Inference and Representation

DS-GA-1005, CSCI-GA.2569

Joan Bruna
Courant Institute of Mathematical Sciences
Center for Data Science
NYU

Celestial Mechanics

CAP. XXIV.

COPERNICI

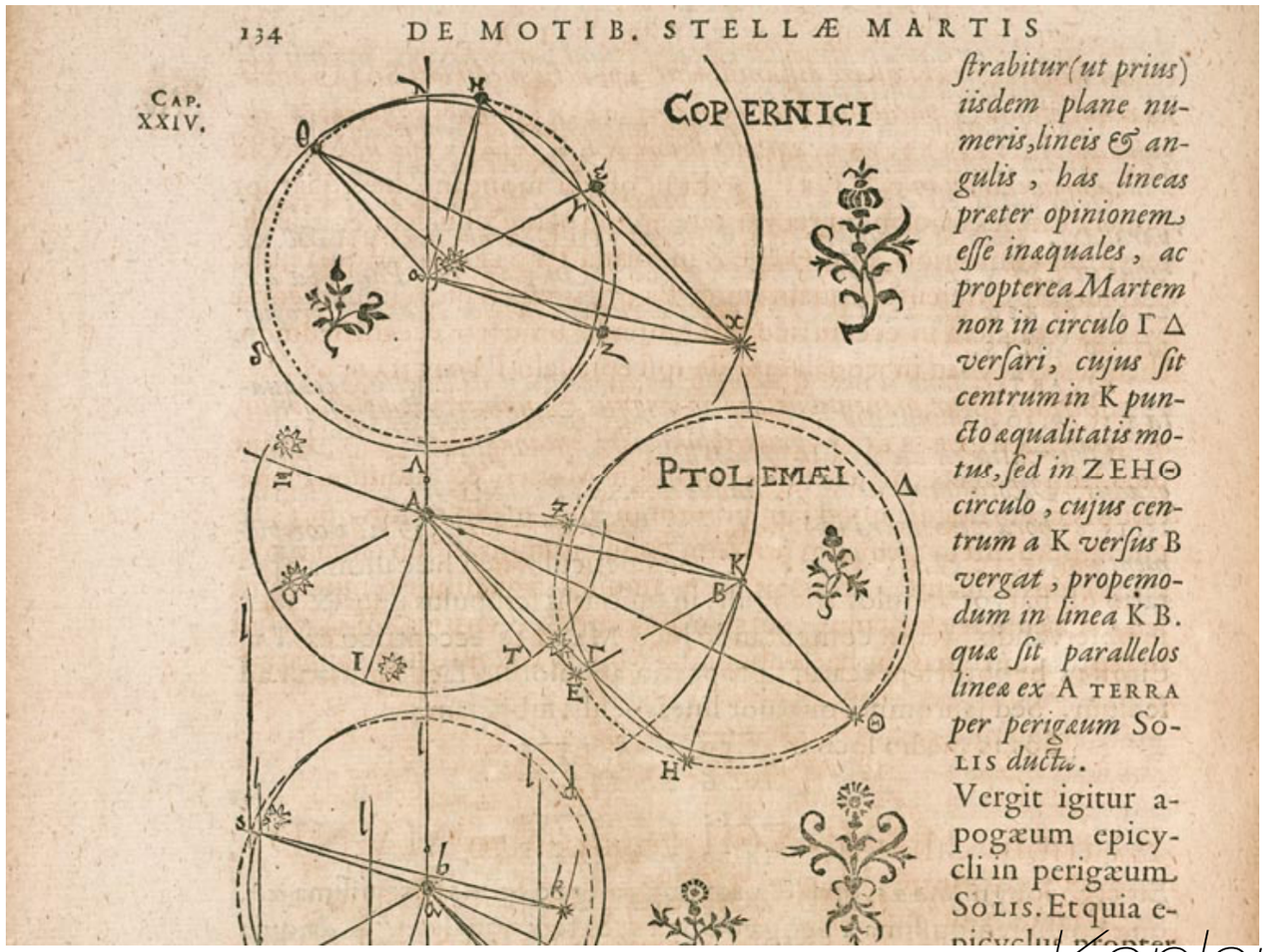
PTOLEMÆI

ſtrabitur (ut prius) iisdem plane numeris, lineis & angulis, has lineas præter opinionem, eſſe inæquales, ac propterea Martem non in circulo Γ Δ verſari, cujus ſit centrum in K *puncto æqualitatis motus, ſed in* ZEHΘ *circulo, cujus centrum a* K *verſus* B *vergat, propemodum in linea* KB. *quæ ſit parallelos lineæ ex* A TERRA *per perigæum* SOLIS *ductæ.*

Vergit igitur apogæum epicycli in perigæum SOLIS. Et quia epicyclus propter

Kepler, 17th Century

Celestial Mechanics



Kepler, 17th Century

- Determine the dynamics of planets, moons and stars given partial, noisy observations, and given partial, noisy mathematical model.
- Scientific Method: Build a model that can assign probabilities to observable events, and reject it whenever likelihood is too small.

Science = Model + Data

- Observations $x_1, \ldots, x_n$.
  - E.g. x_1: position of Jupiter at noon.
    x_2: position of Jupiter at midnight.
    x_3: size of the Moon at noon.
    ...

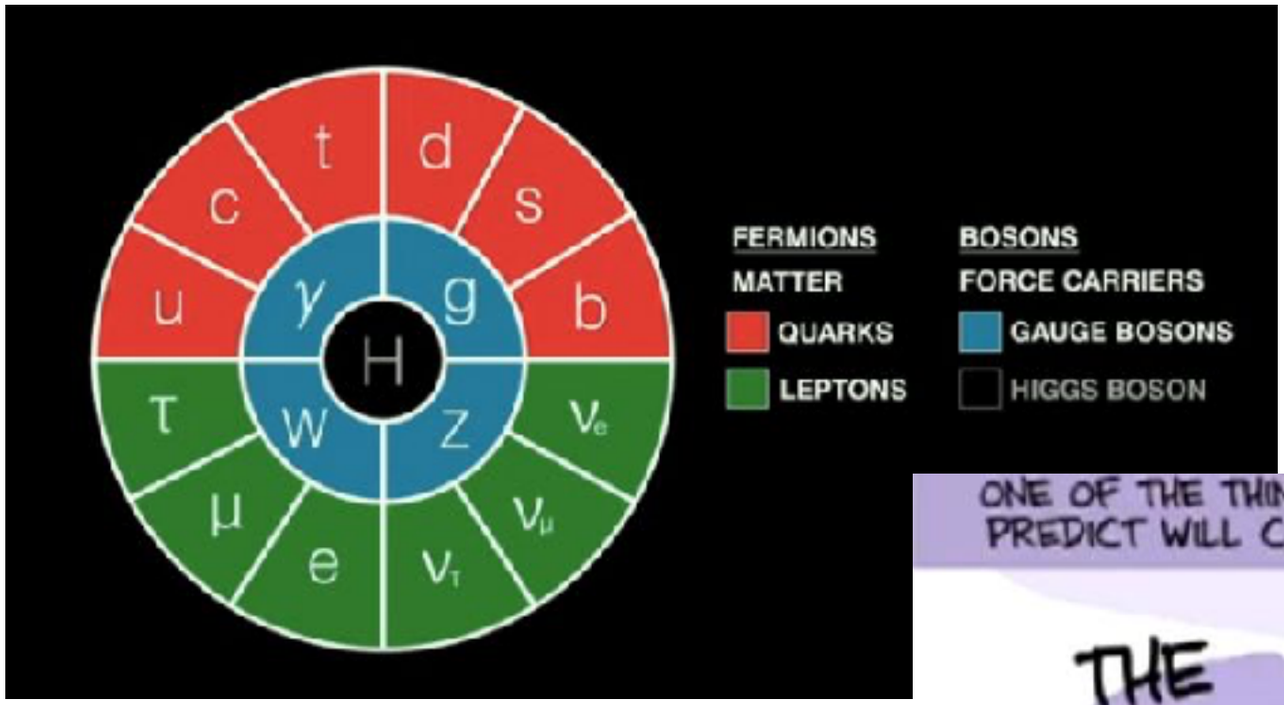
Science = Model + Data

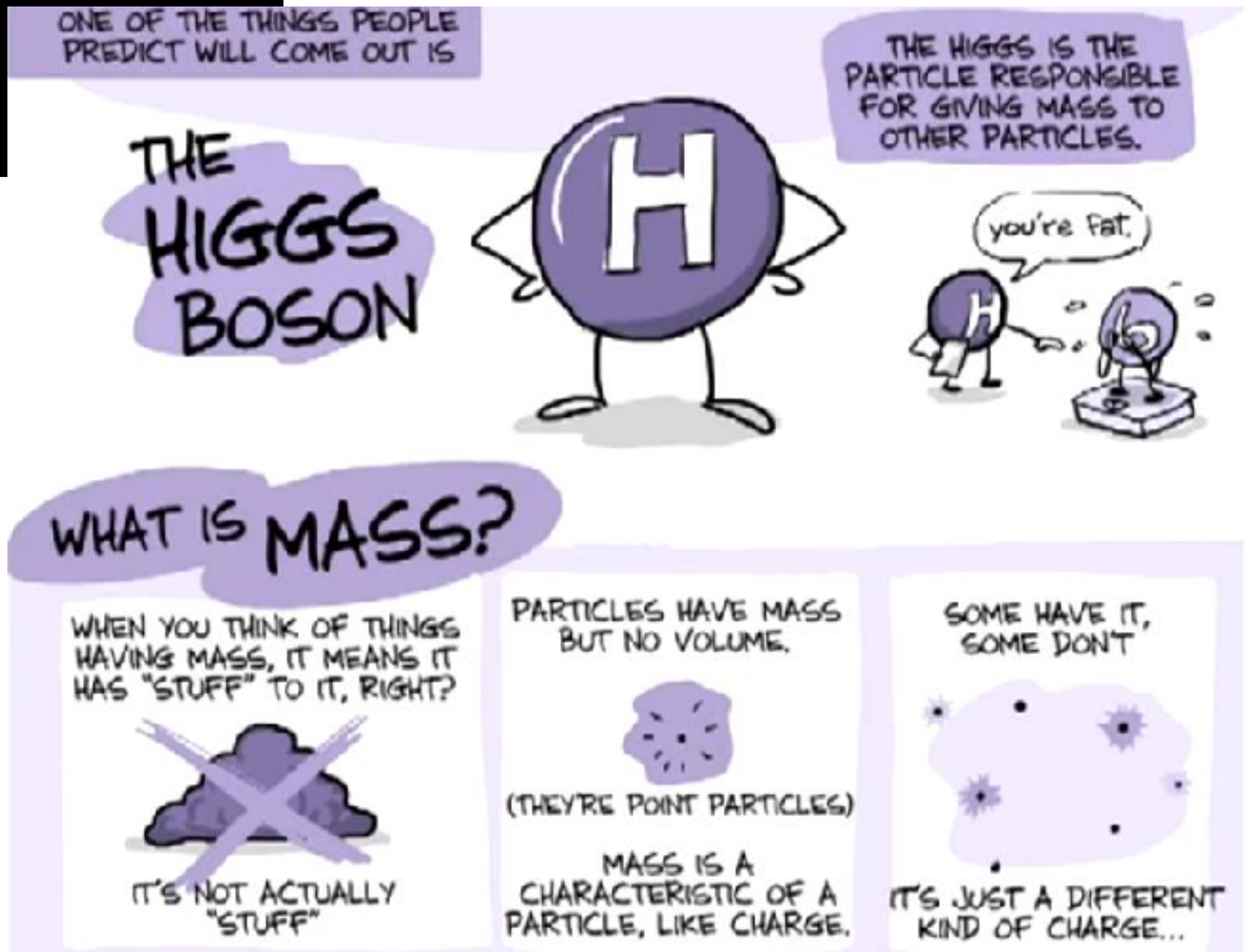
- Observations $x_1, \ldots, x_n$.
  - E.g. x_1: position of Jupiter at noon.
    x_2: position of Jupiter at midnight.
    x_3: size of the Moon at noon.
    ...
- Density models:

  Model A: Joint probability distribution
  $p_A(x_1, \ldots, x_n)$. (Solar system gravitates around Earth)
  Model B: Joint probability distribution
  $p_B(x_1, \ldots, x_n)$. (Solar system gravitates around Sun)

- Theories/Models are refuted from data by comparing likelihoods
  - Hypothesis testing, Likelihood ratios.

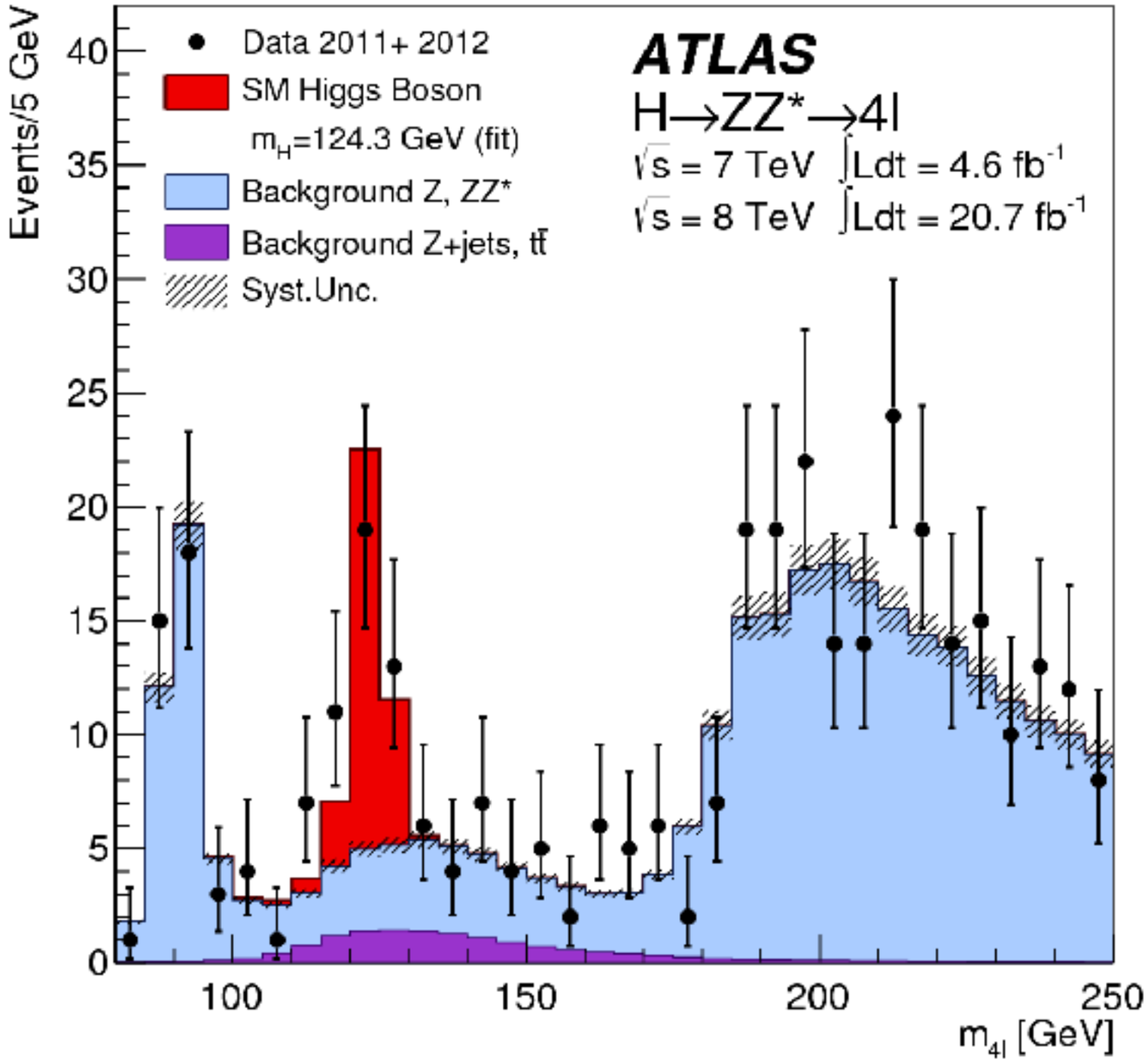
Higgs Boson


t
d
c
s
u
γ
g
b
H
τ
W
Z
ν_e
μ
e
ν_τ
ν_μ
FERMIONS
MATTER
QUARKS
LEPTONS
BOSONS
FORCE CARRIERS
GAUGE BOSONS
HIGGS BOSON


ONE OF THE THINGS PEOPLE PREDICT WILL COME OUT IS
THE HIGGS BOSON
THE HIGGS IS THE PARTICLE RESPONSIBLE FOR GIVING MASS TO OTHER PARTICLES.
you're fat.
WHAT IS MASS?
WHEN YOU THINK OF THINGS HAVING MASS, IT MEANS IT HAS "STUFF" TO IT, RIGHT?
IT'S NOT ACTUALLY "STUFF"
PARTICLES HAVE MASS BUT NO VOLUME.
(THEY'RE POINT PARTICLES)
MASS IS A CHARACTERISTIC OF A PARTICLE, LIKE CHARGE.
SOME HAVE IT, SOME DON'T
IT'S JUST A DIFFERENT KIND OF CHARGE...

