Readings: K&F 19.2, 19.3

EM Algorithm & Learning Problems in Real Applications



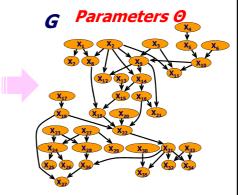
Lecture 13 – May 9, 2011 CSE 515, Statistical Methods, Spring 2011

Instructor: Su-In Lee

University of Washington, Seattle

MLE in Bayesian Networks

Recall that when learning from complete data,

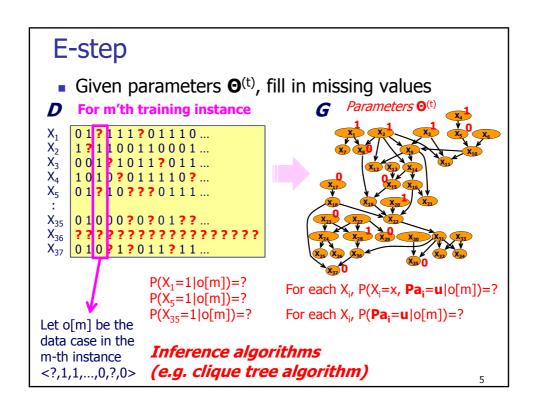


- We would first collect sufficient statistics for each CPD.
- We can estimate parameters that maximize the likelihood with respect to these statistics.
 - For table CPDs: $\theta_{X_i=x|\mathbf{Pa}_i=\mathbf{u}}^{MLE} = \frac{M[X_i = x, \mathbf{Pa}_i = \mathbf{u}]}{M[\mathbf{Pa}_i = \mathbf{u}]}$

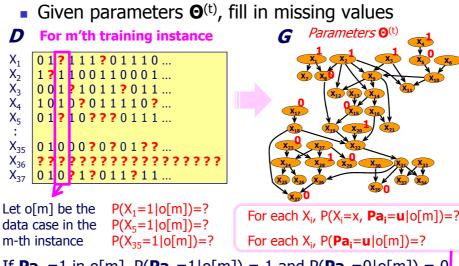
Expectation Maximization (EM) Parameter estimation when D has missing data 01?111?01110... X_1 X_2 1 ? 1 1 0 0 1 1 0 0 0 1 ... X_3^- 001?1011?011... 1010?011110?... 01?10???0111... 01000?0?01??... X_{36} ?????????????? X₃₇ 010?1?011?11... • Set initial set of parameters $\Theta^{(1)} = \Theta_0$ Iterate E-step and M-step until convergence In the t-th iteration,

E-step: Given Θ^(t), fill in missing values

M-step: Given complete data, learn parameters Θ^(t+1)



E-step – expected counts



If $Pa_i = 1$ in o[m], $P(Pa_i = 1|o[m]) = 1$ and $P(Pa_i = 0|o[m]) = 0$ If $Pa_i = ?$ in o[m], $0 \le P(Pa_i = 1|o[m]) \le 1$

"Soft" (expected) counts

E-step cont. & M-step

- Compute sufficient statistics:
- If D is complete data,

$$M[X_i = x, \mathbf{Pa}_i = \mathbf{u}] = \sum_{m} \mathbf{1}(X_i = x, \mathbf{Pa}_i = \mathbf{u} \mid o[m])$$

Given "soft" counts (expected sufficient statistics; ESS),

$$\overline{M}_{\theta^{(t)}}[X_i = x, \mathbf{Pa}_i = \mathbf{u}] = \sum_{m} P(X_i = x, \mathbf{Pa}_i = \mathbf{u} \mid o[m], \theta^{(t)})$$

$$\overline{M}_{\theta^{(t)}}[\mathbf{Pa}_i = \mathbf{u}] = \sum_{m} P(\mathbf{Pa}_i = \mathbf{u} \mid o[m], \theta^{(t)})$$

 M-step: Treat the ESS as those from complete data, and set the parameters to the MLE with respect to the ESS

$$\theta_{X_i=x|\mathbf{Pa}_i=\mathbf{u}}^{(t+1)} = \frac{\overline{M}_{\theta^{(t)}}[X_i = x, \mathbf{Pa}_i = \mathbf{u}]}{\overline{M}_{\theta^{(t)}}[\mathbf{Pa}_i = \mathbf{u}]}$$

Expectation Maximization (EM)

- Formal Guarantees:
 - $L(D:\Theta^{(t+1)}) \ge L(D:\Theta^{(t)})$
 - Each iteration improves the likelihood (read Andrew Ng's lecture note on EM)
 - If $\Theta^{(t+1)} = \Theta^{(t)}$, then $\Theta^{(t)}$ is a stationary point of L(D: Θ)
 - Usually, this means a local maximum
- Main cost:
 - Computations of expected counts in E-Step
 - Requires inference for each instance in training set
 - Exactly the same as in gradient ascent!

