LECTURE 8: PROBABILISTIC GRAPHICAL AND HIERARCHICAL BAYESIAN MODELS

- Probabilistic graphical models (Bayesian and Markov networks)
- Hierarchical Bayesian models
- Motivation: we want to write down the probability of the data d given some parameters θ we wish to determine. But the relation between the two is difficult to write in a closed form. For example, the parameters determine some probability distribution function (PDF) of perfect data *x*, but what we measure is d, a noisy version of *x*, and noise is varying between measurements.
- The main goal of this lecture is to derive automatic rules that will give correct answer in complicated inference situations: a way to formalize statistical inference

LECTURE 8: ADVANCED BAYESIAN CONCEPTS

- We can introduce s as latent variables and model them together with θ. Then θ can be viewed as hyperparameters for s. The advantage is that at each stage PDF is easier to write down. However, we now have a lot of parameters to determine, most of which we do not care about.
- Modern trend in statistics is to use the hierarchical modeling approach, enabled by advances in MC, specially HMC.
- We can also try to marginalize over *x* analytically: convolve true PDF with noise PDF and do this for each measurement. This works, but requires doing the convolution integrals. The advantage is fewer variables, just *θ*.

Graphical Models for Probabilistic and Causal Reasoning

- We would like to describe the causal flow of events such that we can generate (simulate) events in a probabilistic setting (a flowchart of generating data)
- We can describe this with directed acyclic graphs (DAG)
- Typically we divide the process into components each of which generates a single variable x (given all other variables), which we can generate using random number generator for p(x)
- We can also use the same process to describe inference of latent (unobserved) variables from data
- This also goes under the name of Bayesian networks or Belief networks
- probabilistic graphical models (PGM): a more general class of networks that includes Bayesian networks and Markov networks

Approach of Bayesian Networks/PGMs

- We infer the causal (in)dependence of variables
- Write factorized joint probability distributions
- Perform data analysis by posterior inference
- Once we have BN we can do the posterior analysis using MCMC or variational methods (next lecture)
- One way to think about BN: can we realistically simulate the data? If yes then we have a well defined BN, because we specify a simulation with a bunch of randomly drawn variables followed by deterministic rules that lead to data

PGM Rules

- Each circle is a probability distribution for the variable inside it
- Each arrow is a conditional dependence



p(a, b, c) = p(c|b)p(b|a)p(a)



PGM Rules

- Each solid point is a fixed variable (pdf is a delta function)
- Each plate contains conditionally independent variables: repetition, compressed notation for many nodes



Breaking causality down into components



Independent causes of Catching cold

Health \perp Sick colleague \perp Temperature \perp Rain

Credit: Slides from B. Leistedt

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Breaking causality down into components



p(C, S, H, T, R) = p(C | S, H, T, R) p(S, H, T, R)p(S, H, T, R) = p(S) p(H) p(T) p(R)

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p(C, S, H, T, R, J, W) = p(C | S, H, T, R, J, W) $x p(S, H, T, R | J, W) \times p(J, W)$ p(C | S, H, T, R, J, W) = p(C | S, H, T, R) p(S, H, T, R | J, W) = p(S|J, W) p(H|J) p(T|W) p(R|W) p(J, W) = p(J)p(W)Each circle has its own p Each circle has its own p Each arrow has its own letter after |

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Example

• Write down corresponding probability expressions for this graph



p(A, B, C, D, E, F) = x p(F|E) p(D|B, E, C) x p(E) p(C|A, B) p(A) p(B)

PGM Rules: Observables and Inference

- Each shaded (or double) circle implies an observable (*c*), everything else (*a*,*b*) is not an observable, but a latent (hidden) variable
- If we want to determine latent variables (*a*,*b*) from observables we do posterior inference (inverse problem requires Bayes rule)





$$p(a, b, c) = p(c|a, b)p(b|a)p(a)=p(a, b|c)p(c)$$

$$\underbrace{p(a,b|c)}_{\text{posterior}} \propto \underbrace{p(c|a,b)}_{\text{likelihood}} \underbrace{p(b|a)p(a)}_{\text{prior}}$$

