Neural Machine Translation Improvements Using Back-Translation, and Applications in CNN-based Protein-Ligand Docking Evaluation

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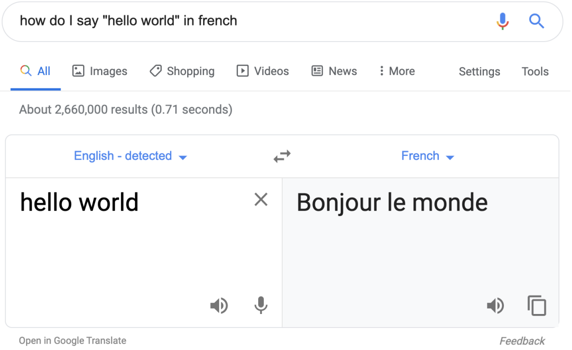
Machine Translation

- Computationally intensive means of bridging and interconverting language pairs



Types of Machine Translation [3]

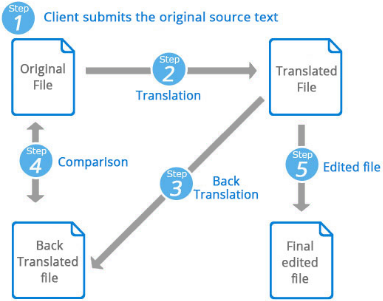
- Traditional Rules-Based Machine Translation:
    - Language organized into a corpus, or collections of known words or statements
    - Run through patterns, grammar, and lexicons
    - Reorganize against syntactic structures (ADJ-N-V-ADV)
- Statistical Machine Translation
    - No lexical or grammatical foreknowledge
    - References previous translations from database
- Neural Machine Translation
    - Data is processed into multiple layers iteratively using parallel processing and hardware acceleration
    - Algorithm use allows linguistic rules to be developed from previous models
    - Structured on encoding/decoding associated with human sensory processing

Essential Question

What if Language Data is Sparse?

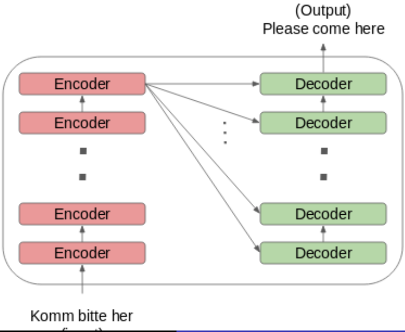
Back Translation

- Training a "Target to Source" pathway
- Monolingual language sets bridged together with synthetic data



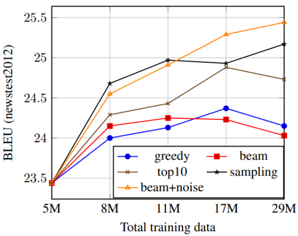
Edunov, Ott, Auli, and Grangier (2018) [1]

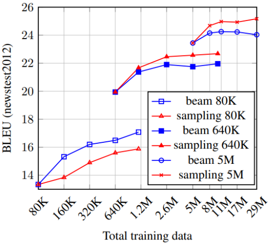
- WMT-2018 English-German Competitive Set w/o 250 word sentences or longer (226M sentences)
- Training Set: 52K sentence pairs
- 6 encode/decode blocks, 4096 feed-foward layers ("Big Transformer")



Edunov, et.al. Results (2018)

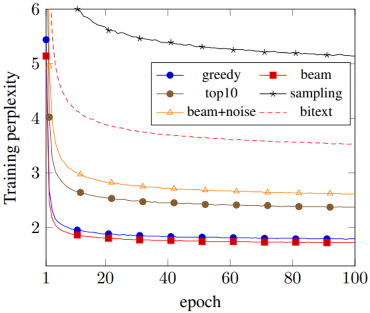
- BLEU(Bilingual Evaluation Understudy)
  - Individually translated segments are compared to a qualified reference
  - Individual scores are averaged against whole corpus
- Bitext- The alignment of relevant words and patterns
- Adding synthetic data (beam+noise and sampling) perform best





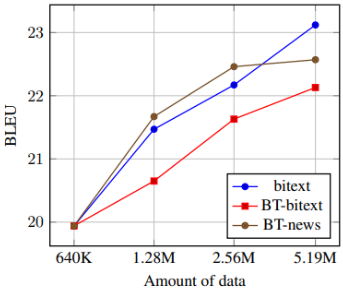
Edunov, et.al. Results (2018)

- Perplexity - how well a model predicts a sample
  - Greedy and Beam do not introduce synthetic data

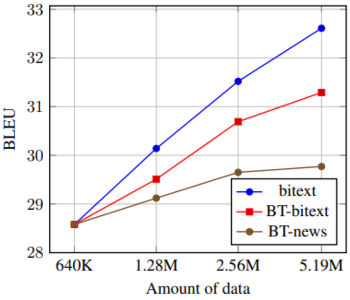


Edunov, et.al. Examining Synthetic Data

- subsample with: remaining data, aligned back-translated bitext, and raw-backtranslated data
- Back-Translated data performs almost as well as the bitext in comparison to raw newstest2012 set and a hybrid set



(a) newstest2012



(b) valid-mixed

Edunov, et.al Conclusions

- Back Translation is effective at augmenting datasets with respect to machine translation
- Synthetic data mostly increased performance
- Future work entails optimized selection of helpful synthetic data

