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Major Goals: Our research objectives are two-fold: (1) We will generate “high-order FEM” appropriate dimensional-reduction feature extraction methods such as vortex cores which can be accomplished as part of an in situ data processing pipeline. (2) Given the exploratory nature inherent in analyzing and visualizing transient phenomena, we will specify the regions of interest in an in situ fashion within a simulation field based upon the visualization objective, extract and transmit relevant high-order FEM modal information to our visualization system, and then reconstruct the visualization features of interest.

Accomplishments: Since the start of the grant, we have focused on feature detection in high-order fields. This has involved five main focus areas: 1) implementing and understanding how line-SIAC (L-SIAC) filters can be used to increase smoothness in the numerical solution prior to rendering, without compromising the simulation results. 2) Updating the L-SIAC filter to accommodate the types of meshes commonly encountered in the bulk of engineering scenarios (which would be meshes that are isotropic and/or mildly anisotropic). 3) Accelerating L-SIAC filtering for these applications. 4) Use of the L-SIAC filter as a preprocessing tool prior to topological analysis. 5) The creation of a new L-SIAC filter – the Non-Uniform Knot L-SIAC Filter (NUK L-SIAC Filter) to allow us to handle strongly anisotropic meshes as encountered in adaptive mesh refinement scenarios. All five areas are summarized in this final report.

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Article Title: Adaptive Characteristic Length for L-SIAC Filtering of FEM Data
Authors: Ashok Jallepalli, Robert Haimes, Robert M. Kirby
Keywords: cG (continuous Galerkin) · dG (discontinuous Galerkin) · Higher order methods · Higher order data · Smoothness increasing accuracy conserving filter (SIAC filter) · Line SIAC (L-SIAC)
Abstract: Treating discontinuities at element boundaries is a significant problem in understanding highorder FEMsimulation data since the physics used to model the simulation is often continuous. Recently, the family of SIAC filters, especially the L-SIAC filter, has been gaining popularity for its use in postprocessing. The computationalmath community, with its focus on improving the theoretical aspects of the SIAC filter, has applied the filter only on simple, fairly uniform unstructured meshes, where the largest element in the mesh is less than or equal to twice the smallest element. In many engineering applications, the unstructured meshes have varying orders of mesh resolution, but there is no literature for adapting the characteristic length of the SIAC filter to address these real-world simulation data. The central contribution of this paper is an algorithm used to calculate the characteristic length dynamically at any point in the mesh. We demonstrate that our approach has a lower error
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Authors: Ashok Jallepalli, Robert M. Kirby
Keywords: Line-SIAC (L-SIAC) filtering · Gauss quadrature · Discontinuous Galerkin (dG) · Continuous Galerkin (cG)
Abstract: Visualizing high-order finite element simulation data using current visualization tools has many challenges: discontinuities at element boundaries, interpolating artifacts, and evaluating derived quantities. These challenges have been addressed by postprocessing the simulation data using the L-SIAC filter. However, the time required to postprocess using this filter needs to be addressed to enable using it on large datasets. In this work, we introduce an efficient technique to speed-up the L-SIAC filter and alternateways to gain further speed-up at the cost of accuracy. This method is also ideal to postprocess at regularly spaced locations, which would be suitable for standard visualization software. Our results show that our method can achieve up to two orders of magnitude speed-up as compared to our interpretation of the technique presented in Docampo-Sánchez (SIAM J Sci Comput 39(5):A2179–A2200, 2017).
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Authors: Ashok Jallepalli, Joshua A. Levine, Robert M. Kirby
Keywords: High-Order Finite Element Methods, Filtering Techniques, Scalar Field Visualization, Topological Analysis
Abstract: High-order finite element methods (HO-FEM) are gaining popularity in the simulation community due to their success in solving complex flow dynamics. There is an increasing need to analyze the data produced as output by these simulations. Simultaneously, topological analysis tools are emerging as powerful methods for investigating simulation data. However, most of the current approaches to topological analysis have had limited application to HO-FEM simulation data for two reasons. First, the current topological tools are designed for linear data (polynomial degree one), but the polynomial degree of the data output by these simulations is typically higher (routinely up to polynomial degree six). Second, the simulation data and derived quantities of the simulation data have discontinuities at element boundaries, and these discontinuities do not match the input requirements for the topological tools. One solution to both issues is to transform the high-order data to achieve low-order, cont
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Article Title: On the Treatment of Field Quantities and Elemental Continuity in FEM Solutions
Authors: Ashok Jallepalli, Julia Docampo-Sanchez, Jennifer K. Ryan, Robert Haimes, Robert M. Kirby
Keywords: Field Quantities, Elemental Continuity, FEM
Abstract: As the finite element method (FEM) and the finite volume method (FVM), both traditional and high-order variants, continue their proliferation into various applied engineering disciplines, it is important that the visualization techniques and corresponding data analysis tools that act on the results produced by these methods faithfully represent the underlying data. To state this in another way: the interpretation of data generated by simulation needs to be consistent with the numerical schemes that underpin the specific solver technology. As the verifiable visualization literature has demonstrated: visual artifacts produced by the introduction of either explicit or implicit data transformations, such as data resampling, can sometimes distort or even obfuscate key scientific features in the data. In this paper, we focus on the handling of elemental continuity, which is often only continuous or piecewise discontinuous, when visualizing primary or derived fields from FEM or FVM simulatio
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Authors: Ashok Jallepalli
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Partners

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I certify that the information in the report is complete and accurate:
Signature: Robert M. Kirby II
Signature Date: 3/1/22 11:58AM

Visualization of Discontinuous Galerkin Based High-Order Methods
Proposal Number W911NF1510222
Professor Robert M. Kirby, School of Computing, University of Utah and Mr. Robert Haimes,
Department of Aeronautics & Astronautics, Massachusetts Institute of Technology

The use of simulation science as a means of scientific inquiry is increasing at a tremendous rate. The process of mathematically modeling physical phenomena, estimating key modeling parameters, numerically approximating the solution, and computationally solving the resulting algorithm has inundated the scientific and engineering worlds, allowing for rapid advances in our understanding and utilization of the world around us. The efficacy of simulation science has been, in part, due to two critical components: (1) the identification and minimization of the error budget (e.g. modeling, discretization and uncertainty errors), and equally importantly, (2) evaluation mechanisms (such as visualization) by which the investigator assimilates the data produced through simulation. The latter allows for further refinement of the simulation science process (through model correction, increased numerical resolution, or algorithm debugging, etc.) and makes possible scientific statements about the physical phenomena being investigated.

Tremendous effort has been exerted over many decades in the pursuit of numerical methods that are both *flexible* and *accurate*, hence providing sufficient fidelity to be employed in the numerical solution of a large number of models, and sufficient analysis of accuracy to allow researchers to focus their attention on model refinement and uncertainty quantification. High-order finite element methods (also known as spectral/*hp* element methods), using either the continuous Galerkin or discontinuous Galerkin formulation, have reached a level of sophistication that allows them to be commonly applied to a diverse set of real-life engineering problems in computational solid mechanics, fluid dynamics, acoustics and electromagnetics. Many of the physical problems of interest are, unfortunately, not steady-state --- leading to simulations that must run for a long time (days, weeks and in some cases months). Thus, in the absence of creative solutions, datasets can easily consume all available storage and networking resources. Examples of such simulations within fluid dynamics include all simulations in which the fluid is in transition or fully turbulent. With regards to ARO interests, problems in turbo-machinery and rotorcraft, where aspects of the geometry are rotating and/or sliding past one other, fall into this category. High-order finite element methods are now beginning to be used to simulate these physical systems due to their inherent ability to capture complex structures (such as vortices) with little numerical dissipation and dispersion. The transient nature of these simulations complicates the data handling (post processing requires the time history) and renders single snap-shots of the solution insufficient to understand the time-varying nature of the physics.

Objective

Our research objectives are two-fold: (1) We will generate "high-order FEM" appropriate dimensional-reduction feature extraction methods such as vortex cores which can be accomplished as part of an *in situ* data processing pipeline. (2) Given the exploratory nature inherent in analyzing and visualizing transient phenomena, we will specify the regions of interest in an *in situ* fashion within a simulation field based upon the visualization objective, extract and transmit relevant high-order FEM modal information to our visualization system, and then reconstruct the visualization features of interest.

Approach

There is now a growing acceptance in the simulation and visualization communities that co-processing (*in situ* processing) is the most effective and least intrusive way to understand the results from transient simulations. Pioneering work in this arena was performed by Haimes in pV3. Nektar++, a publicly available high-order FEM code co-architected by Kirby can be used as a test-bed for designing high-order aware *in situ* methods. We are leveraging both of these former efforts in our current work.

Our approach is that an exploratory visualization methodology for high-order finite element transient data that exploits the high-order nature of the data, in its native form, provides a visual representation that introduces no (or quantifiable) approximation error due to the visualization technique. There are many possible reasons why this thesis is beneficial to the high-order finite element community. The proposed visualization techniques (1) use the data in its native form, hence helping to allay the computational scientists' concern that information is being lost when current visualization techniques are applied; (2) allow the computational scientists to focus their efforts on elimination of other sources of error (modeling errors, numerical errors, etc.) because it eliminates visualization approximation error.

Scientific Opportunities and Barriers

The major scientific barrier we are attempting to overcome is the fact that most flow analysis and visualization software is designed assuming the input is traditional low-order FEM and/or finite volume data. As the Army and other researchers move to high-order methods, it is necessary to update the simulation through analysis to visualization pipeline. This provides a scientific opportunity for us: to use our knowledge of the development of high-order (simulation methods) and new simulation analysis tools on the applied mathematics side to help inform and update the simulation-to-visualization pipeline. In doing so, we arrive at visualizations that faithfully represent the simulation data that is being portrayed.

Significance

The proposed research impacts three areas: the mathematical sciences, the computer sciences, and the interdisciplinary bridge lying between these two areas. The high-order finite element community will benefit from this effort through the proposed development of algorithms, which accurately and efficiently render simulation results. The visualization community will benefit through the exposure to the high-order finite element community and, in particular, the numerical methods prevalently found there. Other current projects funded by ARO's program in computational mathematics that use high-order finite elements will find immediate utility of the algorithms and implementations discussed herein (e.g. projects funded at Brown University, RPI, University of Wyoming, and the Army Rotorcraft Research Area, etc.).

Accomplishments

Since the start of the grant, we have focused on feature detection in high-order fields. This has involved five main focus areas: 1) implementing and understanding how line-SIAC (L-SIAC) filters can be used to increase smoothness in the numerical solution prior to rendering, without compromising the simulation results. 2) Updating the L-SIAC filter to accommodate the types of meshes commonly encountered in the bulk of engineering scenarios (which would be meshes that are isotropic and/or mildly anisotropic). 3) Accelerating L-SIAC filtering for these applications. 4) Use of the L-SIAC filter as a preprocessing tool prior to topological analysis. 5) The creation of a new L-SIAC filter – the Non-Uniform Knot L-SIAC Filter (NUK L-SIAC Filter) to allow us to handle strongly anisotropic meshes as encountered in adaptive mesh refinement scenarios. All five areas are summarized in this final report.

Results of Focus Area 1: In this section, we highlight images from our study presented in our first TVCG paper [J1]. The abstract for this work is given below.

Abstract: As the finite element method (FEM) and the finite volume method (FVM), both traditional and high-order variants, continue their proliferation into various applied engineering disciplines, it is important that the visualization techniques and corresponding data analysis tools that act on the results produced by these methods faithfully represent the underlying data. To state this in another way: the interpretation of data generated by simulation needs to be consistent with the numerical schemes that underpin the specific solver technology. As the verifiable visualization literature has demonstrated: visual artifacts produced by the introduction of either explicit or implicit data transformations, such as data resampling, can sometimes distort or even obfuscate key scientific features in the data. In this paper, we focus on the handling of elemental continuity, which is often only C^0 continuous or piecewise discontinuous, when visualizing primary or derived fields from FEM or FVM simulations. We demonstrate that traditional data handling and visualization of these fields introduce visual errors. In addition, we show how the use of the recently proposed line-SIAC filter provides a way of handling elemental continuity issues in an accuracy-conserving manner with the added benefit of casting the data in a smooth context even if the representation is element discontinuous.

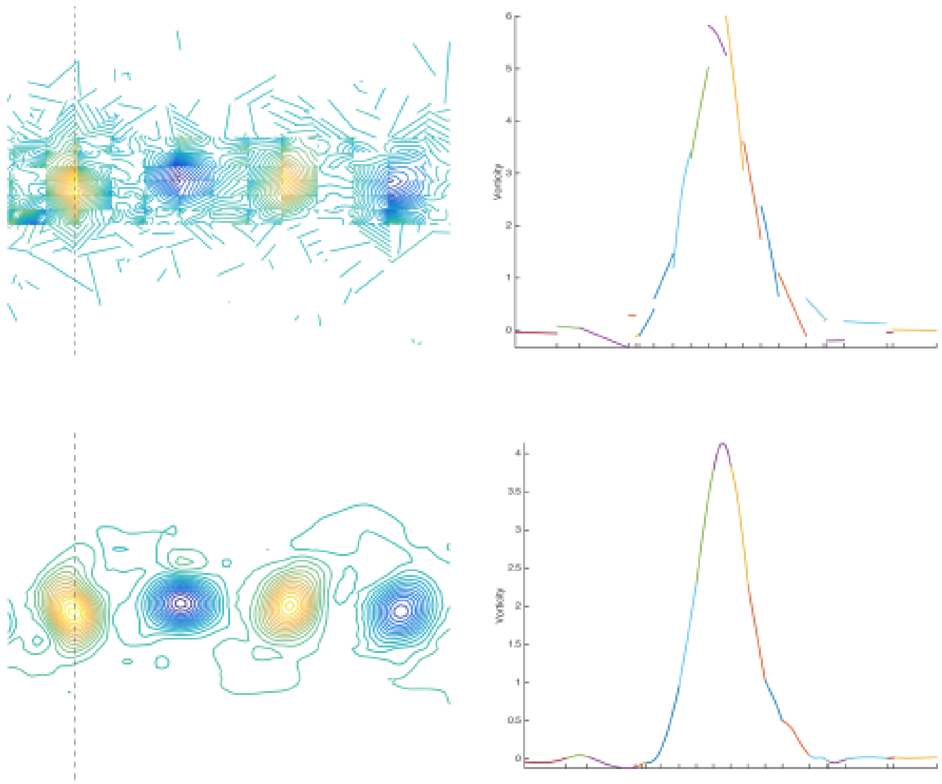


Figure 1: Images from Cylinder Flow. Comparison between calculating vorticity using dG data vs L-SIAC. The first row of images are calculated using raw dG data at fine grid resolution. Second Row of images are vorticity calculated L-SIAC.

Figure 2: Large-Eddy Simulation (LES) for the formation and evolution of a wingtip vortex. The wing is a 3D extrusion of a NACA 0012 airfoil section with a rounded wing tip and a blunt trailing edge. Angle of attack =12. The green cube shown in the vortex, downstream from the tip, indicates the selected region that will be used to more closely examine the vorticity field.

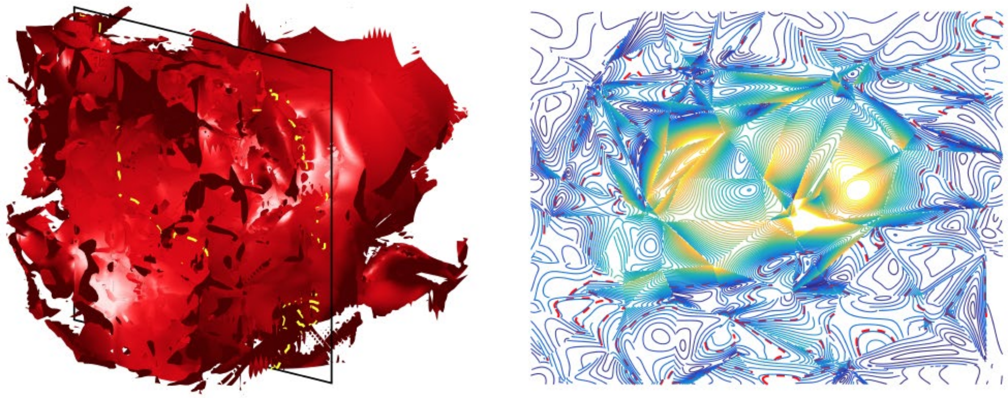


Figure: Before filtering. Left (isocontour), Right (slice).

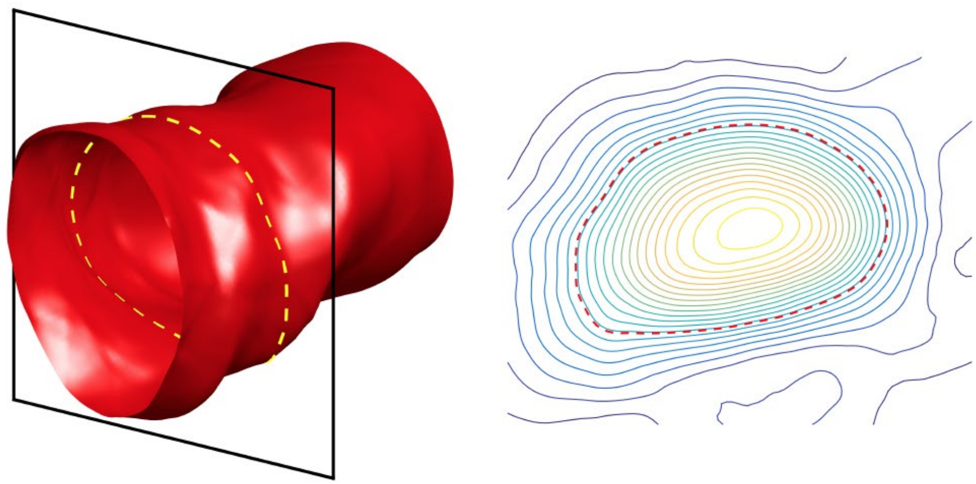


Figure: Before filtering. Left (isocontour), Right (slice).

Results of Focus Area 2: In this section, we highlight images from our dynamic L-SIAC paper [J2]. The abstract for this work is given below.

Abstract: Treating discontinuities at element boundaries is a significant problem in understanding high-order FEM simulation data since the physics used to model the simulation is often continuous. Recently, the family of SIAC filters, especially the L-SIAC filter, has been gaining popularity for its use in postprocessing. The computational math community, with its focus on improving the theoretical aspects of the SIAC filter, has applied the filter only on simple, fairly uniform unstructured meshes, where the largest element in the mesh is less than or equal to twice the smallest element. In many engineering applications, the unstructured meshes have varying orders of mesh resolution, but there is no literature for adapting the characteristic length of the SIAC filter to address these real-world simulation data. The central contribution of this paper is an algorithm used to calculate the characteristic length dynamically at any point in the mesh. We demonstrate that our approach has a lower error and is computationally faster than using maximum edge length over the mesh.

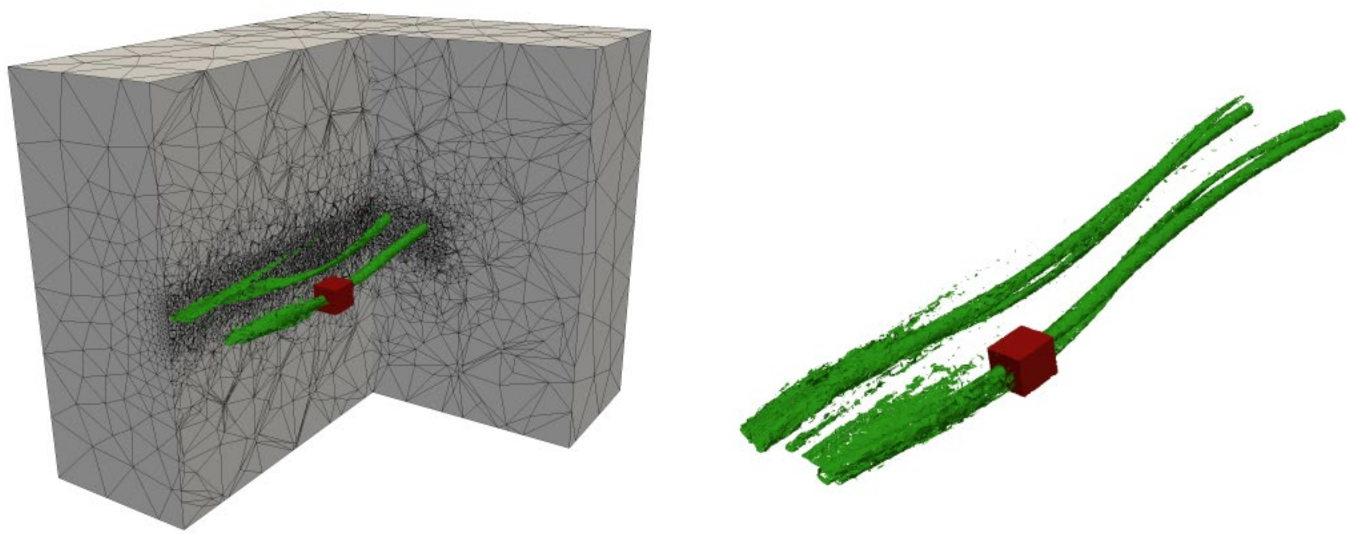


Figure: Simulation output for counter-rotating vortices from high order simulation. Note the variation of element sizes from the region of interest to boundaries. The L-SIAC filter needs to be scaled dynamically to obtain meaningful results.

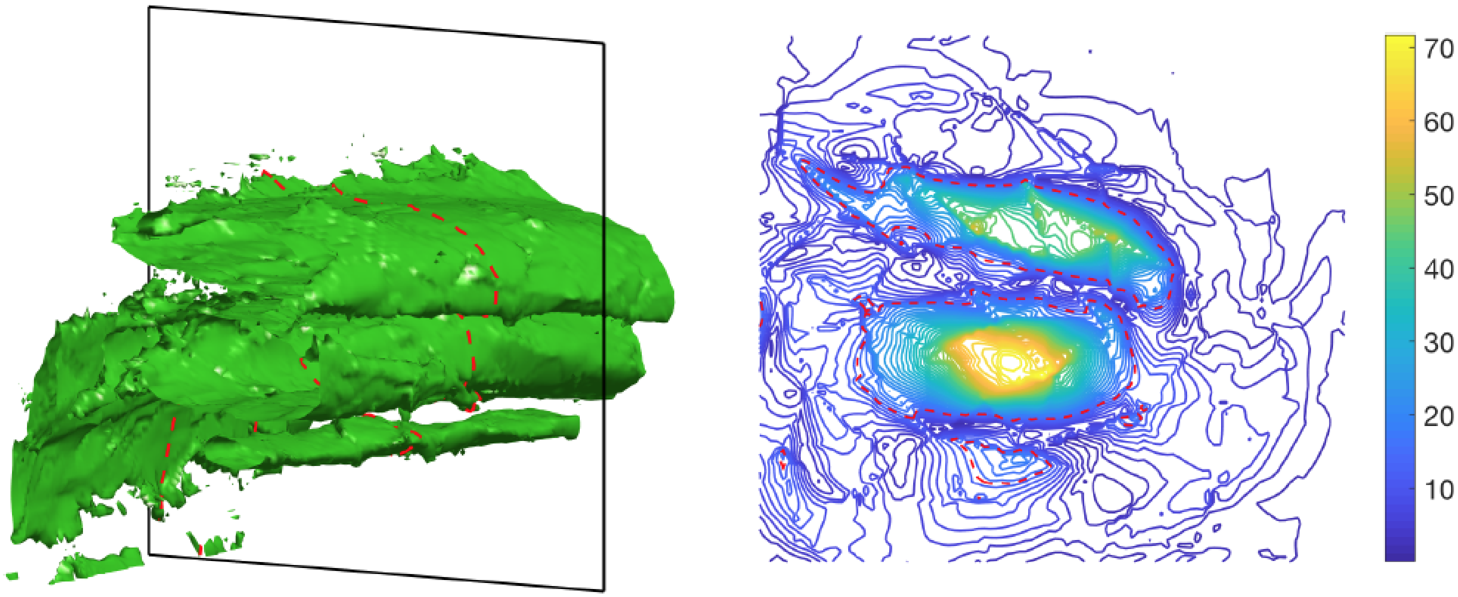


Figure 10: On the left of the image above, we show vortex tube taken from a three-dimensional contour-rotating vortex from Figure 9. The black lines represent the cutting plane for analysis. On the right, we show a contour plot of vorticity computing in an element-wise fashion from the raw data. Note data is noisy, but we observe two iso-contours indicated by dotted redlines.

