Recommendation system for scientific tools and workflows

Master thesis

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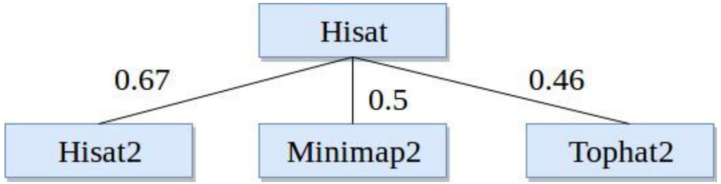
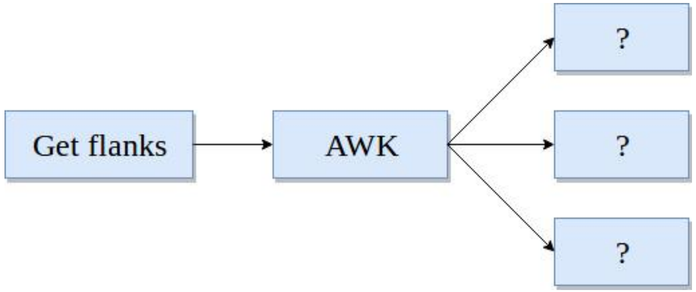
Recommendation system

1. Find similar scientific tools



2. Predict tools for workflows



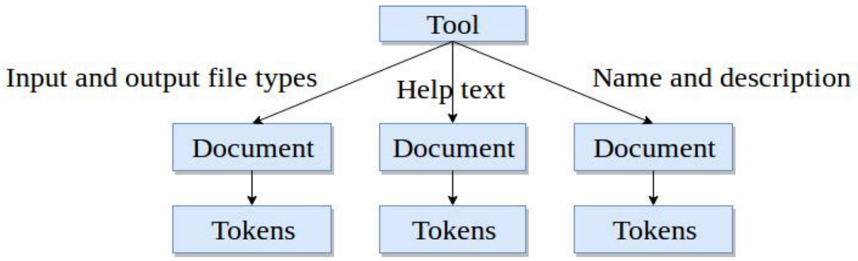
1. Find similar scientific tools

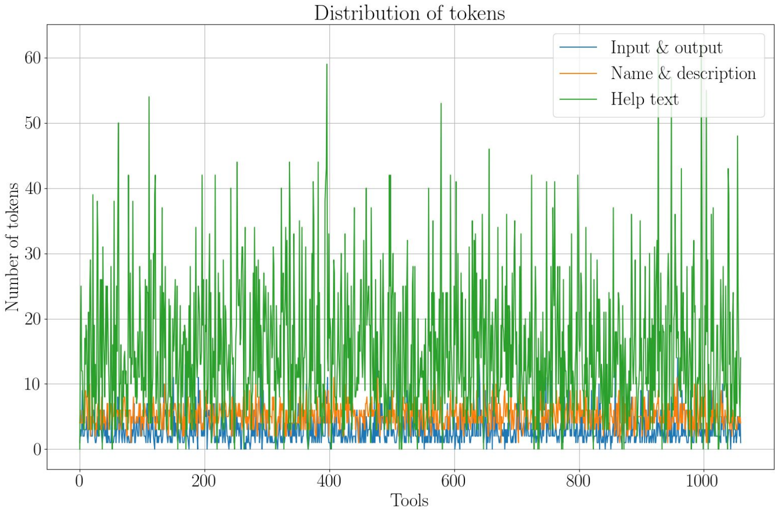
- Compute similarity among tools
- Recommend similar tools
- Replace a tool by its similar tool
- Provide more options for data processing

Approach

1. Collect tools metadata (~ 1,050 tools)
2. Clean metadata - stemming and stopwords
3. Learn vectors for tools
4. Compute similarity among vectors
5. Combine similarity matrices

Tool, documents and tokens





Paragraph (document) vector

- Neural network approach*
- A dense vector for each paragraph
- Similar tools have similar vectors
- Encode variable length paragraphs
- Each tool has three paragraphs (documents)

*https://cs.stanford.edu/~quocle/paragraph_vector.pdf
Input/output file types - https://dl.acm.org/citation.cfm?id=1704810 (bestmatch25)

Similarity scores

- Jaccard index (input and output file types)
- Cosine angle (name and description and help text)
- Compute similarity matrix
- Three similarity matrices
- Simple - average the matrices
- Better - learn weights

$$j = \frac{A \cap B}{A \cup B}$$

$$x \cdot y = |x| \times |y| \times \cos\theta$$

Jaccard index: https://link.springer.com/article/10.1007/BF02365362
Cosine angle similarity: https://www.itl.nist.gov/div898/software/dataplot/refman2/auxillar/cosdist.htm

Optimisation

- Gradient descent
- Learn weights on similarity scores

$$Error(w^k) = \frac{1}{N} \times \sum_{j=1}^{N} [w^k \times SM^k - SM_{ideal})^2]_j$$

$$Gradient(w^k) = \frac{\partial Error}{\partial w^k} = \frac{2}{N} \times ((w^k \times SM^k - SM_{ideal}) \cdot SM^k)$$