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EM – Practical Considerations

- Initial parameters
 - Highly sensitive to starting parameters Θ₀
 - Choose randomly
 - Choose by guessing from another source
- Stopping criteria
 - Small change in data likelihood
 - Small change in parameters
- Avoiding bad local maxima
 - Multiple restarts
 - Early pruning of unpromising starting points

Partially Observed Data: Parameter Estimation

- Log-likelihood function is not concave
- Methods for learning: EM and Gradient Ascent
 - Exploit inference for learning
- Challenges
 - Exploration of a complex likelihood/posterior
 - More missing data ⇒ many more local maxima
 - Cannot represent posterior ⇒ must resort to approximations
 - Inference
 - Main computational bottleneck for learning
 - Learning large networks ⇒ exact inference is infeasible ⇒ resort to approximate inference

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Structure Learning w. Missing Data

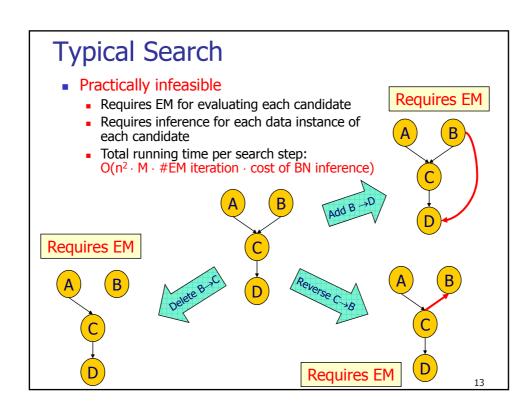
- Distinguish two learning problems
 - Learning structure for a given set of random variables
 - Introduce new hidden variables (K&F 19.5)
 - How do we recognize the need for a new variable?
 - Where do we introduce a newly added hidden variable within G?
 - Open ended and less understood...

Structure Learning w. Missing Data

- Theoretically, there is no problem
 - Define score, and search for structure that maximizes it

$$Score_{BIC}(G:D) = l(\hat{\theta}_G:D) - \frac{\log M}{2}Dim(G)$$

- Likelihood term will require gradient ascent or EM
- Practically infeasible
 - Typically we have O(n²) candidates at each search step



Structural EM

- Basic idea: use expected sufficient statistics to learn structure, not just parameters
 - Use current network to complete the data using EM
 - Treat the completed data as "real" to score candidate structures
 - Pick the candidate network with the best score
 - Use the previous completed counts to evaluate networks in the next step
 - After several steps, compute a new data completion from the current network

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Structural EM

- Set the initial parameters $\Theta^{(1)}=\Theta_0$, structure $G^{(1)}=G_0$
- Iterate:
 - Given parameters/structure $\Theta^{(t)}$ and $G^{(t)}$, fill in missing values with estimates \rightarrow D*
 - Given the complete data D*, learn structure G(t+1)
 - Given the complete data D^* and structure $G^{(t+1)}$, learn parameters $\Theta^{(t+1)}$

Structural EM Benefits

- Many fewer EM runs
- Score relative to completed data is decomposable!
 - Utilize same benefits as structure learning w. complete data
 - Each candidate network requires fewer re-computations
 - Here savings is large since each sufficient statistics computation requires inference
- As in EM, we optimize a simpler score
- Can show improvements and convergence

$$Score_{\mathit{BIC}}(\left\langle G,\theta_{\mathit{G}}\right\rangle : D) - Score_{\mathit{BIC}}(\left\langle G^{\mathcal{Q}},\theta_{\mathit{G}}^{\mathcal{Q}}\right\rangle : D) \qquad \begin{array}{c} \mathsf{D}^{+} \colon \mathsf{Data} \ \mathsf{imputed} \ \mathsf{a} \\ \mathsf{few} \ \mathsf{iterations} \ \mathsf{ago} \\ \\ \geq E_{\mathit{Q}} \Big[Score_{\mathit{BIC}}(\left\langle G,\theta_{\mathit{G}}\right\rangle : D^{+}) \Big] - E_{\mathit{Q}} \Big[Score_{\mathit{BIC}}(\left\langle G^{\mathcal{Q}},\theta_{\mathit{G}}^{\mathcal{Q}}\right\rangle : D^{+}) \Big] \\ \end{array}$$

