Machine Learning & Data Mining
CS/CNS/EE 155

Lecture 13:

Probabilistic Models

Announcements

- Probability Recitation Tonight!

Topic Overview

Supervised Learning

Linear Models	Overfitting	Loss Functions
Non-Linear Models	Learning Algorithms & Optimization	Probabilistic Modeling

Unsupervised Learning

Today

- Basic Probabilistic Models
  - Naïve Bayes
  - Estimation
  - Sampling

- Brief Overview of Advanced Probabilistic Models

- Thursday: Hidden Markov Models

Generative Probabilistic Models

- Models joint distribution of x and y: $P(x,y)$

- Can make predictions via Bayes Rule:

$$P(y \mid x) = \frac{P(x,y)}{P(x)} = \frac{P(x \mid y)P(y)}{P(x)}$$

Prediction = choose y with maximal P(y|x)

- Can infer marginal distributions:

$$P(y) = \sum_x P(y,x) \qquad P(x) = \sum_y P(y,x)$$

Example

- P(x,y) sums to 1
  - Joint distribution

- P(x=Homework) ??
  - **Answer: 0.5**
  - "Marginalize out the y"

y	x	P(x,y)
Y= SPAM	Help!	0.15
y= NOT	Help!	0.1
y= SPAM	Homework	0.05
y= NOT	Homework	0.45
Y= SPAM	Winner!	0.2
Y= NOT	Winner!	0.05

Margin distribution of P(x)

$$P(x) = \sum_{y} P(y,x)$$

Example #2

- P(x,y) sums to 1
  - Joint distribution

- P(y=SPAM|x=Help!) ??
  - **Answer: 0.6**
  - P(x,y) = 0.15
  - P(x) = 0.25

y	x	P(x,y)
Y= SPAM	Help!	0.15
y= NOT	Help!	0.1
y= SPAM	Homework	0.05
y= NOT	Homework	0.45
Y= SPAM	Winner!	0.2
Y= NOT	Winner!	0.05

$$P(y \mid x) = \frac{P(x,y)}{P(x)} \quad P(x) = \sum_y P(y,x)$$

Example #3

- P(x,y) sums to 1
  - Joint distribution

- P(x=Help!|y=NOT) ??
  - **Answer: 0.17**
  - P(x,y) = 0.1
  - P(y) = 0.6

y	x	P(x,y)
Y= SPAM	Help!	0.15
y= NOT	Help!	0.1
y= SPAM	Homework	0.05
y= NOT	Homework	0.45
Y= SPAM	Winner!	0.2
Y= NOT	Winner!	0.05

$$P(x \mid y) = \frac{P(x,y)}{P(y)} \qquad P(y) = \sum_x P(y,x)$$

Training

- Goal is to learn P(x,y)
  - What is objective function?

- **Maximum Likelihood!**

$$\text{argmax}\, P(S) = \text{argmax} \prod_i P(x_i, y_i)$$

$$= \text{argmin} \sum_i -\log P(x_i, y_i)$$

  - Just frequency counts!
  - 6 parameters

y	x	P(x,y)
Y= SPAM	Help!	0.15
y= NOT	Help!	0.1
y= SPAM	Homework	0.05
y= NOT	Homework	0.45
Y= SPAM	Winner!	0.2
Y= NOT	Winner!	0.05

$$S = \left\{ (x_i, y_i) \right\}_{i=1}^{N}$$

Training

- ## Goal is to learn P(x,y)
  - What is objective function?

- ## **Maximum Likelihood!**

$$\text{argmax } P(S) = \text{argmax} \prod_i P(x_i, y_i)$$

$$= \text{argmin} \sum_i -\log P(x_i, y_i)$$

y	x	P(x,y)
Y= SPAM	Help!	0.15
y= NOT	Help!	0.1
y= SPAM	Homework	0.05
y= NOT	Homework	0.45
Y= SPAM	Winner!	0.2
Y= NOT	Winner!	0.05

Interpretation: Given model structure, find that parameterization that best explains data

$$\left.\begin{array}{c} \\ \\ \end{array}\right\}_{i=1}^{N}$$

Training Derivation

- Define:
$$P(x,y) = \frac{w_{x,y}}{\sum_{x',y'} w_{x',y'}}$$

Just a re-parameterization

$$\operatorname{argmin} \sum_i -\log P(x_i, y_i) = \operatorname*{argmin}_w \sum_i \left[-\log w_{x_i,y_i} + \log \sum_{x',y'} w_{x',y'} \right]$$

\# training examples (x,y)

$$\partial_{w_{x,y}} = -\frac{N_{x,y}}{w_{x,y}} + \frac{N}{\sum_{x',y'} w_{x',y'}} \;\Rightarrow\; \frac{N_{x,y}}{N} = \frac{w_{x,y}}{\sum_{x',y'} w_{x',y'}} \;\Rightarrow\; P(x,y) = \frac{N_{x,y}}{N}$$

Frequency of (x,y) in training set!

Regularization

- Hallucinate data!

Prior Probability of observing (x,y)

$$P(x,y) = \frac{N_{x,y} + \lambda P_{x,y}}{N + \lambda}$$

Regularization Strength

- aka: "pseudo counts"

y	x	P(x,y)
Y= SPAM	Help!	0.15
y= NOT	Help!	0.1
y= SPAM	Homework	0.05
y= NOT	Homework	0.45
Y= SPAM	Winner!	0.2
Y= NOT	Winner!	0.05

Generative vs Discriminative

- Generative models
  - Models both y AND x
  - P(x,y)

What are Benefits and Drawbacks?