Posterior Inference

- Here D, F are data
- C, E parameters
- A, B fixed parameters



P(Parameters|Data, Model) = p(C, E | D, F, A, B)= p(F|E) p(D|C, E) p(C |A, B) p(E) p(A) p(B)

We need all these conditional PDFs (probability distribution functions): *p*(F|E), *p*(D|C,E), *p*(C|A,B), *p*(E), note that *p*(A) and *p*(B) are delta functions (fixed parameters)

- An upper case non-bold letter indicates a single random variable ('RV'). The same letter lower cased with a super script indicates a specific value that RV may take. For example, X = x¹ is the *event* the RV X took on the value x¹. We call this event an **assignment**. The set of unique values an RV may take is Val(X). So we might have Val(X) = {x⁰, x¹} in this case.
- A bold upper case letter indicates a *set* of RVs (like X) and a bold lower case letter indicates a set of values they may take. For example, we may have X = {A, B} and x = {a³, b¹}. Then the event X = x is the event that A = a³ happens and B = b¹ happens. Naturally, Val(X) is the set of all possible unique joint assignments to the RVs in X.
- If you see x (or y or z etc...) within a probability expression, like P(x|····) or P(···· |x), that's *always* an abbreviation of the event 'X = x'.
- Perhaps confusingly, we also abbreviate the event 'X = x' as 'X', though this isn't a clean abbreviation. Omission of x means one of two things: either we mean this for *any* given x or for *all* possible x's. As an example for the latter case, 'calculate P(X)' would mean calculate the set of probabilities P(X = x) for all x ∈ Val(X).
- $\sum_{\mathbf{X}} f(\mathbf{X})$ is shorthand for $\sum_{\mathbf{x} \in Val(\mathbf{X})} f(\mathbf{X} = \mathbf{x})$. This is similarly true for $\prod_{\mathbf{X}} (\cdot)$ and $\operatorname{argmin}_{\mathbf{X}} (\cdot)$. Look out for this one it can sneak in there and change things considerably.

Duane Rich blog https://www.quora.com/What-are-probabilistic-graphical-models-and-why-are-they-useful

Bayesian network: conditional independence

Conditional independence



$$P_B(X_1, \dots, X_n) = \prod_{i=1}^n P_B(X_i | \operatorname{Pa}_{X_i}^G)$$
 Chain rule

Example from Koller & Friedman

Given subsets of RVs X,Y and Z from $\mathcal X,$ we say X is conditionally independent of Y given Z if

$$P(\mathbf{x}, \mathbf{y}|\mathbf{z}) = P(\mathbf{x}|\mathbf{z})P(\mathbf{y}|\mathbf{z})$$

for all $x \in Val(X)$, $y \in Val(Y)$ and $z \in Val(Z)$. This is stated as 'P satisfies $(X \perp Y|Z)_{[3]}$ '

$$P_B(I, D, G, S, L) = P_B(I)P_B(D)P_B(G|I, D)P_B(S|I)P_B(L|G)$$

So we would calculate a given assignment as:

$$P_B(i^1, d^0, g^2, s^1, l^0) = P_B(i^1)P_B(d^0)P_B(g^2|i^1, d^0)P_B(s^1|i^1)P_B(l^0|g^2)$$

=0.3 \cdot 0.6 \cdot 0.08 \cdot 0.8 \cdot 0.4
=0.004608

The BN graph, just those nodes and edges, implies a set of CI statements regarding it's accompanying P_B .

 $(L \perp I, D, S|G)$ $(S \perp D, G, L|I)$ $(G \perp S|I, D)$ $(I \perp D)$ $(D \perp I, S)$

14

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Markov Network

- Not every probabilistic model can be represented by Bayesian N. •
- Markov networks: edges are undirected •
- We divide the graph into complete subgraphs •
- simple CI •



 $P(A, B, C, D) = \frac{1}{7}\phi_1(A, B)\phi_2(B, C)\phi_3(C, D)\phi_3(D, A)$

Gibbs rule



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Markov Network

- Φ₁ are Boltzmann factors exp(-H_i), describing interaction energy H_i between neighboring spins, P_M is Boltzmann factor for total energy, Z is partition function, i.e. the sum of the Boltzmann factors over all configurations
- In statistical physics, once we have Z we can derive macroscopic quantities we are interested in (like mean energy, mean magnetization etc.)
- As we discussed in previous lecture, rather than evaluating Z brute force (which is often impossible), we sample over regions of high posterior probability using MCMC
- There are other PGMs: e.g. chain graphical models contain both directed and undirected links

