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The XM Tool Project:

The use of non-linear statistical models for Air Quality Forecasting

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XM Tool Project

Mandate:

- Develop and evaluate new non-linear tools for post-processing of air quality forecasts of O₃, NO₂, and PM_{2.5}

Purpose:

- Supports AQHI forecast program

Key Objectives:

- Improved guidance for air quality episodes.
- Improve timing of air quality episodes.
- Improve overall model forecast skill.

List of Predictors

Predictors

84 AQ Model Predictors

3 **Persistence Predictors**

27 **Antecedent Predictors**

Persistence Predictors

OBS at Hr 00

Antecedent Predictors

Lag 24/48/72 hrs

Max

Min

OBS

AQ Model Predictor types

- Meteorological Variables
- Sine Julian Day
- Day of the week
- NO2, O3, PM2.5
- Spatial Average, Min, Max

6 AQ Sites Tested

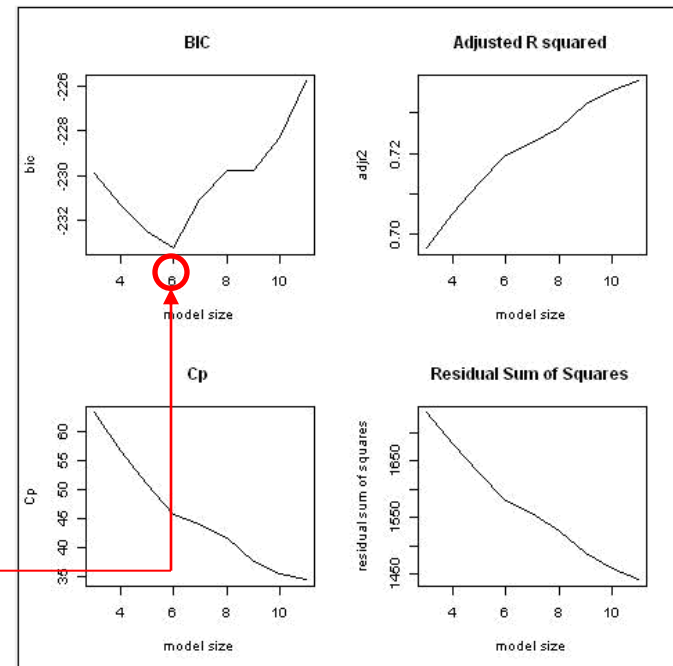
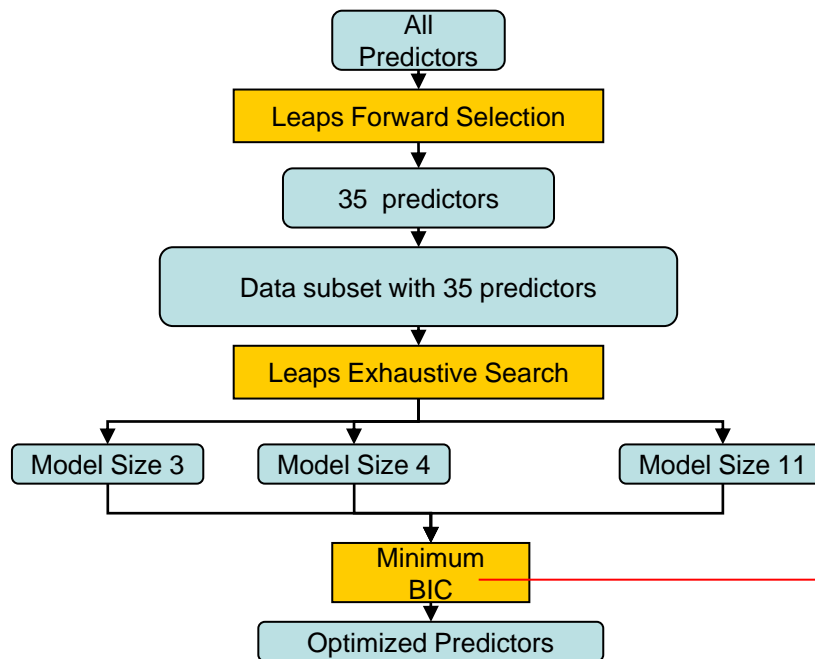
- Halifax
- Montreal
- Toronto
- Winnipeg
- Edmonton
- Vancouver

