Predicting batch queue job wait times for informed scheduling of urgent HPC workloads

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Urgent computing

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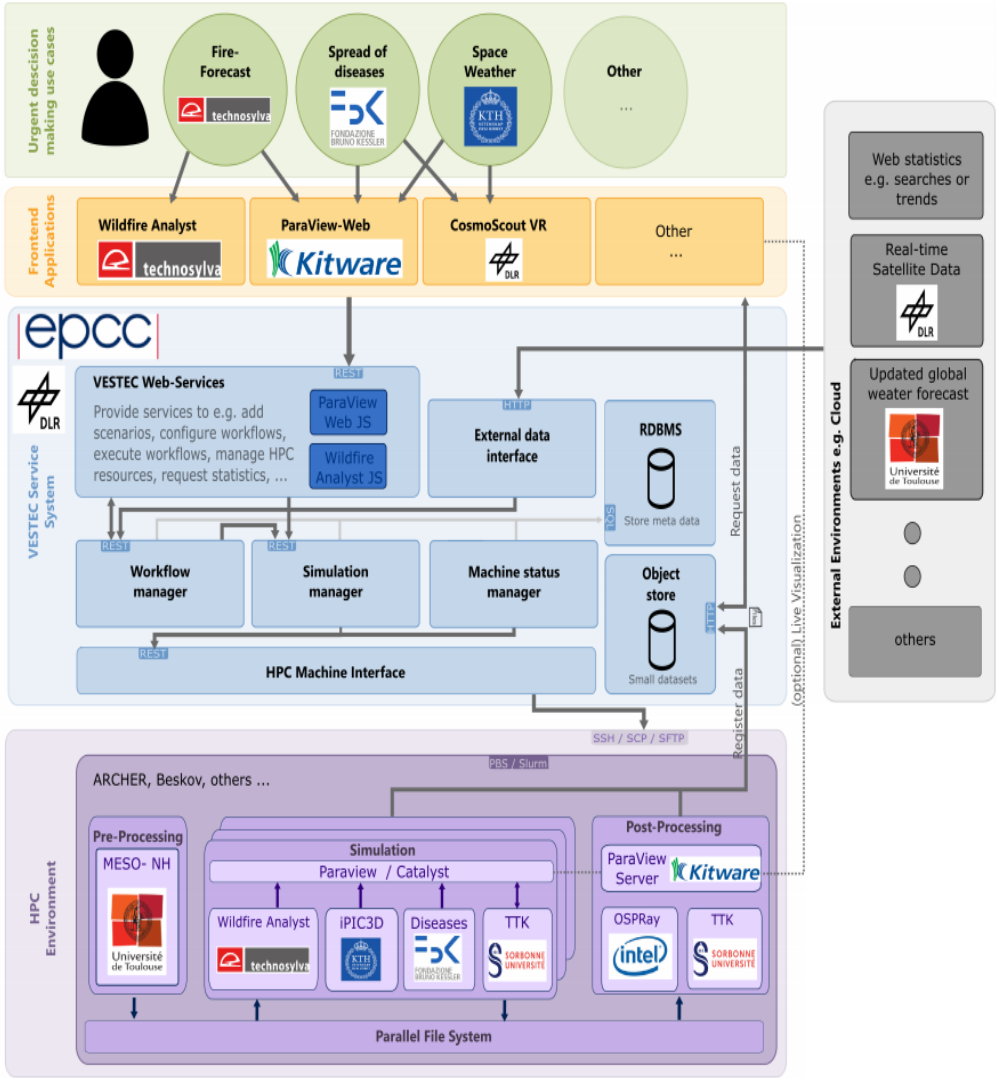
VESTEC system: Urgent computing



- The VESTEC system federates over numerous HPC machines
- Run job on which machine is most suited
  - To address limitations in batch queue for this sort of workload
- However accurate job placement is required to make correct choices

Machines used in this work

ARCHER2: HPE Cray EX, 5860 nodes, 314880 jobs in the standard queue and 73472 jobs in the short queue

Cirrus: HPE/SGI 8600 system with 280 nodes, 582200 jobs

4-cabinet: Early ARCHER2 HPC Cray EX, 1000 nodes, 373560 jobs

Slurm's queue prediction

- Tracked the lifetime of all jobs submitted on ARCHER2 and Cirrus over two week period