- Discriminative models
  - Models y GIVEN x
  - P(y|x)
  - E.g., Logistic Regression

Generative vs Discriminative

- ## Generative:
  - Models all of P(x,y)
  - Prediction via Bayes Rule
    - Tolerates missing data

- ## Discriminative:
  - Only models P(y|x)
  - Directly models prediction task
    - Cannot naturally tolerate missing data

y	x	P(x,y)
Y= SPAM	Help!	0.15
y= NOT	Help!	0.1
y= SPAM	Homework	0.05
y= NOT	Homework	0.45
Y= SPAM	Winner!	0.2
Y= NOT	Winner!	0.05

Discriminative Models Make Better Predictions

- Directly learn to optimize prediction goal:
  - Aka: directly learn: $P(y \mid x)$
  - E.g., minimize log-loss

- Generative Models require combining multiple estimated values:

$$P(y \mid x) = \frac{P(x, y)}{P(x)}$$

What if there are so many different x that P(x) underflows?

  - Training objective does not maximize accuracy.

Generative Models are Joint Models

- Fully specify probability distribution of P(x,y)

- Can draw samples from P(x,y)
  - R = uniform([0,1])   Built-in function in python, Matlab, etc.
  - If(R < 0.15)
    - x=help!, y=SPAM
  - Elseif(R < 0.25)
    - x=help!, y=NOT
  - ...

y	x	P(x,y)
Y= SPAM	Help!	0.15
y= NOT	Help!	0.1
y= SPAM	Homework	0.05
y= NOT	Homework	0.45
Y= SPAM	Winner!	0.2
Y= NOT	Winner!	0.05

Generative Models can Tolerate Missing Values

- We can model the probability of missing feature value
  - We will see this specifically for Naïve Bayes.

- Discriminative models cannot tolerate missing values
  - If you don't observe an input feature, you lose all guarantees

Generative Models are more Elegant?

- Many find generative models more elegant

- Tell a "complete" story about the data

- Useful if we can't decide what is the prediction task a priori

- E.g., train model first, pick what is the y later

Naïve Bayes

Modeling a Feature Vector

- Single y
  - (e.g., binary)

- Vector of x (D-dimensional)
  - Simplest case, each x^d binary
  - E.g., presence/absence of word

- Model P(x,y)

Example

- Binary y
- 2 binary x's

- "Probability table"

- **What's wrong with this approach?**

y	x^1=Winner!	x^2=Homework	P(x,y)
SPAM	1	1	0.01
NOT	1	1	0.01
SPAM	0	1	0.03
NOT	0	1	0.35
SPAM	1	0	0.25
NOT	1	0	0.05
SPAM	0	0	0.2
NOT	0	0	0.1

Example

- Binary y

- 2 binary x's

- "Probability table"

- **Wha**
  this

y	x^1=Winner!	x^2=Homework	P(x,y)
SPAM	1	1	0.01
NOT	1	1	0.01
SPAM	0	1	0.03
NOT	0	1	0.35
SPAM	1	0	0.25
NOT	1	0	0.05
			0.2
			0.1

**Model Complexity is Exponential
w.r.t. the length of x!**

Naïve Bayes Formulation

- Posits a generating model:
  - Single y
  - Multiple x features
  - **Only keep track of:**
    - **P(y), P(x^d|y)**
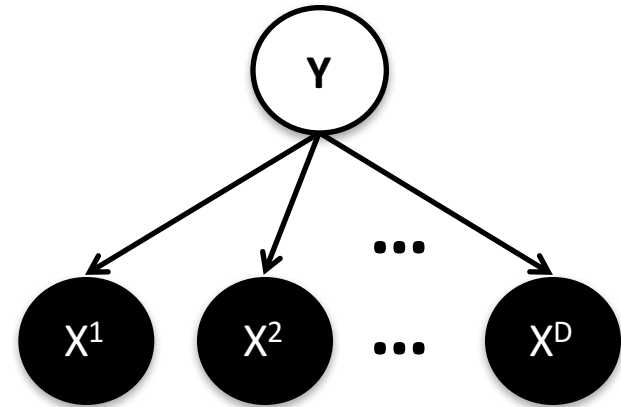
Graphical Model Diagram

$$P(x, y) = P(x \mid y)P(y) = P(y) \prod_d P(x^d \mid y)$$

Each x^d is conditionally independent given y. "Naïve" independence assumption!

Why is Naïve Bayes Convenient?

- Compact representation

- Easy to compute any quantity
  - $P(y|x)$, $P(x^d|y)$, …

- Easy to estimate model components
  - $P(y)$, $P(x^d|y)$

- Easy to sample

- Easy to deal with missing values

Example Model (Discrete)

- Each x^d binary
  - E.g., presence or absence of word

P(x|y)

	x^1=Homework	x^2=Winner!
y=SPAM	$P(x^1|y)$=0.2	$P(x^2|y)$=0.5
y=NOT	$P(x^1|y)$=0.6	$P(x^2|y)$=0.1

P(y)

P(y)	
y=SPAM	0.7
y=NOT	0.3
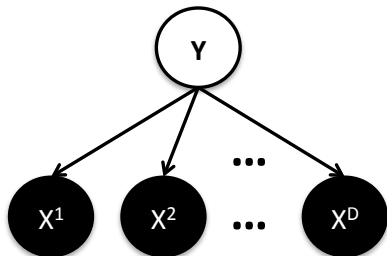
$$P(x,y) = P(x \mid y)P(y) = P(y)\prod_d P(x^d \mid y)$$

Example Model (Discrete)

- Each x^d binary
  - E.g., presence or absence of word

P(x|y)

	x¹=Homework	x²=Winner!
y=SPAM	$P(x^1|y)=0.2$	$P(x^2|y)=0.5$
y=NOT	$P(x^1|y)=0.6$	$P(x^2|y)=0.1$

Model Complexity is Linear w.r.t. the length of x!

