Learning Parameters using EM: incomplete data

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1. Initialize parameters
2. Compute **pseudo counts** for each variable

$$\theta^*_{k|\mathbf{pa}} = \frac{\sum_{i=1}^{m} P(k, \mathbf{pa}|X_i)}{\sum_{i=1}^{m} P(\mathbf{pa}|X_i)}$$

junction tree algorithm

3. **Set parameters to the (completed) ML estimates**
4. If not converged, iterate to 2

Probabilistic Graphical Models*

Bayesian Networks - Learning

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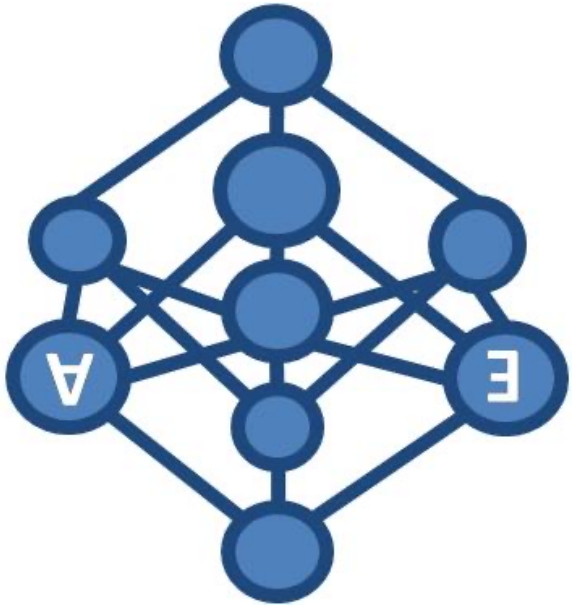

*Thanks to Carlos Guestrin, Pedro Domingos and many others for making their slides publically available

What you need to know so far about learning

- Different Learning Settings
  - Fully vs. partially observable variables
  - Structure known vs. unknown
  - Latent variables vs. scientific discovery
- Maximum Likelihood and Decomposable Scores
- EM and Gradient-based ML parameter estimation
  - Update rules for binomial and multinomial vars

What's next

- Bayesian Parameter Estimation

Bayesian Estimation

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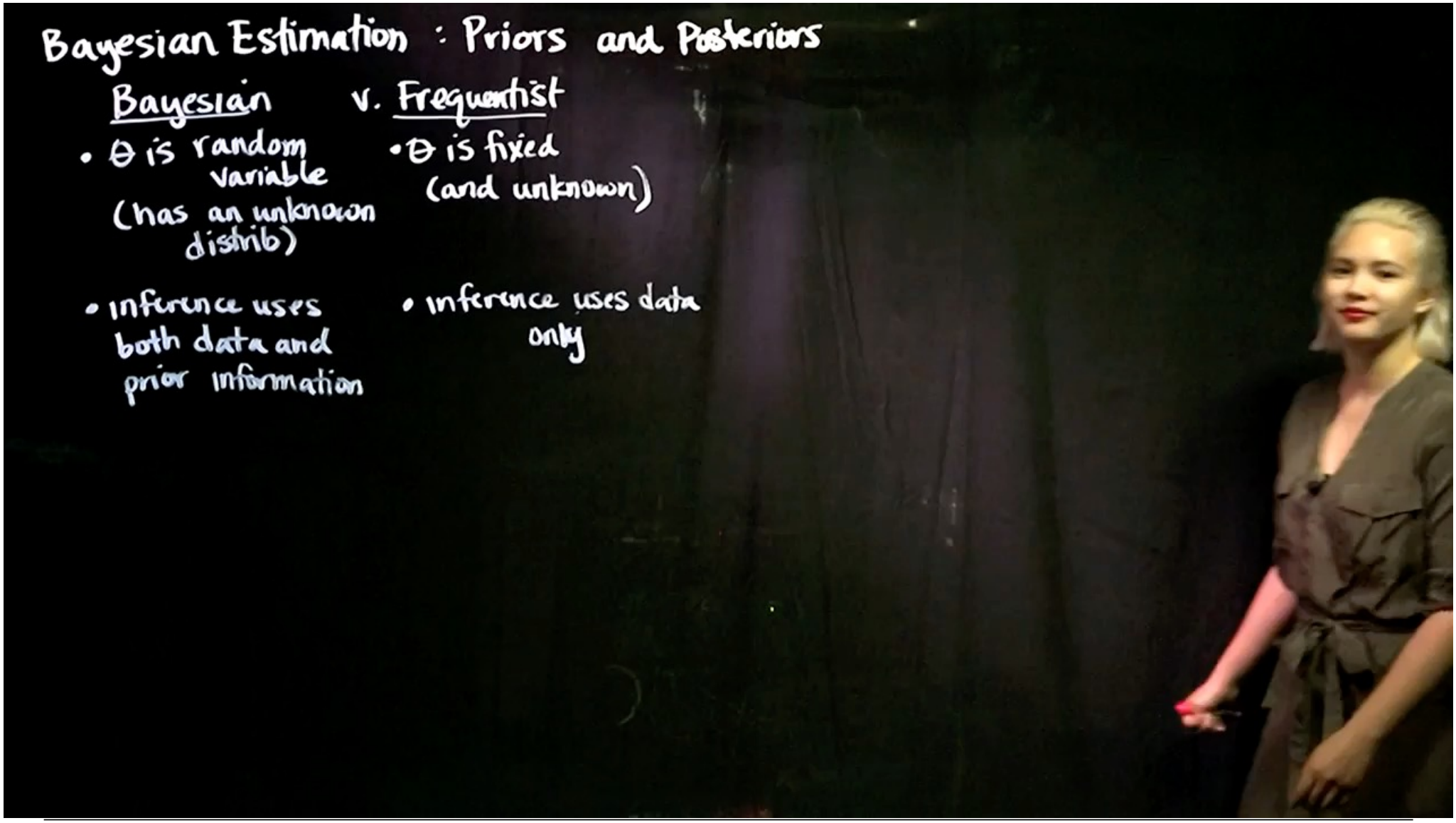
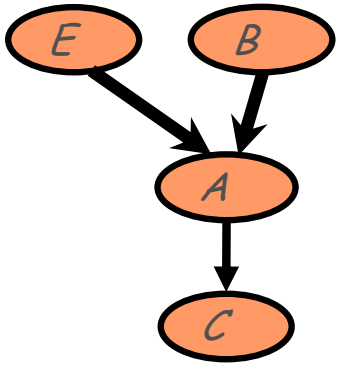


Bayesian Inference

- Recall, training data has the form:

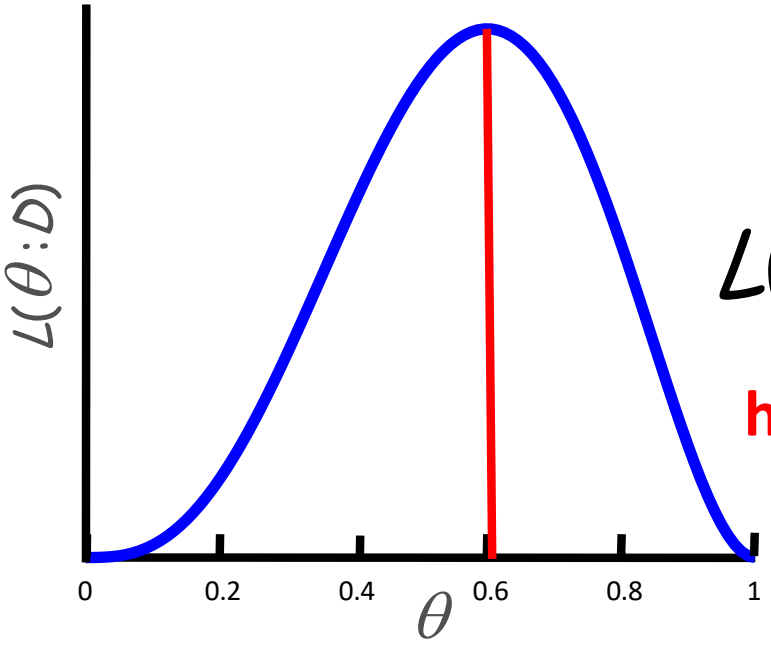
$$D = \begin{bmatrix} E[1] & B[1] & A[1] & C[1] \\ . & . & . & . \\ . & . & . & . \\ E[M] & B[M] & A[M] & C[M] \end{bmatrix}$$



Recall, Likelihood Function for Multinomials

$$L(\theta : D) = P(D \mid \theta) = \prod_m P(x[m] \mid \theta)$$

- The likelihood for the sequence H, T, T, H, H is



$$L(\theta : D) = \theta \cdot (1-\theta) \cdot (1-\theta) \cdot \theta \cdot \theta$$

head is more likely

General case:

$$L(\Theta : D) = \prod_{k=1}^{K} \theta_k^{N_k}$$

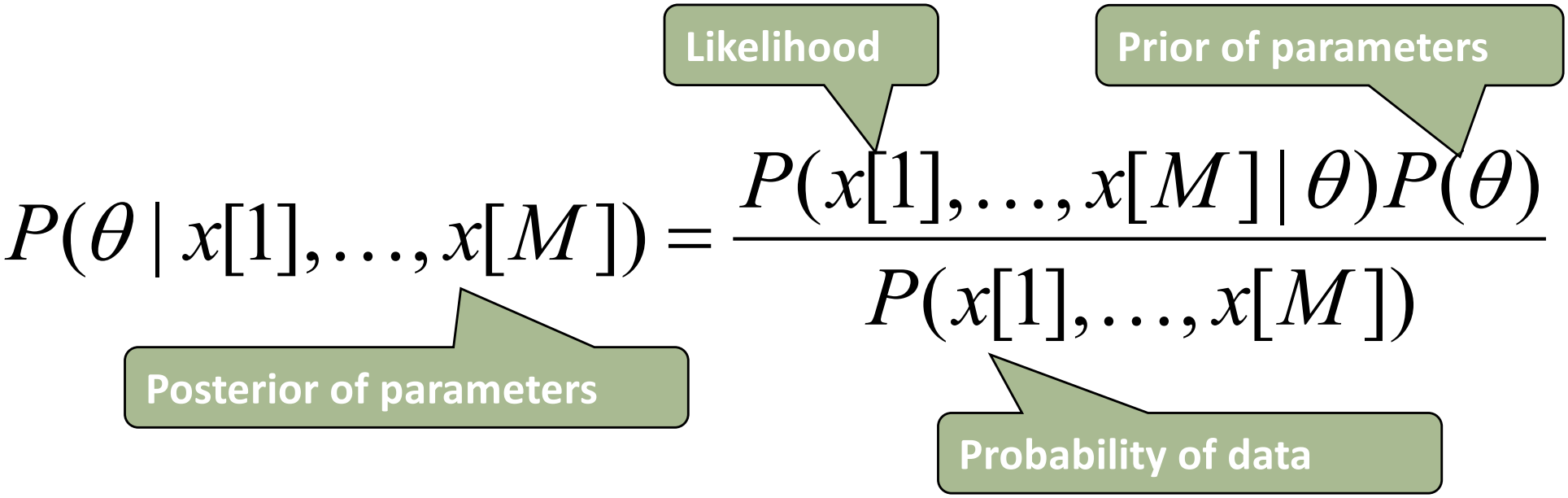
Count of k^{th} outcome in D

Probability of k^{th} outcome

$$LL(\Theta : D) = \sum_{k=1}^{K} N_k \cdot \log \theta_k$$

Now, what is Bayesian Inference?

- In contrast to MLE, it **represents uncertainty about parameters using a probability distribution over parameters and data**
- It is **"Learning by inference" using Bayes' rule**

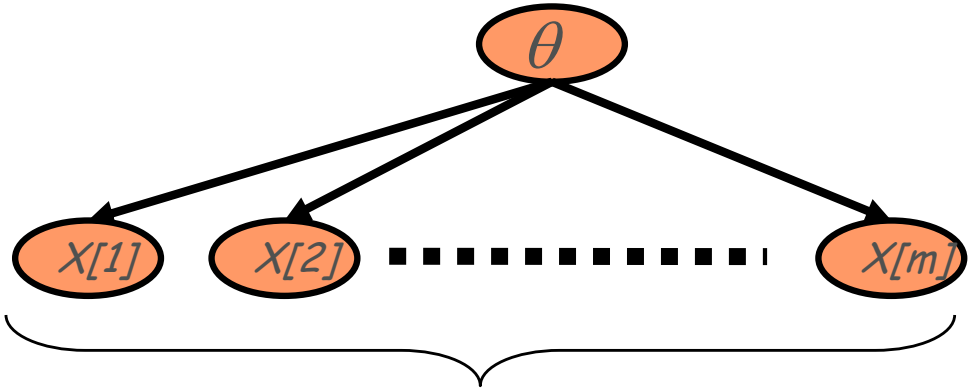


Bayesian Estimation

https://www.youtube.com/watch?v=TUgqL9c1jik

Bayesian Inference (for the Heads/Tails Example)

- Represent Bayesian distribution as Bayesian net



- **Thus, the values of X are independent given θ (which we do not know though)**

$$P(x[m] \mid \theta) = \theta$$ (keep this in mind!)

- Bayesian prediction is inference in this network

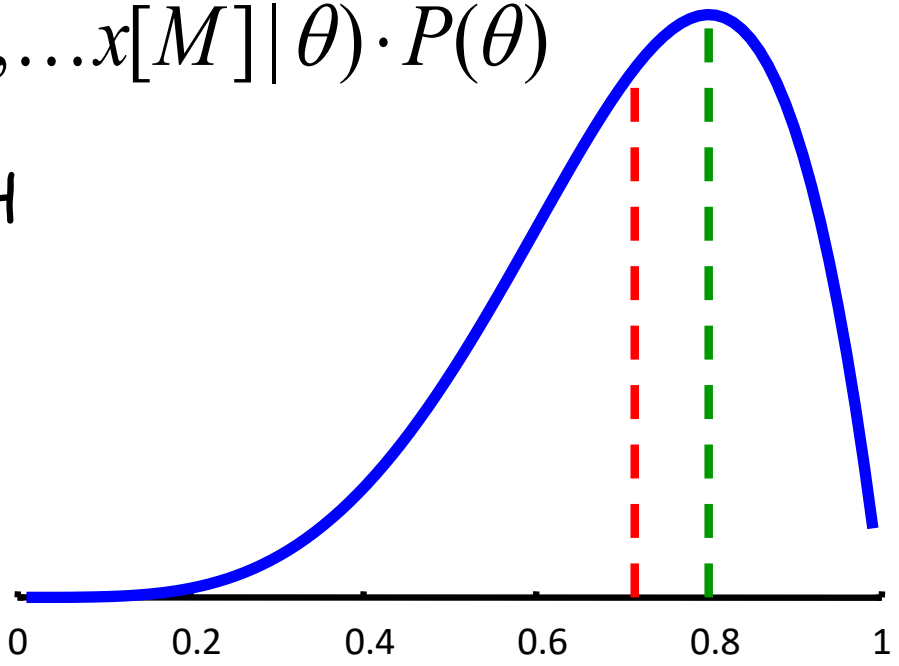
Example: Binomial Data

- Prior: uniform for θ in [0,1]

  $\Rightarrow$ $P(\theta \mid D) \propto$ the likelihood $L(\theta : D)$

$$P(\theta \mid x[1],\ldots x[M]) \propto P(x[1],\ldots x[M] \mid \theta) \cdot P(\theta)$$

$(N_H, N_T) = (4,1)$, e.g., H,T,H,H,H



- **MLE for $P(X = H)$ is 4/5 = 0.8**
- **Bayesian prediction is**

$$P(x[M+1] = H \mid D) = \int \theta \cdot P(\theta \mid D) d\theta = \frac{5}{7} = 0.7142\ldots$$

We do not know theta! So, we have to integrate over all values. Bayesian prediction = Inference in the extended network

Why is this the case?

We start with

- $P(\theta)$ - **prior distribution** about the values of θ
- $P(x_1, \ldots, x_n/\theta)$ - **likelihood** of examples given a known value θ

Given examples $x_1, \ldots, x_n$, we can compute **posterior distribution** on θ

$$P(\theta \mid x_1, \ldots x_n) = \frac{P(x_1, \ldots x_n \mid \theta) P(\theta)}{P(x_1, \ldots x_n)}$$

Where the **marginal likelihood** is

$$P(x_1, \ldots x_n) = \int P(x_1, \ldots x_n \mid \theta) P(\theta) d\theta$$

Binomial Distribution aka Laplace Est.

- In this case the unknown parameter is $\theta = P(H)$

- Simplest **prior** $P(\theta) = 1$ for $0 < \theta < 1$
- **Likelihood** $P(x_1, \ldots x_n \mid \theta) = \theta^k (1-\theta)^{n-k}$

  where k is number of heads in the sequence
- **Marginal Likelihood**:

$$P(x_1, \ldots x_n) = \int_0^1 \theta^k (1-\theta)^{n-k} \, d\theta$$

- Now, we use **integration by parts**

Recap: Integration by parts

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First, start with the Product Rule for differentiation.

$$\frac{d}{dx}(uv) = u\frac{dv}{dx} + v\frac{du}{dx}$$

Integrate both sides of the equation to obtain:

$$\int \frac{d}{dx}(uv)\,dx = \int u\frac{dv}{dx}\,dx + \int v\frac{du}{dx}\,dx$$

$$uv = \int u\,dv + \int v\,du$$

and by manipulating the equation we get … (see next page)

The Fundamental Theorem of Calculus tells us that if we take the derivative of the integral, then we are left with the original function. The derivative and the integral "cancel" each other out.

$$\int u\,dv = uv - \int v\,du$$

This is the formula for Integration by Parts.

Just as the Substitution Method could be thought of as the Chain Rule for integration, Integration by Parts could also be thought of as the Product Rule for integration.

When using this formula, we need to choose which part of the integrand (what we are taking the integral of) is u, and which part of it is dv.

When choosing u and dv, we want to find a u that will be simplified after we take its derivative, and a dv that won't be too complex after integrating it.

