CPSC 440: Advanced Machine Learning Log-Linear Models

Mark Schmidt

University of British Columbia

Winter 2022

Last Time: Undirected Graphical Models

• We discussed undirected graphical models

$$p(x_1, x_2, \dots, x_d) \propto \prod_{c \in \mathcal{C}} \phi_c(x_c),$$

which write joint distribution as product of non-negative potentials over subsets c.

The most common variant is pairwise UGMs,

$$p(x_1, x_2, \dots, x_d) \propto \left(\prod_{j=1}^d \phi_j(x_j)\right) \left(\prod_{(i,j)\in\mathcal{E}} \psi_{ij}(x_i, x_j)\right),$$

which includes Markov chains and multivariate Gaussians as special cases.

- In tree-structured graphs (no loops), common inference operations are $O(dk^2)$.
 - By generalizing the methods used for Markov chains.
 - But runtime is exponential in "treewidth" for graphs with loops.

Vancouver Rain Data: DAG vs. UGM

• We previously considered the "Vancouver Rain" dataset:

	Day 1	Day 2	Day 3	Day 4	Day 5	Day 6	Day 7	Day 8	Day 9	
Month (0	0	0	1	1	0	0	1	1	
Month 2	1	0	0	0	0	0	1	0	0	
Month 3	1	1	1	1	1	1	1	1	1	
Murith 4	1	1	1	1	0	0	1	1	1	
Months		0	0	0	1	1	0	0	0	
Month	0	1	1	0	0	0	0	1	1	

• We previously fit this with a Markov chain under the DAG factorization:

$$p(x_1, x_2, \dots, x_d) = p(x_1) \prod_{j=2}^d p(x_j \mid x_{j-1}),$$

where we used tabular potentials (so learning was counting).

Vancouver Rain Data: DAG vs. UGM

• Consider fitting a Markov chain under the UGM factorization:

$$p(x_1, x_2, \dots, x_d) \propto \left(\prod_{j=1}^d \phi_j(x_j)\right) \left(\prod_{j=2}^d \phi_{j,j-1}(x_j, x_{j-1})\right).$$

• Consider the following UGM parameterization (for $x_j \in \{-1, +1\}$):

$$\phi_j(x_j) = \exp(w_j x_j), \quad \phi_{ij}(x_i, x_j) = \exp(v_{ij} x_i x_j),$$

where w_j is a node weight, v_{ij} is an edge weight, and we have used lsing edges.

• We use the exponential function to make the potentials non-negative.

• We call this a log-linear model: logarithms of potentials are linear.

- Ising potentials can reflect how strongly neighbours are attracted/repulsed.
- For the rain data, we would expect $v_{ij} > 0$ (adjacent days likely to have same value).
- For the rain data, it makes sense to tie w_j across j and v_{ij} across (i, j) values.

Vancouver Rain Data: DAG vs. UGM

• Our log-linear model of the rain data under the Ising parameterization:

$$p(x_1, x_2, \dots, x_d \mid w, v) \propto \left(\prod_{j=1}^d \exp(wx_j)\right) \left(\prod_{j=2}^d \exp(vx_j x_{j-1})\right)$$
$$= \exp\left(\sum_{j=1}^d wx_j + \sum_{j=2}^d vx_j x_{j-1}\right)$$
$$= \exp\left(w\sum_{j=1}^d x_j + v\sum_{j=2}^d x_j x_{j-1}\right)$$
$$= \exp\left(\left[\frac{w}{v}\right]^T \left[\sum_{j=2}^d x_j x_{j-1}\right]\right),$$

which is an exponential family in canonical form.

- NLL will be convex in terms of w and v, derivative of NLL has simple form.
- If we did not tie parameters, we would have a statistic for each time.

Log-Linear UGM NLL and Gradient (Rain Data)

 \bullet Our convex NLL over n training examples is

$$f(w,v) = -w \sum_{i=1}^{n} \sum_{j=1}^{d} x_{j}^{i} - v \sum_{i=1}^{n} \sum_{j=2}^{d} x_{j}^{i} x_{j-1}^{i} + n \log Z(w,v),$$

and we typically train log-linear models using gradient descent.

