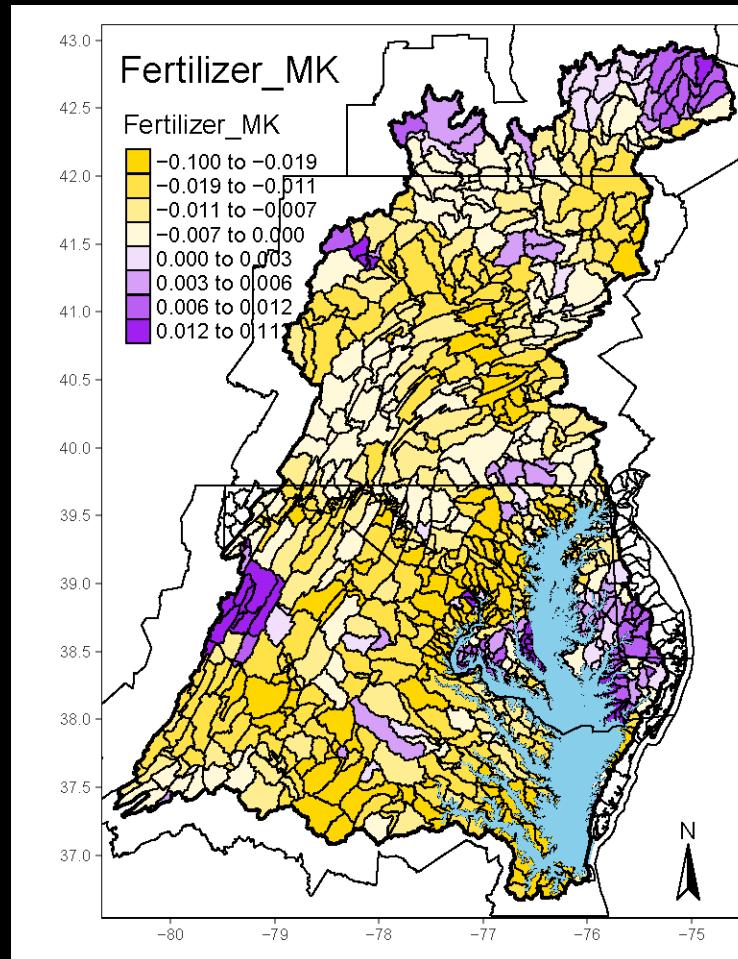
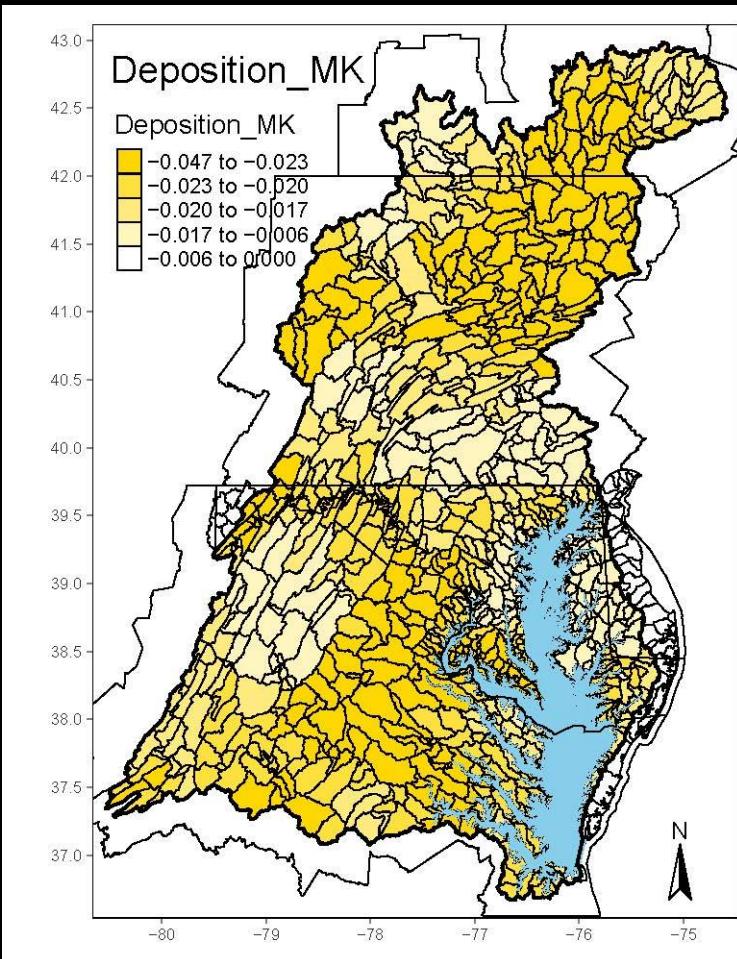
3. Prediction of nitrogen trend clusters for the entire watershed **(Prediction)**



