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AdaLab - 2018

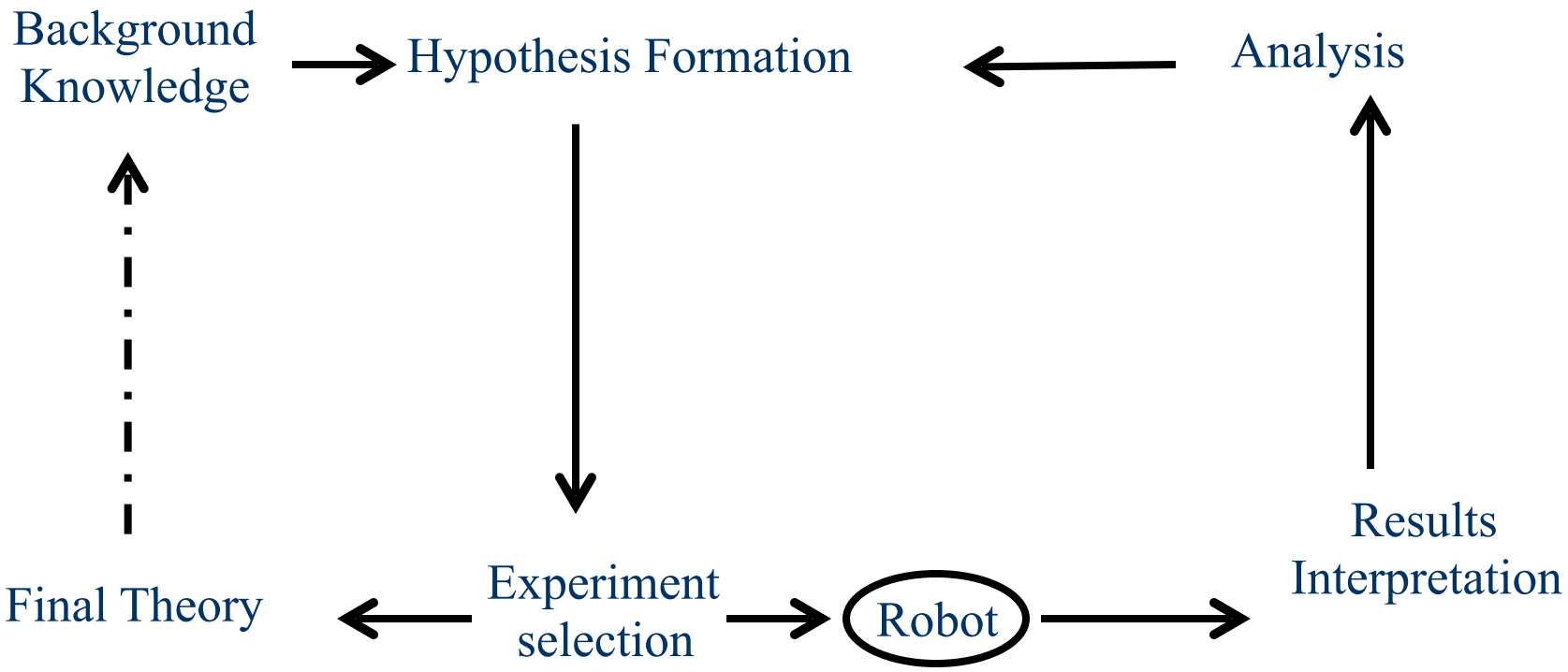
AdaLab

Aims

- To develop a framework for semi-automated and automated knowledge discovery by teams of human and robot scientists.
- This collaborations will produce scientific knowledge more efficiently than either could alone.
- To make scientific research more efficient: cheaper, faster, better.

The Concept of a Robot Scientist

Computer systems capable of originating their own experiments, physically executing them, interpreting the results, and then repeating the cycle.