• The derivative with respect to w has simple form but requires inference,

$$\nabla_w f(w, v) = -\sum_{i=1}^n \sum_{j=1}^d x_j^i + n \sum_{j=1}^d p(x_j = 1 \mid w, v).$$

where in Markov chains all marginals can be obtained from forward-backward.

- The gradient with respect to v is similar, using pairwise marginals.
- If you did the forward pass to compute $\log Z(w,v)$, autodif could do backward pass.
- At solution, we will that $p(x_j = 1)$ is frequency of this happening in data.
 - And $p(x_j = x_{j-1})$ matching frequency in data from the Ising edge parameter.

Log-Linear NLL and Gradient (General Case)

• We often write log-linear UGMs in an exponential family form

$$p(x \mid w) = \frac{\exp\left(w^T F(x)\right)}{Z(w)},$$

where the feature functions F(x) count the number of times we use each w_j .

- Examples of feature functions, and potentails for categoricals, in bonus.
- This leads to a convex NLL (first term is linear, second is a big log-sum-exp),

$$-\log p(x \mid w) = -w^T F(x) + \log(Z(w)),$$

• The gradient has a simple form but requires inference,

$$\nabla_w - \log p(x \mid w) = -F(x) + \mathbb{E}_{x \mid w}[F(x)],$$

which is #P-hard in general graphs.

• So we need to consider approximations when learning.

.

Approximate Learning: Pseudo-Likelihood

- A popular approximation to the NLL is pseudo-likelihood.
 - "Fast, convex, and crude."
- Pseudo-likelihood turns learning into d single-variables problem (similar to DAGs),

$$p(x_{1}, x_{2}, \dots, x_{d}) \approx \prod_{j=1}^{d} p(x_{j} \mid x_{-j}) = \prod_{j=1}^{d} p(x_{j} \mid x_{\mathsf{nei}(j)})$$

Approximate Learning: Marginal Approximations

• Another way to approximate the NLL is with approximate inference.

- **(**) Deterministic variational approximations of $\mathbb{E}[F(x)]$ (we will cover these later).
 - Approximate p by a simpler q, and compute expectation for q.
- **2** Monte Carlo approximation of $\mathbb{E}[F_j(x)]$ given current parameters w:

$$\nabla f(w) = -F(x) + \mathbb{E}[F(x)]$$

$$\approx -F(x) + \underbrace{\frac{1}{t} \sum_{i=1}^{t} F(x^{i})}_{i=1},$$

Monte Carlo approx

based on samples from $p(x \mid w)$.

• Unfortunately, usually we also cannot generate IID samples efficiently.

Approximate Learning with MCMC Marginal Approximation

- An innefficient approach to using MCMC approximation of gradient:
 - **①** At iteration k, we want to sample from $p(x \mid w^k)$.
 - Start from some x^0 , sample x^1 , sample x^2 , and so on.
 - Treat the last sample x^k from the Markov chain as an IID sample.
 - **②** Update the parameters using x^k to get an unbiased gradient approximation,

$$w^{k+1} = w^k + \alpha_k (F(x) - F(x^k)),$$

- If the Markov chain is run long enough, can show convergence using standard stochastic gradient descent arguments.
 - But have to run MCMC on each iteration of the SGD method.

Younes Algorithm ("Persistent Contrastive Divergence")

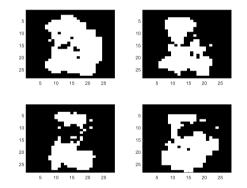
- Younes algorithm (also known as "persistent contrastive divergence"):
 - **①** At iteration k, we want to sample from $p(x \mid w^k)$.
 - Set $x^0 = x^{k-1}$, sample x^1 , sample x^2 , and so on.
 - Treat the last sample x^k from the Markov chain as an IID sample.
 - **②** Update the parameters using x^k to get an unbiased gradient approximation,

$$w^{k+1} = w^k + \alpha_k (F(x) - F(x^k)),$$

- In Younes algorithm, you do not need to run Markov chain to stationarity.
 - Usually you only run MCMC for 1 or a small number of iterations.
 - This gives a biased estimate, but is much faster than running MCMC to stationarity.
 - And with small-enough step-size, can show convergence.