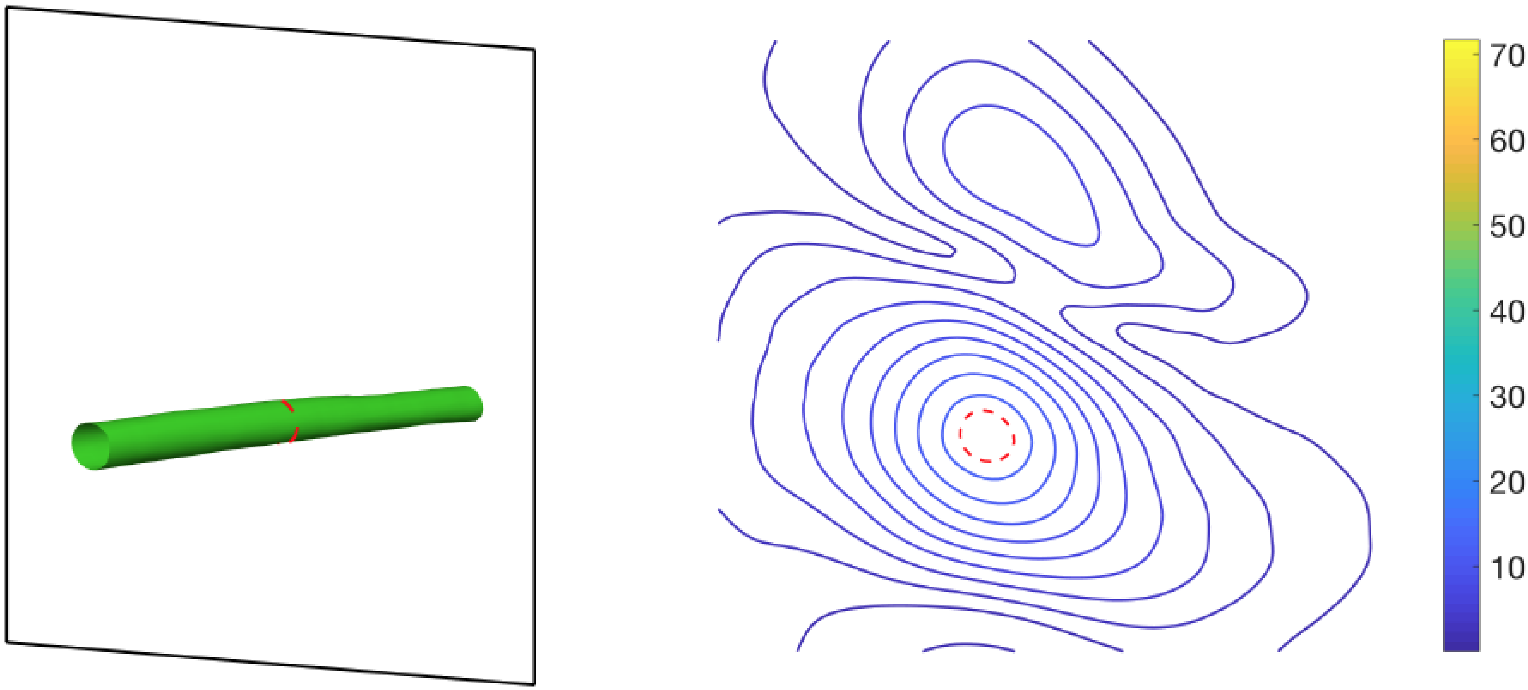


Figure 11: The above vortex tube is obtained by applying the L-SIAC filter using constant characteristic length equal to local maximum edge length. We observe the noise is reduced, but there is only one iso-contour indicated by dotted redline.

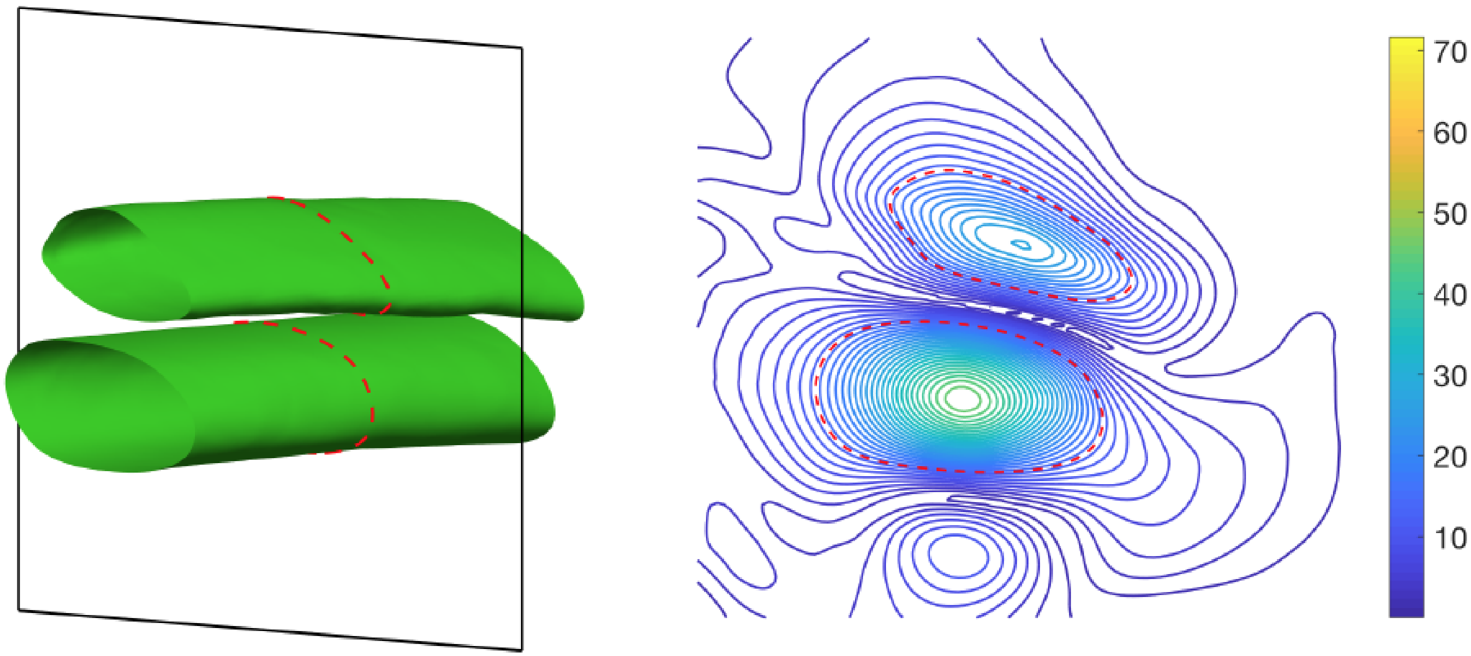


Figure 12: The above vortex tube is obtained by applying the L-SIAC filter using adaptive characteristic length proposed by us. We observe along with the reduction of noise; we can detect the two iso-contours indicated by the dotted red lines.

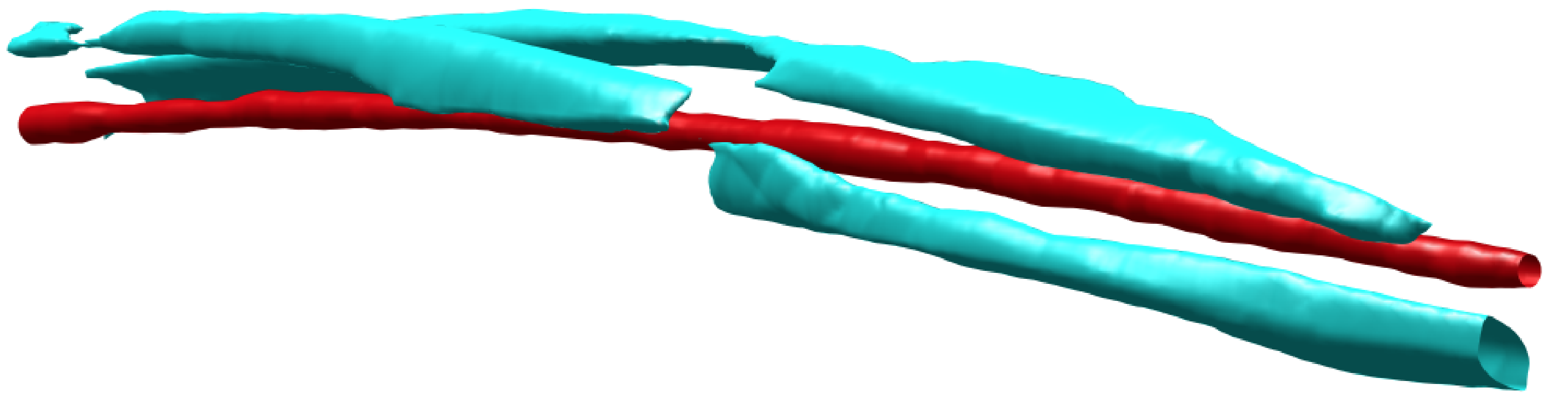


Figure 13: The red iso-surface is the primary vortex with Lambda-2 value of 8000, and cyan iso-surface represents the secondary counter rotating vortex with Lambda-2 value of -750. For this visualization, we have used the adaptive scaling of L-SIAC filter combined with efficient implantation of the L-SIAC filter.

Results of Focus Area 3: In this section, we highlight in a table the results of our acceleration attempts. This resulted in the following paper [J3]. The abstract for this work is given below.

Abstract: Visualizing high-order finite element simulation data using current visualization tools has many challenges: discontinuities at element boundaries, interpolating artifacts, and evaluating derived quantities. These challenges have been addressed by postprocessing the simulation data using the L-SIAC filter. However, the time required to postprocess using this filter needs to be addressed to enable using it on large datasets. In this work, we introduce an efficient technique to evaluate the L-SIAC filter and alternate ways to gain further speed-up at the cost of accuracy. This method is also ideal to postprocess at regularly spaced locations, which would be suitable for standard visualization software.

Speed-up	Algorithm 1				Algorithm 2			
Mesh	10^2	10^4	10^2	10^4	10^2	10^4	10^2	10^4
$\mathcal{P}^2$	Q=4		Q=30		Q=4		Q=6	
21^2	5.63	144.70	5.22	44.99	4.72	21.82	4.62	19.13
41^2	2.67	158.60	2.64	69.81	2.55	37.22	2.13	31.97
81^2	1.92	162.85	1.91	111.21	1.86	73.48	1.86	65.35
161^2	1.87	175.36	1.76	155.34	1.90	136.13	1.89	128.69
$\mathcal{P}^3$	Q=6		Q=40		Q=6		Q=10	
21^2	8.73	124.94	8.29	32.70	6.10	16.21	5.28	12.20
41^2	3.86	147.71	3.67	38.74	3.49	23.31	3.32	16.40
81^2	2.24	156.50	2.22	70.95	2.23	43.40	1.92	32.05
161^2	1.94	176.53	1.70	127.75	1.97	97.12	1.70	79.17
$\mathcal{P}^4$	Q=8		Q=50		Q=8		Q=14	
21^2	11.68	98.83	9.13	22.67	6.23	13.43	5.05	8.94
41^2	5.34	120.01	4.04	24.95	4.21	16.87	3.26	10.70
81^2	2.73	136.46	2.63	39.72	2.60	28.61	2.49	18.89
161^2	2.10	167.24	2.10	89.06	2.11	62.80	2.08	44.94

Table 1: The speedup obtained by our new Algorithms compared to current technique to calculate L-SIAC filter on a uniform structured mesh.

Results of Focus Area 4: In this section, we highlight the results of our empirical study that show the diverse behavior of data transformation methodologies and their downstream effect on feature detection (using topological analysis as the case study). This work was presented at IEEE VIS 2019 and published in TVCG 2020 [J4].

Abstract: High-order finite element methods (HO-FEM) are gaining popularity in the simulation community due to their success in solving complex flow dynamics. There is an increasing need to analyze the data produced as output by these simulations. Simultaneously, topological analysis tools are emerging as powerful methods for investigating simulation data. However, most of the current approaches to topological analysis have had limited application to HO-FEM simulation data for two reasons. First, the current topological tools are designed for linear data (polynomial degree one), but the polynomial degree of the data output by these simulations is typically higher (routinely up to polynomial degree six). Second, the simulation data and derived quantities of the simulation data have discontinuities at element boundaries, and these discontinuities do not match the input requirements for the topological tools. One solution to both issues is to transform the high-order data to achieve low-order, continuous inputs for

topological analysis. Nevertheless, there has been little work evaluating the possible transformation choices and their downstream effect on the topological analysis. We perform an empirical study to evaluate two commonly used data transformation methodologies along with the recently introduced L-SIAC filter for processing high-order simulation data. Our results show diverse behaviors are possible. We offer some guidance about how best to consider a pipeline of topological analysis of HO-FEM simulations with the currently available implementations of topological analysis.

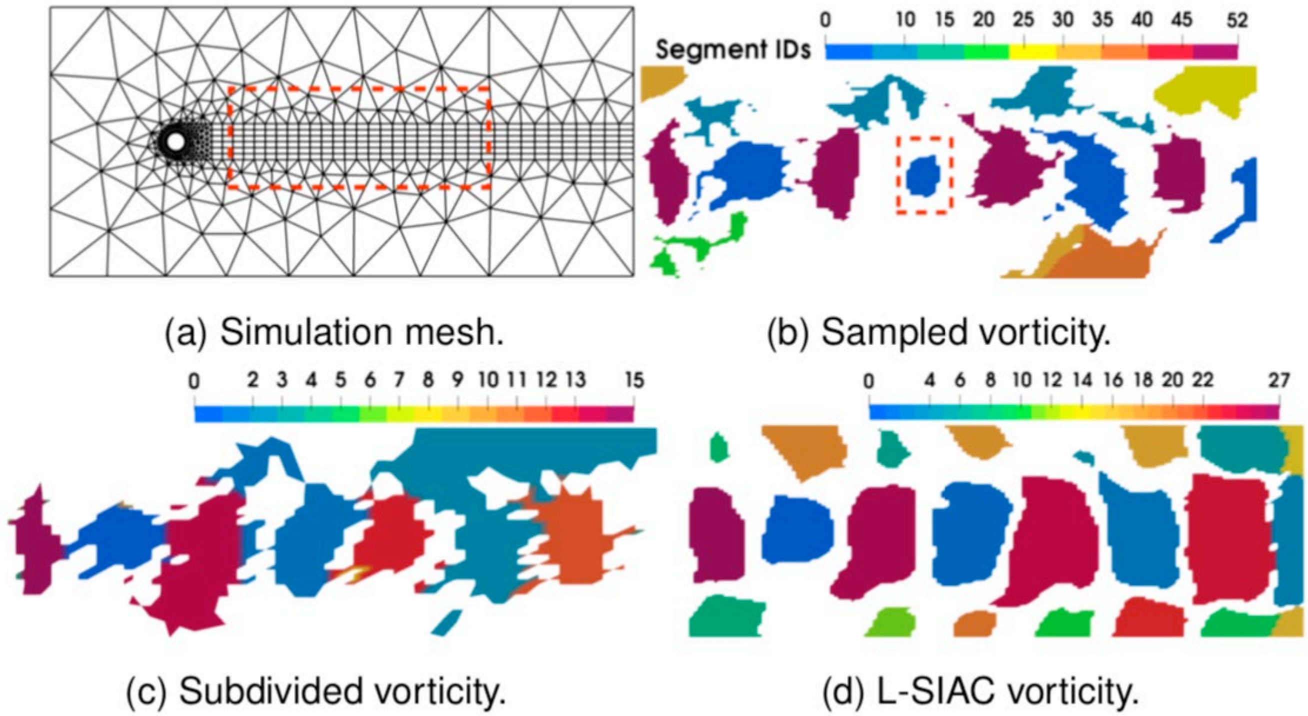
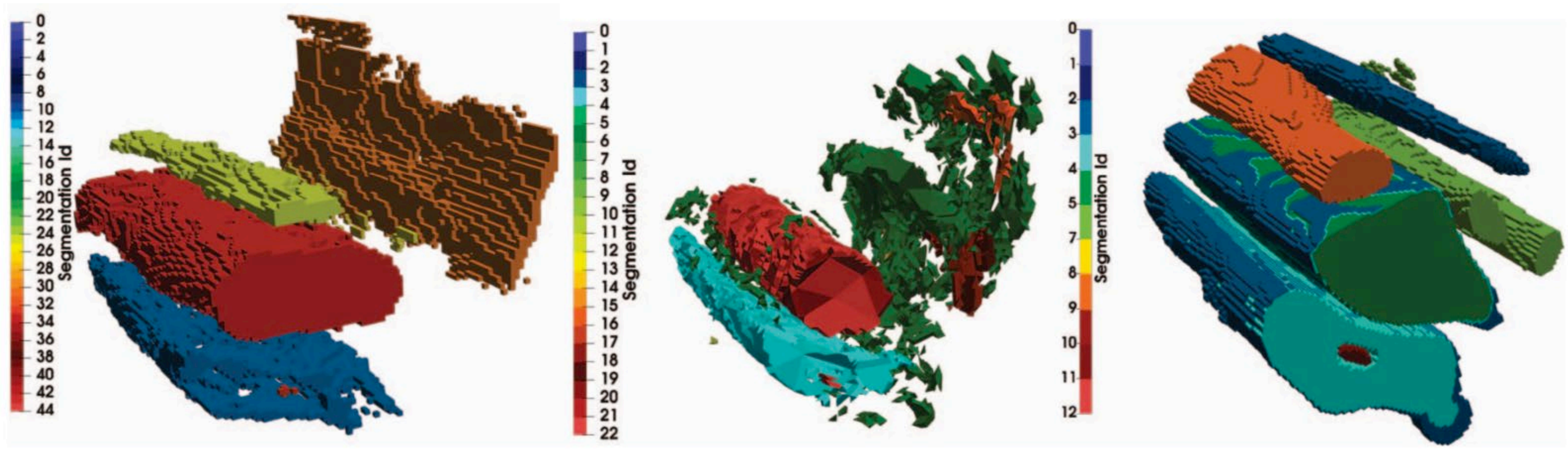


Fig. 16: Segmentation of the vorticity for the flow past a cylinder shown in (a). The segmentation for the sampled and the subdivided vorticity are computed using the contour tree along with a persistence threshold of 0.04. In the case of L-SIAC vorticity, the value of persistence threshold used is 0.001.



(a) Sampled vorticity. (b) Subdivided vorticity. (c) L-SIAC vorticity.

Fig. 1: Topological segmentation of counter-rotating vortex sampled using different methodologies discussed in the paper and by filtering the contour tree for segments that resemble vortex-like structures. The number, shape, and boundaries of the segments are different for the three techniques.

Results of Focus Area 5: In this section, we highlight the results of our most recent efforts – the formulation and implementation of a Non-Uniform Knot (NUK) L-SIAC filter. This filter is designed for use on highly anisotropic meshes. We anticipating submitting a publication to the Journal of Computational Physics (JCP) this summer [J5]. Within our draft manuscript, we compare and contrast our work with our previously published dynamic adaptive L-SIAC filter [J2].

Abstract: As the finite element method (FEM) and the finite volume method (FVM), both their traditional and high-order variants, continue their proliferation into various applied engineering disciplines, adaptive mesh refinement and optimization strategies have increased in their importance when solving real-world computational fluid mechanics applications. The post-processing and visualization of the resulting flow fields present two significant analysis and visualization challenges. The first challenge is the handling of elemental continuity, which is often only C^0 continuous (in continuous Galerkin methods) or piecewise discontinuous (in discontinuous Galerkin methods). The second challenge is that, depending on the flow regime and the geometric configurations for which adaptive meshing strategies are used, the meshes generated are often highly anisotropic. The (uniform knot) line-SIAC (L-

SIAC) filter has been proposed as a way of handling elemental continuity issues in an accuracy-conserving manner with the added benefit of casting the data in a smooth context even if the representation is element discontinuous. In this paper, we demonstrate that the state-of-the-art adaptive L-SIAC filter, designed for anisotropic meshes, suffers degradation in the quality of the post-processed solution when applied to the types of highly anisotropic meshes produced through adaptive mesh refinement and optimization. Hence, a new *Non-Uniform Knot (NUK)* L-SIAC filter is proposed that automatically conforms to the underlying mesh anisotropy. We demonstrate that the new filter behaves similarly to the adaptive L-SIAC filter when applied to uniform and mildly anisotropic meshes, and furthermore we show the superiority of the NUK L-SIAC filter when applied to highly anisotropic meshes. The newly formulated filter is applied to 2D canonical scalar fields and used to visualize 2D and 3D fluid flow simulation results.

In the figure below, we compare the raw dG solution to the adaptively filtered solution and the new NUK filtered solution. In the top-left panel, we show the mesh over which the simulation was accomplished. In the top-right panel, we show a visualization of the "raw" dG-based vorticity contours. In the left-bottom panel, we show the result of applying the dynamic adaptive filter [J2] to this flow field. In the right-bottom panel, we show the result of our newly implemented NUK L-SIAC filter. The adapted mesh has distinct anisotropic regions in the boundary layer as well as in the wake of the main airfoil element over the flap. The vorticity computed directly from the dG solution has discontinuities in the contour lines. However, applying the adaptive L-SIAC filter to compute vorticity for this case degrades the quality in the solution in the wake region. Also of note, the filter width does not fit in the computational domain in the cove of the main airfoil element leading to the white region in the adaptive L-SIAC (bottom-left panel). The degradation in the solution in the wake and the filter width limitations motivates the need for an improve L-SIAC filter for anisotropic meshes. The NUK L-SIAC filter proposed as part of this grant yields an enhanced smooth image of the vorticity.

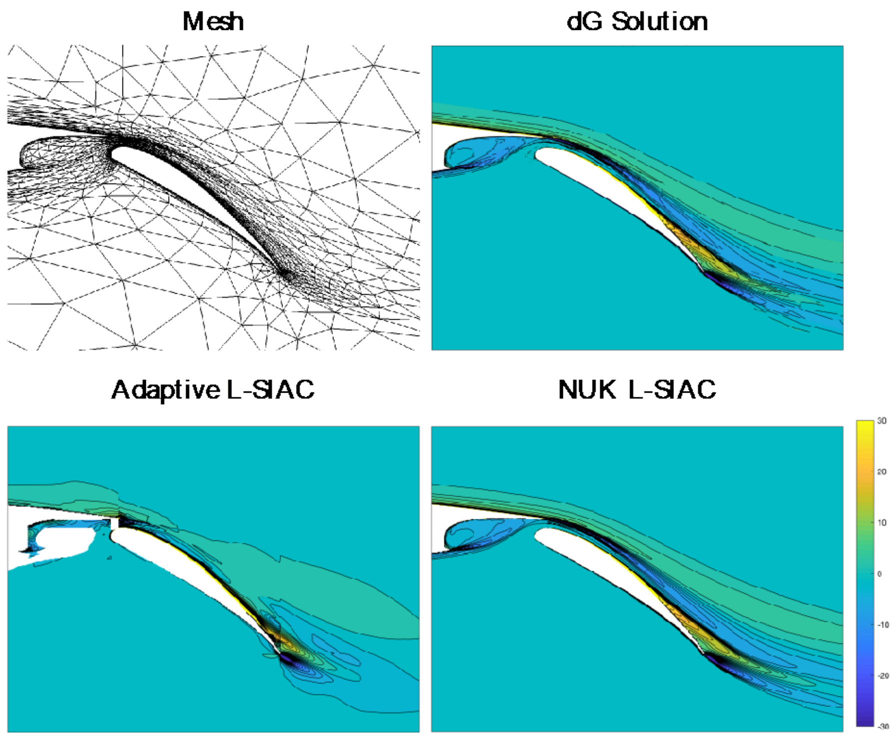


Figure 1: Voticity from a P^2 dG RANS solution for a multi-element airfoil from Ref. [14, 15].

Collaborations and Leveraged Funding

For the work presented in Focus Area 4, we collaborated with the Joshua A. Levine at University of Arizona to combine the data postprocessed using L-SIAC filter with TTK (Topological Tool Kit). This work shed light into the effect of data transformations on feature detection and the importance of L-SIAC filter as a post processor tool to facilitate feature detection on high-order methods. For the work presented in Focus Area 5, in addition to collaboration with co-PI Haimes, we engaged with Computational Fluid Dynamics (CFD) specialist Dr. Marshall Galbraith (MIT).

Open-Source Contributions

The code for the L-SIAC filter with its capabilities discussed in this report is available as a postprocessing module in the Nektar++ software. The postprocessing tool can be used as a data transformation tool to introduce continuity at interelement boundaries and transform high-order simulation data to low-order visualization data that can be used with the current visualization software.

Conclusions

Visualization is often employed as part of the simulation science pipeline. It is the lens through which scientists often examine their data for deriving new science, and is the lens used to view modeling and discretization interactions within their simulations. As such, visualization techniques need to be designed not only to elucidate the features or phenomena of interest within the data, but also to be compatible and complementary with the type and means of generating the data. One such category of simulation data, high-order finite element methods (also known as spectral/*hp* element methods) using either the continuous Galerkin or discontinuous Galerkin formulation, has reached a level of sophistication such that they are now commonly applied to a diverse set of real-life engineering problems. Visualizations of high-order finite element results that do not respect the *a priori* knowledge of how the data were produced and which do not provide a quantification of the visual error produced may undermine the scientific process as isolating where errors and assumptions are introduced into the process is critical.

Technology Transfer

None to report at this time.

Future Plans

The short-term future goal is to move our prototype high-order vortex core extraction code into Nektar++. This would allow us to proceed on two fronts: 1) we would begin to test our vortex core methods on various high-order data sets already available (and/or produced to match Army Rotorcraft conditions) and 2) We can initiate the connection between Nektar++ and the communication code developed by co-PI Haimes. This would allow on-the-fly extraction, communication, and visualization. We are currently working to extend all our results (as published in our IEEE TVCG paper) to work on highly anisotropic meshes (resulting in the new NUK L-SIAC filter), and hope to submit that work to the Journal of Computational Physics [J5] in the Summer of 2021.