P(y)

	P(y)
y=SPAM	0.7
y=NOT	0.3

$$P(x,y) = P(x \mid y)P(y) = P(y)\prod_d P(x^d \mid y)$$

Making Predictions

$$P(y \mid x) = \frac{P(x, y)}{P(x)}$$

$$= \frac{P(x \mid y)P(y)}{P(x)}$$

$$= \frac{P(y)}{P(x)} \prod_d P(x^d \mid y)$$

$$\propto P(y) \prod_d P(x^d \mid y)$$
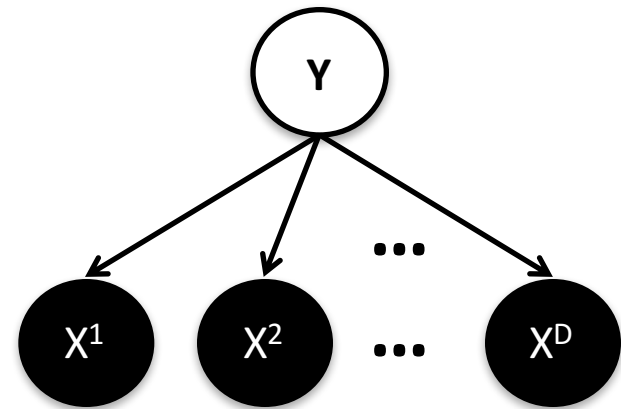
Graphical Model Diagram

Model components we keep track of.

Example Prediction

- Suppose:

$$P(y = 1) = 0.3 \qquad P(x \mid y = 1) = 0.05$$

$$P(y = -1) = 0.7 \qquad P(x \mid y = -1) = 0.001$$

- Then:

$$P(y = 1 \mid x) = \frac{0.3 * 0.05}{0.3 * 0.05 + 0.7 * 0.001} \approx 0.96$$

$$P(y \mid x) \propto P(y) \prod_d P(x^d \mid y) = P(y) P(x \mid y)$$

Example Prediction #2

- What if we want to compute: $P(x^1 | x^{2:D}, y)$

- **Simple!** $P(x^1 | y)$

- It's an explicitly defined model component:

$$P(x, y) = P(x | y)P(y) = P(y)\prod_d P(x^d | y)$$

Example Prediction #3

- What if we want to compute: $P(x^1 \mid x^{2:D})$

$$P(x^1 \mid x^{2:D}) = \frac{P(x)}{P(x^{2:D})} = \frac{\sum_y P(y)P(x \mid y)}{\sum_y P(y)P(x^{2:D} \mid y)}$$

"Marginalizing out the y"

Why is the numerator smaller than the denominator?

$$P(x, y) = P(x \mid y)P(y) = P(y)\prod_d P(x^d \mid y)$$

Marginalization in Matrix Form

Often faster than writing for loops!

O

	x¹=Homework	x²=Winner!
y=SPAM	$P(x^1=1|y)=0.2$	$P(x^2=1|y)=0.5$
y=NOT	$P(x^1=1|y)=0.6$	$P(x^2=1|y)=0.1$

P

	P(y)
y=SPAM	0.7
y=NOT	0.3

- Compute $P(x^d=1)$:

$$P(x^d = 1) = \left[O^T P \right]_d \longleftarrow \text{d-th row}$$

$$P(x^d = 1) = \sum_y P(x^d = 1 | y) P(y)$$

Missing Values

- What if we don't observe x^2?
- Predict $P(y=\text{SPAM}|x^1)$

We can marginalize out the missing values!

$$P(y \mid x^1) = \sum_{x^{2:D}} P(y, x^{2:D} \mid x^1) = \sum_{x^{2:D}} \frac{P(x, y)}{P(x^1)}$$

How to efficiently sum over multiple missing values?

	x^1=Homework	x^2=Winner!
y=SPAM	$P(x^1=1|y)=0.2$	$P(x^2=1|y)=0.5$
y=NOT	$P(x^1=1|y)=0.6$	$P(x^2=1|y)=0.1$

	P(y)
y=SPAM	0.7
y=NOT	0.3

Conditional Independence to the Rescue!

$$P(y \mid x^1) = \sum_{x^{2:D}} P(y, x^{2:D} \mid x^1) = \sum_{x^{2:D}} \frac{P(x,y)}{P(x^1)}$$

From previous slide

$$P(x,y) = P(y) \prod_d P(x^d \mid y)$$

Definition of Naïve Bayes

$$\sum_{x^{2:D}} P(x,y) = P(y) \sum_{x^{2:D}} \prod_d P(x^d \mid y)$$

$$= P(y) P(x^1 \mid y) \prod_{d \in [2,D]} \sum_{x^d} P(x^d \mid y)$$

Swap Product & Sum due to independence!

$$= P(y) P(x^1 \mid y)$$

Marginalizes to 1!