Markov Network example: Boltzmann machine

- Binary variables xi=(-1,1)
- $H=\sum_{i < j} W_{ij} X_i X_j + \sum_i b_i X_i$
- P=exp(-H)
- $Z=\Sigma$ all states exp(-H)
- Weights wij, bias bi
- Example: Ising model of spins on a lattice
- Φ_{ij}=-(x_i-x_j)²/2kT if i neighbor of j: spins prefer to be aligned
- Below critical temperature (Curie T_c) all spins aligned: emergent behavior where a phase transition emerges out of a weak local constraint





Example: image cleaning

• Taken from Barber: Bayesian reasoning and machine learning

Example 114 (Bayesian image denoising). Consider a binary image, where x describes the state of the clean pixels (± 1 encoding). We assume a noisy pixel generating process that takes each clean pixel x_i and flips its binary state:

$$p(y|x) = \prod_{i} p(y_i|x_i), \quad p(y_i|x_i) \propto e^{\gamma y_i x_i}$$

(28.4.3)

The probability that y_i and x_i are in the same state is $e^{\gamma}/(e^{\gamma} + e^{-\gamma})$. Our interest is to the posterior distribution on clean pixels p(x|y). In order to do this we need to make an assumption as to what clean images look like. We do this using a MRF

$$p(x) \propto e^{\sum_{i \sim j} w_{ij} x_i x_j}$$
(28.4.4)

for some settings of $w_{ij} > 0$, with $i \sim j$ indicating that *i* and *j* are neighbours. This encodes the assumption that clean images tend to have neighbouring pixels in the same state. An isolated pixel in a different state to its neighbours is unlikely under this prior. We now have the joint distribution

$$p(x, y) = p(x) \prod_{i} p(y_i|x_i)$$
 (28.4.5)

see fig(28.3), from which the posterior is given by

$$p(x|y) = \frac{p(y|x)p(x)}{\sum_{x} p(y|x)p(x)} \propto e^{\sum_{i \sim j} w_{ij}x_ix_j + \sum_{i} \gamma y_ix_i}$$
(28.4.6)

Quantities such as the MAP state (most a posteriori probable image), marginals $p(x_i|y)$ and the normalisation constant are of interest.



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Hierarchical Bayesian Models

- PGMs encode a hierarchical causal structure: D depends on C which depends on A
- In many problems we have hierarchical structure of parameters
- For example, we measure some data *d*, which are noisy and related to some underlying true values *x*, but what we want is the parameters that determine their distribution *θ*.
- *d*: observable
- Variables that are not observed are called latent variables: θ , x
- Variables we do not care about are called *nuisance variables*: *x*.
 We want marginalize over them to determine *θ*

Exchangeability

- When we do not know anything about latent variables x_i we can place them on equal footing: $p(x_1, x_2, ..., x_J)$ is invariant under permutation of (1, 2, ..., J) indexes.
- Their joint probability distribution cannot change upon exchanging *x_i* with *x_j*...
- A simple way to enforce this is to say $p(x_1, x_2, ..., x_J) = \prod_{j=1}^{J} p(x_i | \theta)$
- This does not always work (e.g. a die has 6 exchangeable x_i, but their values must add to 1), but works in large J limit (de Finetti theorem).

Example



- y_i's : measurements of the temperature in a room
- σ_i: Gaussian noise
- x_i's : true temperature
- α: parameter parametrizing the true distribution of temperatures.
- S : some selection effect (e.g., no measurement if temperature is < 0 degrees)

Marginalization over Latent Variables



We are interested in inferring α We need to **marginalize over** the latent x_i's, numerically or analytically

$$p(\alpha|\{y_i, \sigma_i\})$$

$$\propto \prod_i p(y_i|\alpha, \sigma_i)p(\alpha)$$

$$= \prod_i \int p(y_i, x_i|\alpha, \sigma_i)p(\alpha)dx_i$$

$$= \prod_i \int p(y_i|x_i, \alpha, \sigma_i)p(x_i|\alpha, \sigma_i)p(\alpha)dx_i$$

$$= \prod_i \int p(y_i|x_i, \sigma_i)p(x_i|\alpha)p(\alpha)dx_i$$

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Additional Complication: Noise in x

- We now observe noisy versions of the x_i's, with known Gaussian noises γ_i's
- The x_i's are now latent parameters.
 - They need to be estimated or marginalized over.