Publications for the last five years

- [J1] Ashok Jallepalli, Julia Docampo-Sanchez, Jennifer K. Ryan, Robert Haimes and Robert M. Kirby, "On the Treatment of Field Quantities and Elemental Continuity in FEM Solutions", *IEEE Transactions on Visualization and Computer Graphics* (IEEE Visualization Issue), Volume 24, Issue 1, pages 903-912, 2017.
- [J2] Ashok Jallepalli, Robert Haimes and Robert M. Kirby, "Adaptive Characteristic Length for L-SIAC Filtering of FEM Data", Journal of Scientific Computing, 79 (1), pages 542-563, 2018.
- [J3] Ashok Jallepalli and Robert M. Kirby, "Efficient Implementation of the Line-SIAC Filter", SIAM Journal of Scientific Computing, 80 (2), pages 743-761, 2018.
- [J4] Ashok Jallepalli, Joshua A. Levine, and Robert M. Kirby, "The Effect of Data Transformations on Scalar Field Topological Analysis of High-Order FEM Solutions", *IEEE Transactions on Visualization and Computer Graphics* (IEEE Visualization Issue), Volume 26, Issue 1, pages 162-172, 2020.
- [J5] Ashok Jallepalli, Marshall Galbraith, Robert Haimes and Robert M. Kirby, "Non-uniform Knot (NUK) SIAC Post-processing of Flow Fields Produced Through Unstructured Grid Adaptation and Optimization", *Journal of Computational Physics*, In Preparation, 2021.

Number of graduate and undergraduate students, and postdocs supported for the last two years

- Mr. Ashok Jallepalli – PhD Student at Utah. Primary worked on LSIAC.
- Mr. Mahid Rasouli – PhD Student at Utah. Helped on the simulation side (for numerical results)
- Ms. Vidhi Zala – PhD Student at Utah. Helped test the L-SIAC software.

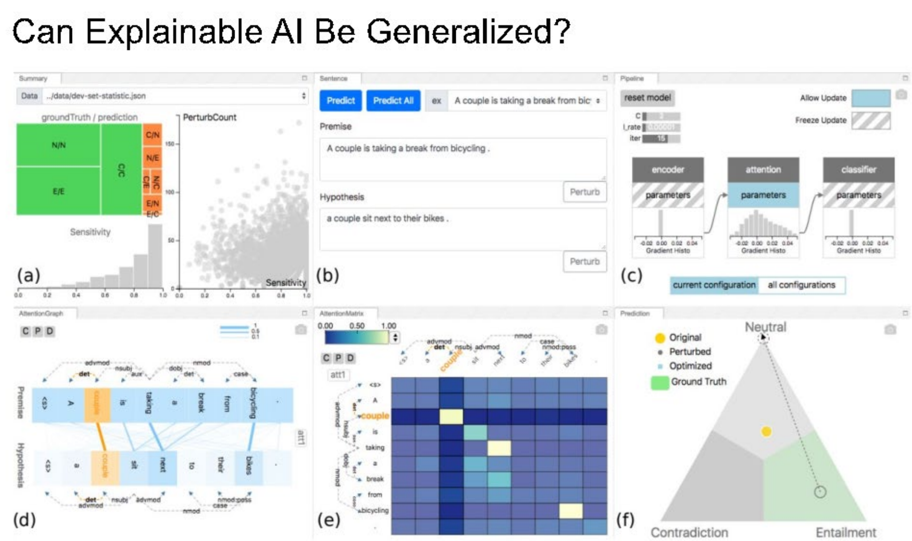
Supplemental Project: Explainable AI Through Visualization and Model Interrogation

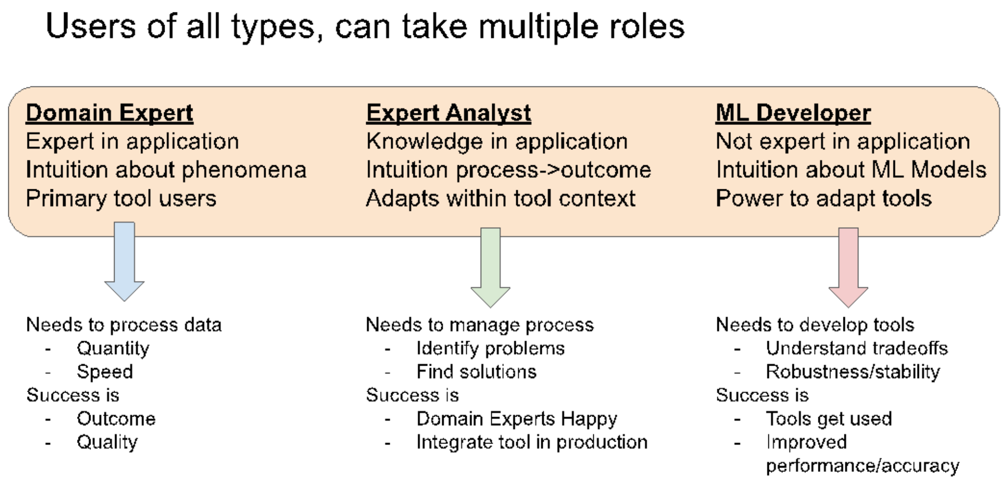
PI: Robert M. (Mike) Kirby and co-PI Valerio Pascucci

In the Spring of 2021, we submitted a request for extended funds to be used for a small project on Explainable AI. This work is in collaboration with Professor Valerio Pascucci (SCI Institute, University of Utah).

Executive Summary: As scientific research fully embraces the fourth paradigm, data-intensive science, it is only natural that decision science would follow. The field of artificial Intelligence and Machine Learning (AI/ML) has moved to the forefront of options used by decision-makers to create data-driven outcome predictions. Correspondingly, it is now important to develop strategies and tools that enable explainable AI/ML: ways of supporting and encouraging trust-building around AI/ML- driven outcome predictions. In this supplementary project, we propose that interactive visualization and interrogation tools play an important role in enabling explainable AI/ML. We propose a six month pilot project to investigate the use of various interactive visualization strategies designed for AI/ML model exploration, interrogation and explanation.

Two slides from our more general presentation (presented to Dr. Simon Su, CISD/ARL on 9 June 2021 are presented below. The full presentation will be provided to Dr. Mike Coyle.





Personnel:

- Dr. Attila Gyulassy – Researcher at the SCI Institute.
- Mr. Samuel Leventhal – PhD Student at Utah: funding was used to support this student as he designed and developed the tools shown in the presentation.
- Mr. Zhimin Li – PhD Student at Utah: additional student within Prof. Pascucci's group who worked with Mr. Leventhal.

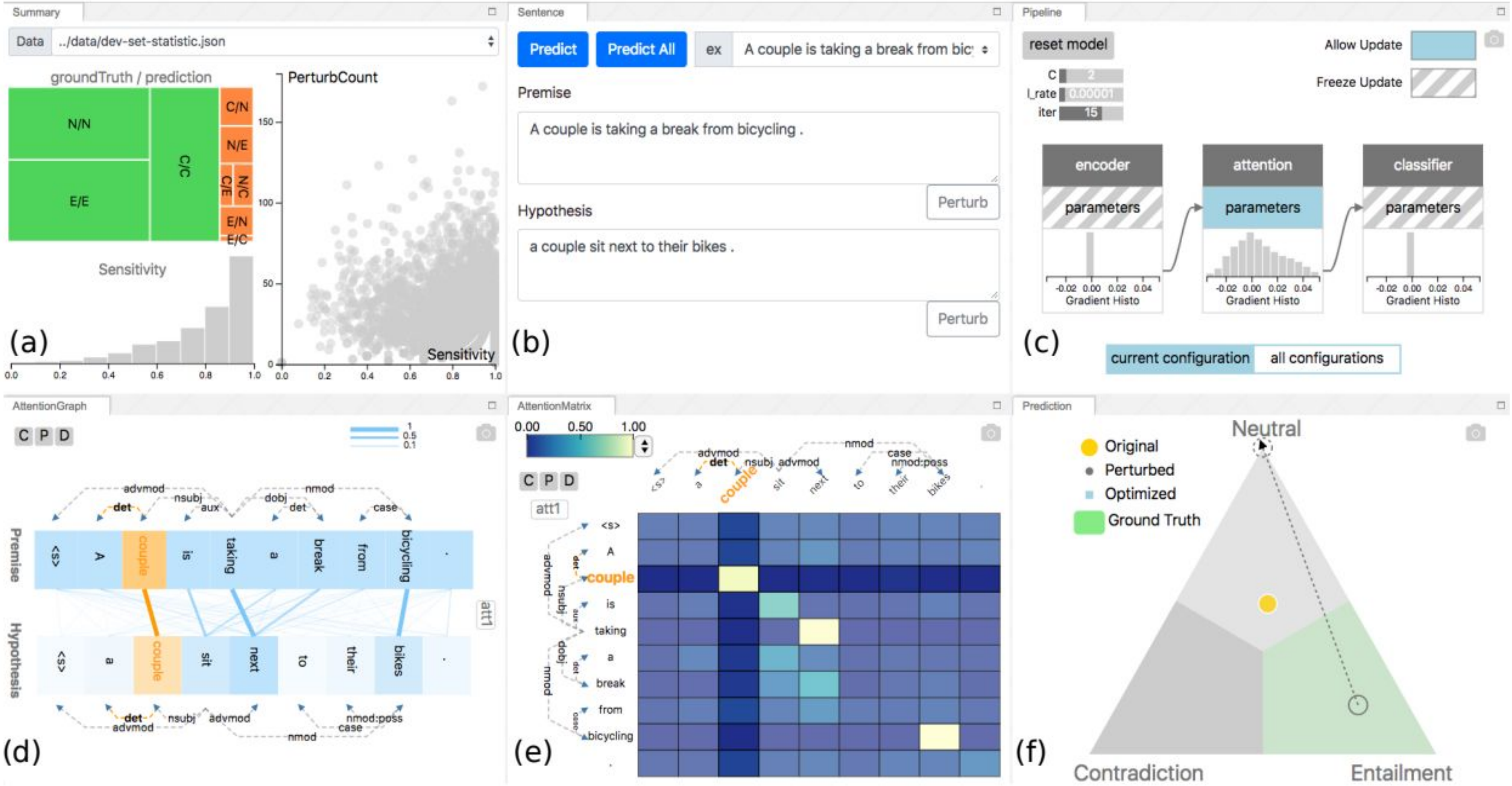
Interactive Exploration for Understanding AI

With a case study in topological feature labeling

Mike Kirby, Valerio Pascucci, Attila Gyulassy, Samuel Leventhal, Zhimin Li

www.sci.utah.edu

Can Explainable AI Be Generalized?



AI Learns “the best” function for the task, given input

f () → cat

f (

) → 

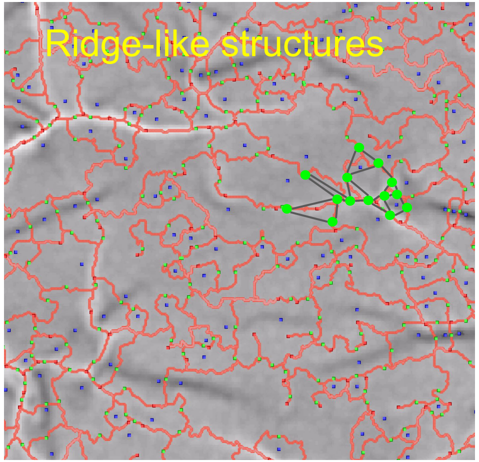
f () → 

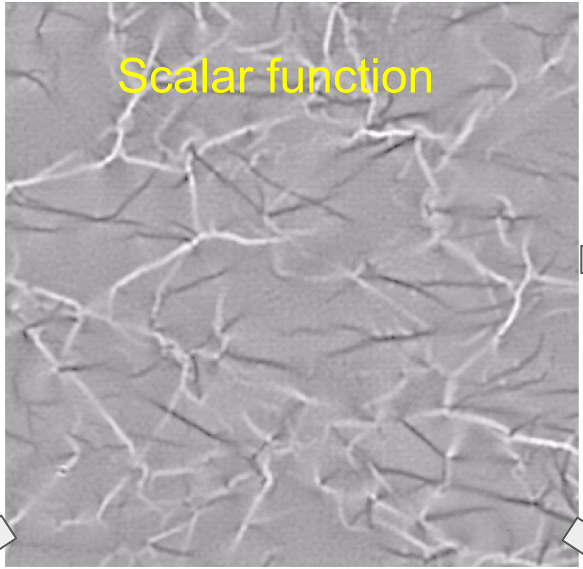
$$f : X \rightarrow Y$$

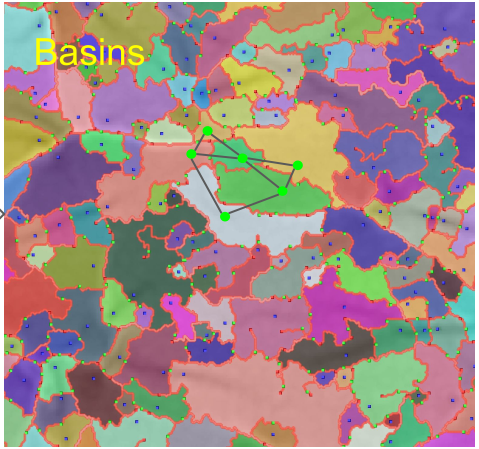
Minimize error on seen data (training)

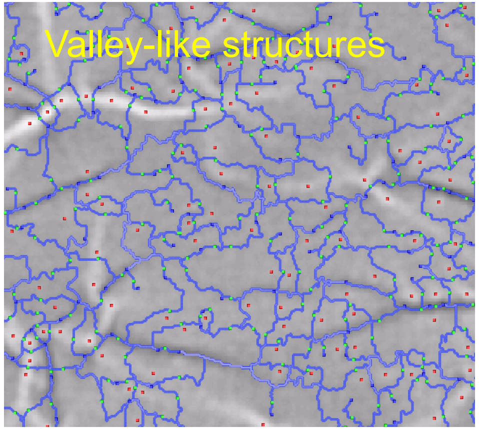
Running Case Study: learning to pick domain-specific features from topological priors, like a domain expert

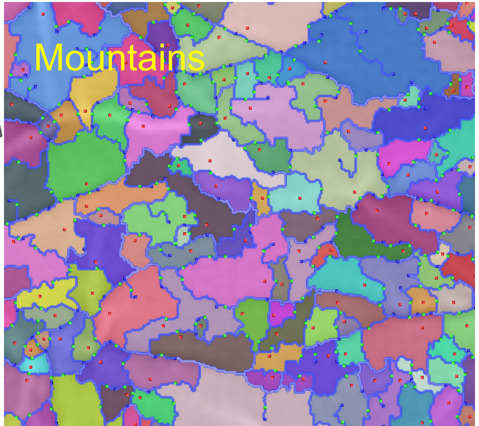
Morse-Smale complex is a reduced representation of a scalar function











Nodes can represent:
critical points, arcs, regions, (volumes 3d)

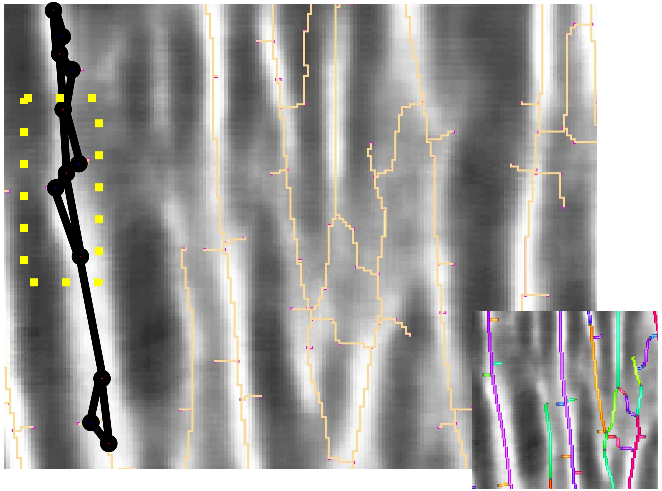
- Any attributes measured per feature
- Intrinsic geometry (size, orientation, curvature,...)

Edges represent where features touch

- Can have measured attributes
- Intrinsic geometry
- Relative geometry

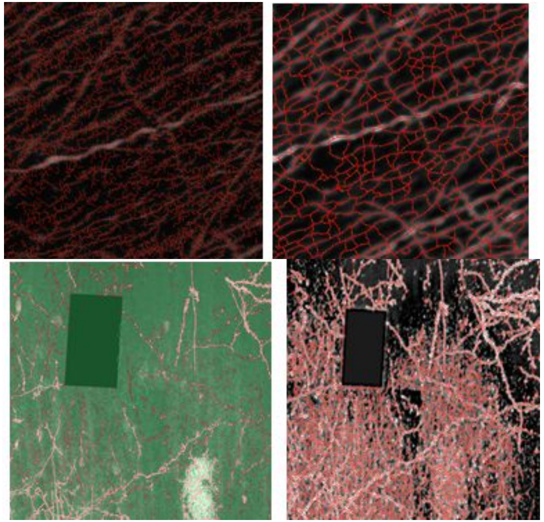
New generic method for many applications

Fault identification
Geologic interpretation



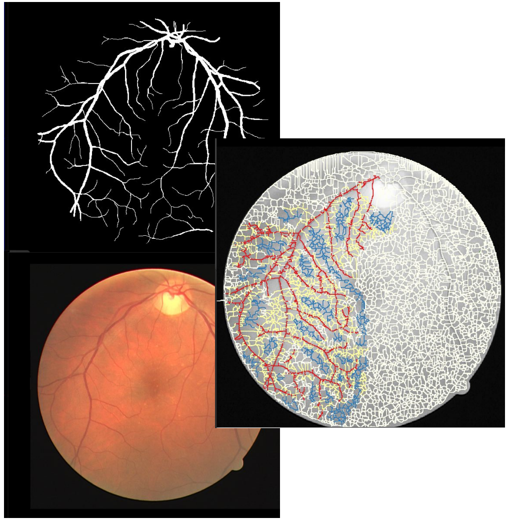
Can we identify which topological pieces correspond to faults, and which are not?

Tracing neurons
Connectomics



Can we automate neuron tracing, picking the dendrites/axons from the background artifacts?

Blood vessel segmentation
Retinal degeneration

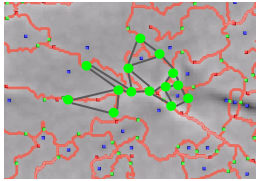


Can we identify which topological priors trace out blood vessels?

Compute topology and represent as samples graph with high-dimensional features

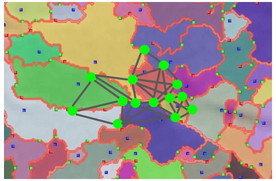
Types | **Example** | **Ex. Tasks**

Polyline graph
- Nodes rep polylines
- Arcs between polylines that touch



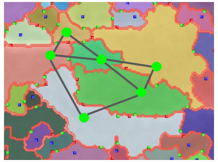
Identify blood vessels
Identify axon/dendrite
Identify cracks

Separator graph
- Nodes rep polylines
    - Encode neighbors?
- Arcs: clique of region boundaries



Identify cell boundaries
Identify fiber boundaries

Region graph
- Nodes rep 2d patches
- Arcs: polylines between regions



Separate cells from bg
Separate fiber from bg
Identify voids
Identify salt bodies

Nodes

gId

Arcs

gId	n0	n1

MSC Geom Database

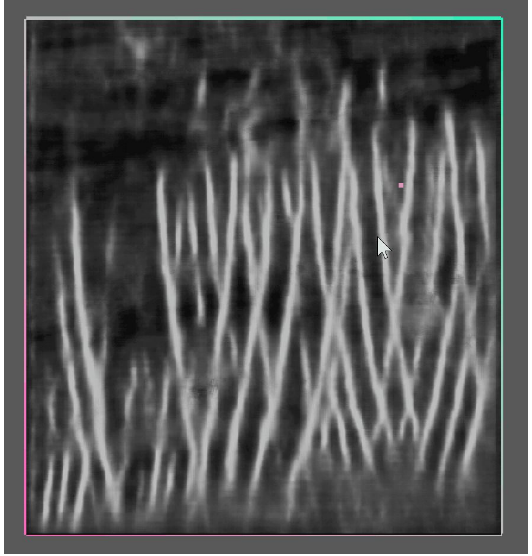
gid	dim	p0	p1	...

MSC Att Database

gId	a0	a1	...

Machine model to augment human interpretation

- Replicate a domain expert in labeling data
- General for multiple application areas



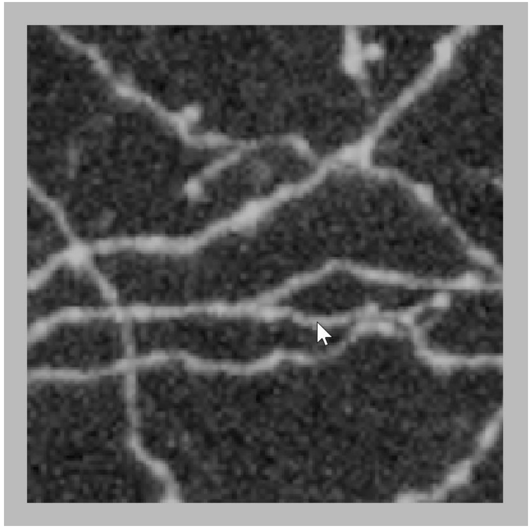
Fault Probability

Brighter structures

More vertical

Connect through gaps

Shape



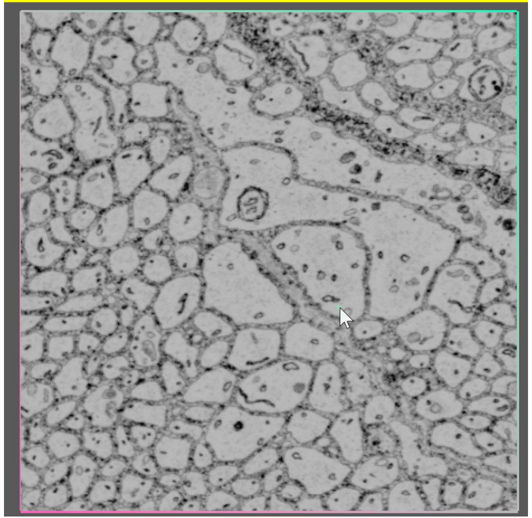
2-Photon Neurites

Axons, dendrites

Relative brightness

Cross gaps

Ignore isolated



EM Tissue

Membrane vs. Cell body

Shape

Dark vs. Light

Outside vs. Inside

Users of all types, can take multiple roles

Domain Expert
Expert in application
Intuition about phenomena
Primary tool users

Needs to process data
- Quantity
- Speed

Success is
- Outcome
- Quality

Expert Analyst
Knowledge in application
Intuition process->outcome
Adapts within tool context

Needs to manage process
- Identify problems
- Find solutions

Success is
- Domain Experts Happy
- Integrate tool in production

ML Developer
Not expert in application
Intuition about ML Models
Power to adapt tools

Needs to develop tools
- Understand tradeoffs
- Robustness/stability

Success is
- Tools get used
- Improved performance/accuracy

Users of all types, can take multiple roles

Domain Expert
Expert in application
Intuition about phenomena
Primary tool users

Expert Analyst
Knowledge in application
Intuition process->outcome
Adapts within tool context

ML Developer
Not expert in application
Intuition about ML Models
Power to adapt tools

Needs

offs

lity

Succ

performance/accuracy

A Toolchain with Explainable AI educates users for all roles

Questions a user may need to answer

How much can I trust a model/set of predictions?

Can I anticipate the outcome of a sample given a model?

Why did the model give me the result it did?

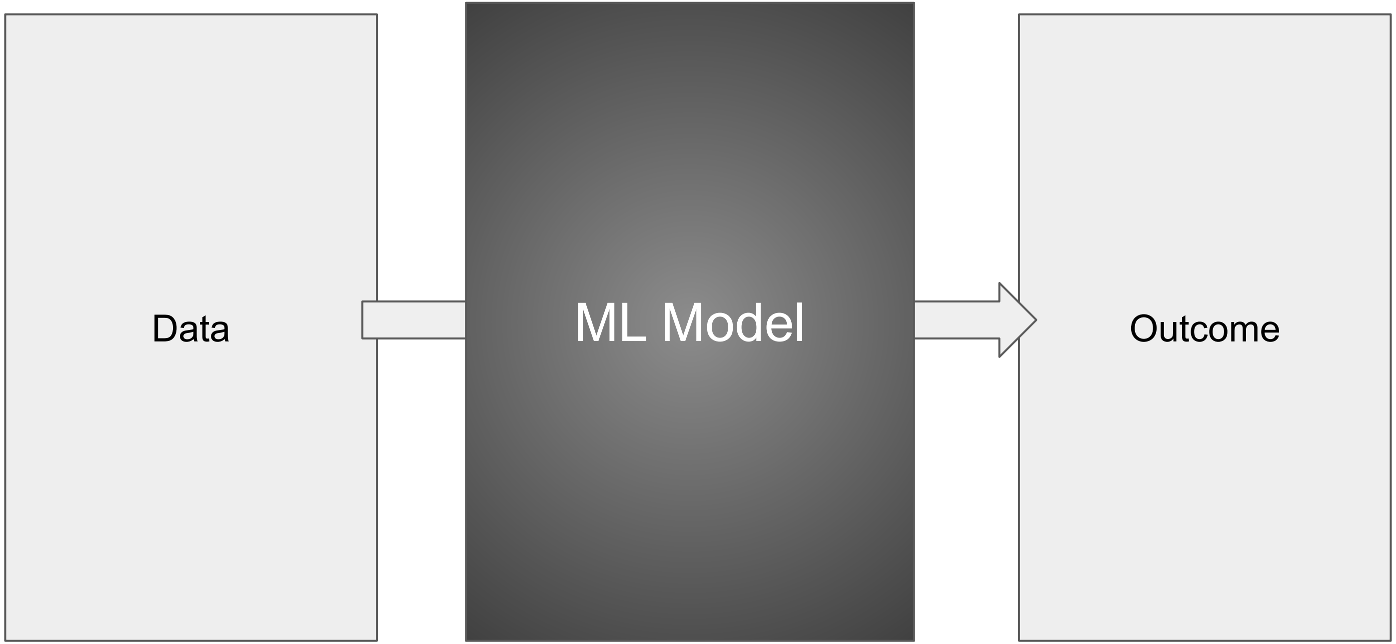
How stable is the prediction?