An SEM step that improves in D+ space, improves real score

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LEARNING PROBLEMS IN REAL APPLICATIONS

 ${\sf CSE~515-Statistical~Methods-Spring~2011}$

Learning Problems in Real Applications

- Robotics, AI, Natural Language Processing, Computational Biology, Computer Vision...
- Robotic mapping
- Collaborative filtering
- Part-of-speech tagging
 - Presented by Nathan Imse
- Peptide identification in MSMS
 - Presented by John Halloran
- Finding tumor-specific mutations
 - Presented by Kris Weber
- Text classification
 - Collective classification of web pages
- Computer vision
 - Image segmentation and de-noising

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Problem Statement

- Robotic mapping: acquiring a spatial model of a robot's environment. (Sebastian Thrun, 2002)
 - Maps are commonly used for robot navigation (e.g. localization).
 - Robots must posses sensors (sonar, laser, radar, GPS, etc) to be able to perceive the outside world.
 - All sensors are subject to errors, often referred to as measurement noise.



Howard et al. Towards 3D mapping in large urban environments, Intelligent Robots and Systems, 2004.

- Object maps
 - A family mapping algorithms addresses the problem of building maps composed of basic geometric shapes or objects, such as lines, walls and so on.
 - Let's focus on one by Thrun et al. (2004) that explicitly tries to use the probabilistic model to capture the structure in the environment.

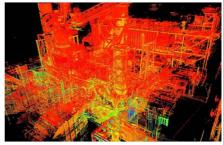
Training Data

Robotic Mapping

- Data: A point cloud representation of an indoor environment.
 - The point cloud can be obtained by collecting a sequence of point clouds, measured along a robot's motion trajectory.







Images from: 3D laser scanning and survey http://www.applycapnor.com/products--services/3d-laserscanning-and-survey/

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Goals

Robotic Mapping

- Goal: Take the points obtained over the trajectory and fit the points using polygons, to derive a 3D map of the surfaces in the robot's environment.
 - However, the noise in the laser measurements, combined with the errors in localization, leads adjacent polygons to have slightly different surface normals, giving rise to a very jagged representation of the environment.





Polygonal map generated from raw data. The display without texture shows the level of noise involved. In particular, it illustrates the difficulty of separating the door from the nearby wall. Thrun et al. (2004)

 Probabilistic model: Fit a more compact representation of the environment to the data, reducing the noise and providing a smoother, more realistic output.

Modeling

Robotic Mapping

- The model consists of a set of 3D planes $p_1, ..., p_K$, each characterized by two parameters (α_k, β_k)
 - α_k: a unit-length vector in R³ that encodes the plane's surface normal vectors
 - β_k: a scalar that denotes its distance to the origin of the global coordinate system.

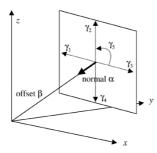


Illustration of the parameters in the planar surface model Thrun et al. (2004)

• The distance of any point **x** to the plane is

$$d(\mathbf{x}, p_k) = |\alpha_k \mathbf{x} - \beta_k|$$

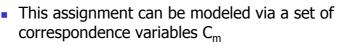
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Probabilistic Model

Robotic Mapping

• Each point x_m belongs to one of the planes $p_1,...,p_K$.







- C_m=k if the measurement point x_m was generated by the k-th plane p_k.
- C_m is not observed (hidden variable)

observed

- Define $P(\mathbf{X}_m | C_m = k : \theta_k) \propto N(d(\mathbf{x}, p_k) : 0, \sigma^2)$
 - Allow an additional value C_m=0 that encodes points that are not generated by any of the planes

Learning

Robotic Mapping

- Define $P(\mathbf{X}_m = \mathbf{x} \mid C_m = k : \theta_k) \propto N(d(\mathbf{x}, p_k) : 0, \sigma^2)$
 - Allow an additional value C_m=0 that encodes points that are not generated by any of the planes



• Goal: the assignment of points to planes (C_m for all m's), the parameters (α_k , β_k) that characterize the planes.



- EM algorithm
 - E-step: computes the assignment to the correspondence variables C_m's by assigning the weight of each point proportionately to its distance to each of them.
 - M-step: recomputes the parameters of each plane to fit the points assigned to it.