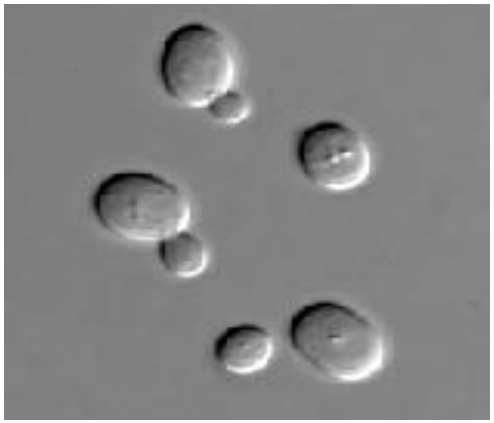


Eve: Robot Scientist

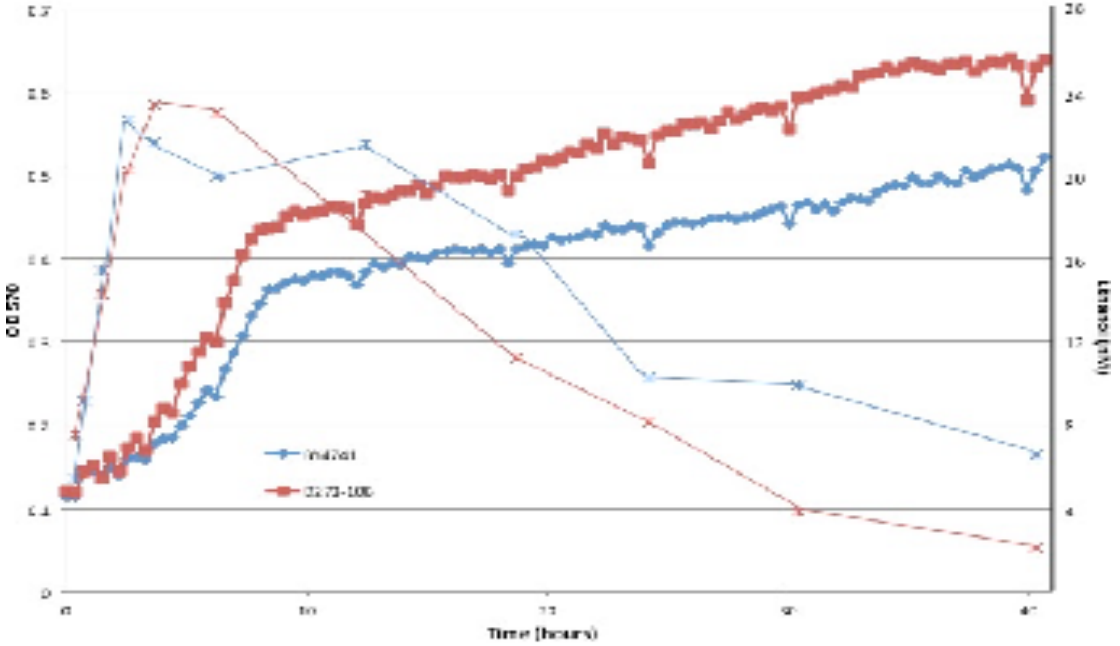
Application area: the diauxic shift

- Yeast (*S. cerevisiae*).
- Transition between growth phases:

1) turn glucose into ethanol.
2) turn ethanol into CO_2.