Higgs Boson Discovery

- What does "discovery" mean in this context?



Fundamental Scientific Pipeline

- How to construct such models to explain large systems?
  - Representation Challenge: How to parametrize ?

$$p(x_1, \ldots, x_n) = f_\theta(x_1, \ldots, x_n)$$

Fundamental Scientific Pipeline

- How to construct such models to explain large systems?
  - Representation Challenge: How to parametrize ?

$$p(x_1, \ldots, x_n) = f_\theta(x_1, \ldots, x_n)$$

- How to adjust the parameters of such models to best explain the data?
  - Learning Challenge: How to fit θ to the data?

Fundamental Scientific Pipeline

- How to construct such models to explain large systems?
  - Representation Challenge: How to parametrize ?

$$p(x_1, \ldots, x_n) = f_\theta(x_1, \ldots, x_n)$$

- How to adjust the parameters of such models to best explain the data?
  - Learning Challenge: How to fit θ to the data?

- How to evaluate likelihoods under the model?
  - Inference Challenge

Fundamental Scientific Pipeline

- How to construct such models to explain large systems?
  - Representation Challenge: How to parametrize ?

$$p(x_1, \ldots, x_n) = f_\theta(x_1, \ldots, x_n)$$

- How to adjust the parameters of such models to best explain the data?
  - Learning Challenge: How to fit θ to the data?

- How to evaluate likelihoods under the model?
  - Inference Challenge
  - In most interesting cases, exact inference will be computationally intractable.

Fundamental Scientific Pipeline

- How to construct such models to explain large systems?
  - Representation Challenge: How to parametrize ?

$$p(x_1, \ldots, x_n) = f_\theta(x_1, \ldots, x_n)$$

- How to adjust the parameters of such models to best explain the data?
  - Learning Challenge: How to fit θ to the data?

- How to evaluate likelihoods under the model?
  - Inference Challenge
  - In most interesting cases, exact inference will be computationally intractable.
  - Major Topic of the course: develop computationally efficient approximate inference.

Applications: Modeling Text Data

- Topic Models allow us to infer, interpret large texts

Poisoning by ice-cream.

No chemist certainly would suppose that the same poison exists in all samples of ice-cream which have produced untoward symptoms in man. Mineral poisons, copper, lead, arsenic, and mercury, have all been found in ice cream. In some instances these have been used with criminal intent. In other cases their presence has been accidental. Likewise, that vanilla is sometimes the bearer, at least, of the poison, is well known to all chemists. Dr. Bartley's idea that the poisonous properties of the cream which he examined were due to putrid gelatine is certainly a rational theory. The poisonous principle might in this case arise from the decomposition of the gelatine ; or with the gelatine there may be introduced into the milk a ferment, by the growth of which a poison is produced.

But in the cream which I examined, none of the above sources of the poisoning existed. There were no mineral poisons present. No gelatine of any kind had been used in making the cream. The vanilla used was shown to be not poisonous. This showing was made, not by a chemical analysis, which might not have been conclusive, but Mr. Novie and I drank of the vanilla extract which was used, and no ill results followed. Still, from this cream we isolated the same poison which I had before found in poisonous cheese (*Zeitschrift für physiologische chemie*, x,

RNA Editing and the Evolution of Parasites

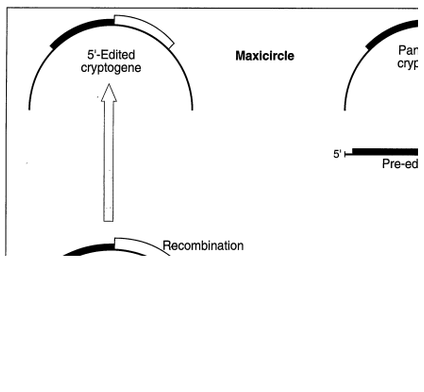
Larry Simpson and Dmitri A. Maslov

The kinetoplastid flagellates, together with their sister group of euglenoids, represent the earliest extant lineage of eukaryotic organisms containing mitochondria (*1*). Within the kinetoplastids, there are two major groups, the poorly studied bodonids-cryptobiids, which consist of both free-living and parasitic cells, and the better known trypanosomatids, which are obligate parasites (*2*).

Perhaps because of the antiquity of the trypanosomatid lineage, these cells possess several unique genetic features (see accompanying Perspective by Nilsen)—one of which is RNA editing of mitochondrial transcripts. This RNA editing function (*3*–*7*) creates open reading frames in "cryptogenes" by insertion (or occasional deletion) of uridine (U) residues at a few specific sites within the coding region of an mRNA (5′-editing) or at multiple specific sites throughout the mRNA (pan-editing). The

tral, but there is disagreement on the nature of the primary parasitic host. The "invertebrate first" model (*10*, *11*) states that the initial parasitism was in the gut of pre-Cambrian invertebrates. Coevolution of parasite and host would have led to a wide distribution of trypanosomatids in insects and leeches. In this theory, digenetic life cycles (alternating invertebrate and vertebrate hosts) evolved later as a result of the acquisition by some hemipterans and dipterans of the ability to feed on the blood

tion
arthr
netic
woul
the a
In
pothe
mito
quen
Crithi
cent
nucle
as an
tical
Trypa
the l
by th
fish
tutes
trypa
branc
separ



Chaotic Beetles

Charles Godfray and Michael Hassell

Ecologists have known since the pioneering work of May in the mid-1970s (*1*) that the population dynamics of animals and plants can be exceedingly complex. This complexity arises from two sources: The tangled web of interactions that constitute any natural community provide a myriad of different pathways for species to interact, both directly and indirectly. And even in isolated populations the nonlinear feedback processes present in all natural populations can result in complex dynamic behavior. Natural populations can show persistent oscillatory dynamics and chaos, the latter characterized by extreme sensitivity to initial conditions. If such chaotic dynamics were common in nature, then this would have important ramifications for the management and conservation of natural resources. On page 389 of this issue, Costantino *et al.* (*2*) provide the most convincing evidence to date of complex dynamics and chaos in a biological population—of the flour beetle, *Tribolium castaneum* (see figure).

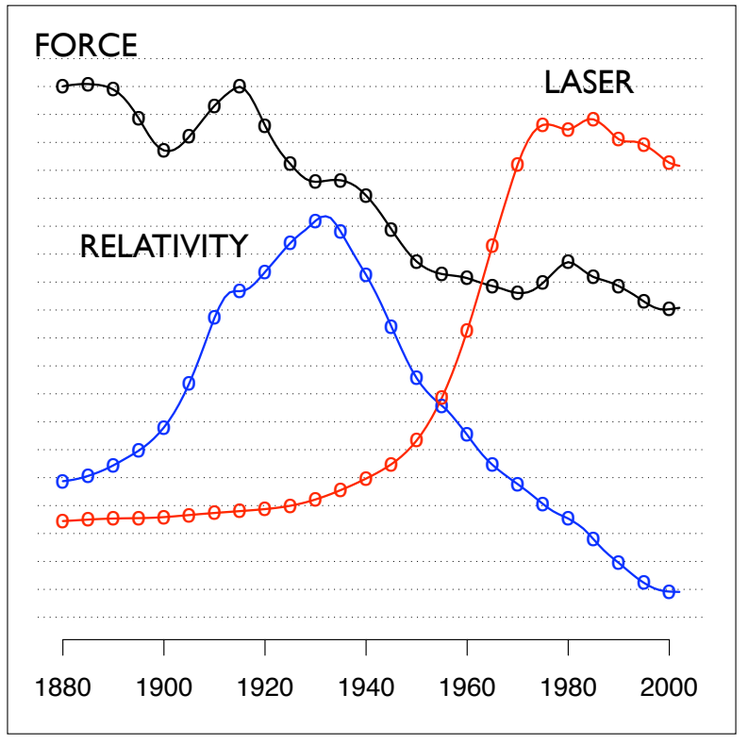
It has proven extremely difficult to demonstrate complex dynamics in populations in the field. By its very nature, a chaotically fluctuating population will superficially resemble a stable or cyclic population buffeted by the normal random perturbations experienced by all species. Given a long enough time series, diagnostic tools from nonlinear mathematics can be used to identify the telltale signatures of chaos. In phase space, chaotic trajectories come to lie on "strange attractors," curious geometric objects with fractal structure and hence noninteger dimension. As they move over the surface of the attractor, sets of adjacent trajectories are pulled apart, then stretched and folded, so that it becomes impossible to predict exact population densities into the future. The strength of the mixing that gives rise to the extreme sensitivity to initial conditions can be measured mathematically estimating the Liapunov exponent, which is positive for chaotic dynamics and nonpositive otherwise. There have been many attempts to estimate attractor dimension and Liapunov exponents from time series data, and some candidate chaotic population have been identified (some insects, rodents, and most convincingly, human childhood diseases), but the statistical difficulties preclude any broad generalization (*3*).

The authors are in the Department of Biology, Imperial College at Silwood Park, Ascot, Berks, SL5 7PZ UK. E-mail: m.hassell@ic.ac.uk

Cannibalism and chaos. The flour beetle, *Tribolium castaneum*, exhibits chaotic population dynamics when the amount of cannibalism is altered in a mathematical model.

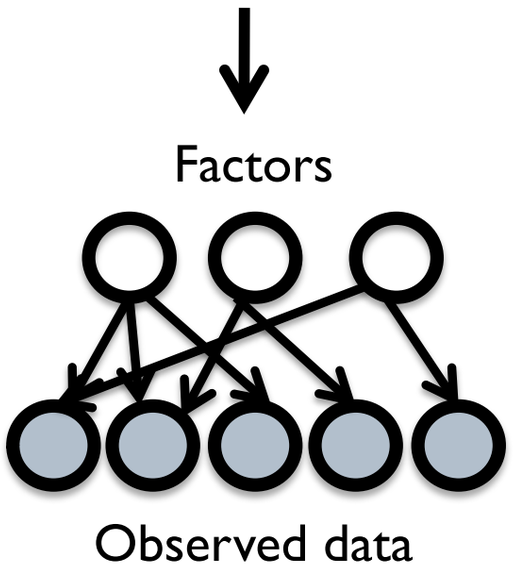
An alternative approach is to parameterize population models with data from natural populations and then compare their predictions with the dynamics in the field. This technique has been gaining popularity in recent years, helped by statistical advances in parameter estimation. Good ex-

human	evolution	disease	computer
genome	evolutionary	host	models
dna	species	bacteria	information
genetic	organisms	diseases	data
genes	life	resistance	computers
sequence	origin	bacterial	system
gene	biology	new	network
molecular	groups	strains	systems
sequencing	phylogenetic	control	model
map	living	infectious	parallel
information	diversity	malaria	methods
genetics	group	parasite	networks
mapping	new	parasites	software
project	two	united	new
sequences	common	tuberculosis	simulations



Applications: Survey Data

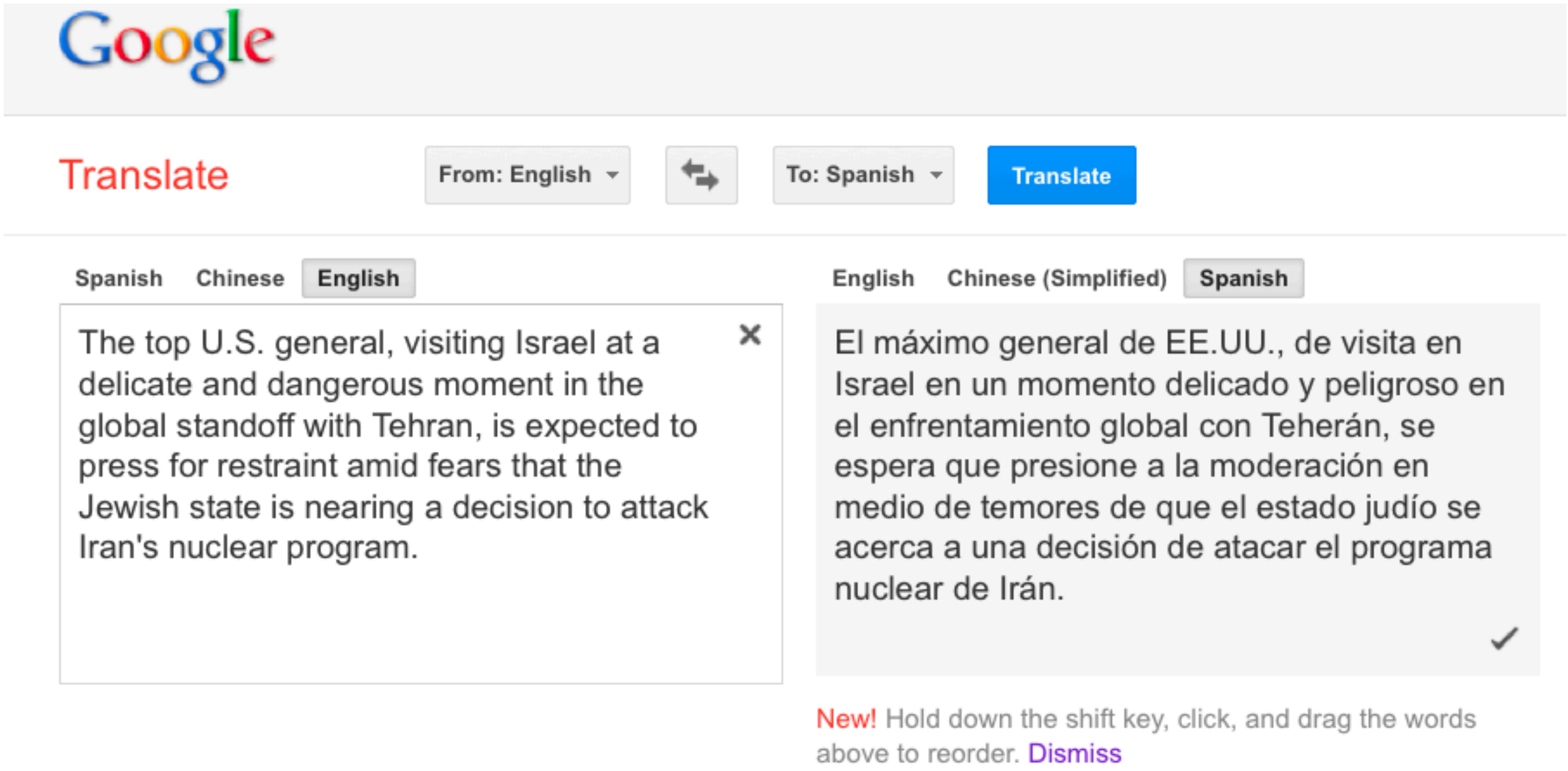
1 0 0 1 1 0 0 0 1
1 1 0 1 1 0 0 1 0
0 1 0 1 0 0 1 0 0
1 0 0 0 1 0 0 1 1
0 1 0 1 0 0 1 1 0



- Social surveys with questions such as
  - Should tax rate be progressive?
  - Do you support the BLM movement?
  - Should affirmative action be used in college admissions?
- Goal is to automatically discover relevant factors, e.g.
  - Socioeconomic status
  - Health
  - Political values
- Factor Analysis models infer underlying beliefs/ traits of survey data

Applications: Modeling Sequential Data

- Automatic Machine Translation

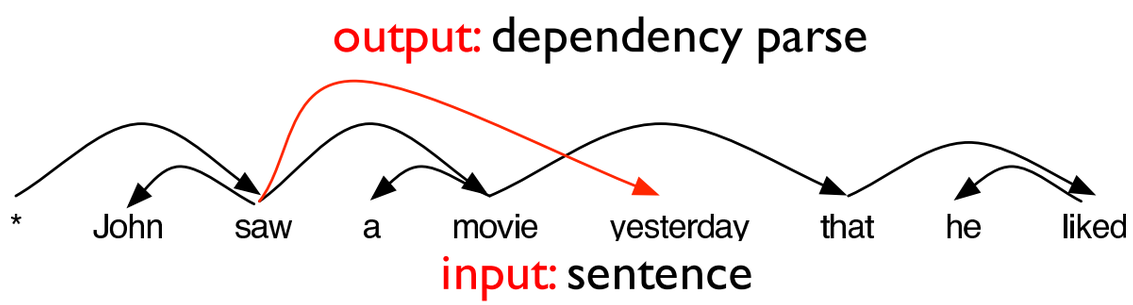


– nowadays mostly based on recurrent neural network models.