Explanatory Variables for River Segments



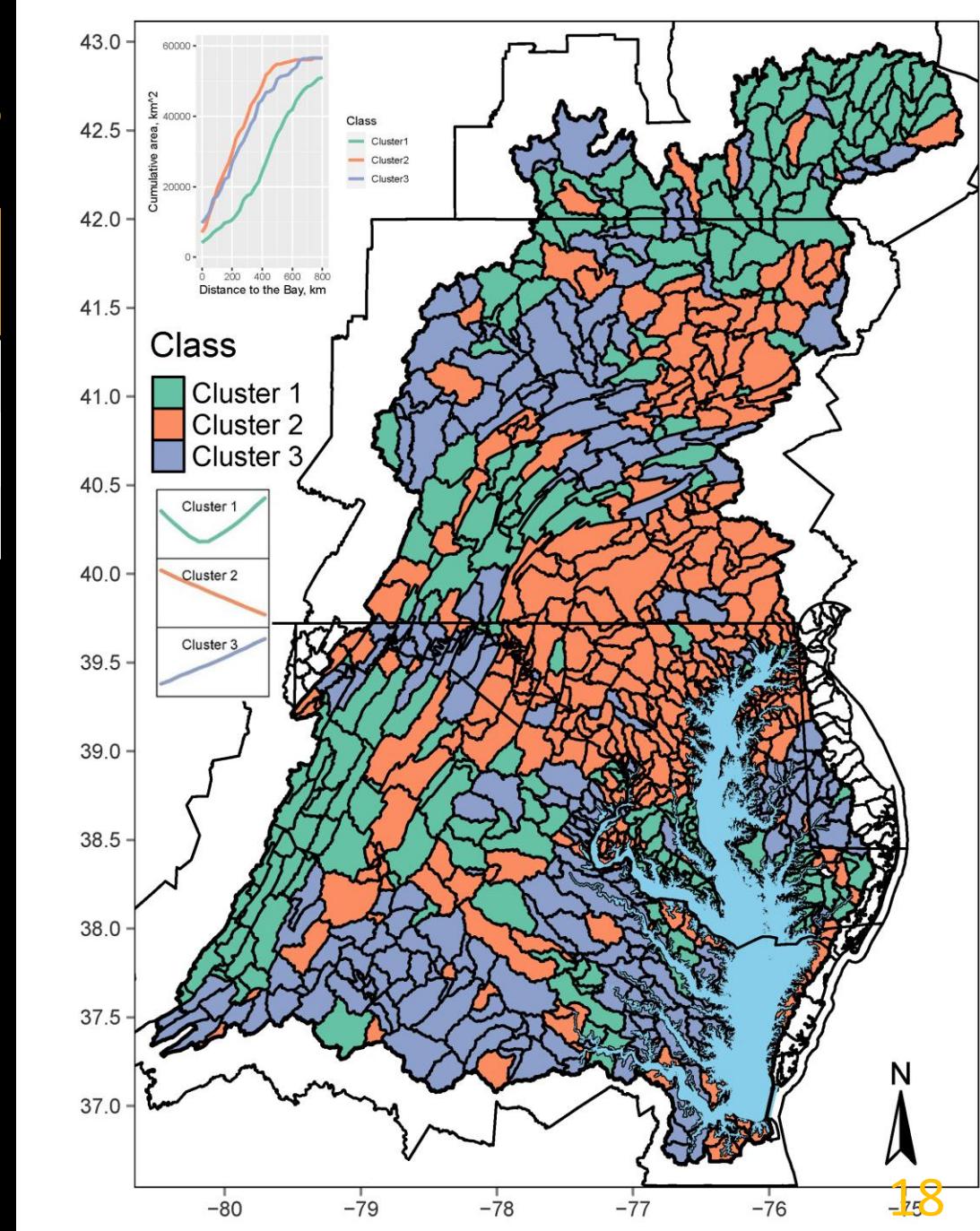
Explanatory Variables for River Segments



Predictions for River Segments

Cluster	No. of Segments	High Likelihood	Medium Likelihood	Low Likelihood
Cluster 1	293 (30%)	103	138	51
Cluster 2	392 (40%)	227	122	43
Cluster 3	295 (30%)	128	117	50

- These predictions are useful for watershed managers to understand trends across the watershed, including unmonitored areas.
- Combined with the effects of the model features, these predictions may inform managers on choosing priority watersheds toward water-quality improvement.