Pairwise UGM on MNIST Digits

• Samples from a lattice-structured pairwise UGM trained on MNIST:



- Training: 100k stochastic gradient w/ Gibbs sampling steps with $\alpha_t = 0.01$.
- $\bullet\,$ Samples are iteration 100k of Gibbs sampling with fixed w.

Log-Linear Models

Conditional Random Fields

Outline

1 Log-Linear Models

2 Conditional Random Fields

Motivation: Rain Data with Month Information

• Our Ising UGM model for the rain data with tied parameters,

$$p(y_1, y_2, \dots, y_k \mid w, v) \propto \exp\left(\sum_{c=1}^k wy_c + \sum_{c=2}^k vy_c y_{c-1}\right),$$

where I have switched the variable names from x_j to y_c (but model is same).

- First term will refelct that "not rain" is a more likely.
- Second term reflects that consecutive days are more likely to be the same.
 This model is equivalent to a Markov chain model.
- But the model does not reflect that some months are less rainy.
- We can add features that reflect the month (or other information).
 - Multi-label supervised learning, but modeling dependence in labels y_c .
 - Adding fixed features to a UGM is also called a conditional random field (CRF).

Conditional Random Field (CRF) for Rain Data

• A CRF model of rain data, conditioned on 12 "one of k" month features x_j ,

$$p(y_1, y_2, \dots, y_k \mid x, w_0, w, v) \propto \exp\left(\sum_{c=1}^k w_0 y_c + \sum_{c=2}^k v y_c y_{c-1} + \sum_{c=1}^k y_c w^T x\right).$$

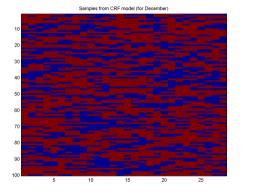
• The potentials in this model over the random variables y_c are:

$$\phi_i(y_i) = \exp\left(w_0 y_i + y_i w^T x\right), \quad \phi_{ij}(y_i, y_j) = \exp(v y_i y_j).$$

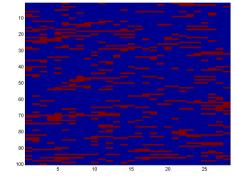
- If we draw the UGM over y_c variables we get a chain structure.
 - So inference can be done using forward-backward.
 - And it's still log-linear so the NLL will be convex.
 - Gradient descent finds global optimum jointly with respect to w_0 , w, and v.

Rain Data with Month Information

• Samples from CRF conditioned on x being December (left) and July (right):



Samples from CRF model (for July)



• Conditional NLL is 16.21, compared to Markov chain which gets NLL 16.81.

• Code for this and a variety of other UGM models is here: https://www.cs.ubc.ca/~schmidtm/Software/UGM.html

Conditional Random Fields (General Case)

• We often write the likelihood for general CRFs in the form

$$p(y \mid \boldsymbol{x}, w) = \frac{1}{Z(\boldsymbol{x}, w)} \exp(w^T F(\boldsymbol{x}, y)),$$

for some parameters \boldsymbol{w} and features $F(\boldsymbol{x},\boldsymbol{y}).$

• The NLL is convex and has the form

$$-\log p(y \mid \boldsymbol{x}, w) = -w^T F(\boldsymbol{x}, y) + \log Z(\boldsymbol{x}, w),$$

and the gradient can be written as

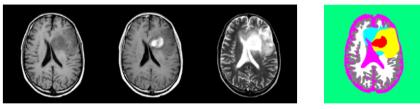
$$-\nabla \log p(y \mid \boldsymbol{x}, w) = -F(\boldsymbol{x}, y) + \mathbb{E}_{y \mid \boldsymbol{x}, w}[F(\boldsymbol{x}, y)],$$

which requires inference for each value of x in training data.

- For rain data need to do run forward-backward 12 times.
- $\bullet\,$ If each example has its own features, need to run it n times.
- So it can make sense to use stochastic gradient if n is large.

Motivation: Automatic Brain Tumor Segmentation

• Task: identification of tumours in multi-modal MRI.