Applications: Structured Output Prediction

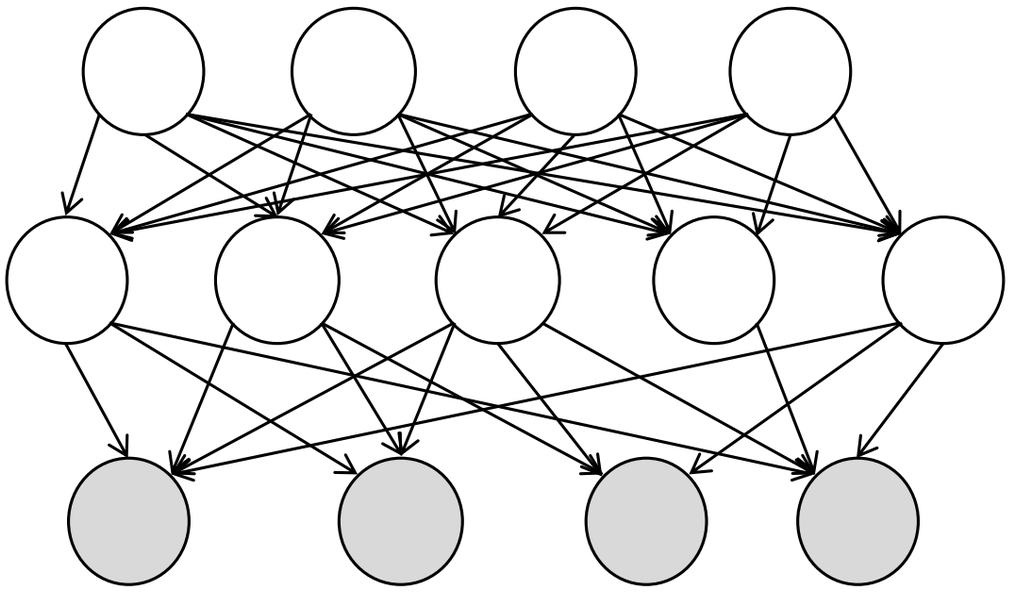
- Image Segmentation

- Natural Language Processing

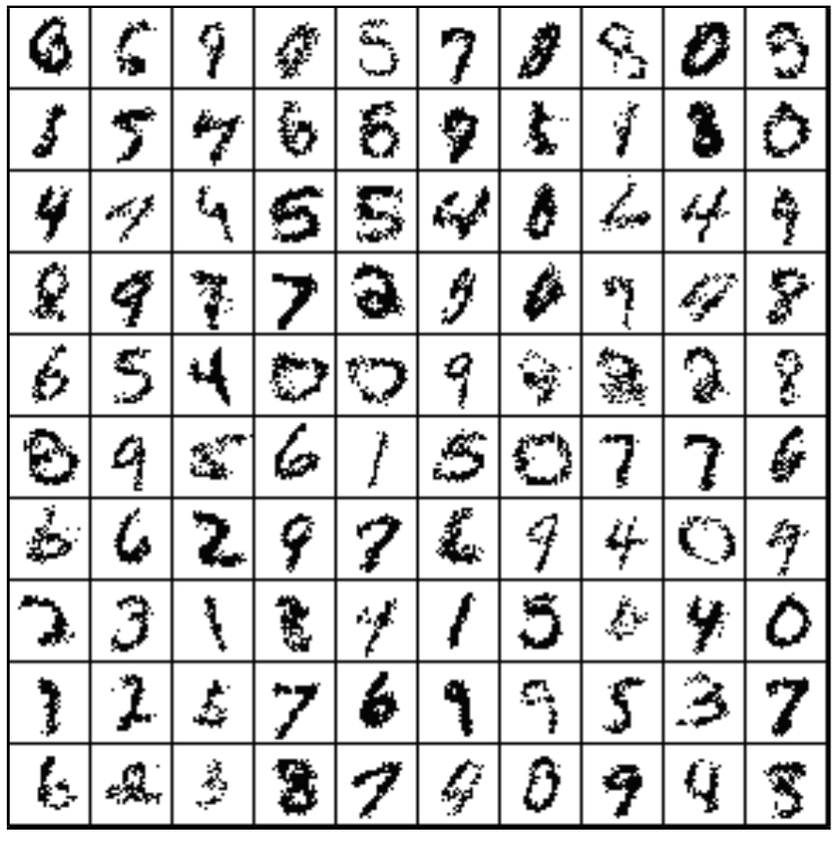


Applications: Modeling Images

- Main challenge: high-dimensionality, complex, long-range dependencies.
  - Deep Generative Models, Autoencoders, Generative Adversarial Networks.

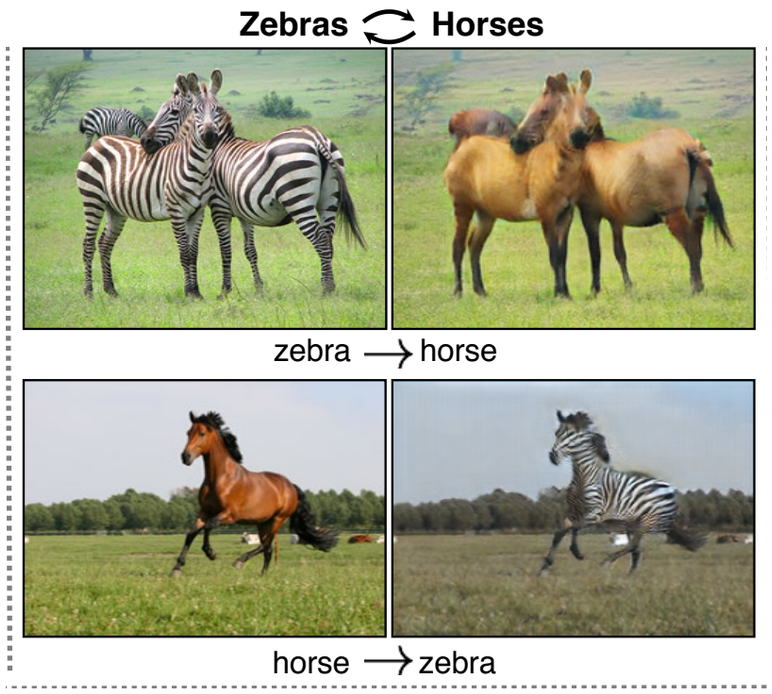


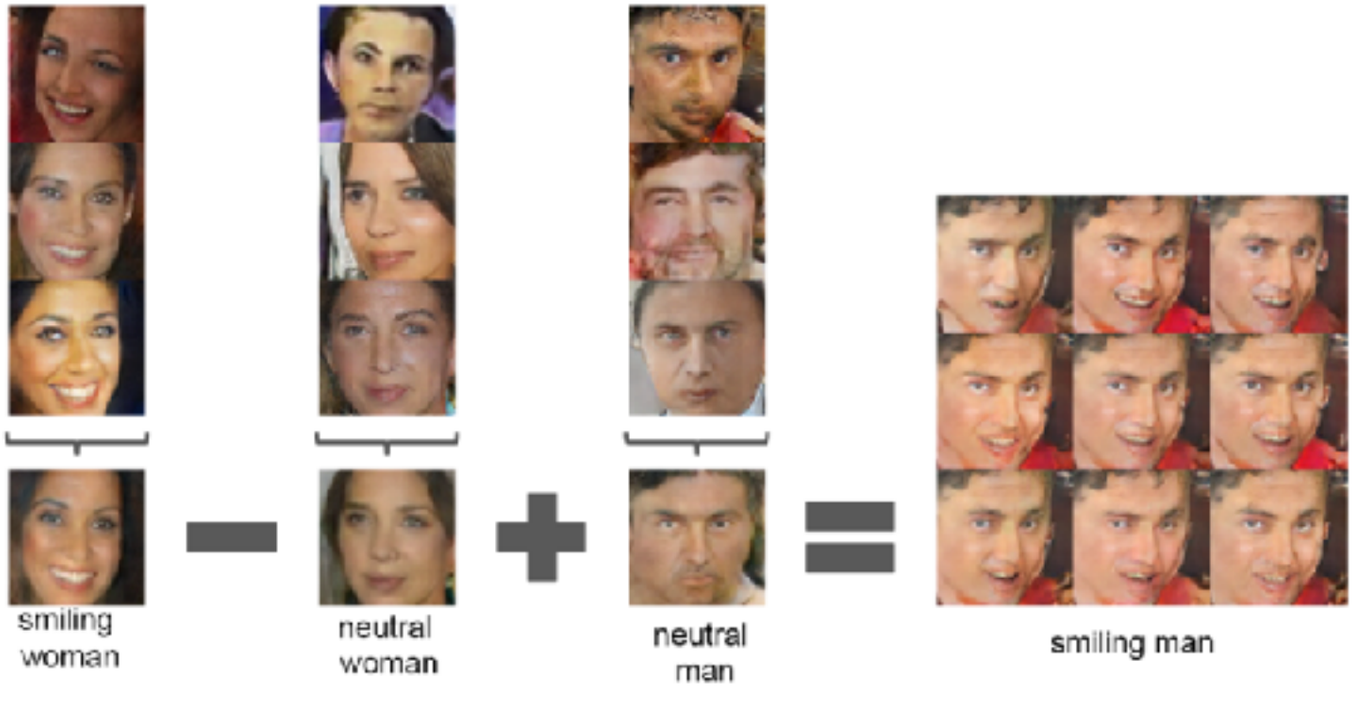
Samples from the model:



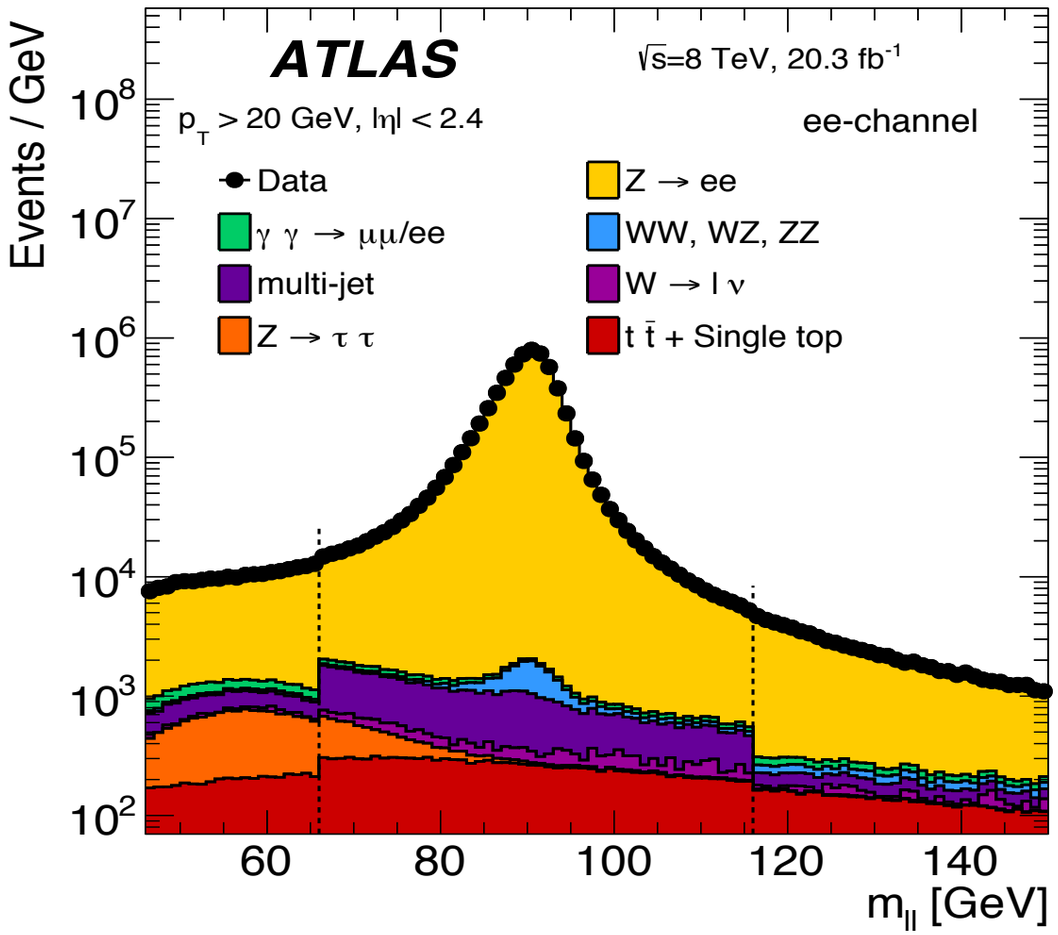
Modern Unsupervised Learning Tasks

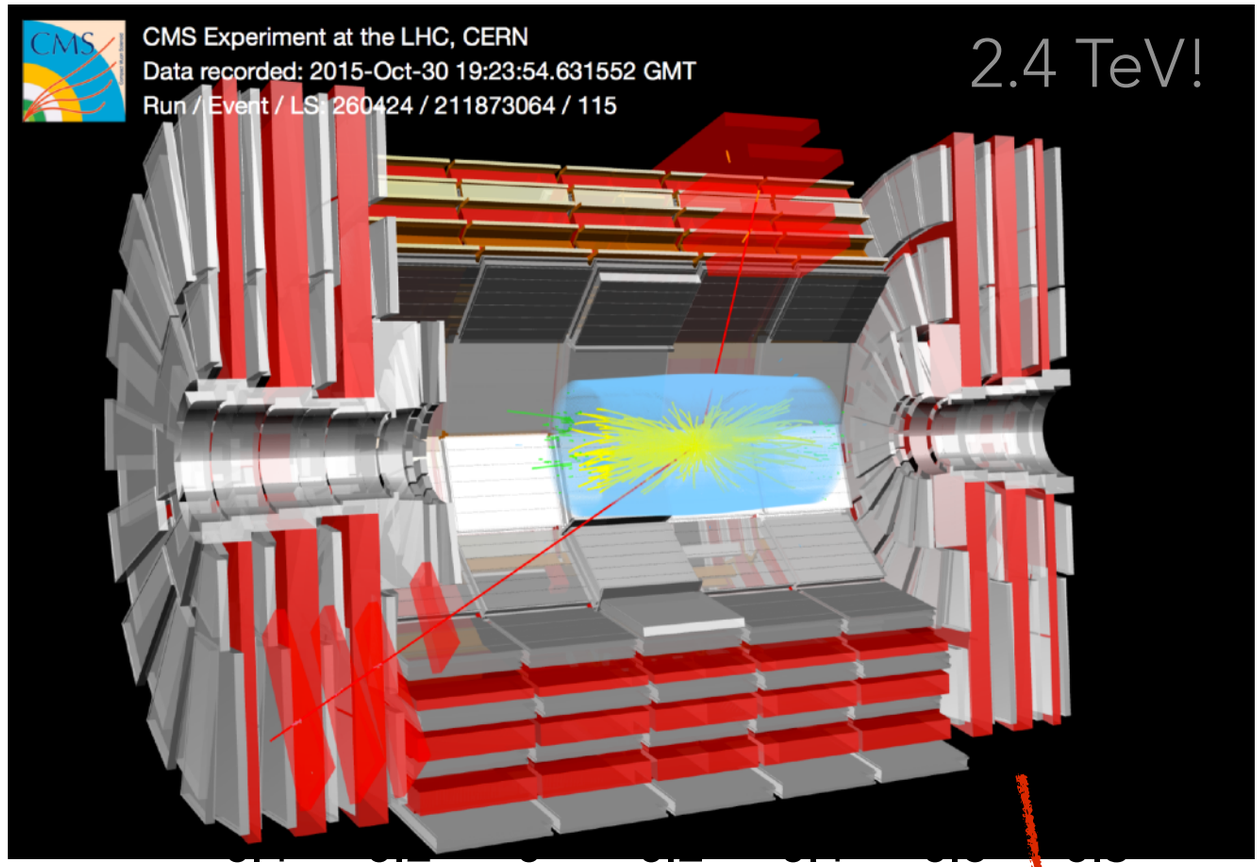
- Adversarial Training
- Domain Adaptation