Marginal Likelihood

$$\int u\,dv = uv - \int v\,du$$

Using **integration by parts** we have:

+ insteat of – because of the derivative of (1-θ), which is -1, due to chain rule of differentiation

$$P(x_1,\dots x_n) = \int_0^1 \underbrace{\theta^k}_{dv}\underbrace{(1-\theta)^{n-k}}_{u} d\theta$$

$$= \underbrace{\frac{1}{k+1}\theta^{k+1}(1-\theta)^{n-k}\Big|_0^1}_{=0} + \frac{n-k}{k+1}\int_0^1 \underbrace{\theta^{k+1}}_{v}\underbrace{(1-\theta)^{n-k-1}}_{du} d\theta$$

$$= \frac{n-k}{k+1}\int_0^1 \theta^{k+1}(1-\theta)^{n-k-1} d\theta$$

Multiply both side by **n choose k**, we have

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}$$

$$\binom{n}{k}\int_0^1 \theta^k(1-\theta)^{n-k} d\theta = \binom{n}{k+1}\int_0^1 \theta^{k+1}(1-\theta)^{n-k-1} d\theta$$

Marginal Likelihood - Cont

$\int x^n\,dx = \frac{x^{n+1}}{n+1} + C \quad (\text{for } n \neq -1)$ (Cavalieri's quadrature formula)

- The recursion terminates when (the initial) $k = n$

Thus

$$\binom{n}{n}\int_0^1 \theta^n (1-\theta)^{n-n}\,d\theta = \int_0^1 \theta^n\,d\theta = \frac{1}{n+1}$$

$$P(x_1,\ldots x_n) = \int_0^1 \theta^k (1-\theta)^{n-k}\,d\theta = \frac{1}{n+1}\binom{n}{k}^{-1}$$

We conclude that the **posterior** is (just plug in all terms and recall that **P(theta)=1**)

$$P(\theta \mid x_1,\ldots x_n) = \frac{P(x_1,\ldots x_n \mid \theta)P(\theta)}{P(x_1,\ldots x_n)} = (n+1)\binom{n}{k}\theta^k (1-\theta)^{n-k}\cdot 1$$

$$P(\theta \mid x_1, \ldots x_n) = \frac{P(x_1, \ldots x_n \mid \theta) P(\theta)}{P(x_1, \ldots x_n)}$$

Bayesian Prediction

- So, we have a **posterior over the parameters**. But how do we predict a probability using this posterior?
- We can think of this as computing the probability of the next element in the sequence

$$P(x_{n+1} \mid x_1, \ldots, x_n) = \int P(x_{n+1}, \theta \mid x_1, \ldots, x_n) d\theta$$

chain rule

$$= \int P(x_{n+1} \mid \theta, x_1, \ldots, x_n) P(\theta \mid x_1, \ldots, x_n) d\theta$$

$$= \int P(x_{n+1} \mid \theta) P(\theta \mid x_1, \ldots, x_n) d\theta$$

  - Assumption: if we know θ, the probability of X_{n+1} is independent of $X_1, \ldots, X_n$

$$P(x_{n+1} \mid \theta, x_1, \ldots, x_n) = P(x_{n+1} \mid \theta)$$

Bayesian Prediction

- Thus, we conclude that

$$P(x_{n+1} = H \mid x_1, \ldots, x_n) = \int P(x_{n+1} \mid \theta) P(\theta \mid x_1, \ldots, x_n) d\theta$$

$$= \int \theta P(\theta \mid x_1, \ldots, x_n) d\theta$$

Plug-in formula for the posterior and move everything out of the intergal that does not depend on theta

$$= (n+1)\binom{n}{k} \int \theta^{k+1} (1-\theta)^{n-k} d\theta$$

Same type of derivation as before

$$= (n+1)\binom{n}{k} \frac{1}{n+2} \binom{n+1}{k+1}^{-1} = \frac{k+1}{n+2}$$

Plugging in the counts from our example (k=4 and n=5) we get the result seen already earlier

$$P(x[M+1] = H \mid D) = \int \theta \cdot P(\theta \mid D) d\theta = \frac{5}{7} = 0.7142\ldots$$

How do we choose the prior?

- Many possible answers…
- **Pragmatic approach:**
  - Want computationally "simple" (and still flexible) prior: conjugate priors

Conjugate Prior

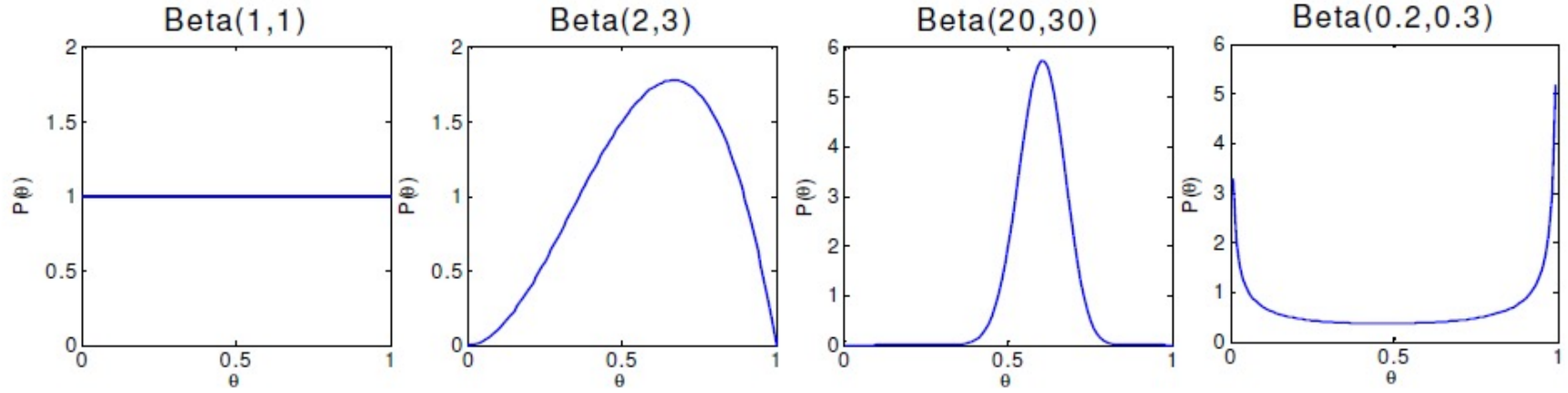
- Consider parametric families of prior distributions:
  - $P(\theta) = f(\theta; \alpha)$
  - α is called "hyperparameters" of prior
- A prior $P(\theta) = f(\theta; \alpha)$ is called **conjugate** for a likelihood function $P(D \mid \theta)$ if $P(\theta \mid D) = f(\theta; \alpha')$
  - Posterior has same parametric form
  - Hyperparameters are updated based on data D

Conjugate for Binomial

- Beta distribution

$$\mathrm{Beta}(\theta; \alpha_H, \alpha_T) = \frac{\theta^{\alpha_H - 1}(1-\theta)^{\alpha_T - 1}}{B(\alpha_H, \alpha_T)}$$

Normalization constant



Posterior for Binomial

- Beta distribution

$$P(\theta) = \text{Beta}(\theta; \alpha_H, \alpha_T) = \frac{\theta^{\alpha_H - 1}(1-\theta)^{\alpha_T - 1}}{B(\alpha_H, \alpha_T)}$$

- Likelihood:

$$P(\mathcal{D} \mid \theta) = \theta^{m_H}(1-\theta)^{m_T}$$

- Posterior:

$$P(\theta|D) \propto P(\theta)P(D|\theta) \propto \theta^{\alpha_H + m_H - 1}(1-\theta)^{\alpha_T + m_T - 1}$$

$$P(\theta|D) = \text{Beta}(\theta; \alpha_H + m_H, \alpha_T + m_T)$$

Bayesian Prediction

- Prior $P(\theta) = \text{Beta}(\alpha_H, \alpha_T)$ Bernoulli: $P(X=H) = \theta$
- Suppose we observe D= {m_H heads, and m_T tails}
- What's P(X=H | D), i.e., prob. that next flip is heads?

$$P(X=H \mid D) = \int \theta \, P(\theta \mid D) \, d\theta = \mathbb{E}[\theta \mid D] = \frac{\alpha_H + m_H}{\alpha_H + \alpha_T + m_H + m_T}$$

Prior = Smoothing

$$\mathbb{E}[\theta] = \frac{m_H + \alpha_H}{m_H + m_T + \alpha_H + \alpha_T} = \frac{m_H + \gamma m'}{m + m'}$$

- Where m' = $\alpha_H + \alpha_T$, and $\gamma = \alpha_H / m'$
- m' is called "equivalent sample size"

➔ "hallucinated" coin flips

$$E[\theta] = \frac{m}{m+m'} \frac{m_H}{m} + \frac{m'}{m+m'} \gamma$$

MLE — prior mean

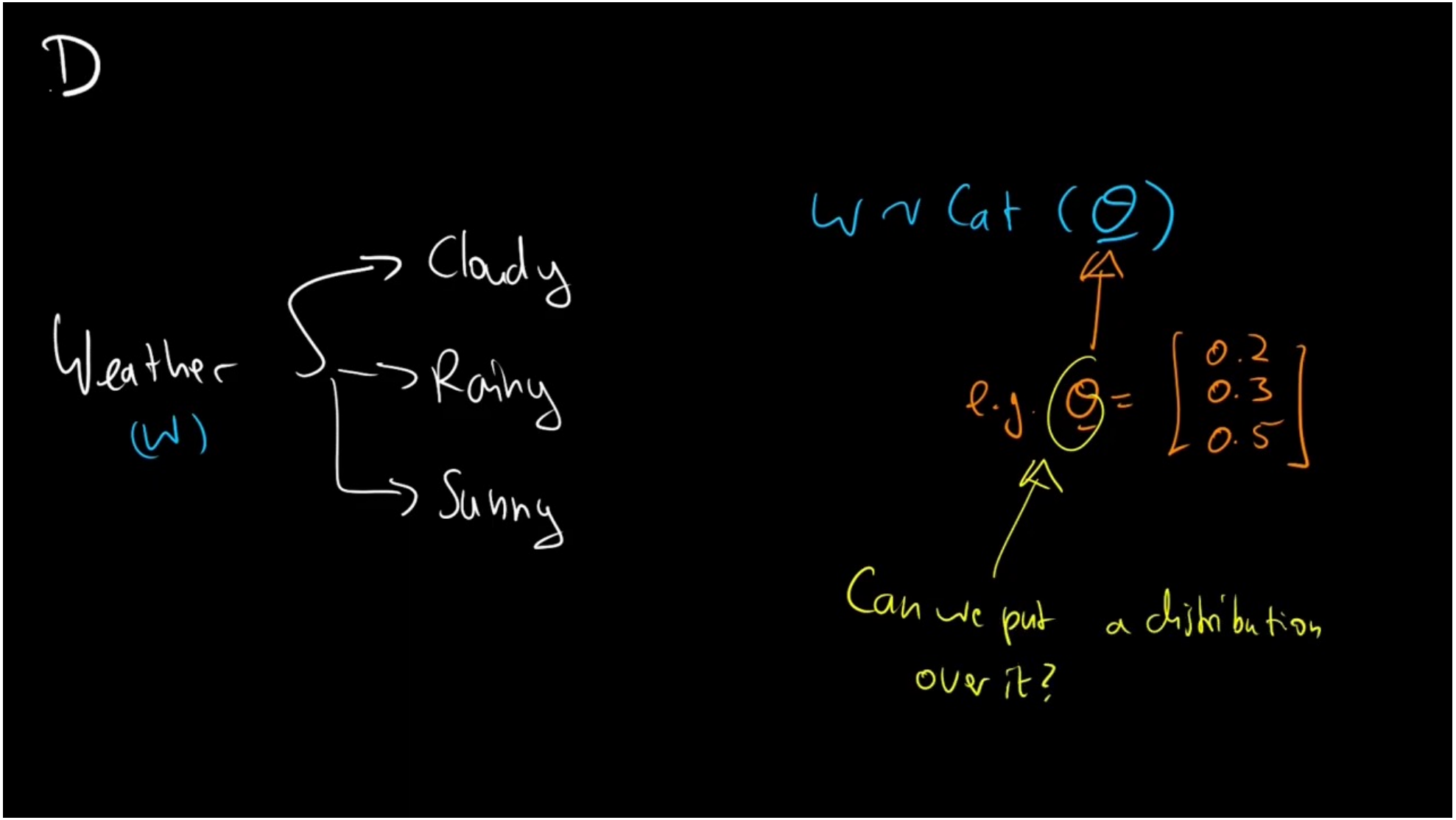
$m \to \infty$: $E[\theta] \to$ MLE — Forget prior

$m = 0$: prior

➔ Interpolate between MLE and prior mean

Conjuagte for Multinomial

https://www.youtube.com/watch?v=gWgsKyEjclw



Conjuagte for Multinomial

- If X∈{1,…,k} has k states:
- Multinomial likelihood

$$P(\mathcal{D} \mid \theta) = \theta_1^{m_1} \theta_2^{m_2} \ldots \theta_k^{m_k}$$

where $\sum_i \theta_i = 1$, $\theta_i \geq 0$

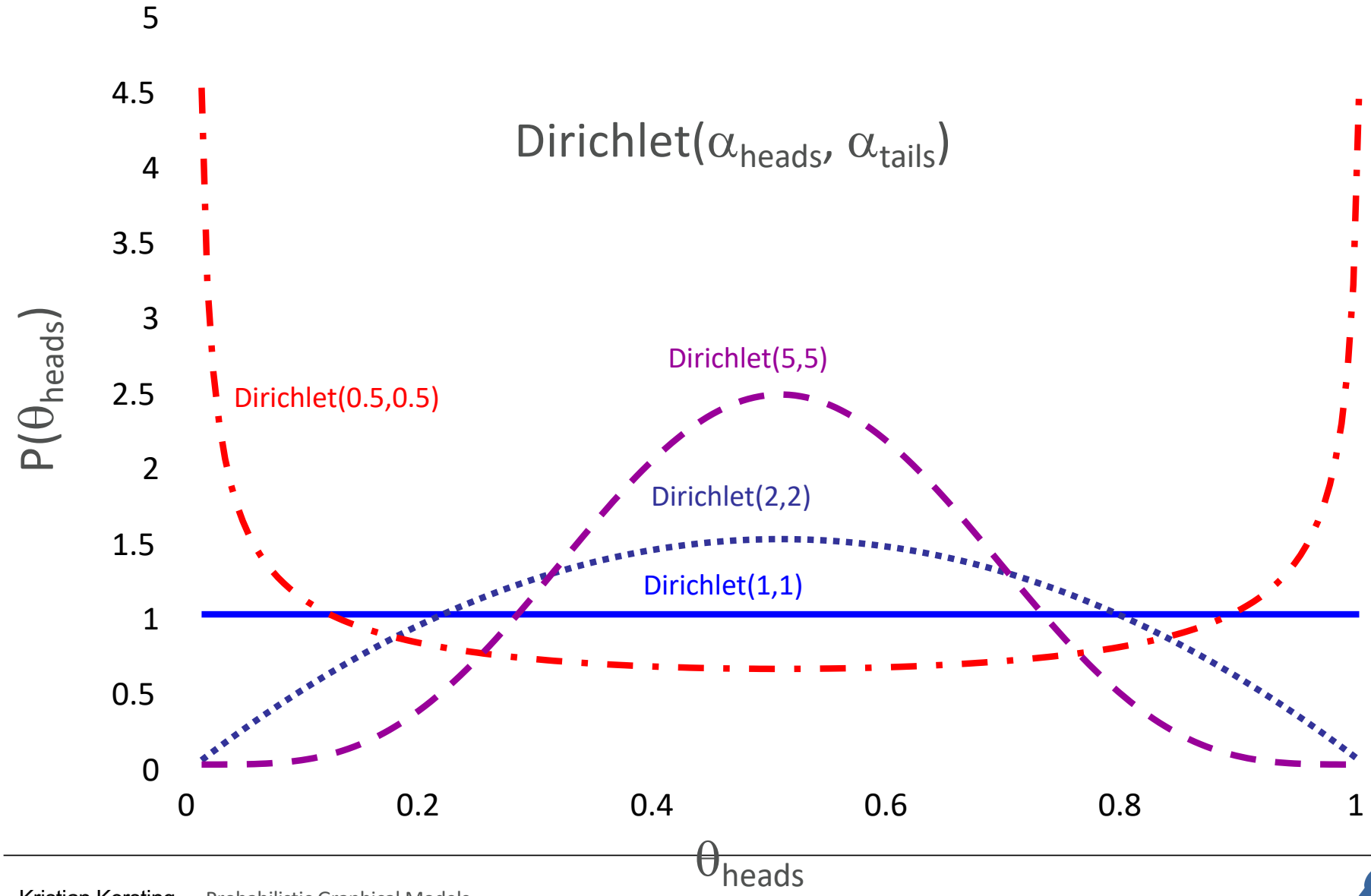
- Conjugate prior: Dirichlet distribution

$$P(\theta) = \mathrm{Dir}(\theta; \alpha_1, \ldots, \alpha_k) = \frac{1}{Z} \prod_i \theta_i^{\alpha_i - 1}$$

- If observe D={m_1 1s, m_2 2s, … m_k ks}, then

$$P(\theta \mid \mathcal{D}) = \mathrm{Dir}(\theta; \alpha_1 + m_1, \ldots, \alpha_k + m_k)$$