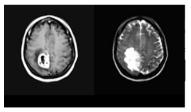
- Applications:
 - Radiation therapy target planning, quantifying treatment response.
 - Mining growth patterns, image-guided surgery.
- Challenges:
 - Variety of tumor appearances, similarity to normal tissue.
 - "You are never going to solve this problem".

Brain Tumour Segmentation with Label Dependencies

• After a lot pre-processing and feature engineering (convolutions, priors, etc.), final system used logistic regression to label each pixel as "tumour" or not.

$$p(y_c \mid x_c) = \frac{1}{1 + \exp(-2y_c w^T x_c)} = \frac{\exp(y_c w^T x_c)}{\exp(w^T x_c) + \exp(-w^T x_c)}$$

• Gives a high "pixel-level" accuracy, but sometimes gives silly results:





- Classifying each pixel independently misses dependence in labels y^i :
 - We prefer neighbouring voxels to have the same value.

Brain Tumour Segmentation with Label Dependencies

• With independent logistic, conditional distribution over all labels in one image is

$$p(y_1, y_2, \dots, y_k \mid x_1, x_2, \dots, x_k) = \prod_{c=1}^k \frac{\exp(y_c w^T x_c)}{\exp(w^T x_c) + \exp(-w^T x_c)}$$
$$\propto \exp\left(\sum_{c=1}^d y_c w^T x_c\right),$$

where here x_c is the feature vector for position c in the image.

• We can view this as a log-linear UGM with no edges,

$$\phi_c(y_c) = \exp(y_c w^T x_c),$$

so given the x_c there is no dependence between the y_c .

Brain Tumour Segmentation with Label Dependencies

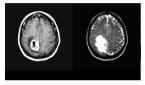
• Adding an Ising-like term to model dependencies between y_i gives

$$p(y_1, y_2, \dots, y_k \mid x_1, x_2, \dots, x_k) \propto \exp\left(\sum_{c=1}^k y_c w^T x_c + \sum_{(c,c') \in E} y_c y_{c'} v\right),$$

- Now we have the same "good" logistic regression model, but v controls how strongly we want neighbours to be the same.
- We can run gradient descent to jointly optimize w and v (convex NLL).
 - So we find the optimal joint logistic regression and Ising model.

Conditional Random Fields for Segmentation

• Recall the performance with the independent classifier:





- The pairwise CRF better modelled the "guilt by association":
 - Trained with pseudo-likelihood, constraining $v \ge 0$.
 - Decoding with "graph cuts" (see bonus lecture).



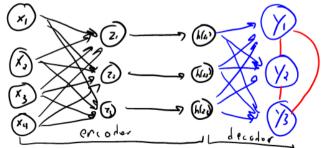
(We were using edge features $x_{cc'}$ too, see bonus (and different λ on edges).)

Combining Neural Networks and UGMs

• Instead of fixed features, you could use a neural network:

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

or you could have an encode-decode model spit out potentials of a UGM:



• These are sometimes called a conditional neural fields or deep structured model.

Multi-Label Classification

• Learned dependencies on a mult-label image classification dataset:

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	-0.0	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	Ο.	04	0.06	0.	00	0.05	-0.0	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	ο.	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	ο.	02	-0.0	0 -0	.06	0.10	0.00	0.04	0.08	0.05			-0.02	0.09	-0.02	0.06	0.03	0.14	0.36	0.06	0.05	0.01	80.0	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	Ο.	03	0.03	-0	.12	0.07	0.08	0.01	0.00	0.02	0.14	0.07		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	-0.0	8 -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	-0.0	5 -0	.35	0.03		-0.03	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	Ο.	01	-0.0	3 -0	.03	0.10		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	Ο.	04	0.02	-0	.46	0.01	-0.0	2 -0.03	0.14	-0.03		-0.00	0.00	0.01	0.04	-0.05	0.06	0.08	-0.04	-0.06		0.09	-0.00	0.06	0.03	0.02
bird	-0	.00	-0.0	6 -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	-0.1	2 -0	.34	0.02	-0.0	2 -0.03	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	-0.0	5 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	-0.0	4 -0	.15	0.08		0.02	0.08	0.04	0.44	0.12										0.11	0.05	0.22	-0.01	0.10
water	-0	.00	-0.0	3 -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	-0.2	1 -0	.01	0.07	0.06	-0.0	7 -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									0.36														0.06	0.08	0.07	0.06
tree	Ο.								0.10													0.00	0.04	0.09	-0.00	0.12
dog	0.	01	-0.0	3 0.	03	0.09	0.08	0.03	0.04	0.06	0.01	0.07										0.04	0.00	0.06	0.05	0.07
sunset	0.	02	-0.0	3 -0	.08	0.09	0.14	0.04	0.05						0.05							0.09	0.06	0.00	0.06	0.10
night							0.06		0.04						-0.07										0.00	
river									0.07																0.07	
	*	603	¢°	×	ý.	280	.0°°	Ф.	Ş2	5	SFA	1ate	°č.	, ³ , 5	5	, ^{°o} c	A PAL	5	43.	30	Cox.	or's oo	606	SS.	24	Ś.
		ng.		de la	. Q	0,00 0,00	4 9	<	t air	A POSS	10. V	.46	3	O ^{ito}	, ¹ 97			, ^c zoł	A BEE	anin,	5.5	00	, y	SUNG	a the second	Striver.
			0	.0		4			97×	2005	~			~Q2		2,			°°	-	. V.O.				0	
									ć.	1				.6	8	`~; _*	ò									

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

Automatic Differentiation (AD) vs. Inference

- Deep structured model gradient combines neural/Markov gradients:
 - **(**) Forward pass through neural network to get \hat{y}_c predictions.
 - Ø Forward message passing to compute normalizing constant.
 - **③** Backwards message passing to compute marginals.
 - Backwards pass through neural network to get all gradients.
- You could skip the last two steps if you use automatic differentiation.
- But with approximate inference, AD may or may not work:
 - AD will work for iterative variational inference methods (which we'll cover later).
 - But it takes way more memory than needed (needs to store all iterations).
 - AD will not tend to work for Monte Carlo methods.
 - Cannot AD through sampling (need 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".

Conditional Random Fields

Combining FCNs and CRFs

• DeepLab used a fully-connected pairwise UGM on top layer of FCN:

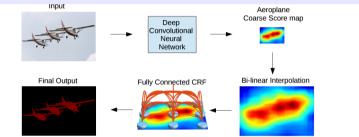


Fig. 1: Model Illustration. A Deep Convolutional Neural Network such as VGG-16 or ResNet-101 is employed in a fully convolutional fashion, using atrous convolution to reduce the degree of signal downsampling (from 32x down 8x). A bilinear interpolation stage enlarges the feature maps to the original image resolution. A fully connected CRF is then applied to refine the segmentation result and better capture the object boundaries.

https://arxiv.org/pdf/1606.00915.pdf

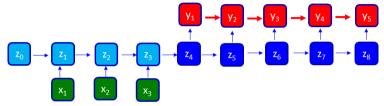
• But most recent version of the paper removed the UGM.

Do we need UGMs in Neural Networks?

- Recall that encode-decode hidden layers already capture label dependencies.
 - So do we need a UGM to explicitly model label dependencies in output layer?
- Factor 1: data size (big vs. small).
 - With a small dataset, it could be helpful to have direct dependencies in model.
 - With a large dataset, the hidden layers should reflect dependencies.
- Factor 2: how you evaluate the model (individual parts or full decoding).
 - If you measure "pixel level" or "word level" error, UGMs may not help.
 - If you measure "whole image" or "whole sentence" error, UGMs may help.
 - Because for example inference can discourage unlikely joint labelings.

Combining RNNs and Graphical Models

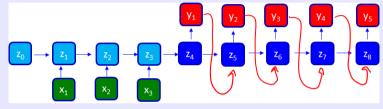
• An example where we use explicit label dependencies is language translation:



- Above model has usual deterministic edges, and DAG edges on labels.
- Can use Viterbi decoding to find best translation in this model.
 - Taking into account probability of seeing neighbouring words.
- But there is not much information in the DAG part of the model.
 - Only modeling dependencies between adjacent words.
- What we really want is to have the label we output affect the hidden state.
 - So that the encoding reflects previously-output words.