Predictions accurate within	ARCHER2		Cirrus	
	initial	best	initial	best
1 minute	5.13%	16.55%	0.42%	4.12%
5 minutes	12.47%	23.51%	0.42%	4.26%
10 minutes	19.91%	30.99%	0.85%	4.40%
30 minutes	41.31%	58.25%	2.69%	11.78%
1 hour	58.40%	70.25%	4.40%	16.34%
2 hours	69.91%	79.17%	8.38%	25.99%
6 hours	81.47%	90.59%	30.11%	52.70%
12 hours	90.45%	94.39%	50.85%	67.90%
24 hours	95.39%	99.31%	77.98%	86.93%

- Around 83% of jobs updated their estimates, and over 50% have five or more estimates
- Can see ARCHER2 is far more accurate than Cirrus here

Basic KNN model

- Trained a basic K-Nearest Neighbours model to act as a foundation for our work
  - Two versions: *basic* uses only the number of nodes and wall time requested, *temporal* also includes submission time and day.

Predictions accurate within	Standard queue		Short queue	
	basic	temporal	basic	temporal
1 minute	9.27%	22.67%	33.53%	66.08%
5 minutes	28.79%	35.53%	46.46%	78.16%
10 minutes	39.53%	41.37%	50.47%	83.76%
30 minutes	52.60%	53.32%	96.73%	92.21%
1 hour	64.37%	61.85%	98.55%	96.18%
2 hours	72.05%	68.68%	99.37%	97.50%
6 hours	83.28%	80.70%	99.67%	99.23%
12 hours	88.31%	87.40%	99.68%	99.67%
24 hours	94.39%	92.68%	100.00%	100.00%

  - Can see correlation between when a job was submitted and accuracy of prediction
  - Short queue is easy to predict for here as jobs are much more similar, the major challenge is standard queue

Basic KNN model

- Trained temporal model for each of our machines
  - 80% of data for training, 20% for testing. However split on days rather then data elements to provide a fair test

Predictions accurate within	ARCHER2	Cirrus	4-cabinet
1 minute	22.67%	51.48%	12.41%
5 minutes	35.53%	61.20%	24.35%
10 minutes	41.37%	65.28%	29.27%
30 minutes	53.32%	75.38%	38.73%
1 hour	61.85%	80.03%	44.87%
2 hours	68.68%	88.47%	55.24%
6 hours	80.70%	93.52%	71.18%
12 hours	87.40%	96.43%	81.31%
24 hours	92.68%	98.49%	89.34%

  - Can see for ARCHER2 more accurate predictions are better than Slurm's estimator but less so for less accurate predictions
  - Cirrus has much better prediction than Slurm's estimator!

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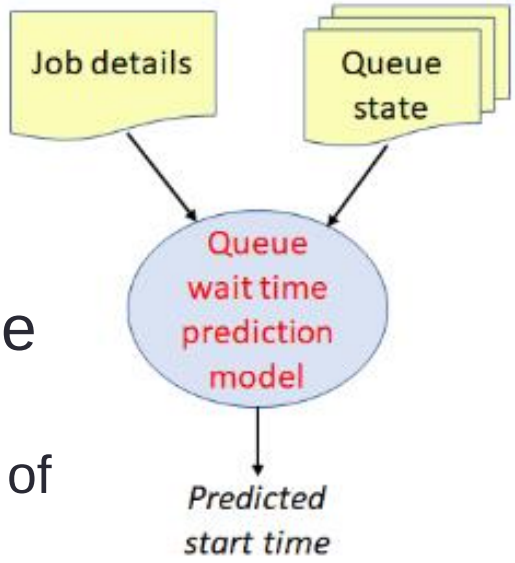
Queue state as an input



- Correlation between time and date is because this represents a state in the queue
  - Provide queue state as input to models based on histograms which are binned to represent pattern of the queue at the time of submission