Sometimes marginalization can be done analytically

$$p(m,s|\{\hat{y}_i, \hat{x}_i, \sigma_i, \gamma_i\})$$

$$= \int d\{x_i\}p(m,s, \{x_i\}|\{\hat{y}_i, \hat{x}_i, \sigma_i, \gamma_i\})$$

$$\propto \prod_{i=1}^N \int dx_i \mathcal{N}\left(\hat{y}_i - mx_i - b; \sigma_i^2\right) \mathcal{N}\left(\hat{x}_i - x_i; \gamma_i^2\right) \quad p(\{x_i\}, m, s)$$

$$\propto \prod_{i=1}^N \mathcal{N}\left(\hat{y}_i - m\hat{x}_i - b; \sigma_i^2 + \gamma_i^2\right) \quad p(s, m)$$

25

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Example: gaussian process with unknown variance and noise

 We have data x, gaussian process that generates s=N(0,S), and gaussian noise with variance N that generates data x. We can write the problem in terms of unknown s and S (ignoring constant terms like 2π and N):

$$\mathcal{L}_p = -\ln p(\boldsymbol{s}, S | \boldsymbol{x}) = \frac{1}{2} \left\{ S^{-1} \boldsymbol{s}^T \boldsymbol{s} + [\boldsymbol{x} - \boldsymbol{s}]^T \boldsymbol{N}^{-1} [\boldsymbol{x} - \boldsymbol{s}] + \ln \det S \right\}$$

• We can also analytically_marginalize over s: doing a gaussian integral over *p*,

$$p(S|\boldsymbol{x}) = \int d\boldsymbol{s} p(\boldsymbol{s}, S|\boldsymbol{x})$$

we find

$$-\ln p(S|\boldsymbol{x}) = \frac{1}{2} \left[\ln \det(\boldsymbol{S} + \boldsymbol{N}) + \boldsymbol{x}^T (\boldsymbol{S} + \boldsymbol{N})^{-1} \boldsymbol{x} \right]$$

• No s dependence left, just data x and hyperparameter S

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We should also put hyperpriors onto parameters

- We have hyperprior Σ: each parameter should have a prior, which can be noninformative
- A proper PGM should start with hyperpriors and end with observables



Another Extension: Mixture Models

- Mixture models try to fit the data with a mixture of components
- For example, we can fit multiple lines to the data assuming the data are drawn from one of the components





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Mixture Model for Outliers

- Suppose we have data that can be fit to a linear regression, apart from a few outlier points
- It is always better to understand the underlying generative model of outliers
- But suppose we just want to identify them



Let us model this as a Gaussian

$$p(x_i, y_i, e_i \mid \theta) \propto \exp\left[-\frac{1}{2e_i^2}(y_i - y(x_i \mid \theta))^2\right]$$

• We get a poor fit to the data, goodness of fit is poor (we will discuss more formally what that means in the next lecture)



30

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Let us model this as a double Gaussian

$$p(\{x_i\}, \{y_i\}, \{e_i\} \mid \theta, \{g_i\}, \sigma, \sigma_b) = \frac{g_i}{\sqrt{2\pi e_i^2}} \exp\left[\frac{-(y(x_i \mid \theta) - y_i)^2}{2e_i^2}\right] + \frac{1 - g_i}{\sqrt{2\pi\sigma_B^2}} \exp\left[\frac{-(y(x_i \mid \theta) - y_i)^2}{2\sigma_B^2}\right]$$

- Now we allow the model to have a nuisance parameter 0 < g_i <1 for each data point: g_i = 0 indicates an outlier. We can also allow σ_b to be a nuisance parameter to marginalize over (or just make it a large number)
- We can define an outlier (circle) whenever posterior $E(g_i) < 0.5$
- prior on gi: we can adopt a noninformative (uniform) prior, or we could have adopted a double peaked prior (one peaked at 0 one at 1) to force the solutions into 0 or 1: this does buy not us that much when compared to simply using $E(g_i) < 0.5$ criterion.