MLR approaches

	UMOS-AQ	XM version
<i>Technique</i>	MLR	MLR
<i>Predictors</i>	AQ model + Persistence	AQ model + Persistence and/or Antecedents
<i>Predictor Selection</i>	Forward Stepwise Regression	Leaps Minimum BIC (Ken Lau)
<i>Seasonality</i>	2 season	1 season
<i>QA/QC</i>	Min, Max, rate	Min, Max, rate
<i>Minimum cases</i>	250	250
<i>Updatable</i>	Yes	Not yet

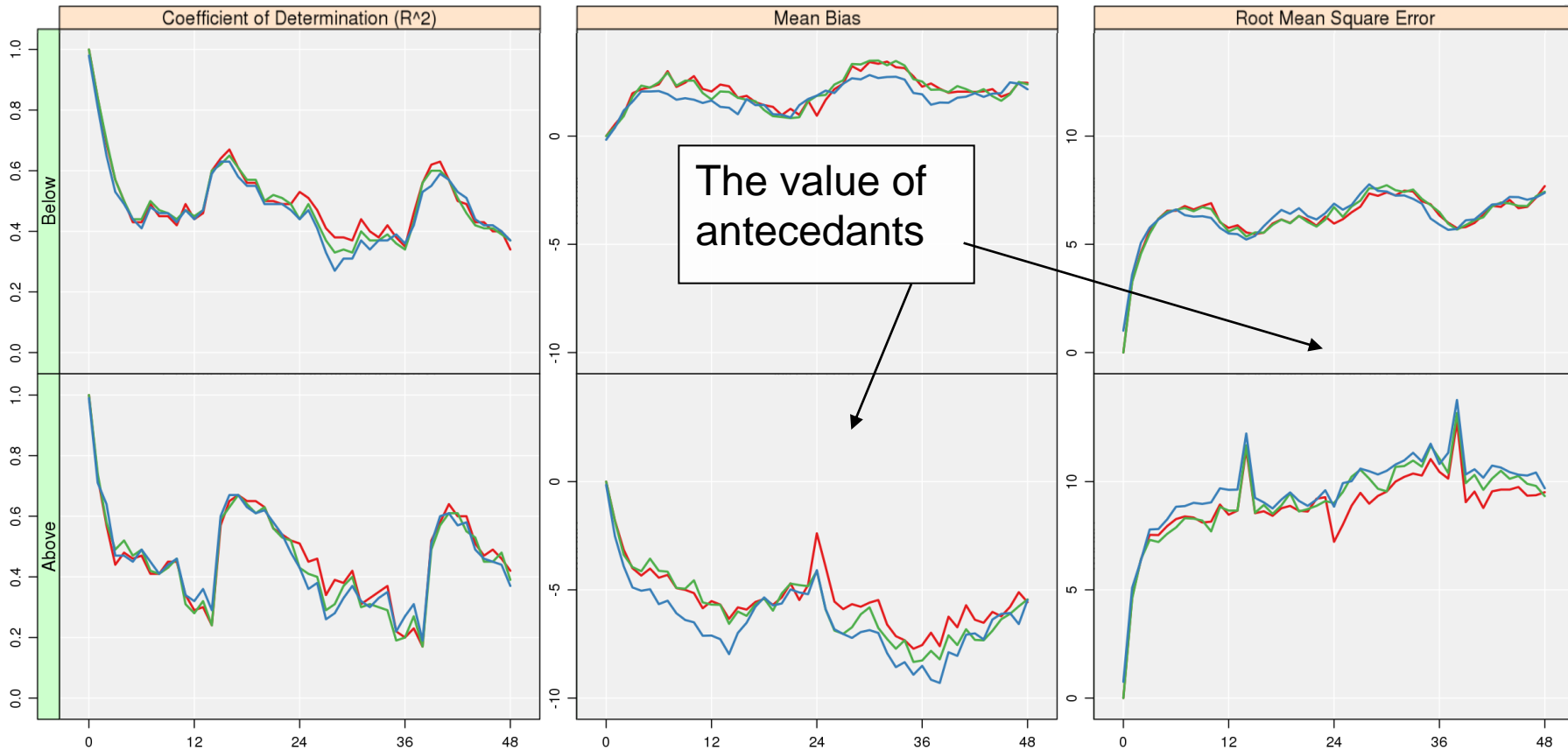
Flow Diagram for Leaps BIC Selection

- Leaps Package in R Statistical programming language
- Use combination of Forward and Exhaustive Search