- w.r.t. perturbation of training, sample, model?

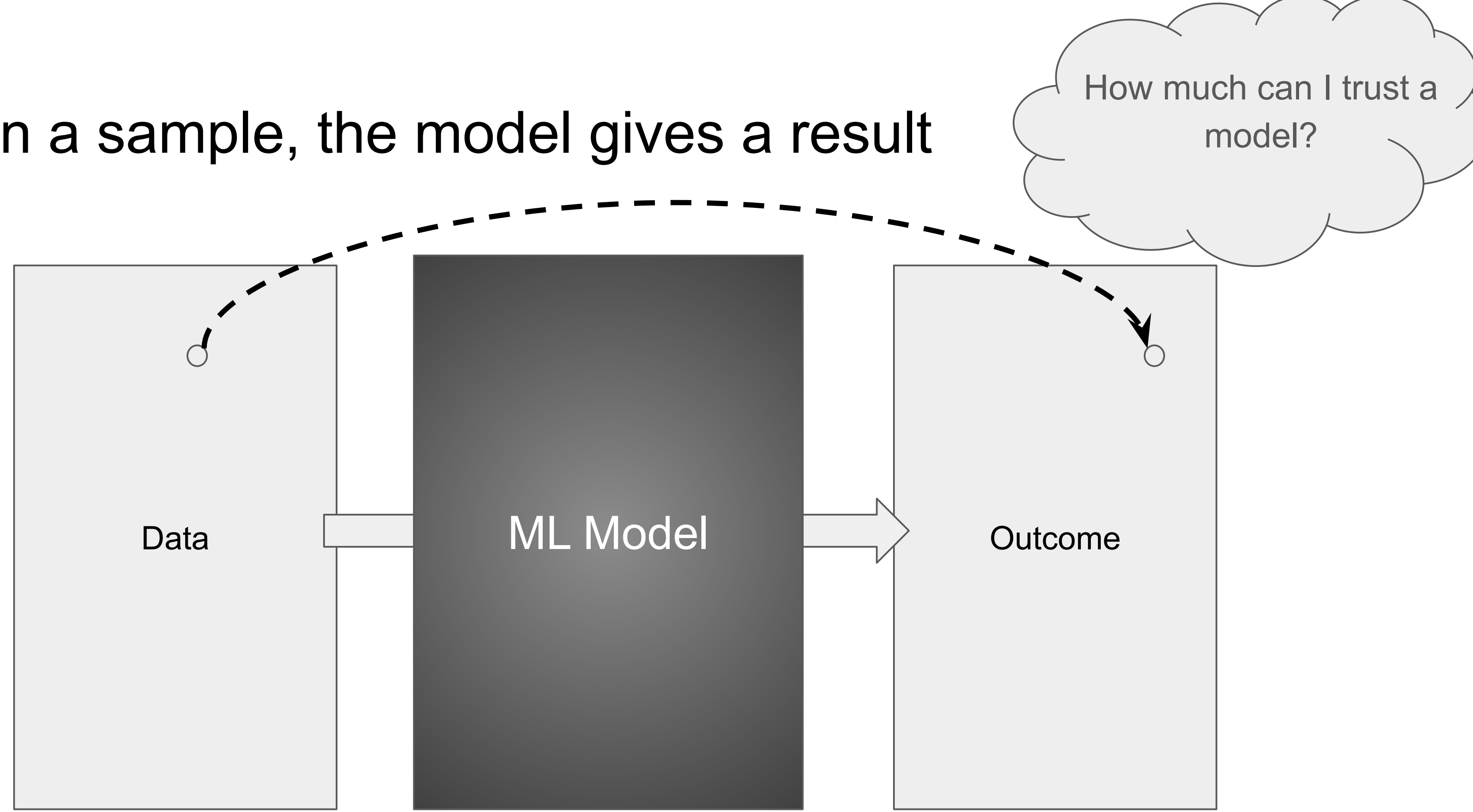
Could I have changed something to get a better prediction for the kinds of phenomena I am interested in?

Level 0: Explaining a trained black box model

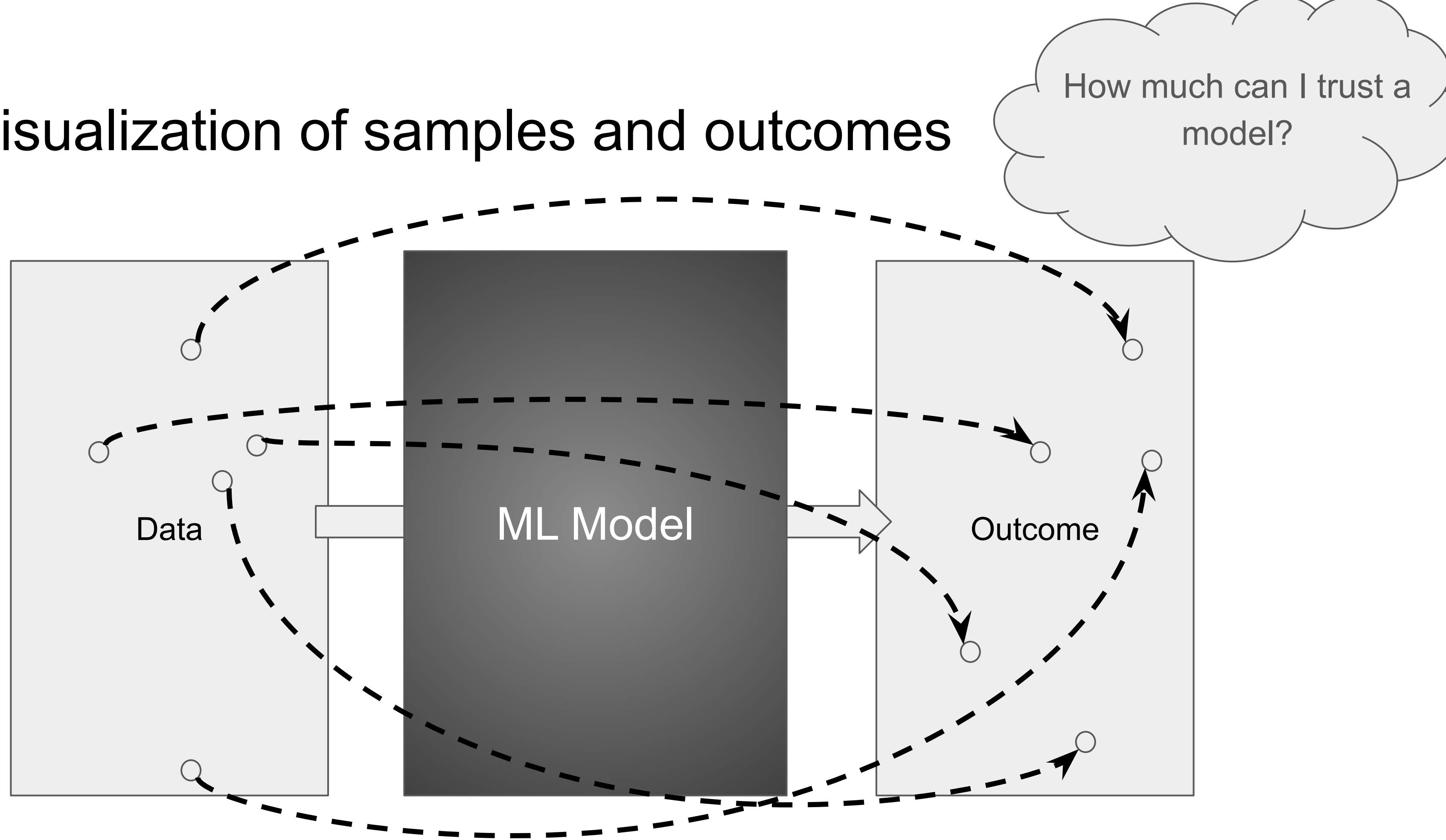
ML can be an opaque process to a user



Given a sample, the model gives a result



Co-visualization of samples and outcomes



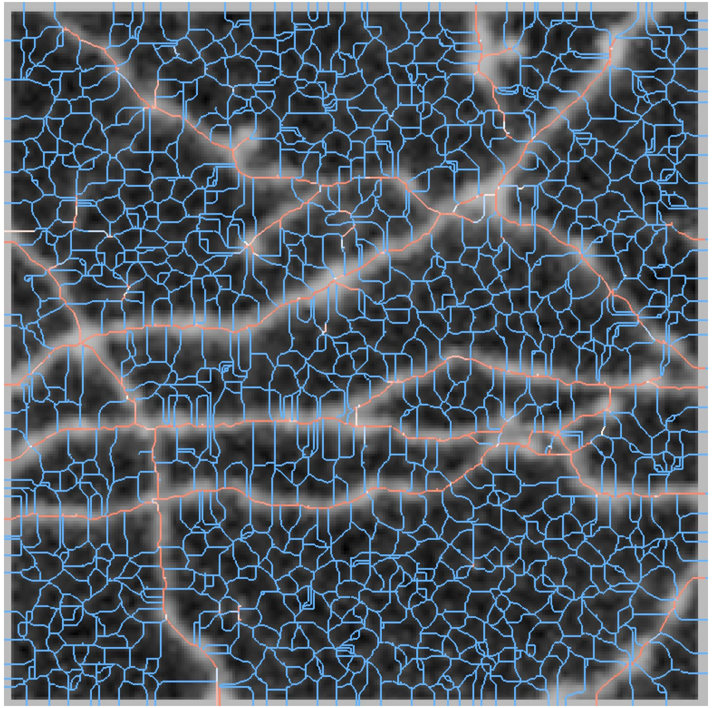
Case Study: Co-visualize results on top of samples

sample->outcome

outcome->sample

<u>Visualization uses:</u>
Context to show outliers

Turn on-off outcomes



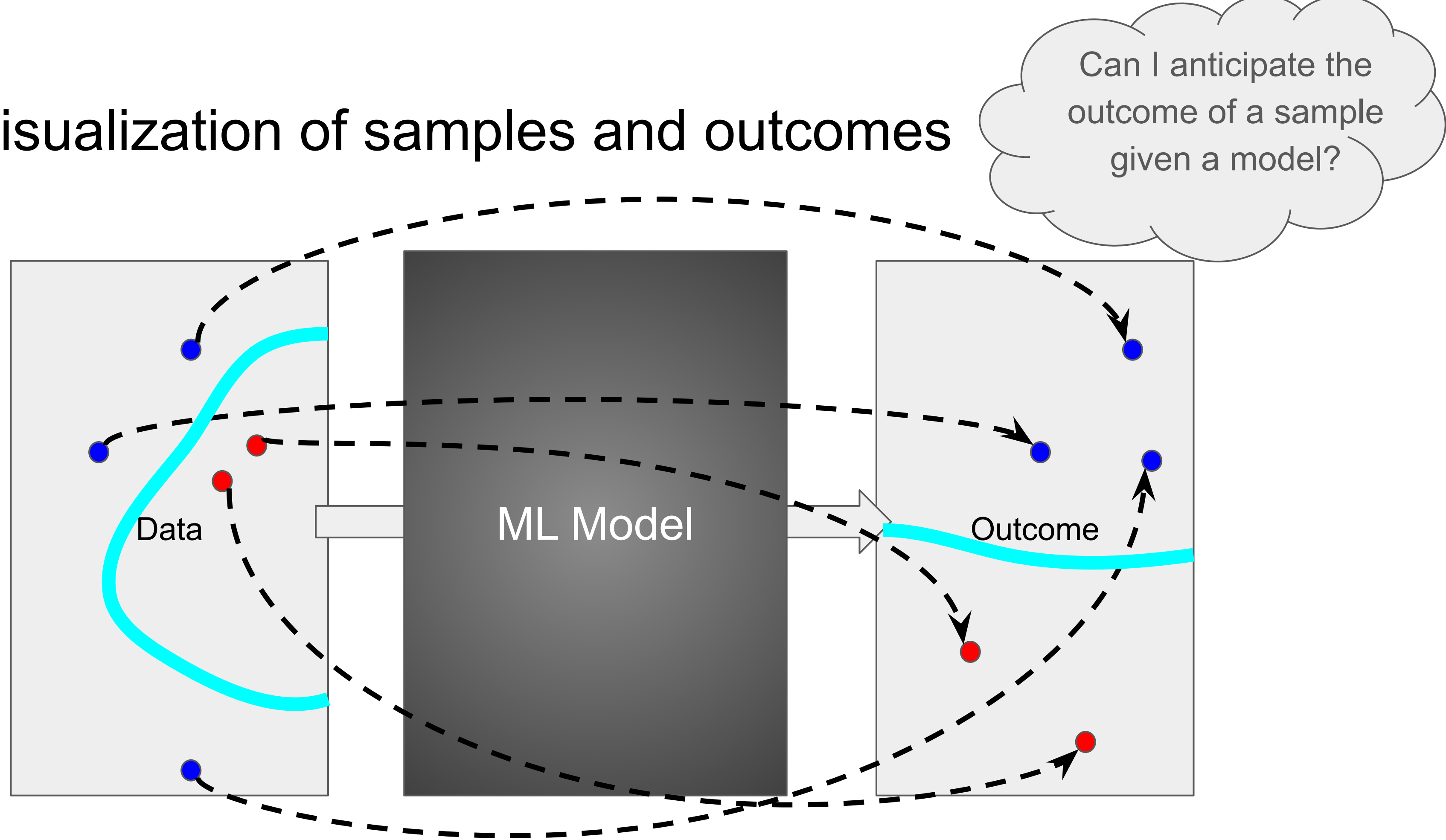
How much can I trust a model?

<u>Added to Vis Tool:</u>

Capability to load various outcomes

Color by class/prediction value

Co-visualization of samples and outcomes



Case Study: Co-visualize results on top of samples

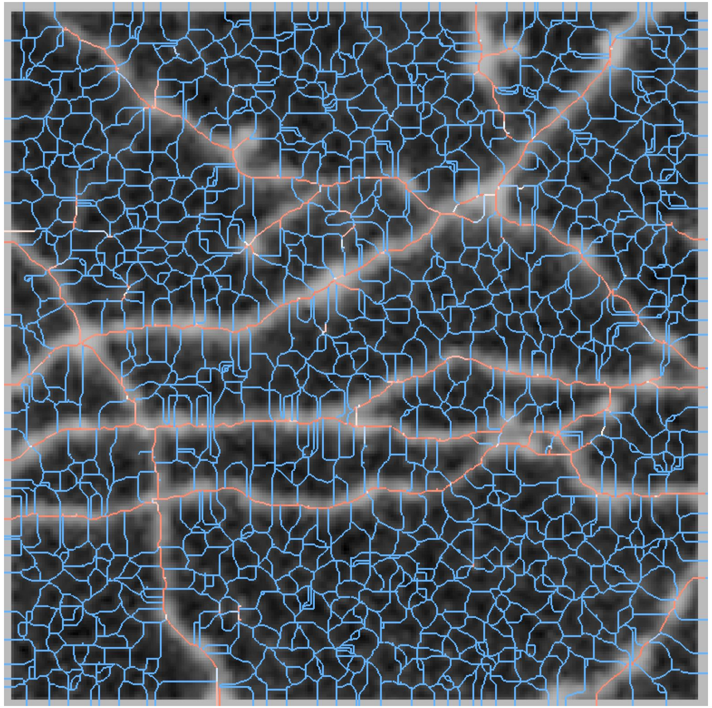
Can I anticipate the outcome of a sample given a model?

sample->outcome

outcome->sample

<u>Visualization uses:</u>
Context to show outliers

Turn on-off outcomes



Case Study: Co-visualize results on top of samples, and high dimensional exploration.

Can I anticipate the outcome of a sample given a model?

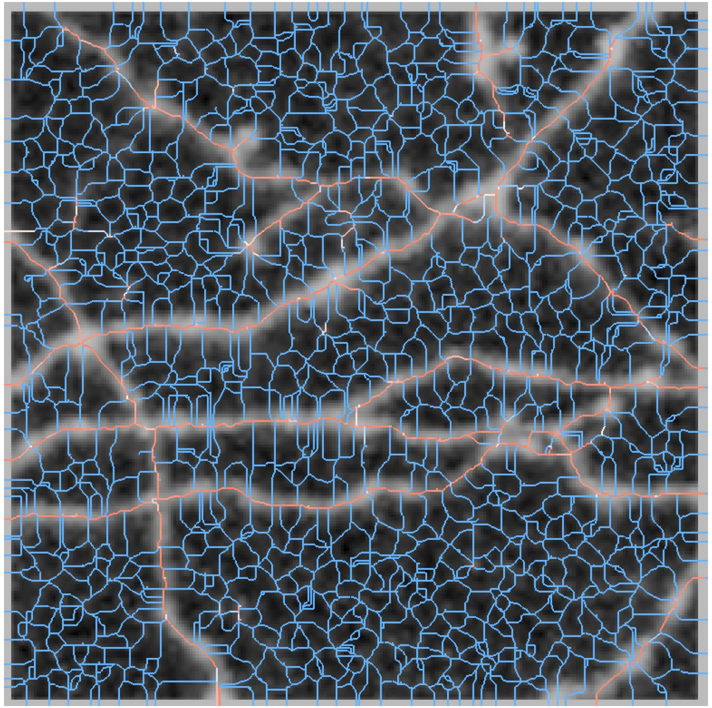
sample->outcome

outcome->sample

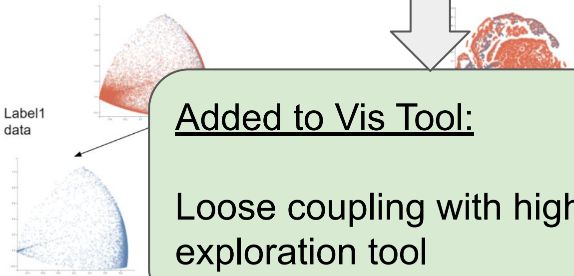
<u>Visualization uses:</u>
Context to show outliers

Turn on-off outcomes

Brushing samples for deeper dive



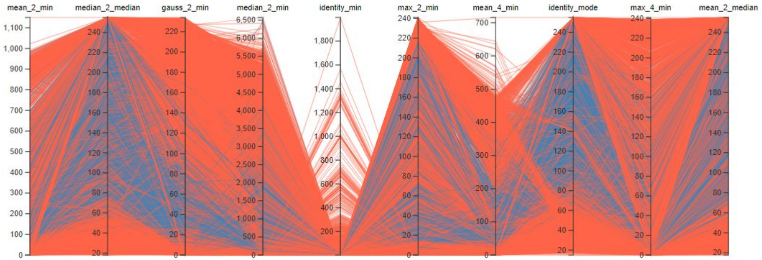
Regression: PCA, TSNE



<u>Added to Vis Tool:</u>

Loose coupling with high-dim exploration tool

Parallel coordinates



Case Study: Co-visualize results on top of samples, and high dimensional exploration.

Can I anticipate the outcome of a sample given a model?

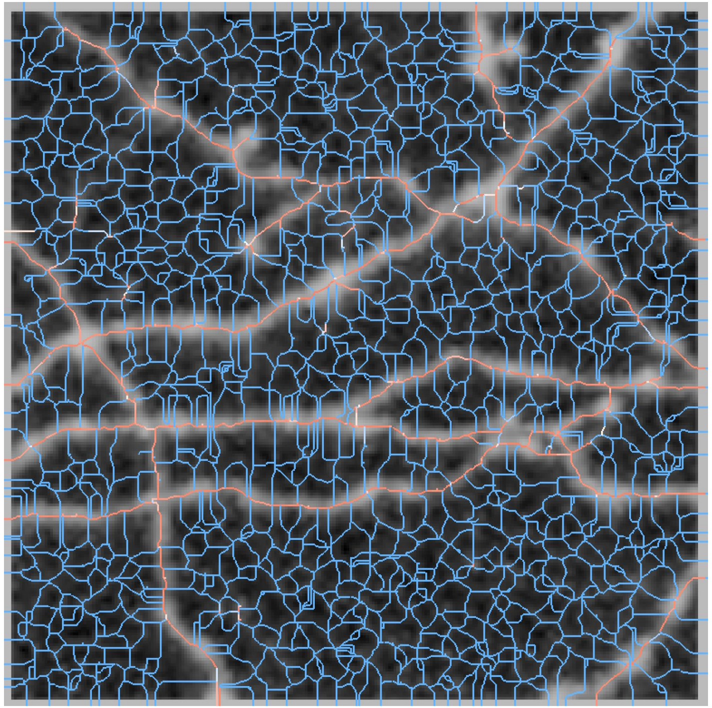
sample->outcome

outcome->sample

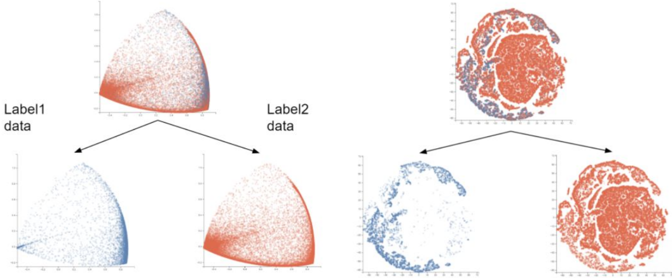
<u>Visualization uses:</u>
Context to show outliers

Turn on-off outcomes

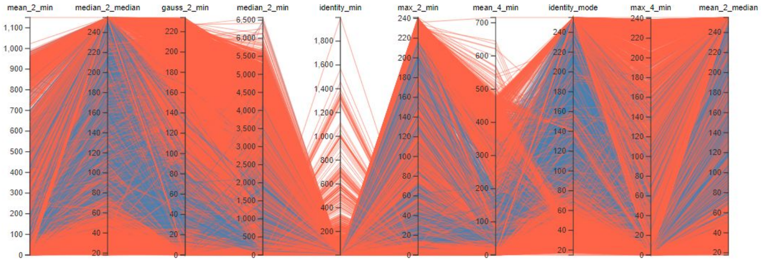
Brushing samples for deeper dive



Regression: PCA, T-SNE



Parallel coordinates



Case Study: Co-visualize results on top of samples, and high dimensional exploration.

Why did the model give me the result it did?

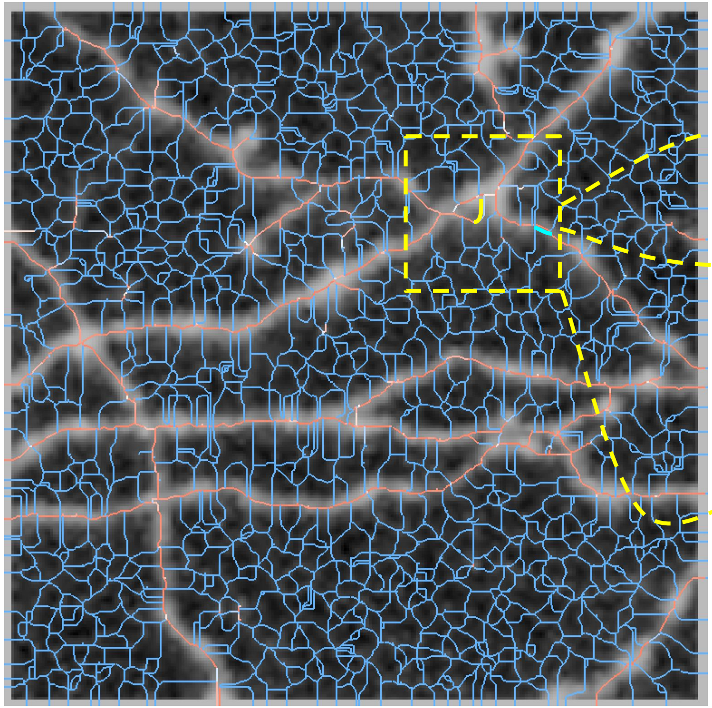
sample->outcome

outcome->sample

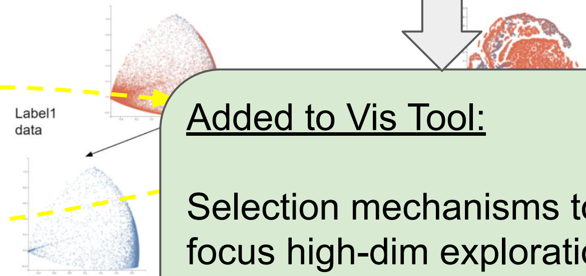
<u>Visualization uses:</u>
Context to show outliers

Turn on-off outcomes

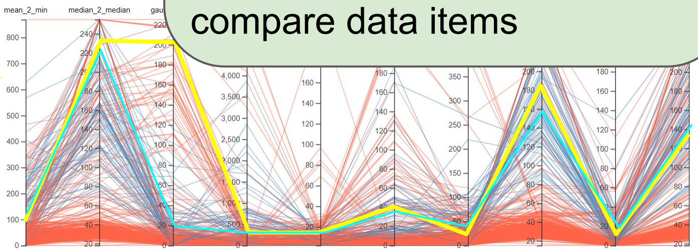
Brushing samples for deeper dive



Regression: PCA, T SNE



Parallel c



<u>Added to Vis Tool:</u>

Selection mechanisms to focus high-dim exploration

Multi-label selections to compare data items

Case Study: Co-visualize results on top of samples, and high dimensional exploration.

