CPSC 440: Advanced Machine Learning

Deep Structured Models

Mark Schmidt

University of British Columbia

Winter 2021

Backpropagation as Message-Passing

- Computing the gradient in neural networks is called backpropagation.
  - Derived from the chain rule and memoization of repeated quantities.
- We're going to view backpropagation as a message-passing algorithm.
- Key advantages of this view:
  - It's easy to handle different graph structures.
  - It's easy to handle different non-linear transformations.
  - It's easy to handle multiple outputs (as in structured prediction).
  - It's easy to add non-deterministic parts and combine with other graphical models.

Backpropagation Forward Pass

- Consider computing the output of a neural network for an example i,

$$y^i = v^T h(W^3 h(W^2 h(W^1 x^i)))$$
$$= \sum_{c=1}^{k} v_c h\left(\sum_{c'=1}^{k} W^3_{c'c} h\left(\sum_{c''=1}^{k} W^2_{c''c'} h\left(\sum_{j=1}^{d} W^1_{c''j} x^i_j\right)\right)\right).$$

  where we've assume that all hidden layers have k values.
  - In the second line, the h functions are single-input single-output.

- The nested sum structure is similar to our message-passing structures.

- However, it's easier because it's deterministic: no random variables to sum over.
  - The messages will be scalars rather than functions.

Backpropagation Forward Pass

- Forward propagation through neural network as message passing:

$$
\begin{aligned}
y^i &= \sum_{c=1}^{k} v_c h\left(\sum_{c'=1}^{k} W^3_{c'c} h\left(\sum_{c''=1}^{k} W^2_{c''c'} h\left(\sum_{j=1}^{d} W^1_{c''j} x^i_j\right)\right)\right) \\
&= \sum_{c=1}^{k} v_c h\left(\sum_{c'=1}^{k} W^3_{c'c} h\left(\sum_{c''=1}^{k} W^2_{c''c'} h(M_{c''})\right)\right) \\
&= \sum_{c=1}^{k} v_c h\left(\sum_{c'=1}^{k} W^3_{c'c} h(M_{c'})\right) \\
&= \sum_{c=1}^{k} v_c h(M_c) \\
&= M_y,
\end{aligned}
$$

where intermediate messages are the z values.

Backpropagation Backward Pass

- The backpropagation backward pass computes the partial derivatives.
  - For a loss f, the partial derivatives in the last layer have the form

$$\frac{\partial f}{\partial v_c} = z_c^{i3} f'(v^T h(W^3 h(W^2 h(W^1 x^i)))),$$

where

$$z_{c'}^{i3} = h\left(\sum_{c'=1}^{k} W_{c'c}^3 h\left(\sum_{c''=1}^{k} W_{c''c'}^2 h\left(\sum_{j=1}^{d} W_{c''j}^1 x_j^i\right)\right)\right).$$

  - Written in terms of messages it simplifies to

$$\frac{\partial f}{\partial v_c} = h(M_c) f'(M_y).$$

Backpropagation Backward Pass

- In terms of forward messages, the partial derivatives have the forms:

$$\frac{\partial f}{\partial v_c} = h(M_c)f'(M_y),$$

$$\frac{\partial f}{\partial W^3_{c'c}} = h(M_{c'})h'(M_c)w_c f'(M_y),$$

$$\frac{\partial f}{\partial W^2_{c''c'}} = h(M_{c''})h'(M_{c'})\sum_{c=1}^{k} W^3_{c'c}h'(M_c)w_c f'(M_y),$$

$$\frac{\partial f}{\partial W^1_{jc''}} = h(M_j)h'(M_{c''})\sum_{c'=1}^{k} W^2_{c''c'}h'(M_{c'})\sum_{c=1}^{k} W^3_{c'c}h'(M_c)w_c f'(M_y),$$

which are ugly but notice all the repeated calculations.