Dirichlet Priors - Example



Dirichlet visualization

https://www.youtube.com/watch?v=CEVELIz4WXM&t=425s

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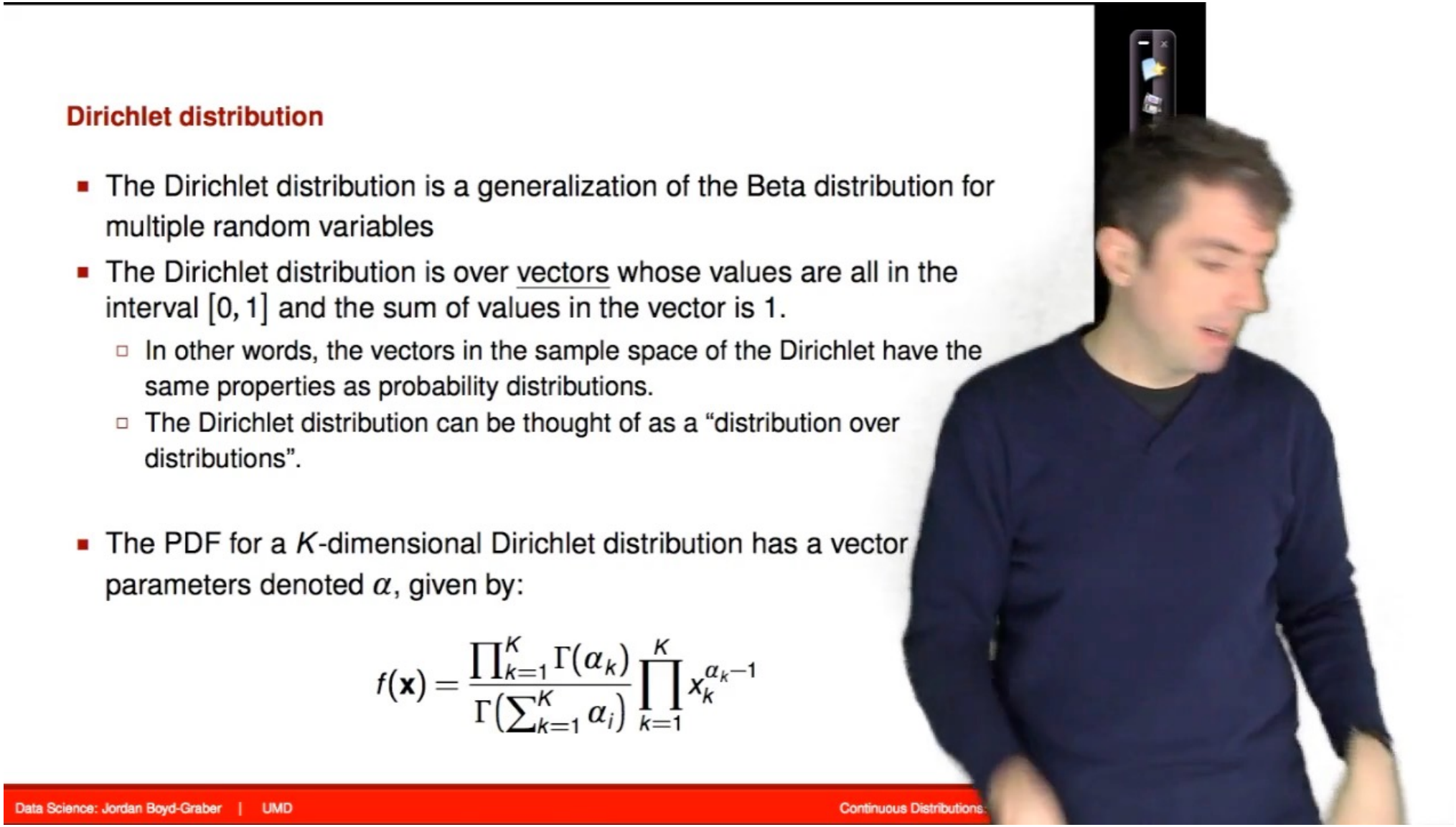


Dirichlet Priors (cont.)

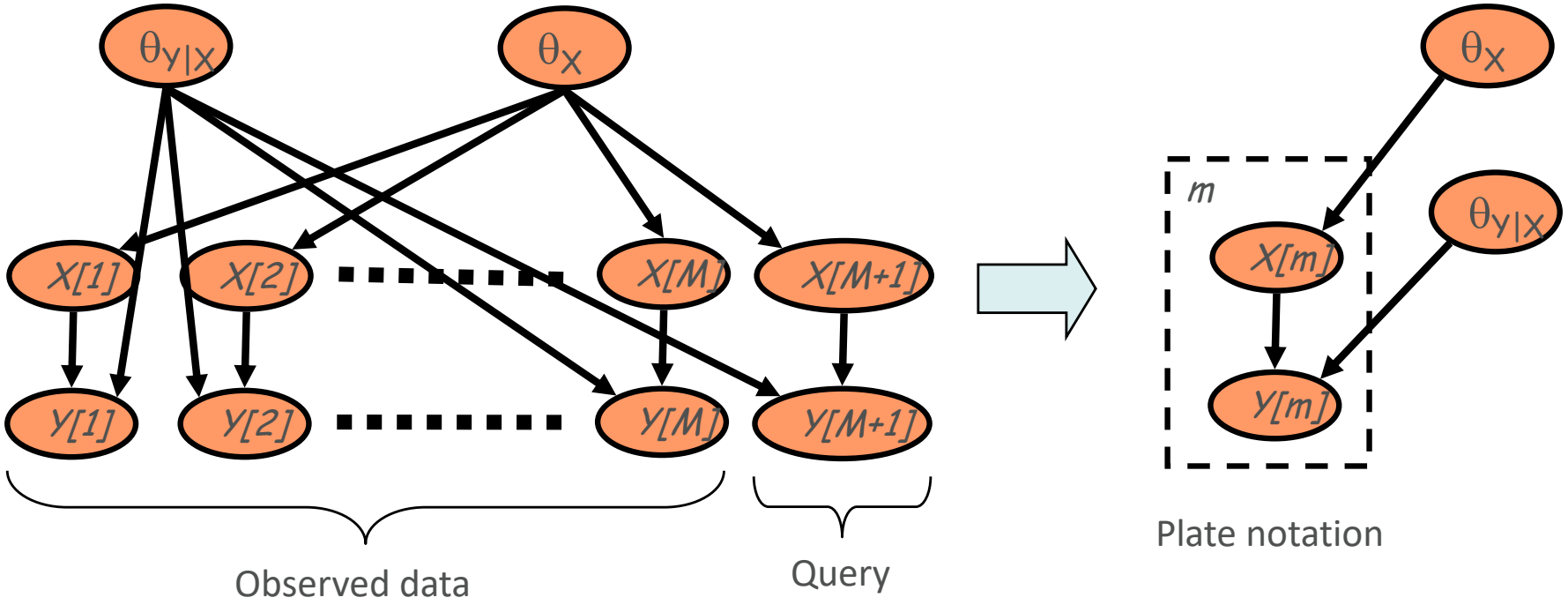
- If $P(\Theta)$ is Dirichlet with hyperparameters $\alpha_1,\ldots,\alpha_K$

$$P(X[1]=k)=\int \theta_k \cdot P(\Theta)d\Theta=\frac{\alpha_k}{\sum_\ell \alpha_\ell}$$

- Since the posterior is also Dirichlet, we get

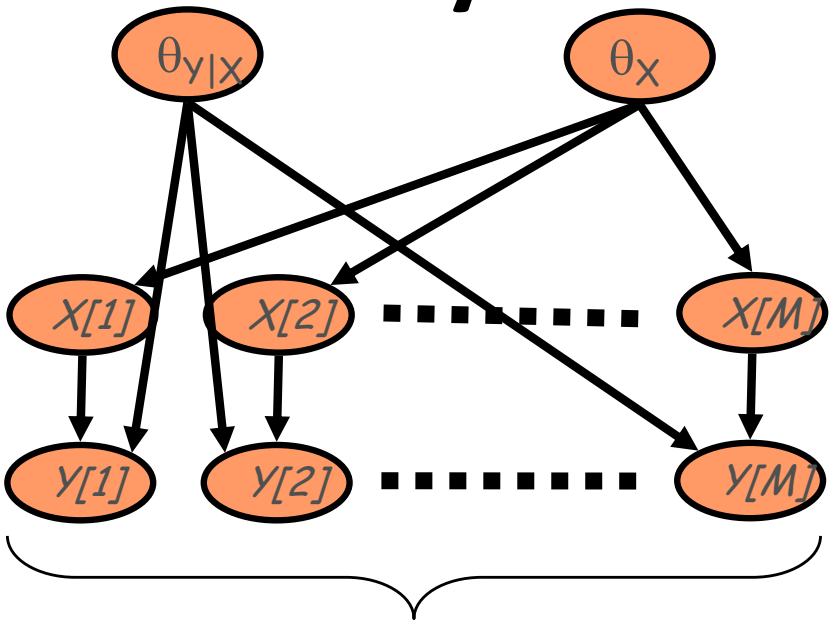
$$P(X[M+1]=k\mid D)=\int \theta_k \cdot P(\Theta\mid D)d\Theta=\frac{\alpha_k+N_k}{\sum_\ell(\alpha_\ell+N_\ell)}$$

Bayesian Nets & Bayesian Prediction



- Priors for each parameter group are independent
- Data instances are independent given the unknown parameters (so to say the “Bayesian iid”)

Bayesian Nets & Bayesian Prediction



- We can also "read" from the network:

Complete data ⇒

posteriors on parameters are independent

- Can compute posterior over parameters separately!

Learning Parameters: Summary

- Estimation relies on **sufficient statistics**
  - For multinomials: counts $N(x_i, pa_i)$
  - Parameter estimation

$$\hat{\theta}_{x_i|pa_i} = \frac{N(x_i, pa_i)}{N(pa_i)}$$

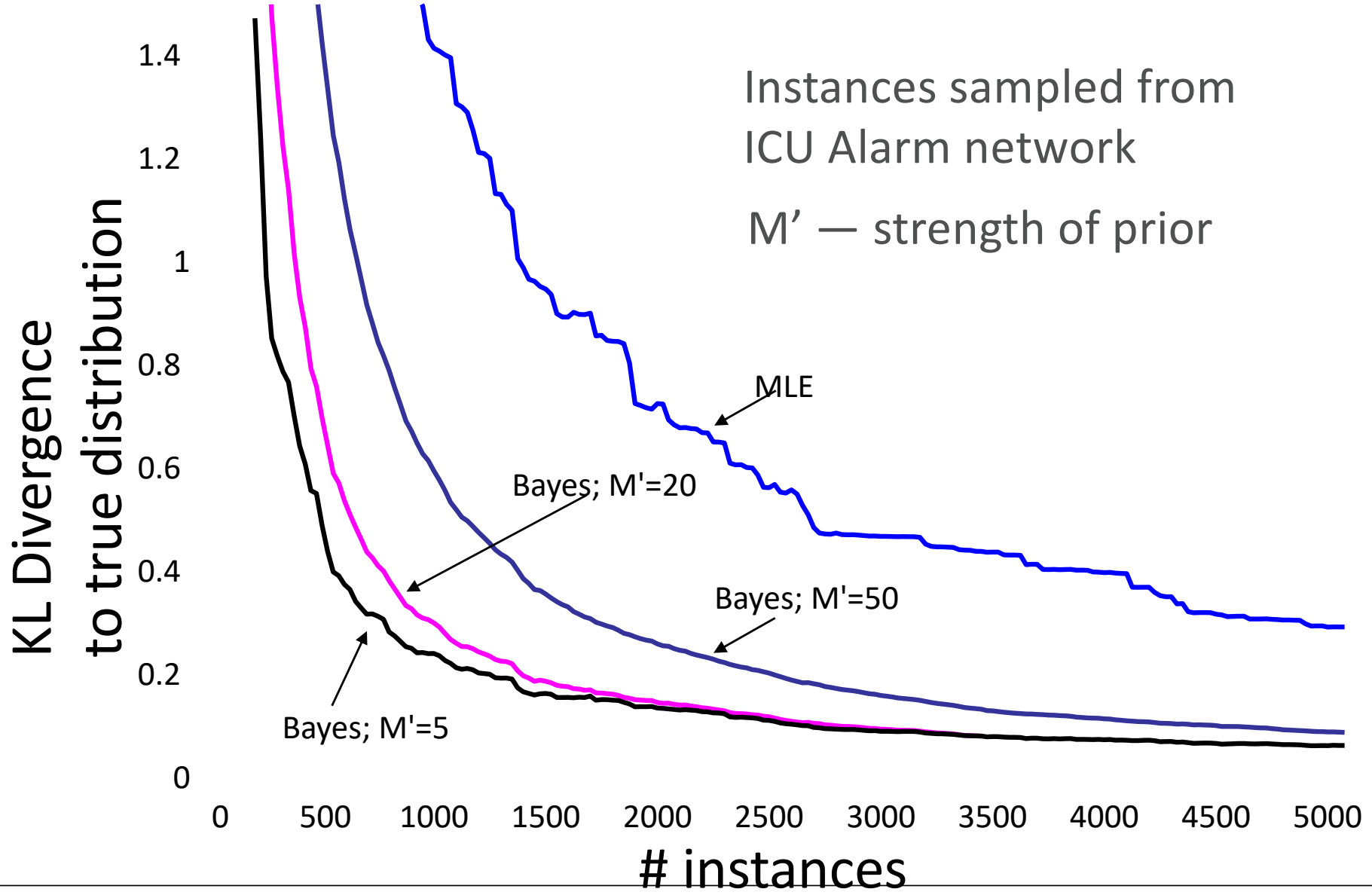
MLE

$$\tilde{\theta}_{x_i|pa_i} = \frac{\alpha(x_i, pa_i) + N(x_i, pa_i)}{\alpha(pa_i) + N(pa_i)}$$

Bayesian (Dirichlet)

- Both are asymptotically equivalent and consistent

Learning Parameters: Case Study



So far

- Where do the numbers come frome?
  - Expectation-Maximization (EM)
  - Gradient
  - Bayesian learning

What's next

- Structure Learning/Model Selection
  - Constrained-based
  - Score-based

- But first
  - I-equivalence, perfect maps etc.

Recap : Building BNs from independence properties

- From d-separation we learned:
  - Start from local Markov assumptions, obtain all independence assumptions encoded by graph
  - For most *P*'s that factorize over *G*, I(*G*) = I(*P*)
  - All of this discussion was for a given *G* that is an I-map for *P*

Recap: I-Map to Factorization

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G is I-map of P → obtain → P factorizes according to G

- Start with a topological ordering, wlog $X_1,\ldots,X_n$
- Apply chain rule

$$P(X_1,\ldots,X_n) = P(X_1)P(X_2 \mid X_1)\ldots P(X_n \mid X_1,\ldots,X_{n-1})$$

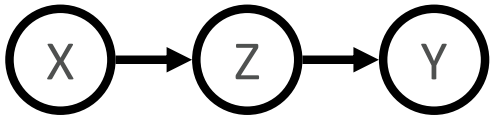
- Consider $P(X_i \mid X_1,\ldots,X_{i-1})$
- We know that $\mathrm{Pa}(X_i) \subseteq \{X_1,\ldots,X_{i-1}\}$, i.e., there are no descendants of Xi in X1,…Xi-1
- Hence, due to local Markov assumption

$$P(X_i \mid X_1,\ldots,X_{i-1}) = P(X_i \mid \mathrm{Pa}(X_i))$$

Recap: D-Separation

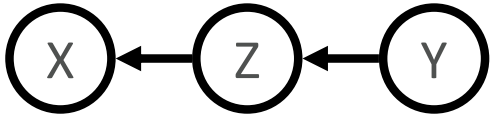
Local Markov Assumption: A variable X is independent of ist non-descendants given its parents and only ist parents:
$(X_i \perp \text{NonDescendants}_{X_i} \mid \text{Pa}_{X_i})$

Indirect causal effect:



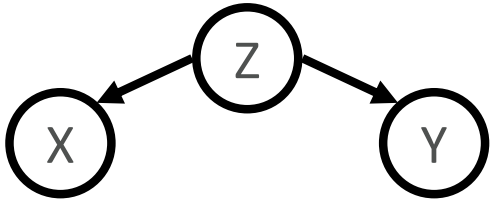
$$X \perp Y \mid Z$$
$$\neg X \perp Y$$

Indirect evidential effect:



$$X \perp Y \mid Z$$
$$\neg X \perp Y$$

Common cause:

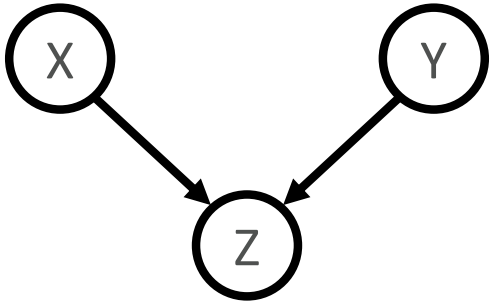


$$X \perp Y \mid Z$$
$$\neg X \perp Y$$

Represent all the same distributions

inverted

(v-structure)
Common effect:



$$X \perp Y$$
$$\neg X \perp Y \mid Z$$

Recap : Building BNs from independence properties

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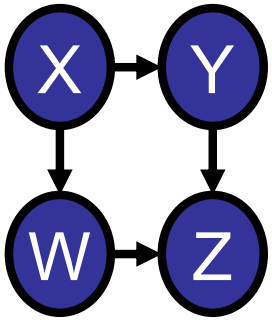
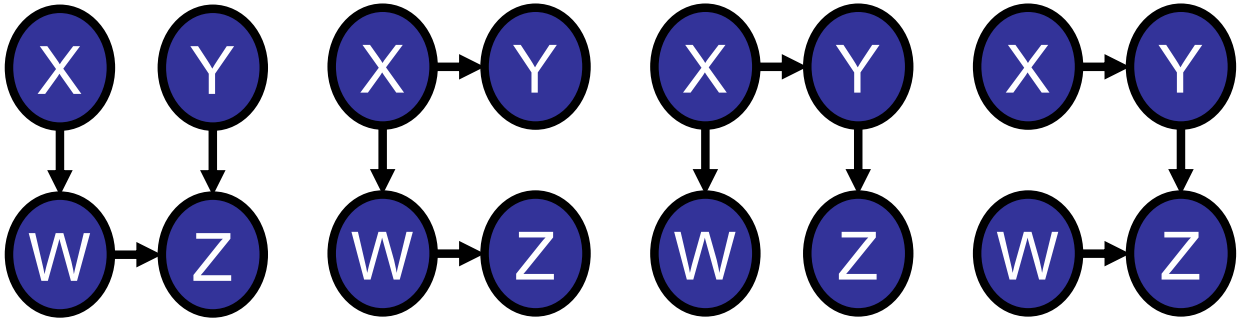
- From d-separation we learned:
  - Start from local Markov assumptions, obtain all independence assumptions encoded by graph
  - For most *P*'s that factorize over *G*, I(*G*) = I(*P*)
  - All of this discussion was for a given *G* that is an I-map for *P*
- **Now, given a *P*, how can I get a *G*?**
  - i.e., give me the independence assertions entailed by *P*
  - However, many *Gs* are "equivalent".
  - How do we represent this?
  - Most of this discussion is not about practical algorithms, but useful concepts that are used by practical algorithms

Minimal I-maps

- Given the independence assertions that are true for *P*, **find G**
- One option:
  - *G* is an I-map for *P*, $I_l(G) \subseteq I(P)$
  - ***G* is as simple as possible**
- *But what do we mean by "simple"?* ***G* is a minimal I-map for *P* if deleting any edges from *G* makes it no longer an I-map**
- Is this a good idea?