Intuition

- Consider the case of 3 variables in x:
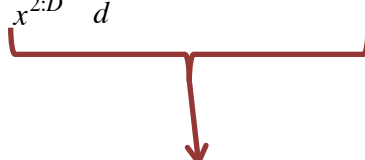
$$\sum_{x^{2:D}} P(x,y) = P(y) \sum_{x^{2:D}} \prod_d P(x^d \mid y) = P(y)P(x^1 \mid y) \prod_{d \in [2,D]} \sum_{x^d} P(x^d \mid y) = P(y)P(x^1 \mid y)$$

$$= \sum_{x^2 \in \{0,1\}} \sum_{x^3 \in \{0,1\}} P(x^2 \mid y)P(x^3 \mid y)$$

$$= P(x^2 = 0 \mid y)P(x^3 = 0 \mid y) + P(x^2 = 0 \mid y)P(x^3 = 1 \mid y)$$
$$+ P(x^2 = 1 \mid y)P(x^3 = 0 \mid y) + P(x^2 = 1 \mid y)P(x^3 = 1 \mid y)$$

$$= \left(P(x^2 = 0 \mid y) + P(x^2 = 1 \mid y) \right)\left(P(x^3 = 0 \mid y) + P(x^3 = 1 \mid y) \right)$$

$$= 1$$

Comparison with Logistic Regression

Missing Values Setting

- ## Naïve Bayes
  - Can query any distribution: $P(y|x)$, $P(y|x^1)$, $P(x^1|x^2)$
  - Training just requires counting (next slide)
  - Not optimized for classification accuracy

- ## Logistic Regression
  - Can only query $P(y|x)$
  - Training requires optimization procedure
  - Trained to minimize log-loss of $P(y|x)$

One Empirical Comparison

MODEL	1ST	2ND	3RD	4TH	5TH	6TH	7TH	8TH	9TH	10TH
BST-DT	0.580	0.228	0.160	0.023	0.009	0.000	0.000	0.000	0.000	0.000
RF	0.390	0.525	0.084	0.001	0.000	0.000	0.000	0.000	0.000	0.000
BAG-DT	0.030	0.232	0.571	0.150	0.017	0.000	0.000	0.000	0.000	0.000
SVM	0.000	0.008	0.148	0.574	0.240	0.029	0.001	0.000	0.000	0.000
ANN	0.000	0.007	0.035	0.230	0.606	0.122	0.000	0.000	0.000	0.000
KNN	0.000	0.000	0.000	0.009	0.114	0.592	0.245	0.038	0.002	0.000
BST-STMP	0.000	0.000	0.002	0.013	0.014	0.257	0.710	0.004	0.000	0.000
DT	0.000	0.000	0.000	0.000	0.000	0.000	0.004	0.616	0.291	0.089
LOGREG	0.000	0.000	0.000	0.000	0.000	0.000	0.040	0.312	0.423	0.225
NB	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.030	0.284	0.686

- Measure how frequently each model places
  - 1st, 2nd, 3rd, etc.

- Only generative model (Naïve Bayes) is in last place

"An Empirical Comparison of Supervised Learning Algorithms"
Caruana, Niculescu-Mizil, ICML 2006

Training

- Maximum Likelihood of Training Set:

$$\text{argmax}\, P(S) = \text{argmax} \prod_i P(x_i, y_i) \qquad S = \left\{ (x_i, y_i) \right\}_{i=1}^{N}$$

$$= \text{argmin} \sum_i -\log P(x_i, y_i)$$

– Subject to Naïve Bayes assumption on structure of P(x,y)
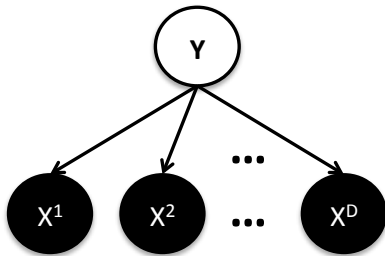
Only need to estimate P(y) and each P(x^d|y)!

$$P(x, y) = P(x \mid y) P(y) = P(y) \prod_d P(x^d \mid y)$$

Just Counting!

$$P(y = SPAM) = \frac{N_{y=SPAM}}{N}$$

Frequency of SPAM documents in training set

$$P(x^1 = 1 \mid y = SPAM) = \frac{N_{y=SPAM \wedge x^1=1}}{N_{y=SPAM}}$$

Frequency of word x1 appearing in SPAM documents in training set

Regularization

- Add "pseudo counts"
  - aka hallucinate some data

$$P(y = SPAM) = \frac{N_{y=SPAM} + \lambda P_{y=SPAM}}{N + \lambda}$$

Often just set pseudo counts to uniform distribution!

$$P(x^1 = 1 \mid y = SPAM) = \frac{N_{y=SPAM \wedge x^1=1} + \lambda P_{x^1=1 \mid y=SPAM}}{N_{y=SPAM} + \lambda}$$

Sampling

- ## Can sample from distribution
  - Definition of Generative Model

- ## Can draw samples from P(x,y)
  - First sample y:
    - Random uniform variable R
    - Set y=SPAM if R < P(y=SPAM) & y=NOT otherwise
  - Then sample each x^d:
    - Sample uniform variable R
    - Set x^d=1 if R < P(x^d=1|y) & x^d=0 otherwise
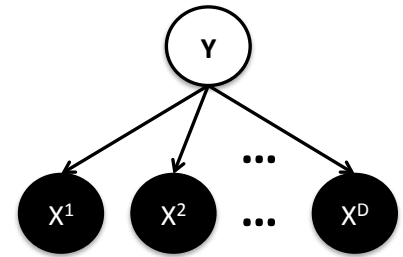
Built-in function in python, Matlab, etc.