Backpropagation Backward Pass

- It's again simpler using appropriate messages

$$\frac{\partial f}{\partial v_c} = h(M_c) f'(M_y),$$

$$\frac{\partial f}{\partial W^3_{c'c}} = h(M_{c'}) h'(M_c) w_c V_y,$$

$$\frac{\partial f}{\partial W^2_{c''c'}} = h(M_{c''}) h'(M_{c'}) \sum_{c=1}^{k} W^3_{c'c} V_c,$$

$$\frac{\partial f}{\partial W^1_{jc''}} = h(M_j) h'(M_{c''}) \sum_{c'=1}^{k} W^2_{c''c'} V_{c'},$$

where $M_j = x_j$.

Backpropagation as Message-Passing

- The general forward message for child c with parents p and weights W is

$$M_c = \sum_p W_{cp} h(M_p),$$

  which computes weighted combination of non-linearly transformed parents.
  - In the first layer we don't apply h to x.
- The general backward message from child c to *all* its parents is

$$V_c = h'(M_c) \sum_{c'} W_{cc'} V_{c'},$$

  which weights the "grandchildren's gradients".
  - In the last layer we use f instead of h.
- The gradient of W_{cp} is $h(M_c)V_p$, which works for general graphs.

Automatic Differentiation

- Automatic differentiation:
  - Input is code that computes a function value.
  - Output is code computing is one or more derivatives of the function.

- Forward-mode automatic differentiation:
  - Computes a directional derivative for cost of evaluating function.
    - So computing gradient would be d-times more expensive than function.
  - Low memory requirements.
  - Most useful for evaluating Hessian-vector products, $\nabla^2 f(w)d$.

- Reverse-mode automatic differentiation:
  - Computes gradient for cost of evaluating function.
  - But high memory requirements: need to store intermediate calculations.
    - Backpropagation is (essentially) a special case.
- Reverse-mode is replacing "gradient by hand" (less time-consuming/bug-prone).

Combining Neural Networks and CRFs

- Previously we saw conditional random fields like

$$p(y \mid x) \propto \exp\left(\sum_{c=1}^{k} y_c v^T x_c + \sum_{(c,c')\in E} y_c y_{c'} w\right),$$

  which can use logistic regression at each location c and Ising dependence on y_c.

- Instead of logistic regression, you could put a neural network in there:

$$p(y \mid x) \propto \exp\left(\sum_{c=1}^{k} y_c v^T h(W^3 h(W^2(W^1 x_c))) + \sum_{(c,c')\in E} y_c y_{c'} w\right).$$

- Sometimes called a conditional neural field or deep structured model.
- Backprop generalizes:
  1. Forward pass through neural network to get $\hat{y}_c$ predictions.
  2. Belief propagation to get marginals of y_c (or Gibbs sampling if high treewidth).
  3. Backwards pass through neural network to get all gradients.

Multi-Label Classification

- Consider multi-label classification:

http://proceedings.mlr.press/v37/chenb15.pdf

- Flickr dataset: each image can have multiple labels (out of 38 possibilities).

- Use neural networks to generate “factors” in an undirected model.
  - Decoding undirected model makes predictions accounting for label correlations.

Multi-Label Classification

- Learned correlation matrix:

	female	people	indoor	baby	sea	portrait	transport	flower	sky	lake	structures	bird	plant life	food	male	clouds	water	animals	car	tree	dog	sunset	night	river
female	0.00	0.68	0.04	0.06	0.02	0.24	0.03	−0.00	−0.01	0.01	0.04	−0.00	−0.05	−0.01	0.07	−0.01	−0.00	−0.12	0.04	0.01	0.01	0.02	0.04	0.02
people	0.68	0.00	0.06	0.06	−0.00	0.36	0.03	−0.08	−0.05	−0.03	0.02	−0.06	−0.12	−0.05	0.74	−0.04	−0.03	−0.21	0.01	−0.03	−0.03	−0.03	0.05	−0.03
indoor	0.04	0.06	0.00	0.05	−0.06	0.07	−0.12	−0.07	−0.35	−0.03	−0.46	−0.02	−0.34	0.11	0.02	−0.15	−0.14	−0.01	−0.07	−0.21	0.03	−0.08	0.06	−0.03
baby	0.06	0.06	0.05	0.00	0.10	0.11	0.07	0.09	0.03	0.10	0.01	0.10	0.02	0.09	0.06	0.08	0.07	0.07	0.08	0.06	0.09	0.09	0.08	0.10
sea	0.02	−0.00	−0.06	0.10	0.00	0.04	0.08	0.05	0.16	0.17	−0.02	0.09	−0.02	0.06	0.03	0.14	0.36	0.06	0.05	0.01	0.08	0.14	0.06	0.10
portrait	0.24	0.36	0.07	0.11	0.04	0.00	0.01	0.03	−0.02	0.05	−0.02	0.04	−0.01	0.03	0.12	0.02	0.01	−0.07	0.05	0.05	0.03	0.04	0.07	0.05
transport	0.03	0.03	−0.12	0.07	0.08	0.01	0.00	0.02	0.14	0.07	0.14	0.04	0.05	0.03	0.06	0.08	0.07	−0.03	0.36	0.10	0.04	0.05	0.04	0.07
flower	−0.00	−0.08	−0.07	0.09	0.05	0.03	0.02	0.00	0.02	0.07	−0.03	0.07	0.34	0.04	−0.04	0.04	0.04	0.02	0.05	0.06	0.06	0.06	0.02	0.07
sky	−0.01	−0.05	−0.35	0.03	0.16	−0.02	0.14	0.02	0.00	0.12	0.22	0.04	0.24	−0.02	−0.00	0.44	0.12	−0.04	0.10	0.30	0.01	0.23	0.05	0.11
lake	0.01	−0.03	−0.03	0.10	0.17	0.05	0.07	0.07	0.12	0.00	−0.00	0.09	0.09	0.07	0.01	0.12	0.26	0.06	0.06	0.10	0.07	0.12	0.07	0.18
structures	0.04	0.02	−0.46	0.01	−0.02	−0.02	0.14	−0.03	0.22	−0.00	0.00	0.01	0.04	−0.05	0.06	0.08	−0.04	−0.06	0.14	0.09	−0.00	0.06	0.03	0.02
bird	−0.00	−0.06	−0.02	0.10	0.09	0.04	0.04	0.07	0.04	0.09	0.01	0.00	0.04	0.07	−0.01	0.06	0.09	0.26	0.06	0.05	0.07	0.09	0.05	0.09
plant life	−0.05	−0.12	−0.34	0.02	−0.02	−0.01	0.05	0.34	0.24	0.09	0.04	0.04	0.00	−0.03	−0.07	0.09	0.01	0.01	0.08	0.68	0.02	0.05	−0.07	0.10
food	−0.01	−0.05	0.11	0.09	0.06	0.03	0.03	0.04	−0.02	0.07	−0.05	0.07	−0.03	0.00	−0.01	0.03	0.03	0.03	0.05	0.01	0.06	0.06	0.04	0.07
male	0.07	0.74	0.02	0.06	0.03	0.12	0.06	−0.04	−0.00	0.01	0.06	−0.01	−0.07	−0.01	0.00	0.00	−0.01	−0.10	0.04	−0.02	0.01	0.00	0.06	0.01
clouds	−0.01	−0.04	−0.15	0.08	0.14	0.02	0.08	0.04	0.44	0.12	0.08	0.06	0.09	0.03	0.00	0.00	0.09	−0.00	0.07	0.11	0.05	0.22	−0.01	0.10
water	−0.00	−0.03	−0.14	0.07	0.36	0.01	0.07	0.04	0.12	0.26	−0.04	0.09	0.01	0.03	−0.01	0.09	0.00	0.05	0.02	0.03	0.05	0.10	0.03	0.27
animals	−0.12	−0.21	−0.01	0.07	0.06	−0.07	−0.03	0.02	−0.04	0.06	−0.06	0.26	0.01	0.03	−0.10	−0.00	0.05	0.00	0.02	0.00	0.22	0.03	−0.01	0.05
car	0.04	0.01	−0.07	0.08	0.05	0.05	0.36	0.05	0.10	0.06	0.14	0.06	0.08	0.05	0.04	0.07	0.02	0.02	0.00	0.11	0.06	0.08	0.07	0.06
tree	0.01	−0.03	−0.21	0.06	0.01	0.05	0.10	0.06	0.30	0.10	0.09	0.05	0.68	0.01	−0.02	0.11	0.03	0.00	0.11	0.00	0.04	0.09	−0.00	0.12
dog	0.01	−0.03	0.03	0.09	0.08	0.03	0.04	0.06	0.01	0.07	−0.00	0.07	0.02	0.06	0.01	0.05	0.05	0.22	0.06	0.04	0.00	0.06	0.05	0.07
sunset	0.02	−0.03	−0.08	0.09	0.14	0.04	0.05	0.06	0.23	0.12	0.06	0.09	0.05	0.06	0.00	0.22	0.10	0.03	0.08	0.09	0.06	0.00	0.06	0.10
night	0.04	0.05	0.06	0.08	0.06	0.07	0.04	0.02	0.05	0.07	0.03	0.05	−0.07	0.04	0.06	−0.01	0.03	−0.01	0.07	−0.00	0.05	0.06	0.00	0.07
river	0.02	−0.03	−0.03	0.10	0.10	0.05	0.07	0.07	0.11	0.18	0.02	0.09	0.10	0.07	0.01	0.10	0.27	0.05	0.06	0.12	0.07	0.10	0.07	0.00

