

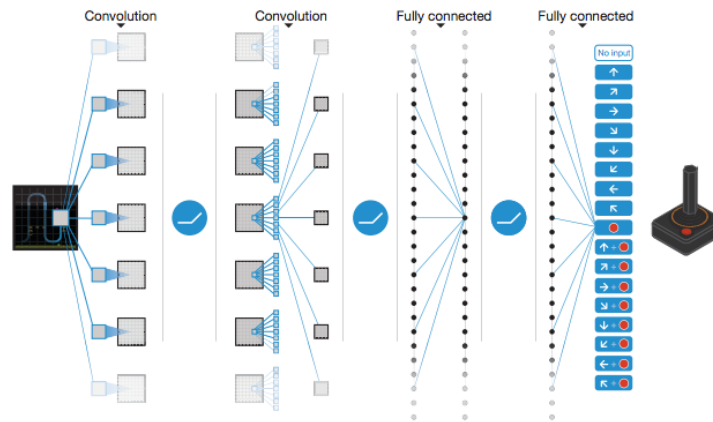
# **TTIC 31230, Fundamentals of Deep Learning**

David McAllester, April 2017

## **Deep Graphical Models**

# Review: Deep Q Networks (DQN)

Q-network  $Q_{\Theta}(s, a)$



$$\Theta \leftarrow \Theta + \eta \nabla_{\Theta} (Q_{\Theta}(s_t, a_t) - R_t)^2$$

$$\pi(s) \leftarrow \underset{a}{\operatorname{argmax}} Q_{\Theta}(s, a)$$

## Review: Asynchronous Advantage Actor-Critic (A3C)

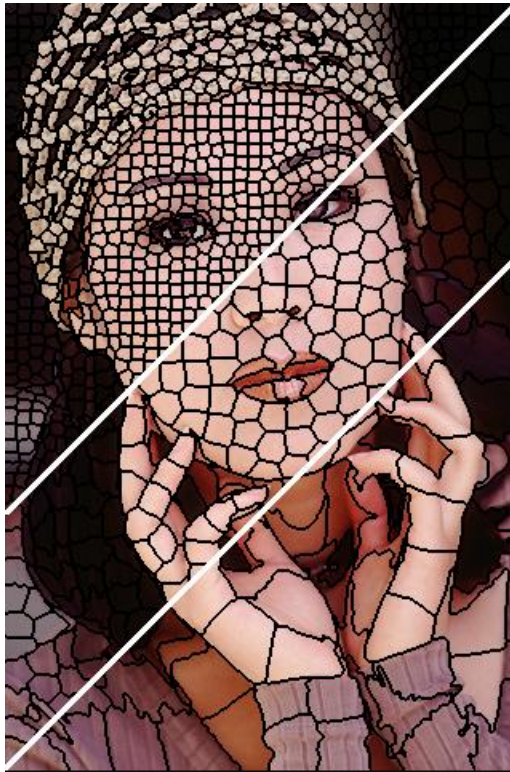
Policy network  $\pi_{\Phi}(a|s)$   
State value network  $V_{\Psi}(s)$

$$\Phi \ += \ \eta \left( \nabla_{\Phi} \ln \pi_{\Phi}(a_t|s_t) \right) (R_t - V_{\Psi}(s_t))$$

$$\Psi \ -= \ \eta \nabla_{\Psi} (V_{\Psi}(s_t) - R_t)^2$$

# Deep Graphical Models

## Image Segmentation with Superpixels



[Achanta et al.]

We want to assign each superpixel a semantic label. Maybe “face”, “hand”, or “hat”. (More typically “person”, “car”, “road”, “building” or “background”).

## Exponential Softmax

If we have  $K$  superpixels and  $N$  possible semantic labels we have  $N^K$  possible semantic labelings.

We will define a probability distribution over the semantic labelings with an **exponential softmax**.

## Segmentation Features

We have  $K$  superpixels and  $N$  possible semantic labels.

We define  $KN$  features  $U_{k,n}$  where  $U_{k,n} = 1$  if segment  $k$  has label  $n$  and 0 otherwise.

