CS 533: Natural Language Processing

More Pretrained Transformers, Latent-Variable Generative Models

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Review: Pretrained Transformers

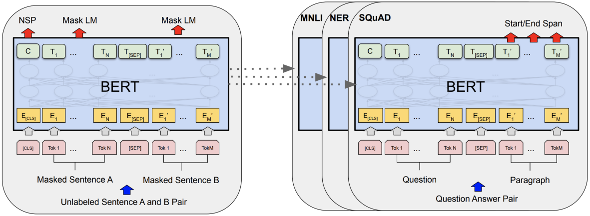
- Language models with Transformer architecture
- **Unsupervised transfer learning** (aka. "self-supervised" learning)
  1. Pretrain on a ton of raw text
  2. Finetune on a downstream task with modest supervision
- Enormous improvement over baselines trained from scratch on many NLU tasks
- Landmark: BERT (Devlin et al., 2019)
  - **Masked language modeling** (MLM)
  - "*this is too [MASK] to fit*" $\rightarrow$ "*big*"
  - Amenable to the full force of deep bidirectional self-attention in Transformer encoders

Some BERT Extensions

- RoBERTa (Liu et al., 2019)
  - A **R**obustly **o**ptimized **BERT** pretraining approach
  - Same as BERT but much more thoroughly optimized
  - Dynamic masking, no next sentence prediction (i.e., only MLM loss), BPE instead of wordpiece tokenization (thus language agnostic), trained with larger batch sizes for longer on more data
  - Very significant improvement, e.g., GLUE score
    - BERT (340m parameters): 80.5
    - RoBERTa (355m parameters): 88.1
    - Human: 87.1
- ALBERT (Lan et al., 2019)
  - **A L**ite **BERT**
  - Reduce number of parameters by: (1) Token embedding dimension bottleneck ($\ll$ hidden dimension), (2) Tying Transformer parameters across layers
  - Catch: The model is smaller but slower! Larger hidden dim
  - GLUE score 89.4 with ensembling

Pretraining Encoder-Decoder Models

- BERT only pretrains a Transformer *encoder*
  - Limited to simple downstream tasks like text classification, tagging, span finding



Pre-training Fine-Tuning

  - Critically, cannot be directly used for text generation
- How can we pretrain a Transformer *decoder*?
  - Can certainly just train it as a standard left-to-right LM (e.g., GPTs). But then no deep bidirectional self-attention
  - Is there a way to pretrain encoder & decoder jointly and get the best of both worlds?

BART (Lewis et al., 2019)

- Pronounced *bahrt* (vs. *burt* for BERT)
- Transformer encoder-decoder model trained as a *denoising autoencoder*
  - **Input.** $\text{Corrupt}(\text{text})$
  - **Output.** text
- Special cases
  - $\text{Corrupt}(\text{text}) = \varnothing$: $\approx$GPT
  - $\text{Corrupt}(\text{text}) = \text{MaskTokens}(\text{text})$: $\approx$BERT
  - $\text{Corrupt}(\text{text}) = \text{Permute}(\text{text})$: $\approx$XLNet (Yang et al., 2019)
- Great deal of flexibility in noise. Example: "text infilling", a span-level generalization of MLM
  - Span lengths sampled from $\text{Poisson}(\lambda = 3)$, *entire* span replaced by single [MASK], e.g.,

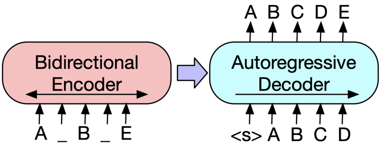
    $\text{Corrupt}($*There Is No Plan to Stop Chemical Weapons in Syria*$)$

    $=$ *There Is No Plan to [MASK] in Syria*

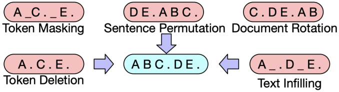
  - Model must learn to infer span lengths in denoising

BART Pretraining

- Best of both worlds
  1. Encoder: Deep bidirectional self-attention over corrupted text
  2. Decoder: Autoregressive prediction of *uncorrputed* text



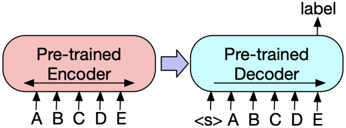
- Explored a vareity of noise schemes



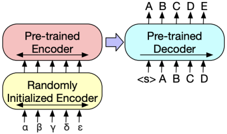
  - Token/span masking is again found to be crucial
  - Final choice: Text infilling + sentence-level shuffling
  - No single noise best for all: Performance highly task-dependent. E.g., for perplexity null corruption (plain left-to-right LM) sometimes best.