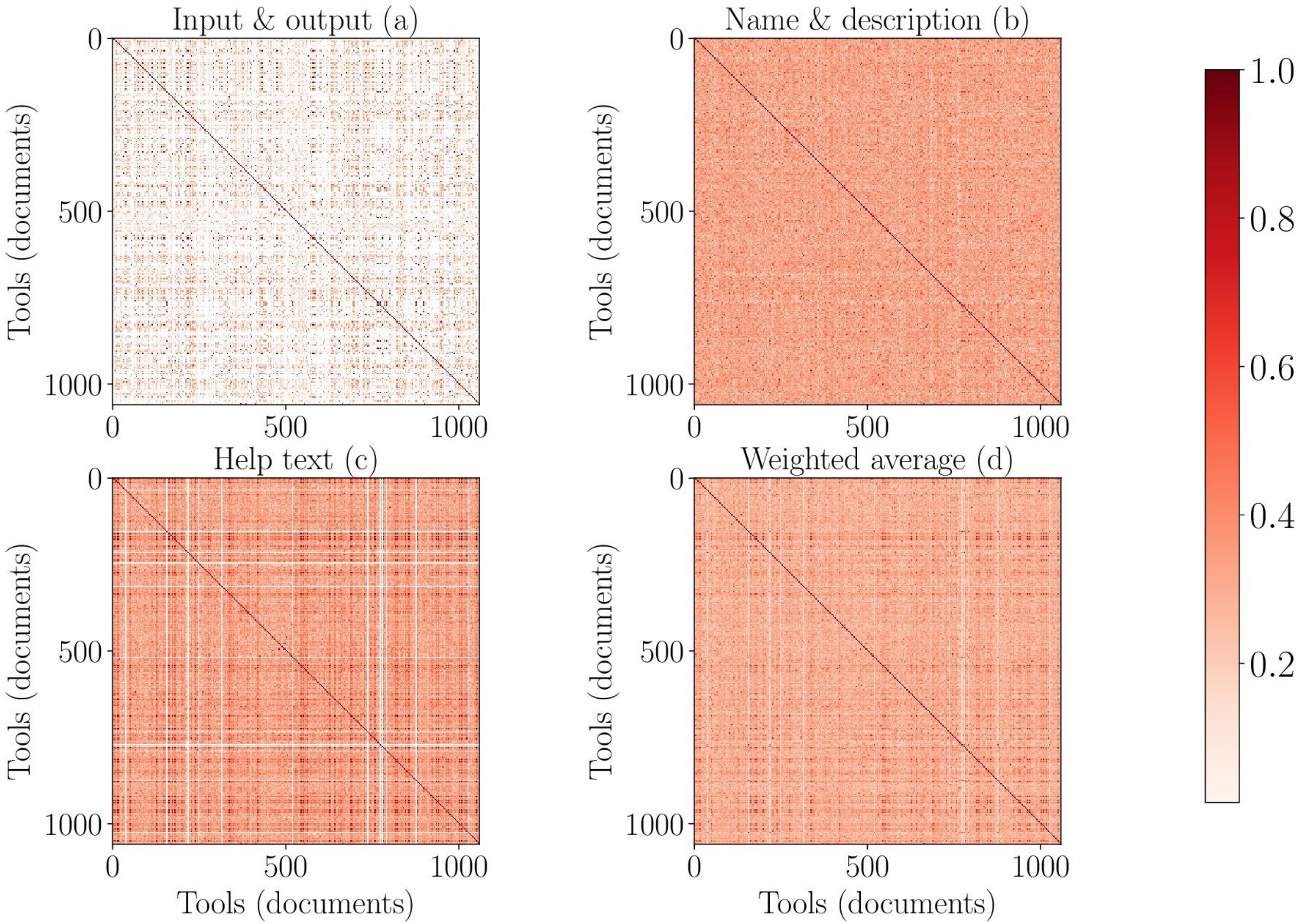
$$w^k = w^k - \eta \times Gradient(w^k)$$

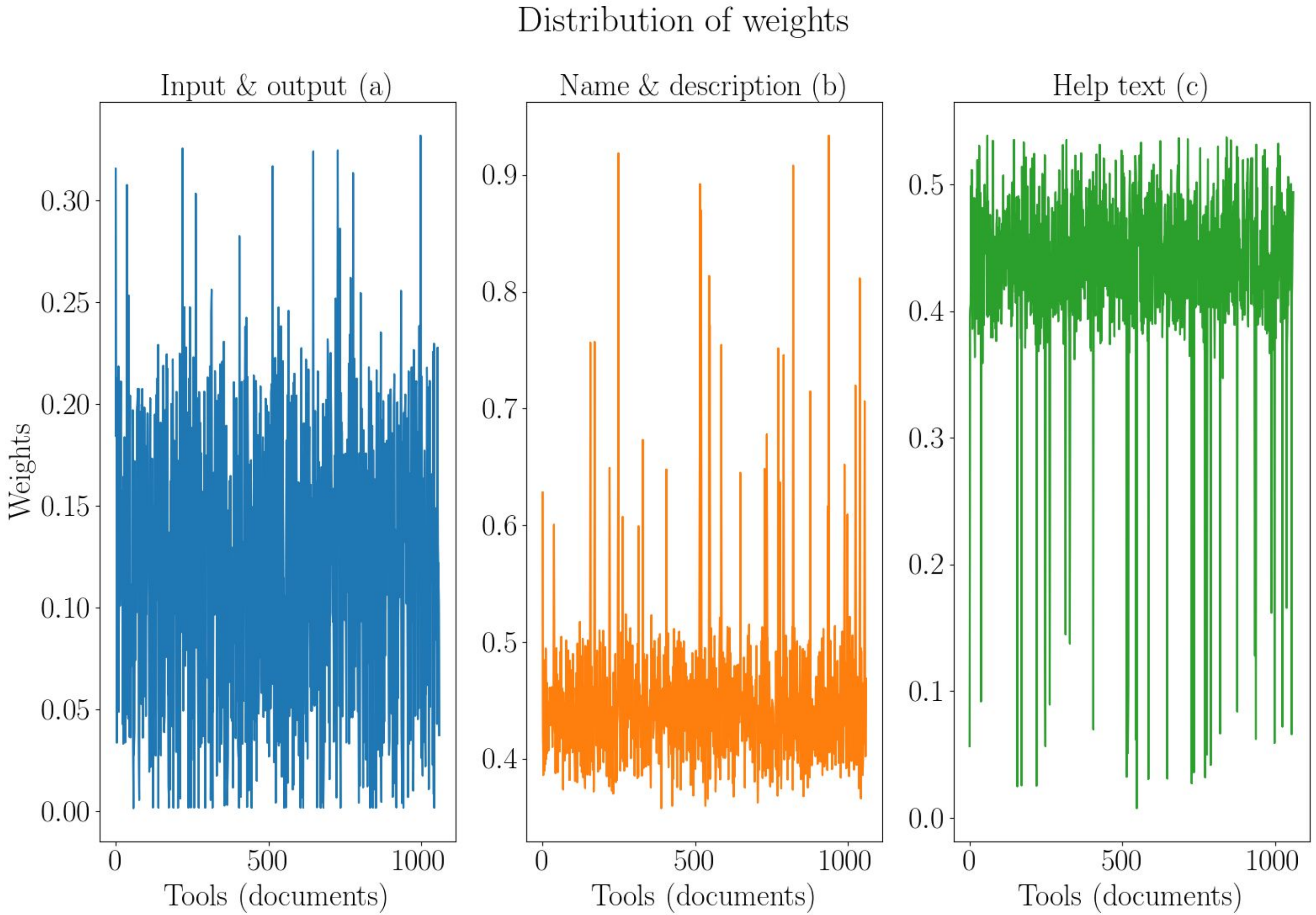
- Obtain a weighted average similarity matrix

SM_{ideal} is 1.0 as the maximum value of similarity measures can be at most 1.0

Gradient descent: https://developers.google.com/machine-learning/crash-course/reducing-loss/gradient-descent

Similarity matrices



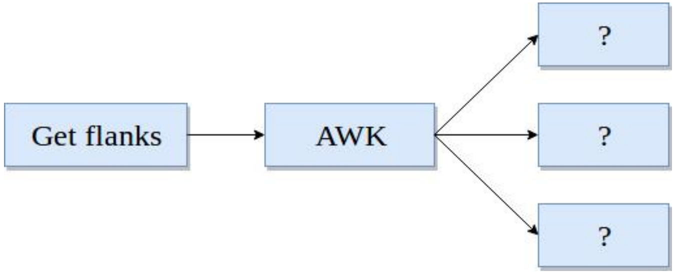

Distribution of weights
Input & output (a)
Name & description (b)
Help text (c)
Weights
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.4
0.5
0.6
0.7
0.8
0.9
0.0
0.1
0.2
0.3
0.4
0.5
0
500
1000
Tools (documents)
Tools (documents)
Tools (documents)