Why did the model give me the result it did?

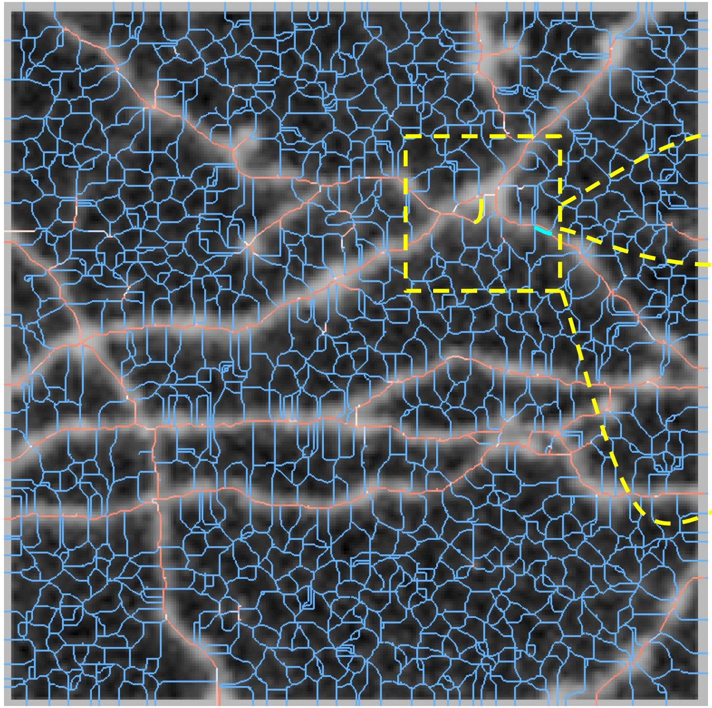
sample->outcome

outcome->sample

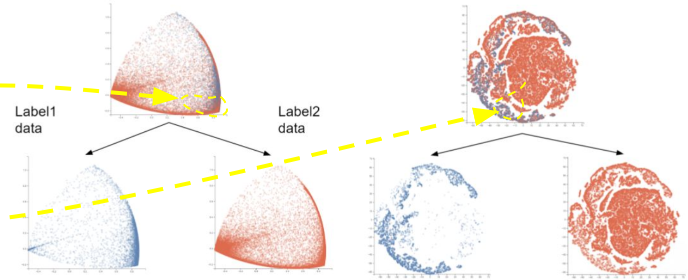
<u>Visualization uses:</u>
Context to show outliers

Turn on-off outcomes

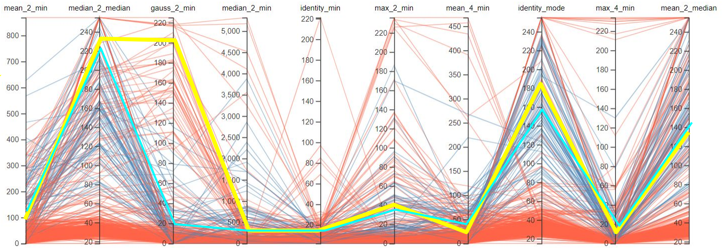
Brushing samples for deeper dive



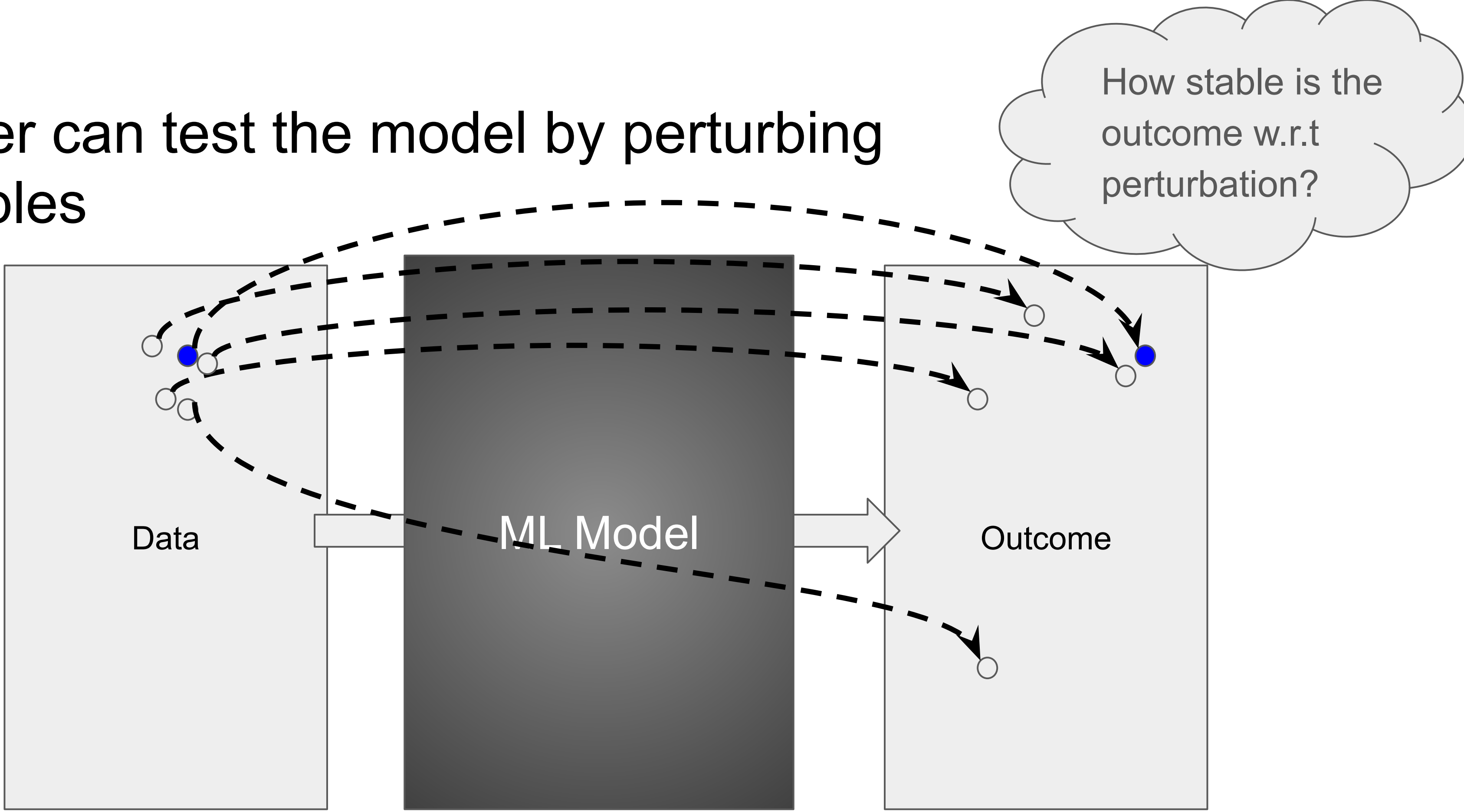
Regression: PCA, T-SNE



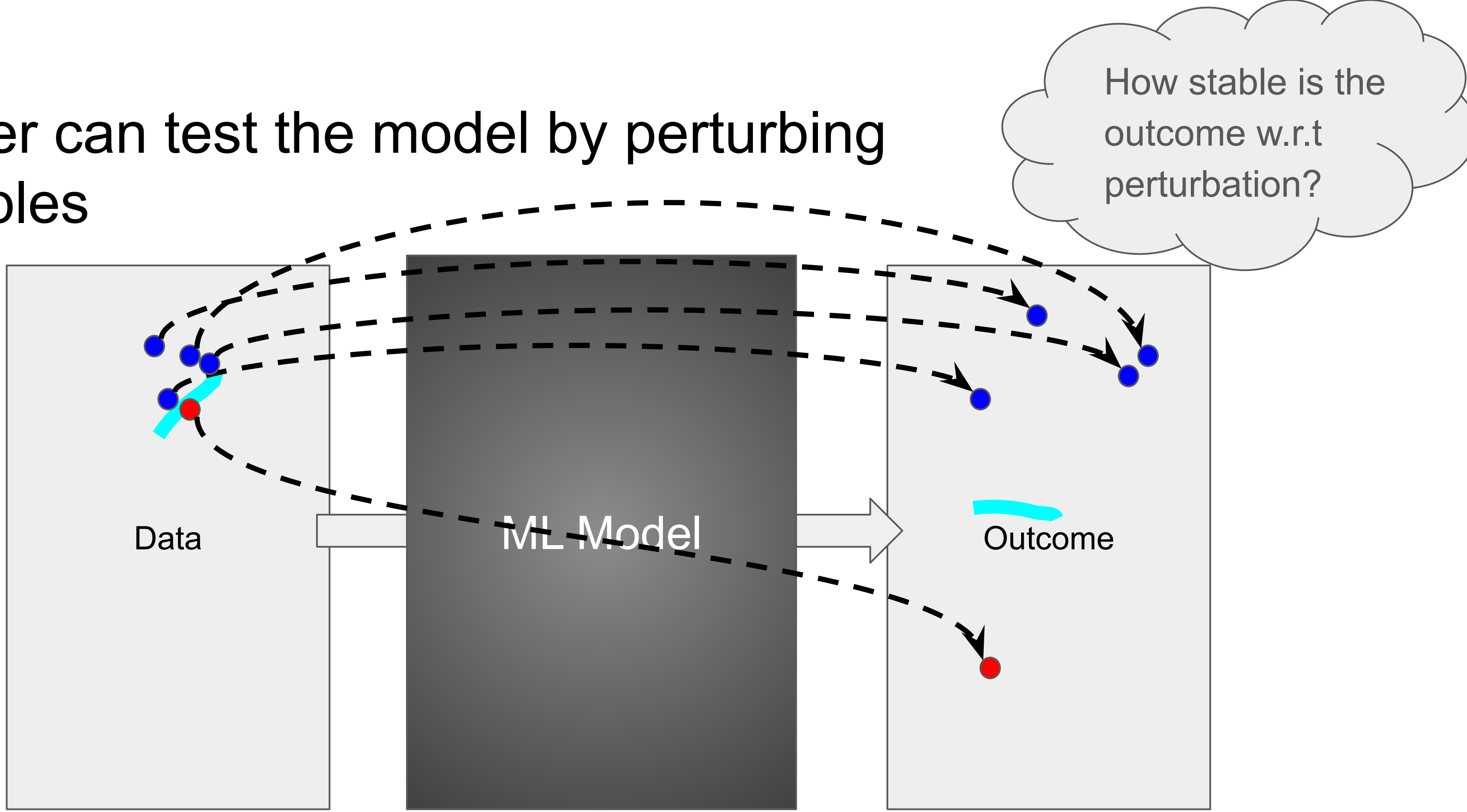
Parallel coordinates



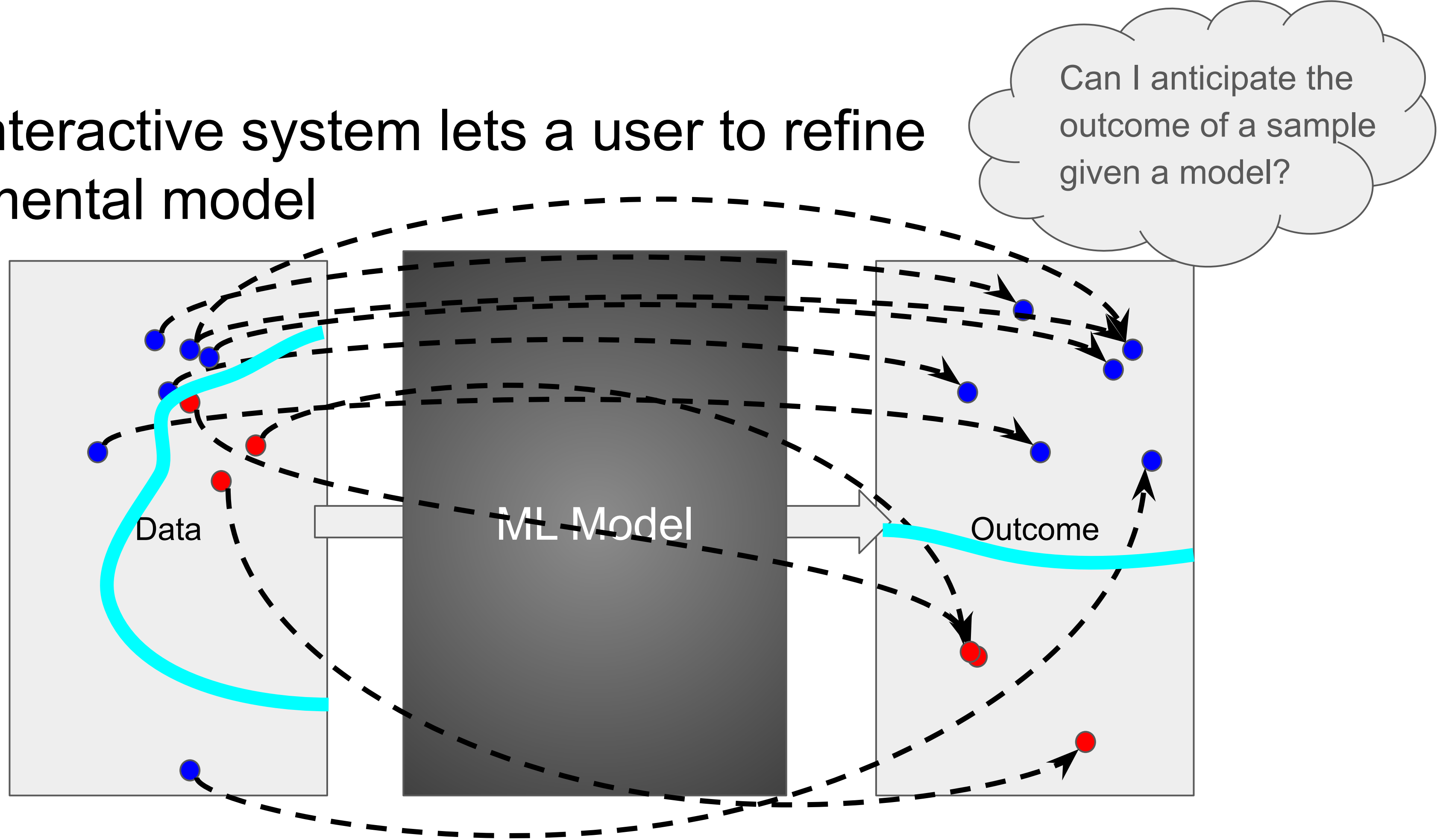
A user can test the model by perturbing samples



A user can test the model by perturbing samples



An interactive system lets a user to refine the mental model



Case Study: Co-visualize perturbations

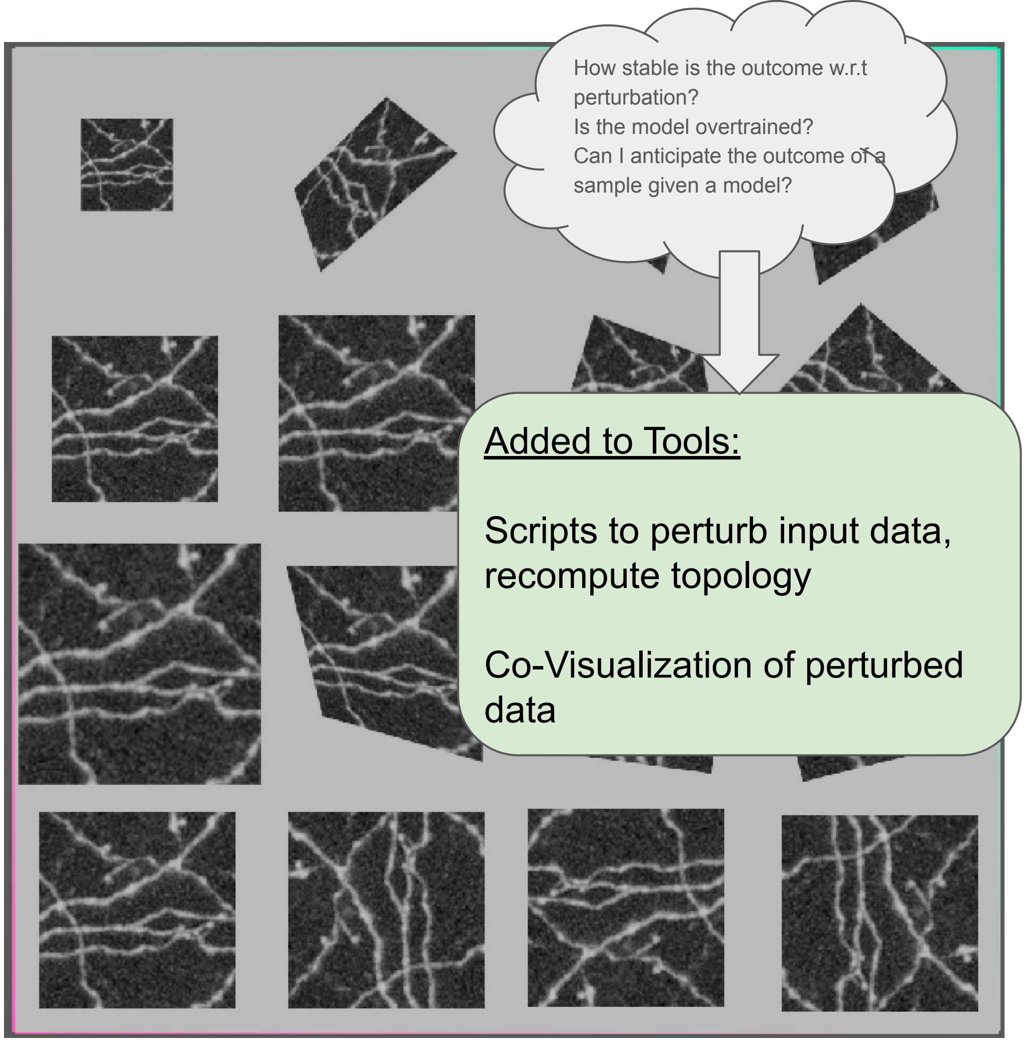
Generate perturbations

- Modify images
- Recompute topological elements

<u>Visualization utilizes:</u>

Interactive zoom to compare

Simple mental model to map perturbations (context)



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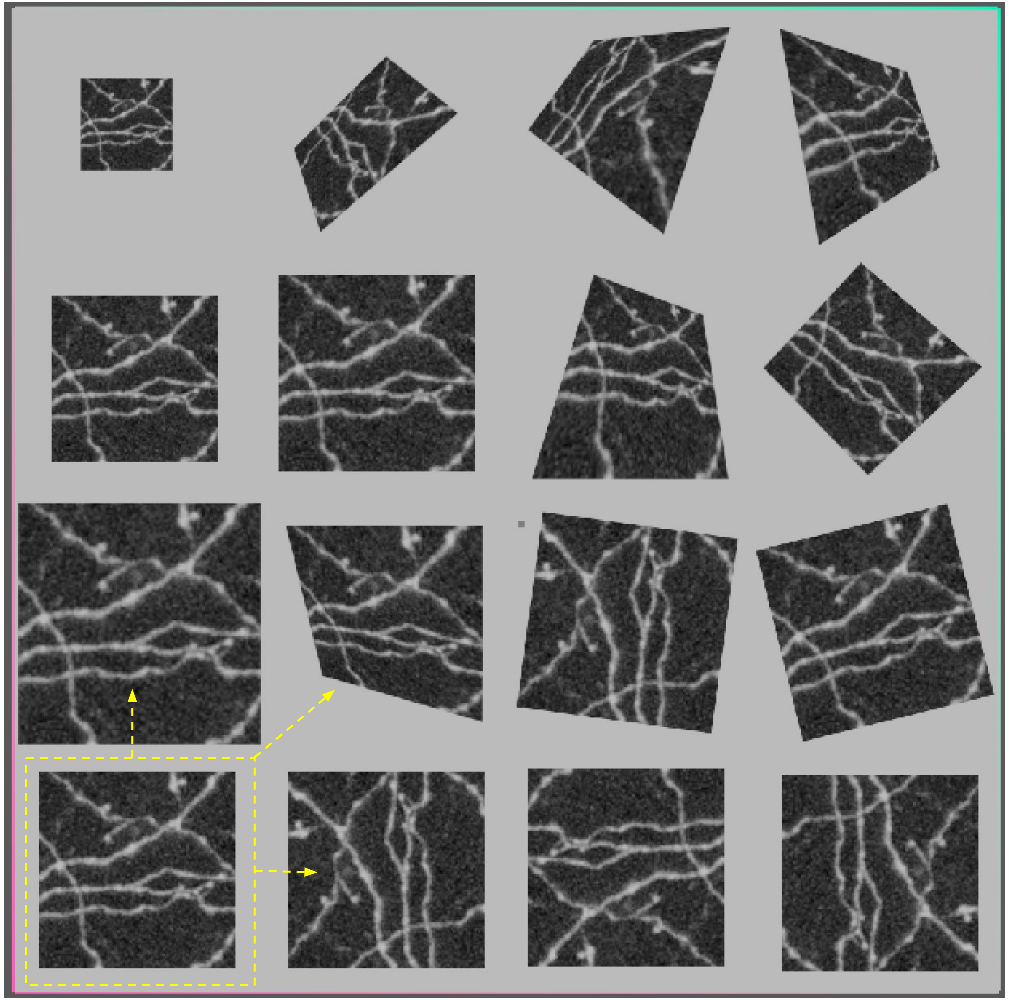

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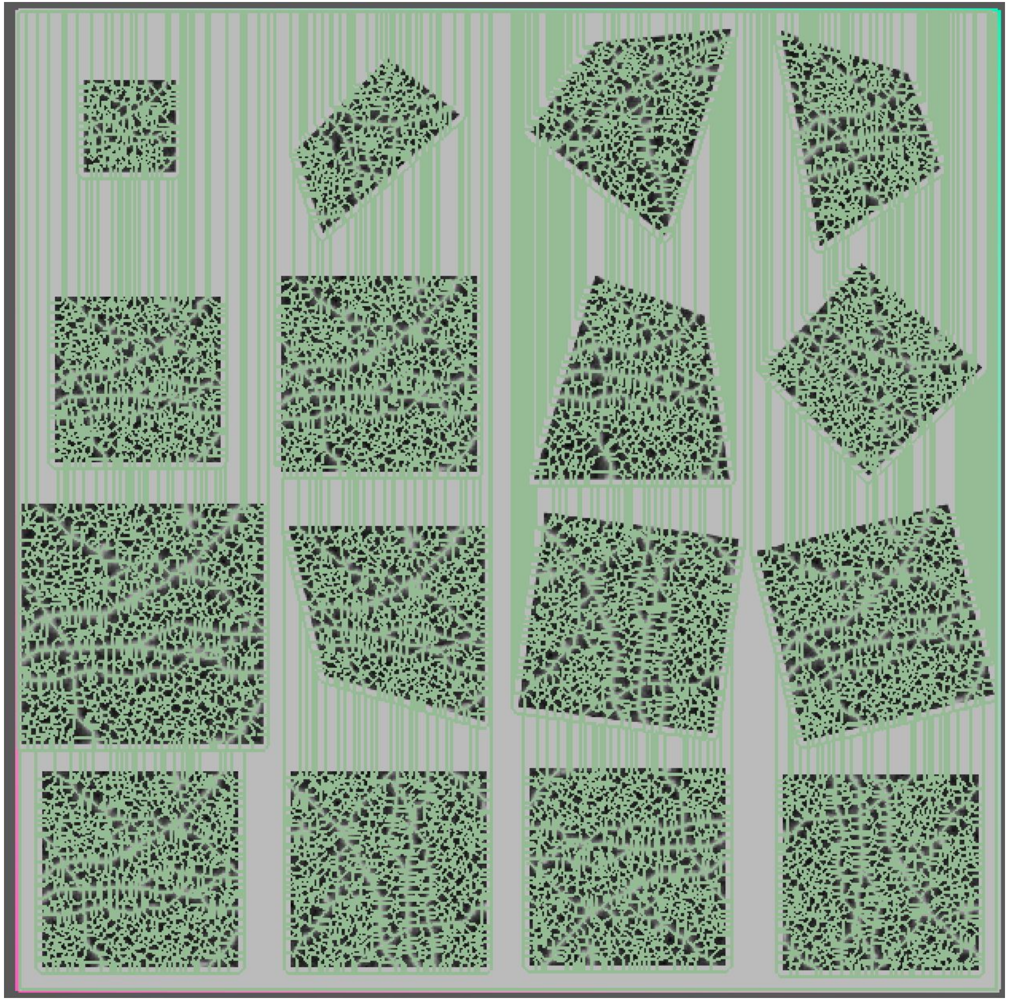