BART Finetuning

- Text-level classification
  1. Feed input text to encoder (if sentence pair, concatentated)
  2. Feed the *same* text to decoder conditioning on the encoding
  3. Use the last top hidden state of the decoder to classify



- Token-level classification (e.q., SQuAD-style QA, tagging): Same as text-level classification, only use top decoder hidden states as contextual token embeddings
- Conditional text generation: Directly finetune
- MT: Add a few randomly initialized encoder layers at input.

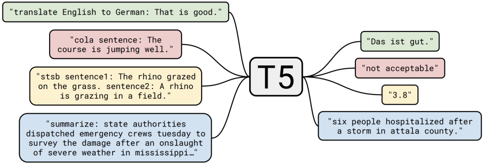


Details of BART

- Number of parameters $406m$ (vs. $355m$ of RoBERTa which has 24 encoder layers)
  - 12 Transformer encoder/decoder layers, dimension 1024
  - GPT-2 style BPE tokenization: Shared embs $E \in \mathbb{R}^{50265 \times 1024}$
- Pretraining
  - Noise: Text infilling + sentence-level shuffling. Input is a document. 30% tokens masked, sentences shuffled.
  - Closely follows RoBERTa: Same pretraining data (160gb of news, books, stories, web), $500k$ updates w/ batch size 8000
- Classification result: Matches RoBERTa
  - BART's generation capabilities don't come at the expense of classification performance
- At the same time, significant improvement on conditional text generation
  - Abstractive summarization (R1): CNN/DailyMail 42.13 $\rightarrow$ 44.16, XSum 38.81 $\rightarrow$ 45.14
  - MT (BLEU): WMT16 Ro-En 36.80 $\rightarrow$ 37.96

T5 (Raffel et al., 2020)

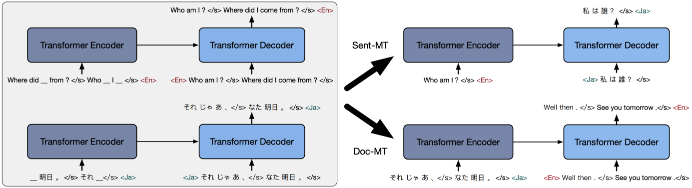
- **T**ext-**T**o-**T**ext **T**ransfer **T**ransformer
  - Concurrent work with BART on pretraining Transformer encoder-decoder model
  - Also based on large-scale denoising autoencoding, using a carefully cleaned version of the Common Crawl web scrapes
  - Additionally pretrained on a diverse set of *supervised* tasks framed as seq2seq problems



- Complementary insights confirming BART's findings
  - Denoising encoder-decoder more effective than decoder LM
  - For noise, token masking crucial
- One of the very top performers on GLUE/SuperGLUE
  - 11 billion parameters: 90.3 GLUE, 89.3 SuperGLUE

Multilingual/Domain-Specific Pretrained Transformers

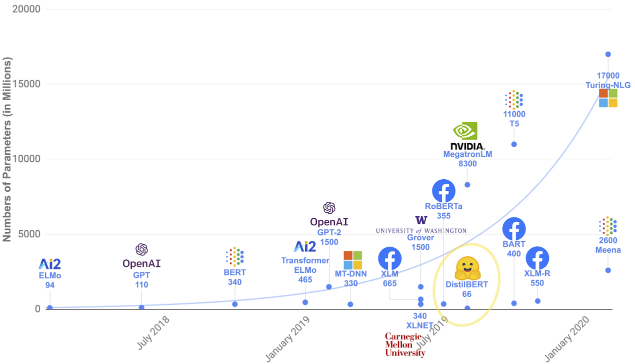
- Multilingual BERT: Released along with the original BERT
  - Same as BERT but trained on a union of Wikipedia dumps in 104 languages
  - Enables zero-shot cross-lingual model transfer (Pires et al., 2019): Finetune in language A, evaluate in language B
- Multilingual BART (mBART) (Liu et al., 2020)
  - Same as BART but trained on 25 languages extracted from Common Crawl with language identifier