MLR for O3: Persistence + Antecedents

Statistics TEST Set
All Season GEM15 Hourly Forecast of O3 for 75% Quantile
Station Combine
MLR w/ Pers+Ante — MLR w/ Pers — UMOs-AQ —



Forecast Hour
Test data from May 30, 2011 to Oct 28th, 2011
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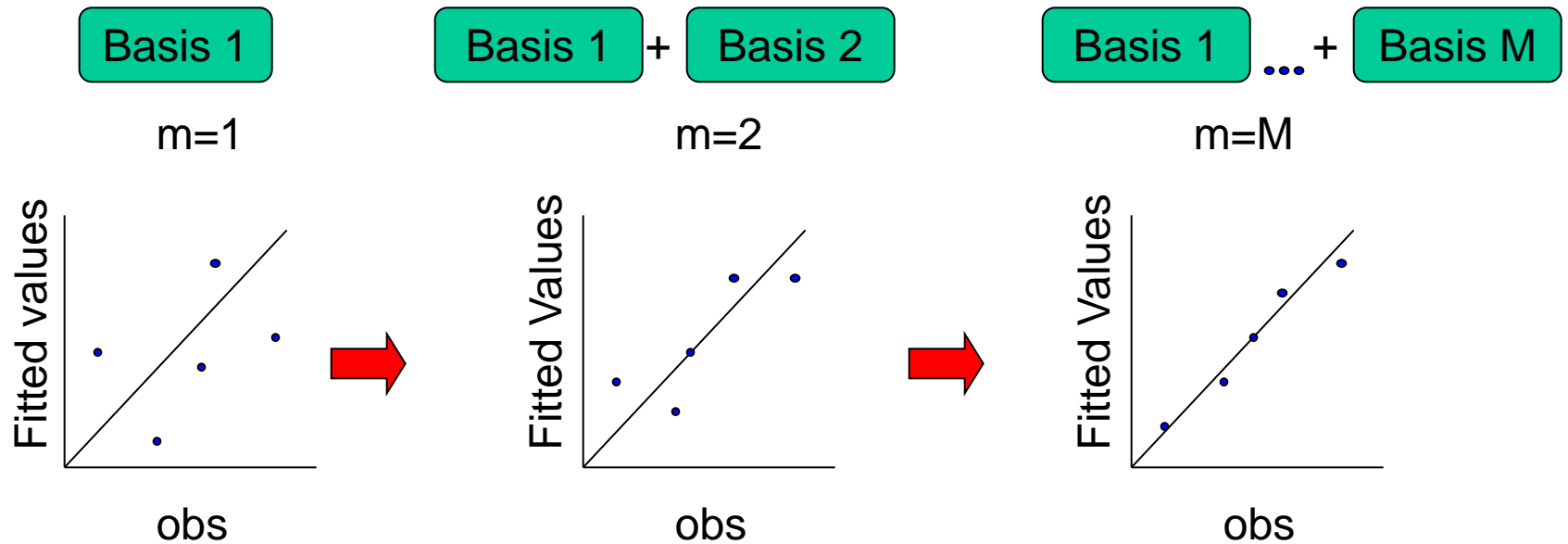
Techniques Tested

Method Tested	Status	Comments
Modified MLR with BIC predictors	Prototype	
Boosted Regression	Minor refinements	Optimization routine needed
Bayesian Neural Network	Needs Refinements	Revise predictors Matlab code
Support Vector Regression	Needs Refinement	
Neural Network with cross-validation	Rejected	Data loss
MDA	Rejected	
CART	Rejected	



Generalized Boosted Regression Model (GBM)

- Iterative Regression method
- Minimizes a certain loss function
- Applicable to many techniques [MLR, CART, SVR, ...]



