LECTURE 10: ADVANCED BAYESIAN CONCEPTS

- Probabilistic graphical models (Bayesian 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.

LECTURE 10: ADVANCED BAYESIAN CONCEPTS

- We can introduce x as latent variables and model them together with θ. Then θ can be viewed as hyperparameters for x. 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 Casual Reasoning

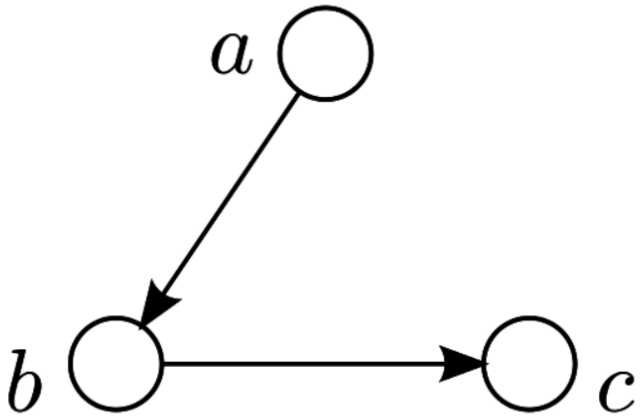
- We would like to describe the causal flow of events such that we can generate (simulate) events in a probabilistic setting (a flowchart of generating data)
- We can describe this with directed acyclic graphs (DAG)
- Typically we divide the process into components each of which generates a single variable 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 and probabilistic graphical models (PGM)

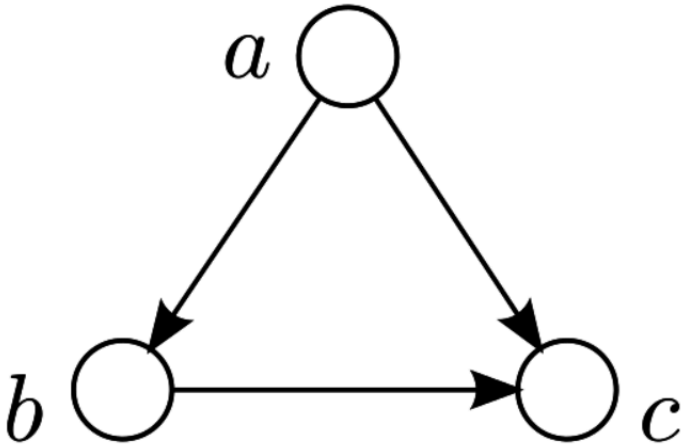
Approach of Bayesian Networks/PGMs

- We infer the causal (in)dependence of variables
- Write factorized joint probability distributions
- Perform data analysis by posterior inference