Sampling Example

- ## Sample P(y)
  - R = 0.5, so set y = SPAM
- ## Sample P(x^1|y=SPAM)
  - R = 0.1, so set x^1 = 1
- ## Sample P(x^2|y=SPAM)
  - R = 0.9, so set x^2 = 0
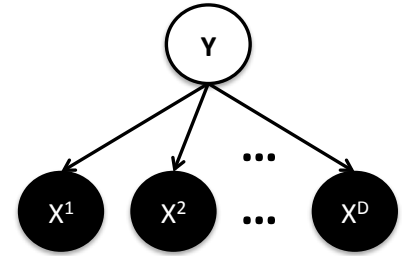
Can be done in either order

	x^1=Homework	x^2=Winner!
y=SPAM	P(x^1=1|y)=0.2	P(x^2=1|y)=0.5
y=NOT	P(x^1=1|y)=0.6	P(x^2=1|y)=0.1

	P(y)
y=SPAM	0.7
y=NOT	0.3

Sampling Example #2

- Sample P(y)
  - R = 0.9, so set y = NOT
- Sample $P(x^1|y=NOT)$
  - R = 0.5, so set $x^1 = 1$
- Sample $P(x^2|y=NOT)$
  - R = 0.05, so set $x^2 = 1$
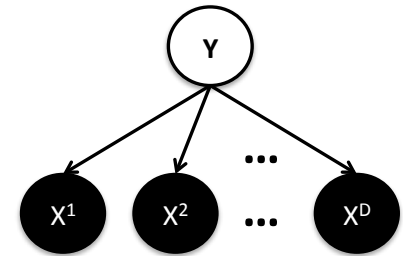
	x^1=Homework	x^2=Winner!
y=SPAM	$P(x^1=1|y)=0.2$	$P(x^2=1|y)=0.5$
y=NOT	$P(x^1=1|y)=0.6$	$P(x^2=1|y)=0.1$

	P(y)
y=SPAM	0.7
y=NOT	0.3

Recap: Naïve Bayes

- Probabilistic Generative Model

- Make strong independence assumptions
  - Compact representation
  - Easy to train
  - Easy to compute various probabilities
  - Not the most accurate for standard prediction
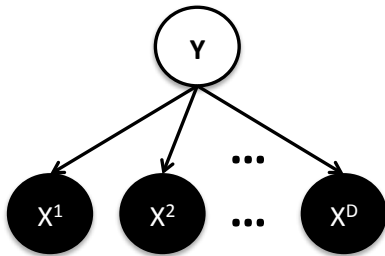
$$P(x, y) = P(x \mid y)P(y) = P(y)\prod_{d} P(x^d \mid y)$$

Invent Your Own Model

- Naïve Bayes is a special case of Bayesian Network

- Here's another one I just made up:

$$P(x, y) = P(x \mid y)P(y)$$

$$= P(x \mid y)P(y^1 \mid y^2)P(y^2)$$

$$= P(y^1 \mid y^2)P(y^2)P(x^D \mid y^1, y^2) \prod_{d \in [1, D-1]} P(x^d \mid y^1)$$
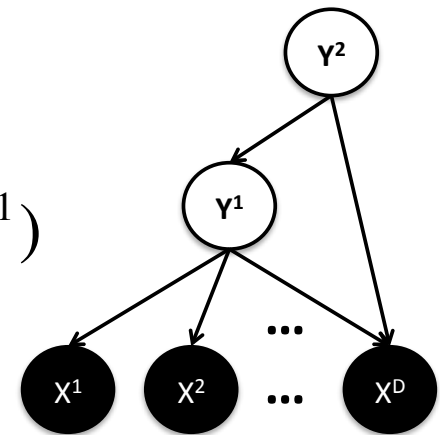
Some Other Probabilistic Models

Gaussian Naïve Bayes

- Same independence structure as Naïve Bayes
  - But probability functions are now Gaussians
    - (Instead of discrete lookup tables.)

  - y is binary: $P(y)$ the same

  - Each x^d is continuous:

$$P(x^d \mid y) \sim N(\mu_{d,y}, \sigma)$$
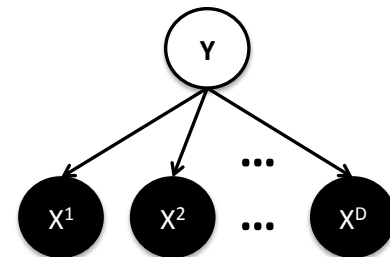
Hidden Markov Models
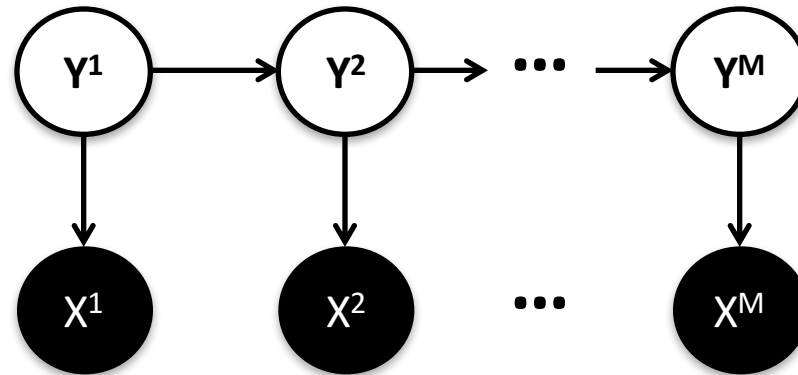
- Generative model of sequences