Summary and conclusion

- Collect and clean tools metadata
- Learn vector for each tool
- Compute and combine similarity matrices
- Less data for name and description attribute
- No true similarity
- Exclude low similarity values
- Run analysis on larger set of tools
- Compute similar tools using workflows

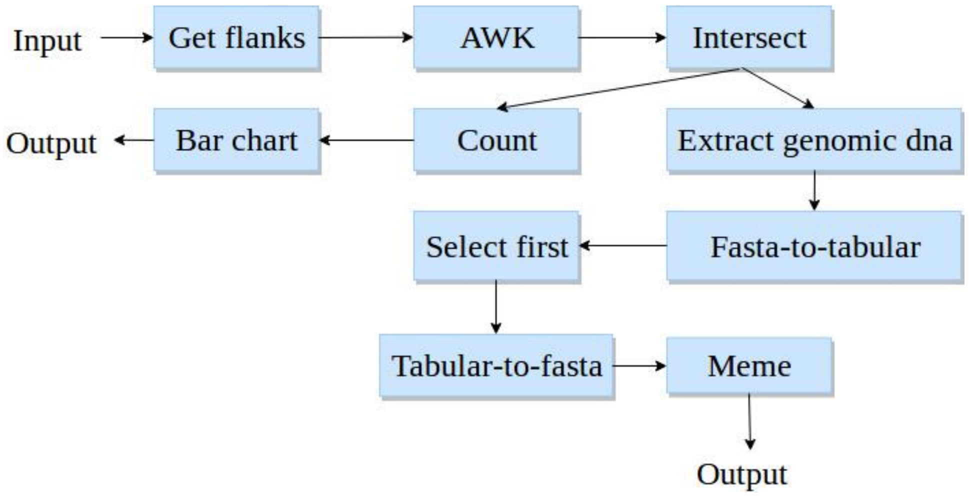
2. Predict tools in workflows

- Tough to assemble workflows
- Tools compatibility issues
- Loss of computation time
- Thousands of tools



Workflows

- Workflow - a directed acyclic graph
- Paths in a workflow

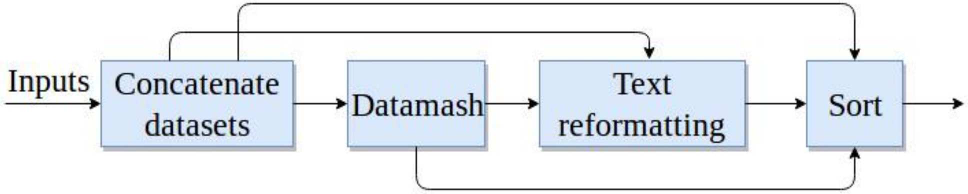


- 193,000 workflows
- 900,000 paths
- Maximum 25 tools in a path

Directed acyclic graph: https://cran.r-project.org/web/packages/ggdag/vignettes/intro-to-dags.html

Higher order dependency

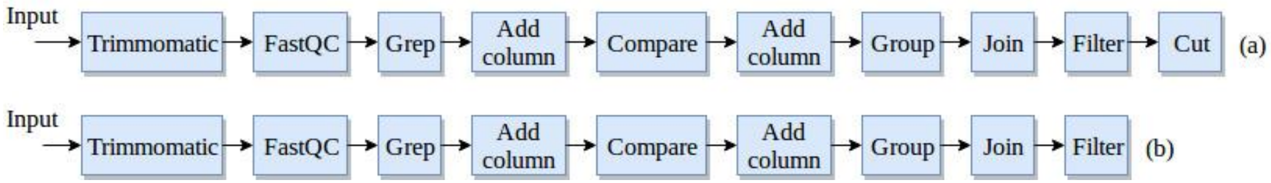
- Not dependent only on immediate parent
- Dependent on all previous tools



Higher order dependency: https://arxiv.org/pdf/1506.06268.pdf
https://arxiv.org/pdf/1508.03113.pdf