PGM Rules

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



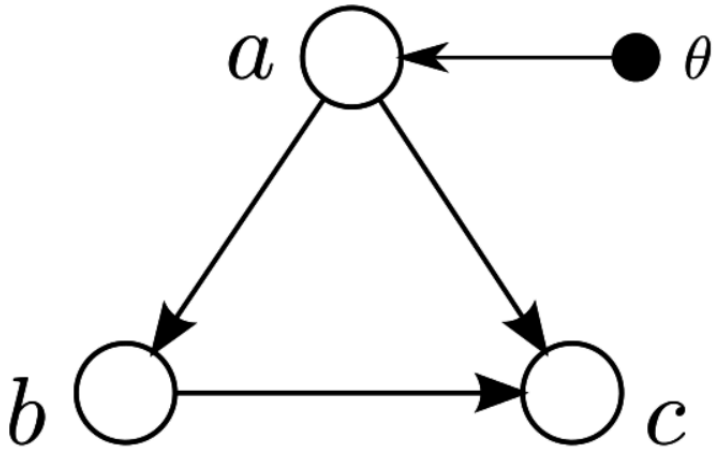


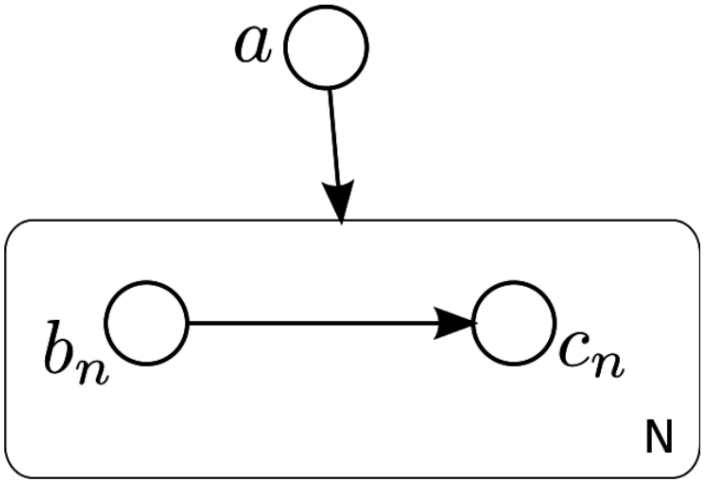
$$p(a,b,c) = p(c|b)p(b|a)p(a)$$

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

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

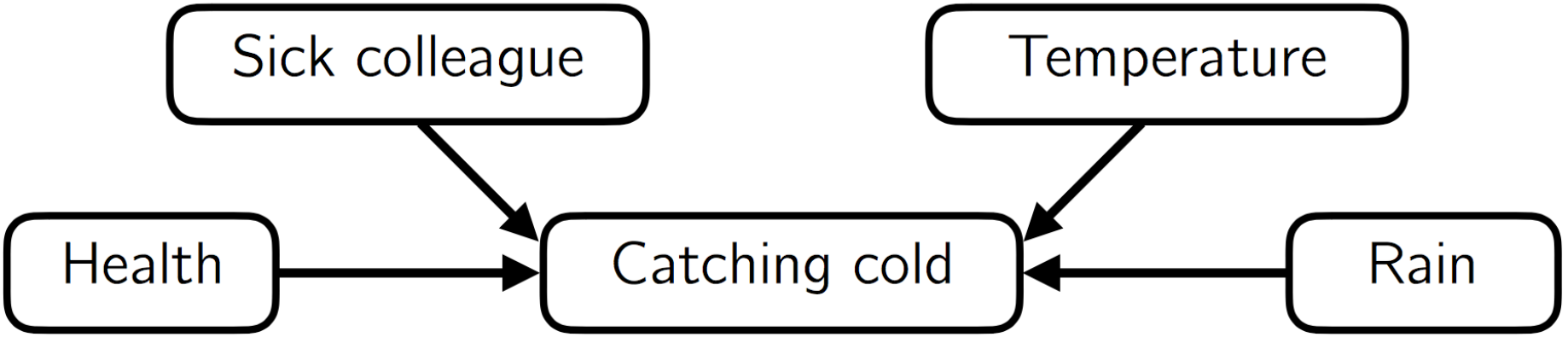




$$p(a, b, c) = p(c|a, b)p(b|a)p_\theta(a)$$

$$p(a, \mathbf{b}, \mathbf{c}) = \prod_{n=1}^{N} [p(c_n|a, b_n)p(b_n|a)]\, p(a)$$

Breaking casality down into components

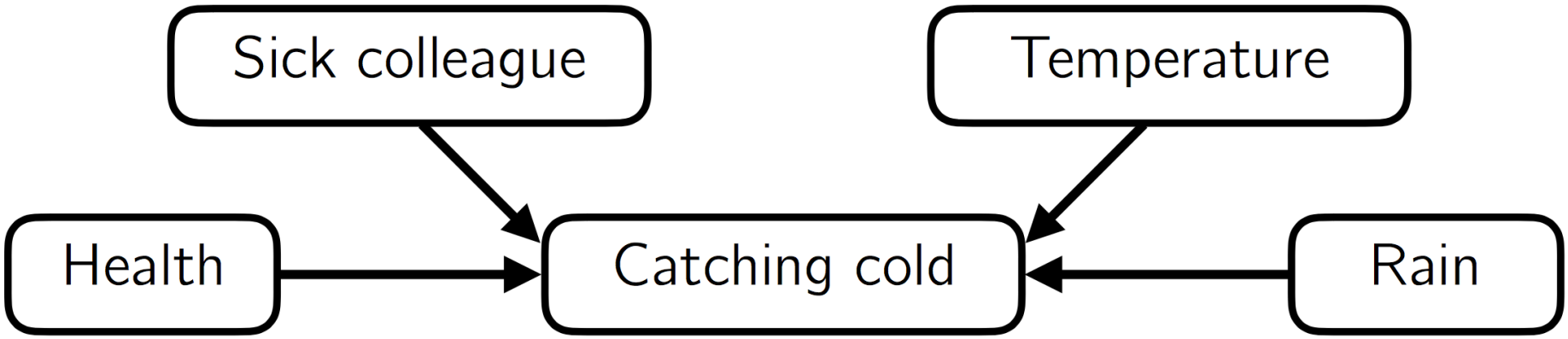


Independent causes of Catching cold

$$\text{Health} \perp \text{Sick colleague} \perp \text{Temperature} \perp \text{Rain}$$