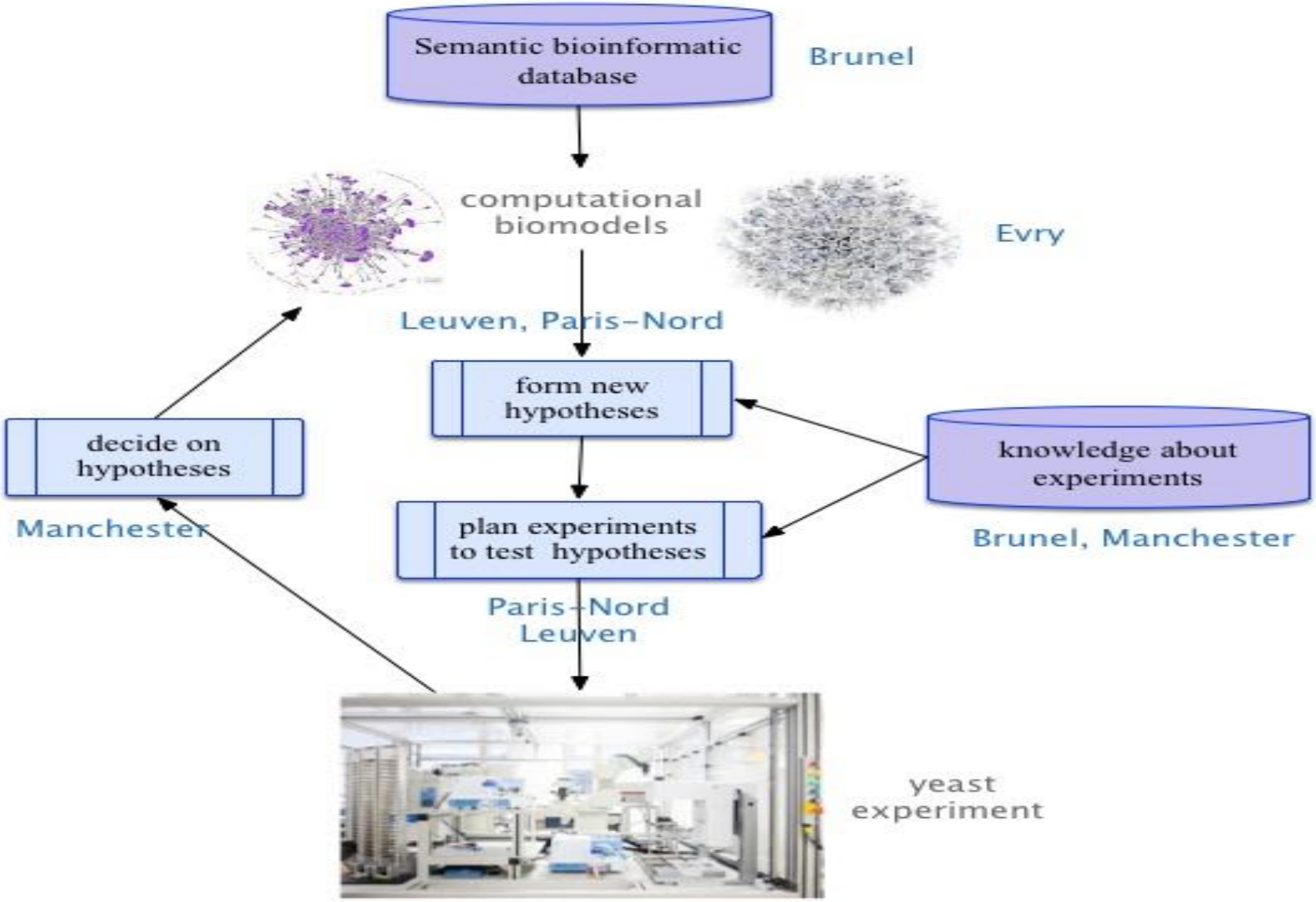
- Cancer
- Ageing



Key Challenges

- Scientific knowledge is inherently uncertain.
- Within the AdaLab framework we are developing Bayesian methods that make inferences and plan experiments under uncertainty. We developed an ontology for representing uncertain knowledge.
- Systems biology deals with extremely complex phenomenas, and integrates computational modelling, experimentation, and biological interpretation.
- AdaLab, as an AI system, is designed to automate such cycles of investigations.