Training Data

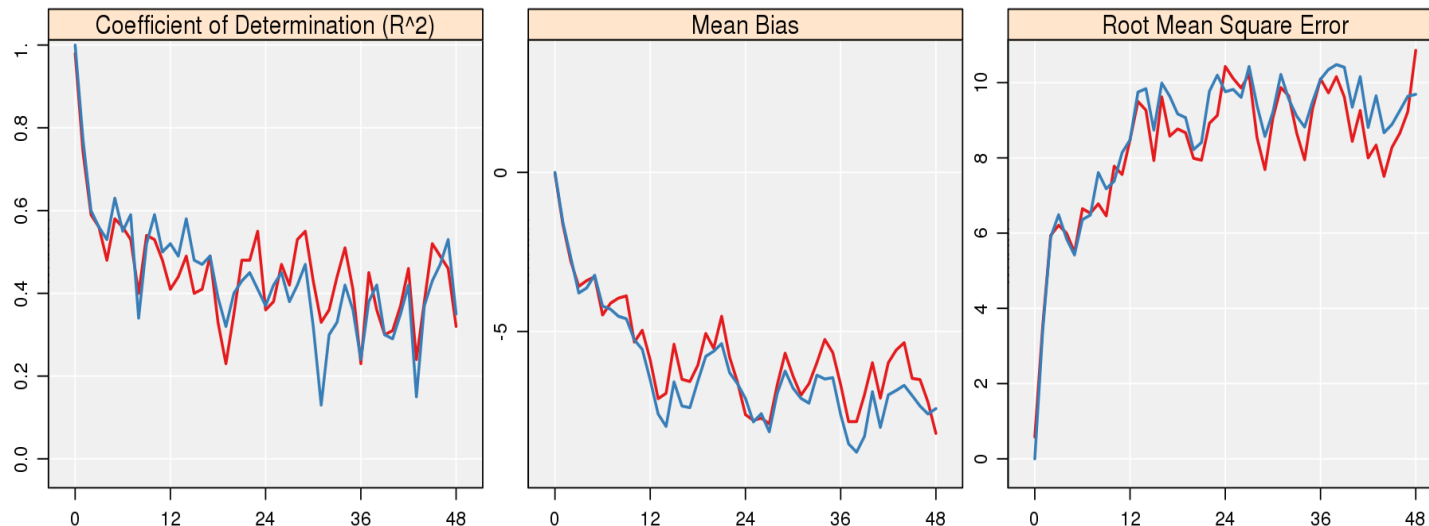
Verification Results for Above 75th Percentile cases

Statistics TEST Set All Season GEM15 Hourly Forecast of O3 for 75% Quantile Station 00030120