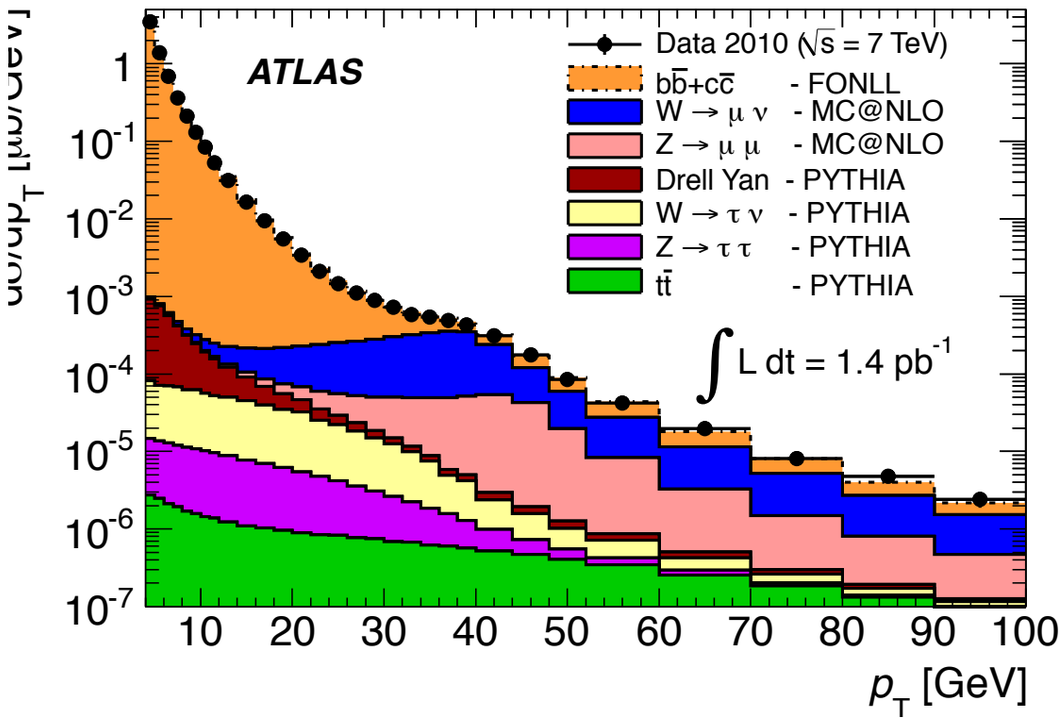


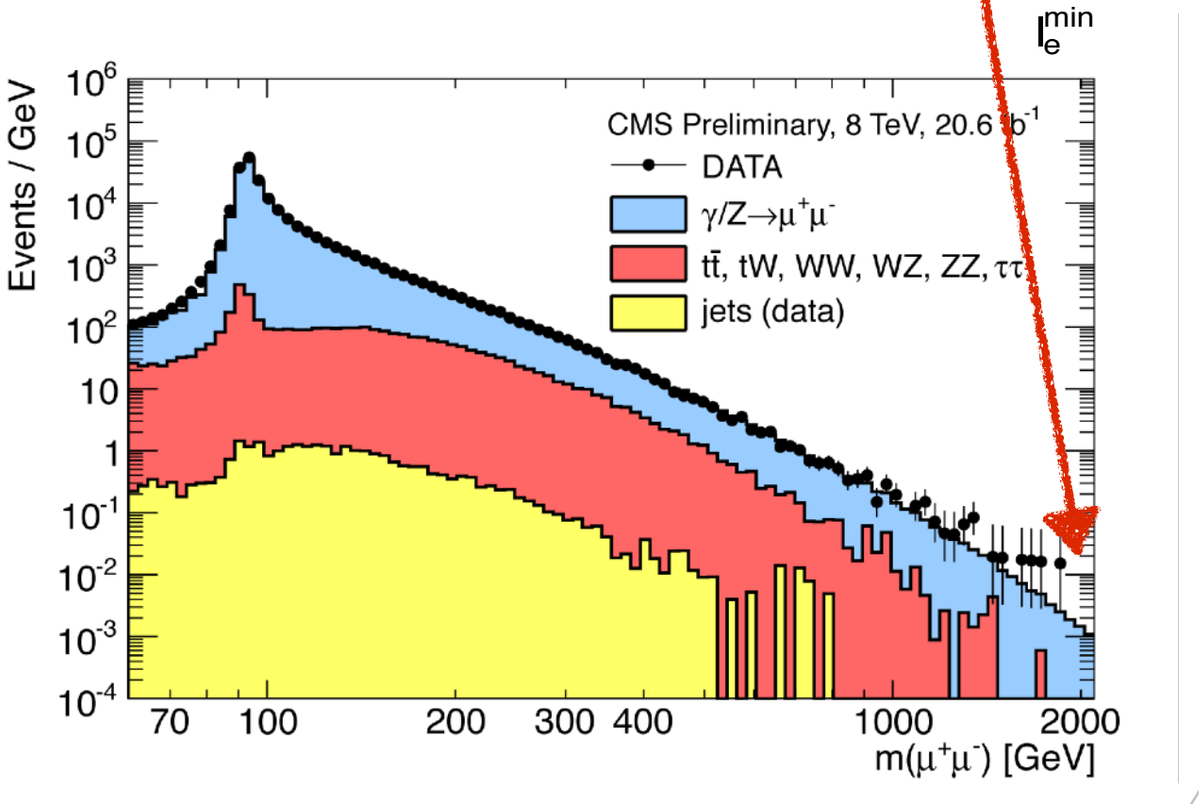


Applications: Particle Physics

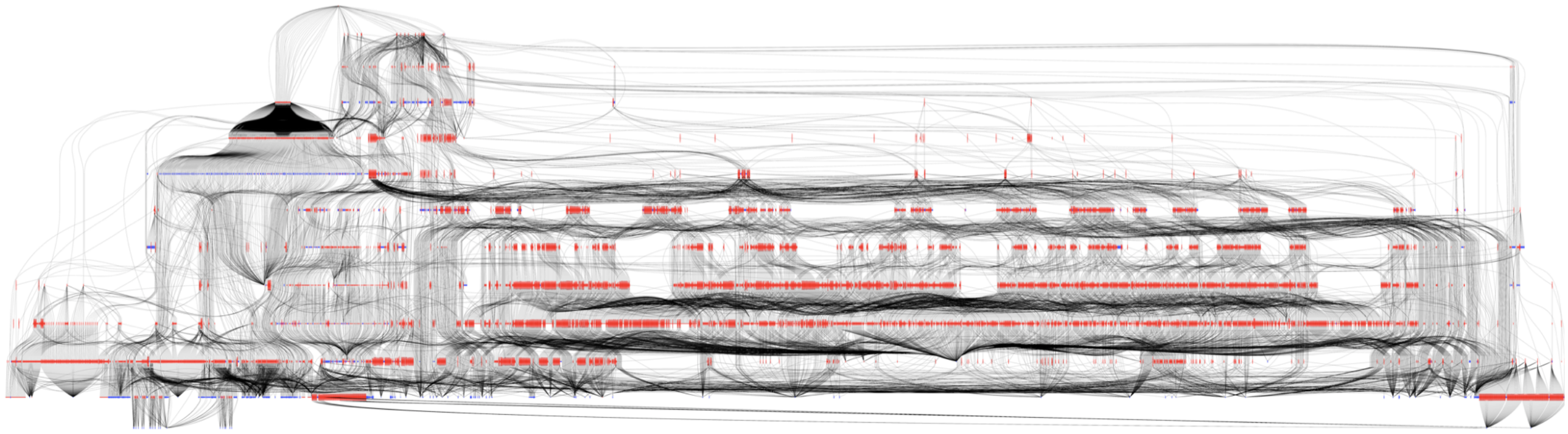








Applications: Particle Physics



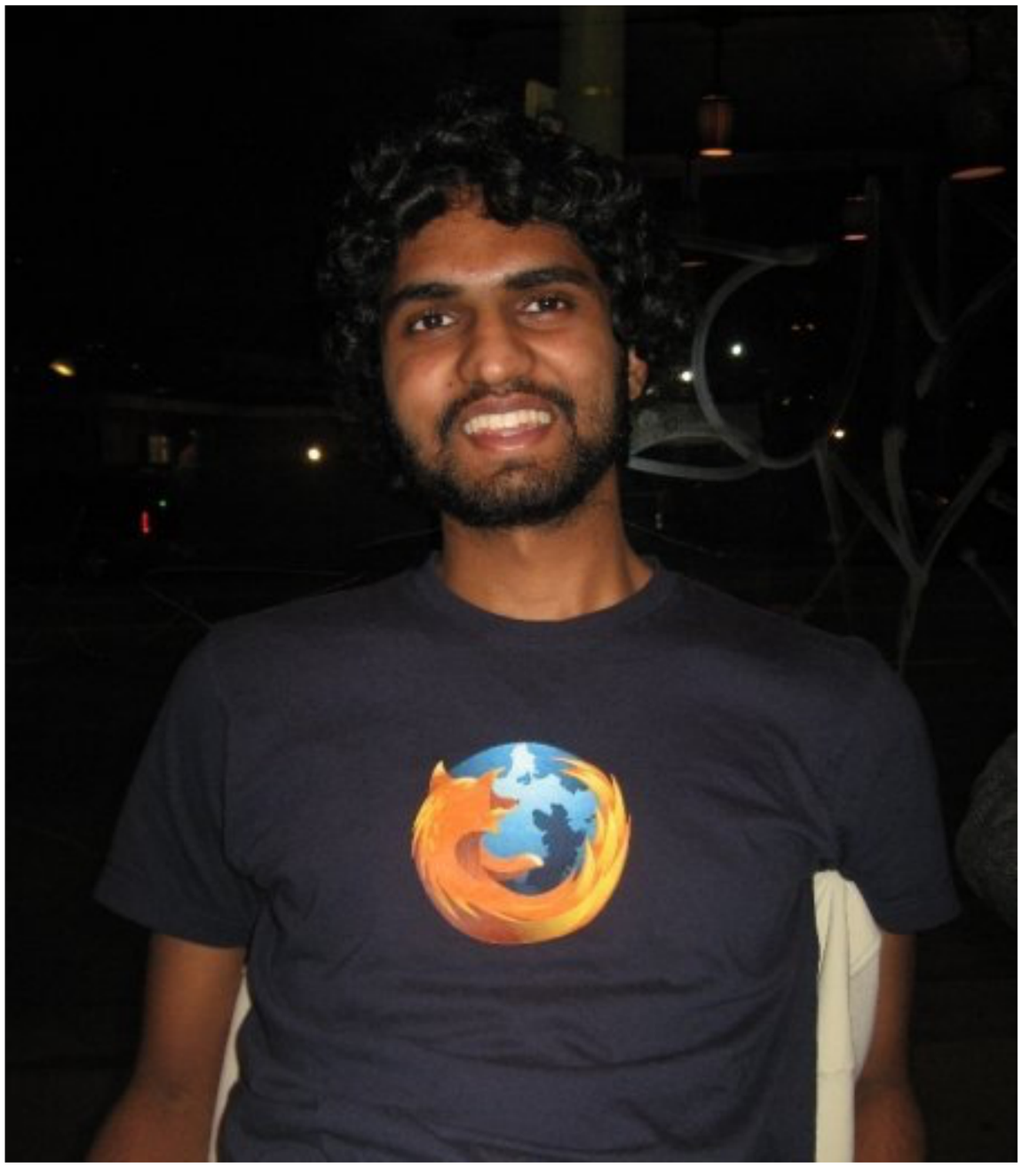
$$\mathbf{f}_{\text{tot}}(\mathcal{D}_{\text{sim}}, \mathcal{G}|\boldsymbol{\alpha}) = \prod_{c \in \text{channels}} \left[\text{Pois}(n_c|\nu_c(\boldsymbol{\alpha})) \prod_{e=1}^{n_c} f_c(x_{ce}|\boldsymbol{\alpha}) \right] \cdot \prod_{p \in \mathbb{S}} f_p(a_p|\alpha_p)$$

Syllabus Overview

- Definitions, Directed Graphical Models and Bayesian Networks (lect1)
- Undirected Graphical Models. Markov Random Fields (lect2)
- Topic Models and Bayesian Non-parametrics (lect 3)
- Principal Component Analysis with Applications (lect 4)
- Expectation-Maximization. MCMC (lect 5)
- Variational Inference (lect 6)
- Structured Output Prediction (lect 7)
- Sequential Models (lect 8)
- Boltzmann Machines, Variational Autoencoders (lect 9)
- Modeling images. GANs, Flows and Autoregressive (lect 10)
- Modern unsupervised learning with GANs and VAEs (lect 11)

Guest Lectures

- Rajesh Ranganath (next week)
  - Machine Learning, Variational Inference, ML for Healthcare.



Logistics

- Website: https://joanbruna.github.io/ir18/
- Piazza (you need to sign up): https://joanbruna.github.io/ir18/ piazza.com/nyu/fall2018/dsga1005csciga2569

- Required Readings for each lecture posted to course website.
- Books
  - Machine Learning: a probabilistic perspective, by Kevin Murphy (available online)
  - Mike Jordan's notes on Probabilistic Graphical Models.
- Office Hours
  - Tuesdays 3pm-5pm (office 612)
- Lab/Recitation: Monday, 4:55-6:35pm in 60 FA 110

Prerequisites and Grading

- Pre-requisite: DS-GA-1003/CSCI-GA 2567 Machine Learning and Computational Statistics)
- Grading
  - Problem Sets: 40%
  - Midterm Exam: 25%
  - Final Project: 30%
  - Class/Lab participation: 5%

Prerequisites and Grading

- Pre-requisite: DS-GA-1003/CSCI-GA 2567 Machine Learning and Computational Statistics)
- Grading
  - Problem Sets: 45%
  - Midterm Exam: 25%
  - Final Project: 25%
  - Class/Lab participation: 5%
- Final Project
  - Research project applying tools developed in class.
  - Proposal due by end of October
  - Feedback on proposal early November
  - Project writeup and Poster presentation: end of semester

Recitation: Inverse Curriculum

- Led by Sanyam Kapoor
- Based on the idea of "depth-first learning" by C. Resnick.