Combining RNNs and Graphical Models

• In order for the hidden states to depend on the output, we have this monstrosity:



- This can still be written as a Markov chain, but we cannot do Viterbi decoding.
 - Problem is that the hidden states in decoder become random variables.
 - So the state at each time has discrete and continuous parts (cannot be enumerated).
- To do decoding in this thing, we typically use beam search.
 - Heuristic algorithm that maintains "k best decodings up to time t".
 - Can be arbitrarily bad, but works if decoding is obvious as we go forward in time.
 - The type of edge and decoding strategy is also common with transformers.

Summary

- Log-linear parameterization can be used to learn UGMs:
 - Maximum likelihood is convex, but requires normalizing constant and inference.
- Approximate UGM learning:
 - Change objective function: pseudolikelihood.
 - Approximate marginals: Monte Carlo or variational methods.
 - Younes algorithm for using MCMC within SGD.
- Conditional random fields generalize logistic regression:
 - Multi-label model that explicitly models label dependencies.
- Combining CRFs with deep learning.
 - You can learn features and and the explicit label dependencies.
- Next time: a universal model for continuous density estimation.

Example: Ising Model of Rain Data

• E.g., for the rain data we could parameterize our node potentials using

$$\log(\phi_i(x_i)) = \begin{cases} w_1 & \text{no rain} \\ 0 & \text{rain} \end{cases}$$

- Why do we only need 1 parameter?
 - Scaling $\phi_i(1)$ and $\phi(2)$ by constant doesn't change distribution.
- In general, we only need (k-1) parameters for a k-state variable.
 - But if we're using regularization we may want to use k anyways (symmetry).

Example: Ising Model of Rain Data

• The Ising parameterization of edge potentials,

$$\log(\phi_{ij}(x_i, x_j)) = \begin{cases} w_2 & x_i = x_j \\ 0 & x_i \neq x_j \end{cases}$$

• Applying gradient descent gives MLE of

$$w = \begin{bmatrix} 0.16\\ 0.85 \end{bmatrix}, \quad \phi_i = \begin{bmatrix} \exp(w_1)\\ \exp(0) \end{bmatrix} = \begin{bmatrix} 1.17\\ 1 \end{bmatrix}, \quad \phi_{ij} = \begin{bmatrix} \exp(w_2) & \exp(0)\\ \exp(0) & \exp(w_2) \end{bmatrix} = \begin{bmatrix} 2.34 & 1\\ 1 & 2.34 \end{bmatrix},$$

preference towards no rain, and adjacent days being the same.

• Average NLL of 16.8 vs. 19.0 for independent model.

Conditional Random Fields

Full Model of Rain Data

• We could alternately use fully expressive edge potentials

$$\log(\phi_{ij}(x_i, x_j)) = \begin{bmatrix} w_2 & w_3 \\ w_4 & w_5 \end{bmatrix}$$

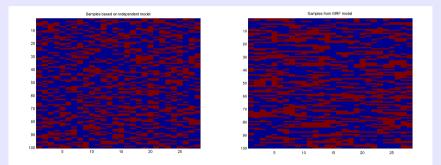
but these don't improve the likelihood much.

- We could fix one of these at 0 due to the normalization.
 - But we often don't do this when using regularization.
- We could also have special potentials for the boundaries.
 - Many language models are homogeneous, except for start/end of sentences.

Example: Ising Model of Rain Data

Independent model vs. chain-UGM model with tied nodes and Ising tied edges:

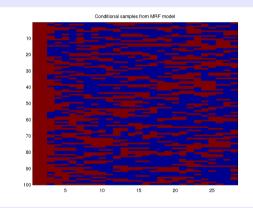
• For this dataset, using untied or general edges doesn't change likelihood much.