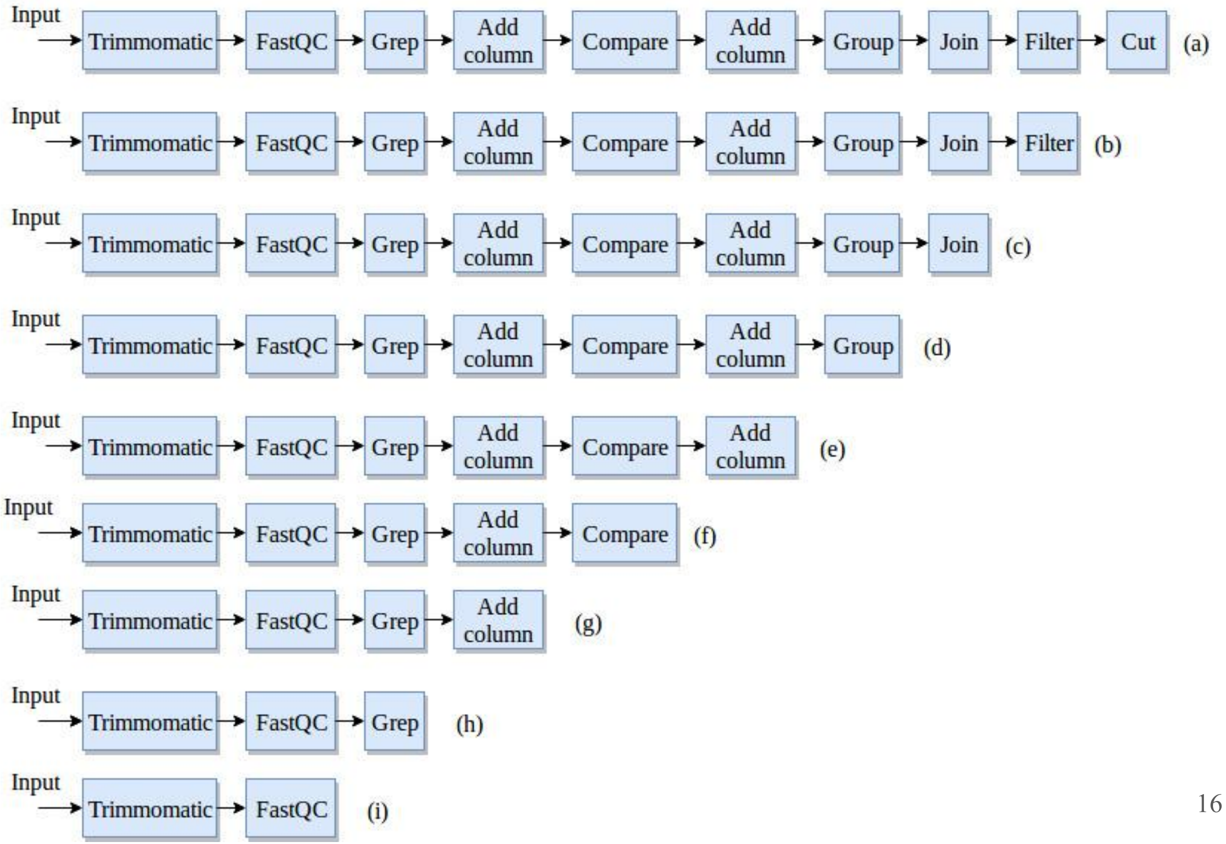
Workflow preprocessing

- No decomposition



Workflow preprocessing

- Keep first tool fixed

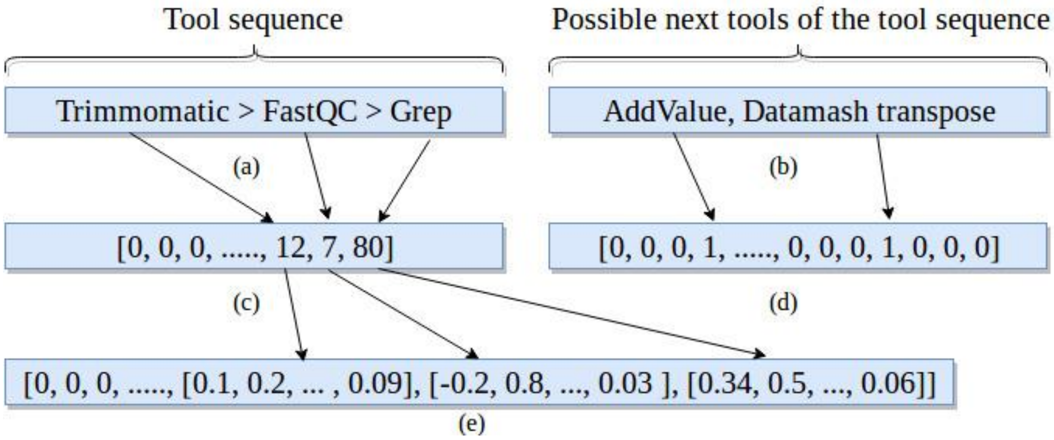


Recurrent neural network

- Classifier to learn on sequential data
- Multilabel, multiclass classification
- Recurrent neural network - Gated recurrent units
- Learn long-range dependencies
- Two hidden layers, one embedding layer and one output layer
- Cross-entropy loss
- Root mean square propagation (rmsprop) optimiser
- Sigmoid output activation
- 80% training paths, 20% test paths

Recurrent neural network: https://arxiv.org/pdf/1412.3555.pdf

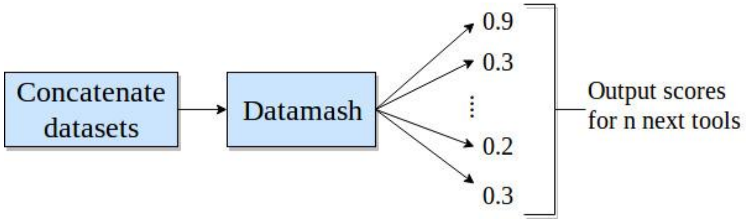
Embedding and label vectors



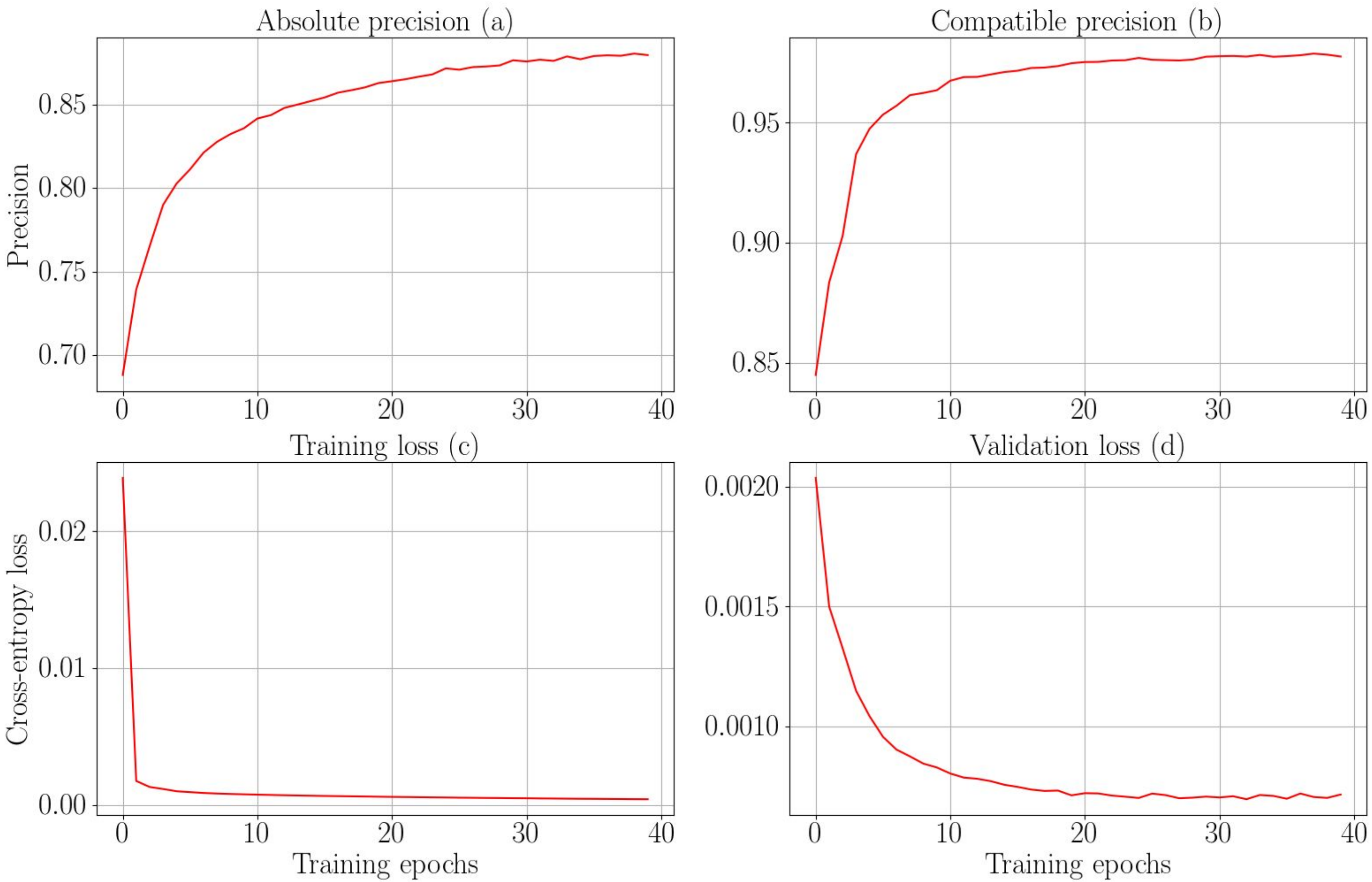
Embedding layer: https://keras.io/layers/embeddings/