- Two topics (6 weeks + 6 weeks):
  - Normalizing Flows
  - Inference and Representation in RL

Basic Definitions and Notation

- A central object of this class is a joint probability distribution over a high-dimensional space.
- To simplify, we start with a discrete space. Assume random variables $X_1, \ldots, X_n$, each defined over a discrete space of q symbols: $\mathcal{X} = \{a_1, \ldots, a_q\}$

Basic Definitions and Notation

- A central object of this class is a joint probability distribution over a high-dimensional space.
- To simplify, we start with a discrete space. Assume random variables $X_1, \ldots, X_n$, each defined over a discrete space of q symbols: $\mathcal{X} = \{a_1, \ldots, a_q\}$
- Joint probability distribution of random vector $\mathbf{X} = (X_1, \ldots, X_n)$ is a mapping $p : \mathcal{X} \otimes \cdots \otimes \mathcal{X} \rightarrow [0, 1]$ that computes

$$p(X_1 = a_{i_1}, \ldots, X_n = a_{i_n}) \quad \text{for all } i_1, \ldots i_n \in \{1, q\}.$$

  - Normalized measure $\sum_{x \in \mathcal{X}^n} p(x) = 1$

Basic Definitions and Notation

- A central object of this class is a joint probability distribution over a high-dimensional space.
- To simplify, we start with a discrete space. Assume random variables $X_1, \ldots, X_n$, each defined over a discrete space of q symbols: $\mathcal{X} = \{a_1, \ldots, a_q\}$
- Joint probability distribution of random vector $\mathbf{X} = (X_1, \ldots, X_n)$ is a mapping $p : \mathcal{X} \otimes \cdots \otimes \mathcal{X} \rightarrow [0, 1]$ that computes

$$p(X_1 = a_{i_1}, \ldots, X_n = a_{i_n}) \text{ for all } i_1, \ldots i_n \in \{1, q\}.$$

  - Normalized measure $\sum_{x \in \mathcal{X}^n} p(x) = 1$
- A *Probabilistic Model* is one such distribution, typically indexed by parameters $\theta \in \mathbb{R}^s$ that are fit to the data: p_θ
  - Two statistical paradigms
    - Parametric/ low-dimensional statistics: s fixed as n increases
    - Non-parametric / high-dimensional statistics: s increases with n.

Curse of Dimensionality

- How large is the space of multivariate distributions as a function of n?
  - Discrete case: the number of possible outcomes is q^n : exponential dependency.
  - Continuous case: under regularity assumptions, same phenomena.

Curse of Dimensionality

- How large is the space of multivariate distributions as a function of n?
  - Discrete case: the number of possible outcomes is q^n : exponential dependency.
  - Continuous case: under regularity assumptions, same phenomena.
- **Generic joint distribution: given by $\theta \in \mathbb{R}_+^{q^n}$:** parameters of a multinomial distribution.
- Estimation from m samples:

$$\hat{\theta}_j = \frac{1}{m} \sum_{i \leq m} \mathbf{1}\{x_i = (a_{j_1} \dots a_{j_n})\} \ .$$

Curse of Dimensionality

- How large is the space of multivariate distributions as a function of n?
  - Discrete case: the number of possible outcomes is q^n : exponential dependency.
  - Continuous case: under regularity assumptions, same phenomena.
- **Generic joint distribution: given by $\theta \in \mathbb{R}_+^{q^n}$:** parameters of a multinomial distribution.
- Estimation from m samples:

$$\hat{\theta}_j = \frac{1}{m} \sum_{i<m} \mathbf{1}\{x_i = (a_{j_1} \dots a_{j_n})\} \ .$$

- $$\frac{\mathbb{E}(\|\theta - \hat{\theta}\|^2)}{\|\theta\|^2} = \frac{\sum_j \theta_j(1-\theta_j)}{m\|\theta\|^2} \simeq \frac{\|\theta\|^{-2}}{m}$$

Curse of Dimensionality

- How large is the space of multivariate distributions as a function of n?
  - Discrete case: the number of possible outcomes is q^n : exponential dependency.
  - Continuous case: under regularity assumptions, same phenomena.
- **Generic joint distribution: given by $\theta \in \mathbb{R}_+^{q^n}$:** parameters of a multinomial distribution.
- Estimation from m samples:

$$\hat{\theta}_j = \frac{1}{m} \sum_{i<m} \mathbf{1}\{x_i = (a_{j_1} \dots a_{j_n})\} \ .$$

- $$\frac{\mathbb{E}(\|\theta - \hat{\theta}\|^2)}{\|\theta\|^2} = \frac{\sum_j \theta_j(1-\theta_j)}{m\|\theta\|^2} \simeq \frac{\|\theta\|^{-2}}{m}$$

- But $\|\theta\|^{-2} \sim q^n$

Curse of Dimensionality

- How large is the space of multivariate distributions as a function of n?
  - Discrete case: the number of possible outcomes is q^n : exponential dependency.
  - Continuous case: under regularity assumptions, same phenomena.
- Estimation of a generic multivariate distribution is therefore intractable: **statistical intractability.**
- Inference of conditional probabilities is **computationally intractable**

$$p(\text{pneumonia} = 1 \mid \text{cough} = 1, \text{fever} = 1, \text{vomiting} = 0)$$

Curse of Dimensionality

- How large is the space of multivariate distributions as a function of n?
  - Discrete case: the number of possible outcomes is q^n: exponential dependency.
  - Continuous case: under regularity assumptions, same phenomena.
- Estimation of a generic multivariate distribution is therefore intractable: **statistical intractability.**
- Inference of conditional probabilities is **computationally intractable**

$$p(\text{pneumonia} = 1 \mid \text{cough} = 1, \text{fever} = 1, \text{vomiting} = 0)$$

- Therefore, we need to make assumptions about reality, and consider probabilistic models with smaller number of parameters.
- Q: How to introduce structure?

Bayes Rule

- Theorem/definition of conditional probability:

$$p(x_1, x_2) = p(x_1)\ p(x_2 \mid x_1)$$

Bayes Rule

- Theorem/definition of conditional probability:

$$p(x_1, x_2) = p(x_1)\ p(x_2 \mid x_1)$$

- Iterating this rule, we obtain

$$\begin{aligned} p(x_1, \ldots, x_n) &= p(x_1)p(x_2, \ldots, x_n \mid x_1) \\ &= p(x_1)p(x_2 \mid x_1)p(x_3, \ldots x_n \mid x_1, x_2) \\ &= \prod_{i=1}^{n} p(x_i \mid x_1 \ldots x_{i-1}) \ . \end{aligned}$$

– the bulk of the terms on the rhs involve $o(n)$ terms.

– variable ordering is arbitrary in general.

– what if we drop some conditioning variables? $(i_j < i)$

$$p_G(x_1, \ldots, x_n) = \prod_{i=1}^{n} p(x_i \mid x_{i_1}, \ldots x_{i_{l_i}}) \ .$$

Example: Naive Bayes

- Consider n discrete features $X_1 \ldots X_n$ and a categorical variable Y

  .

- Suppose the joint distribution

$$p(X_1, \ldots, X_n, Y) = P(Y) \prod_{i=1}^{n} P(X_i \mid Y, X_1, \ldots X_{i-1})$$

  can be simplified to

$$p(X_1, \ldots, X_n, Y) = P(Y) \prod_{i=1}^{n} P(X_i \mid Y)$$

Example: Naive Bayes

- Consider n discrete features $X_1 \ldots X_n$ and a categorical variable Y

.

- Suppose the joint distribution

$$p(X_1, \ldots, X_n, Y) = P(Y) \prod_{i=1}^{n} P(X_i \mid Y, X_1, \ldots X_{i-1})$$

can be simplified to

$$p(X_1, \ldots, X_n, Y) = P(Y) \prod_{i=1}^{n} P(X_i \mid Y)$$

- This means that X_i, X_j are independent given Y .
  - We will write $X_i \perp X_j \mid Y$, and say that they are *conditionally independent*.

Example: Naive Bayes

- Consider n discrete features $X_1 \ldots X_n$ and a categorical variable Y

.

- Suppose the joint distribution

$$p(X_1, \ldots, X_n, Y) = P(Y) \prod_{i=1}^{n} P(X_i \mid Y, X_1, \ldots X_{i-1})$$

can be simplified to

$$p(X_1, \ldots, X_n, Y) = P(Y) \prod_{i=1}^{n} P(X_i \mid Y)$$

- This means that X_i, X_j are independent given Y .
  - We will write $X_i \perp X_j \mid Y$, and say that they are *conditionally independent.*
- Q: Does $X_i \perp X_j \Rightarrow X_i \perp X_j \mid Y \quad ?$
- Q: Does $X_i \perp X_j \mid Y \Rightarrow X_i \perp X_j \quad ?$

Example: Classification with Naive Bayes

- Naive Bayes may be used to classify emails as spam $(Y = 1)$ or not spam $(Y = 0)$.
- By indexing the words on a given vocabulary $1 : n$, we construct

$$X_i = 1 \text{ if word } i \text{ appears in email, } 0 \text{ otherwise.}$$

- Naive Bayes model

$$p(X_1, \ldots, X_n, Y) = p(Y) \prod_{i=1}^{n} p(X_i \mid Y)$$

  – The parameters of the model are estimated with maximum likelihood.

Example: Classification with Naive Bayes

- Naive Bayes may be used to classify emails as spam $(Y = 1)$ or not spam $(Y = 0)$.
- By indexing the words on a given vocabulary $1 : n$, we construct

$$X_i = 1 \text{ if word } i \text{ appears in email, } 0 \text{ otherwise.}$$

- Naive Bayes model

$$p(X_1, \ldots, X_n, Y) = p(Y) \prod_{i=1}^{n} p(X_i \mid Y)$$

  - The parameters of the model are estimated with maximum likelihood.
- Spam Prediction:

$$p(Y = 1 \mid X_1, \ldots X_n) = \frac{P(Y = 1, X_1 = x_1, \ldots, X_n = x_n)}{P(X_1 = x_1, \ldots, X_n = x_n)} \; .$$

  - Conditional Independence assumptions are strong, but resulting model is simple and useful.

Bayesian Networks

- We've seen that reducing the scope of conditional probability is critical in order to beat the curse of dimensionality.

$$p_G(x_1, \ldots, x_n) = \prod_{i=1}^{n} p(x_i \mid x_{i_1}, \ldots x_{i_{l_i}}) \ .$$

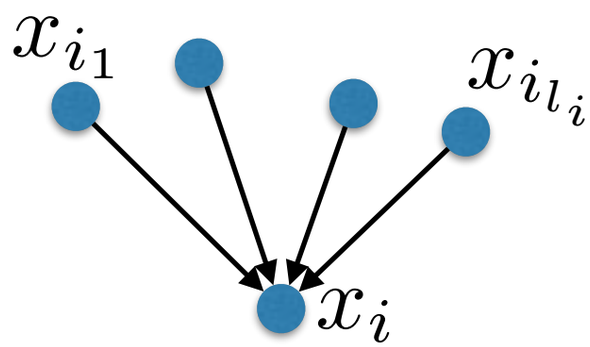
- Q: How to describe those dependencies?

Bayesian Networks

- We've seen that reducing the scope of conditional probability is critical in order to beat the curse of dimensionality.

$$p_G(x_1, \ldots, x_n) = \prod_{i=1}^{n} p(x_i \mid x_{i_1}, \ldots x_{i_{l_i}}) \ .$$

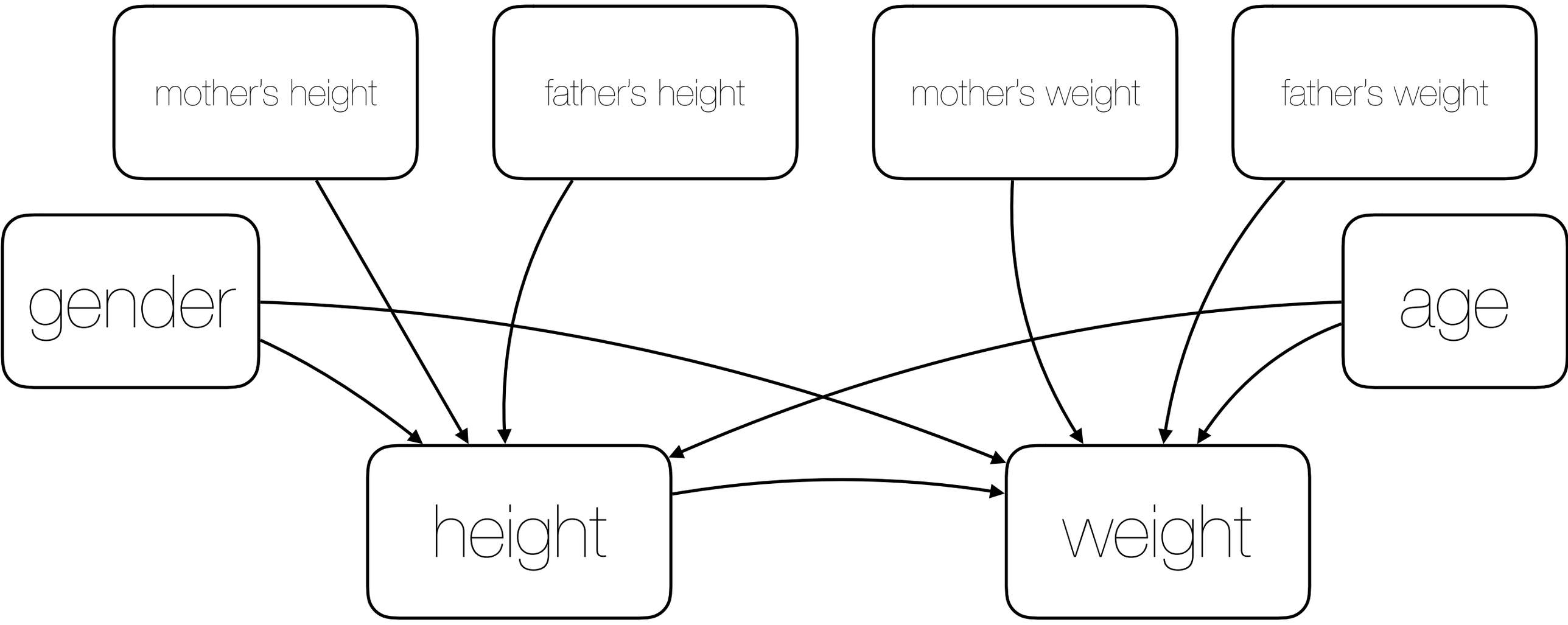
- Q: How to describe those dependencies?
- Given a directed acyclic graph $G = (V, E)$ we encode a model as
  - One node $i \in V$ for each random variable.
  - One conditional probability distribution per node, where conditional factors become the parents in the graph:



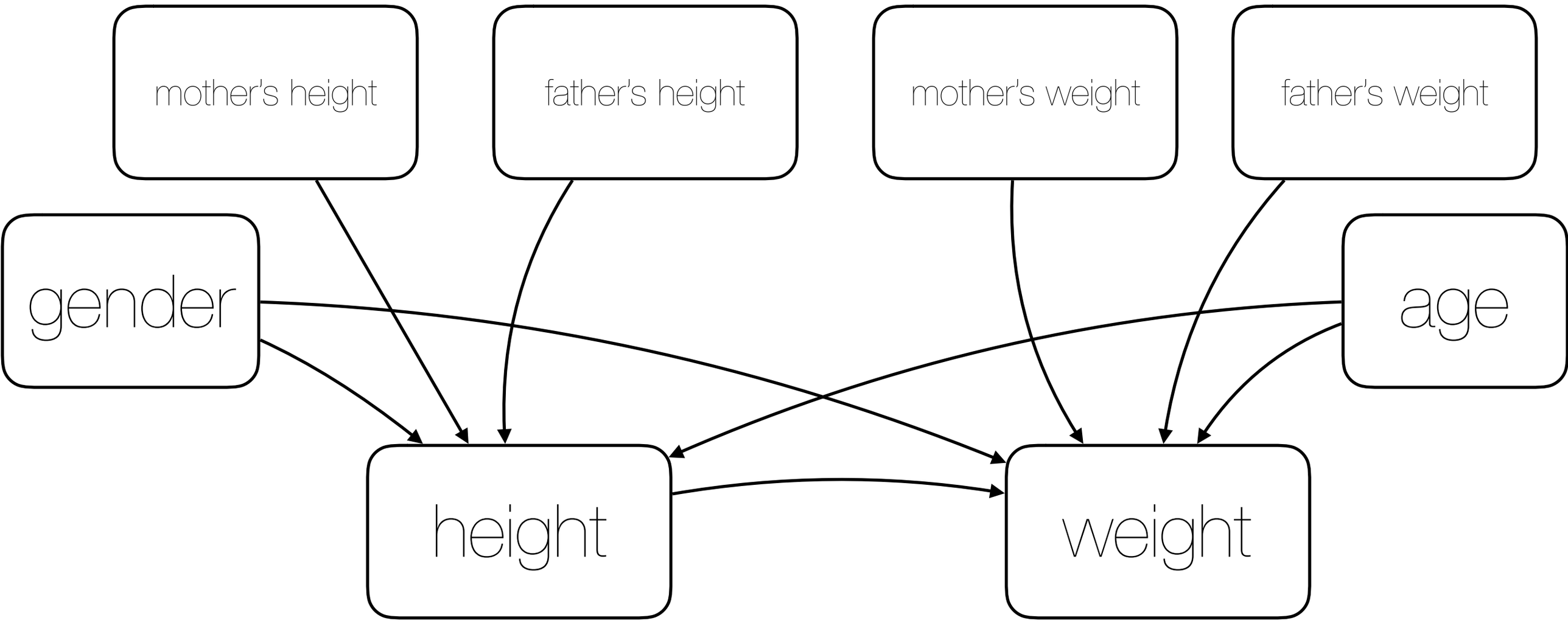
$$\{x_{i_1}, \ldots, x_{i_{l_i}}\} := x_{Pa(i}$$

- Properties of the joint distribution are now expressed in terms of the graph.
  - algorithms for inference
  - complexity questions.