Obtaining Minimal I-maps

Example: if  is an minimal I-map

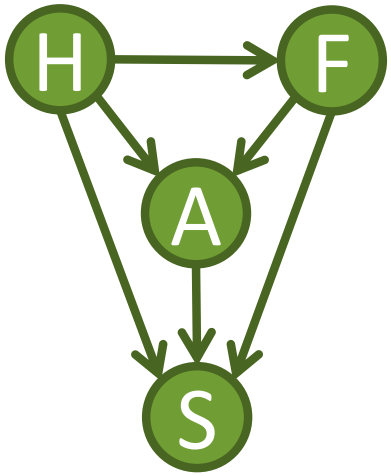
- Then: 

are not minimal-maps

Obtaining Minimal I-maps

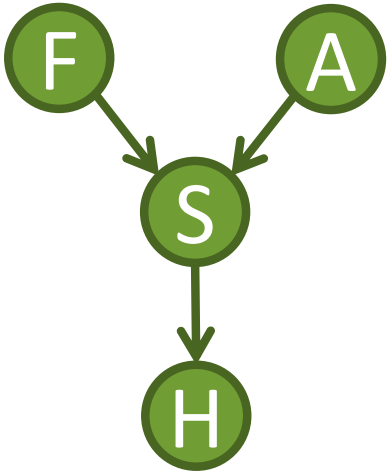
Flu, Allergy, SinusInfection, Headache

2 3 4 1



Flu, Allergy, SinusInfection, Headache

1 2 3 4



Both are minimal I-maps (if we remove an edge, they are not I-maps anymore) but the left-hand side BN is much more complicated!

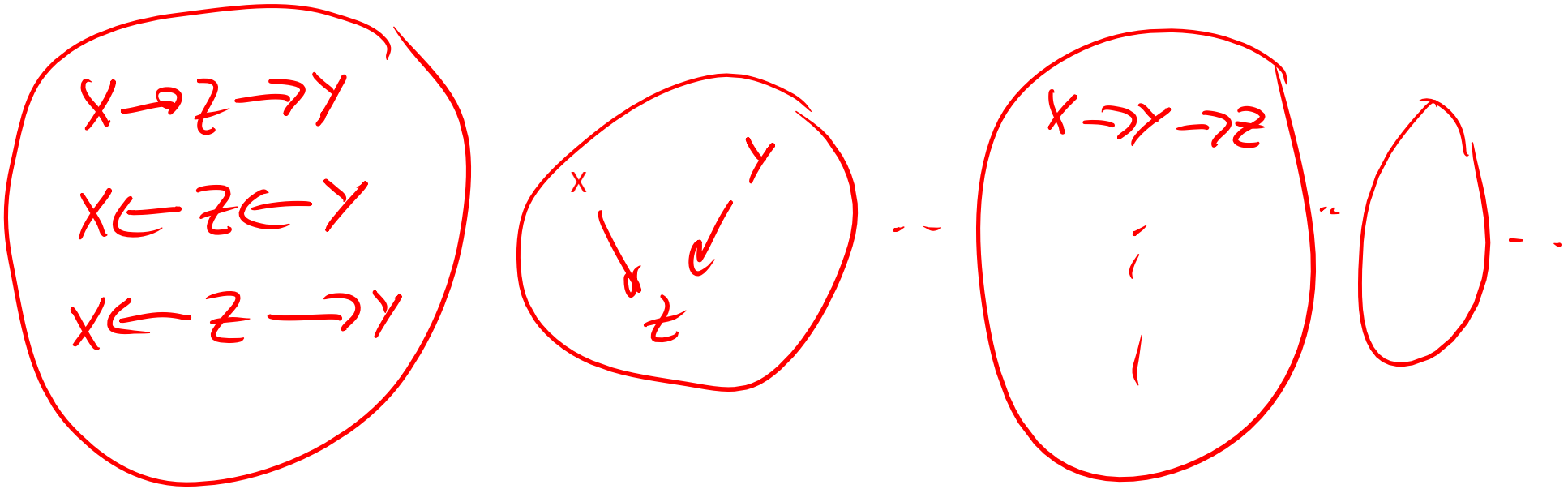
Perfect maps (P-maps)

- I-maps are not unique and often not simple enough
- Define "simplest" *G* differently
  - **A BN structure *G* is a perfect map for *P* if I(*P*) = I(*G*)**
- Our new goal is now:
  - Find a perfect map!
  - Must address **equivalent BNs**

Perfect maps (P-maps)

I-Equivalence

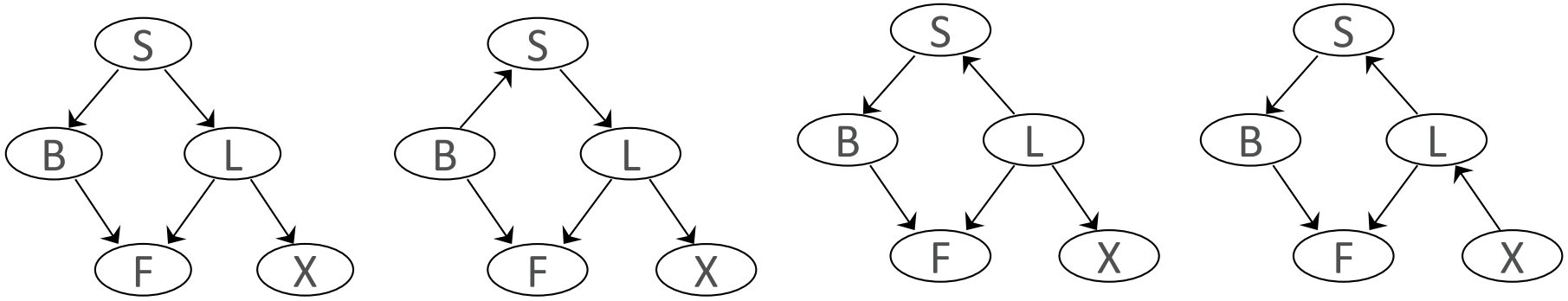
- **Two graphs G_1 and G_2 are I-equivalent if $I(G_1) = I(G_2)$**
- **However, p-maps are not unique**
- **Equivalence class** of BN structures
  - Mutually-exclusive and exhaustive partition of graphs



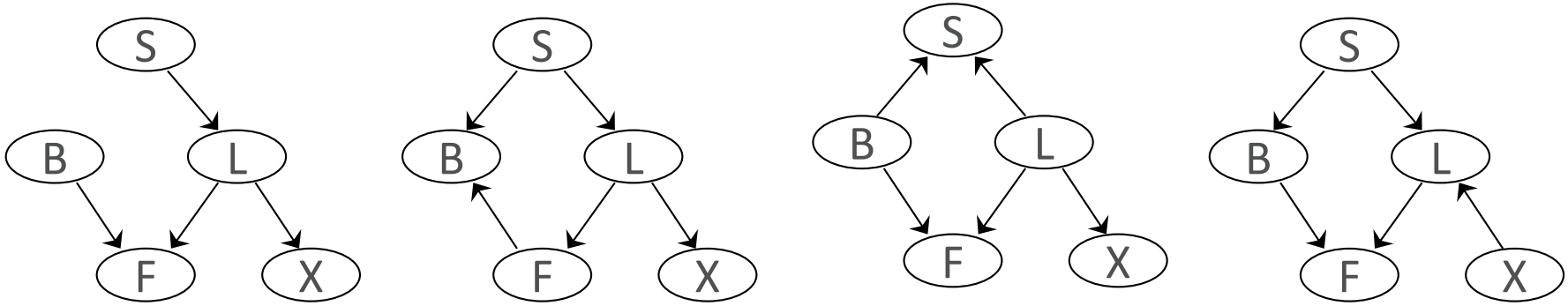
- **How do we characterize these equivalence classes?**

Examples of I-Equivalence

The following four DAGs are Markov equivalent and are said to form a Markov equivalence class.

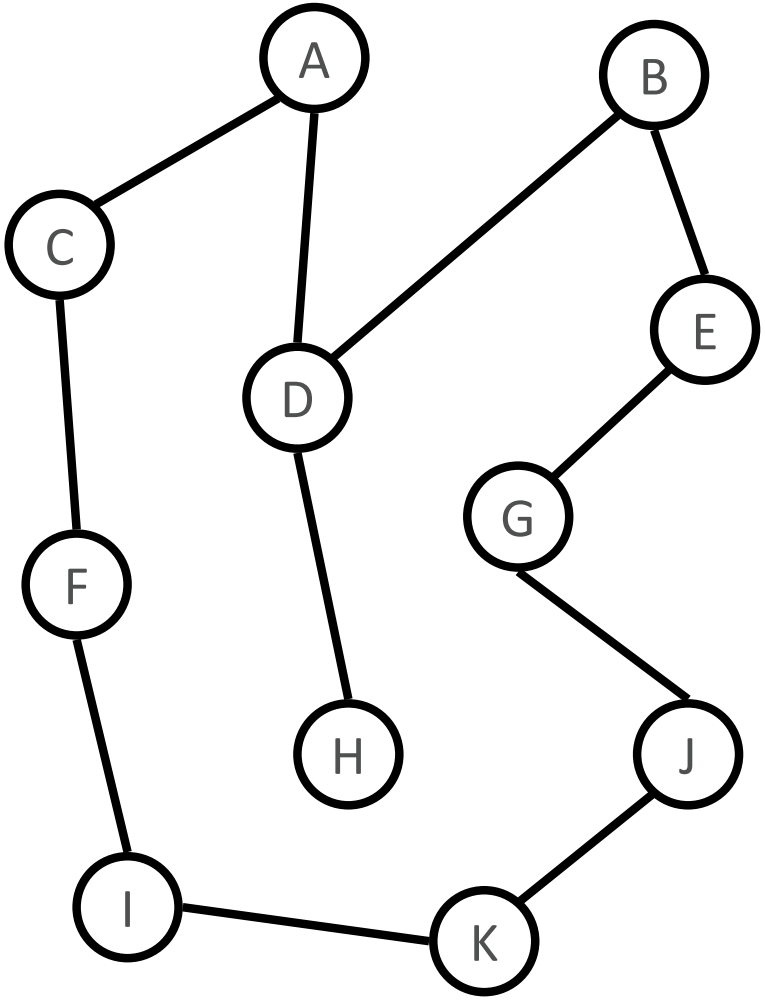


The following four DAGs are not Markov equivalent to those given above:



Skeleton of a BN

- Skeleton of a BN structure G is an undirected graph over the same variables that has an edge X–Y for every X->Y or Y->X in G (as we used it already for trails)
- (Little) Lemma: Two I-equivalent BN structures must have the same skeleton
- Proof via trials

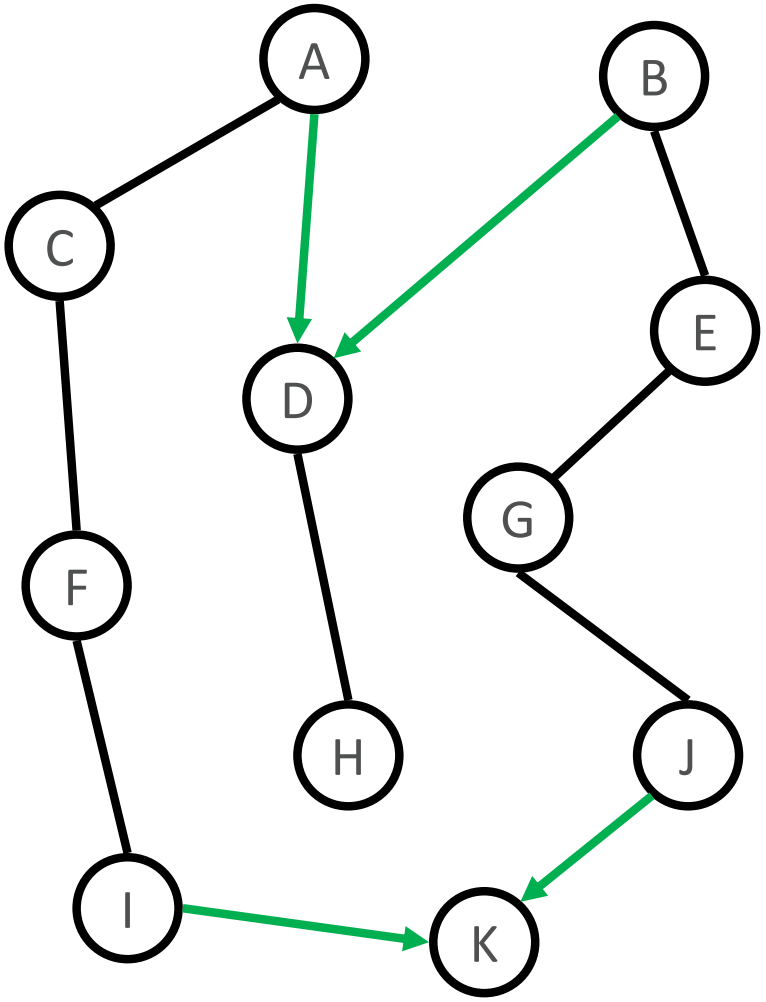


What about the other „direction“?

What about V-structures?

- **V-structures are key property of BN structure** (as used for d-separation)

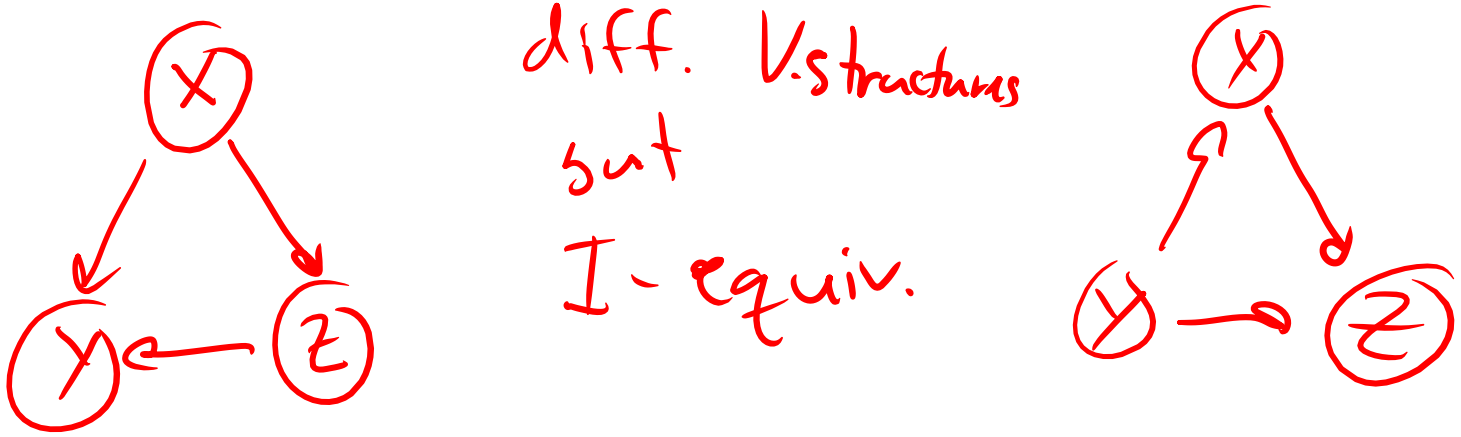
- **Theorem: If** G_1 and G_2 have the same skeleton and V-structures, **then** G_1 and G_2 are I-equivalent
- Proof via trials and rules of d-separation



Same V-structures not necessary

- **Theorem: If** G_1 and G_2 have the same skeleton and V-structures, **then** G_1 and G_2 are I-equivalent

- Though sufficient, same V-structures not necessary, i.e., no **iff**



Actually, for the "none-necessity", any complete graph can be considered. They are I-equivalent but they do not have the same V-structures

Immoralities & I-Equivalence

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- Key concept is not V-structure, but "**immoralities**" (unmarried parents 😞)
  - **X -> Z <– Y, with no arrow between X and Y**
- Important pattern: **X and Y independent given their parents, but not given Z**
- (If edge exists between X and Y (moralized), we have *covered* the V-structure)
- **Theorem:**

  G_1 and G_2 have the same skeleton and immoralities if and only if G_1 and G_2 are I-equivalent

Obtaining a P-map

- **Step 1: Given the independence assertions that are true for *P***
  - Obtain skeleton
  - Obtain immoralities
- We have found the right equivalence class
- **Step 2: From skeleton and immoralities, obtain every (and any) BN structure from the equivalence class**

Identifying the skeleton

- When is there an edge between X and Y?
  - Difficult to answer

- When is there no edge between X and Y?
  - Local Markov Assumption
  - Exists $\mathbf{U} \subseteq \mathbf{X} - \{X,Y\}$, $|\mathbf{U}| \leq d$, such that $(X \perp Y \mid \mathbf{U})$
  - d maximal number of parents