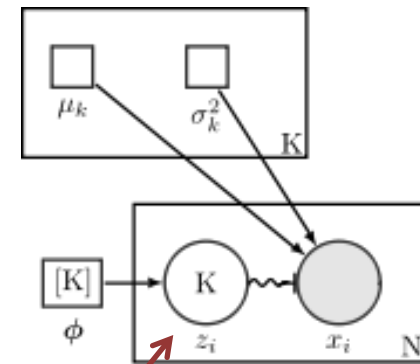$$P(x,y) = P(y^1)P(x^1 \mid y^1)\prod_{j=2}^{M} P(y^j \mid y^{j-1})P(x^j \mid y^j)$$

- (focus of next lecture)

(Gaussian) Mixture Models

- Each data point is associated with a membership to a Gaussian distribution
  - Denoted by z variable

- 1D Example with 3 Gaussians
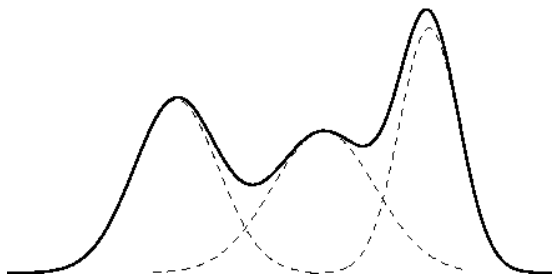
K Gaussian Distributions

N Data Points

Membership variable
per data point

Topic Models
(Latent Dirichlet Allocation)

- Posits that documents can represented as a mixture of topics.
  - K topics, choose K a priori
- Posits that topics can be represented as a mixture of words

Each word corresponds to a specific topic.
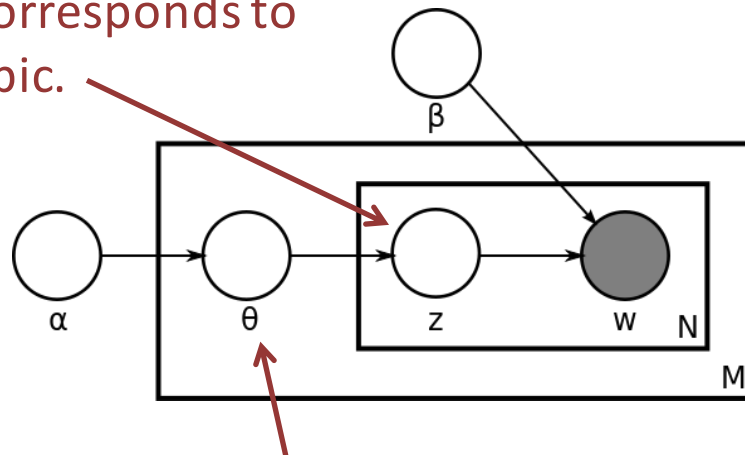
Training set: M documents, each with N words.

Topic mixture of document.

"Latent Dirichlet allocation" by Bkkbrad –
Own work. Licensed under GFDL via Commons –
https://commons.wikimedia.org/wiki/File:Latent_Dirichlet_allocation.svg#/media/File:Latent_Dirichlet_allocation.svg

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Example: LDA analysis of Sarah Palin's emails
(Disclaimer: this was the top result of Google Search "LDA example")

- **Topics**:

- **Trig/Family/Inspiration**: family, web, mail, god, son, from, congratulations, children, life, child, down, trig, baby, birth, love, you, syndrome, very, special, bless, old, husband, years, thank, best, …

- **Wildlife/BP Corrosion**: game, fish, moose, wildlife, hunting, bears, polar, bear, subsistence, management, area, board, hunt, wolves, control, department, year, use, wolf, habitat, hunters, caribou, program, denby, fishing, …

- **Energy/Fuel/Oil/Mining:** energy, fuel, costs, oil, alaskans, prices, cost, nome, now, high, being, home, public, power, mine, crisis, price, resource, need, community, fairbanks, rebate, use, mining, villages, …

- **Gas**: gas, oil, pipeline, agia, project, natural, north, producers, companies, tax, company, energy, development, slope, production, resources, line, gasline, transcanada, said, billion, plan, administration, million, industry, …

- **Education/Waste**: school, waste, education, students, schools, million, read, email, market, policy, student, year, high, news, states, program, first, report, business, management, bulletin, information, reports, 2008, quarter, …

- **Presidential Campaign/Elections**: mail, web, from, thank, you, box, mccain, sarah, very, good, great, john, hope, president, sincerely, wasilla, work, keep, make, add, family, republican, support, doing, p.o, …

http://blog.echen.me/2011/08/22/introduction-to-latent-dirichlet-allocation/

Example: LDA analysis of Sarah Palin's emails
(Disclaimer: this was the top result of Google Search "LDA example")

- Presidential Campaign
- Wildlife
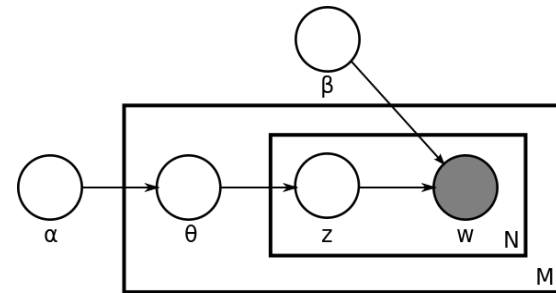
We understand that you have been discussed as a possible choice for the **Vice Presidency**.