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Automatic Differentiation (AD) vs. Inference

- If you use exact inference methods, automatic differentiation will give gradient.
  - You write message-passing code to compute Z.
  - AD modifies your code to compute expectations in gradient.
- With approximate inference, AD may or may not work:
  - AD will work for iterative variational inference methods (which we'll cover later).
  - AD will not tend to work for Monte Carlo methods.
    - Can't AD through sampling (but there exist tricks like "common random numbers").
- Recent trend: run iterative variational method for a fixed number of iterations.
  - AD can give gradient of result after this fixed number of iterations.
  - "Train the inference you will use at test time".

Deep Learning for Structured Prediction (Big Picture)

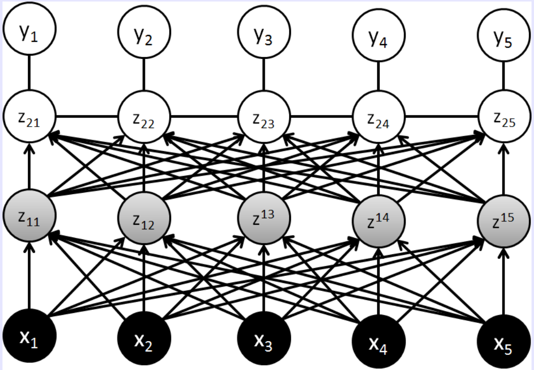
- How is deep learning being used for structured prediction applications?
  - Discriminative approaches are most popular.

- Typically you will send x through a neural network to get representation z, then:
  1. Perform inference on $p(y \mid z)$ (backpropagate using exact/approximate marginals).
     - Neural network learns features, CRF "on top" models dependencies in y_c.
  2. Run m approximate inference steps on $p(y \mid z)$, backpropagate through these steps.
     - "Learn to use the inference you will be using" (usually with variational inference).
  3. Just model each $p(y_c \mid z)$ (treat labels as independent given representation).
     - Assume that structure is already captured in neural network goo (no inference).

- Current trend: less dependence on inference and more on learning representation.
  - "Just use an RNN rather than thinking about stochastic grammars."
  - We're improving a lot at learning features, less so for inference.
  - This trend may or may not reverse in the future...

Neural Networks with Latent-Dynamics

- Instead of modeling y dependencies, could random z values.
  - Like an HMM with neural networks defining the hidden dynamics.



- Combines deep learning, mixture models, and graphical models.
  - "Latent-dynamics model".
  - Previously achieved among state of the art in several applications.

Summary

- Implicit regularization:
  - Some optimization methods may converge to regularized solutions.
- Double descent curves:
  - Weird phenomenon from increasing regularization as you increase complexity.
- Backpropagation can be viewed as a message passing algorithm.
- Combining CRFs with deep learning.
  - You can learn the features and the label dependency at the same time.
- Reducing the reliance on inference is a current trend in the field.
  - Rely on neural network to learn clusters and dependencies.
- Next time: "end-to-end" learning.