Identifying the skeleton

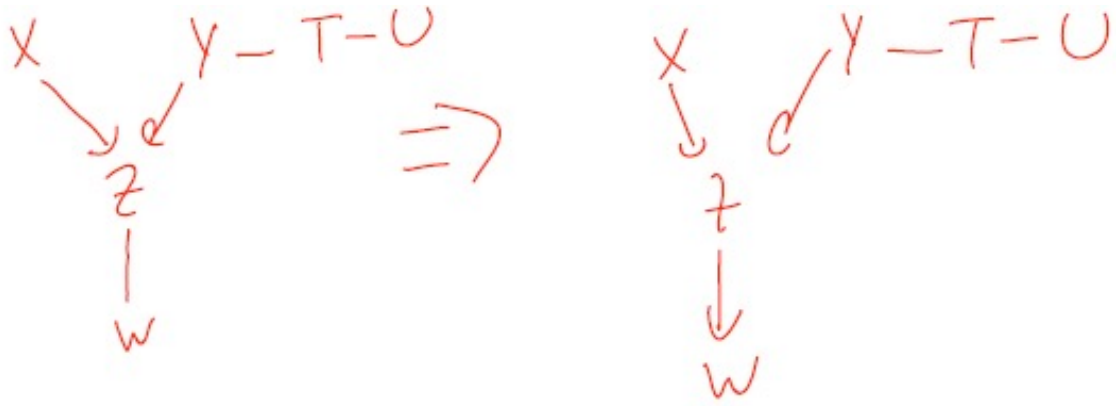
- Assume d<=(n-1) is max number of parents
- For each X_i and X_j
  - $E_{ij} \leftarrow$ true
  - For each $\mathbf{U} \subseteq \mathbf{X} - \{X_i, X_j\}$, $|\mathbf{U}| \leq d$
    - Is $(X_i \perp X_j \mid \mathbf{U})$? // note that we "assume " to know this
      - $E_{ij} \leftarrow$ false
      - break
  - If E_{ij} is true
    - Add edge X – Y to skeleton
- For measuring independence, there are several ways. One considers the mutual information (you will see this later)

Identifying immoralities

- Consider X –Z–Y in skeleton, when should it be an immorality X->Z<-Y? Essentially when X ⊥ Y
- Must be X -> Z <– Y (immorality):
  - When X and Y are **never independent given U,** if Z in **U**
    - Proof: Assume no **Z** exists but X–Z–Y is not an immorality
    - Then, either X→Z→Y or X←Z←Y or X←Z→Y exists
    - But then, we can block X–Z–Y by Z
    - Then, since X and Y are not connected, can find **U** that includes Z such that Ind(X;Y | **W**)
    - Contradiction
- Must **not** be X -> Z <– Y (not immorality):
  - When there exists **U** with Z in **U**, such that X and Y are **independent** given **U**

From immoralities and skeleton to BN structures

- Representing BN equivalence class as a **partially-directed acyclic graph** (PDAG)
- Immoralities force direction on other BN edges



Otherwise we would get another immoral v-structure, which was ruled out by the algorithm

- Full (polynomial-time) procedure exists

What you need to know

- Minimal I-map
  - every *P* has one, but usually many
- Perfect map
  - better choice for BN structure
  - not every *P* has one
  - can find one (if it exists) by considering I-equivalence
  - Two structures are I-equivalent if they have same skeleton and immoralities

Learning With Bayesian Networks

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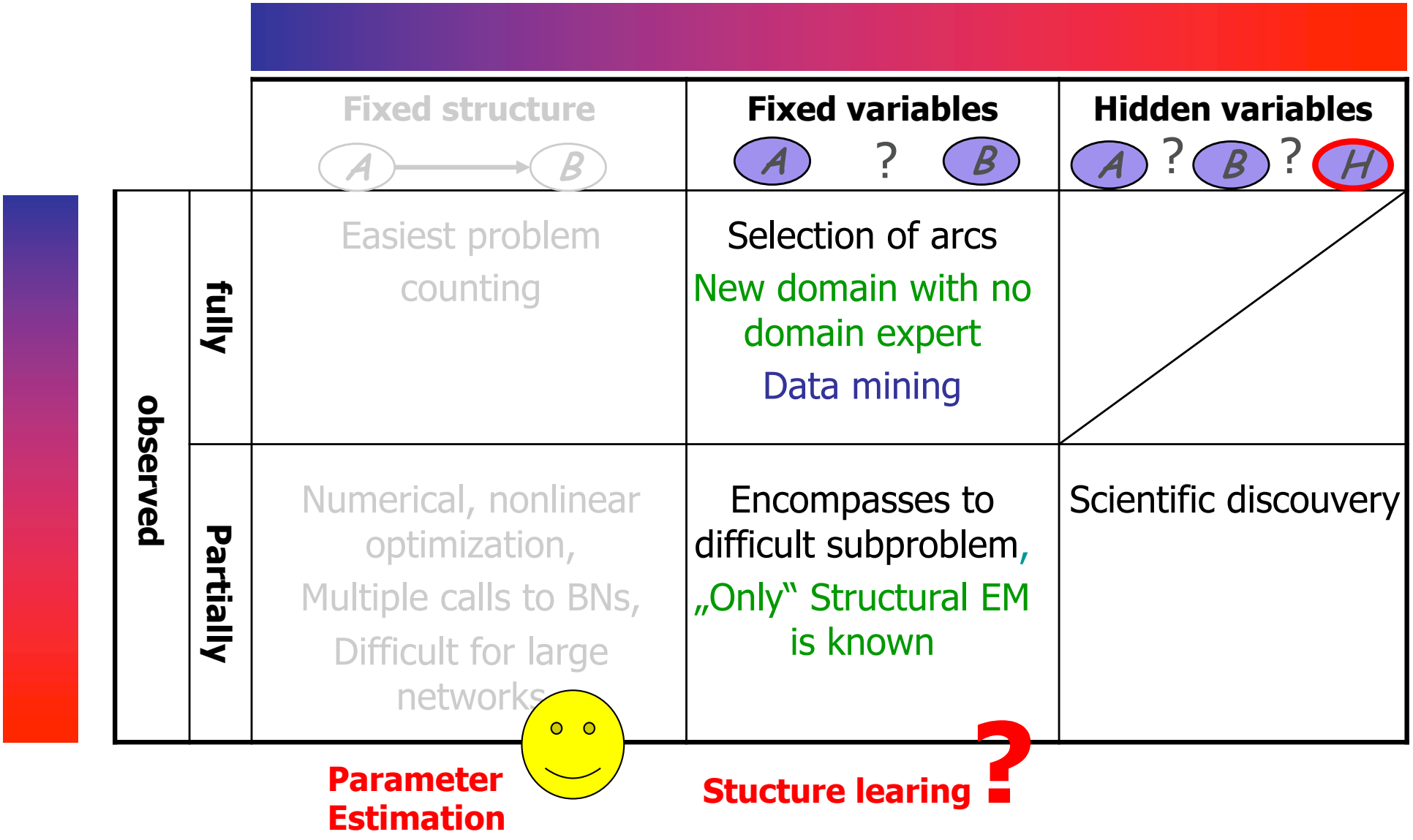
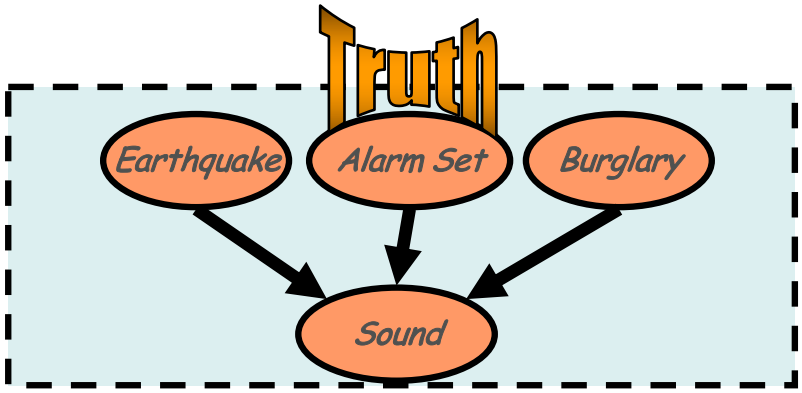
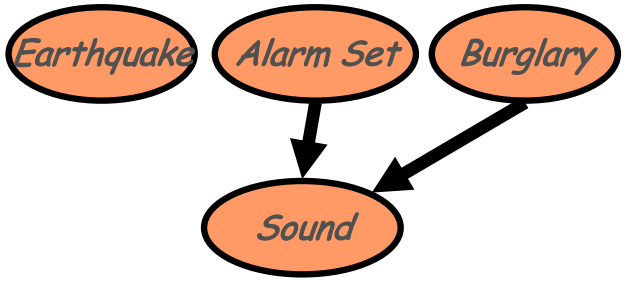


Why Struggle for Accurate Structure?

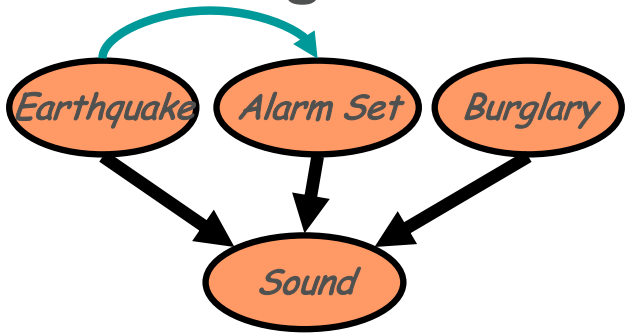


Missing an arc



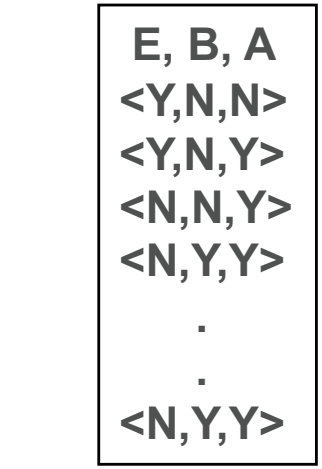
- Cannot be compensated for by fitting parameters
- Wrong assumptions about domain structure

Adding an arc

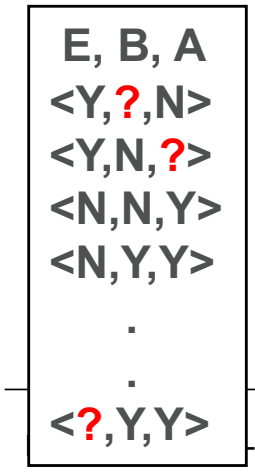


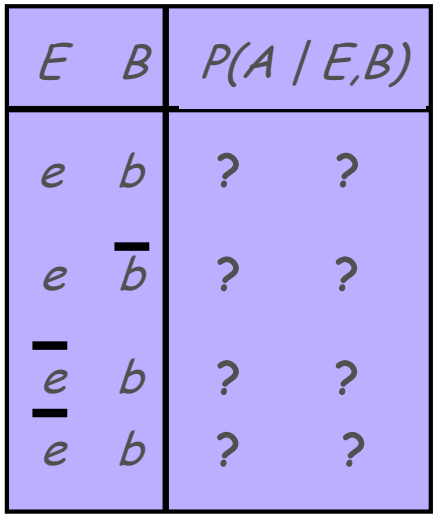
- Increases the number of parameters to be estimated
- Wrong assumptions about domain structure

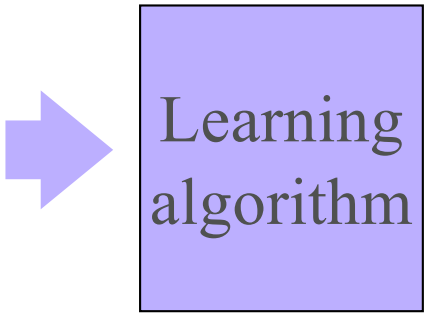
Unknown Structure, (In)complete Data

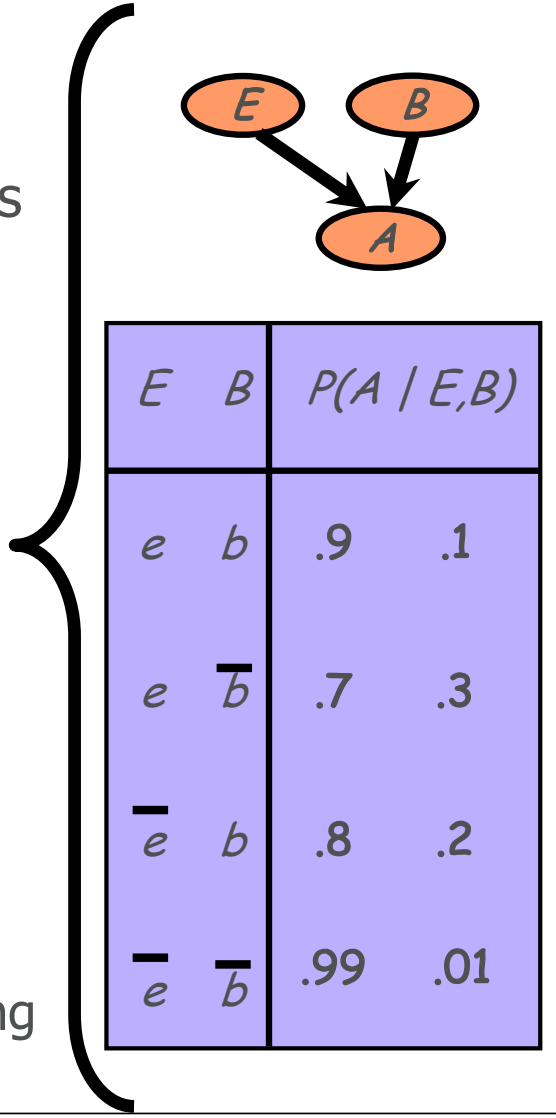


- Network structure is not specified
  - Learnerr needs to select arcs & estimate parameters
- Data does not contain missing values









- Network structure is not specified
- Data contains missing values
  - Need to consider assignments to missing values

Structure Learning

- Two main approaches

1. Constrained-based
2. Score-based

Constraint-Based Learning

- Remember: Optaining a P-Map?
  - Given the independence assertions that are true for *P*
    - Obtain skeleton and then obtain immoralities
  - From skeleton and immoralities, obtain every (and any) BN structure from the equivalence class
- Only now, we do **not** have I(X,Y|Z) statements
- **Basic task:**
  - Determine whether two variables are independent
  - Well studied question in statistics

Testing Independence

- Null hypothesis H0 is
  - Data was sampled from P(X,Y)=P(X)*P(Y)

- Need a procedure that will Accept or Reject H0
- Use χ^2 -test
  - χ^2 (X,Y) ~ I(X,Y)* N * ln(4) where I(X,Y) is the mutual information
- Or directly mutual information

$$\hat{P}(x_i, x_j) = \frac{\text{Count}(x_i, x_j)}{m} \qquad \hat{I}(X_i, X_j) = \sum_{x_i, x_j} \hat{P}(x_i, x_j) \log \frac{\hat{P}(x_i, x_j)}{\hat{P}(x_i)\hat{P}(x_j)}$$

Score-based Learning

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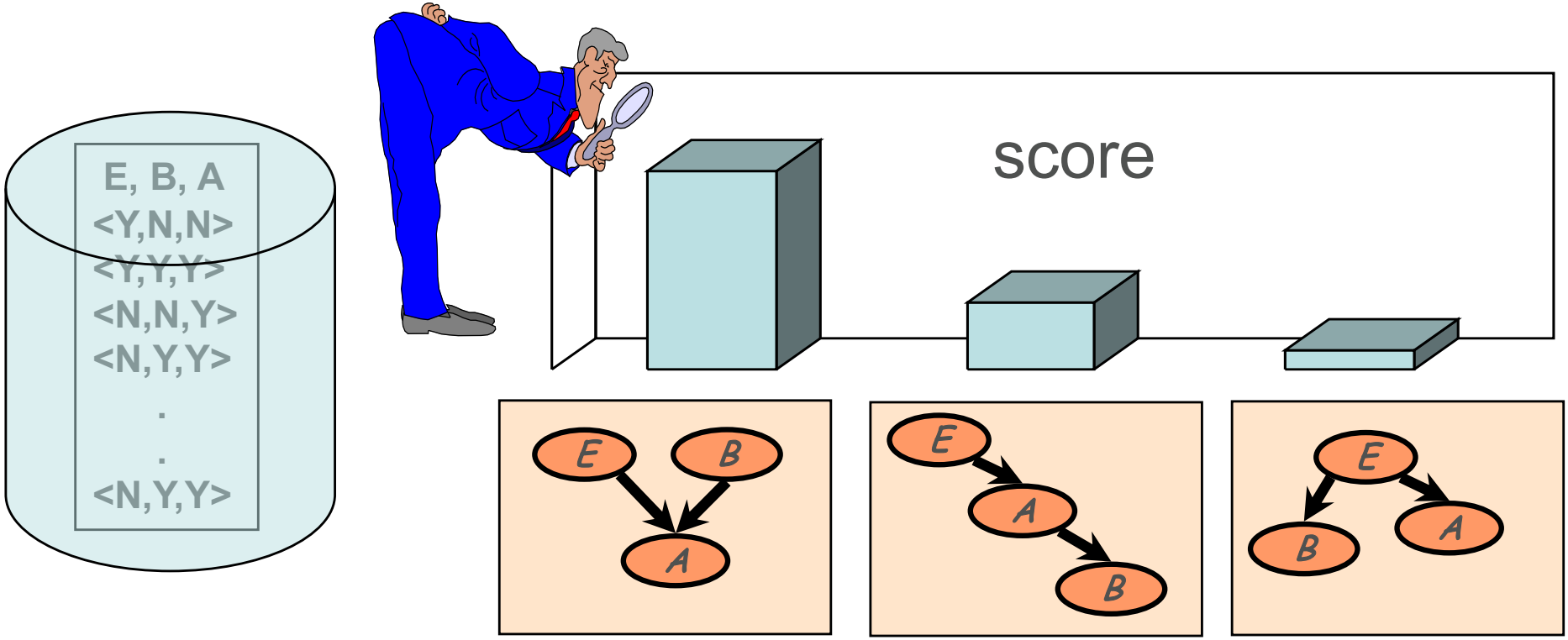
Define scoring function that evaluates how well a structure matches the data