Credit: Slides from B. Leistedt

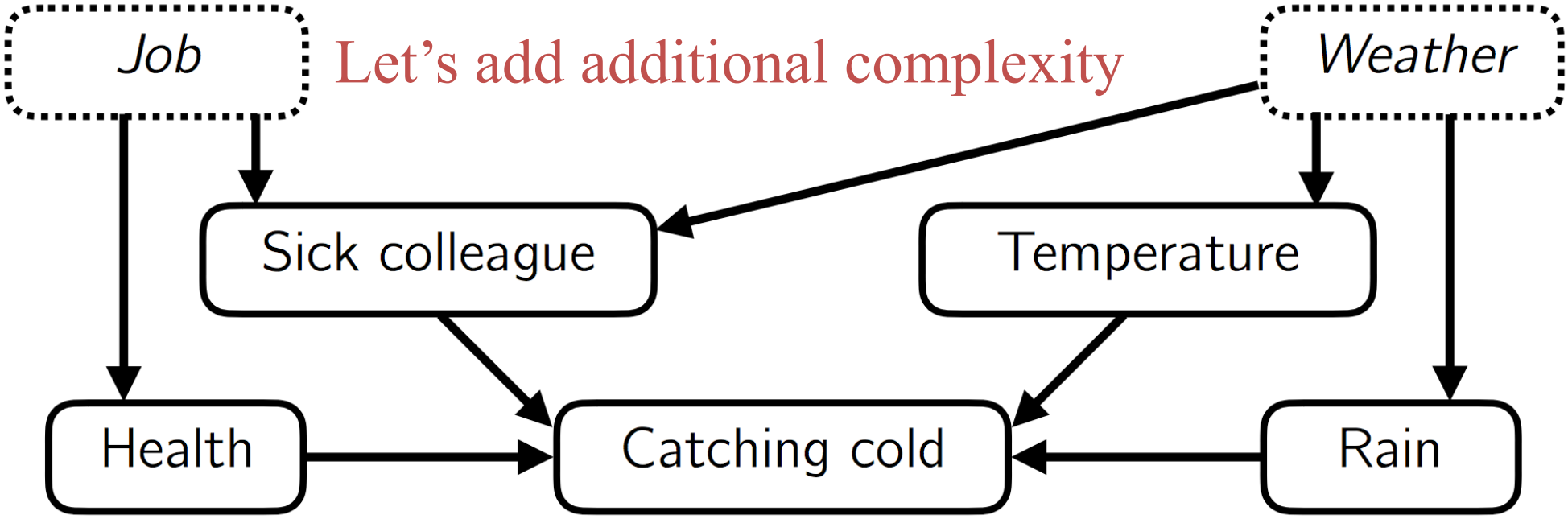
Breaking casality down into components



$$p(C, S, H, T, R) = p(C \mid S, H, T, R)\, p(S, H, T, R)$$

$$p(S, H, T, R) = p(S)\, p(H)\, p(T)\, p(R)$$

Credit: Slides from B. Leistedt



$$p(C, S, H, T, R, J, W) = p(C \mid S, H, T, R, J, W) \times p(S, H, T, R \mid J, W) \times p(J, W)$$

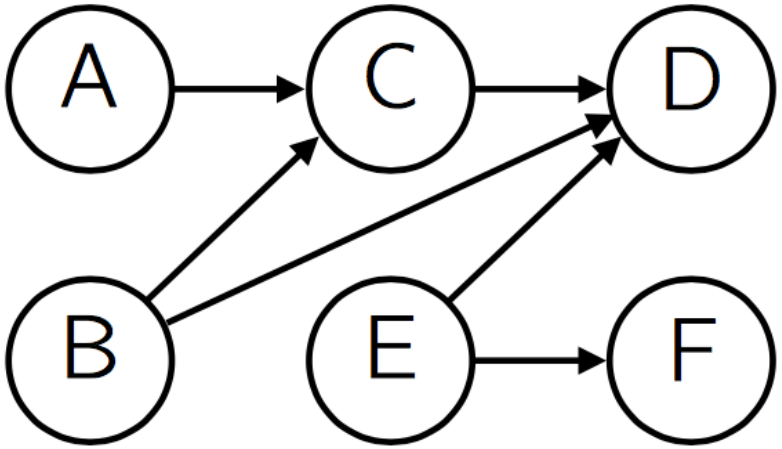
$$p(C \mid S, H, T, R, J, W) = p(C \mid S, H, T, R)$$

