Sensitivity Analysis for Dimensionality Reduction in Agent-Based Modeling

Bianca Granato and Nicole Y.K. Li-Jessen
McGill University, Montreal, Canada

McGill
Quantitative Life Sciences | Sciences quantitatives du vivant

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Thank you!

Nicole Li-Jessen

Patrick, Mika, Christian, Lisa, Grace, Chelsea

Key Definitions

- **Agent-Based Model (ABM)**
  - Numerical simulation of dynamical systems
  - Multiple, independent entities = **Agents**
  - Non-linear individual- or group-level responses
  - Emergent behaviour from local interactions
  - Agents act according to equations or conditional statements = **Rules**
  - Virtual world landscape and boundary = **Environment**

Key Definitions

- **Uncertainty Analysis**
  - Estimates output variance and confidence bounds
- **Sensitivity Analysis**
  - Systematically change each parameter's value to estimate their contribution to output variance
  - Can improve agreement with data, reduce computational cost for calibration and verification, and suggest causal mechanisms
  - Local vs. global sensitivity analysis
  - Model-free methods vs. model-based methods

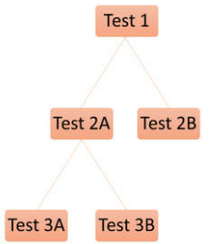
ABM in biomedicine: challenges

- **Challenges**
  - Lack of training examples and/or incomplete data sets
  - Hundreds of parameters, many with **unknown values**
  - Many systems with non-convex solutions
  - Computationally expensive to evaluate
    - Sensitivity Analysis, Calibration, Verification…
- **Machine Learning for Sensitivity Analysis**
  - Reduce number of parameters before Calibration and Verification

Random Forests

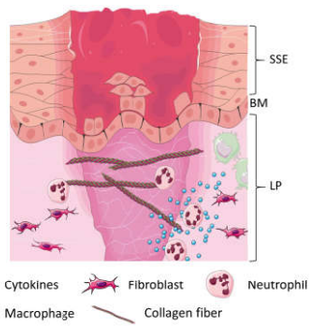
- Ensemble of decision trees applied to random subsets of data through bootstrapping, then aggregated
- For each decision tree:
  - Randomly select data points
  - Randomly select subset of features
  - For a given node in a tree, split if the score of daughter nodes are better than mother node's

  E.g. information gain or lower Gini index



Highlight paper: Garg et al. (2019)

- **System modeled:** vocal folds, the voice organ in the throat
- **Problem of interest:** predicting risk of vocal fold scarring after surgery



Response to tissue damage in the superficial layers of the vocal folds, which is composed of the stratified squamous epithelium (SSE), basement membrane (BM), and lamina propria (LP).

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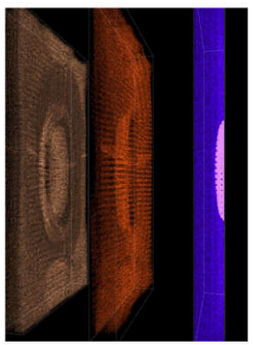
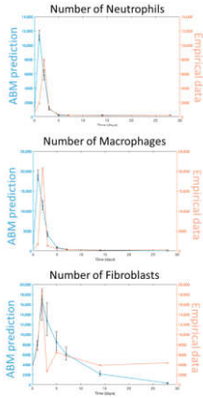
- **Simulation:** tissue regeneration response over 4 weeks
- **Model inputs:** initial wound size
- **Model outputs:** number of fibroblasts, neutrophils and macrophages



Screenshot of model output. Distribution of macrophages (brown, left), neutrophils (red, centre), fibroblasts (blue, right), and tissue damage (pink, right area). Image adapted from Seekhao, N. et al. (2018). doi:10.3389/fphys.2018.00304

Highlight paper: Garg et al. (2019)

- **Sensitivity Analysis:** *RandomForest* (R package) with 5,000 iterations and 213 input parameters
- **Dimensionality Reduction:** top 3 parameters with highest mean GINI impurity decrease for the first 4 time points = 24 parameters remained



Empirical (right axis, red) and simulated (left axis, blue) population trajectory of neutrophils (top), macrophages (middle) and fibroblasts (bottom). Y-axis represents time in days. Image adapted from Garg, A. et al. (2019). doi: 10.3390/app9152974