Search for a structure that maximizes the score

Likelihood Score for Structure

$$\ell(G:D) = \log L(G:D) = M \sum_i \left(I(X_i; Pa_i^G) - H(X_i) \right)$$

Mutual information between X_i and its parents

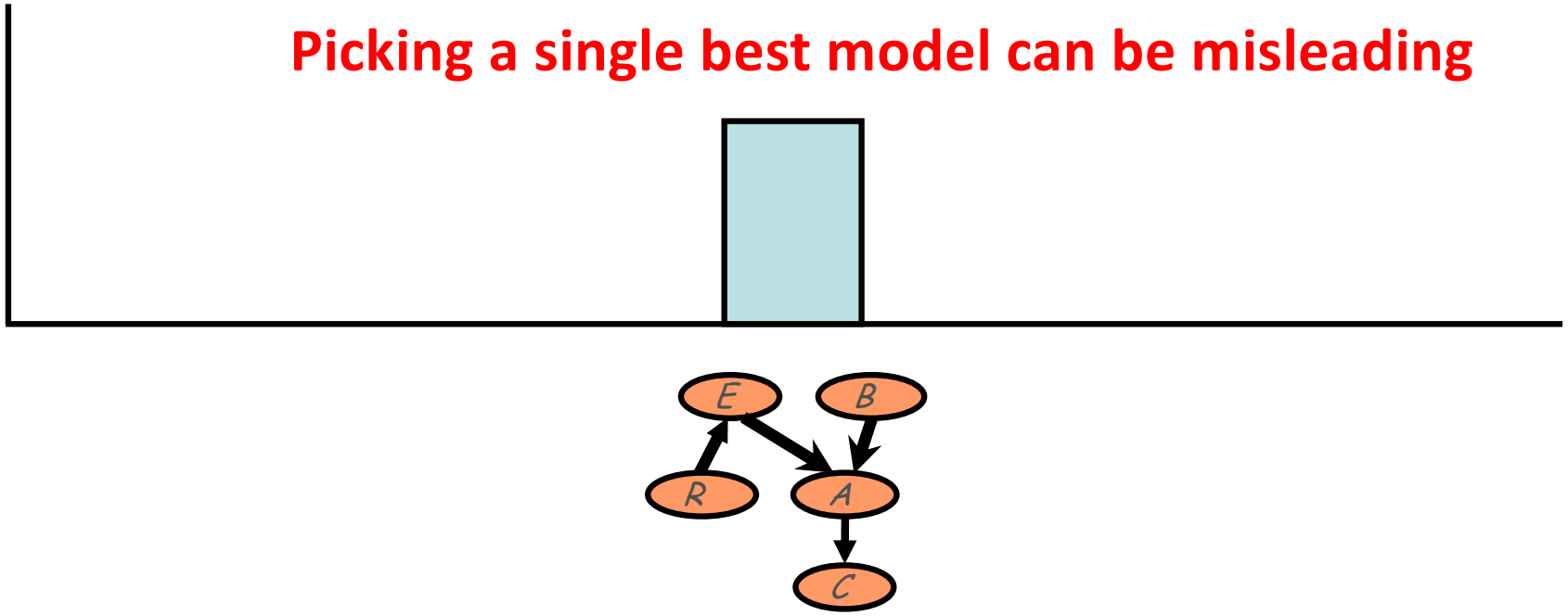
Entropy X_i

- Larger dependence of X_i on $Pa_i \Rightarrow$ higher score

- Adding arcs always helps
  - $I(X; Y) \leq I(X; \{Y,Z\})$
  - Max score attained by fully connected network
  - Overfitting: A bad idea…

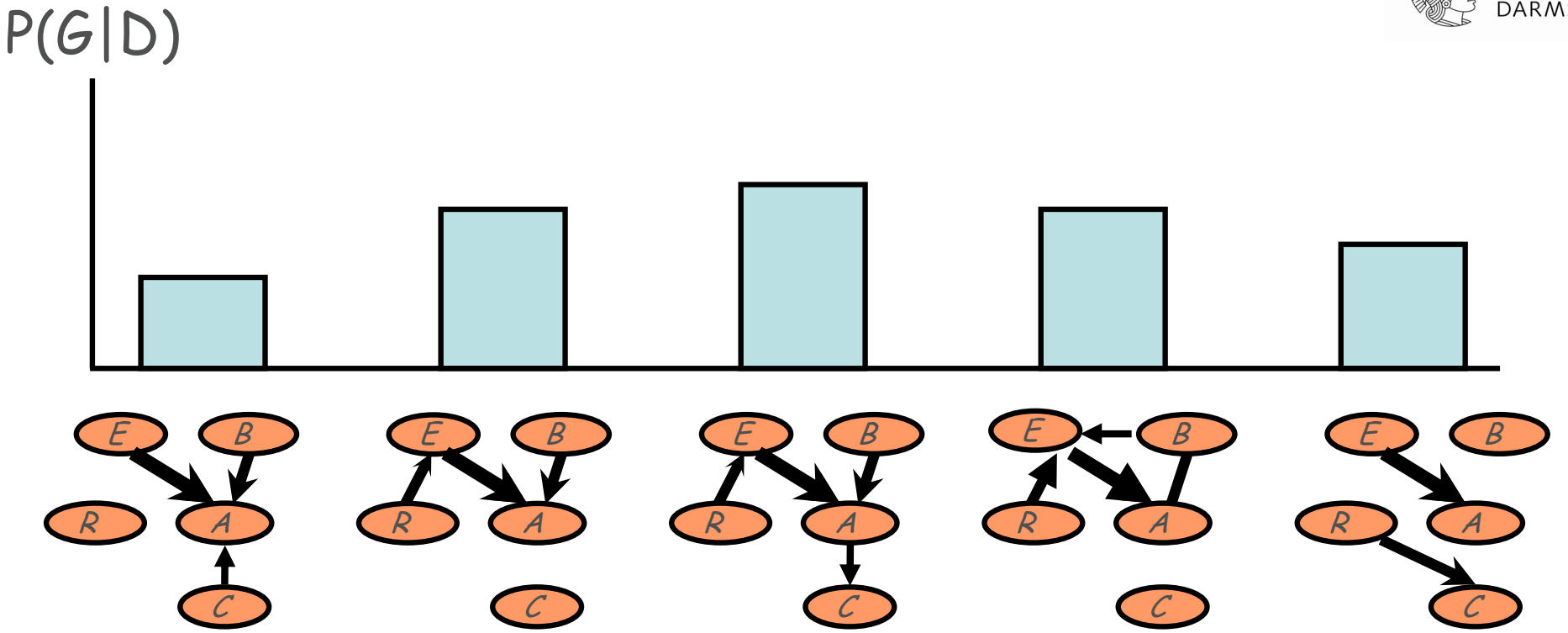
Bayesian Score

$P(G|D)$



- Current practice: model selection
  - Pick a single high-scoring model
  - Use that model to infer domain structure

Bayesian Score



Problem

- Small sample size ⇒ many high scoring models
- Answer based on one model often useless

Bayesian Score

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Likelihood score: $L(G:D) = P(D \mid G, \hat{\theta}_G)$

Max likelihood params

Bayesian approach:

- Deal with uncertainty by assigning probability to all possibilities

$$P(D \mid G) = \int P(D \mid G, \theta) P(\theta \mid G)\, d\theta$$

Marginal Likelihood

Likelihood

Prior over parameters

$$P(G \mid D) = \frac{P(D \mid G) P(G)}{P(D)}$$

Bayesian Score

- Bayesian has difficult integrals
- For Dirichlet prior, can use simple Bayes information criterion (BIC) approximation

- **Theorem:** for Dirichlet prior, and a BN with Dim(*G*) independent parameters, *as* $m \to \infty$*:*

$$\log P(D \mid G) = \log(D \mid G, \theta) - \frac{\log M}{2} \dim(G) + O(1)$$

Bayesian Information Criterion (BIC)

$$\log P(D \mid G) = \ell(G : D) - \frac{\log M}{2} \dim(G) + O(1)$$

$$= \underbrace{M \sum_i \left(I(X_i; Pa_i^G) - H(X_i) \right)}_{\text{Fit dependencies in empirical distribution}} - \underbrace{\frac{\log M}{2} \dim(G)}_{\text{Complexity penalty}} + O(1)$$

- As M (amount of data) grows,
  - Increasing pressure to fit dependencies in distribution
  - Complexity term avoids fitting noise
- Asymptotic equivalence to MDL score
- Bayesian score/BIC is **consistent**
  - Observed data eventually overrides prior

Structure Search as Optimization

Input:

- Training data
- Scoring function (MDL, BIC, …)
- Set of possible structures

Output:

- A network that maximizes the score

Learning Trees (complete data)

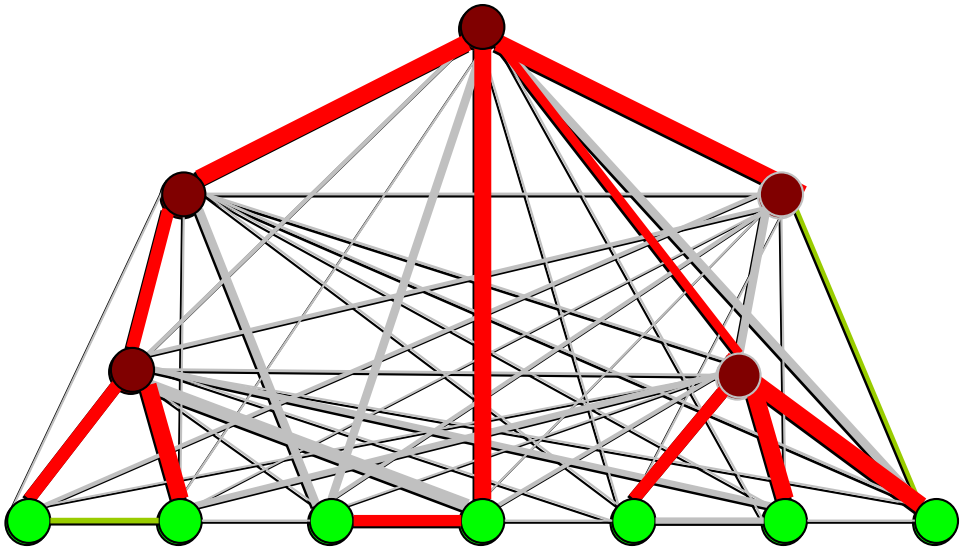
https://www.youtube.com/watch?v=8N0HsrBY7WI&t=3629s

Vibhav Gogate, UT Dallas

Learning Bounded Treewidth Models

- Good news: Models with treewidth 1 can be learned optimally in polynomial time! Recall that such Bayesian networks are called Singly-connected Bayesian networks and their primal graph is a tree.
- Bad news: Models having treewidth > 1 are NP-hard to learn.

Learning Trees (complete data)



- Can find optimal tree structure in $O(n^2 \log n)$ time: just find the max-weight spanning tree
- If some of the variables are hidden, problem becomes hard again, but can use EM to fit mixtures of trees

Heuristic Search

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- Define a search space:
  - search states are possible structures
  - operators make small changes to structure
- Traverse space looking for high-scoring structures
- Search techniques:
  - Greedy hill-climbing
  - Best first search
  - Simulated Annealing
  - ...

Theorem: Finding maximal scoring structure with at most k parents per node is NP-hard for $k > 1$

Typically: Local Search

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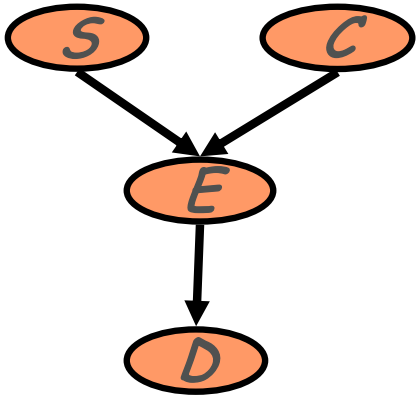
- Start with a given network
  - empty network, best tree , a random network
- At each iteration
  - Evaluate all possible changes
  - Apply change based on score
- Stop when no modification improves score



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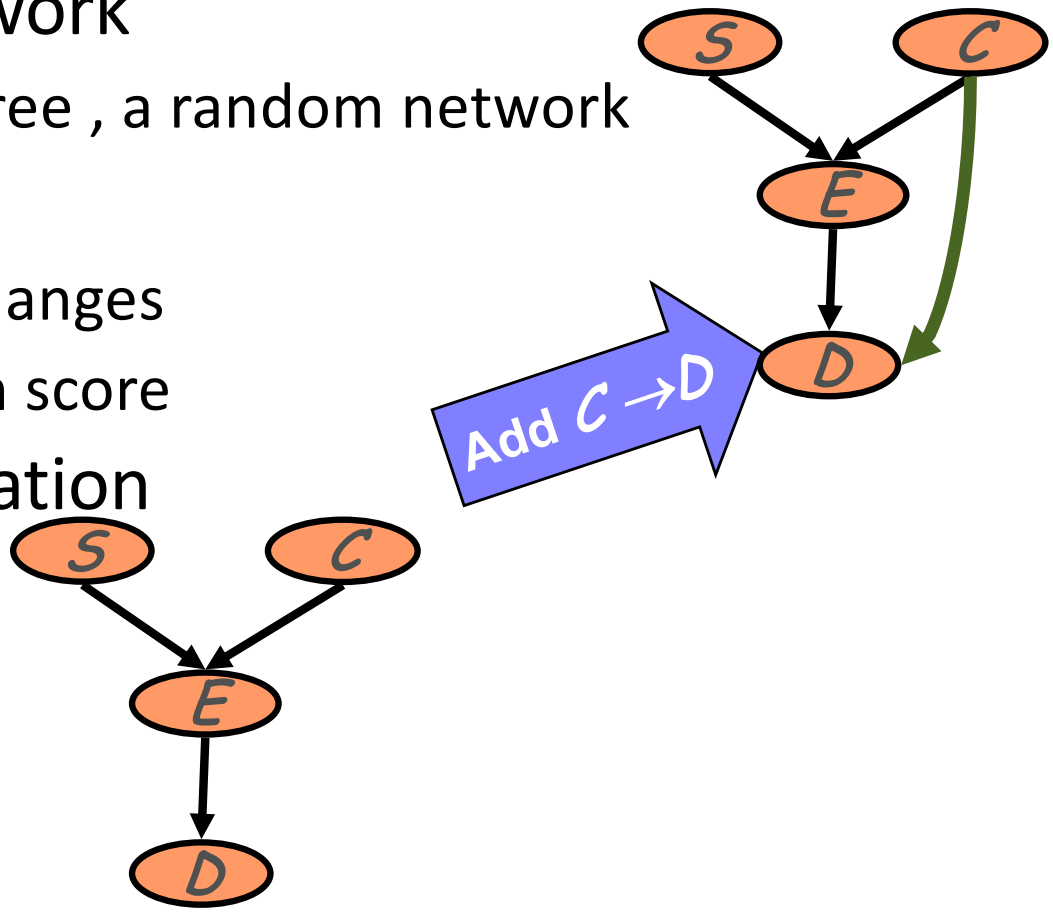

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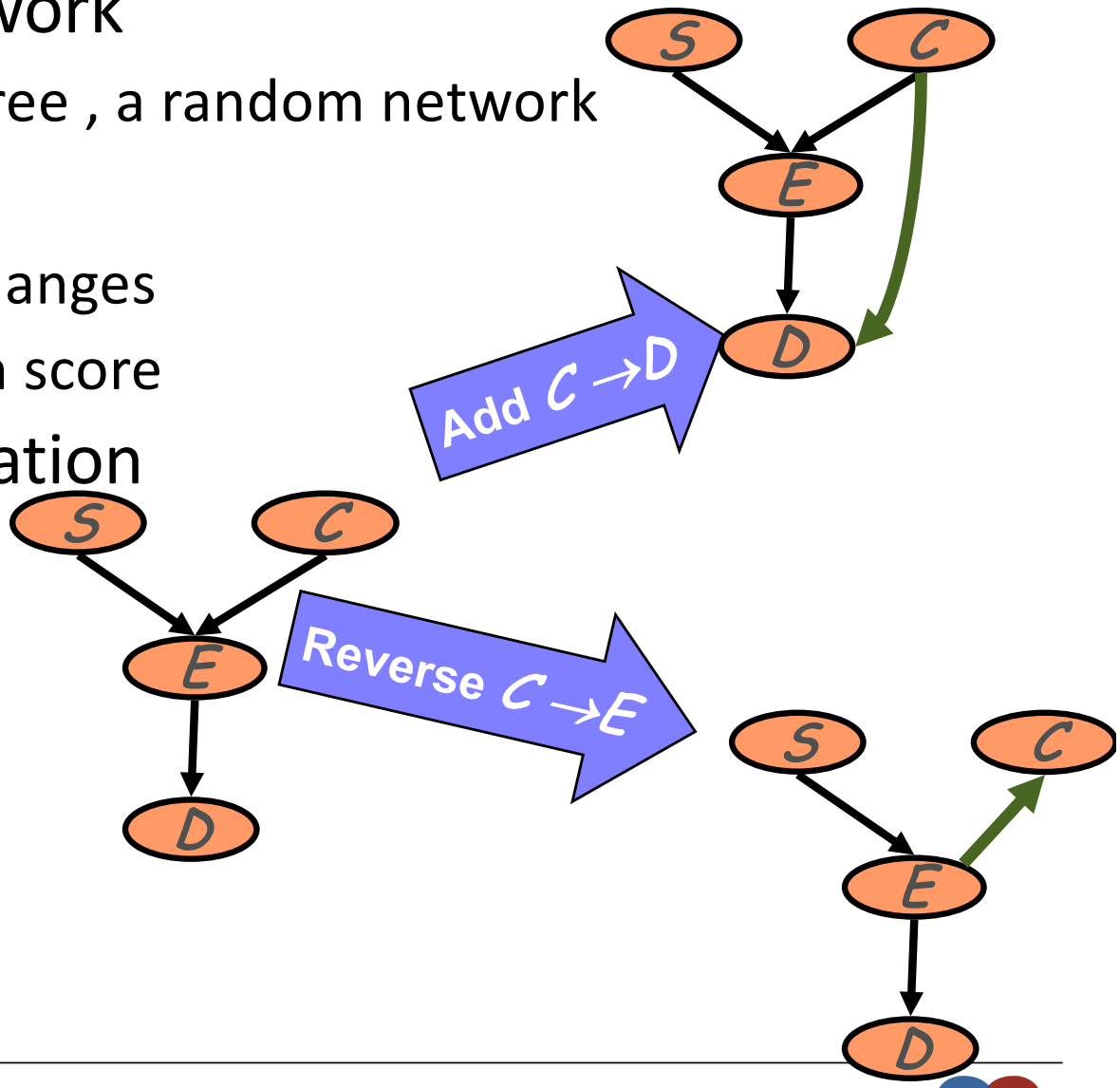