  - Directly transferrable to MT tasks, huge improvement (esp for low-resource languages)
- Domain specific BERTs: BioBERT (Lee et al., 2019) for biomedical text, SciBERT (AI2) for scientific text

The Model Size Problem

- Pretrained LMs growing rapidly in size



(Image Credit: TensorFlow Blog)

  - Impossible to train except industry, difficult to use
  - Focus of NLP shifted too much on sheer engineering (brainless usage of larger models)
  - Also bad for the environment: Training a BERT on GPU emits as much CO_2 as a trans-American flight (Strubell et al., 2019)

Model Compression/Knowledge Distillation (KD)

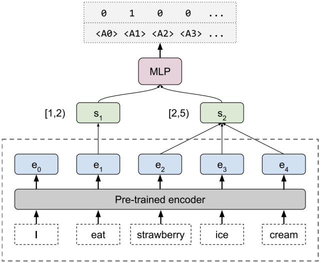
- KD: Train a big "teacher" model p_{teacher}, learn a small "student" model p_θ by minimizing

$$J(\theta) = -\frac{1}{N} \sum_{i=1}^{N} \sum_{y \in \mathcal{Y}} p_{\text{teacher}}(y|x_i) \log p_\theta(y|x_i)$$

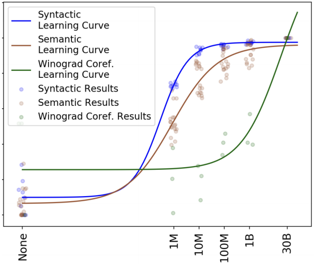
- Form of regularization, in particular label smoothing
  - If $p_{\text{teacher}}(y_i|x_i) = 1$ then back to usual cross entropy. Can be controlled by softmax temperature (Hinton et al., 2015)
  - Big models have capacity to induce broader patterns, make small models mimic rather than figure out on their own
- Example: DistilBERT (Sanh et al., 2020)
  - Teacher: BERT-base ($110m$). Student: BERT-base with half of layers removed ($67m$)
  - 40% smaller, 60% faster, GLUE score down by 79.5 $\rightarrow$ 77.0
- Can also sample from teacher (e.g., if y is a sequence)
  - KD: Use teacher predictions not gold labels (Kim and Rush, 2016)

What Does a Pretrained LM Know?

- **Probing.** Freeze pretrained model, train a classifier on top for simplified linguistic tasks (POS tagging, NER, semantic role labeling, etc.)
  - The more it "contains" linguistic knowledge, the better probing performance
- Easily solved even with small-scale pretraining
- In contrast, NLU tasks require billions of pretraining tokens before working



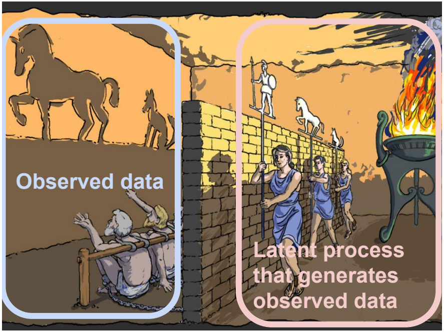
(Tenney et al., 2019)



(Zhang et al., 2020)

Introducing Latent Variables in Generative Models

- Generative models (e.g., LMs) define $p_\theta(x)$
  - The only random variable is observation x
- Idea: Introduce additional variable z and explicitly model an unseen generative process
  - We believe the process to be true (or at least useful for something), even though we don't observe it



(Original Image: 4edges/Wikimedia Commons)

Latent-Variable Generative Models (LVGMs)

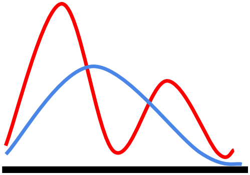
- p_θ defining a *joint* distribution over observation $x \in \mathcal{X}$ and latent variable $z \in \mathcal{Z}$

$$p_\theta(x, z) = \underbrace{\kappa_\theta(x|z)}_{\text{conditional likelihood}} \times \underbrace{\pi_\theta(z)}_{\text{prior}}$$