Conclusions

- Machine learning approaches – i.e., hierarchical clustering and random forest – can be combined to better understand the regional patterns and drivers of TN trends in large river monitoring networks.
- We explicitly incorporated temporal trends in agricultural fertilizer, manure, and agricultural input as well as agricultural surplus, providing evidence that improved nutrient management has resulted in declines in agricultural nonpoint sources, which in turn contributed to water quality improvement.
- Water-quality improvements are more likely in watersheds underlain by carbonate rocks but less likely in watersheds in the Coastal Plain.
- Results show degrading trends in forested watersheds, suggesting new and/or remobilized sources of N.
- Although we aimed for parsimony, models may be improved with additional features, e.g., management practice, legacy N, and riparian buffers.

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Thank you!

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REGIONAL PATTERNS AND DRIVERS OF NITROGEN TRENDS IN A HUMAN-IMPACTED WATERSHED AND MANAGEMENT IMPLICATIONS

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²CHESAPEAKE BAY PROGRAM

³U.S. ENVIRONMENTAL PROTECTION AGENCY

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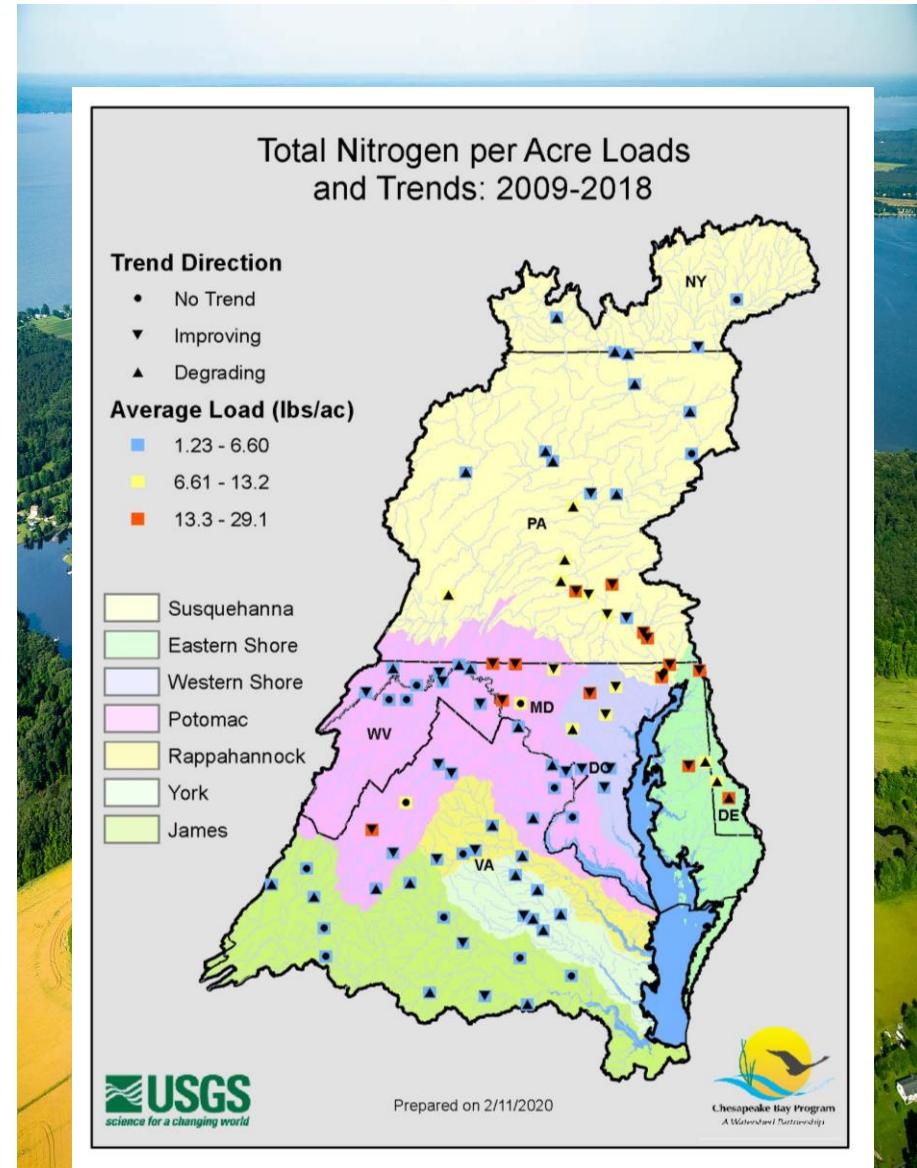
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OBJECTIVE AND MOTIVATIONS