Typically: Local Search

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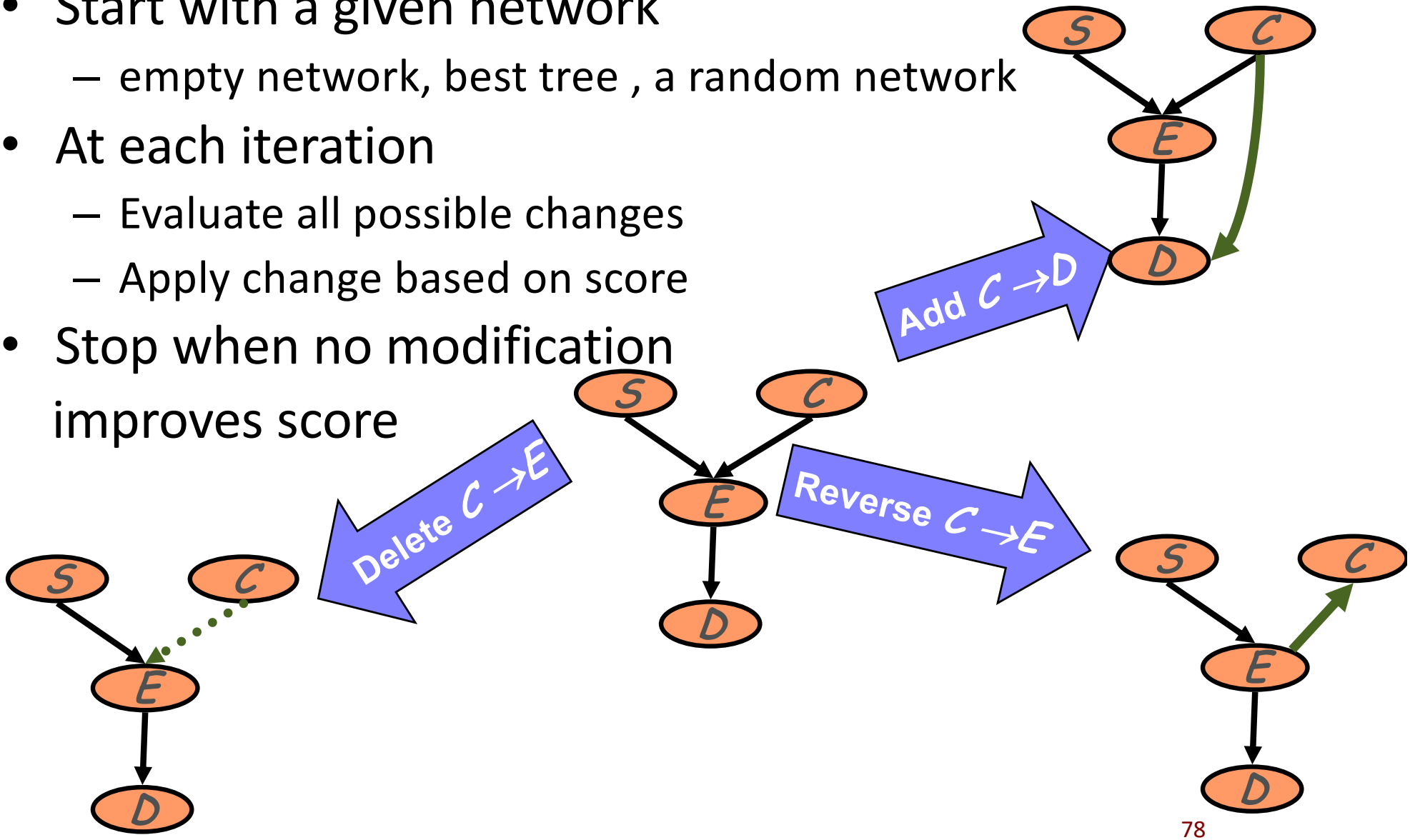
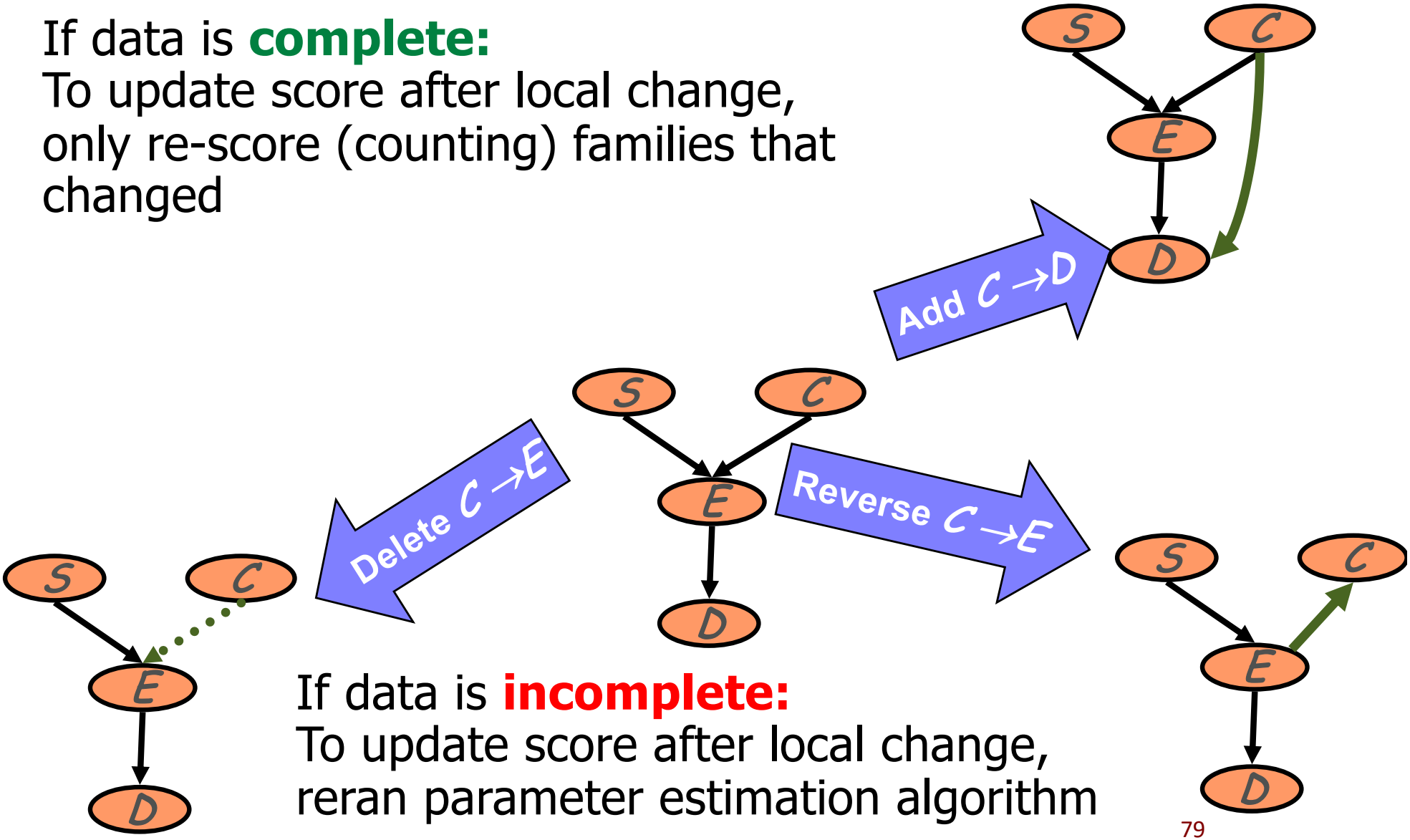


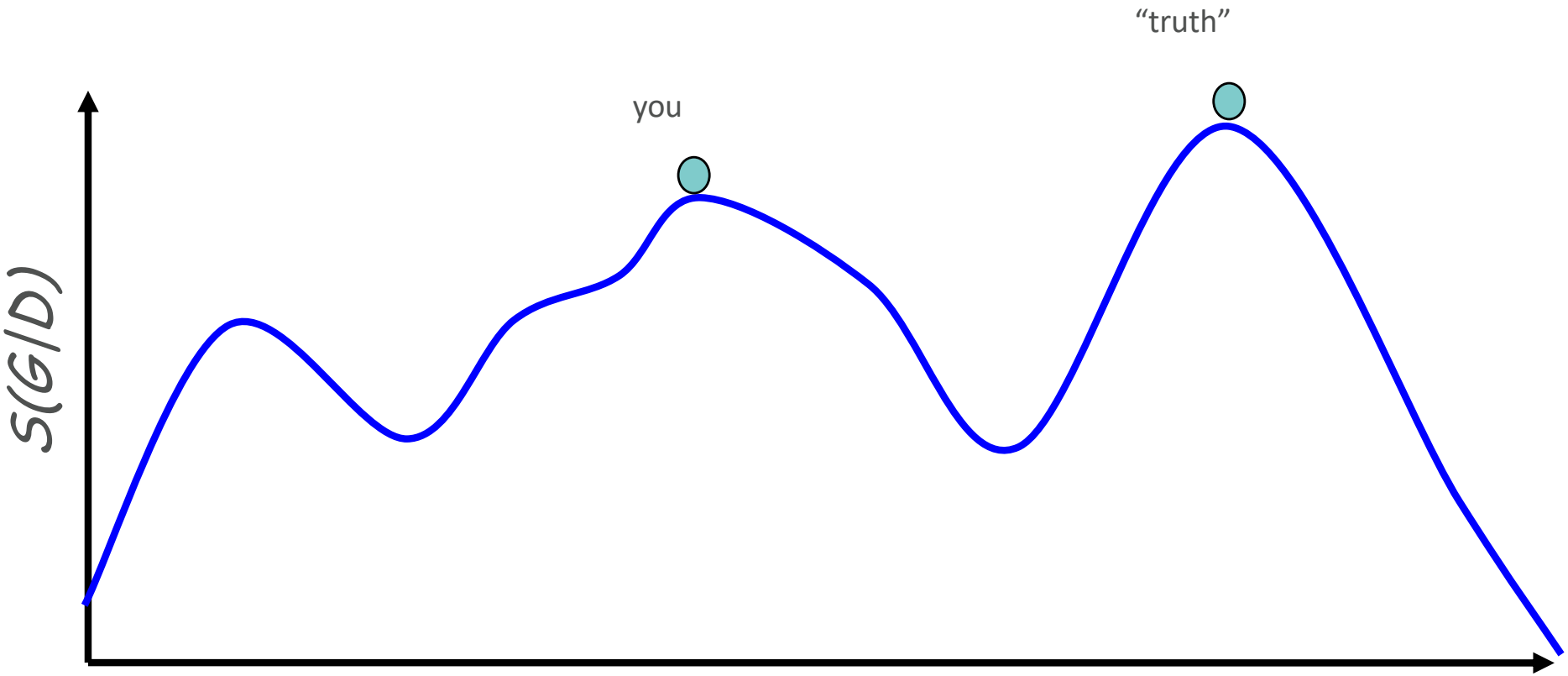
Typically: Local Search

If data is **complete:**
To update score after local change, only re-score (counting) families that changed



If data is **incomplete:**
To update score after local change, reran parameter estimation algorithm

Other Problem with local search



Easy to get stuck in local optima

Local Search in Practice

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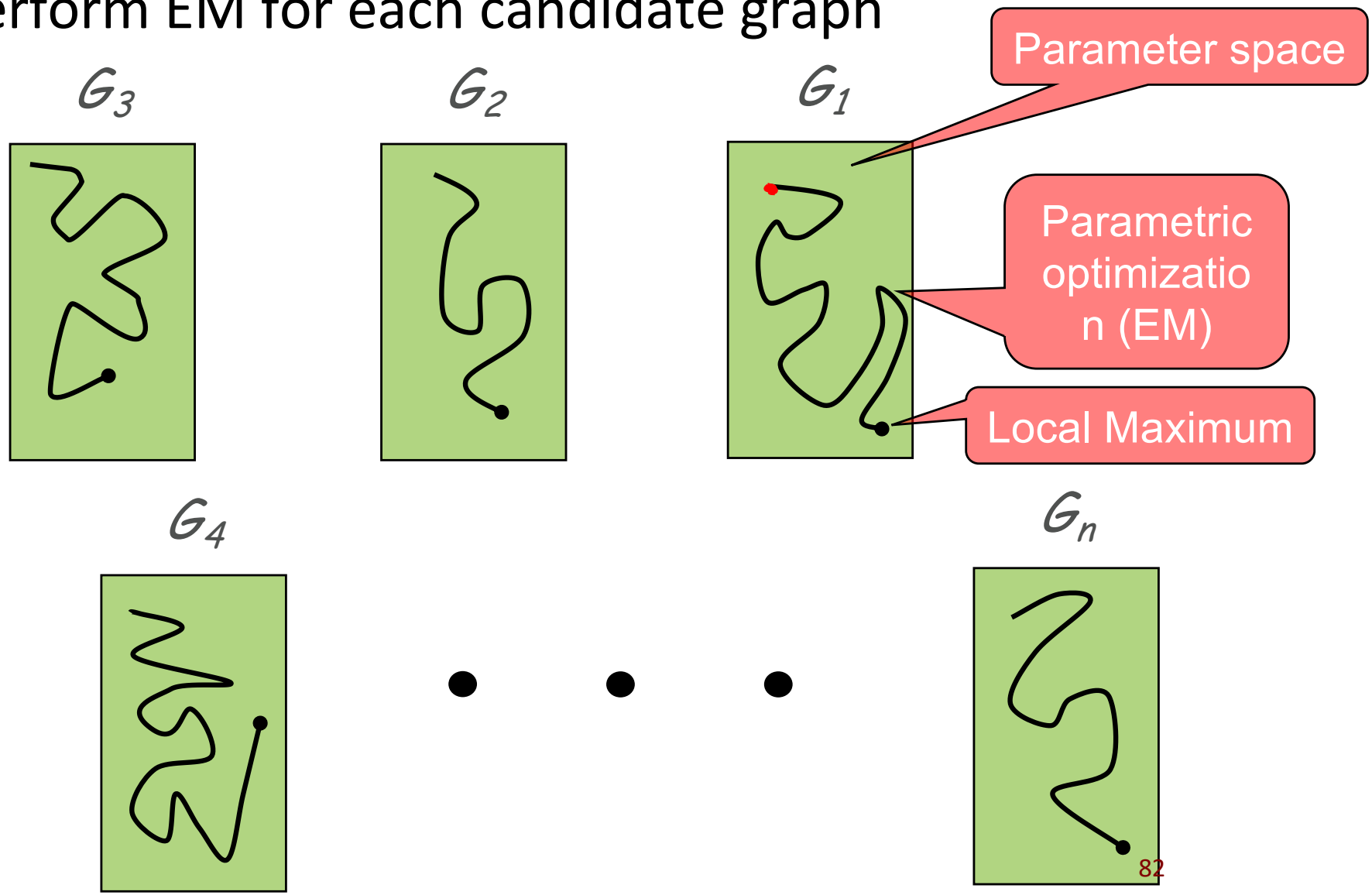
- Local search can get stuck in:
  - **Local Maxima:**
    - All one-edge changes reduce the score
  - **Plateaux:**
    - Some one-edge changes leave the score unchanged

- So, standard heuristics can escape both
  - Random restarts
  - TABU search
  - Simulated annealing

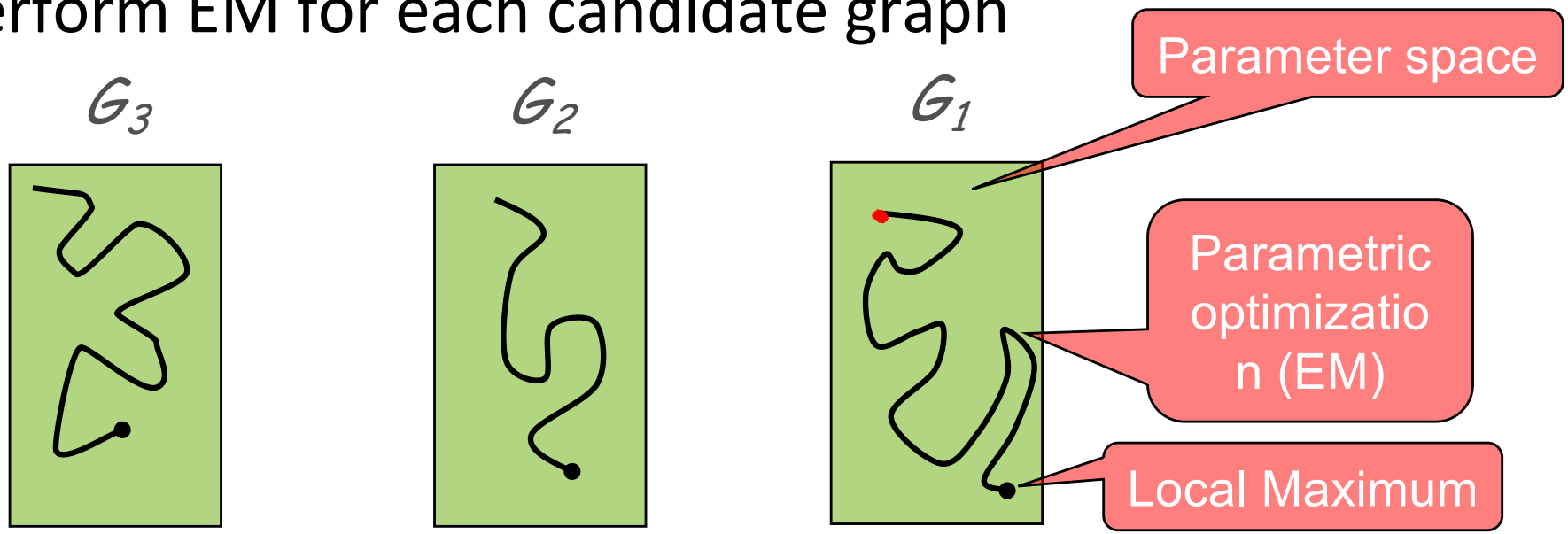
Local Search in Practice

- Perform EM for each candidate graph



Local Search in Practice

- Perform EM for each candidate graph



- Computationally expensive:
  - Parameter optimization via EM — non-trivial
  - Need to perform EM for all candidate structures
  - Spend time even on poor candidates