Example


mother's height
father's height
mother's weight
father's weight
gender
age
height
weight

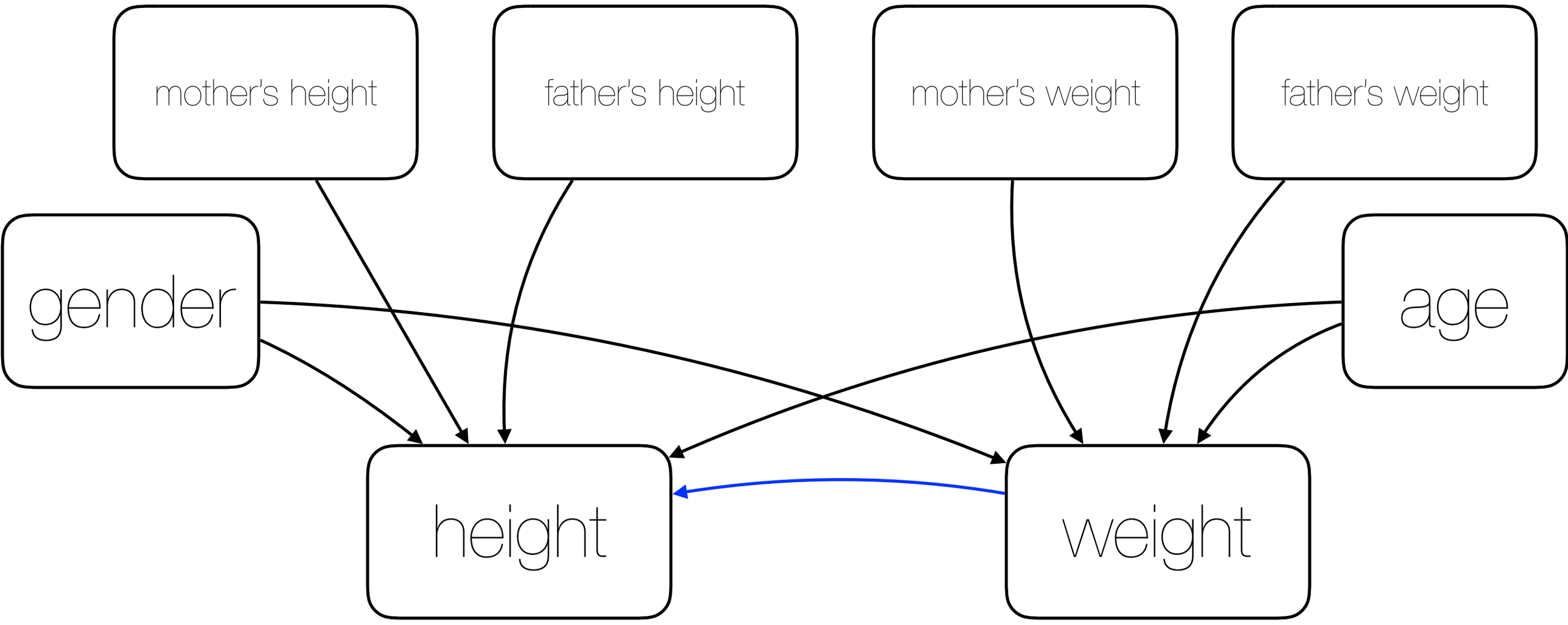
Example



$$p(X_1, \ldots, X_n) = \prod_{i \in V} p(X_i \mid X_{Pa(i)})$$

$$p(MH, FH, MW, FW, G, A, H, W) =$$
$$= p(G)p(A)p(MH)p(FH)p(MW)p(FW)$$
$$p(H \mid MH, FH, G, A)p(W \mid H, MW, FW, G, A)$$

Example



$$p(X_1, \ldots, X_n) = \prod_{i \in V} p(X_i \mid X_{Pa(i)})$$

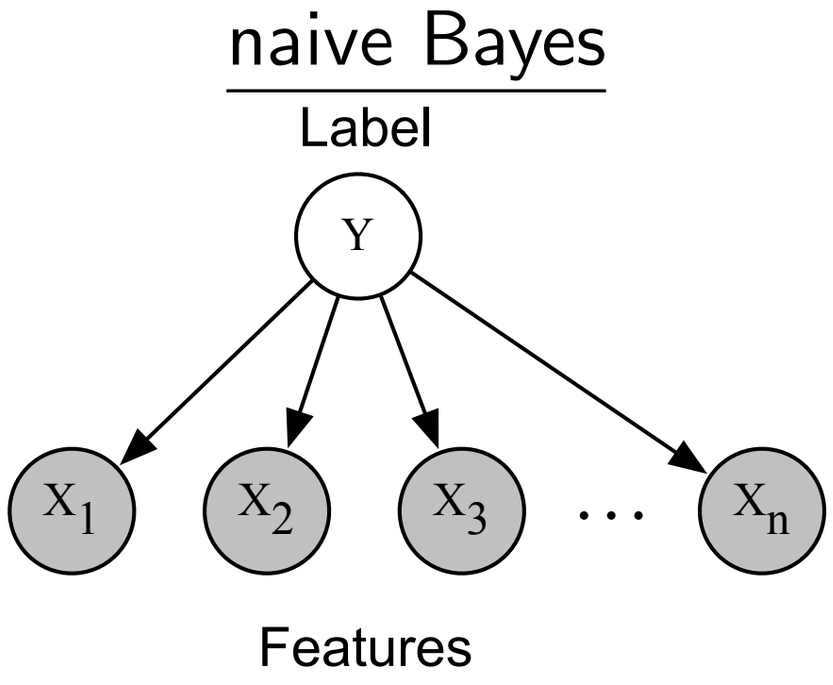
$$p(MH, FH, MW, FW, G, A, H, W) =$$

$$= p(G)p(A)p(MH)p(FH)p(MW)p(FW)$$

$$p(W \mid MH, FH, G, A)p(H \mid W, MW, FW, G, A)$$

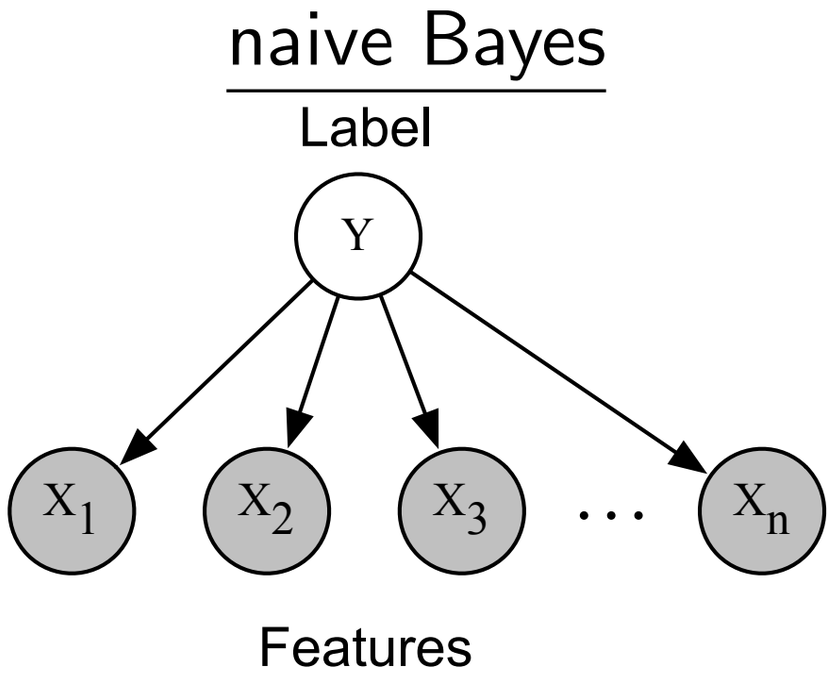
same model!

Representing partially observed models



- Observing variables = shading nodes
- Posterior inference: $p(Y \mid X_1 = x_1, \ldots, X_n = x_n)$

Representing partially observed models



- Observing variables = shading nodes
- Posterior inference: $p(Y \mid X_1 = x_1, \ldots, X_n = x_n)$
- Also, we can use a Bayesian network as a generative process:
  1. Sample $y \sim p(Y)$
  2. For each i, sample $x_i \sim p(X_i \mid Y = y)$.

Conditional Independence

- Reminder:

$$X_i \perp X_j \mid Y \text{ if } p(X_i, X_j \mid Y) = p(X_i \mid Y) p(X_j \mid Y)$$

  - equivalently, $p(X_i \mid X_j, Y) = p(X_i \mid Y)$ whenever $p(X_j) > 0$.

- A generic joint distribution has no independence assumptions. Which associated graph?

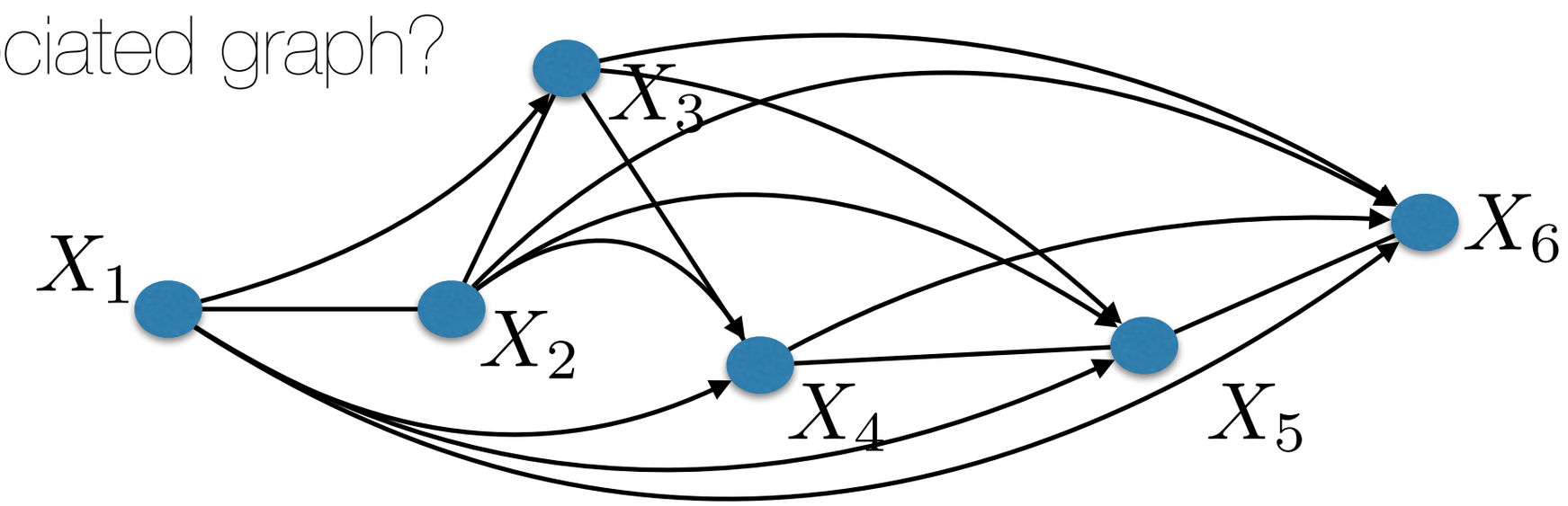
Conditional Independence

- Reminder:

$$X_i \perp X_j \mid Y \text{ if } p(X_i, X_j \mid Y) = p(X_i \mid Y)p(X_j \mid Y)$$

  - equivalently, $p(X_i \mid X_j, Y) = p(X_i \mid Y)$ whenever $p(X_j) > 0$.

- A generic joint distribution has no independence assumptions. Which associated graph?



  - Fully connected directed graph.

Conditional Independence

- In a specific graphical model, conditional probabilities have missing terms:

$$p(X_i \mid X_{i_1}, \ldots, X_{i_{l_i}}) \text{ instead of } p(X_i \mid X_1, \ldots, X_{i-1})$$

- Thus

$$X_i \perp X_j \mid X_{Pa(i)} \text{ for } j < i,\ j \notin Pa(i).$$

Conditional Independence

- In a specific graphical model, conditional probabilities have missing terms:

$$p(X_i \mid X_{i_1}, \ldots, X_{i_{l_i}}) \text{ instead of } p(X_i \mid X_1, \ldots, X_{i-1})$$