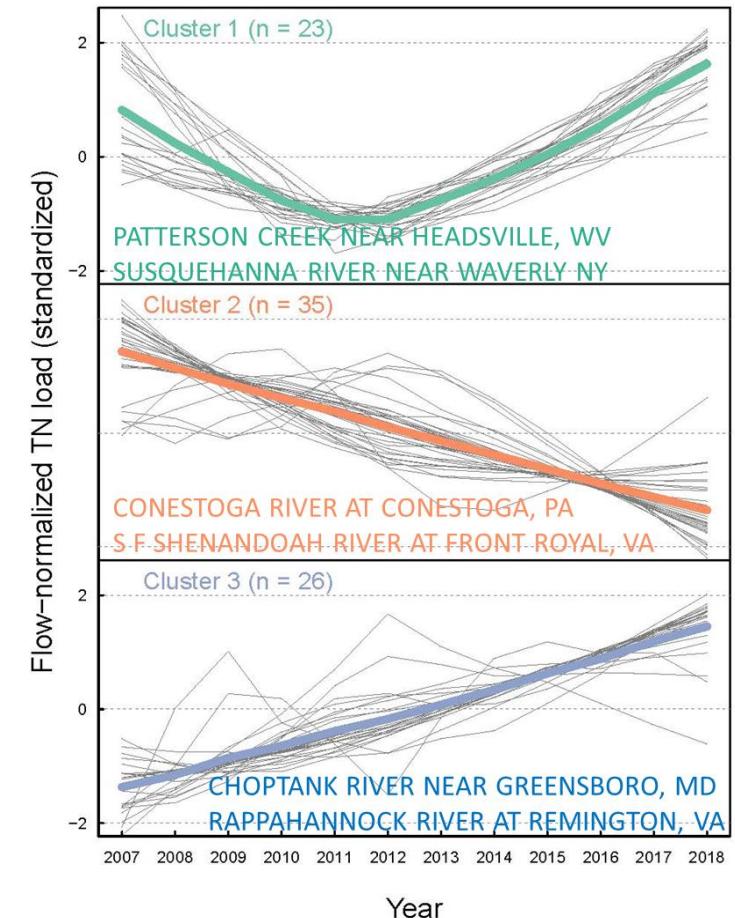
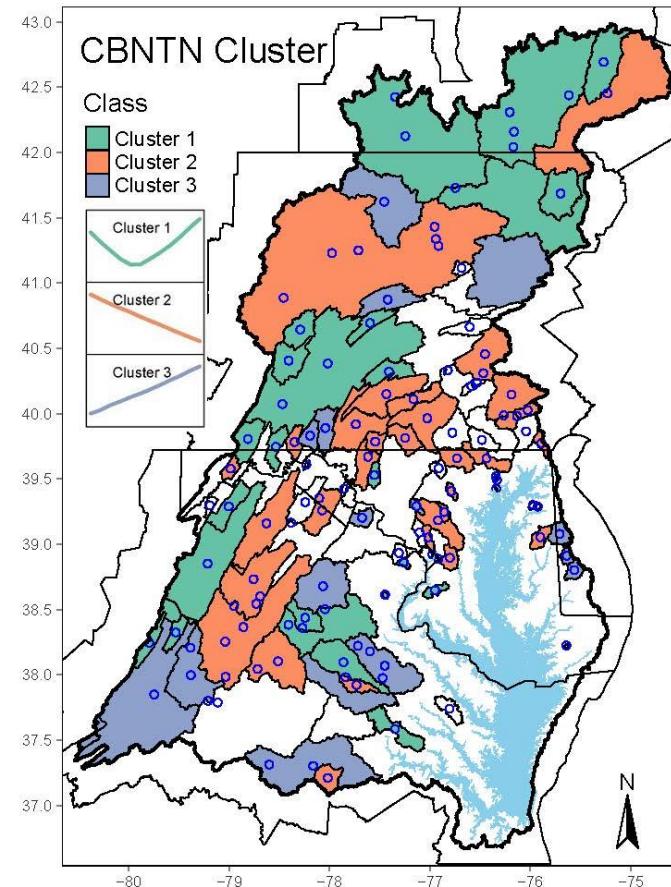
- To reveal regional patterns and drivers of total nitrogen (TN) trends using advanced machine learning approaches -- combined use of hierarchical clustering and random forest (RF).
 - Cover the Nontidal Monitoring Network (NTN).
 - Examine the similarity in TN trend signals and responses to natural and anthropogenic drivers.
 - Analyze short-term trends in order to incorporate newly established stations.
 - Incorporate important Agricultural variables.
 - Provide predictions for unmonitored areas.