$\Rightarrow$ In practice, considers only a few candidates

Structural EM

[Friedman et al. 98]

Recall, in complete data we had

- Decomposition $\Rightarrow$ efficient search

Idea:

- Instead of optimizing the real score…
- Find **decomposable** alternative score
- Such that maximizing new score

$\Rightarrow$ improvement in real score

Structural EM

[Friedman et al. 98]

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Idea:

- Use current model to help evaluate new structures

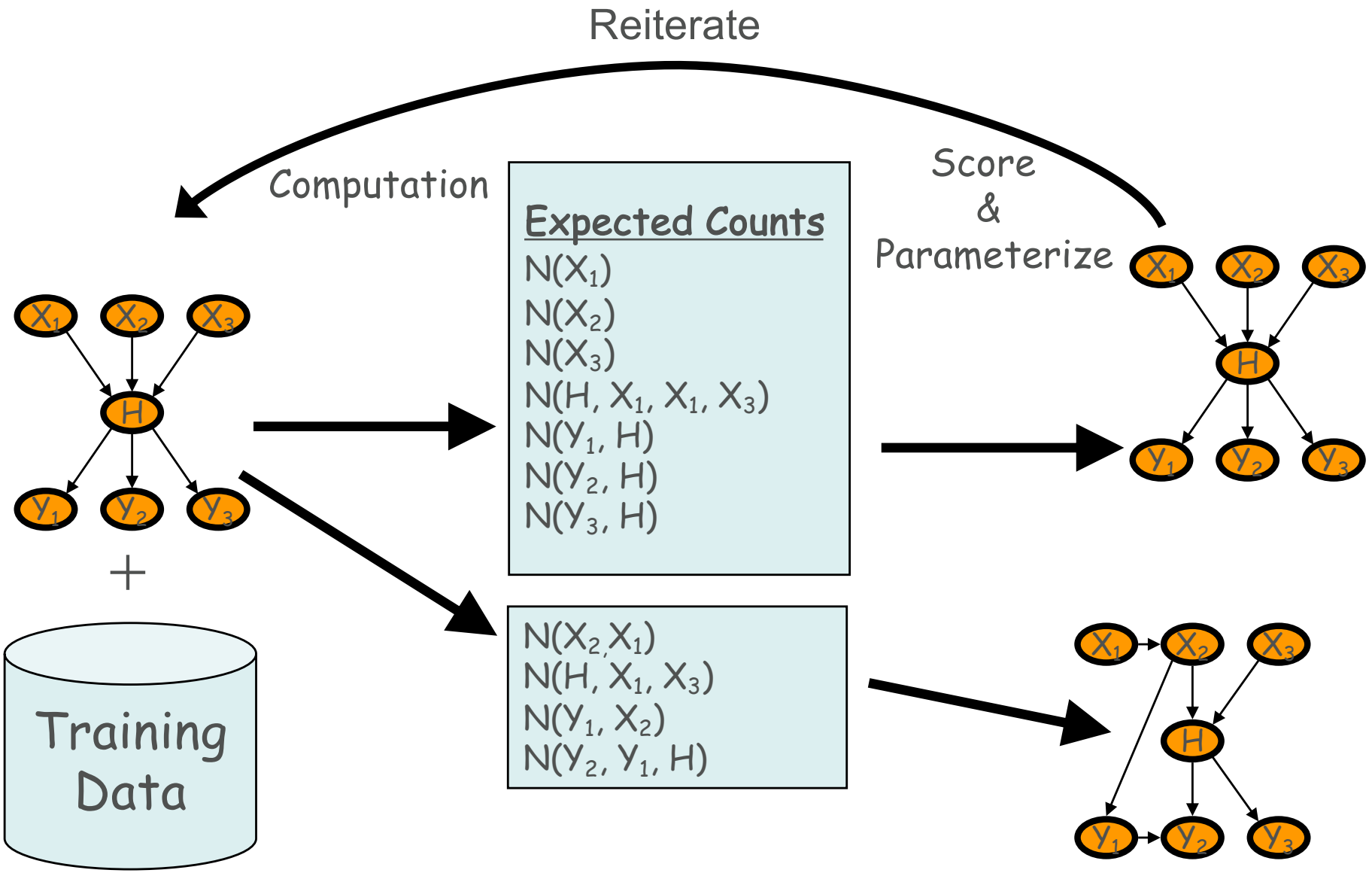
Outline:

- Perform search in (Structure, Parameters) space
- At each iteration, use current model for finding
  - Better scoring parameters: “parametric” EM step

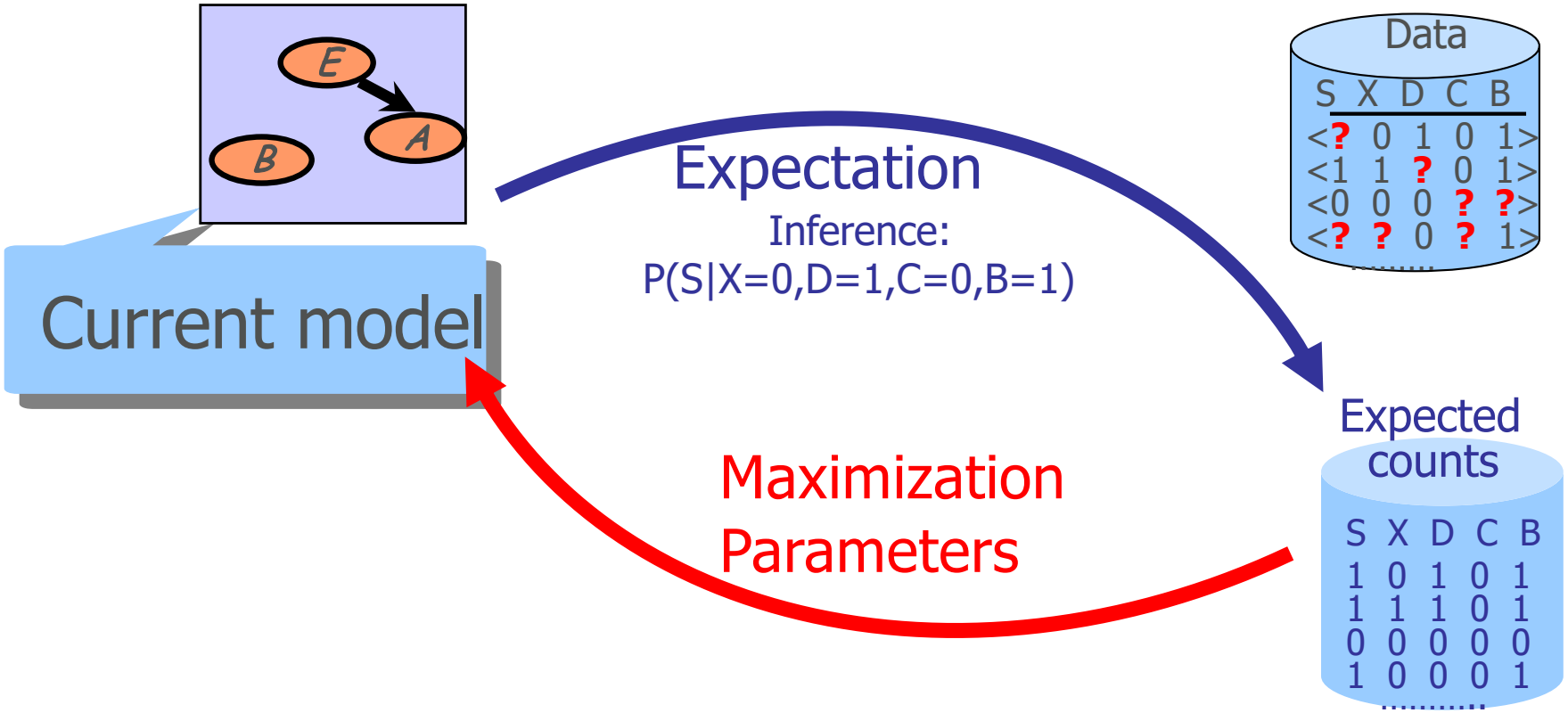
  or
  - Better scoring structure: “structural” EM step

Structural EM

[Friedman et al. 98]

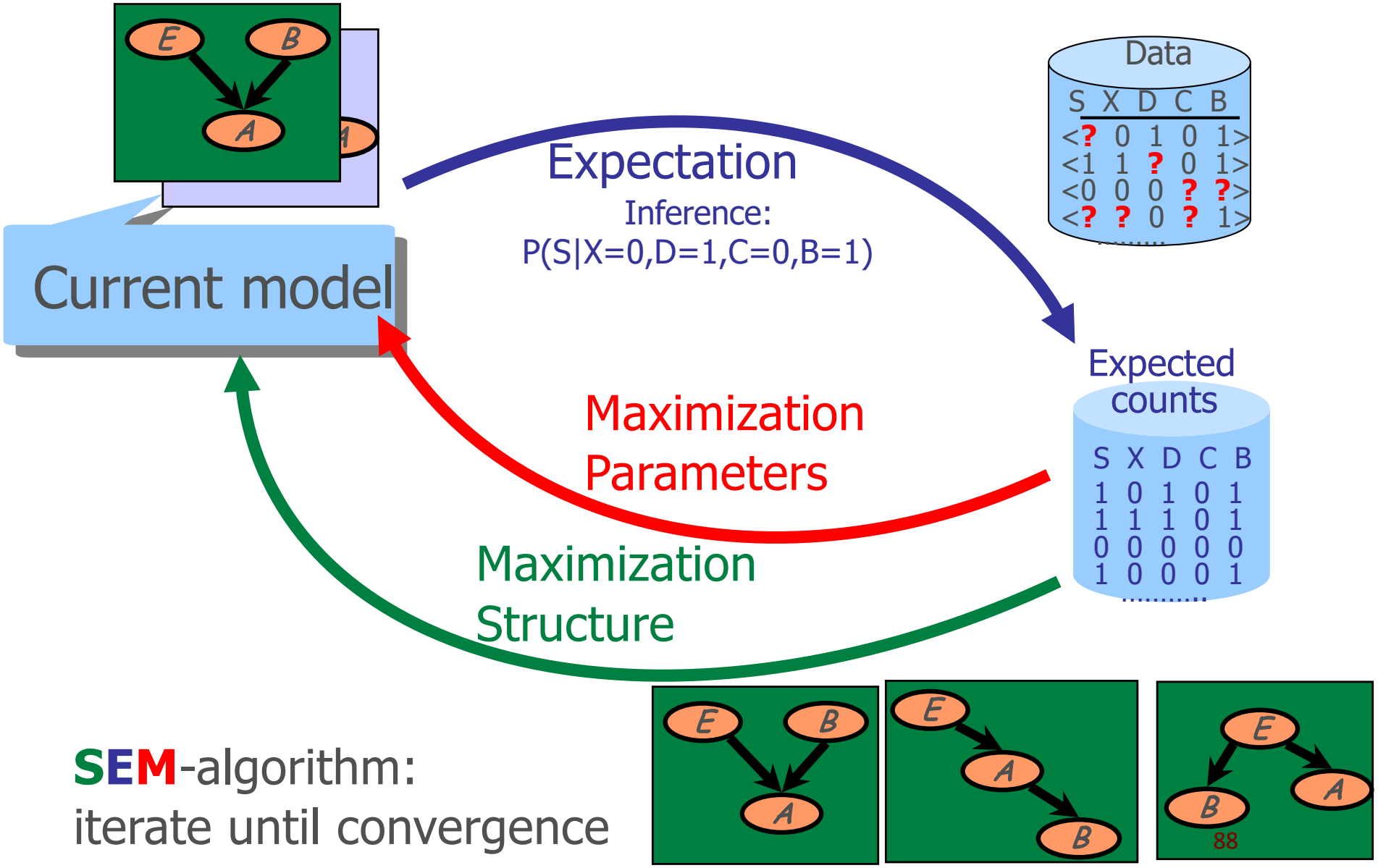


Structure Learning: incomplete data



EM-algorithm:
iterate until convergence

Structure Learning: incomplete data



SEM-algorithm:
iterate until convergence

Structure Learning: Summary

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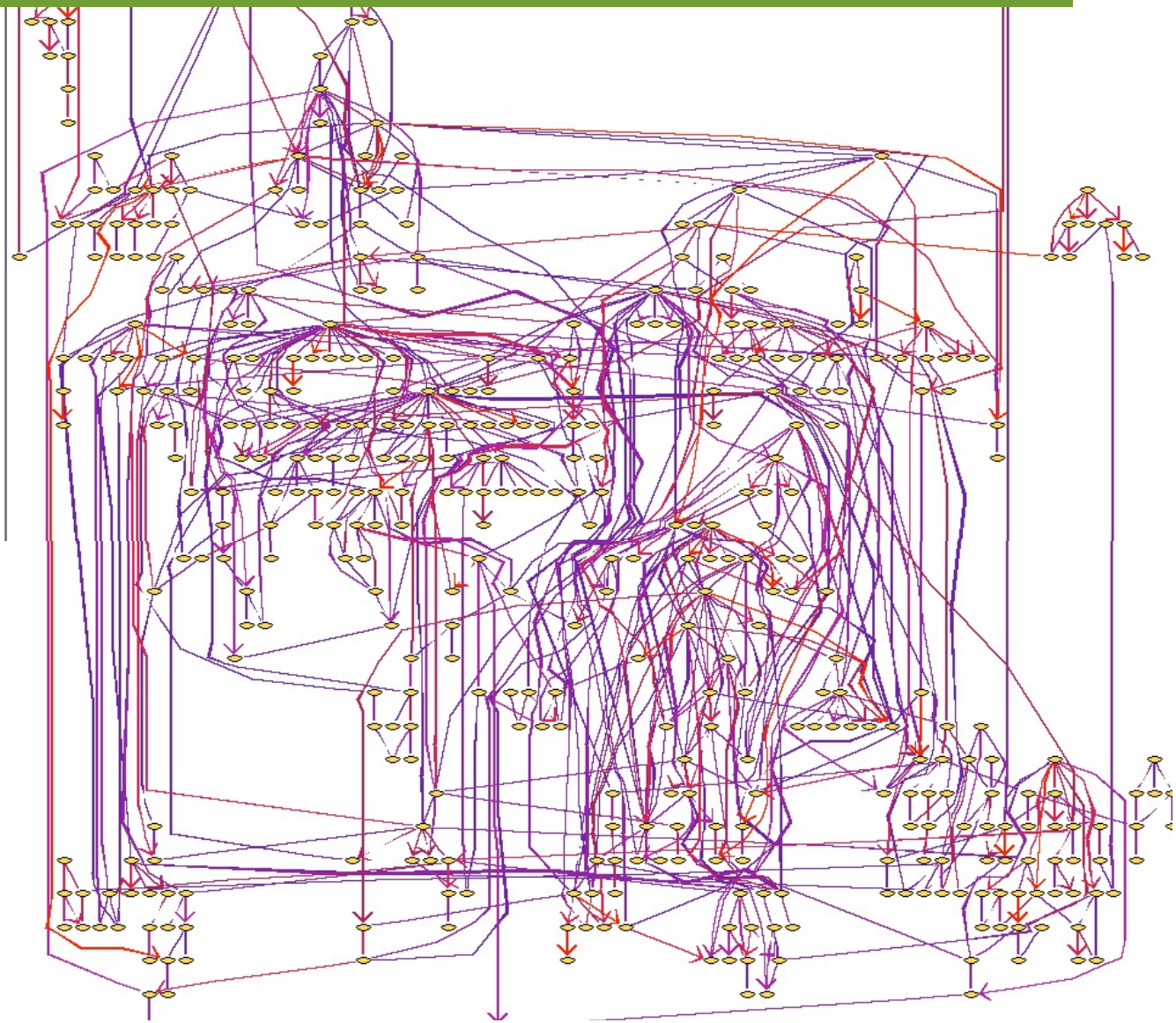
- Expert knowledge + learning from data
- Structure learning involves parameter estimation (e.g. EM)
- Optimization w/ score functions
  - likelihood + complexity penality = MDL
- Local traversing of space of possible structures:
  - add, reverse, delete (single) arcs
- Speed-up: Structural EM
  - Score candidates w.r.t. current best model

Structure learning success stories: gene regulation network (Friedman et al.)

Yeast data

[Hughes et al 2000]

- 600 genes
- 300 experiments



Structure learning success stories II: Phylogenetic Tree Reconstruction (Friedman et al.)

Input: Biological sequences

Human CGTTGC…

Chimp CCTAGG…

Orang CGAACG…

….

Output: a phylogeny

Uses structural EM,
with max-spanning-tree
in the inner loop