Ken GBM BIC Long Per All Season Optimum2



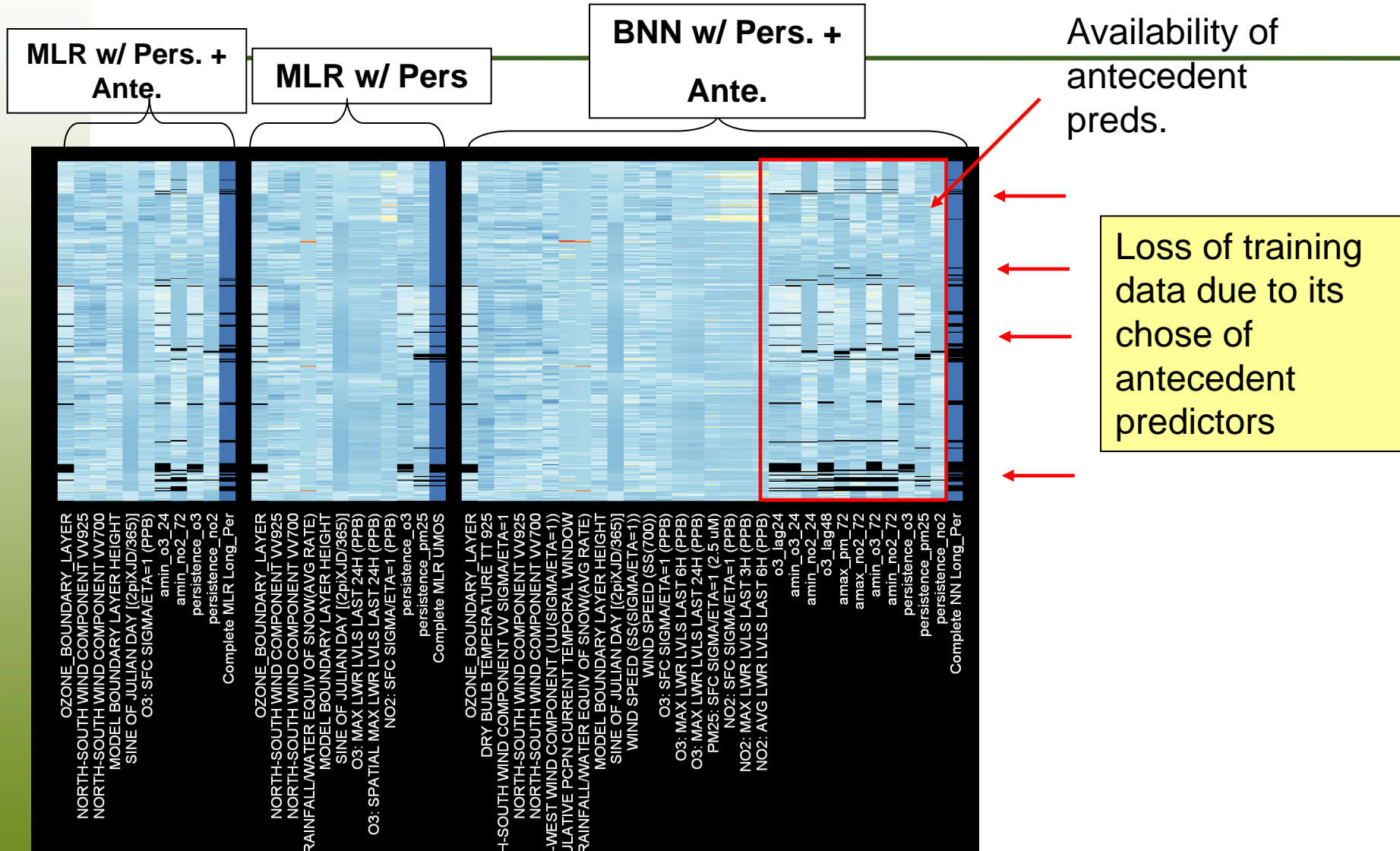
Ken MLR BIC Long Per All Season



Shrinkage: 0.001 Iterations: 6000 Interactions: 9

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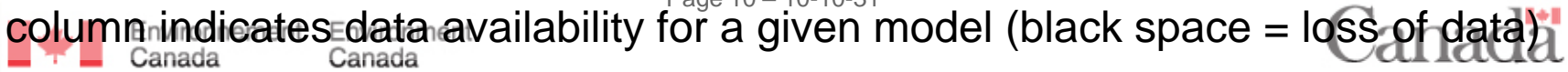
Impact of Data Loss on Predictor Selection



Availability of antecedent preds.

Loss of training data due to its chose of antecedent predictors

* Last column indicates data availability for a given model (black space = loss of data)



Non-Linear Auto-Regression (prelim)

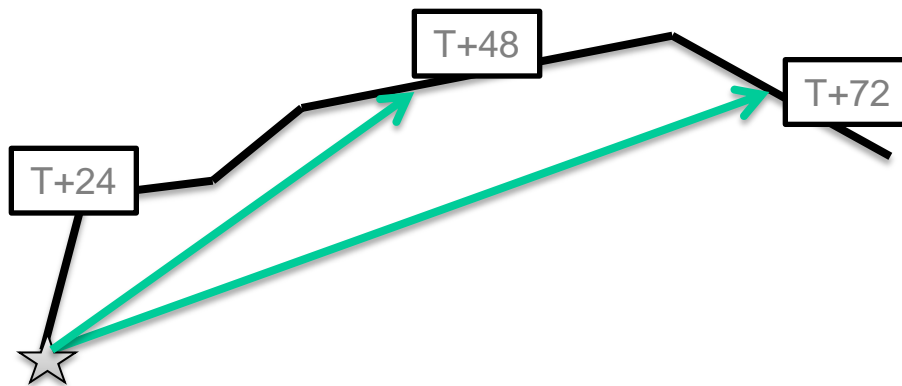
Approach: Relates trends in the Predictors and Predictand to improve the forecast accuracy

- Poster by Sean Perry

Trajectories (prelim)

Approach:

- Improve pattern recognition for transport events
- 7 launch heights (below 3km).
- Trace forward and backwards trajectories (00Z)