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Results I

 Notice that the map in (b) is smoother and appears to be visually more accurate than the one in (a)



Thrun et al. A Real-time EM Algorithm for Acquiring Multi-Planar Maps of Indoor Environments with Mobile Robots.
IEEE Transactions on Robotics and Automation, 2004.

(a) 3D map generated from raw sensor data

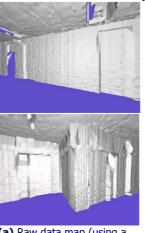


(b) 3D map generated using the EM algorithm 25

Results II

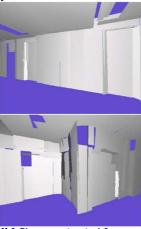
Robotic Mapping

- Maps generated in real-time, of office environments
- Notice that the map in (b) is smoother and appears to be visually more accurate than the one in (a)



Thrun et al. A Real-time EM Algorithm for Acquiring Multi-Planar Maps of Indoor Environments with Mobile Robots.
IEEE Transactions on Robotics and Automation, 2004.

(a) Raw data map (using a high-accuracy range finder)

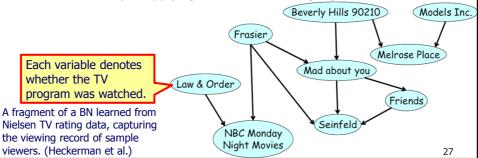


(b) Planes, extracted from the map using EM 26

Problem Statement

Collaborative Filtering

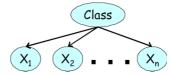
- In many marketing settings, we want to provide to a user a recommendation of an item that he might like, based on previous items that he has bought or liked...
- Collaborative filtering: Use the observed preferences of other users to try and determine the preferences for any other user.
 - Learn the dependency structure between different purchases, as observed in the population.
 - For example, applying a structure learning algorithm can result in:



Probabilistic Model

Collaborative Filtering

- A different application of BN learning to the collaborative filtering data task utilized a Bayesian clustering approach.
- Cluster variable C denotes subpopulations of customers.
 - C is not observed (hidden variable)



- Variable X_i indicates whether the user purchased item i.
 - Item i that the user did not purchase is assigned X_i=x_i⁰.
- The individual purchases X_i of each user are taken to be conditionally independent given the user's cluster assignment C.
- Training Data
 - Each user is a training instance
 - For each user, we have values on purchase variables X_i 's, not on C_i .

Results I

Collaborative Filtering

- Learning: EM algorithm
 - E-step: Fill in the missing values on C
 - M-step: Learn parameters in $P(X_1|C),...,P(X_n|C)$
- Experiment
 - Applied to a data set of people browsing the MSNBC website.
 - Each article is associated with a binary rv X_i which takes the value x¹ if the user followed the link to the article.
- Results
 - Four largest clusters found by Bayesian clustering applied to MSNBC news browsing data. For each cluster, the table below shows the three news articles whose probability of being browsed is highest.

Cluster 1 (36 percent)

E-mail delivery isn't exactly guaranteed Should you buy a DVD player? Price low, demand high for Nintendo Cluster 3 (19 percent)

Umps refusing to work is the right thing Cowboys are reborn in win over eagles Did Orioles spend money wisely? Cluster 2 (29 percent)

757 Crashes At Sea

Israel, Palestinians Agree To Direct Talks Fuhrman Pleads Innocent To Perjury Cluster 4 (12 percent)

Cluster 4 (12 percent)

The truth about what things cost Fuhrman Pleads Innocent To Perjury Real Astrology

Hidden Markov Models for Part of Speech Tagging

Nathan Imse njimse@uw.edu

What Is Part of Speech Tagging?

- Labeling words based on their function
 - Nouns: person, place, thing
 - Verb: action
 - Adjective: describes a noun
- Tagsets often have anywhere from 10-90 tags

Nouns	Verbs	Adjectives
Cat, dog, ball, car, zoo, human, book	Book, chase, is, cook, live, sleep, sing	Red, big, heavy, human, short, cold, smelly

Why Tag the Part of Speech?