- Very general definition
  - Can be discrete, continuous, or mixed
  - x can be structured, z can be structured, or both
- Why introduce latent variables?
  1. Clear generative story: Sample $z \sim \pi_\theta(z)$, then $x \sim \kappa_\theta(\cdot|z)$
  2. *Marginal* observation distribution can be more expressive
  3. Latent variables can be useful: Controllable generation (i.e., change z to get x we want), z natural representation of x

Marginal Observation Distribution

- LVGM defines a marginal distribution m_θ over $\mathcal{X}$
  - If z is discrete: $m_\theta(x) = \sum_{z \in \mathcal{Z}} p_\theta(x, z)$
  - If z is continuous: $m_\theta(x) = \int_{z \in \mathcal{Z}} p_\theta(x, z) dz$
  - If z is mixed: sum/integrate out appropriate dimensions
- m_θ can express a larger family of distributions
- Example: Bimodal distribution over $\mathcal{X} = \mathbb{R}$ cannot be expressed by any single Gaussian $\mathcal{N}(\mu, \sigma^2)$



- But can be expressed by a mixture of two Gaussians:

$$m_\theta(x) = \pi_1 \mathcal{N}(\mu_1, \sigma_1^2)(x) + \pi_2 \mathcal{N}(\mu_2, \sigma_2^2)(x)$$

Discrete latent variable $\mathcal{Z} = \{1, 2\}$

Better Explanation of Data

- Suppose iid samples from unknown $\mathbf{pop}$ over $\{a, b\}^{10}$ look like

$$x^{(1)} = (a, a, a, a, a, a, a, a, a, a) \qquad x^{(2)} = (b, b, b, b, b, b, b, b, b, b)$$
$$x^{(3)} = (a, a, a, a, a, a, a, a, a, a) \qquad x^{(4)} = (b, b, b, b, b, b, b, b, b, b)$$
$$x^{(5)} = (a, a, a, a, a, a, a, a, a, a) \qquad x^{(6)} = (b, b, b, b, b, b, b, b, b, b)$$

- Bag-of-words model $p_\theta(x) = \prod_{j=1}^{10} p_\theta(x_j)$?
  - The model's independence assumption is clearly wrong!
  - Poor data fit: At most $p_\theta(x^{(i)}) = 2^{-10} < 0.001$ for each i
- LVGM $m_\theta(x) = \sum_{z \in \{1,2\}} \pi_\theta(z) \times \prod_{j=1}^{10} \kappa_\theta(x_j|z)$
  - The model makes the right assumption (draw a latent "topic" z and draw observation conditioned on z).
  - Can achieve $m_\theta(x^{(i)}) = 2^{-1}$ for each i with only twice more parameters
  - Also likely to generalize better (i.e., higher log liklihood of future samples)

Example LVGMs

- **HMMs**: $z \in \mathcal{Z}^T$ (unobserved label sequence), $x \in \mathcal{V}^T$ (sentence)

$$p_\theta(x, z) = \prod_{t=1}^{T+1} t_\theta(z_t | z_{t-1}) \times \prod_{t=1}^{T} o_\theta(x_t | z_t)$$

- **Gaussian LM**: $z \in \mathbb{R}^d$ ("thought vector"), $x \in \mathcal{V}^T$ (sentence)

$$p_\theta(x, z) = \mathcal{N}(0_d, I_{d \times d})(z) \times \prod_{t=1}^{T+1} p_\theta(x_t | x_{<t}, z)$$

- **Document hashing**: $z \in \{0, 1\}^d$ ("hash code"), $x \in \mathbb{R}^V$ (TFIDF document encoding)

$$p_\theta(x, z) = \prod_{j=1}^{d} \mathrm{Bernoulli}(\lambda_j)(z_j) \times \prod_{k=1}^{V} p_\theta(x_k | z)$$

Marginal Log Likelihood

- Training objective: Maximize marginal log likelihood (MLL)

$$L(\theta) = \mathop{\mathbf{E}}_{x \sim \mathbf{pop}} [\log m_\theta(x)]$$

  (Equivalent to cross entropy minimization, but convenient to frame as maximization for later)
- Requires the ability to calculate marginal probability of x!