Result of Gaussian 2 Mixture Model



Note that this may not be what we want: outliers may be a source of information, so labeling them and discarding may destroy useful information

Pooling

- In previous example we have assumed each event has its own gi without any connection between them. In the context of drawing data from separate experiments (which is not the case in this example) this is called no pooling.
- We could have also used g_i = g, which is to say that all data are drawn from the same pdf: complete pooling in the context of separate experiments. Then we do not determine g_i for each data point, instead we use the data to determine 1-g as the outlier fraction (g=3/19 on previous slide). This allows us to determine σ_b from the data (σ_b=30+/- 10 on previous slide)
- Or we could have grouped data into separate groups each with its own prior, if we have a priori reasons to separate them into such groups: partial pooling. For example, outliers with x<40 have a different prior than outliers with x>40 on previous slide

Alternatives: Robust Analysis

- So far we used L2 norm, justified by Gaussian error distribution, as in the least squares fit. We used a mixture of Gaussians to treat outliers
- If we know the error probability distribution we can use it instead: Gaussian is the most compact and any other distribution will reduce sensitivity to outliers
- This can be related to changing the norm



Error PDF

- Suppose we know PDF of the error P=e(- ρ) $P = \prod_{i=0}^{N-1} \{ \exp[-\rho(y_i, y \{x_i | \mathbf{a}\})] \Delta y \}$
- We then want to minimize $\sum_{i=0}^{N-1} \rho(y_i, y \{x_i | \mathbf{a}\})$
- If this is only a function of difference between model and data we can minimize over **a**

•
$$\sum_{i=0}^{N-1} \rho\left(\frac{y_i - y(x_i | \mathbf{a})}{\sigma_i}\right) \quad \psi(z) \equiv \frac{d\rho(z)}{dz}$$

$$0 = \sum_{i=0}^{N-1} \frac{1}{\sigma_i} \psi\left(\frac{y_i - y(x_i)}{\sigma_i}\right) \left(\frac{\partial y(x_i | \mathbf{a})}{\partial a_k}\right) \qquad k = 0, \dots, M-1$$

M-Estimators and Norms

- Gaussian (L2) $\rho(z) = \frac{1}{2}z^2$ $\psi(z) = z$
- Laplace (double exponential, L1) $\rho(x) = |z| \quad \psi(z) = \operatorname{sgn}(z)$

• Lorentzian (Cauchy)
$$\rho(z) = \log\left(1 + \frac{1}{2}z^2\right)$$
 $\psi(z) = \frac{z}{1 + \frac{1}{2}z^2}$

- All are special cases of Student t: $\rho(z) = log(n+z^2)$
- Student t can also be viewed as a mixture of gaussians with the same mean and variances distributed as inverse- γ^2 with n degrees of freedom
- Norms: Lp norm defined as $||Z||_p = \left(\sum_{i=1}^N |Z_i|^p\right)^{1/p}$
- L2: ridge, L1: lasso

Regularization

- In image processing, machine learning etc. we often work with many more parameters than we can determine from the data: this is a form of non-parametric analysis (i.e. we have many more parameters than we can handle)
- Because of this the parameters will fit noise: overfitting
- If there is no noise by sampling is sparse the parameters will fit the data where measured and the model will make little sense elsewhere: overfitting
- To prevent that we regularize the solutions by imposing some smoothness
- Easiest way to achieve this is to minimize the sum of χ^2 and norm of parameters, with the relative contribution determining the overall level of smoothness
- In Bayesian context we are adding a prior

$$\mathcal{L}_p = -\ln p(s, S | x) = \frac{1}{2} \left\{ S^{-1} s^T s + [x - s]^T N^{-1} [x - s] + \ln \det S \right\}$$

Tikhonov (ridge, L2) Regularization

- We use L2 norm and add it to linear least squares $\|A\mathbf{x} - \mathbf{b}\|^2 + \|\mathbf{\Gamma}\mathbf{x}\|^2$
- Γ can be a general matrix, but for L2 $\Gamma = \alpha I$
- Normal equation solution $\hat{x} = (A^{\top}A + \Gamma^{\top}\Gamma)^{-1}A^{\top}\mathbf{b}$
- SVD solution: $A = U\Sigma V^{\top}$ $\hat{x} = VDU^{\top}b$ $D_{ii} = \frac{\sigma_i}{\sigma_i^2 + \alpha^2}$
- We see that regularization reduces condition number of the matrix: it regularizes it