If each superpixel has  $D$  neighbors we define  $DK/2$  features  $B_{k,k'}$  where  $B_{k,k'} = 1$  (with  $k < k'$ ) if neighboring segments  $k$  and  $k'$  have different labels, and 0 otherwise.

Let  $\Phi(y)$  be the feature vector of segmentation  $y$ .

## Scoring by Weighting Features

We can score a segmentation  $y$  by providing a vector of weights for the features.

$$s_w(y) = w \cdot \Phi(y)$$

We can then define an exponential softmax over the semantic assignments.

$$P_w(y) = \operatorname{softmax}_y s_w(y)$$



## Weight Networks

We will consider a weight network  $W_{\Theta}(x)$  which assigns weights to the features of  $y$ .

$$s_{\Theta}(y|x) = W_{\Theta}(x) \cdot \Phi(y)$$

$$P_{\Theta}(y|x) = \underset{y}{\text{softmax}} \ s_{\Theta}(y|x)$$

## Cross Entropy Training

$$\Theta^* = \underset{\Theta}{\operatorname{argmin}} \operatorname{E}_{(x,y) \sim D} [-\ln P_{\Theta}(y|x)]$$

$$P_{\Theta}(y|x) = \operatorname{softmax}_y s_{\Theta}(y|x)$$

Note that the same equations apply whether  $y$  is drawn from a small set or an exponentially large set.

**It Suffices to Compute  $w.\text{grad}$**

$$w = W_{\Theta}(x)$$

$$P = \text{softmax } s(\cdot|w)$$

$$\ell = -\ln P(y)$$

$$\Theta.\text{grad} = w.\text{grad} \quad \nabla_{\Theta} W(x, \Theta)$$

## Computing $w.\text{grad}$

$$\ell(y|w) = -\ln P(y|w)$$

$$P(y|w) = \frac{1}{Z(w)} e^{w \cdot \Phi(y)}$$

$$Z(w) = \sum_y e^{w \cdot \Phi(y)}$$

$$\ell(y|w) = \ln Z(w) - w \cdot \Phi(y)$$

$$\nabla_w \ell(y|w) = \nabla_w \ln Z(w) - \Phi(y)$$

## Negative Sampling

$$\begin{aligned} -w.\text{grad} &= \Phi(y) - \nabla_w \ln Z(w) \\ &= \Phi(y) - \frac{1}{Z} \sum_{y'} e^{w \cdot \Phi(y')} \Phi(y') \\ &= \Phi(y) - \sum_{y'} \left( \frac{1}{Z} e^{w \cdot \Phi(y')} \right) \Phi(y') \\ &= \Phi(y) - \mathbb{E}_{y' \sim P(\cdot|w)} [\Phi(y')] \end{aligned}$$

We can estimate  $\mathbb{E}_{y' \sim P(\cdot|w)} [\Phi(y')]$  by sampling. This is called **negative sampling**.

**We move toward  $\Phi(y)$  and away from  $\Phi(y')$ .**

# Monte Carlo Markov Chain (MCMC) Sampling

## Metropolis Algorithm

Assume that each  $y$  has a set of  $N$  “neighbors” where the neighbor relation is symmetric.

Pick an initial  $y$  then repeat for the **mixing time**.

1. pick a neighbor  $y'$  of  $y$  uniformly at random.
2. If  $s(y'|w) > s(y|w)$  update  $y = y'$
3. If  $s(y'|w) \leq s(y|w)$  then update  $y = y'$  with probability  $e^{-\Delta s}$ ,  $\Delta s = s(y|w) - s(y'|w)$ .

## Markov Processes and Stationary Distributions

A Markov process is a process defined by a fixed state transition probability  $P(y'|y) = M_{y',y}$ .

Let  $P^t$  the probability distribution for time  $t$ .

$$P^{t+1} = MP^t$$

If every state can be reached from every state (ergodic process) then  $P^t$  converges to a unique **stationary distribution**  $P^\infty$

$$P^\infty = MP^\infty$$

## Correctness of Metropolis

To verify that the Metropolis process has the correct stationary distribution we simply verify that  $MP = P$  where  $P$  is the desired distribution.