$$m_\theta(x) = \mathbf{E}_{z \sim \pi_\theta} [\kappa_\theta(x|z)]$$

- Sometimes we can calculate it exactly (best scenario)
  - z is discrete and $\mathcal{Z}$ is small: $m_\theta(x) = \sum_{z \in \mathcal{Z}} p_\theta(x, z)$ directly computable
  - p_θ makes Markov assumptions: $m_\theta(x)$ computable by dynamic programming (e.g., forward algorithm for HMMs)
- In general, we need to approximate by sampling

Variance Reduction by Importance Sampling

- Have an $x \in \mathcal{X}$, would like to estimate $L_x(\theta) = \log m_\theta(x)$
- Naive scheme: Draw K iid samples $z^{(1)} \ldots z^{(K)} \sim \pi_\theta$ and use $\widehat{L}_x^K(\theta) = (1/K)\sum_{k=1}^K \log \kappa_\theta(x|z^{(k)})$
  - Unbiased: As $K \to \infty$ we have $\widehat{L}_x^K(\theta) \to L_x(\theta)$
  - Problem: High variance. What if $\kappa_\theta(x|z^*) = 1$ for a single $z^* \in \mathcal{Z}$ but $\pi_\theta(z^*)$ is tiny?
- Reduce variance by introducing an **inference network** (aka. approximate posterior) $q_\phi(z|x)$ that tells us which z is "important" for x
- For any choice of q_ϕ (full support)

$$L_x(\theta) \overset{(1)}{=} \log \mathop{\mathbf{E}}_{z \sim q_\phi(\cdot|x)} \left[\frac{p_\theta(x,z)}{q_\phi(z|x)}\right] \overset{(2)}{\geq} \mathop{\mathbf{E}}_{z \sim q_\phi(\cdot|x)} \left[\log \frac{p_\theta(x,z)}{q_\phi(z|x)}\right]$$

(1) Importance sampling, (2) Jensen's inequality (log is concave)

ELBO

- **E**vidence **L**ower **Bo**und

$$\mathrm{ELBO}(\theta, \phi) = \mathop{\mathbf{E}}_{x \sim \mathbf{pop},\, z \sim q_\phi(\cdot|x)} \left[\log \frac{p_\theta(x, z)}{q_\phi(z|x)} \right] \leq L(\theta)$$

- A variational lower bound on MLL ("variational" means optimization-based)
- We are learning *three* distributions
  1. Prior $\pi_\theta(z)$
  2. Conditional likelihood $\kappa_\theta(x|z)$
  3. Approximate posterior $q_\phi(z|x)$: This is an "optimization assistant".
- In fact, the gap is precisely

$$L(\theta) - \mathrm{ELBO}(\theta, \phi) = D_{\mathrm{KL}}(q_\phi || \omega_\theta)$$

where $\omega_\theta(z|x) = \frac{p_\theta(x,z)}{m_\theta(x)}$ is the true posterior probability, thus

$$\mathrm{ELBO}(\theta, \phi) = L(\theta) \quad \Leftrightarrow \quad q_\phi(z|x) = \omega_\theta(z|x) \;\; \forall x, z$$

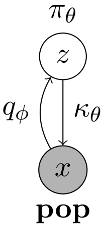
Exact Relationship Between ELBO and MLL

$$
\begin{aligned}
L(\theta) &= \mathop{\mathbf{E}}_{x \sim \mathbf{pop}} \left[\log m_\theta(x) \right] \\
&= \mathop{\mathbf{E}}_{x \sim \mathbf{pop},\ z \sim q_\phi(\cdot|x)} \left[\log m_\theta(x) \right] \\
&= \mathop{\mathbf{E}}_{x \sim \mathbf{pop},\ z \sim q_\phi(\cdot|x)} \left[\log \frac{m_\theta(x)\omega_\theta(z|x)q_\phi(z|x)}{\omega_\theta(z|x)q_\phi(z|x)} \right] \\
&= \underbrace{\mathop{\mathbf{E}}_{x \sim \mathbf{pop},\ z \sim q_\phi(\cdot|x)} \left[\log \frac{p_\theta(x,z)}{q_\phi(z|x)} \right]}_{\mathrm{ELBO}(\theta,\phi)} + \underbrace{\mathop{\mathbf{E}}_{x \sim \mathbf{pop},\ z \sim q_\phi(\cdot|x)} \left[\log \frac{q_\phi(z|x)}{\omega_\theta(z|x)} \right]}_{D_{\mathrm{KL}}(q_\phi || \omega_\theta)}
\end{aligned}
$$