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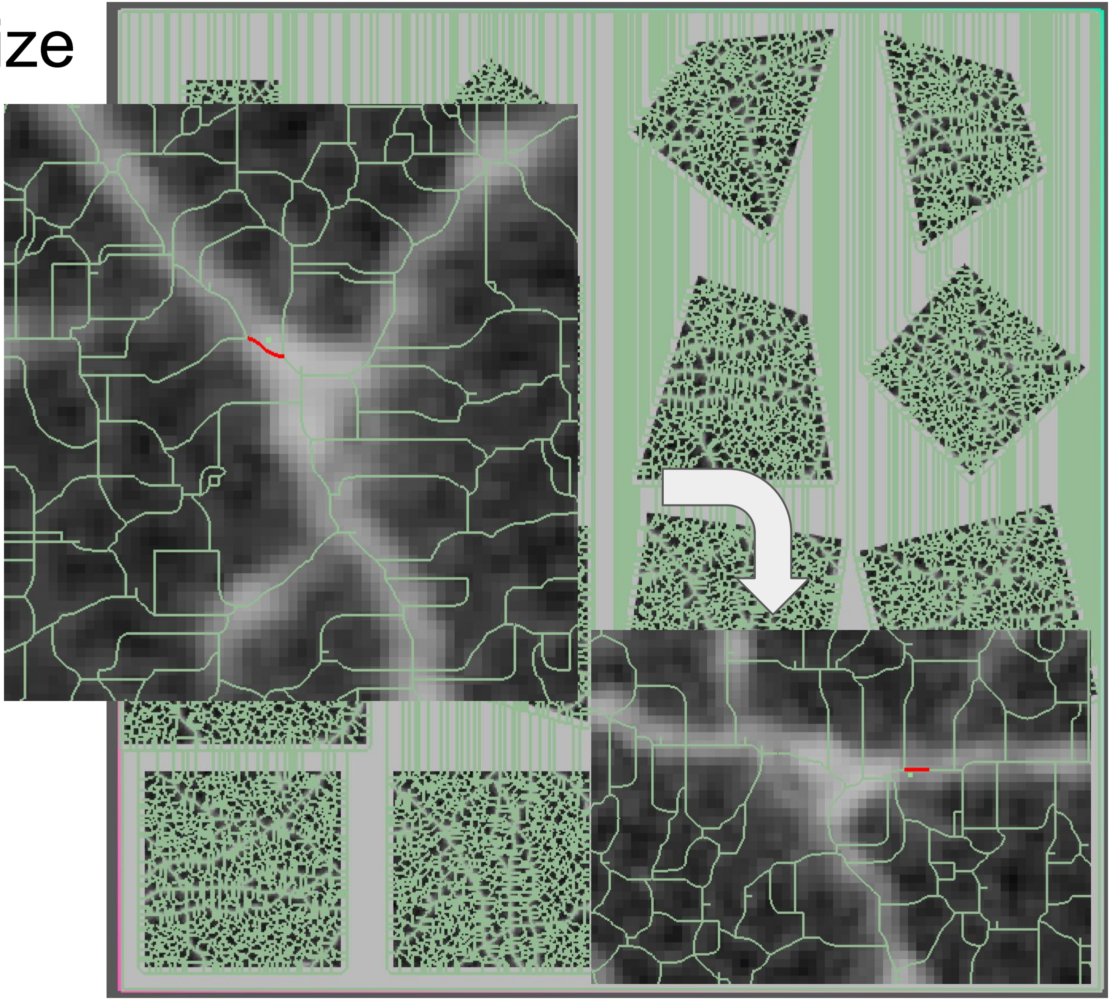

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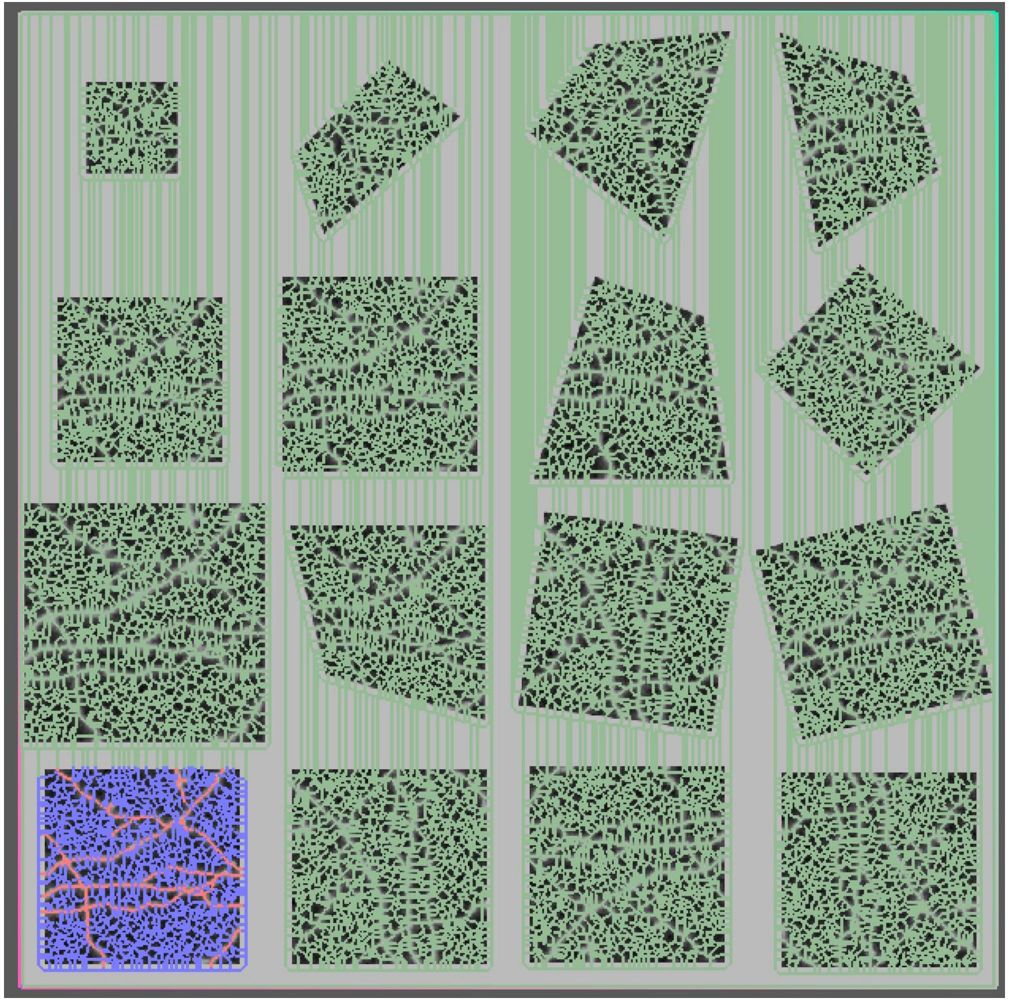

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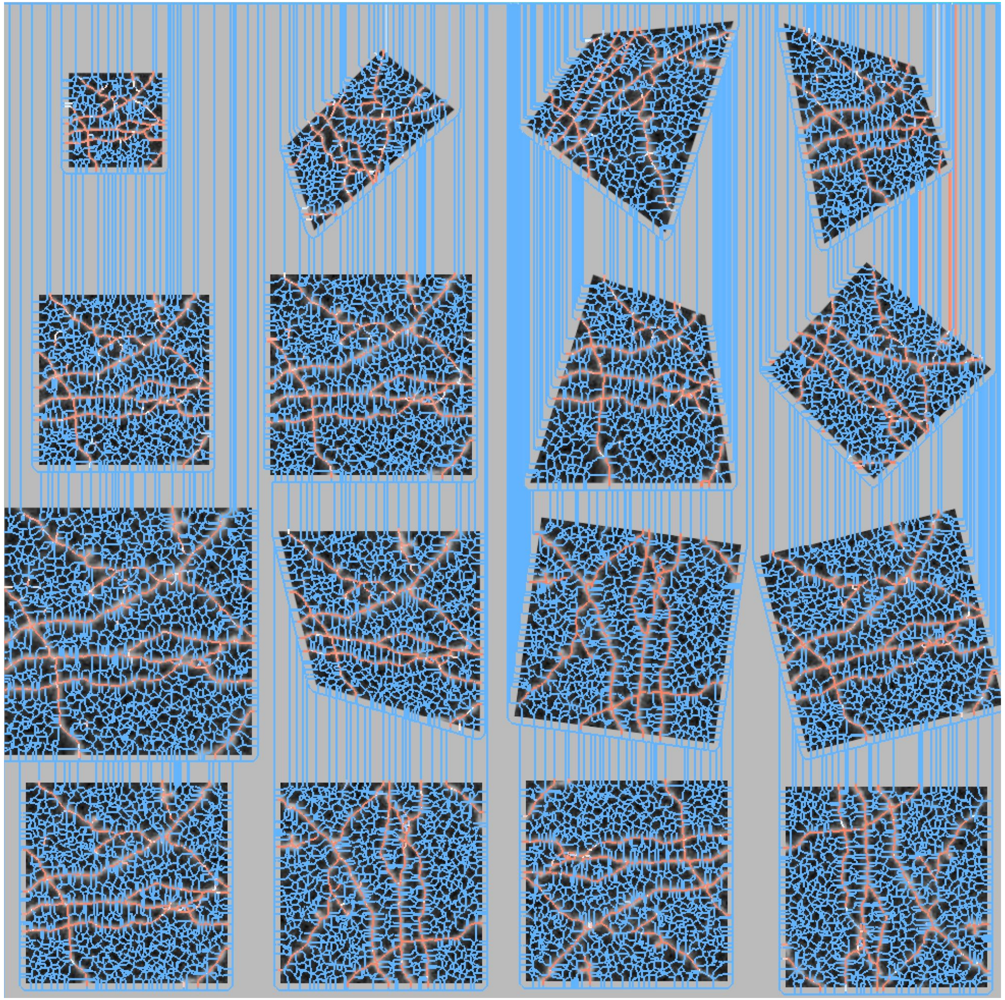

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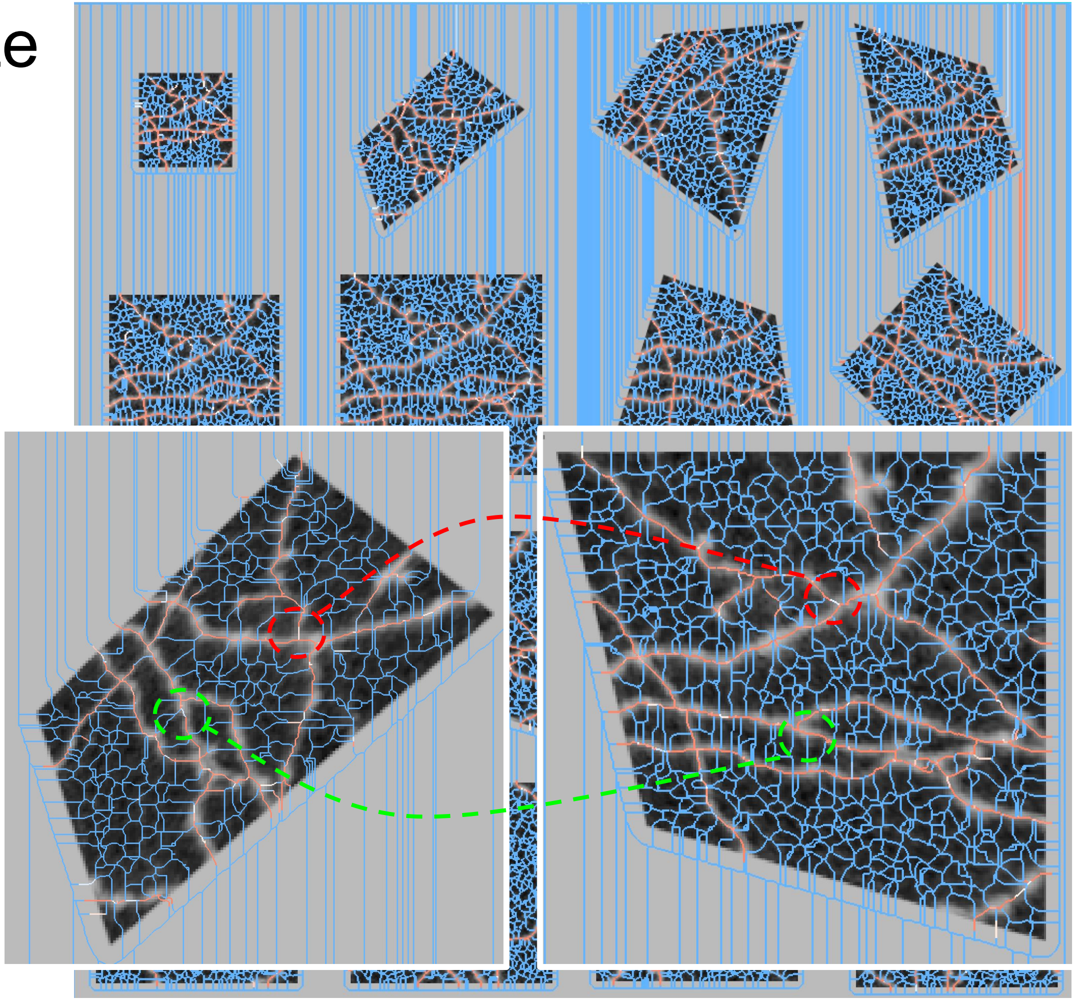
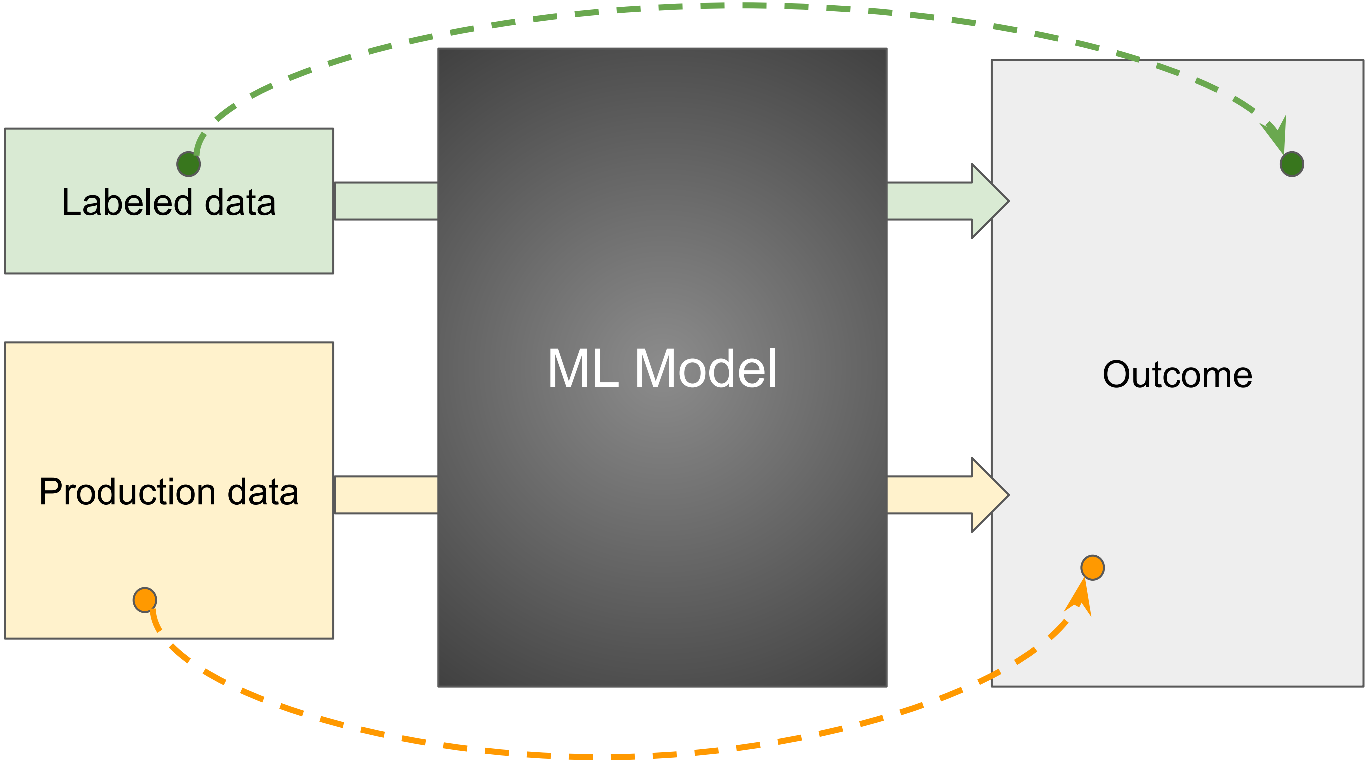
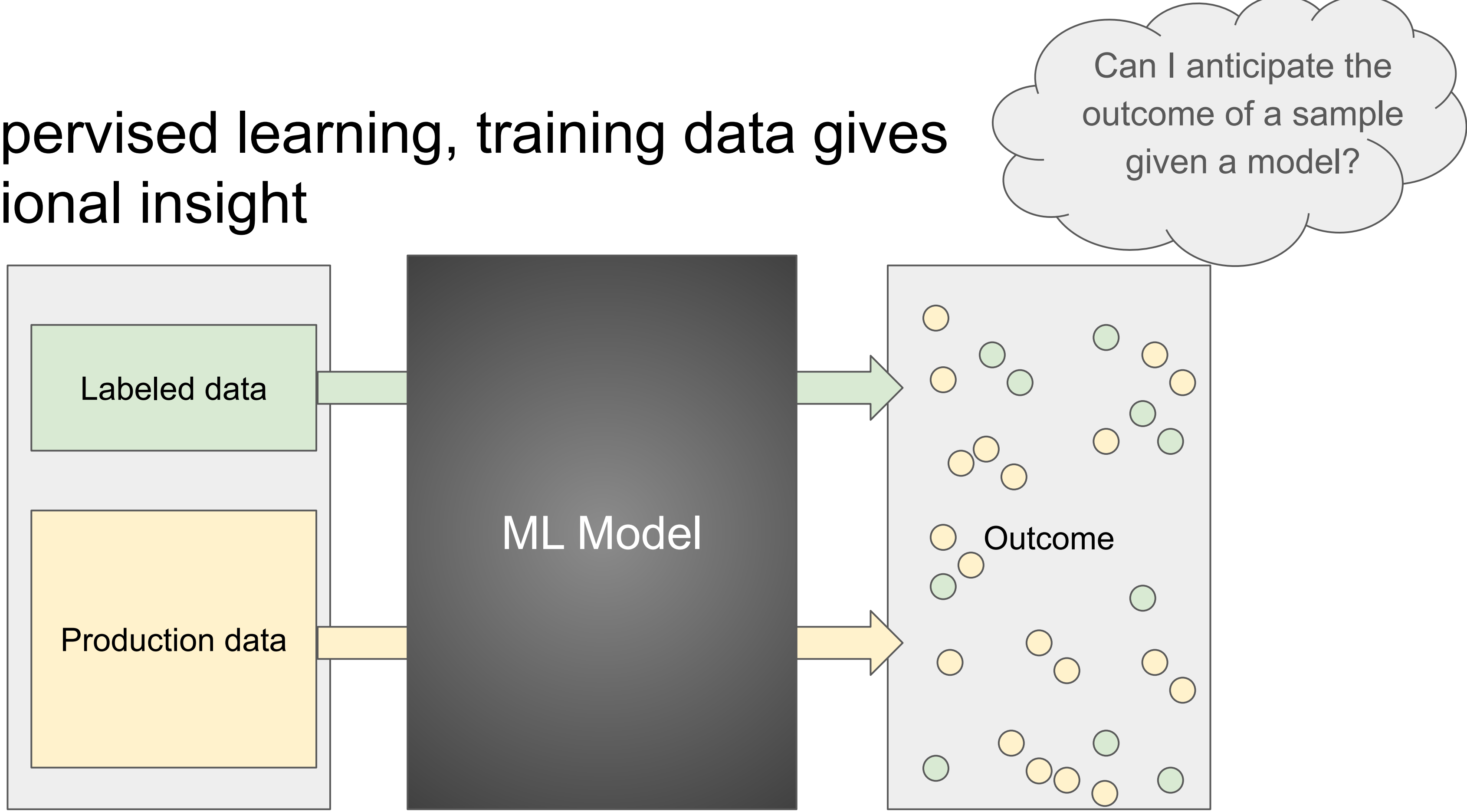


Level 1: Having labeled data

What can a user play with to gain insight/trust?



In supervised learning, training data gives additional insight



Case Study: Visualize mis-labels

Quantitative scores for model

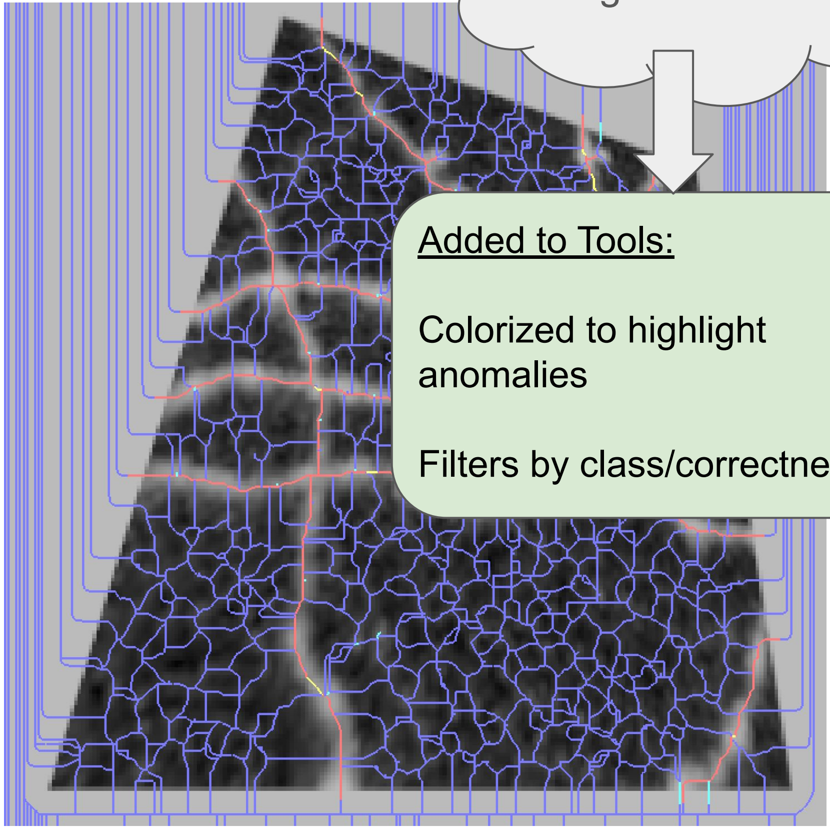
Visualization relies less on context

Have a rapid-labeling tool to produce “ground truth”

<u>Visualization uses:</u>

Color reduces cognitive burden

Simplifies matching



Can I anticipate the outcome of a sample given a model?

<u>Added to Tools:</u>

Colorized to highlight anomalies

Filters by class/correctness

Case Study: Visualize mis-labels

Can I anticipate the outcome of a sample given a model?