Bayesian Regression



• In the Bayesian context we perform regression of coefficients a_j assigning them some prior distribution, such as a gaussian with some precision α . If we also have noise precision β then ln p is

$$\ln p(\mathbf{w}|\mathbf{t}) = -\frac{\beta}{2} \sum_{n=1}^{N} \left(t_n - \mathbf{w}^{\mathrm{T}} \phi(\mathbf{x}_n) \right)^2 - \frac{\alpha}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} + \text{const}$$

- So regularizing parameter is $\lambda = \alpha/\beta$
- How do we set α? It is a hyper-parameter that we can determine separately from the data itself. We will return to this when we discuss gaussian process and regression (lecture 11)

L1 vs. L2 Norm for Regularization

Suppose we have just one linear relation and 2 parameters: we must regularize. We want to find w1 and w2 subject to their linear relation
 E11w1+E12w2 = c1 (normal eq., red line) and minimizing the norm L1 or L2



- We see that L1 norm is minimized at w₁ = 0: L1 norm enforces sparseness, L2 does not
- Bayesian view: Laplace distribution is sharply peaked at 0
- L1 regularization is called LASSO: can both regularize and reduce dimensionality (shrinkage). Least absolute shrinkage and selection operator **40**

Example: Image sampled at discrete points



Input map 10×10 arcmin

Source distribution

Credit: F. Lanusse **41**

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No Regularization Reconstruction



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L2 Norm Regularization



Input map 10 \times 10 arcmin

Binning + Gaussian Smoothing

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L1 Norm Regularization



44

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Linmix: Fitting with correlated errors in x and y

Perform linear regression of y on x when there are measurement errors in both variables. The regression assumes:

eta = alpha + beta * xi + epsilon

x = xi + xerr

y = eta + yerr

Here, (*alpha, beta*) are the regression coefficients, *epsilon* is the intrinsic random scatter about the regression, *xerr* is the measurement error in *x*, and *yerr* is the measurement error in *y*. *epsilon* is assumed to be normally-distributed with mean zero and variance sigsqr. *xerr* and *yerr* are assumed to be normally-distributed with means equal to zero, variances *xsig*² and *ysig*², respectively, and covariance *xycov*. The distribution of *xi* is modeled as a mixture of normals, with group proportions *pi*, means *mu*, and variances *tausqr*. The following graphical model illustrates, well..., the model...

$$U(x,y): \text{ uniform between x and y}$$

Dirichlet distribution f:
$$f(x_1, \dots, x_K; \alpha_1, \dots, \alpha_K) = \frac{1}{B(\alpha)} \prod_{i=1}^K x_i^{\alpha_i - 1}$$

$$\sum_{i=1}^K x_i = 1 \text{ and } x_i \ge 0 \text{ for all } i \in [1, K]$$

This could have been solved by
integrating out latent variables
analytically: this does not change
hierarchical modeling approach

Summary

- The simplest way to write the full probabilistic model is to break it down into individual conditional probabilities, which often includes several levels of hierarchy of parameters
- Doing this is facilitated with the help of directed acyclic graphs (Bayesian networks) or undirected graphs (Markov networks)
- The price one pays is a large number of parameters: one either works with all of them or tries to marginalize analytically over nuisance parameters that are not of interest
- A few typical examples are regression with errors in both variables, regression with outliers etc.
- A more heuristic approach to outliers is robust analysis with M-estimators where the error distribution is generalized beyond gaussian to a Student t distribution
- This is related to the concept of L-norms, where L1 lasso norm corresponds to Laplace distribution which enforces sparsity
- This in turn is related to regularization in the context of image processing with incomplete and noisy data

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Literature

- Numerical Recipes, Press et al., Chapter 15
- Bayesian Data Analysis, Gelman et al., Chapter 5
- <u>https://www.quora.com/What-are-probabilistic-graphical-</u> models-and-why-are-they-useful (7 parts!)