Precision and prediction

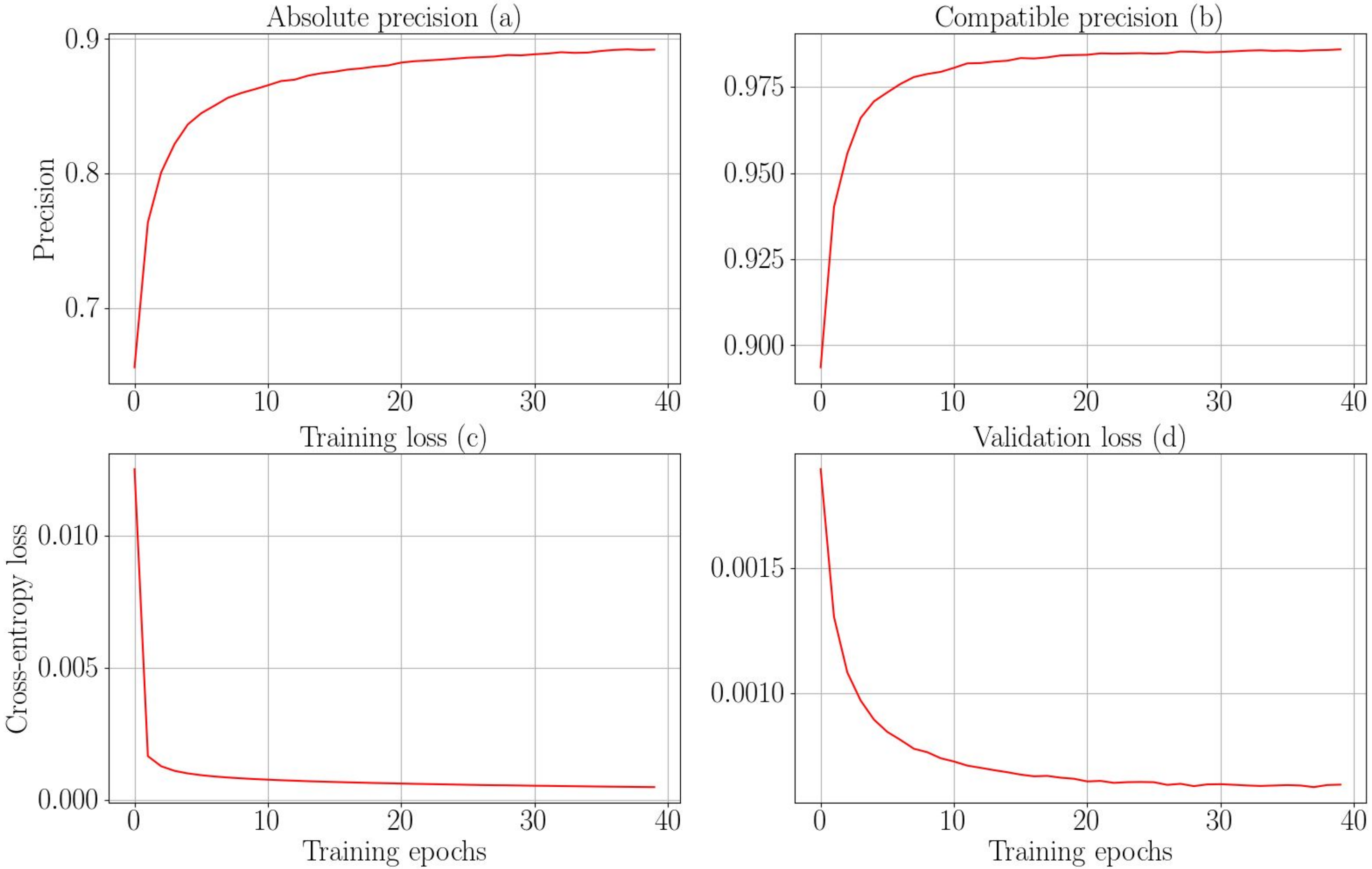
- Absolute precision
- Compatible precision