AdaLab partners & structure



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AdaLab

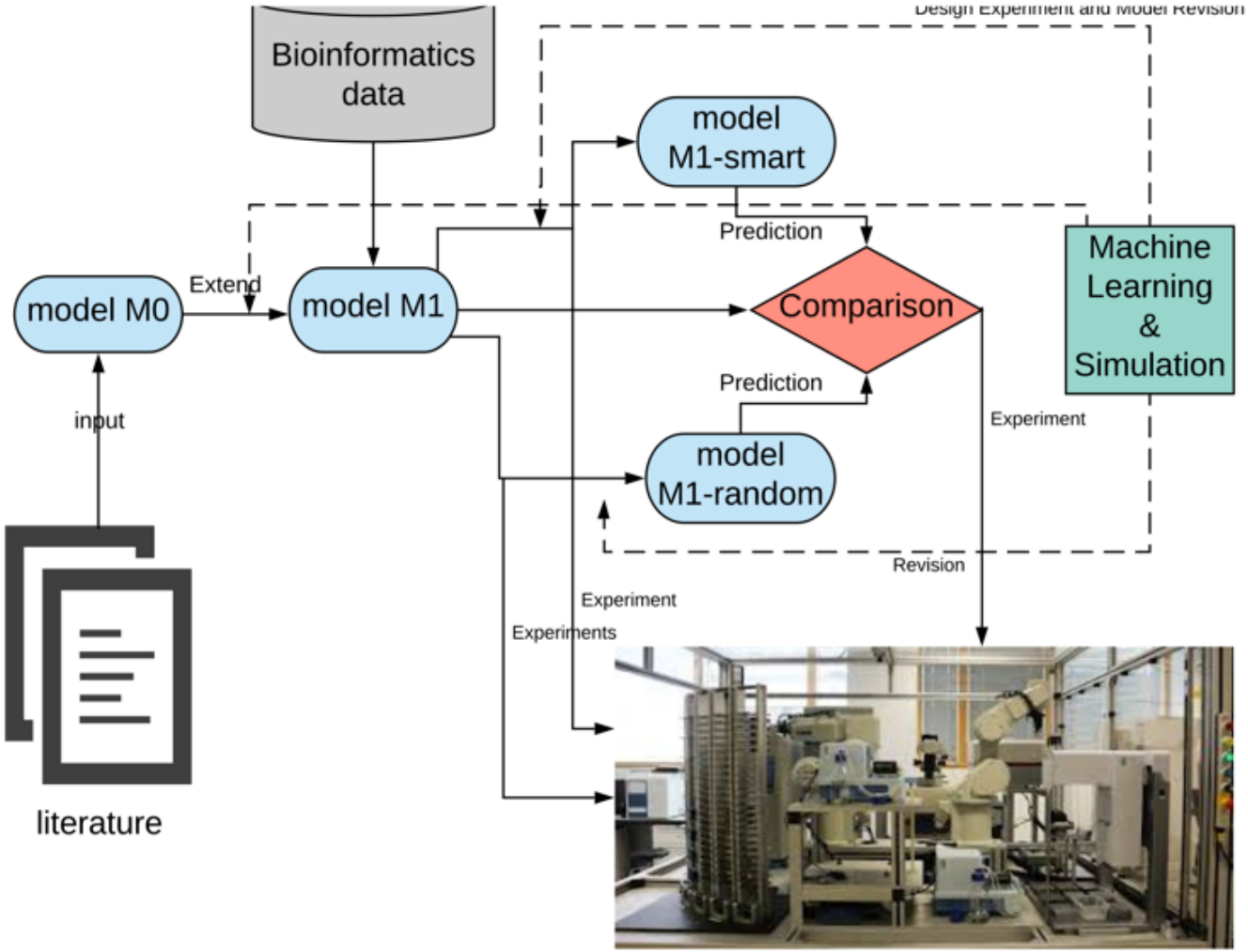
Partners

- Brunel University London (UK): Coordination, knowledge representation, a communication mechanism between robot and human scientists.
- The University of Manchester (UK): Scientific leadership, Eve experimentation, the application.
- KULeuven (Belgium): Machine learning (ILP), probabilistic inference.
- Universite Paris-Nord: Machine learning (active learning), cost minimisation, model revisions
- Universite Evry: bioinformatics and systems biology (development of an integrated metabolic and gene signalling network).

Key Outputs

- Integration of the components for learning, simulation, revision and experimental design into an adaptive laboratory system Adalab.
- Application of AdaLab to improve diauxic shift models: high reduction of prediction error (30% - 75%)

Summary


Design Experiment and Model Revision
Bioinformatics data
model M1-smart
Prediction
Machine Learning & Simulation
model M0
Extend
model M1
Comparison
Prediction
input
Experiment
model M1-random
Revision
Experiment
Experiments
literature
wet lab results