This can be done by checking that under the desired distribution the flow from  $y$  to  $y'$  equals the flow from  $y'$  to  $y$  (**detailed balance**).

For  $s(y) \geq s(y')$

$$\text{flow}(y' \rightarrow y) = \frac{1}{Z} e^{s(y')} \frac{1}{N}$$

$$\text{flow}(y \rightarrow y') = \frac{1}{Z} e^{s(y)} \frac{1}{N} e^{-\Delta s} = \frac{1}{Z} e^{s(y')} \frac{1}{N}$$

Detailed balance is not required in general.



## Negative Sampling with MCMC

Sample  $y' \sim P(\cdot|w)$  using MCMC.

$$-w.\text{grad} \leftarrow \Phi(y) - \Phi(y')$$

**We move toward  $\Phi(y)$  and away from  $\Phi(y')$ .**

# Gibbs Sampling

The Metropolis algorithm wastes time by rejecting proposed moves.

Gibbs sampling avoids this move rejection.

Gibbs sampling applies when  $y$  is a tuple  $(y_1, \dots, y_K)$ .

In semantic segmentation  $y_k$  is the class of superpixel  $k$ .

# Gibbs Sampling

Initialize  $y$

Repeat for the **mixing time**:

1. Select a component  $k$
2. Update  $y_k = y'_k$  where  $y'_k$  is drawn from

$$P(y'_k | y_1, \dots, y_{k-1}, y_{k+1}, \dots, y_K)$$

For the models we are considering  $P(y'_k | y_1, \dots, y_{k-1}, y_{k+1}, \dots, y_K)$  is easily computed (the partition function  $Z$  cancels).

## Correctness Proof

$P(y)$  is a stationary distribution of Gibbs Sampling:

$$\begin{aligned} P^{t+1}(y_1, \dots, y_K) &= \frac{1}{K} \sum_k \frac{P^t(y_k | y_1, \dots, y_{k-1}, y_{k+1}, \dots, y_K)}{P^t(y_1, \dots, y_{k-1}, y_{k+1}, \dots, y_K)} \\ &= \frac{1}{K} \sum_k P^t(y_1, \dots, y_k) \\ &= P^t(y_1, \dots, y_K) \end{aligned}$$

## Negative Sampling with Gibbs

Sample  $y' \sim P(\cdot|w)$  using MCMC.

$$-w.\text{grad} \leftarrow \Phi(y) - \Phi(y')$$

## Pseudolikelihood

In Pseudolikelihood we replace the objective  $\ln P(y|w)$  with the objective  $\ln \tilde{P}(y|w)$  where

$$\tilde{P}(y|w) = \prod_k P(y'_k | y_1, \dots, y_{k-1}, y_{k+1}, \dots, y_K, w)$$

As in Gibbs sampling, we note that these probabilities are easily computed.

$$-w.\text{grad} \leftarrow \nabla_w \ln \tilde{P}(y|w)$$

# Pseudolikelihood

**Algorithm:**

$$\Theta^* = \operatorname{argmin}_{\Theta} \mathbb{E}_{(x,y) \sim D} [-\ln \tilde{P}(y|W(x; \Theta))]$$

**Theorem:**

$$\operatorname{argmin}_{Q(y|x)} \mathbb{E}_{(x,y) \sim D} [-\ln \tilde{Q}(y|x)] = D(y|x)$$

This is called **consistency**.

## Proof of Consistency I

We have

$$\min_{Q(y|x)} \mathbb{E}_{(x,y) \sim D} [-\ln \tilde{Q}(y|x)] \leq \mathbb{E}_{(x,y) \sim D} [-\ln \tilde{D}(y|x)]$$

If we can show

$$\min_{Q(y|x)} \mathbb{E}_{(x,y) \sim D} [-\ln \tilde{Q}(y|x)] \geq \mathbb{E}_{(x,y) \sim D} [-\ln \tilde{D}(y|x)]$$

Then the minimizer (the argmin) is  $D$  as desired.