As **people** who **support** the democratic process and care about protecting our **wildlife** for future generations, we want **you** to know that we don't believe **people** in our states would vote for **you** for any office if they knew your record on these issues.
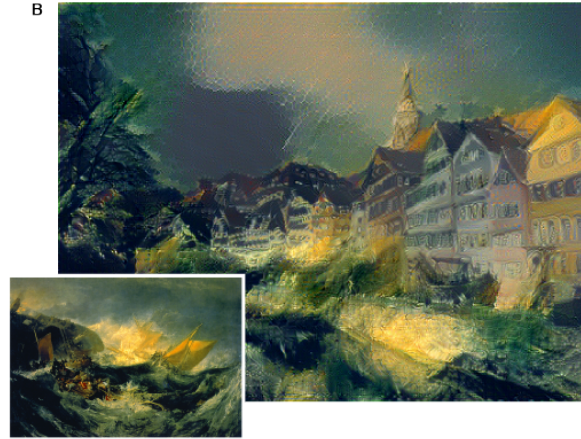
It is troubling that **you** are **now** working to deny more than 50,000 Alaskans a vote on **aerial** killing of **wolves** and **bears** with legislation now **being** considered in the Alaska legislature.
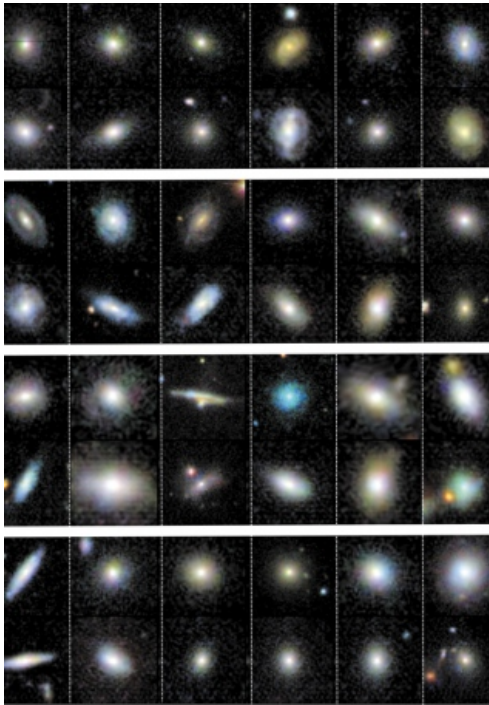
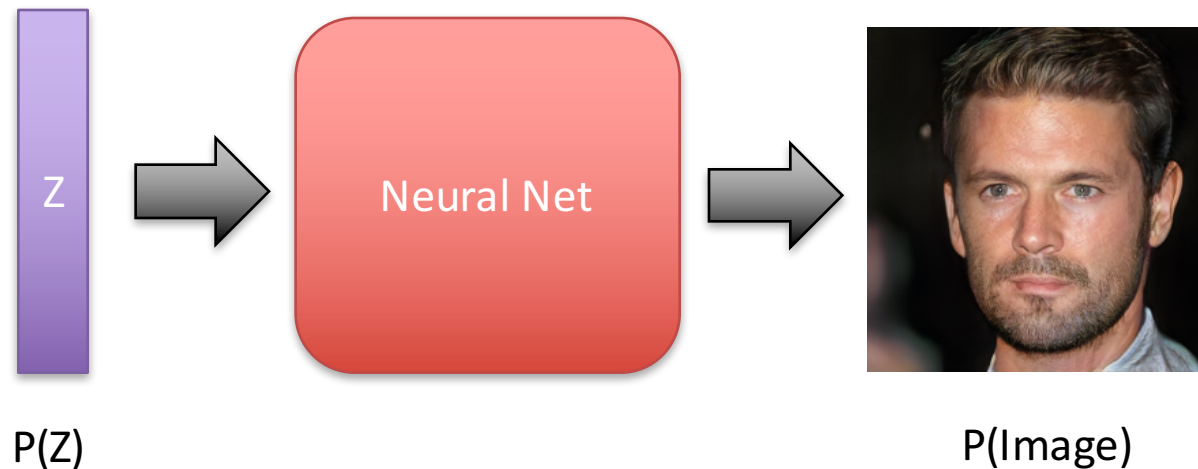# Deep Belief Networks

Generative Adversarial Networks

Learn from unlabeled telescope imagery,
generate new images,
now astronomers have more data