$$p(S, H, T, R \mid J, W) = p(S|J, W)\, p(H|J)\, p(T|W)\, p(R|W)$$

$$p(J, W) = p(J)p(W)$$

Example

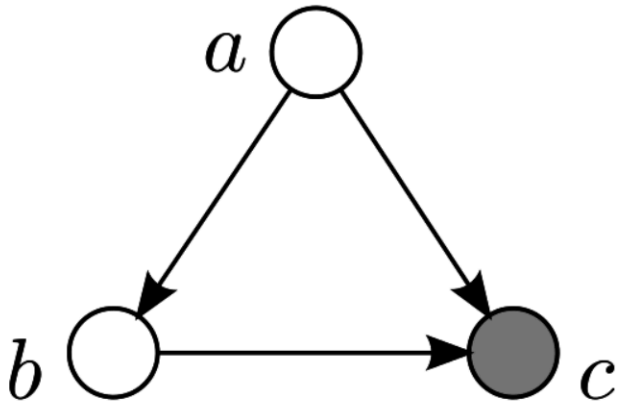
- Write down corresponding probability expressions for this graph and discuss the meaning with your neighbor

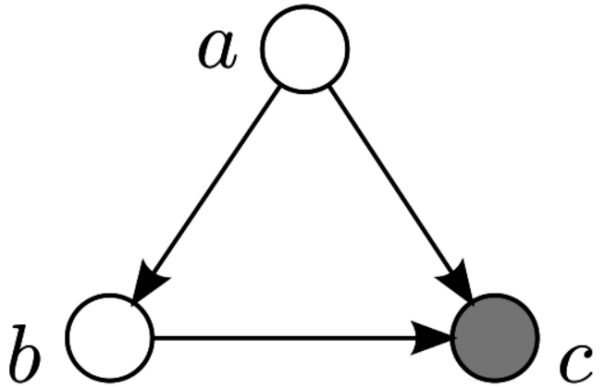


$$p(A, B, C, D, E, F) =$$
$$x\ p(F|E)\ p(D|B, E, C)$$
$$x\ p(E)\ p(C|A, B)\ p(A)\ p(B)$$