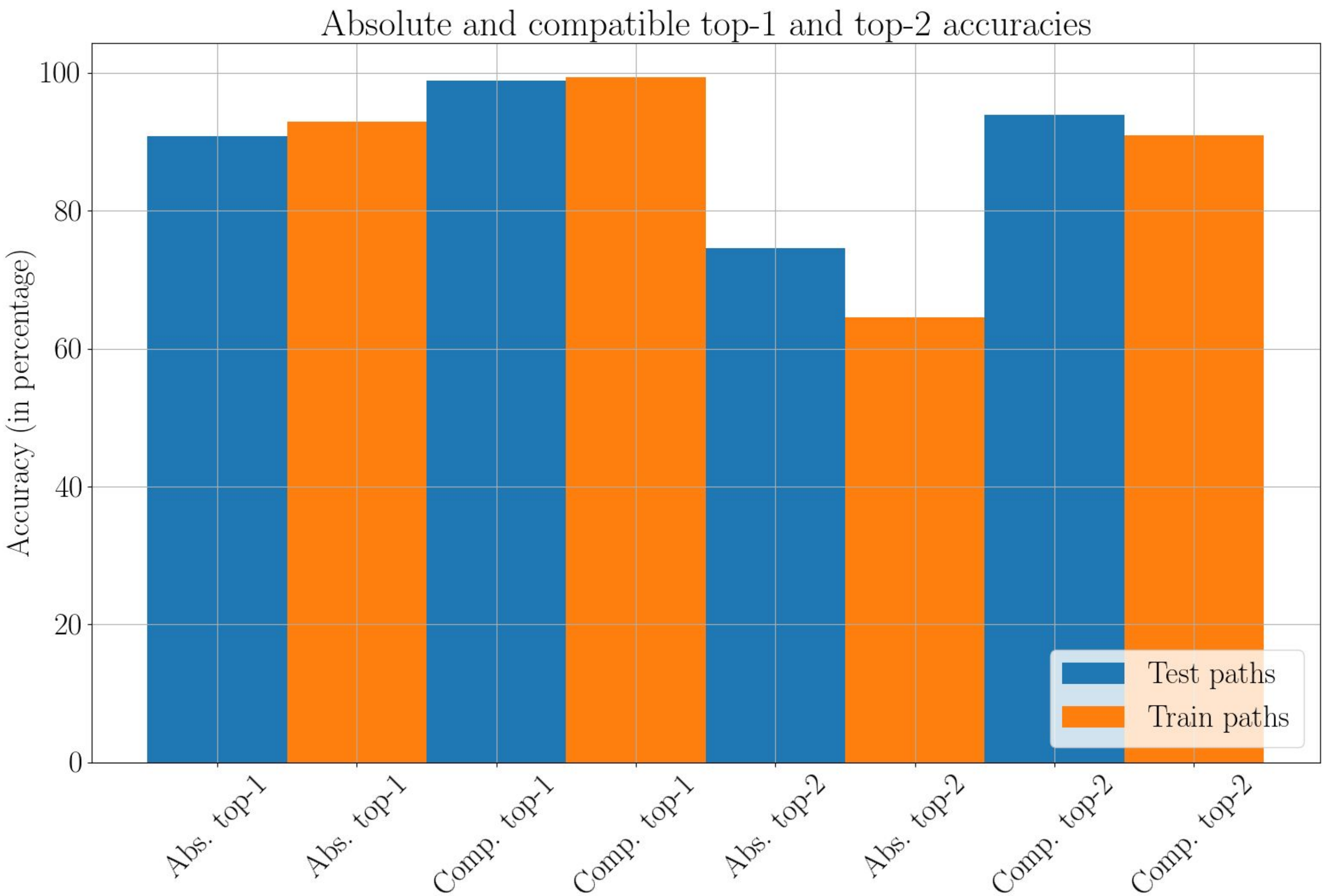


Precision and loss for no decomposition of paths



Precision and loss for decomposition of train and test paths




Absolute and compatible top-1 and top-2 accuracies
Accuracy (in percentage)
0
20
40
60
80
100
Test paths
Train paths
Abs. top-1
Abs. top-1
Comp. top-1
Comp. top-1
Abs. top-2
Abs. top-2
Comp. top-2
Comp. top-2

Summary and conclusion

- Workflows are directed acyclic graphs (193, 000 workflows)
- Extract paths from workflows
- Learn long-range dependencies
- Recurrent neural network (gated recurrent units)
- Multilabel, multiclass classification
- Absolute precision ~90%, compatible precision ~99%
- More workflows, better results

Future work

- Restore original distribution
- Decay prediction over time
- Integrate into Galaxy

Thank you for your attention

Questions?

Supplementary material

Stemming and stopwords

- Stemming - converge all forms of a word into one basic form
- “*Operate, operating, operates, operation, operative, operatives, operational*” into “*oper*” [1]
- Stopwords - “*a, about, above, would, could …*” [2]

1. https://nlp.stanford.edu/IR-book/html/htmledition/stemming-and-lemmatization-1.html
2. https://www.ranks.nl/stopwords

Bestmatch25 (bm25)

- Token frequency (tf)
- Document and inverted document frequency (idf)

$$idf = \log \frac{N}{df}$$

$$\alpha = (1 - b) + \frac{b \cdot |D|}{|D|_{avg}}$$

$$tf^* = tf \cdot \frac{k+1}{k \cdot \alpha + tf}$$

$$bm25 = tf^* \cdot idf$$

https://dl.acm.org/citation.cfm?id=1704810
http://www.staff.city.ac.uk/~sb317/papers/foundations_bm25_review.pdf

Bestmatch25 (bm25) scores

Tools/Tokens	Regress	Linear	Gap	Mapper	Perform
LinearRegression	5.22	4.1	0.0	0.0	3.84
LogisticRegression	3.54	0.0	0.0	0.0	2.61
Tophat2	0.0	0.0	1.47	1.47	0.0
Hisat	0.0	0.0	0.0	0.0	0.0

Latent Semantic Analysis

- Document-token matrix (*X*)
- Singular value decomposition

$$X_{n\times m} = U_{n\times n} \cdot S_{n\times m} \cdot V^T_{m\times m}$$

$$U^T \cdot U = I_{n\times n}$$

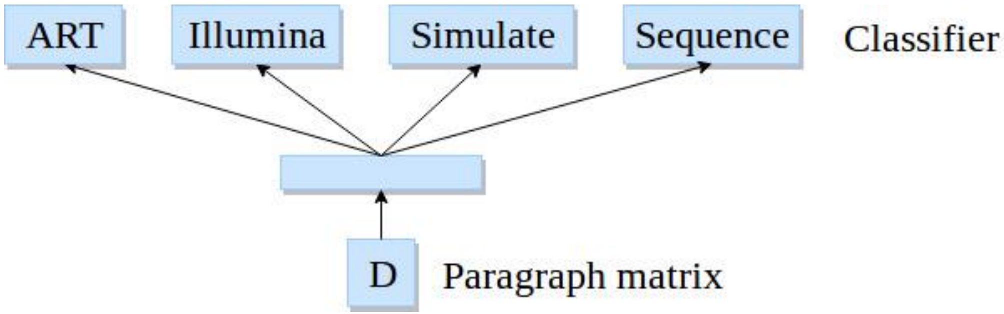
$$V^T \cdot V = I_{m\times m}$$

$$X_{n\times m} = U_k \cdot S_k \cdot V^T_k$$

Paragraph vectors

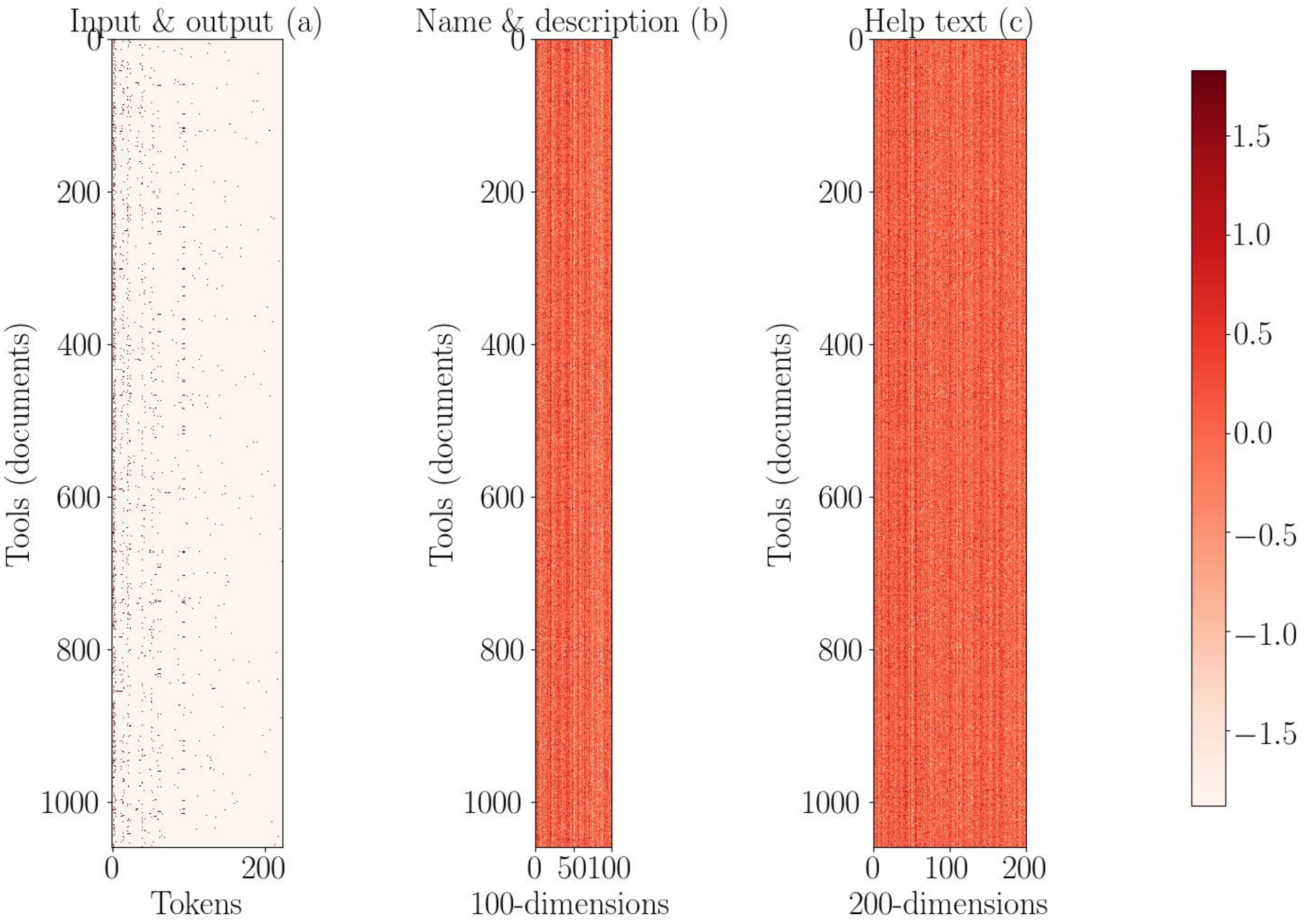
- Softmax classifier
- Backpropagation
- Stochastic gradient descent
- Gensim*