Hoang, Haffari, Koehn, and Cohn

- Iterative Back Translation- feeding back translation back into the model
- Hypothesis: Better Back Translation = Better Synthetic Corpus = Better Translation Quality
- German-English and English-German Scenarios

Hoang, et.al Back Translation [2]

- Worst: 10k iterations
- Best: Convergence

German–English	Back	Final
no back-translation	-	29.6
10k iterations	10.6	29.6 (+0.0)
100k iterations	21.0	31.1 (+1.5)
convergence	23.7	32.5 (+2.9)

English–German	Back	Final
no back-translation	-	23.7
10k iterations	14.5	23.7 (+0.0)
100k iterations	26.2	25.2 (+1.5)
convergence	29.1	25.9 (+2.2)

Hoang, et.al Iterative "Re-Back" Back Translation

- Cycle through inputted back translations multiple times
- High and low resource conditions with shallow and deep architectures
  - Base - parallel data only, not yet back translated, shallow only
  - First - parallel and synthetic data, deep only
  - Final - shallow, deep, and 4-stage ensemble
  - Low Resources only- English-French, English-Farsi

Hoang, et.al High Resource Iterative BT

- Re-back back translation typically outperformed conventional back translation
- Out-performed best translation models of WMT 2017 Competition

German–English	Back*	Shallow	Deep	Ensemble
back-translation	23.7	32.5	35.0	35.6
re-back-translation	27.9	33.6	36.1	36.5
Best WMT 2017	-	-	-	35.1

English–German	Back*	Shallow	Deep	Ensemble
back-translation	29.1	25.9	28.3	28.8
re-back-translation	34.8	27.0	29.0	29.3
Best WMT 2017	-	-	-	28.3

Hoang, et.al Low Resource Iterative BT

- Moses- a Statistical Machine Translation model set, for comparison purposes
- Slight improvements over conventional back translation

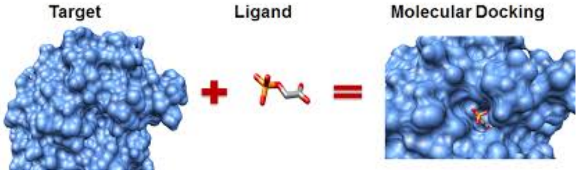
Setting	French–English		English–French		Farsi–English	English-Farsi
	100K	1M	100K	1M	100K	100K
NMT baseline	16.7	24.7	18.0	25.6	21.7	16.4
back-translation	22.1	27.8	21.5	27.0	22.1	16.7
back-translation iterative+1	22.5	-	22.7	-	22.7	17.1
back-translation iterative+2	22.6	-	22.6	-	22.6	17.2
back-translation (w/ Moses)	23.7	27.9	23.5	27.3	21.8	16.8

Hoang, et.al. Conclusions

- Both standard and iterative back-translation is quality dependent, and dependent on sampling
- Iterative back-translation clearly shows improved performance in comparison to standard back translation
- Future considerations will entail developing a unified end-to-end system

How is this Relevant?

- Quantum Mechanical Computations
  - Time and Resource Intensive
- Machine Learning Methods
  - Docking ligands (potential drugs) into a protein and evaluating the pose
  - Pose is evaluated using Convolutional Neural Networks once partitioned into 24Å grid spaces



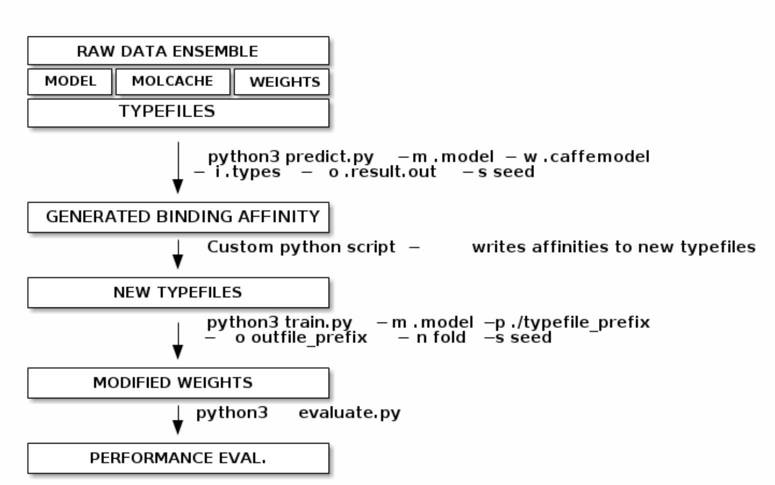
Essential Question

What if Data is Partially Unavailable?

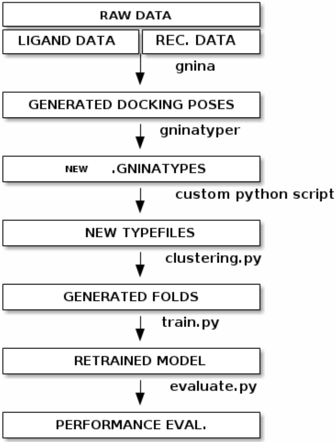
We Can Generate It!

- Project Proposal
  - Evaluate if adding computationally generated data improves model scoring performance
  - Generated Binding Affinities (CrossDock2020 Completeset) and Generated Protein-Ligand docking poses (BindingDB and PDBBind)

How This is Accomplished: Affinities



How This is Accomplished: Poses



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Questions