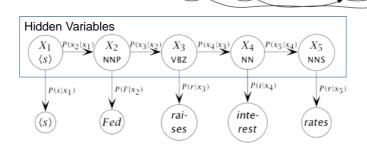
- Named Entity Recognition
 - Extract names of people, companies, and cities from text
- Word Sense Disambiguation
 - Differentiate between different meanings of the same word (e.g. bank, run, book)
- Parsing
 - Build a structure of the sentence with a much simpler grammar (<90 tags vs. 200,000+ words)

HMM Representation: Hidden Variables

• Hidden variables are Part of Speech (POS) tags

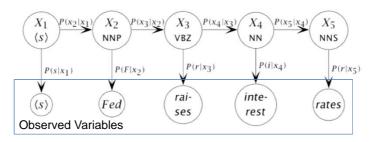
• Edges between POS tags are the probability of one following the other

adjective



HMM Representation: Observed Variables

- Observed variables are words, numbers, punctuation, etc...
- Observed variables are leaves in the network
 - No outgoing edges
- Edge from hidden variable to observed variable is the probability of that observation given that hidden variable



Training and Testing

- Training data consists of annotated text, either in parse trees or in flat text
 - Pierre/NNP Vinken/NNP ,/, 61/CD years/NNS old/JJ ,/, will/MD join/VB the/DT board/NN
- Testing data does not have tags
 - "Fed raises interest rates"
 - Tags are considered "hidden"

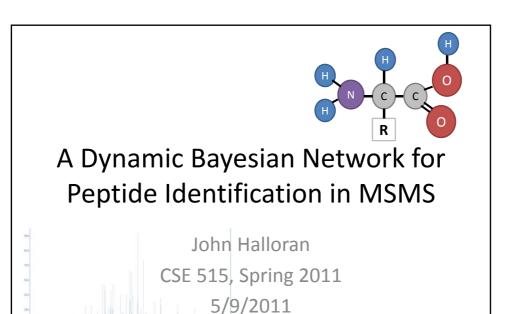
Decoding/Inference

- Viterbi Algorithm is common
 - Dynamic programming
 - Optimal global sequence, with probability
- Implemented for a course last fall
 - Trained on ~1900 sentences from the Wall Street
 Journal
 - 88% accuracy (with smoothing)

	Bigram	Trigram
States	47	2162
Observations	~7900	~7900
Transitions	~890	~99500
Emissions	~8700	~400800

Credit

The diagram of the HMM network as a Bayesian Network on slides 4 & 5 are the work of Andrew McCallum from Umass, Amherst



Problem Statement

- Tandem mass spectrometry
 - Spectrum of measured m/z intensities generated from sample proteins (peptides)
- Given MSMS spectrum, identify peptide which generated spectra
- Typically look up peptides in database of the mapped organism

Model

- Normalize spectra, quantize into B bins
- Model fragmentation event:

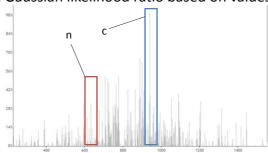
→ IEQFM⁺

Fragment Ions

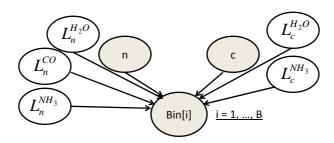
- Candidate Peptide: IEQFMEEMYQDK **

→ EEMYQDK⁺

 Check n=mass(IEQFM⁺), c=mass(EEMYQDK⁺) bins values, calculate Gaussian likelihood ratio based on values



Model



- •n, c, Bin[i] values are observed
- •Loss of CO, NH₃, H₂O(?) Losses are hidden variables (Bernoulli)
- •Peptide length N, N-1 such events: concatenate to form DBN

Training

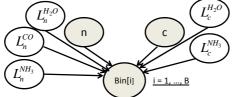
- Learned parameters:
 - Gaussian variances, neutral loss probabilities
- Training Data:
 - 1208 high quality E-coli matches
 - Matches generated combining 7 peptideidentification algorithms
- Parameters trained using EM

Inference

 Candidate peptide C and B bins assigned score of log(P(bins,C)), where:

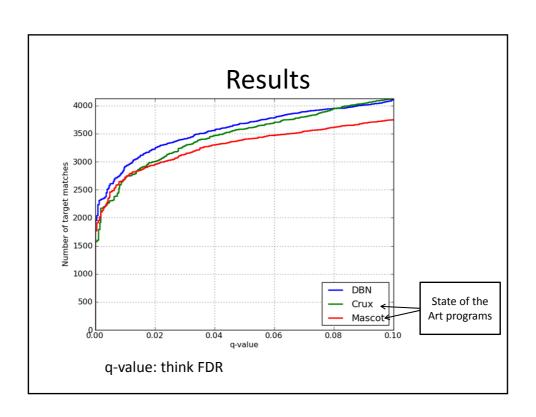
$$P(bins, C) = \prod_{i}^{n-1} \sum_{losses} p(loss) \prod_{j}^{B} p_{I}(b_{j}) \frac{p_{A}(b_{n})}{p_{I}(b_{n})} \frac{p_{A}(b_{c})}{p_{I}(b_{c})}$$

$$Likelihood ratios$$



Results

- Testing performed using decoy database:
 - Permute target database values
 - Good algorithm should score targets high, decoys low
 - Performance metric: false discovery rates (FDR)