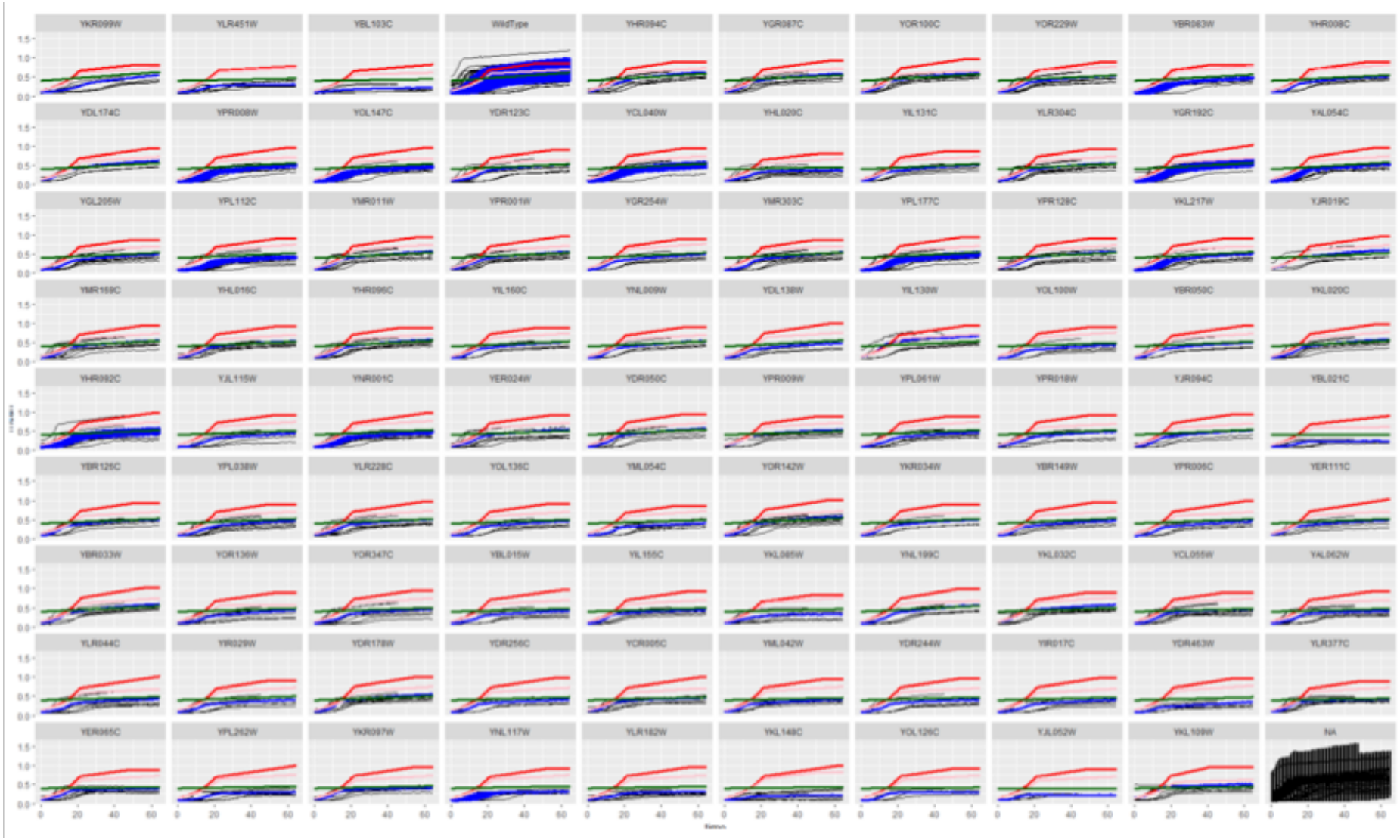
Model revisions: M0-M1

- **M0:** the best existing model - Zimmer model (from hundreds of articles).
- **M1:** is built using an in-house ensemble network inference method, using M0 as prior model, and focusing on subset of genes for extension as the top ones in CoRegNet rankings; + bioinformatics database.
- **Improvements:** The network inference produces many new links that we filter using cross validation on Brauer dataset. **M1 outperforms M0.**

Model revisions: M1 - M smart

- **M1** is considered as a Hypothesis to devise experiments to improve the model. Experiment selection taking into account inconsistencies between various kinds of simulated gene expression (forward /backward) has been implemented.
- Revision from 80 carefully selected experiments
- **Improvements:** M1-smart outperforms M1

Model revisions: M1 - M smart



Model revisions: M1 - M random

- **M1-rand:** a revision of M1 using high-throughput experiments. A random set of 80 genes was selected to identify strains to experiment with.
- Selected 40 experiments for which M1 random and M1 smart disagree most, on these:
- **Improvements:** M1-rand outperforms M1; M1-smart outperforms M1-rand

Next Steps

- **WP2:** Produce a final version of the knowledge representation of the application domain.
- **WP3:** Finalise works on the integrated AdaLab framework and the application.
- **WP4:** Improve the revision and experiment design strategies and to evaluate and validate the learning results with real experiments
- **Overall:** to make all the Adalab components work better together

Dissemination

- Public Engagement
  - London Science Museum Event
  - Interview for Belgian television channel
- Dissemination to non-specialist audiences
  - Project Website and promotional literature
  - Newsletters
  - Public lectures and seminars (e.g. Pint of Science; Pendle Science café; Summer School of Science)
- Dissemination via specialist media
  - Presentations (44 given to date)
  - Journal publications (7 generated to date)
- **International AdaLab Workshop in June 12, 2018 in the Royal Society, London.**

Thanks