1. REGIONAL PATTERNS OF TN LOAD TRAJECTORY (CLUSTERING)

- We used hierarchical cluster analysis to categorize the short-term (2007-2018) TN trends at the Chesapeake NTN stations (84) into three distinct clusters.
- Cluster 2 ($n = 35$) represents a trajectory of long-term decline in TN.





2. REGIONAL DRIVERS OF TN TREND CLUSTERS (RANDOM FOREST)

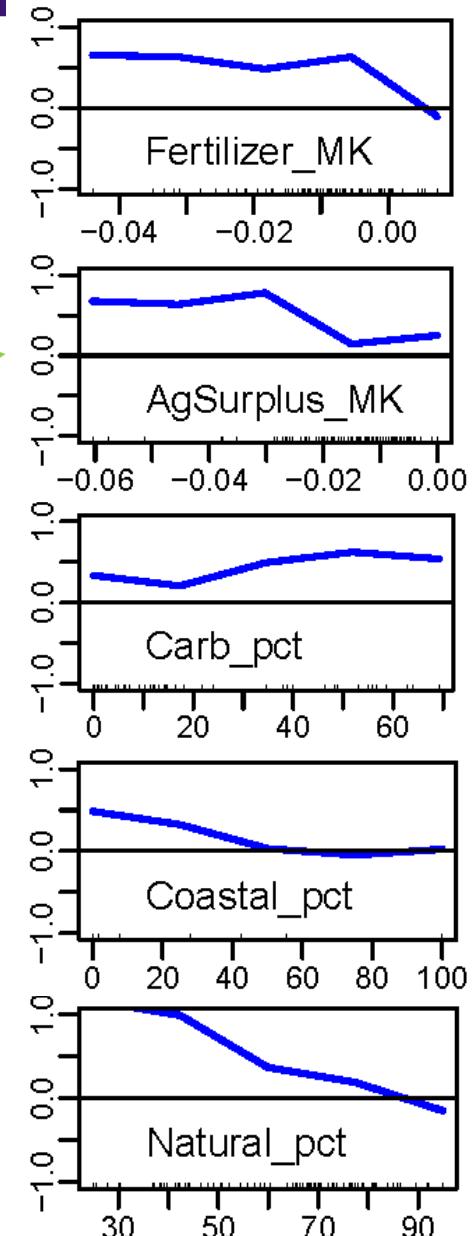
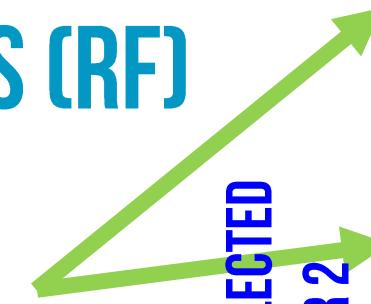
- We developed an exhaustive search algorithm to identify random forest (RF) models that can explain the TN cluster assignment.
- Three RF models selected by the search algorithm each settled on a specific set of features that are most useful to explain a specific cluster.

Model	Model form	OOB accuracy, percent			
		Overall	Cluster1	Cluster2	Cluster3
A	Class ~ Natural_pct + Fertilizer_MK + ValleyRidge_pct + Deposition_MK + Carb_pct	70.5	66.7	68.8	76.0
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2. REGIONAL DRIVERS OF TN TREND CLUSTERS (RF)