- Thus

$$X_i \perp X_j \mid X_{Pa(i)} \text{ for } j < i,\ j \notin Pa(i).$$

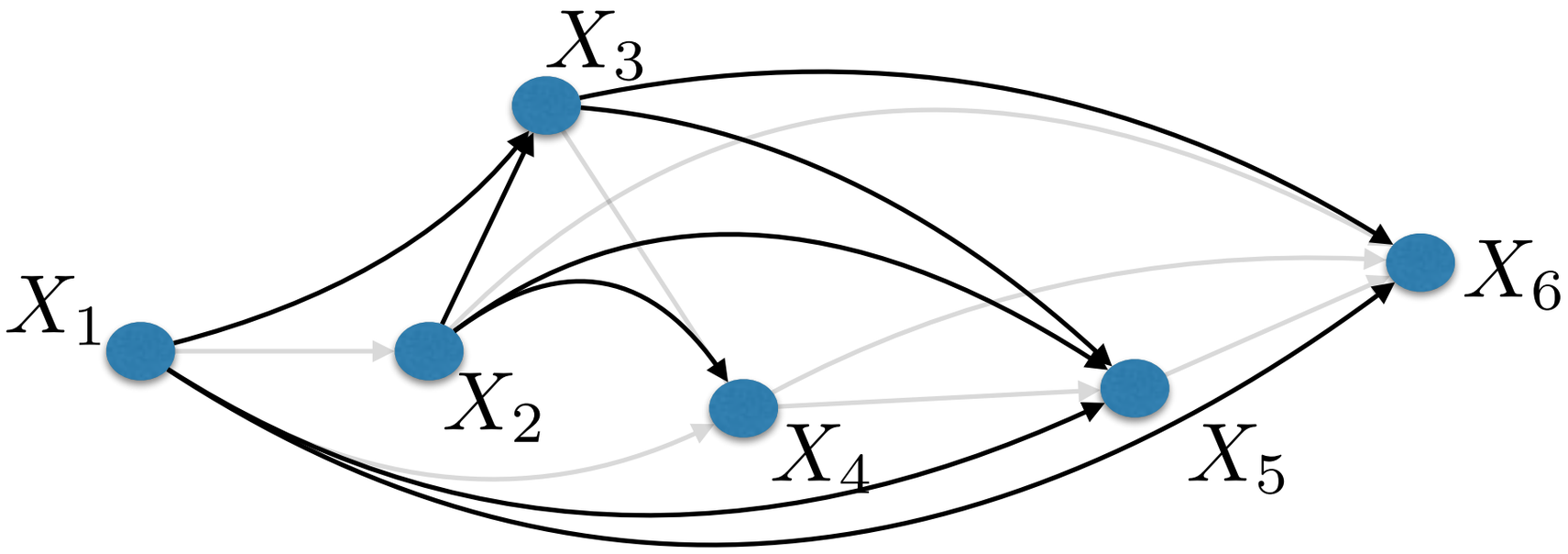
- In fact,

missing variables in the local conditional probabilities

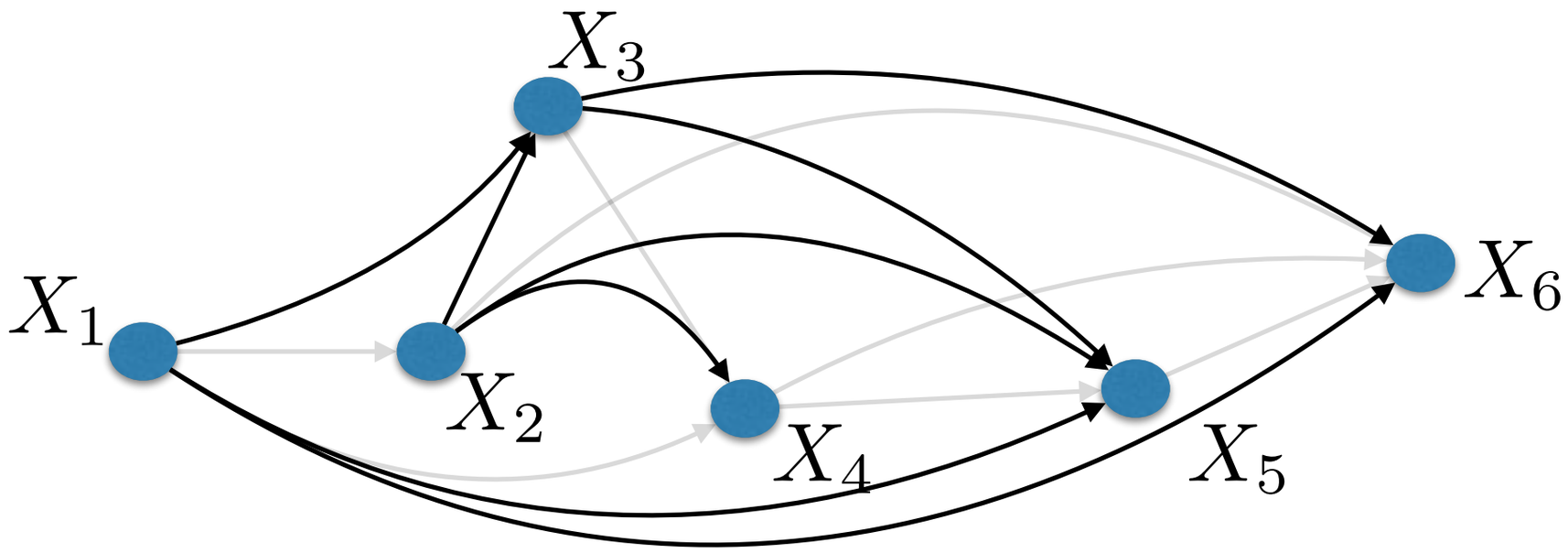
$\Updownarrow$

missing edges in the corresponding graph

Conditional Independence



Conditional Independence



- So, removing edges creates conditional independences:

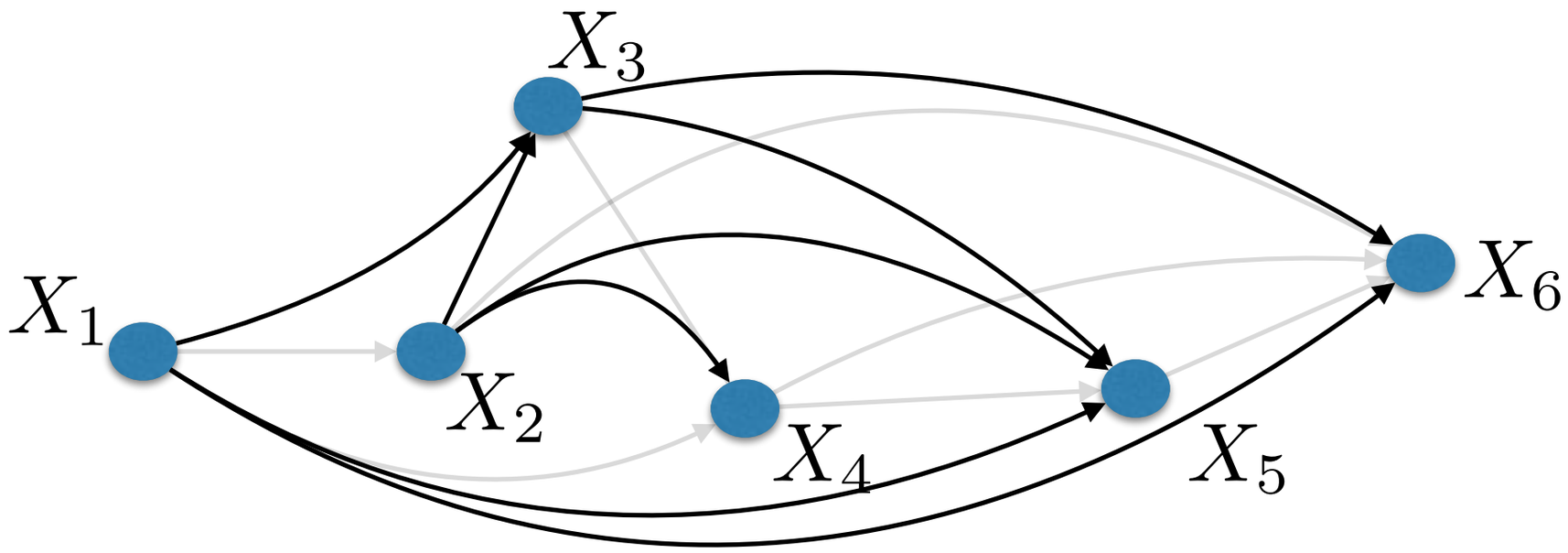
$X_1 \perp X_2 \mid \emptyset$

$X_4 \perp \{X_1, X_3\} \mid X_2$

$X_5 \perp X_4 \mid \{X_1, X_2, X_3\}$

$X_6 \perp \{X_2, X_4, X_5\} \mid \{X_1, X_3\}$

Conditional Independence



- So, removing edges creates conditional independences:

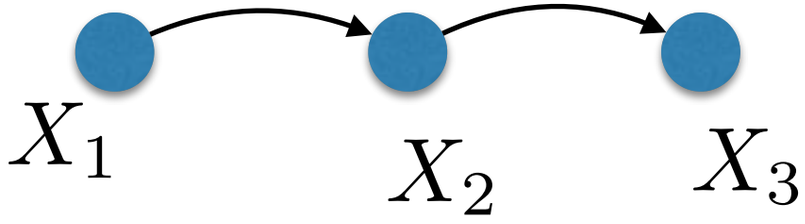
$$X_1 \perp X_2 \mid \emptyset \qquad X_5 \perp X_4 \mid \{X_1, X_2, X_3\}$$

$$X_4 \perp \{X_1, X_3\} \mid X_2 \qquad X_6 \perp \{X_2, X_4, X_5\} \mid \{X_1, X_3\}$$

- **A variable is independent from its non-descendants given its parents.**
- Q: Are there other conditional independence relationships induced by the graphical model?

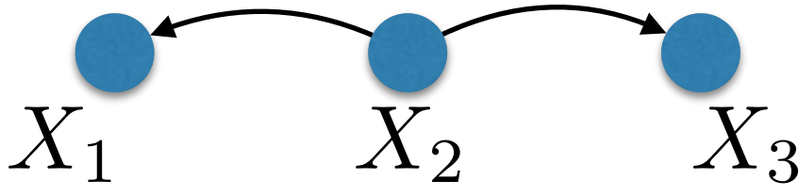
Independence in three-node graphs

- Let's first focus on canonical, small graphical models.



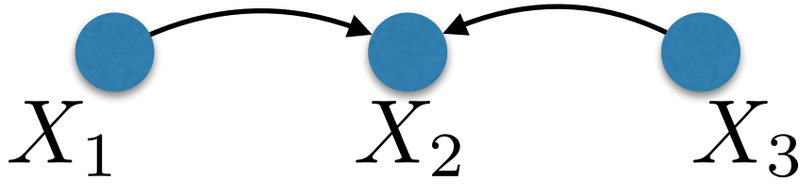
"Cascade":

$X_1 \perp X_3 \mid X_2$



"Common Parent"

$X_1 \perp X_3 \mid X_2$

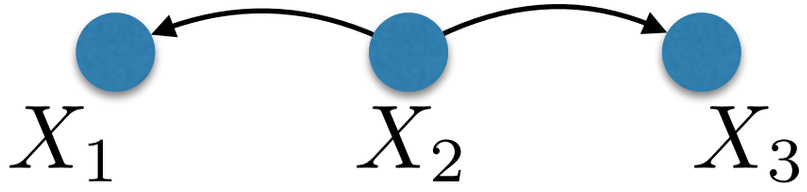


"V-structure"

Explaining away: knowing X2 couples X1 and X3

$X_1 \perp X_3$, but $X_1 \perp X_3 \mid X_2$ is false in general!

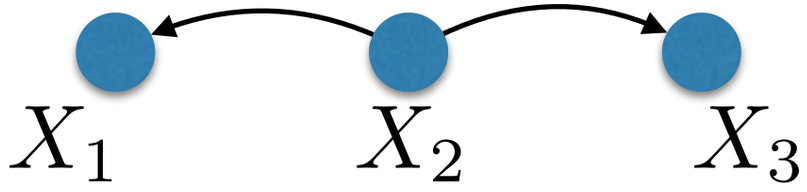
Example: Common Parent



"Common Parent"

$$X_1 \perp X_3 \mid X_2$$

Example: Common Parent



"Common Parent"

$$X_1 \perp X_3 \mid X_2$$

We need to show that if $p(X_1, X_2, X_3)$ factors as

$$p(X_1, X_2, X_3) = p(X_2)p(X_1|X_2)p(X_3|X_2)$$

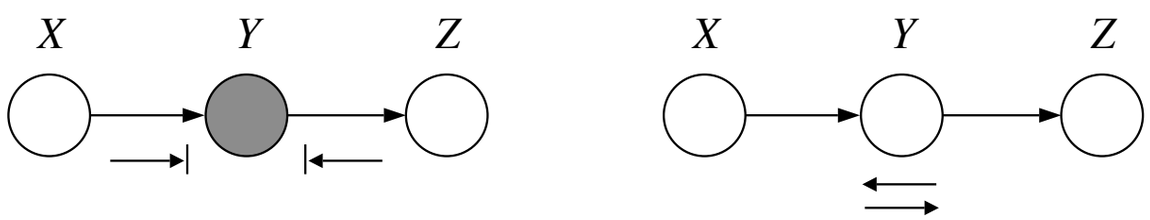
then

$$p(X_1, X_3 \mid X_2) = p(X_1 \mid X_2)p(X_3 \mid X_2)$$

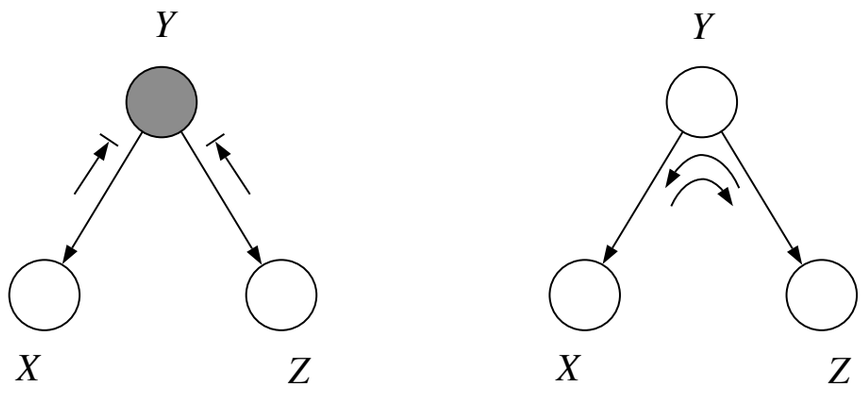
$$p(X_1, X_3 \mid X_2) = \frac{p(X_1, X_2, X_3)}{p(X_2)} = \frac{p(X_2)p(X_1 \mid X_2)p(X_3 \mid X_2)}{p(X_2)} \; \square$$

D-separation

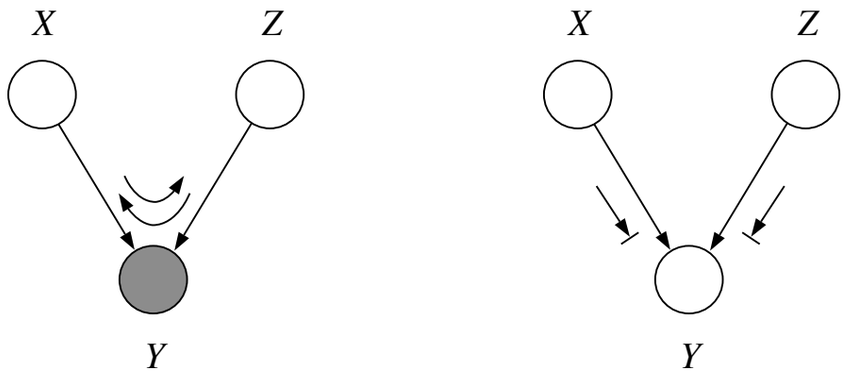
- In a general Bayesian Network, let us describe an algorithm to determine whether $X \perp Z \mid \mathbf{Y}$ by inspecting the graph.
- Idea: Determine an *active path* between X and Z when variables in $\mathbf{Y}$ are observed.
  - Use the canonical three-graphs as local rules:
  - Cascade:



  - Common parent:



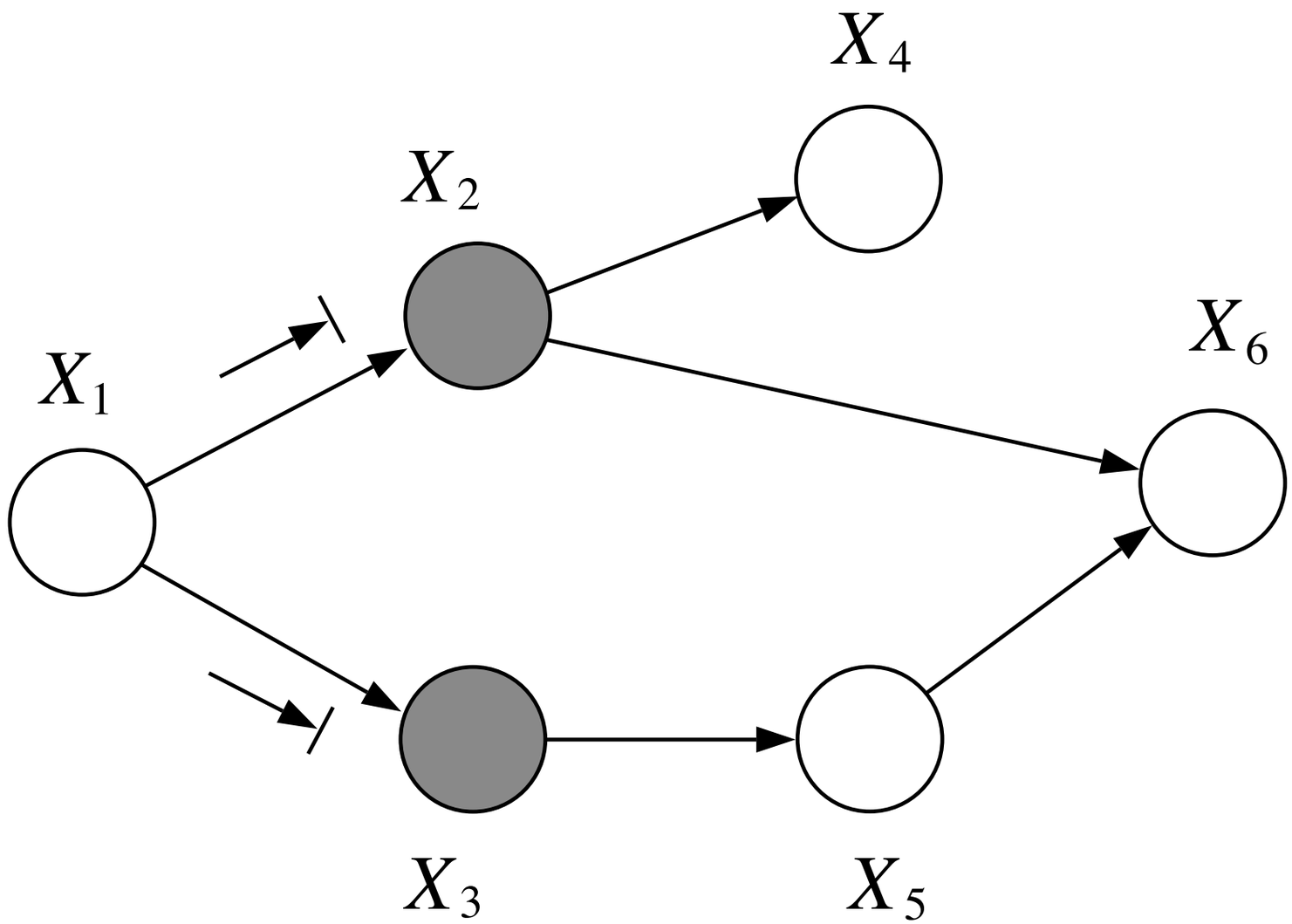
  - V-structure:



D-separation

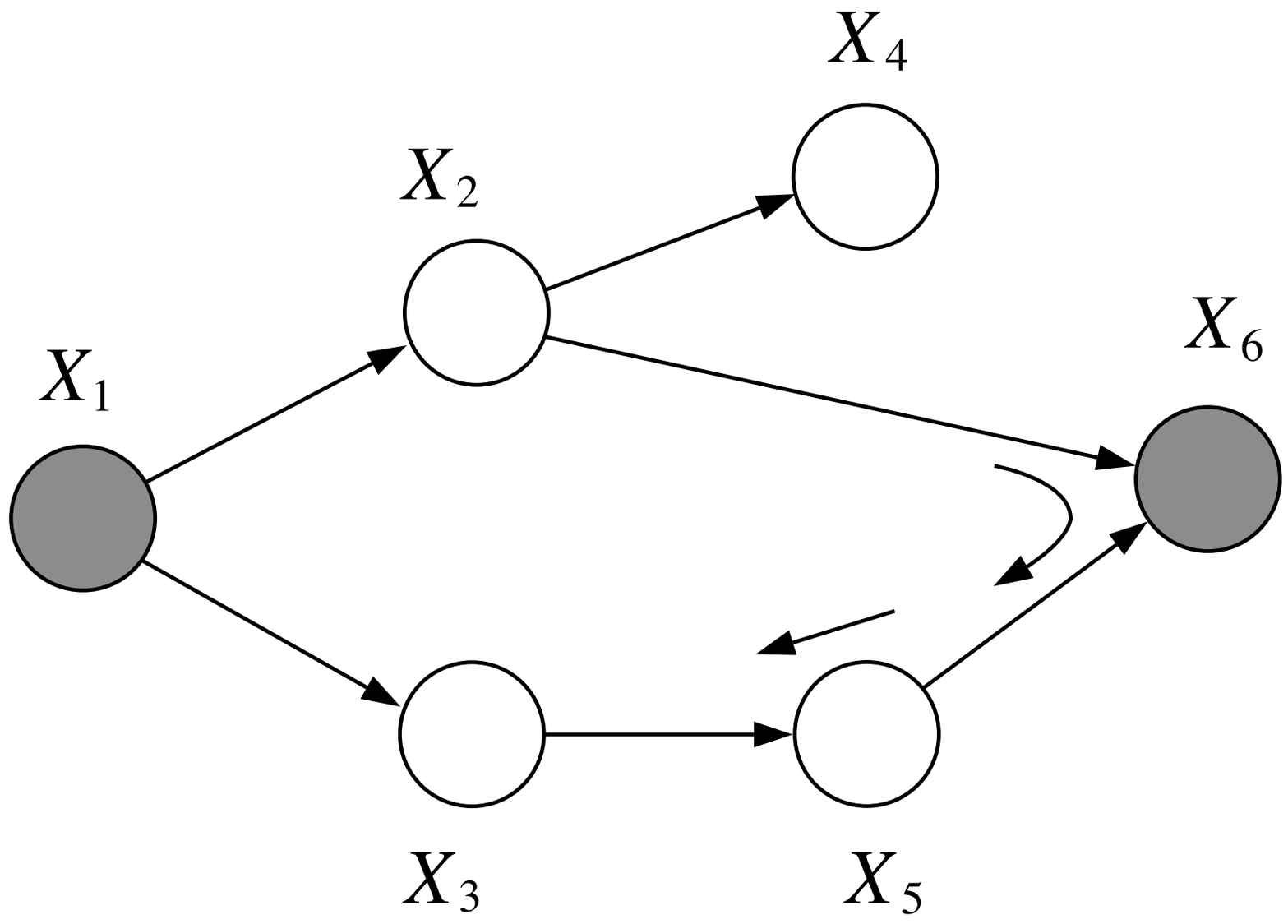
- If no such path exists, then we say that X and Z are d-separated wrt $\mathbf{Y}$, thus $X \perp Z \mid \mathbf{Y}$.
- Also referred as "Bayes Ball" algorithm
  - If we "throw" a ball from X, can it reach Z according to local rules?

D-separation example 1



Is $X_6 \perp X_5 \mid X_2, X_3$? Is $X_4 \perp X_5 \mid X_2, X_3$?

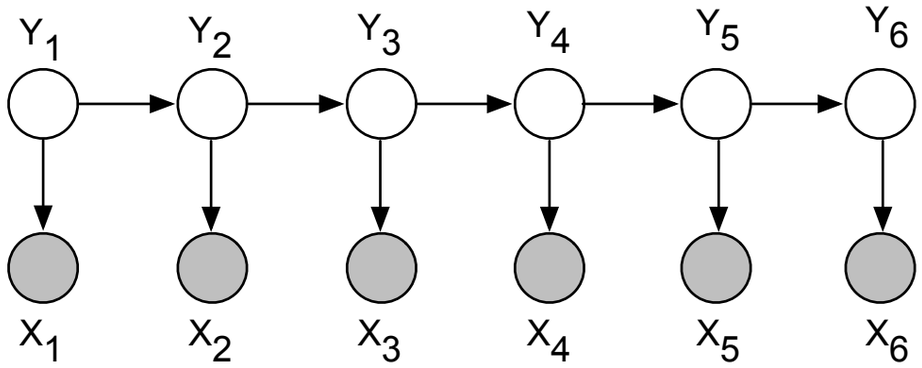
D-separation example 2



Is $X_4 \perp X_5 \mid X_1, X_6$?

What about if X_6 is not observed? I.e., is $X_4 \perp X_5 \mid X_1$?

Hidden Markov Models

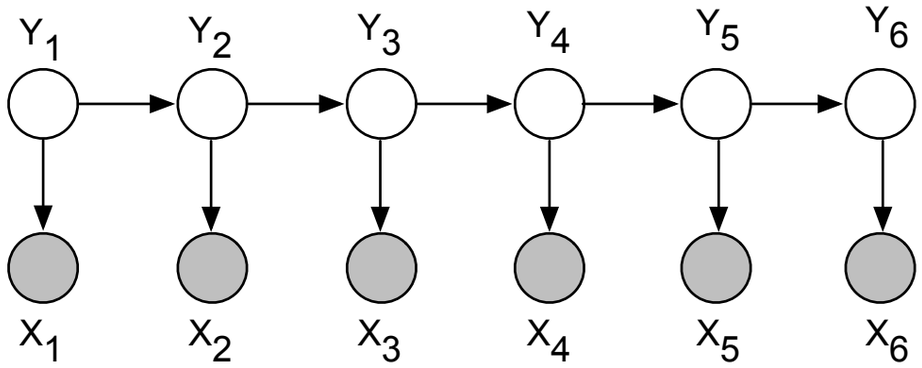


- Very popular (today less so) in speech recognition and part-of-speech tagging.
- State-space model (more on that later in the course).
- Joint distribution

$$p(\mathbf{X}, \mathbf{Y}) = p(Y_1)p(X_1 \mid Y_1) \prod_{t=2}^{T} p(Y_t \mid Y_{t-1}) P(X_t \mid Y_t) \ .$$

  - $p(Y_t \mid Y_{t-1})$ is the *transition* probability kernel.
  - $p(X_t \mid Y_t)$ is the output probability.
- Q: What are the conditional independencies?

Hidden Markov Models



- Very popular (today less so) in speech recognition and part-of-speech tagging.
- State-space model (more on that later in the course).
- Joint distribution

$$p(\mathbf{X}, \mathbf{Y}) = p(Y_1)p(X_1 \mid Y_1) \prod_{t=2}^{T} p(Y_t \mid Y_{t-1}) P(X_t \mid Y_t) \ .$$

  - $p(Y_t \mid Y_{t-1})$ is the *transition* probability kernel.
  - $p(X_t \mid Y_t)$ is the output probability.
- Q: What are the conditional independencies?

$$\text{past} \perp \text{future} \mid \text{present}$$

Independence Maps

- Given a directed acyclic graph G, we denote by $I(G)$ the set of conditional independencies implied by it.
- Given a joint distribution p, we denote by $I(p)$ the set of conditional independencies satisfied by it.

Independence Maps

- Given a directed acyclic graph G, we denote by $I(G)$ the set of conditional independencies implied by it.
- Given a joint distribution p, we denote by $I(p)$ the set of conditional independencies satisfied by it.
- G is an *independence map* of p if $I(G) \subseteq I(p)$.
  - Dense graphs are i-maps of any distribution (why?)

Independence Maps

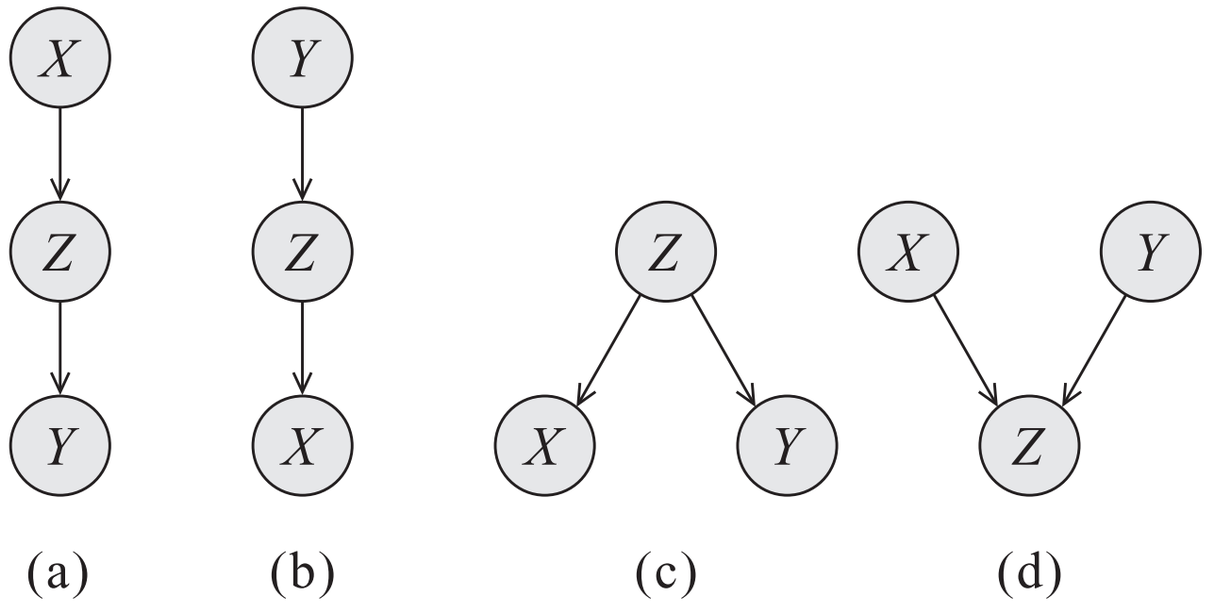
- Given a directed acyclic graph G, we denote by $I(G)$ the set of conditional independencies implied by it.
- Given a joint distribution p, we denote by $I(p)$ the set of conditional independencies satisfied by it.
- G is an *independence map* of p if $I(G) \subseteq I(p)$.
  - Dense graphs are i-maps of any distribution (why?)
- G is a *minimal independence map* if pruning G (thus enlarging $I(G)$) makes it not an i-map.
  - Each node ordering may correspond to a different minimal i-map.
- G is a *perfect independence map* for p if $I(G) = I(p)$
  - Q: Does every distribution have a perfect map?

Independence Maps

- Given a directed acyclic graph G, we denote by $I(G)$ the set of conditional independencies implied by it.
- Given a joint distribution p, we denote by $I(p)$ the set of conditional independencies satisfied by it.
- G is an *independence map* of p if $I(G) \subseteq I(p)$.
  - Dense graphs are i-maps of any distribution (why?)
- G is a *minimal independence map* if pruning G (thus enlarging $I(G)$) makes it not an i-map.
  - Each node ordering may correspond to a different minimal i-map.
- G is a *perfect independence map* for p if $I(G) = I(p)$
  - Q: Does every distribution have a perfect map?
  - $X, Y \sim \mathrm{Ber}(0.5)$, $Z = X \text{ XOR } Y$.

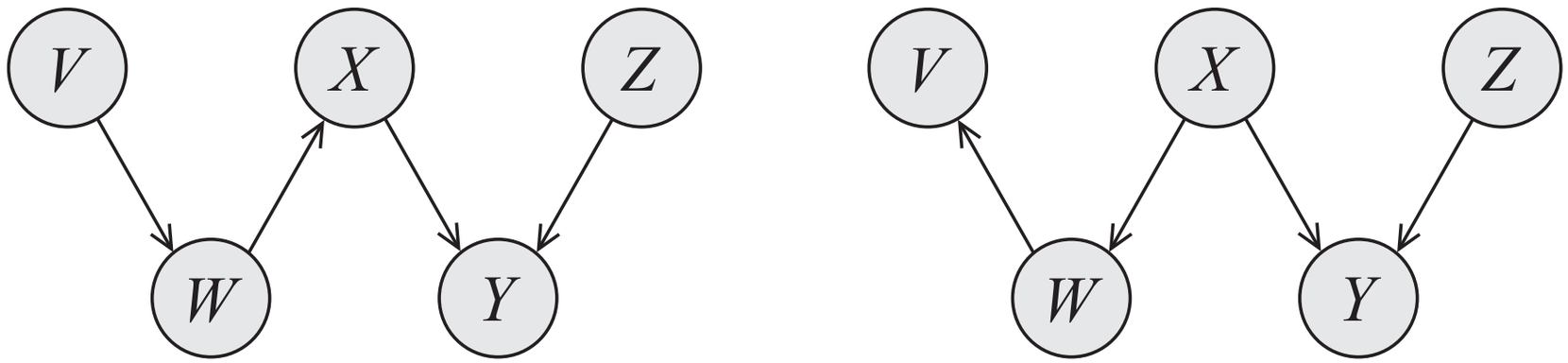
Equivalent Graph Structures

- Two different BNs can be equivalent: they encode the same conditional independence assumptions.
- Which of these are equivalent?



Equivalent Graph Structures

- Two different BNs can be equivalent: they encode the same conditional independence assumptions.
- Are these equivalent?



Lecture 1 Summary

- Bayesian Networks are constructed from a DAG G and a set of local conditional probability distributions.
- BN can be seen as a generative model specified by its topological order.
- Local and global conditional independence properties can be identified with the notion of d-separation.