## Proof of Consistency II

We will prove the case of  $K = 2$ .

Consider **unrelated** distributions  $Q_1(y_1|y_2, x)$  and  $Q_2(y_2|y_1, x)$ .

$$\begin{aligned} & \min_{Q(y|x)} \mathbb{E}_{(x,y) \sim D} [-\ln Q(y_1|y_2, x) - \ln Q(y_2|y_1, x)] \\ & \geq \min_{Q_1, Q_2} \mathbb{E}_{(x,y) \sim D} [-\ln Q_1(y_1|y_2, x) - \ln Q_2(y_2|y_1, x)] \\ & = \min_{Q_1} \mathbb{E}_{(x,y) \sim D} [-\ln Q_1(y_1|y_2, x)] + \min_{Q_2} \mathbb{E}_{(x,y) \sim D} [-\ln Q_2(y_2|y_1, x)] \\ & = \mathbb{E}_{(x,y) \sim D} [-\ln D(y_1|y_2, x)] + \mathbb{E}_{(x,y) \sim D} [-\ln D(y_2|y_1, x)] \\ & = \mathbb{E}_{(x,y) \sim D} [-\ln \tilde{D}(y|x)] \end{aligned}$$

## Contrastive Divergence

**Algorithm (CDk):** Run  $k$  steps of MCMC for  $P_{\Theta}(y|x)$  starting from  $y$  to get  $y'$ .

$$-w.\text{grad} \leftarrow \Phi(y) - \Phi(y')$$

**Theorem:** If  $P_{\Theta}(y|x) = D(y|x)$  then

$$\mathbb{E}_{(x,y) \sim D} [\Phi(y) - \Phi(y')] = 0$$

Here we can take  $k = 1$  — no mixing time required.

## Handling Task Loss

## Different Costs for Different Errors

In inexpensive cancer screening we want **high recall** of cancers but can tolerate **low precision**.

In other words, the cost of a **false negative** is generally considered higher than the cost of a **false positive**.

## Intersection over Union

In visual detection problems one is typically evaluated by **intersection over union**.

$$\mathbf{IOU} = \frac{|\text{true positives} \cap \text{false positives}|}{|\text{true positives} \cup \text{false positives}|} = \frac{P - FN}{P + FP}$$

$$\frac{\partial IOU}{\partial FP} = \frac{-(P - FN)}{(P + FP)^2} = \frac{-\text{IOU}}{P + FP}$$

$$\frac{\partial IOU}{\partial FN} = \frac{-1}{P + FP}$$

## Generic Task Loss

We can consider an arbitrary loss function  $L(y, \hat{y})$  assigning a loss when the true label is  $y$  and the system guesses  $\hat{y}$ .

For example, If  $y$  and  $\hat{y}$  are segmentations then  $\hat{y}$  typically has many errors.

We can then assign a cost  $C_{i,j}$  for labeling a pixel  $i$  when the true label is  $j$ .

## Label Adjustment

$$s_{\Theta}(y|x) = W_{\Theta}(x) \cdot \Phi(y)$$

$$\hat{y}_{\Theta}(x) = \operatorname{argmax}_y s_{\Theta}(y|x)$$

$$\tilde{y}_{\Theta,\epsilon}(x, y) = \operatorname{argmax}_{\tilde{y}} s_{\Theta}(y|x) - \epsilon L(y, \tilde{y}) \quad (\text{adjusted label})$$

$$-w.\text{grad} \leftarrow \Phi(\tilde{y}_{\epsilon}) - \Phi(\hat{y})$$

**Theorem:** For a continuous and smooth data distribution  $D$

$$-\nabla_w \mathbb{E}_{(x,y) \sim D} [L(y, \hat{y}_w)] = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \mathbb{E}_{(x,y) \sim D} [\Phi(\tilde{y}_{w,\epsilon}) - \Phi(\hat{y}_w)]$$

**END**