Quantitative scores for model

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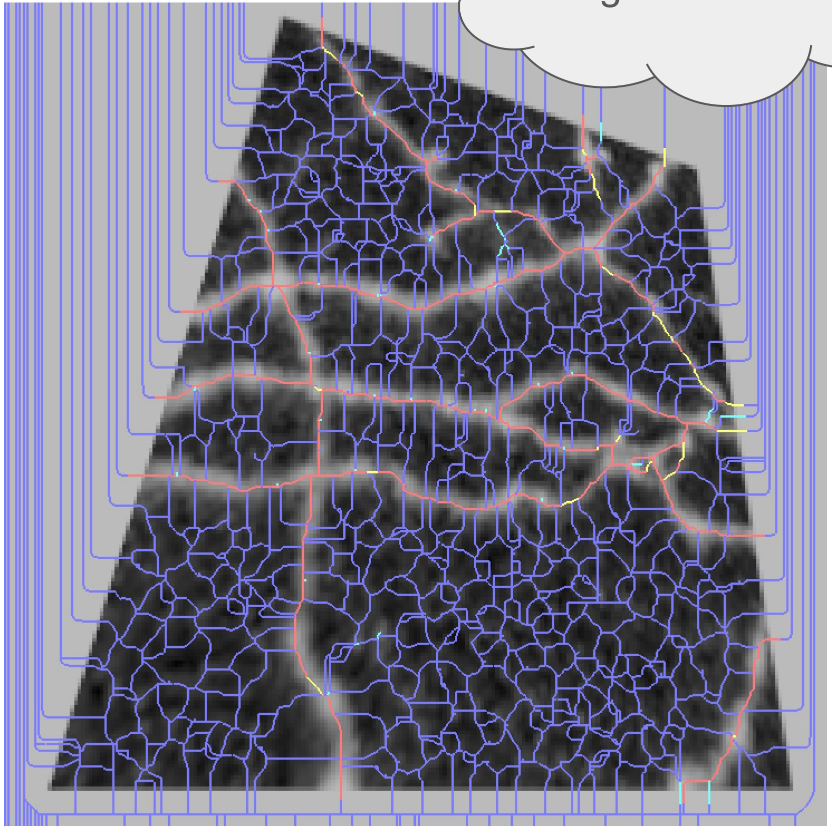

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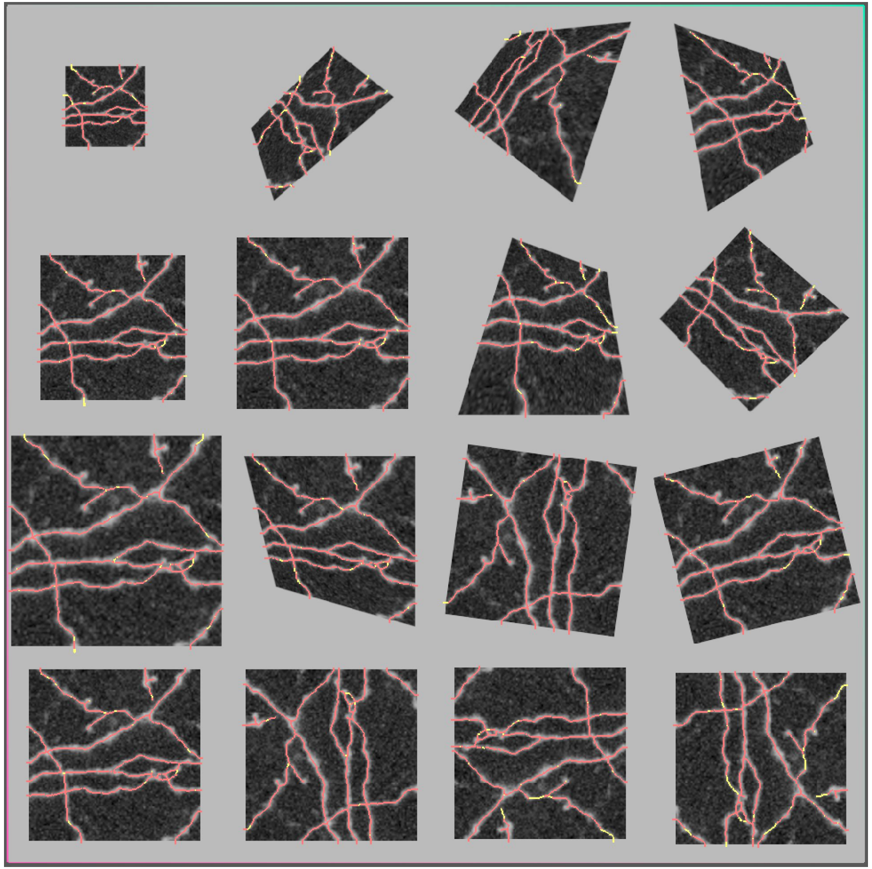


<u>Visualization uses:</u>

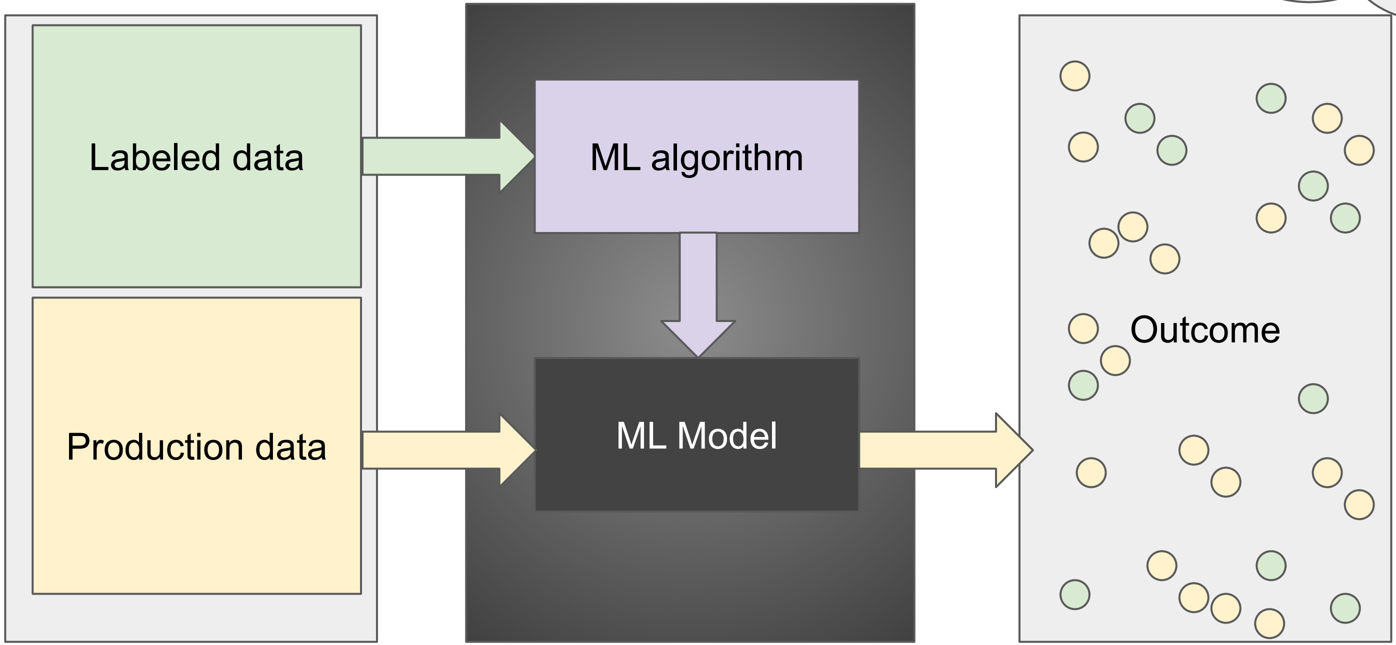
Color reduces cognitive burden

Simplifies matching

Level 2: Allowing re-training model

Training the model with different input sets sheds light on what kinds of samples are needed in training

How stable is the outcome w.r.t perturbation?



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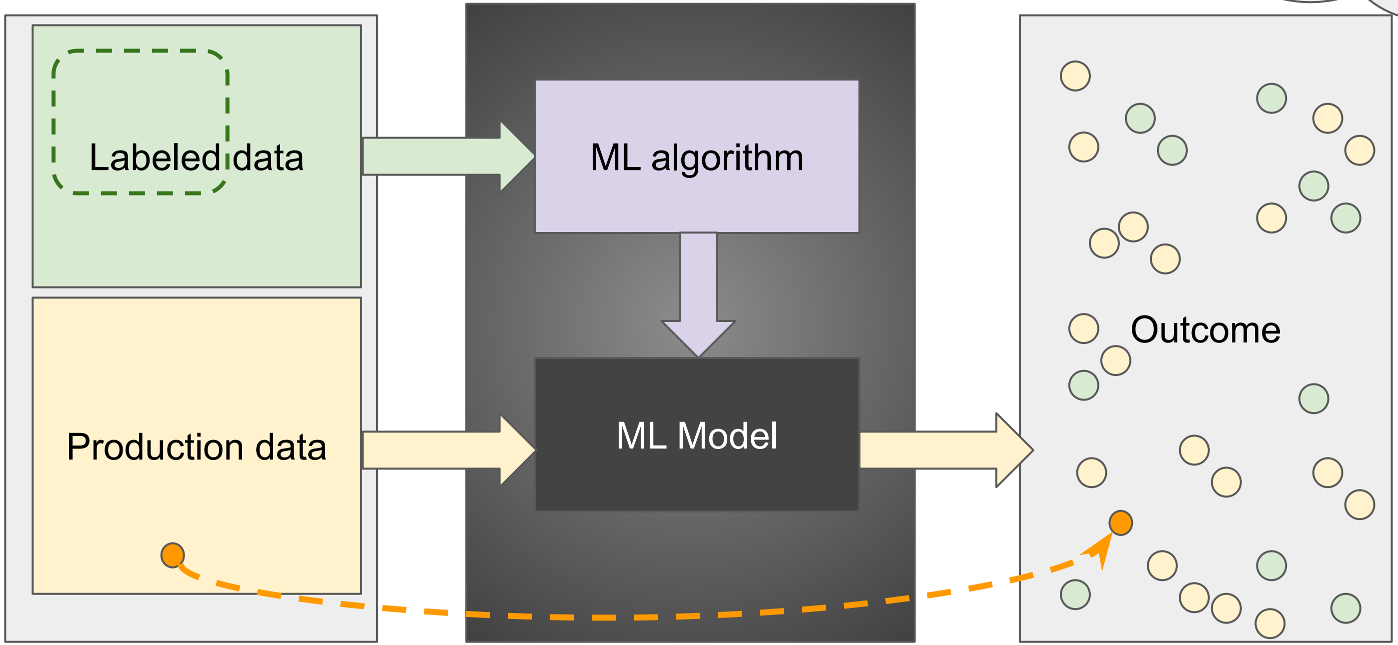

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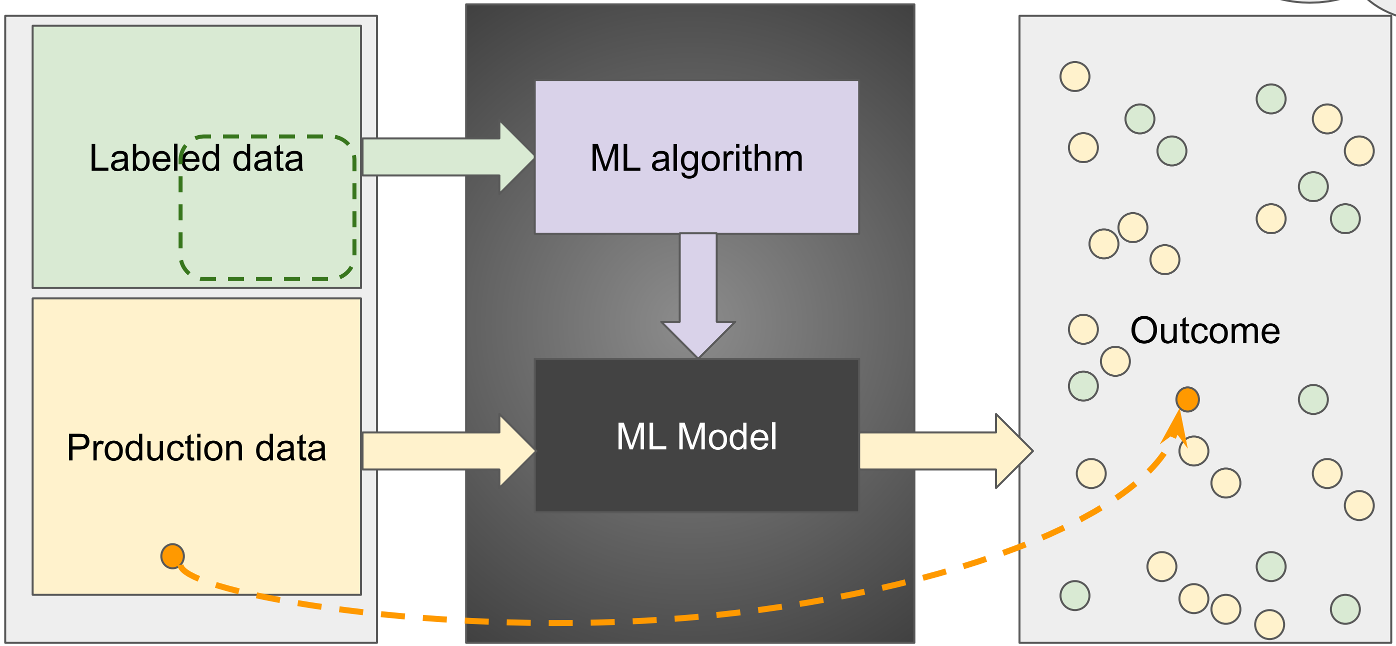
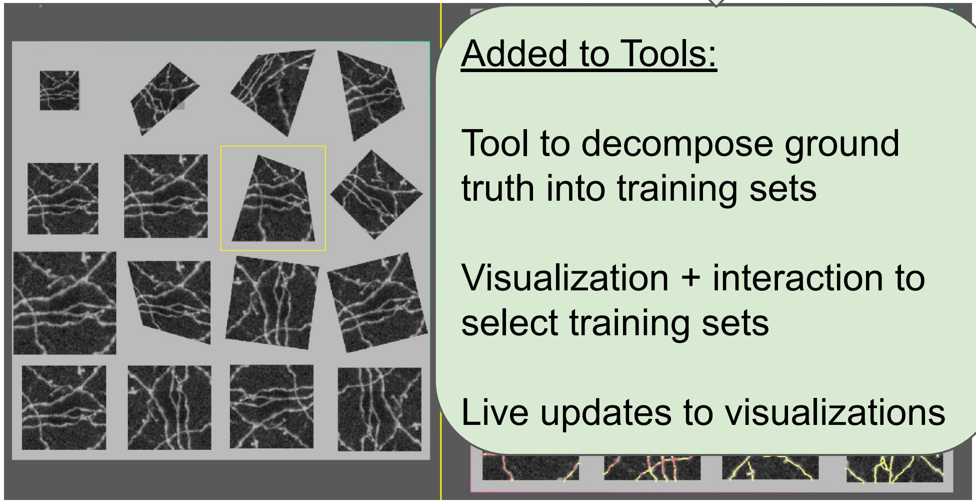


Case Study: Teaching the user what matters in training set

How stable is the outcome w.r.t perturbation?

Fast interactive way of swapping training sets (left)

Interactive visualization of outputs



Added to Tools:

Tool to decompose ground truth into training sets

Visualization + interaction to select training sets

Live updates to visualizations

Visualization relies on:

User interaction in moving over training sets

Live view of results

Case Study: Teaching the user what matters in training set

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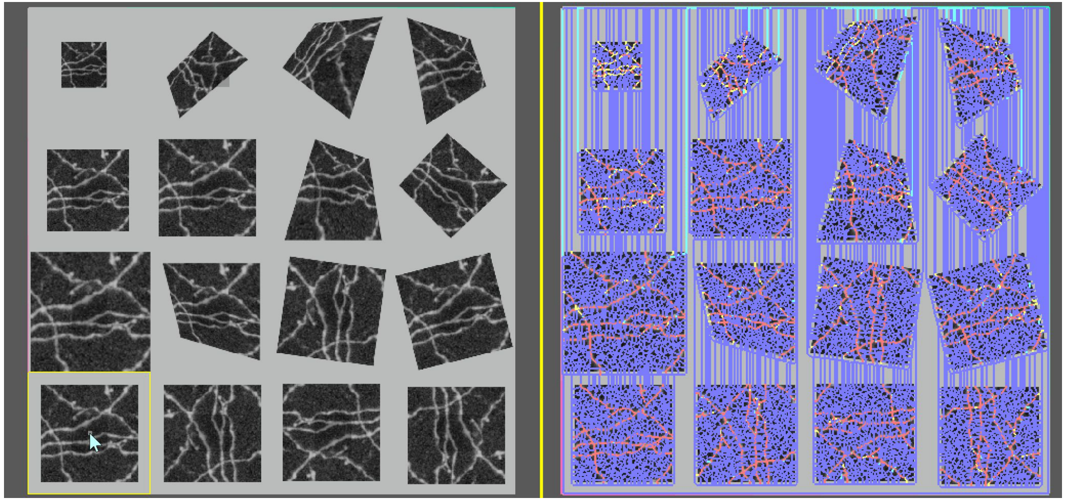

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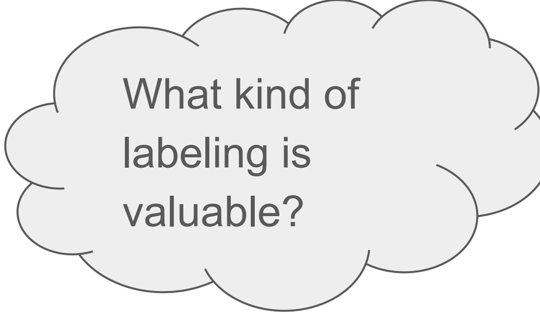

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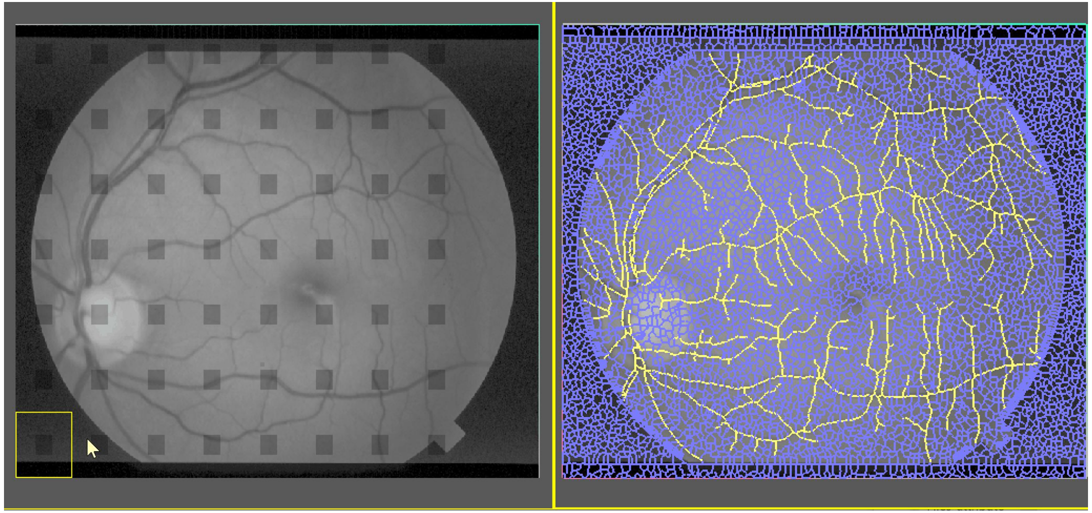


<u>Visualization relies on:</u>

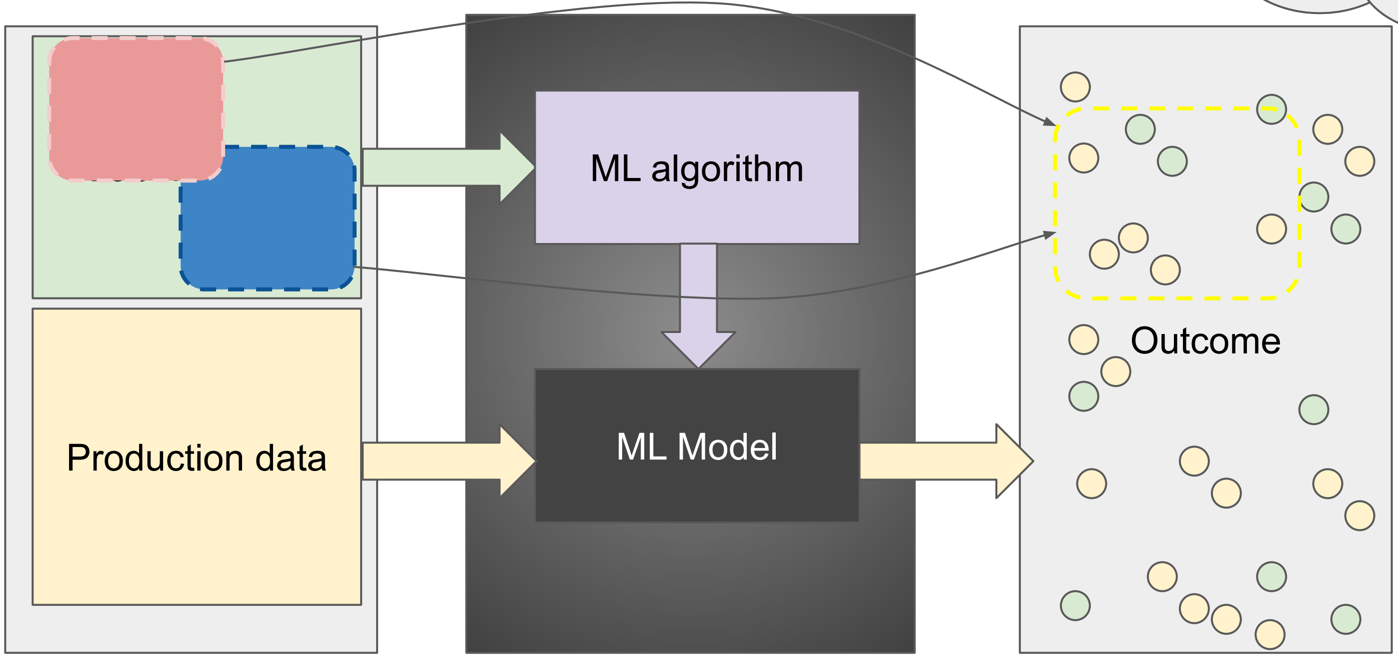
User interaction in moving over training sets

Live view of results

Querying the outcome/samples allows understanding which training gives a better model *for those samples*

How stable is the outcome w.r.t perturbation?

What kind of labeling is valuable?



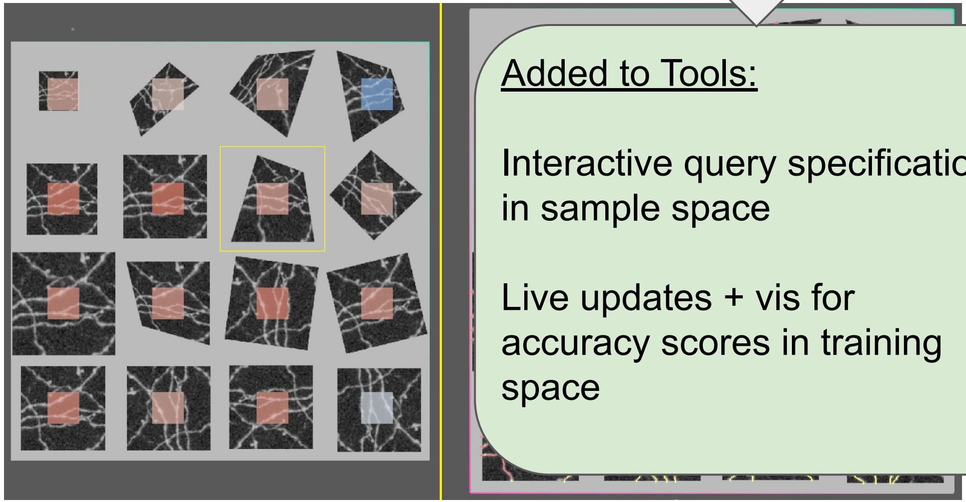
Case Study: Interrogate which training generalizes

Fast interactive way specifying which samples to compute quantitative scores on

Live update for each training region how well it predicts query

How stable is the outcome w.r.t perturbation?

What kind of labeling is valuable?



<u>Added to Tools:</u>

Interactive query specification in sample space

Live updates + vis for accuracy scores in training space

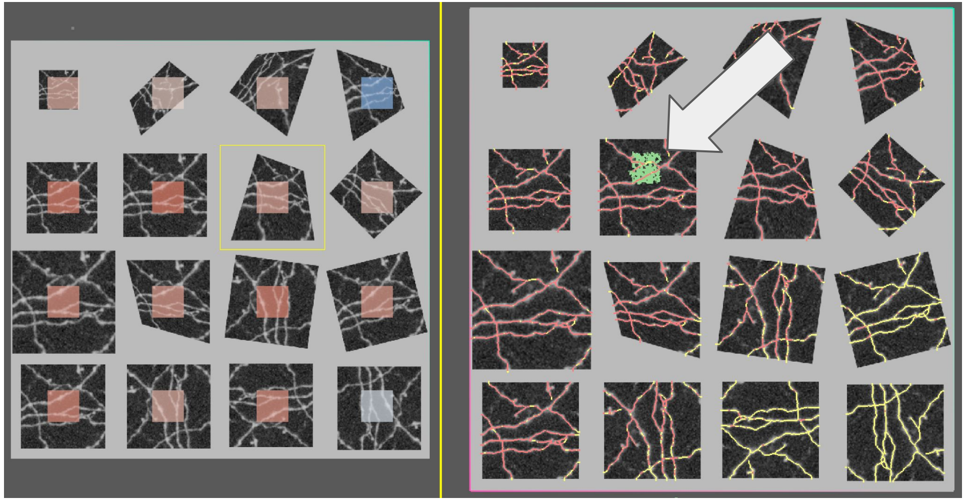
Case Study: Interrogate which training generalizes

How stable is the outcome w.r.t perturbation?

What kind of labeling is valuable?