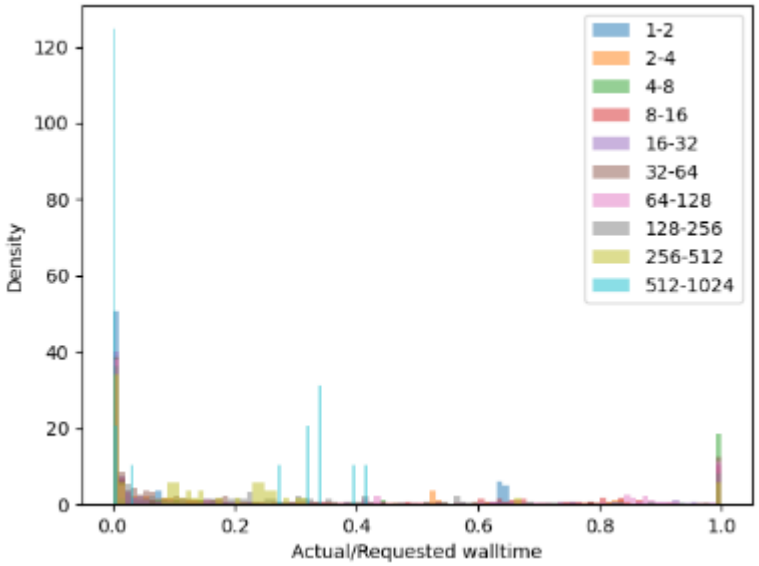
Name	Description
nodes_req	Number of nodes requested by the job
req_wtime	The requested wall time (hours)
day	Day of the week (0-6)
hour	Hour of the day (0-23)
s_q_jobs	The number of queued jobs
s_q_nodes	The total number of nodes requested by the queued jobs
s_q_work*	The total work (nodes × wall time) of the queued jobs
m_q_wait	The median time queued jobs have been waiting for to run (hours)
d_q_nodes[0-7]	Histogram of the nodes requested by queued jobs (8 values)
d_q_work[0-7]*	Histogram of work requested by queued jobs (8 values)
d_q_wait[0-7]	Histogram of wait times for queued jobs (8 values)
s_r_jobs	The number of running jobs
s_r_nodes	The total number of nodes requested by the running jobs
s_r_work*	The total remaining work (nodes × remaining time) of the running jobs
d_r_nodes[0-7]	Histogram of the nodes requested by running jobs (8 values)
d_r_work[0-7]*	Histogram of remaining work of running jobs (8 values)
d_r_remain[0-7]*	Histogram of remaining times for running jobs (8 values)

- This somewhat improved accuracy but still not perfect predictions

Predictions accurate within	ARCHER2	Cirrus	4-cabinet
1 minute	28.52%	63.45%	18.43%
5 minutes	37.09%	69.48%	24.54%
10 minutes	38.81%	72.10%	32.88%
30 minutes	59.34%	76.74%	39.28%
1 hour	61.70%	79.89%	45.00%
2 hours	70.20%	87.70%	62.28%
6 hours	81.74%	91.60%	79.94%
12 hours	88.18%	97.74%	91.44%
24 hours	93.35%	98.73%	92.80%

Stochastic queue state generation

- The challenge is that the amount of work in the queue is unknown
  - Users provide maximum wall times, but these do not necessarily represent the actual wall time of the jobs
    - E.g. on ARCHER2 and 4-cabinet on average 8 times overestimation of job wall time and 6 times on Cirrus.
  - Significantly impacts the overall prediction accuracy



- Therefore generate 100 queue states for each prediction job, each of these comprises randomly generated runtimes but they follow the general distribution of runtimes on the machine so are representative of real jobs.