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



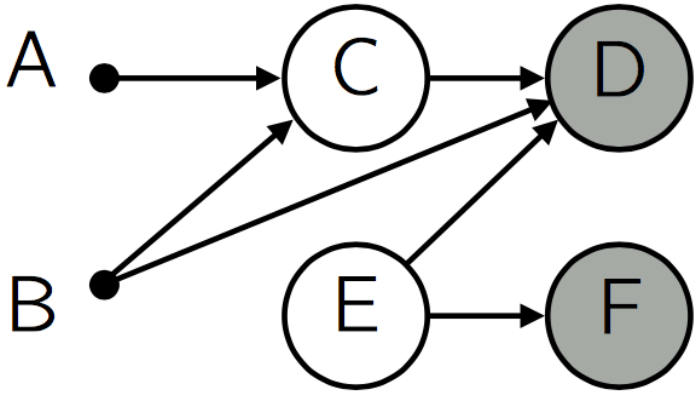


$$p(a,b,c) = p(c|a,b)p(b|a)p(a)$$

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

Posterior Inference

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

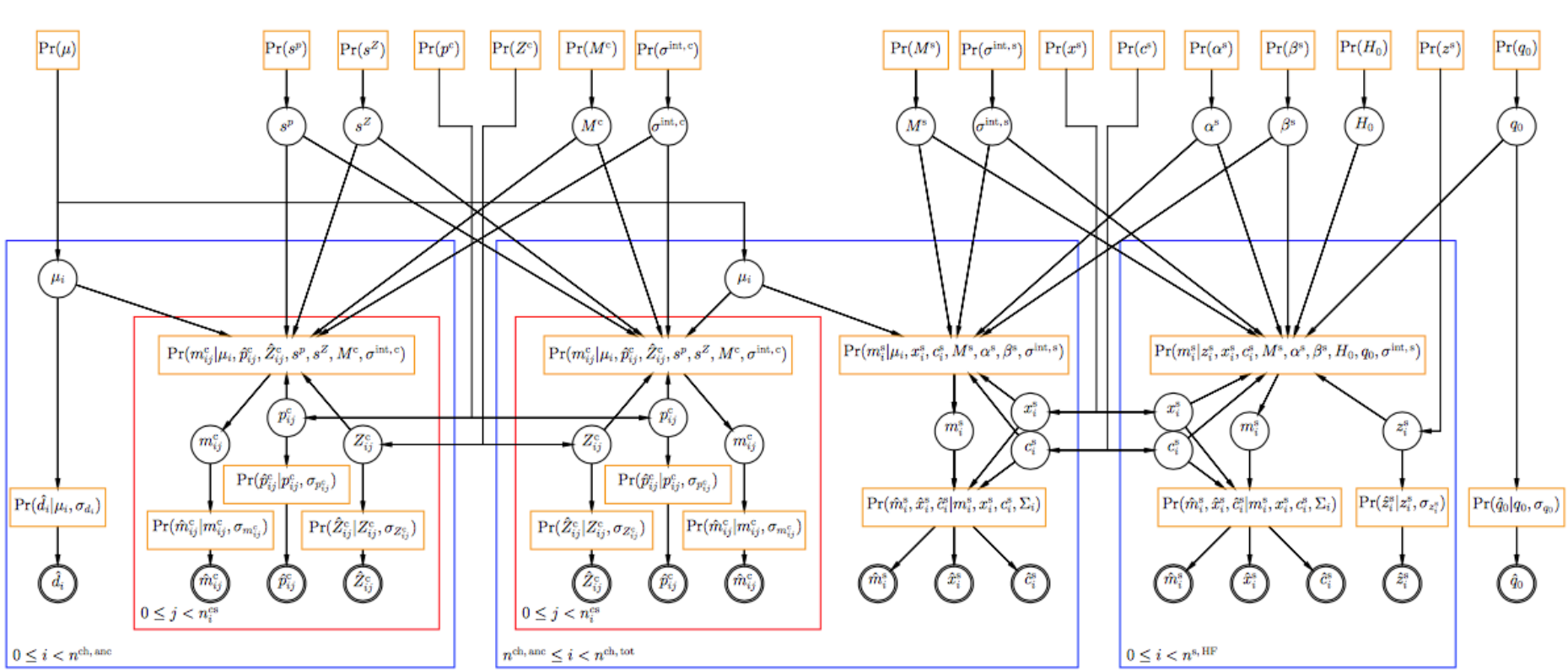


$$P(\text{Parameters}|\text{Data, Model}) = p(C, E \mid D, F, A, B)$$
$$= p(F|E)\, p(D|C, E)\, p(C|A, B)\, p(E)\, p(A)\, p(B)$$

- 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)

A Big PGM (Distance Ladder)