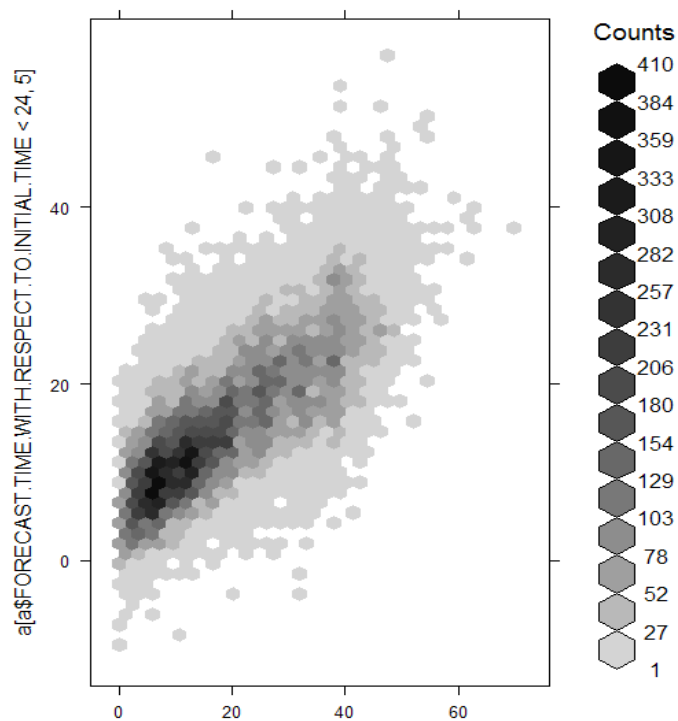
New Predictors

- Height
- Distance
- Bearing

Ozone for Halifax

Trajectory MLR

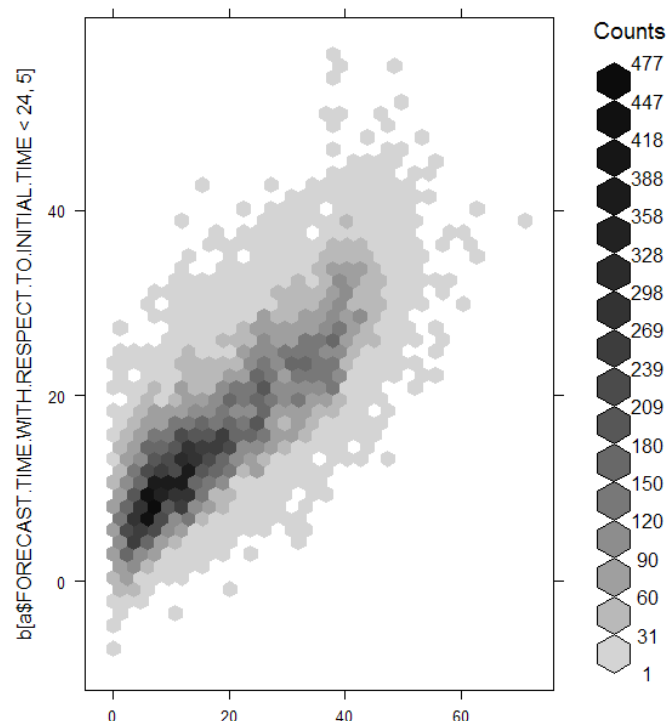
$R^2 = 0.81$ MB= -2.473



a[a\$FORECAST.TIME.WITH.RESPECT.TO.INITIAL.TIME < 24, 4]

MLR

$R = 0.75$ MB= -3.487



b[a\$FORECAST.TIME.WITH.RESPECT.TO.INITIAL.TIME < 24, 4]



Lesson Learned

- Air quality forecast can be improved using statistical techniques
- Linear methods are not the only resource available for this type of work
- Improvement can be achieved by:
 - Applying non-linear techniques
 - Using better predictors
 - Refinement of your data treatment
- Conditional bias still a problem and there is more work needed

Path Forward

- Address data reliability issues
 - Has a greater impact on the non-linear methods
- More predictor testing
 - new GEM-MACH fields (chemistry)
 - Further trajectory testing
- New techniques
 - Recursive NN
 - Fuzzy Logic
- Evaluate learning rates
- Prototypes (early 2013)