Cancer Genomics Problem: Finding tumor-specific mutations

Problem Statement:

Given:

- a human cancer patient
- sample from tumor tissue
- sample from normal tissue
- DNA sequence of both samples

Identify the mutations present in the tumor tissue that are not present in the normal tissue

Background: DNA, Genotypes, Mutations

TAACGCGGTCCCG...

 At the simplest level, we can think of DNA as a sequence of letters from the alphabet, {A,C,G,T}



Genotype AA

Genotype CT

- Humans have 2 copies of each chromosome.
- 10 possible "genotypes" at each position



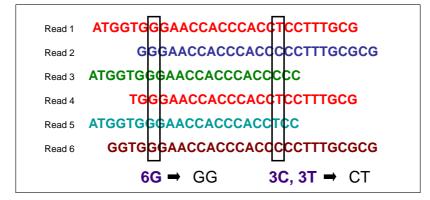
Genotype AT

Genotype CT

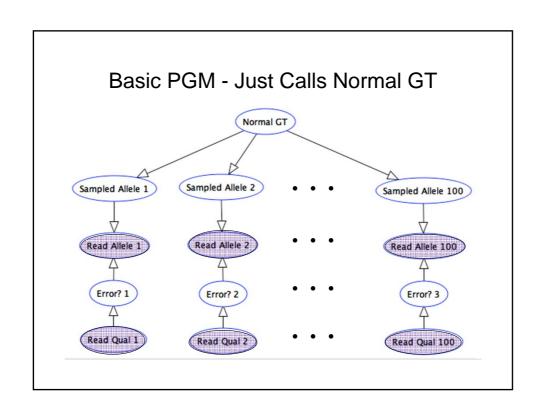
 We are trying to find single base mutations in the tumor DNA

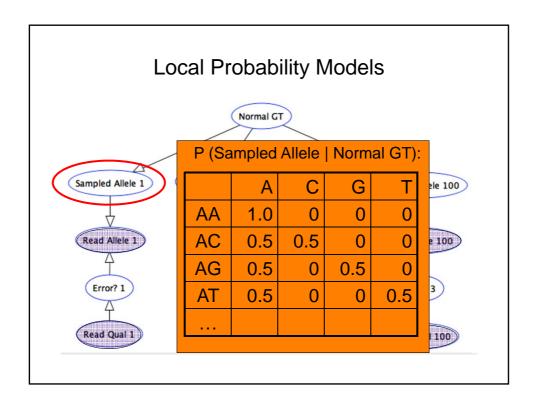
Problem: Call Genotypes from Data

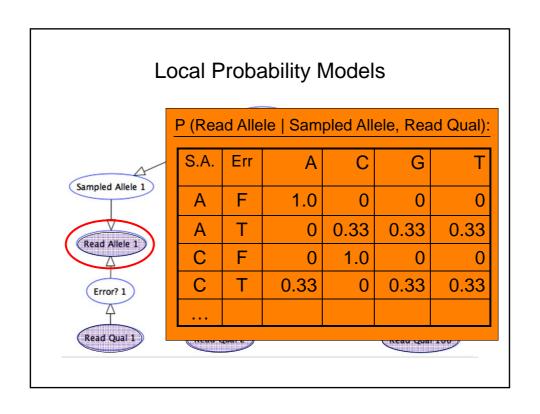
- Our data: lots of overlapping short reads.
- At each position, we count the number of reads for each base...

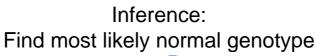


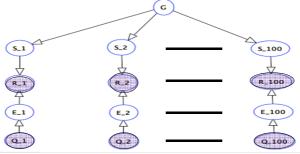
• But the data is noisy: 1C, 9G → CG? or GG?











$$P(G, r_1, \dots, r_{100}, q_1, \dots, q_{100}) = P(G) \prod_{i=1}^{100} \sum_{S_i, E_i} P(q_i) P(E_i | q_i) P(S_i | G) P(r_i | S_i, E_i)$$

Return $\max_{g} P(G, r_1, \dots, r_{100}, q_1, \dots, q_{100})$