Learn from labeled images,
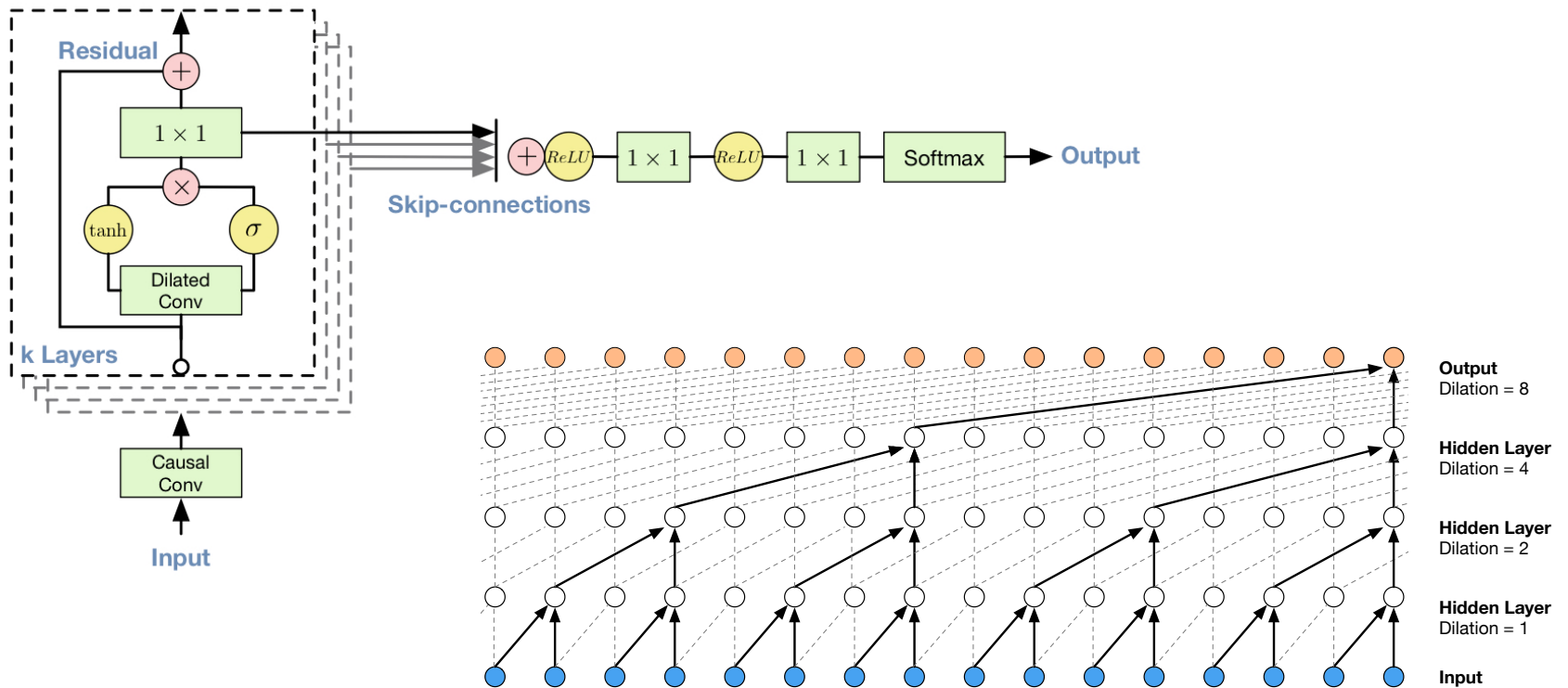condition on "Volcano" and generate new
images, because why not?

http://www.nature.com/news/astronomers-explore-uses-for-ai-generated-images-1.21398?WT.mc_id=FBK_NatureNews

"DeepFake"

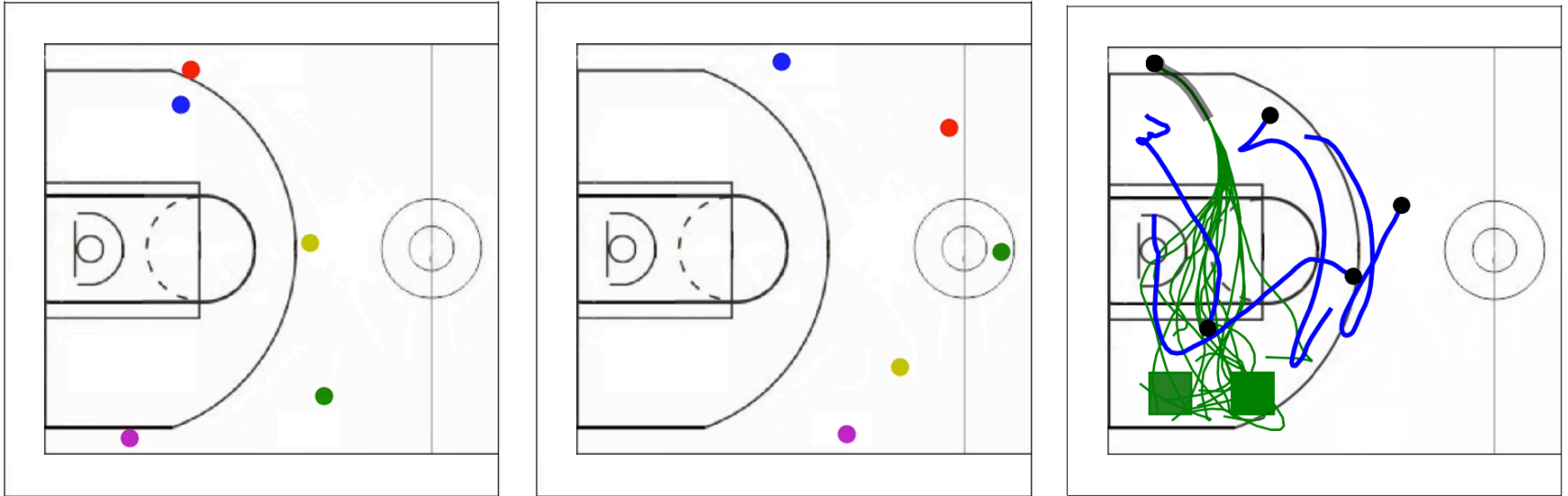P(Z)   P(Image)

Generative Adversarial Network (GAN)
(discussed further in Deep Generative Models lecture)

WaveNet

Generative Multi-Agent Models

- Train trajectories of basketball games
- Generate new trajectories
- https://arxiv.org/abs/1803.07612

Recap: Generative Probabilistic Models

- ## Quantifies Uncertainty
  - Can tolerate missing values

- ## Model represents a "summary" of the data
  - Fit model parameters to data
  - Can use for inspection

- ## Not trained to optimize prediction accuracy

- ## Can generate new samples
  - 10

- ## CS 159: Deep Generative Models (Spring 2019)

Next Two Lectures

- Hidden Markov Models in depth
  - Sequence Modeling
  - Requires Dynamic Programming
  - Implement aspects of HMMs in homework

- Recitation on Probability Tonight!