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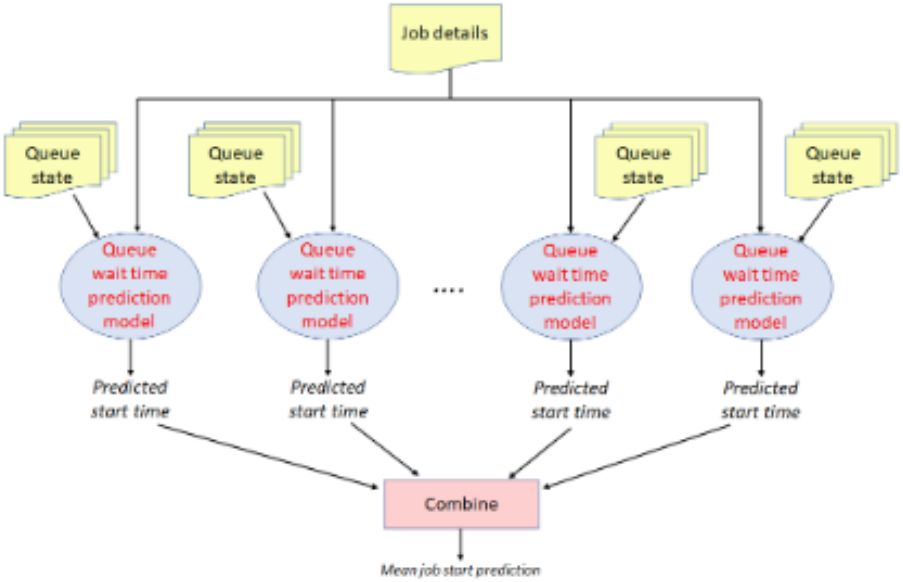
Stochastic queue state generation



- Once generated run each of these random queue states as inputs to our model and then combine predictions to generate the overall mean job start prediction

Predictions accurate within	ARCHER2	Cirrus	4-cabinet
1 minute	41.70%	50.45%	20.41%
5 minutes	54.16%	69.98%	27.16%
10 minutes	61.17%	75.00%	45.00%
30 minutes	69.09%	76.18%	51.48%
1 hour	74.50%	79.65%	60.87%
2 hours	76.12%	89.72%	78.57%
6 hours	87.58%	92.36%	80.98%
12 hours	91.73%	98.05%	93.96%
24 hours	95.00%	99.67%	95.34%

- This improves accuracy further, for the first time we beat Slurm's estimator at all levels of accuracy

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Boosted trees

- K-nearest neighbours (KNN) is a very simple model
  - Instead boosted trees enables us to capture non-linear relationships in the data and has been shown to work well for similar workloads.
  - We use the XGBoost library here

Predictions accurate within	ARCHER2	Cirrus	4-cabinet
1 minute	50.90%	65.86%	30.58%
5 minutes	54.63%	74.44%	42.78%
10 minutes	58.66%	77.55%	55.56%
30 minutes	74.28%	82.76%	65.90%
1 hour	79.74%	86.23%	73.70%
2 hours	82.71%	88.33%	78.69%
6 hours	93.71%	96.55%	85.78%
12 hours	94.47%	98.52%	93.53%
24 hours	97.50%	99.38%	97.23%

  - Improves accuracy but not a silver bullet!

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Combining classification and regression

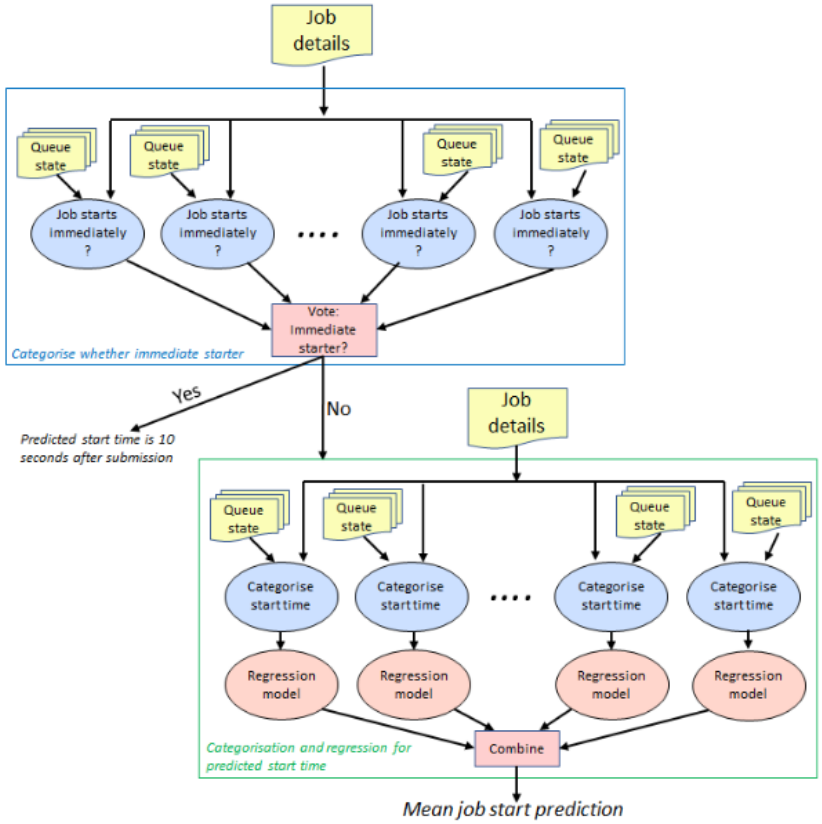
- Can combine classification and regression approaches
  - First classify if jobs are immediate starters (e.g. start in less than 10 seconds) and if so they that is the predicted start time
  - Otherwise categorise as one of seven starting categories