Variational Autoencoders (VAEs) (Kingma and Welling, 2014)

- **VAE.** Maximizing ELBO written as an autoencoding objective

$$\begin{aligned}
\mathrm{ELBO}(\theta, \phi) &= \mathop{\mathbf{E}}_{x \sim \mathbf{pop},\ z \sim q_\phi(\cdot|x)} \left[\log \frac{\kappa_\theta(x|z)\pi_\theta(z)}{q_\phi(z|x)} \right] \\
&= \underbrace{\mathop{\mathbf{E}}_{x \sim \mathbf{pop},\ z \sim q_\phi(\cdot|x)} \left[\log \kappa_\theta(x|z) \right]}_{\text{reconstruction}} - \underbrace{\mathop{\mathbf{E}}_{x \sim \mathbf{pop}} \left[D_{\mathrm{KL}}(q_\phi(\cdot|x) || \pi_\theta) \right]}_{\text{regularization}}
\end{aligned}$$



- Reconstruction term large if $q_\phi(\cdot|x)$ encodes x into z well and $\kappa_\theta(\cdot|z)$ decodes z back to x well
- Regularization term small if $q_\phi(\cdot|x) \approx \pi_\theta$ in expectation

Example: Gaussian VAE for Language Modeling

- Continuous latent space $\mathcal{Z} = \mathbb{R}^d$
- Observation space $\mathcal{X} = \mathcal{V}^*$ (i.e., all sentences)
- Model
  - Prior: $\pi_\theta = \mathcal{N}(0_d, I_{d\times d})$ (no learnable parameters)
  - Conditional likelihood: $\kappa_\theta(x|z) = \prod_{t=1}^{T+1} \kappa_\theta(x_t|x_{<t}, z)$. This can be any conditional word distribution that additionally conditions on $z \in \mathbb{R}^d$
- Inference network: $q_\phi(z|x) = \mathcal{N}(\mu_\phi(x), \mathrm{diag}(\sigma^2_\phi(x)))$ where

$$\begin{bmatrix} \mu_\phi(x) \\ \sigma^2_\phi(x) \end{bmatrix} = \underbrace{\textbf{enc}_\phi(x)}_{\text{any sentence encoder (e.g., LSTM last state)}} \in \mathbb{R}^{2d}$$

- The Gaussian parameterization enables a particularly effective estimation of ELBO
  - KL between Gaussians: Closed form
  - Differentiable sampling by **reparameterization trick**: $z \sim \mathcal{N}(\mu, \sigma^2) \Leftrightarrow z = \mu + \sigma \cdot \epsilon$ where $\epsilon \sim \mathcal{N}(0, 1)$

Example: Gaussian VAE for Language Modeling (Cont.)

- ELBO for a single sentence x for clarity
- KL term:

$$\begin{aligned} D_{\mathrm{KL}}(q_\phi(\cdot|x)||\pi_\theta) &= D_{\mathrm{KL}}(\mathcal{N}(\mu_\phi(x), \mathrm{diag}(\sigma^2_\phi(x)))||\mathcal{N}(0_d, I_{d\times d})) \\ &= \frac{1}{2}\left(\sum_{i=1}^{d}[\sigma^2_\phi(x)]_i + [\mu_\phi(x)]_i^2 - 1 - \log[\sigma^2_\phi(x)]_i\right) \end{aligned}$$

- Reconstruction term: Single-sample estimation, $\epsilon \sim \mathcal{N}(0_d, I_{d\times d})$

$$\mathop{\mathbf{E}}_{z\sim q_\phi(\cdot|x)}[\log \kappa_\theta(x|z)] \approx \underbrace{\log \kappa_\theta(x|\mu_\phi(x) + \sigma_\phi(x) \odot \epsilon)}_{\widehat{R}_x(\theta,\phi)}$$

- Take a gradient step on $\beta D_{\mathrm{KL}}(q_\phi(\cdot|x)||\pi_\theta) - \widehat{R}_x(\theta, \phi)$.