- This is a way to organize the generative probabilistic model



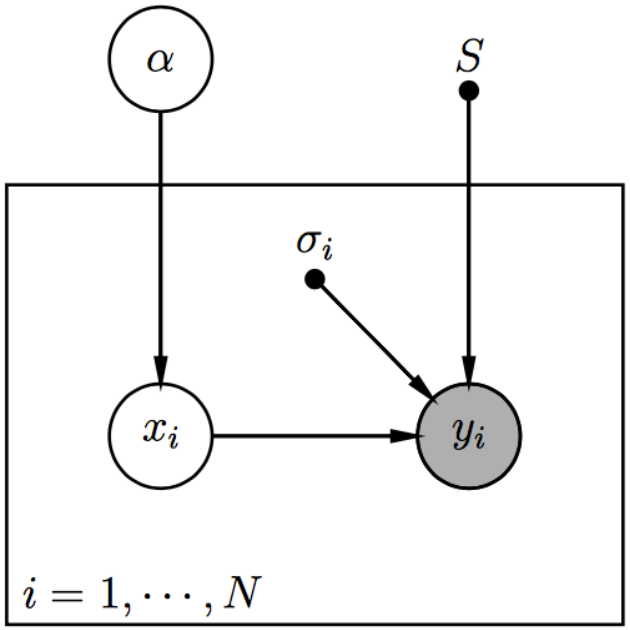
Hierarchical Bayesian Models

- 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

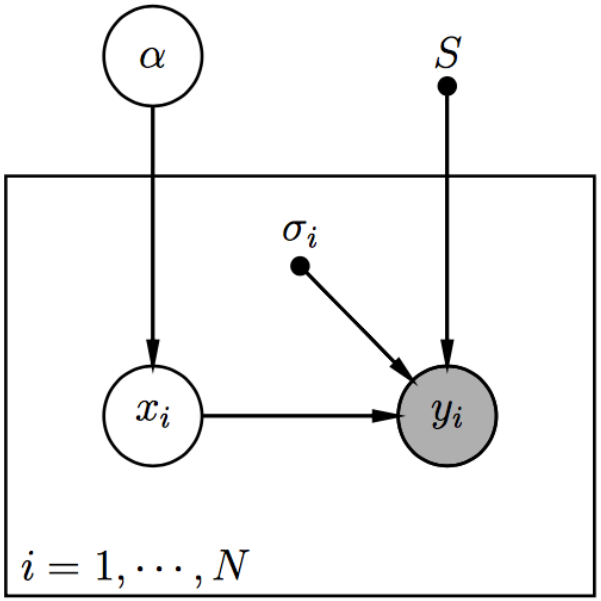
- When we do not know anything about latent variables x_i we can place them on equal footing: $p(x_1,x_2,...x_J)$ is invariant under permutation of (1, 2 , … J) indexes.
- Their joint probability distribution cannot change upon exchanging x_i with x_j …
- A simple way to enforce this is to say $p(x_1,x_2,...x_J) = \Pi_{j=1}^{J} p(x_i|\theta)$
- 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



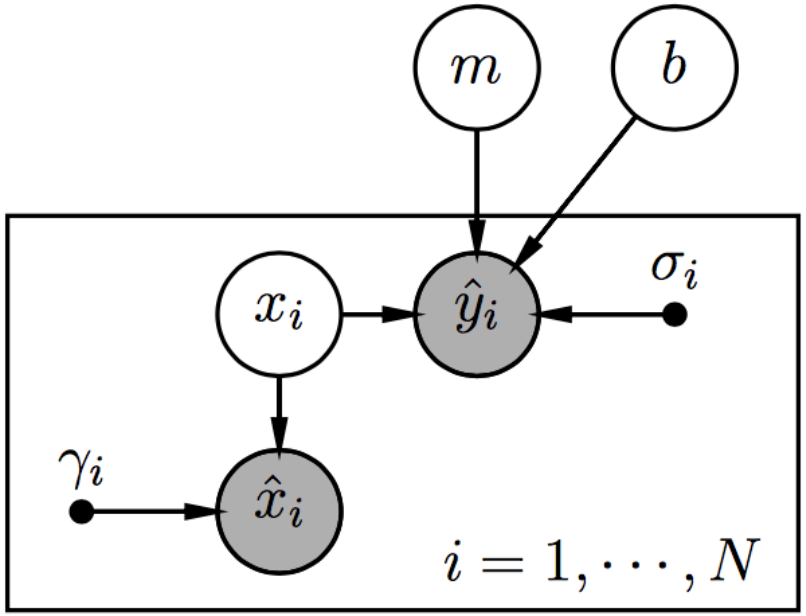
We are interested in inferring $\boldsymbol{\alpha}$

We need to **marginalize over** the latent x_i's, numerically or analytically

$$p(\alpha|\{y_i, \sigma_i\})$$
$$\propto \prod_i p(y_i|\alpha, \sigma_i)p(\alpha)$$
$$= \prod_i \int p(y_i, x_i|\alpha, \sigma_i)p(\alpha)\mathrm{d}x_i$$
$$= \prod_i \int p(y_i|x_i, \alpha, \sigma_i)p(x_i|\alpha, \sigma_i)p(\alpha)\mathrm{d}x_i$$
$$= \prod_i \int p(y_i|x_i, \sigma_i)p(x_i|\alpha)p(\alpha)\mathrm{d}x_i$$

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.