$$\frac{1}{T} \cdot \sum_{t=k}^{T-k} \log p(w_t | w_{t-k}, \ldots, w_{t+k})$$



*https://radimrehurek.com/gensim/models/doc2vec.html
Image adapted from: https://cs.stanford.edu/~quocle/paragraph_vector.pdf

Document-token and paragraph matrices



Optimisation

- Gradient descent
- Mean squared error
- Initial learning rate - 0.05
- Decay learning rate
- Nesterov's accelerated gradient

$$update_{t+1} = \gamma \cdot update_t - \eta \cdot Gradient(w_t + \gamma \cdot update_t)$$

$$w_{t+1} = w_t + update_{t+1}$$

Optimisation

1	0.34	0.65	0.44
0.34	1	...	...
0.65	...	1	...
0.44	...	...	1

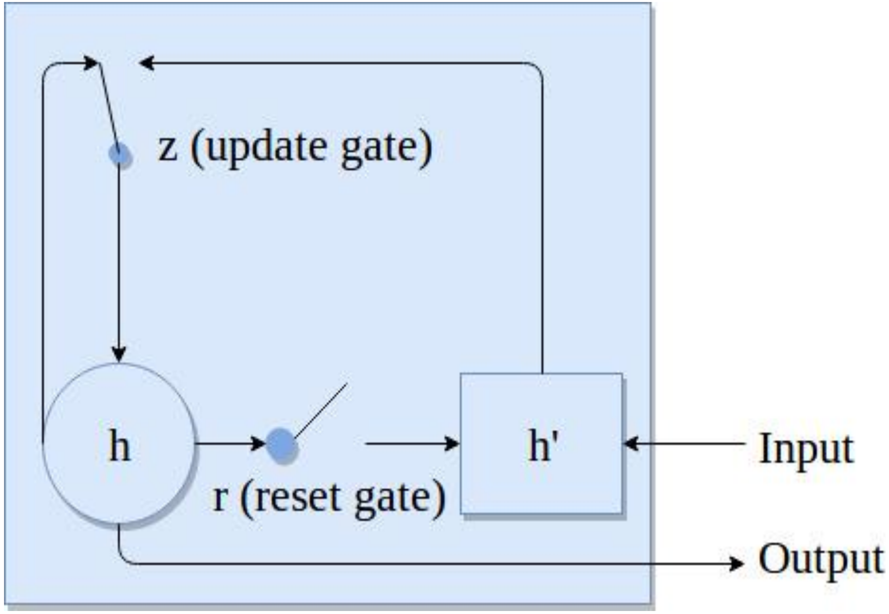
1	0.76	0.63	0.85
0.76	1	...	...
0.63	...	1	...
0.85	...	...	1

1	0.06	0.1	0.17
0.06	1	...	...
0.1	...	1	...
0.17	...	...	1

Visualisers

- Paragraph vectors
- Latent Semantic Analysis (5% of full-rank)

Recurrent neural network



$$h_t = (1 - z_t) \times h_{t-1} + z_t \times h_t^{'}$$

$$z_t = \sigma(W_z \times x_t + U_z \times h_{t-1})$$

$$r_t = \sigma(W_r \times x_t + U_r \times h_{t-1})$$

$$h_t^{'} = \tanh(W \times x_t + U \times (r_t \odot h_{t-1})$$

$$p(x_T | x_1, x_2, \ldots, x_{T-1})$$

RNN: https://arxiv.org/pdf/1412.3555.pdf

Recurrent neural network

- One embedding layer, two hidden layer and one output layer
- Recurrent layer activation - exponential linear unit

$$f(x) = \begin{cases} x, & \text{if}\, x > 0 \\ \alpha \times (e^x - 1), & \text{if}\, x \leq 0, \alpha > 0 \end{cases}$$

- Output activation is sigmoid $f(x) = \frac{1}{1+e^{-x}}$

Exponential linear units: https://arxiv.org/pdf/1511.07289.pdf

Recurrent neural network

- Optimiser - Root mean square propagation (rmsprop)

$$MeanSquare(w,t) = 0.9 \times MeanSquare(w,t-1) + 0.1 \times (\frac{\partial E}{\partial w}(t))^2$$