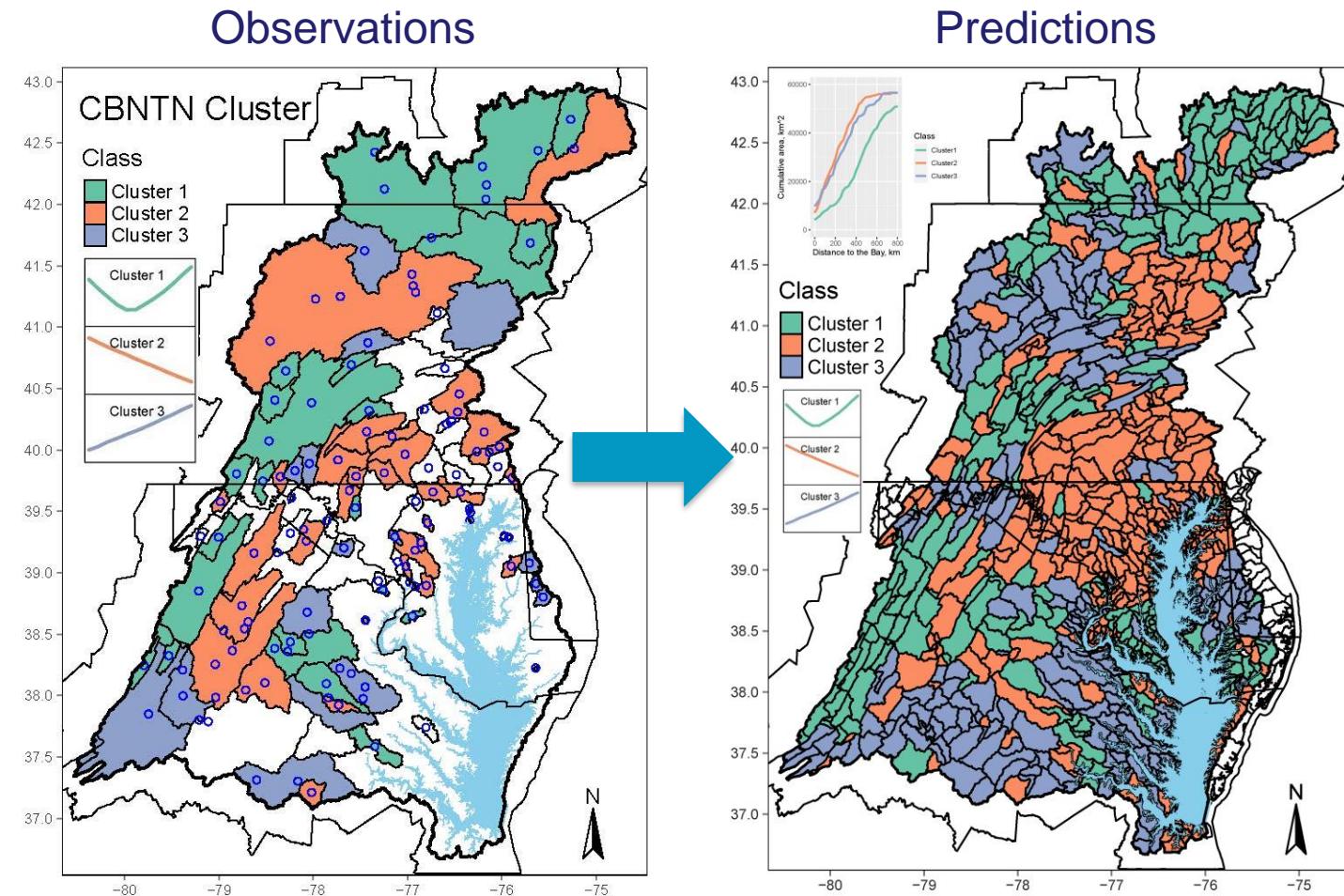
- Improved nutrient management has resulted in declines in agricultural nonpoint sources, which in turn contributed to water quality improvement.
- Water-quality improvements are more likely to occur in watersheds underlain by carbonate rocks, reflecting the relatively quick groundwater transport of this terrain.
- By contrast, water-quality improvements are less likely to occur in watersheds in the Coastal Plain, reflecting the effect of legacy N in groundwater.
- Results show degrading trends in forested watersheds, suggesting new and/or remobilized sources of N that may compromise downstream watershed restoration plans more focused on agricultural and urban areas.





3. PREDICTIONS OF TN TREND CLUSTERS FOR THE ENTIRE WATERSHED

- We applied the RF models to predict short-term trend clusters for the entire Bay watershed at a fine spatial scale (i.e., river segments).
- These predictions are useful for managers to understand trends across the watershed, including unmonitored areas, and to choose priority watersheds toward water-quality improvement.



THANK YOU

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