Fast interactive way specifying which samples to compute quantitative scores on

Live update for each training region how well it predicts query



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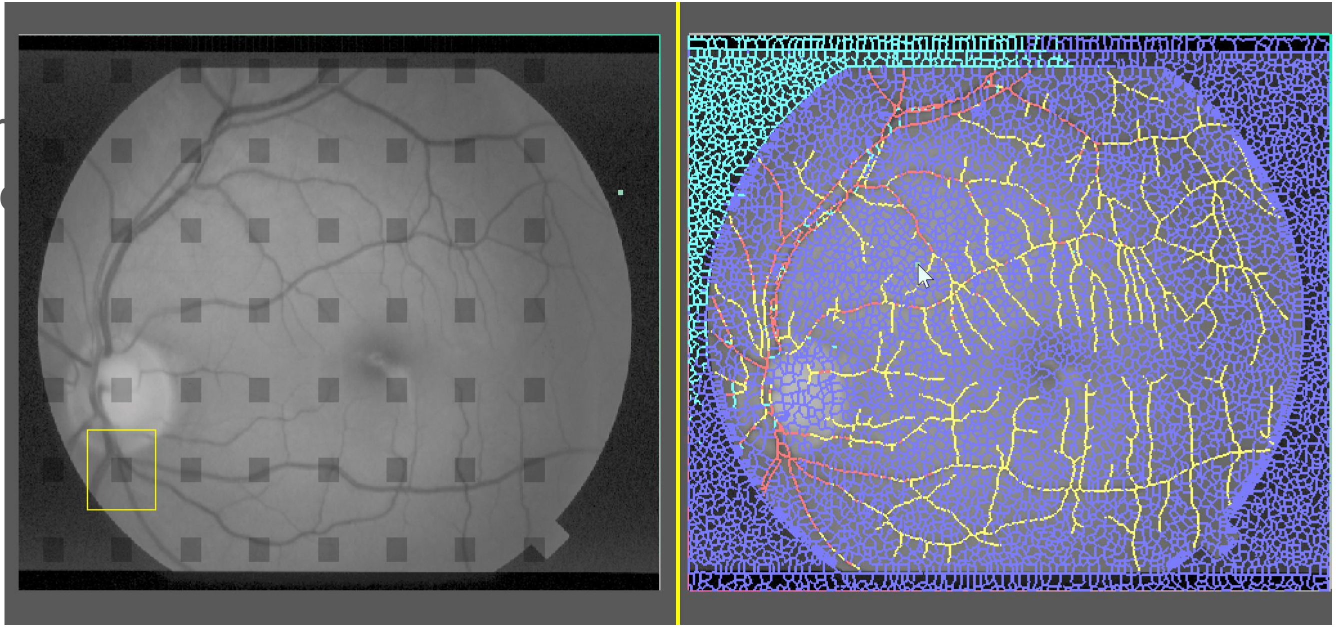
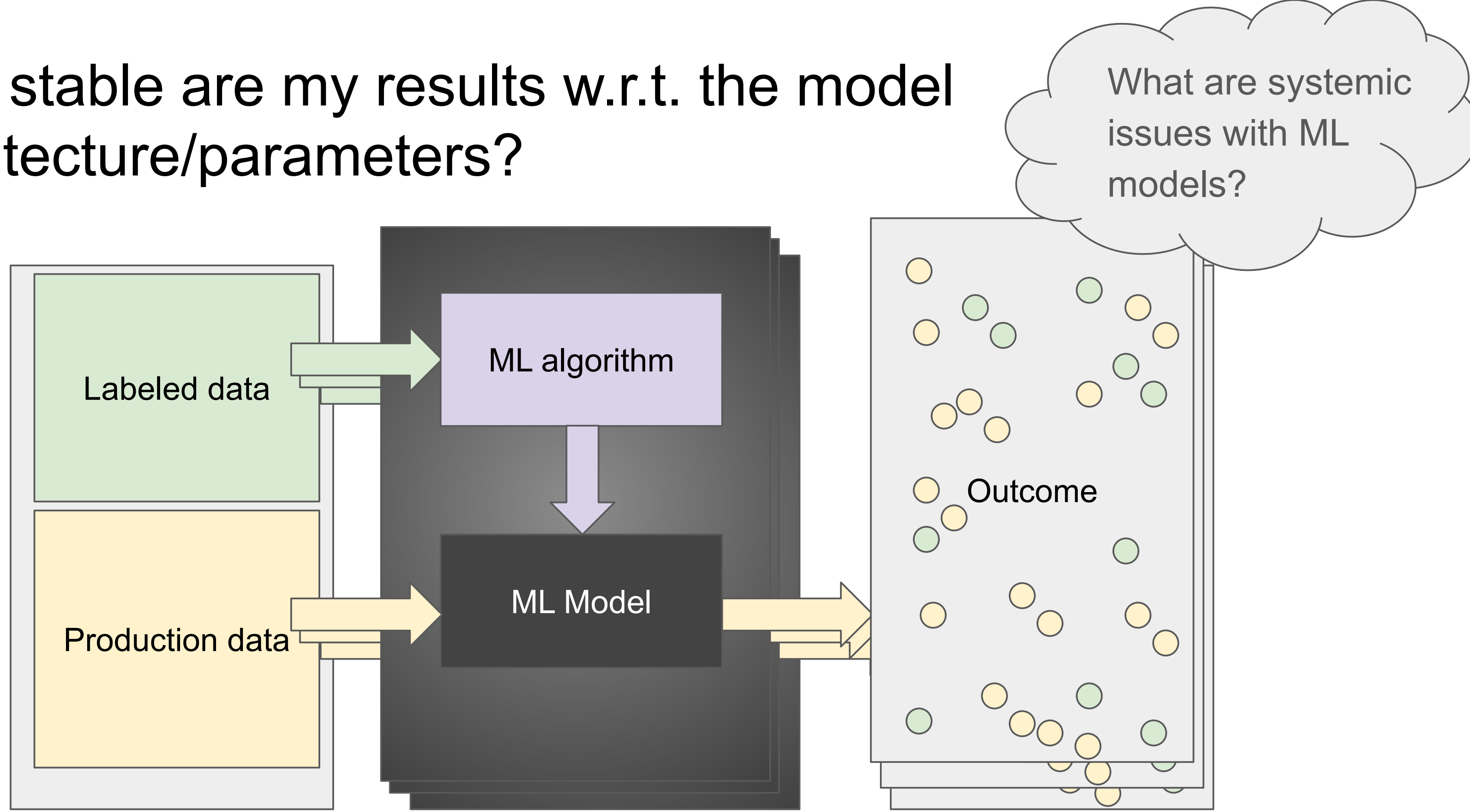


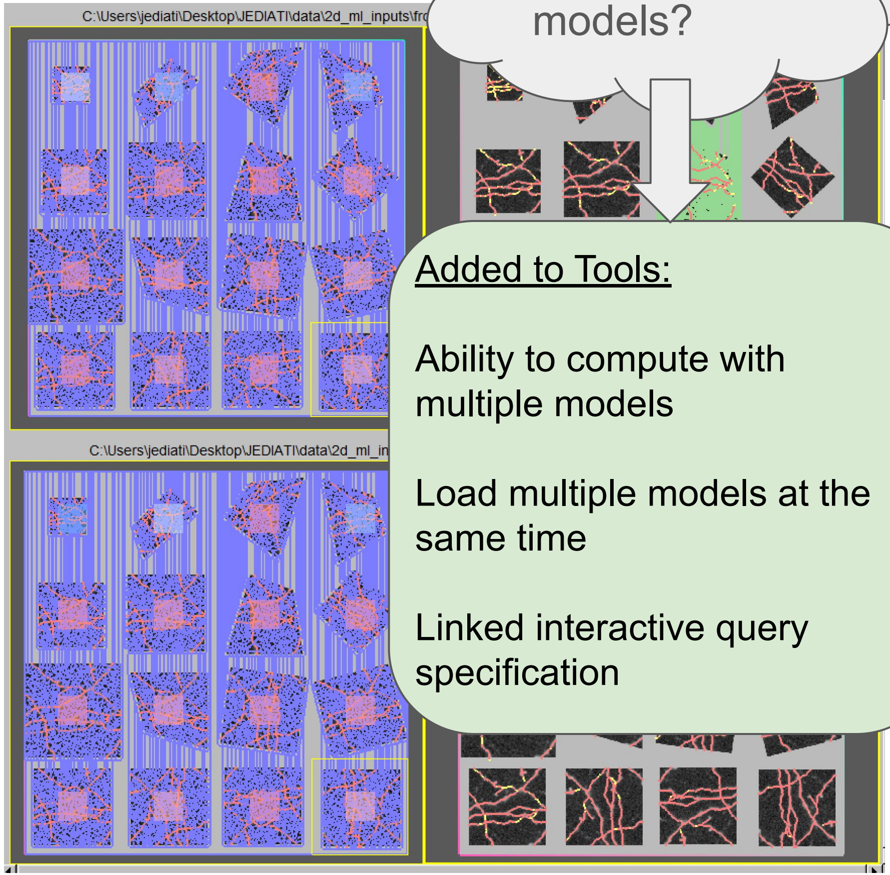
Level 3: Access to multiple/perturbed models

How stable are my results w.r.t. the model architecture/parameters?



Case Study: Live interrogation of multiple models for problem identification or to build trust

- Linked selection of queries
- Linked interaction for visual inspection
- Visual evaluation of sensitivity w.r.t hyperparameter



What are systemic issues with ML models?

<u>Added to Tools:</u>

Ability to compute with multiple models

Load multiple models at the same time

Linked interactive query specification

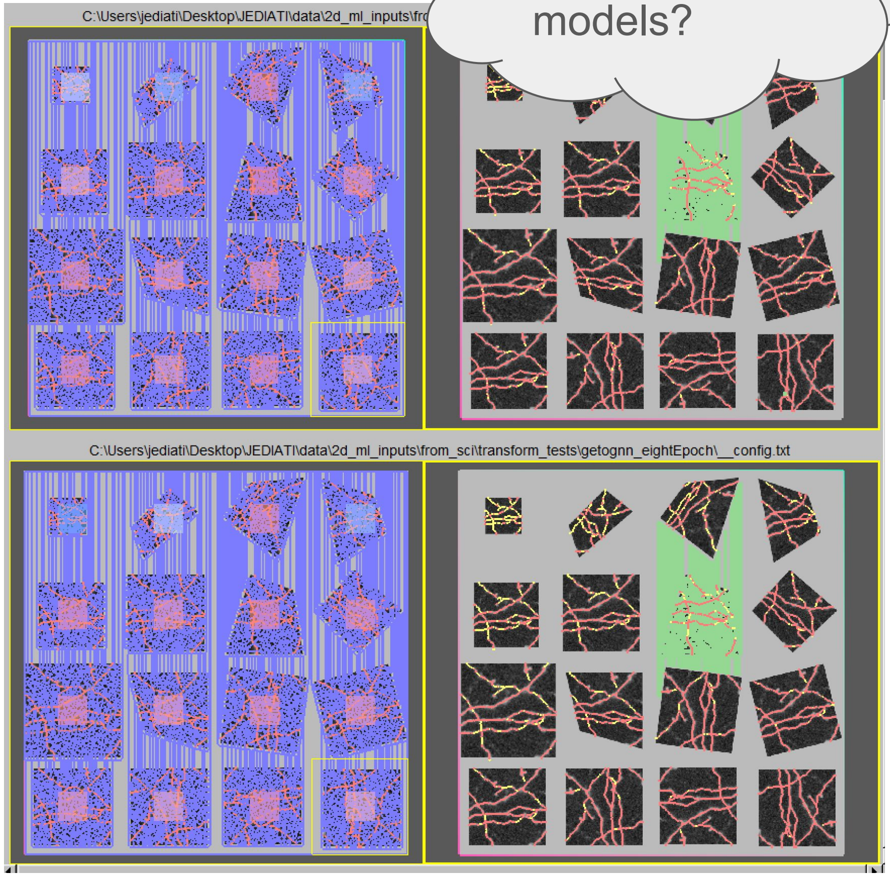
Case Study: Live interrogation of multiple models for problem identification or to build trust

What are systemic issues with ML models?

Linked selection of queries

Linked interaction for visual inspection

Visual evaluation of sensitivity w.r.t hyperparameter



Demos

Project takeaways

Interactive “digging” necessary to explore high-dimensional ML space

Mix of batch and live computation gives interactivity

Domain experts are able to begin intuit and verbalize expectations of models

Domain experts gain a better understanding of how to define phenomena -- and how not to

Analysts get better understanding of processes for success

Developers able to debug and design better models

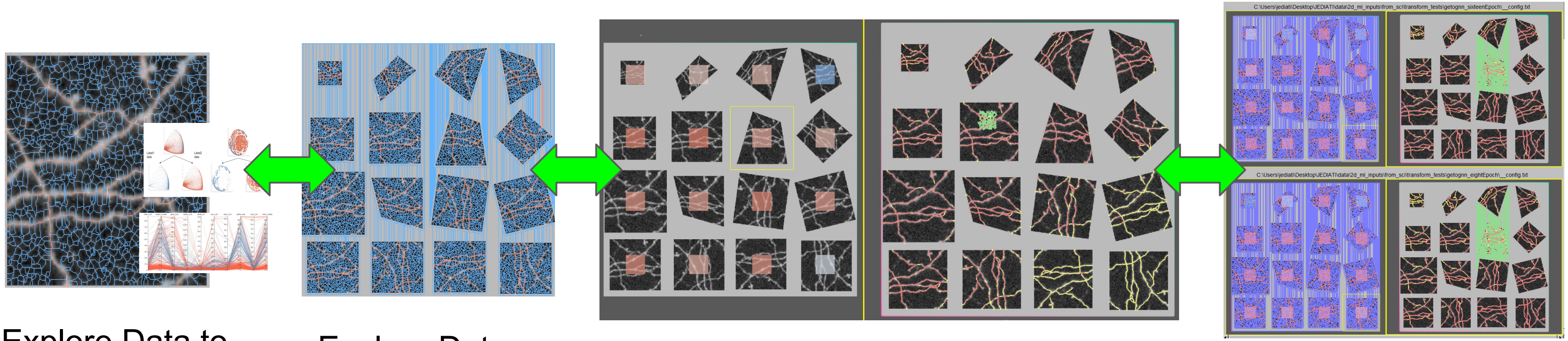
Beginning to generalize development process to list of requirements for explainable AI

Users of all types, can *learn* multiple roles

<u>Domain Expert</u>
Expert in application
Intuition about phenomena
Primary tool users

<u>Expert Analyst</u>
Knowledge in application
Intuition process->outcome
Adapts within tool context

<u>ML Developer</u>
Not expert in application
Intuition about ML Models
Power to adapt tools



Explore Data to Outcome

Explore Data Perturbations

Explore Data + Training Perturbations

Explore Data + Training + System Perturbations

Set of tools to drive explainable ML

Fast ground truth generation tool

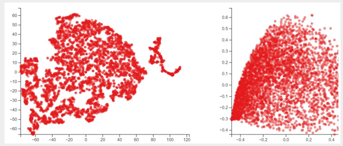
Tool to perturb data

Method to perturb training set

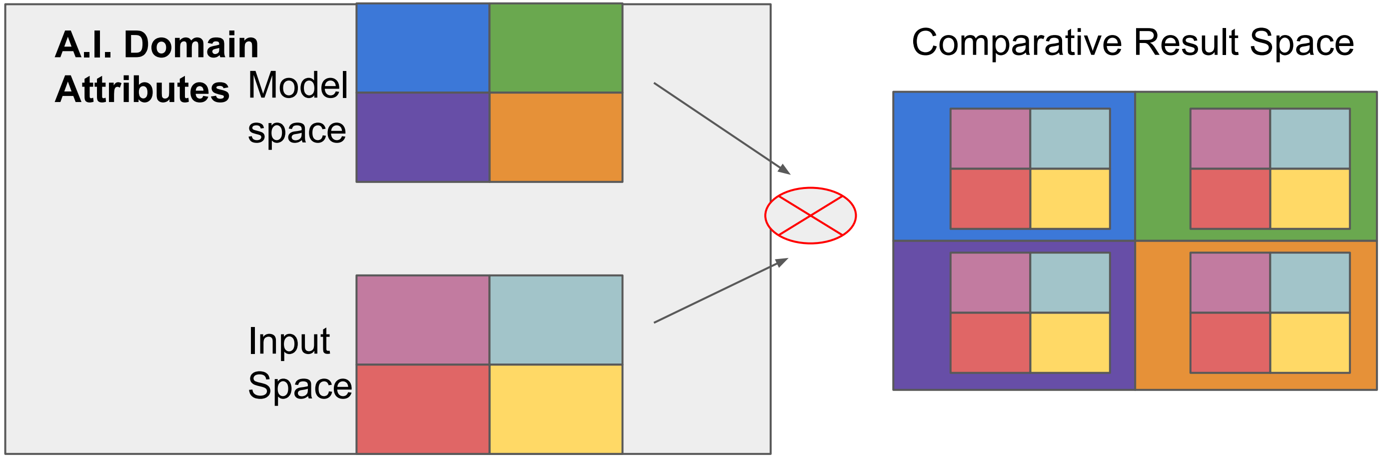
Tool to generate and run perturbed models/architectures

Interactive tool for co-visualization

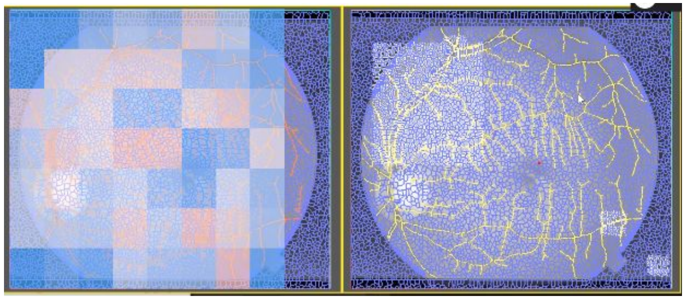
Interactive linked tool for investigation differences in samples



- Ability to navigate a Tensor view of mixed models, mixed training sets, mixed results



- Concurrent visualization of multitudes of scenarios allows us to explore AI behaviour by exploring multiple dimensions of the problem in parallel.



- Fast interactive view of input / model combinations coupled with observed behaviour.

Future directions

Expand on exploratory capabilities

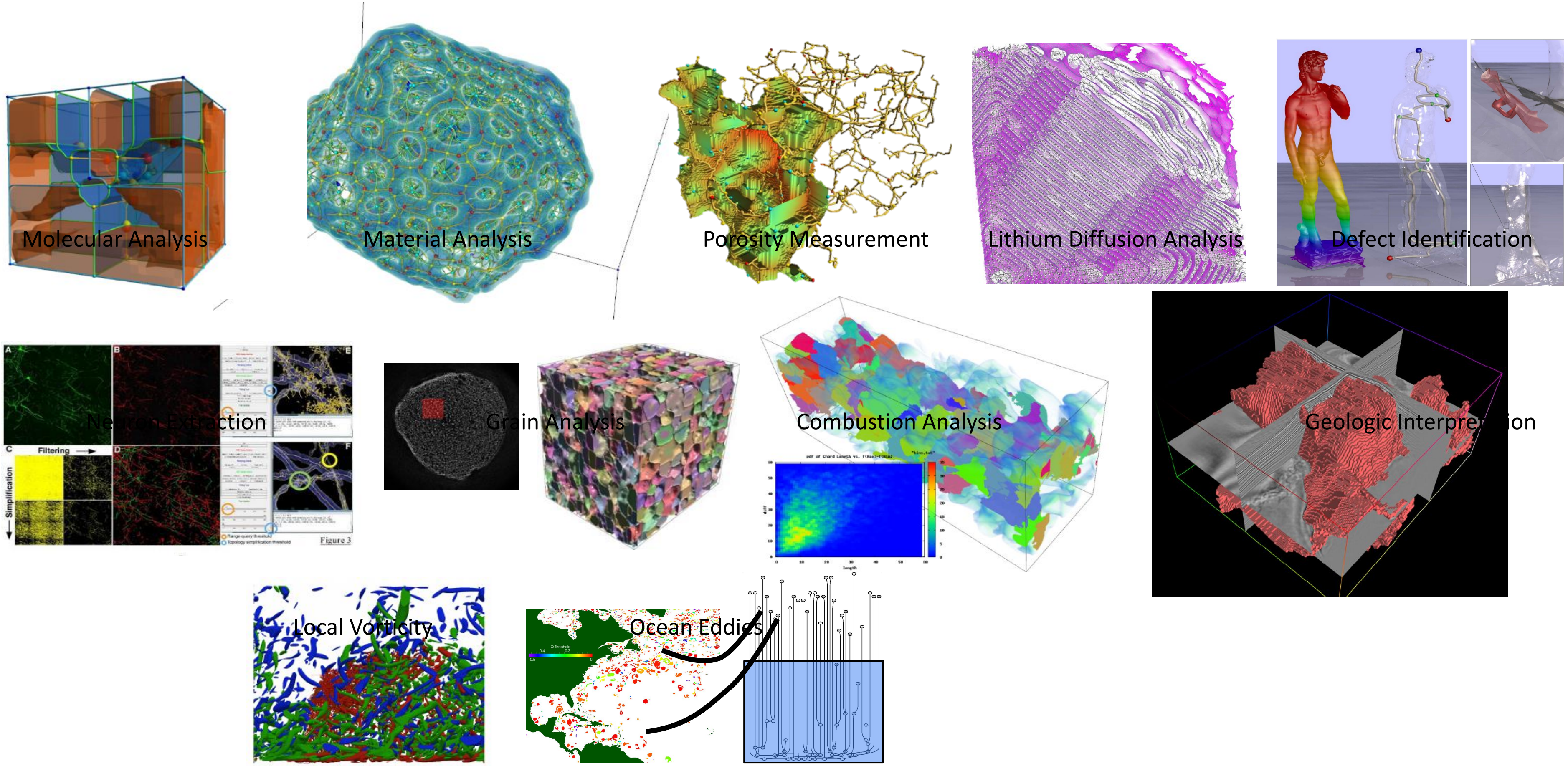
Expand on interface usability, methods of selection

Extend tools in increase scope of what can be varied interactively

Extend to 3d topology

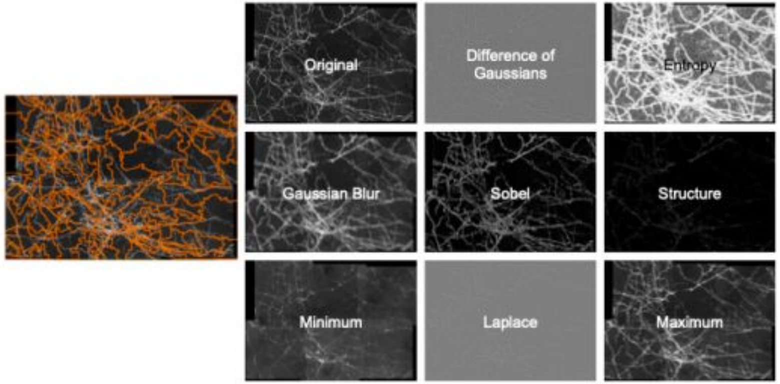
Formalize Explainable AI design patterns

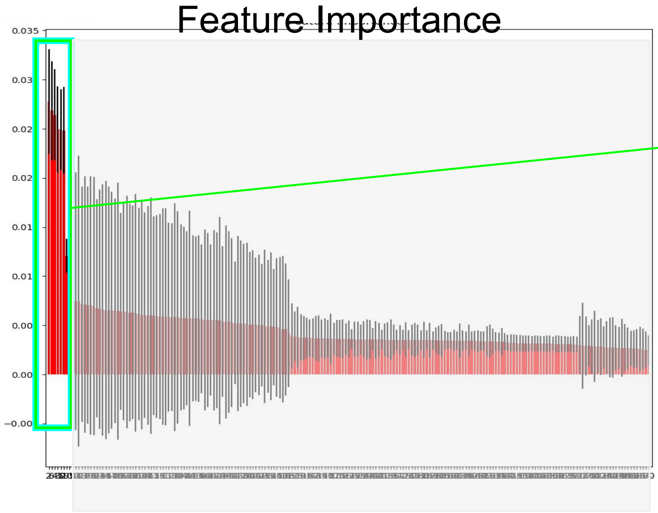
Questions?



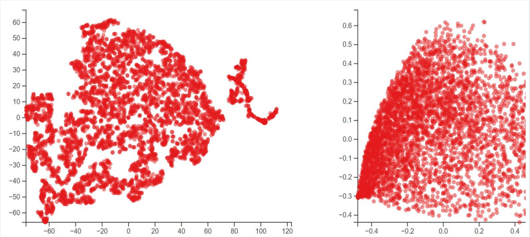
Molecular Analysis
Material Analysis
Porosity Measurement
Lithium Diffusion Analysis
Defect Identification
Filtering
Simplification
Figure 3
Grain Analysis
Combustion Analysis
Geologic Interpre
Local Vorticity
Ocean Eddies

Interactively understand role of features in model behavior





Interactive tool to investigate various impacting features to see how they influence the model or commonalities in the feature space between models



Investigation Meta Goals

Generalize development process to list of requirements for explainable AI

Ability to answer questions depends on how deep a user goes

Level 1: end user

- Perturb the sample - does prediction change?
- Visualization mapping outcome to samples

Level 2: ability to train model

- Perturb training samples
- Visualization mapping outcomes to perturbations of training samples

Challenges

Brand new data representation = no existing labeled data

We don’t know what ML architecture to use

Want to apply to wide variety of applications

Setting the stage...

In many applications, topological features encode phenomena of interest

In practical imaged data, however, while a human eye is good at identifying foreground/background, model-based decisions reach diminishing returns

Can ML help?

Overlay of geometric graph for training and prediction