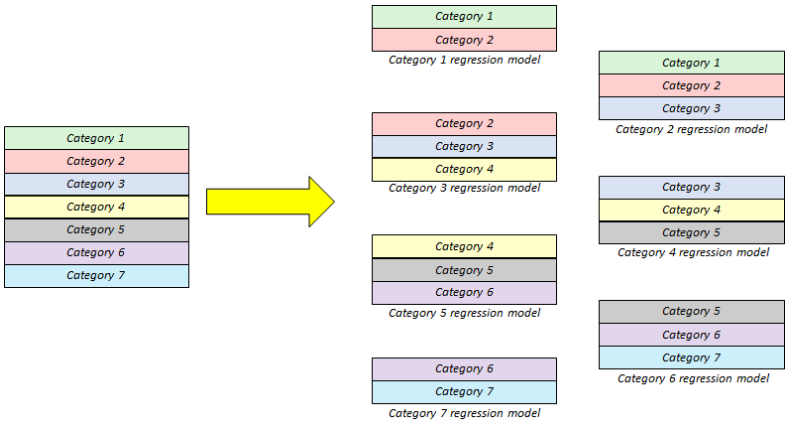
Job start time category	ARCHER2		Cirrus		4-cabinet	
	exact	relaxed	exact	relaxed	exact	relaxed
Immediately	73.81%	-	89.69%	-	88.67%	-
Up to 1 minute	73.60%	83.45%	88.38%	91.48%	68.45%	75.33%
Between 1 and 5 minutes	63.98%	78.93%	75.48%	80.04%	43.26%	69.32%
Between 5 and 10 minutes	61.51%	71.81%	62.79%	78.15%	61.95%	72.10%
Between 10 and 30 minutes	75.90%	89.55%	65.54%	80.26%	71.93%	80.54%
Between 30 minutes and 1 hour	60.54%	82.20%	70.62%	84.16%	71.48%	74.52%
Between 1 and 4 hours	70.91%	74.77%	80.68%	84.55%	77.02%	82.26%
Over 4 hours	80.26%	83.34%	87.03%	93.00%	77.55%	82.85%

  - Exact reports the accuracy of correct predictions being made, relaxed is both correct predictions and those miss-predicted but only in either of the two neighbouring categories

Combining classification and regression

- We undertake these classifications for all one hundred stochastic queue states
- Specific boosted trees regression models are trained for each category (with neighbours) to undertake job start time predictions





Combining classification and regression

- This combination of classification and regression considerably improved our performance across all machines

Predictions accurate within	ARCHER2	Cirrus	4-cabinet
1 minute	63.49%	76.87%	66.25%
5 minutes	71.46%	88.31%	71.89%
10 minutes	75.67%	89.69%	75.29%
30 minutes	81.93%	92.11%	80.37%
1 hour	85.17%	93.55%	83.19%
2 hours	89.11%	95.39%	86.63%
6 hours	95.87%	98.65%	94.74%
12 hours	98.99%	99.68%	99.79%
24 hours	99.93%	100.00%	100.00%

- We can accurately predict start times of around 65% of jobs within 1 minute of actual time on ARCHER2 and 4-cabinet, and over 76% on Cirrus
- This extends to three quarters within 10 minutes on ARCHER2 and 4-cabinet and 89% on Cirrus