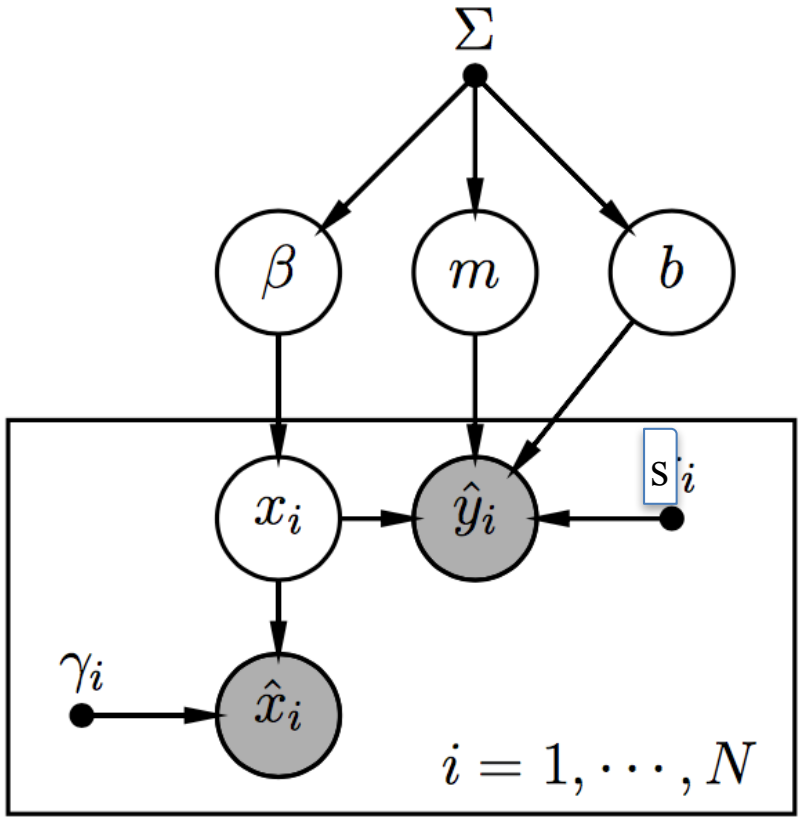


Sometimes marginalization can be done analytically

$$
\begin{aligned}
& p\left(m, s \middle| \{\hat{y}_i, \hat{x}_i, \sigma_i, \gamma_i\}\right) \\
&= \int \mathrm{d}\{x_i\} p\left(m, s, \{x_i\} \middle| \{\hat{y}_i, \hat{x}_i, \sigma_i, \gamma_i\}\right) \\
&\propto \prod_{i=1}^{N} \int \mathrm{d}x_i \mathcal{N}\left(\hat{y}_i - m x_i - b; \sigma_i^2\right) \mathcal{N}\left(\hat{x}_i - x_i; \gamma_i^2\right) \quad p\left(\{x_i\}, m, s\right) \\
&\propto \prod_{i=1}^{N} \mathcal{N}\left(\hat{y}_i - m \hat{x}_i - b; \sigma_i^2 + \gamma_i^2\right) \; p(s, m)
\end{aligned}
$$

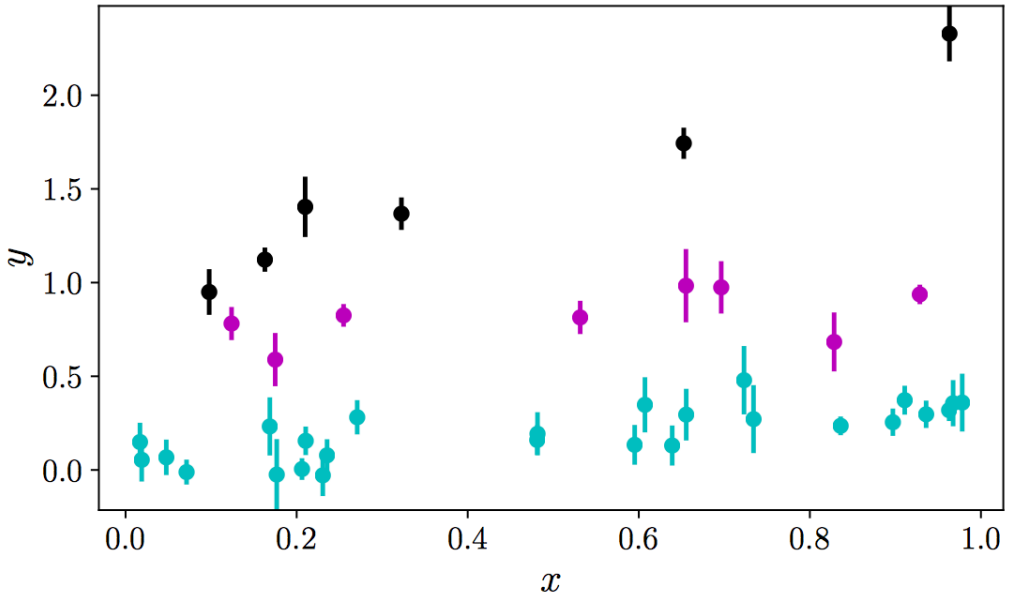
We should also put hyperpriors onto parameters