Conditional Random Fields

Example: Ising Model of Rain Data

Samples from Ising chain-UGM model if it rains on the first day:



Example of Feature Function

- Consider the 2-node 1-edge UGM (1)–(2), where each state has 2 values.
 - So we have potentials $\phi_1(x_1)$, $\phi_2(x_2)$, and $\phi_{12}(x_1,x_2)$ and want to have

$$w^T F(x) = w_{1,x_1} + w_{2,x_2} + w_{1,2,x_1,x_2}.$$

• With no parameter tieing and $x = \begin{bmatrix} 2 & 1 \end{bmatrix}$, our parameter vector and features are

$$w = \begin{bmatrix} w_{1,1} \\ w_{1,2} \\ w_{2,1} \\ w_{2,2} \\ w_{1,2,1,1} \\ w_{1,2,1,2} \\ w_{1,2,2,1} \\ w_{1,2,2,2} \end{bmatrix}, \quad F(x) = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix},$$

Example of Feature Function

• If we instead had Ising potentials (just measuring whether $x_1 = x_2$) we would have

$$w^T F(x) = w_{1,x_1} + w_{2,x_2} + w_{1,2,same},$$

where $w_{1,2,\text{same}}$ is the parameter specifying how much we want $x_1 = x_2$.

• With no parameter tieing and $x = \begin{bmatrix} 2 & 1 \end{bmatrix}$, our parameter vector and features are

$$w = \begin{bmatrix} w_{1,1} \\ w_{1,2} \\ w_{2,1} \\ w_{2,2} \\ w_{1,2.\text{same}} \end{bmatrix}, \quad F(x) = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \\ 0 \end{bmatrix},$$

UGM Training Objective Function

• With log-linear parameterization, NLL for IID training examples is

$$f(w) = -\sum_{i=1}^{n} \log p(x^{i} \mid w) = -\sum_{i=1}^{n} \log \left(\frac{\exp(w^{T}F(x^{i}))}{Z(w)}\right)$$
$$= -\sum_{i=1}^{n} w^{T}F(x^{i}) + \sum_{i=1}^{n} \log Z(w)$$
$$= -w^{T}F(X) + n \log Z(w).$$

where the $F(X) = \sum_{i} F(x^{i})$ are called the sufficient statistics of the dataset.

• Given sufficient statistics F(X), we can throw out the examples x^i .

(only go through data once)

- Function f(w) is convex (it's linear plus a big log-sum-exp function).
 - But notice that Z depends on w

Log-Linear UGM Gradient

• For 1 example x, we showed that NLL with log-linear parameterization is

$$f(w) = -w^T F(x) + \log Z(w).$$

• The partial derivative with respect to parameter w_i has a simple form

$$\nabla_{w_j} f(w) = -F_j(x) + \sum_x \frac{\exp(w^T F(x))}{Z(w)} F_j(x)$$
$$= -F_j(x) + \sum_x p(x \mid w) F_j(x)$$
$$= -F_j(x) + \mathbb{E}[F_j(x)].$$

• Observe that derivative of log(Z) is expected value of feature.

Brain Tumour Segmentation with Label Dependencies

 \bullet We got a bit more fancy and used edge features $x^{ij},$

$$p(y^1, y^2, \dots, y^d \mid x^1, x^2, \dots, x^d) = \frac{1}{Z} \exp\left(\sum_{i=1}^d y^i w^T x^i + \sum_{(i,j) \in E} y^i y^j v^T x^{ij}\right).$$

- For example, we could use $x^{ij} = 1/(1 + |x^i x^j|)$.
 - Encourages y_i and y_j to be more similar if x^i and x^j are more similar.



• This is a pairwise UGM with

$$\phi_i(y^i) = \exp(y^i w^T x^i), \quad \phi_{ij}(y^i, y^j) = \exp(y^i y^j v^T x^{ij}),$$

so it didn't make inference any more complicated.

Log-Linear Models

Conditional Random Fields

Modeling OCR Dependencies

• What dependencies should we model for this problem?