Runtime

- Prediction accuracy is our major concern, but we also must run our predictions within a timely fashion
- All model runs undertaken on a 26-core Intel Xeon Platinum (Skylake) 8170 CPU

Activity	Type	ARCHER2 (seconds)	Cirrus (seconds)	4-cabinet (seconds)
Cumulative Distribution Function (CDF)	Training	264	420	310
Histogram bin identification	Training	6981	11298	7256
Split training and test data including binning	Training	4322	6223	5098
Generating random queue test states	Training	7650	14890	8442
Train Section IV stochastic queue KNN model	Training	20884	70667	33410
Train Section V classification and regression boosted trees models	Training	13574	34589	15911
Single job prediction for Section IV stochastic queue KNN model	Prediction	0.88	0.89	0.89
Single job prediction for Section V classification and regression boosted trees models	Prediction	0.11	0.18	0.10

- Model training takes a long time, but only needs to be done one
- Prediction for our most accurate approach is a tenth of a second per machine

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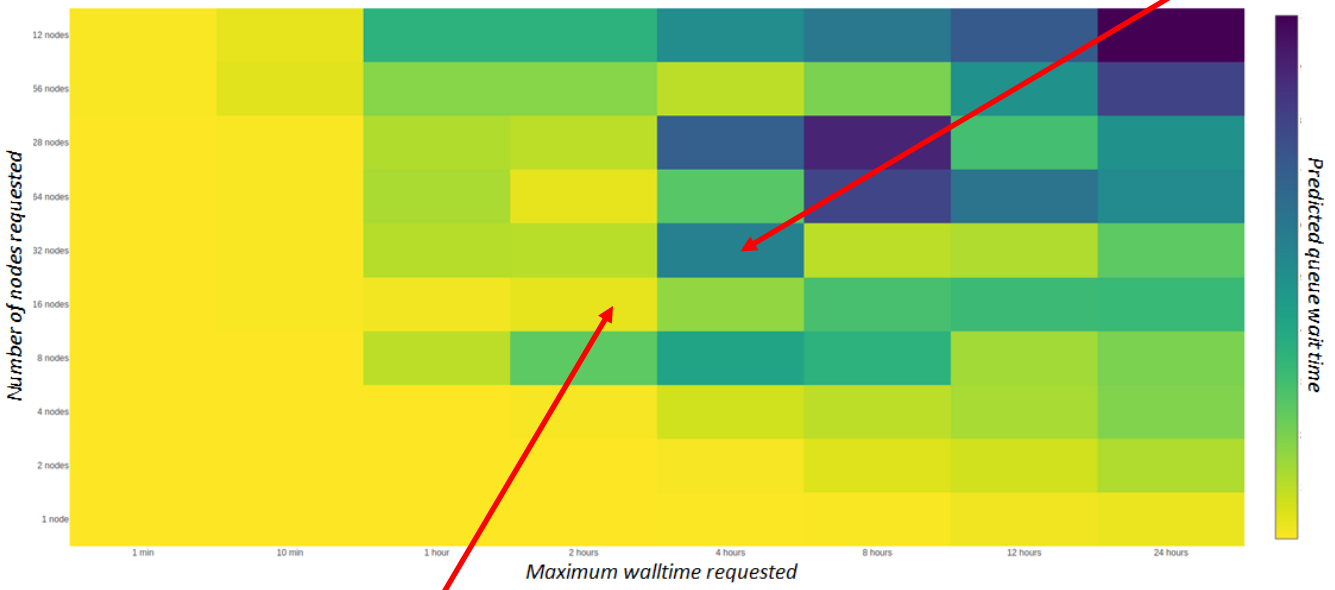
User insights

- Whilst urgent workloads are our major focus, it is also possible to gain insights from running predictions through our models

Avoid requesting 4 hours max wall time with 32 nodes, instead select 8 or 12 hours



With 16 nodes if you can stay at maximum wall time of 2 hours or less, as beyond this there is an increase in job wait time

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Conclusions

- Our approach delivers significantly improved accuracy than Slurm's estimations and previous machine learning approaches

- We use a combination of classification and regression models to most accurately predict the queue wait time
- Whilst our major focus has been for urgent workloads, and the accuracy delivered is reasonable for this, there are also numerous other uses too.

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