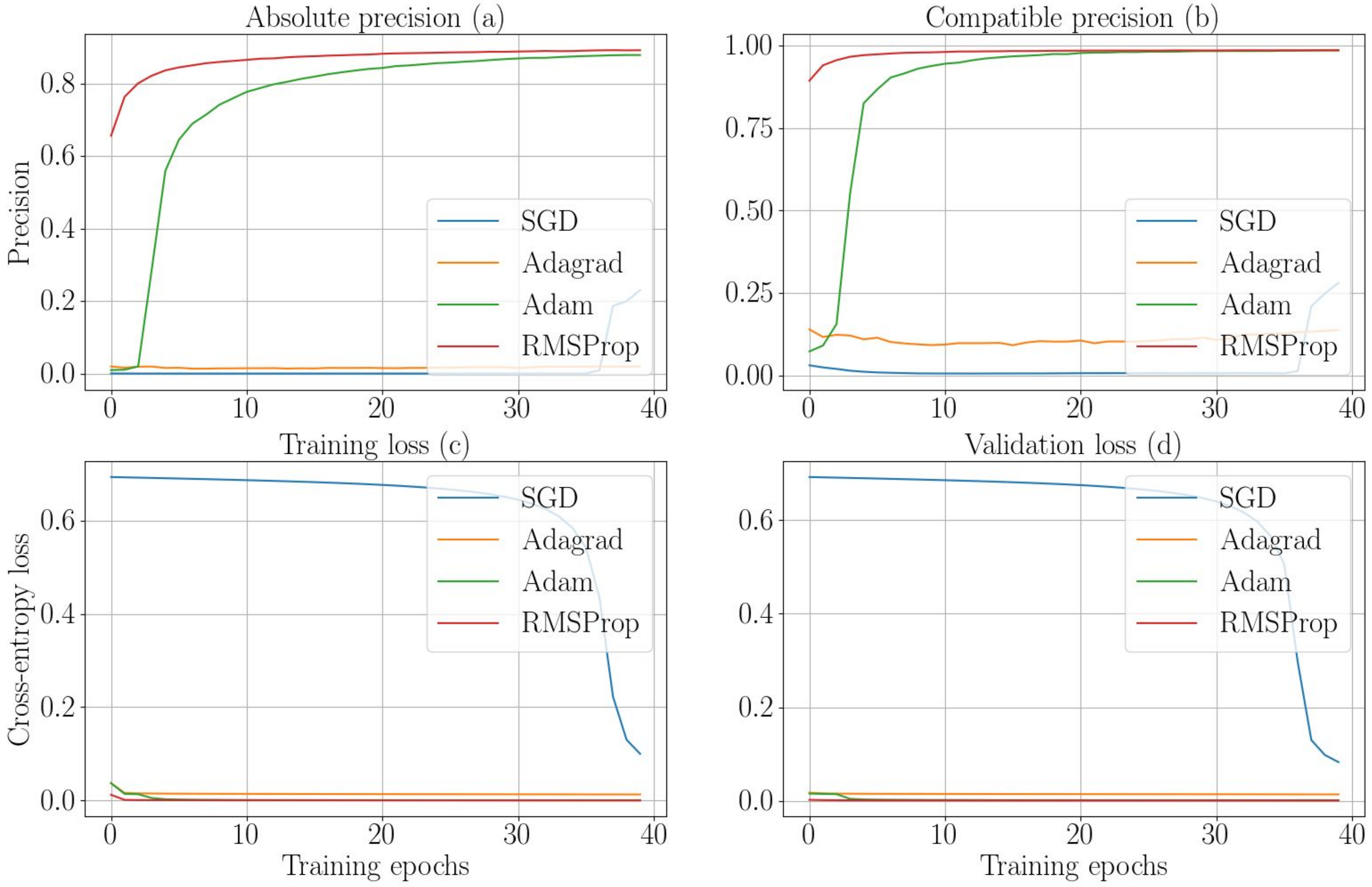
$$w_{t+1} = w_t - \frac{\eta}{\sqrt{MeanSquare(w,t) + \epsilon}} \times \frac{\partial E}{\partial w}(t)$$

- Binary cross-entropy loss

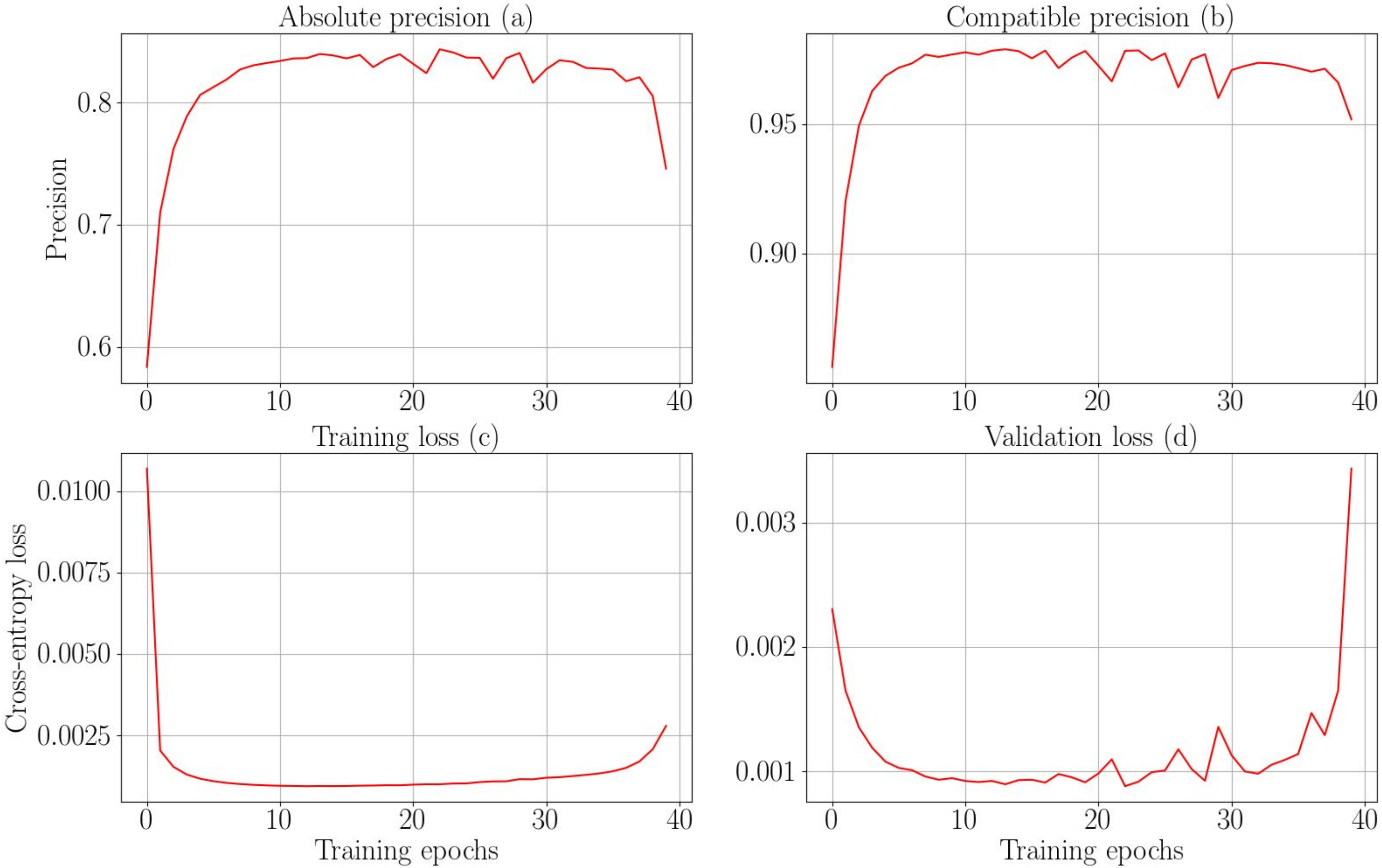
$$loss_{mean} = -\frac{1}{N}(\sum_{i=1}^{N} y_i \times log(p_i) + (1 - y_i) \times log(1 - p_i))$$

RMSProp: https://arxiv.org/pdf/1609.04747.pdf
Binary cross-entropy: https://www.tensorflow.org/api_docs/python/tf/keras/losses/binary_crossentropy

Precision and loss for various optimisers



Precision and loss using neural network with dense layers



Precision and loss using less data