Output: "Paris"

- $\phi(y_c, x_c)$: potential of individual letter given image.
- $\phi(y_{c-1}, y_c)$: dependency between adjacent letters ('q-u').
- $\phi(y_{c-1}, y_c, x_{c-1}, x_c)$: adjacent letters and image dependency.
- $\phi_c(y_{c-1}, y_c)$: inhomogeneous dependency (French: 'e-r' ending).
- $\phi_c(y_{c-2}, y_{c-1}, y_c)$: third-order and inhomogeneous (English: 'i-n-g' end).
- $\phi(y \in \mathcal{D})$: is y in dictionary \mathcal{D} ?

Tractability of Discriminative Models

• Features can be very complicated, since we just condition on the x_c , .

- Given the x_c , tractability depends on the conditional UGM on the y_c .
 - $\bullet\,$ Inference tasks will be fast or slow, depending on the y_c graph.
- Besides "low treewidth", some other cases where exact computation is possible:
 - Semi-Markov chains (allow dependence on time you spend in a state).
 - For example, in rain data the seasons will be approximately 3 months.
 - Context-free grammars (allows potentials on recursively-nested parts of sequence).
 - Sum-product networks (restrict potentials to allow exact computation).
 - "Dictionary" feature is non-Markov, but exact computation still easy.
- We can alternately use our previous approximations:
 - Pseudo-likelihood (what we used).
 - **2** Monte Carlo approximate inference (eventually better but probably much slower).
 - Solutional approximate inference (fast, quality varies).

Structure Learning in UGMs

• Recall that in Ising UGMs, our edge potentials have the form

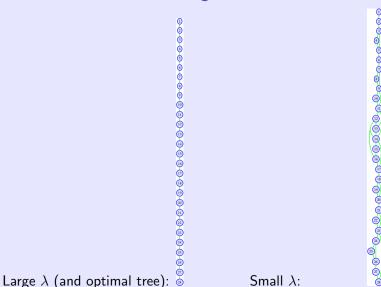
$$\phi_{ij}(x_i, x_j) = \exp(w_{ij} x_i x_j).$$

- If we set w_{ij} = 0, it sets φ_{ij}(x_i, x_j) = 1 for all x_i and x_j.
 Potential just "multiplies by 1", which is equivalent to removing the edge.
- L1-regularization of w_{ij} values performs structure learning in UGM.
- For general log-linear, each edge has multiple parameters $w_{i,j,s,s'}$.
 - In this case we can use "group L1-regularization" for structure learning.
 - Each group will be all parameters $w_{i,j,\cdot,\cdot}$ associated with an edge (i,j).

Log-Linear Models

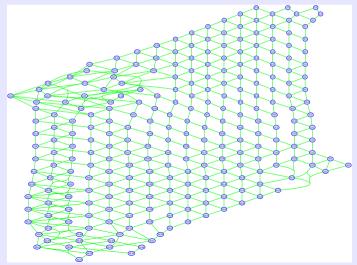
Conditional Random Fields

Structure Learning on Rain Data



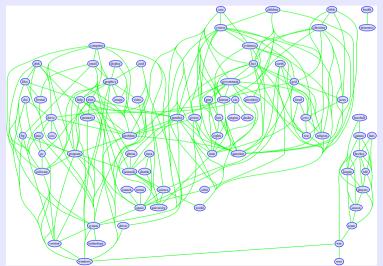
Structure Learning on USPS Digits

Structure learning of pairwise UGM with group-L1 on USPS digits:



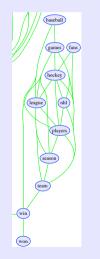
Structure Learning on News Words

Group-L1 on newsgroups data:



Structure Learning on News Words

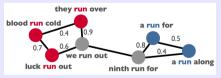
Group-L1 on newsgroups data:





Posterior Regularization

- In some cases it might make sense to use posterior regularization:
 - Regularize the probabilities in the resulting model.
- Consider an NLP labeling task where
 - You have a small amount of labeled sentences.
 - You have a huge amount of unlabeled sentences.
- Maximize labeled likelihood, plus total-variation penalty on $p(y_c \mid x, w)$ values.
 - Give high regularization weights to words appearing in same trigrams:



http://jgillenw.com/conll2013-talk.pdf

- Useful for "out of vocabulary" words (words that don't appear in labeled data).
 - Has been replaced in recent by continuous word representations like word2vec.