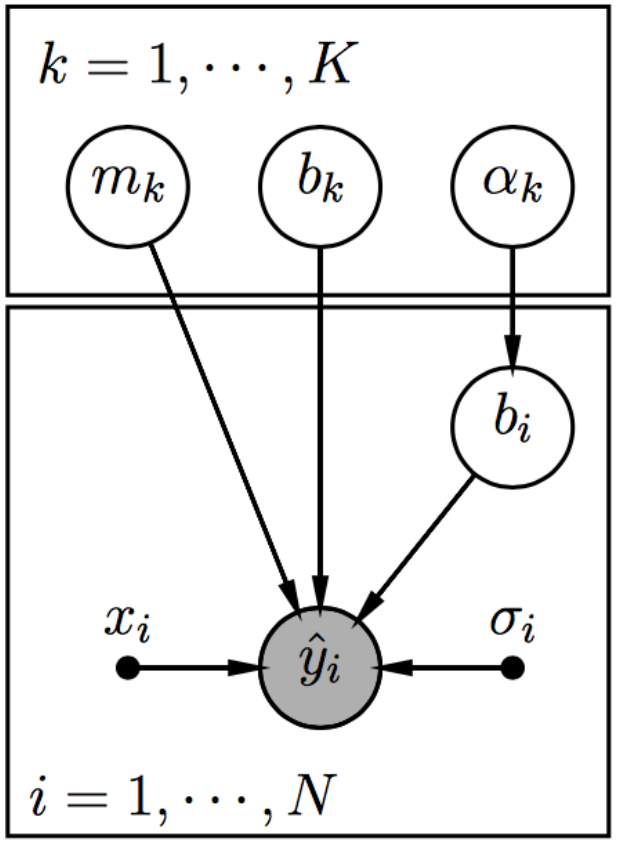
- We have hyperprior Σ
- A proper PGM should start with hyperpriors and end with observables



Another Extension: Mixture Models

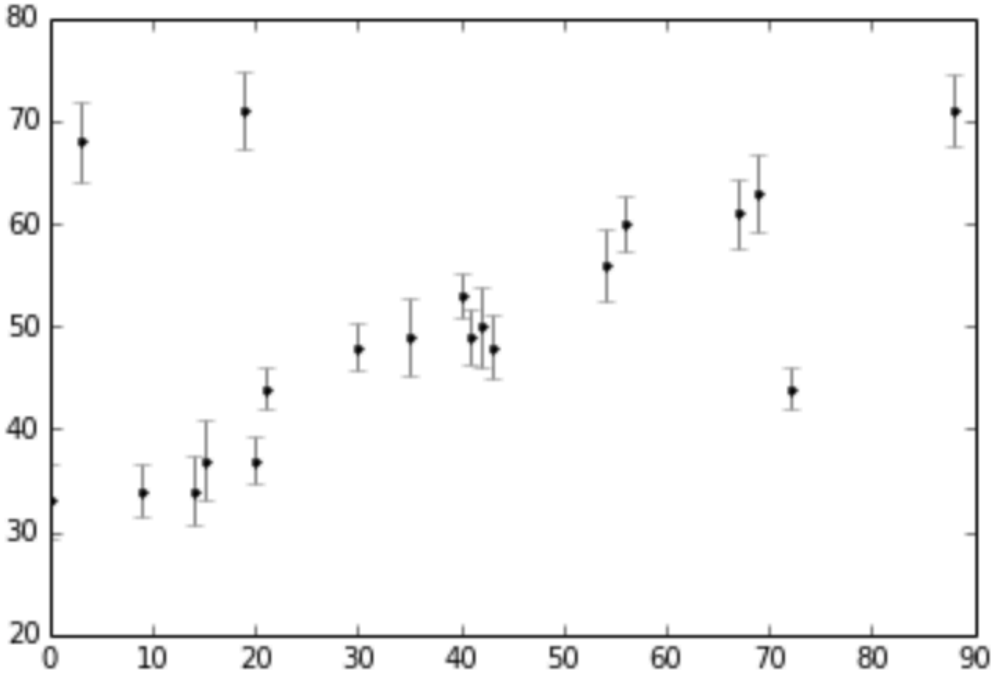
- Mixture models try to fit the data with a mixture of components
- For example, we can fit multiple lines to the data assuming the data are drawn from one of the components





Mixture Model for Outliers

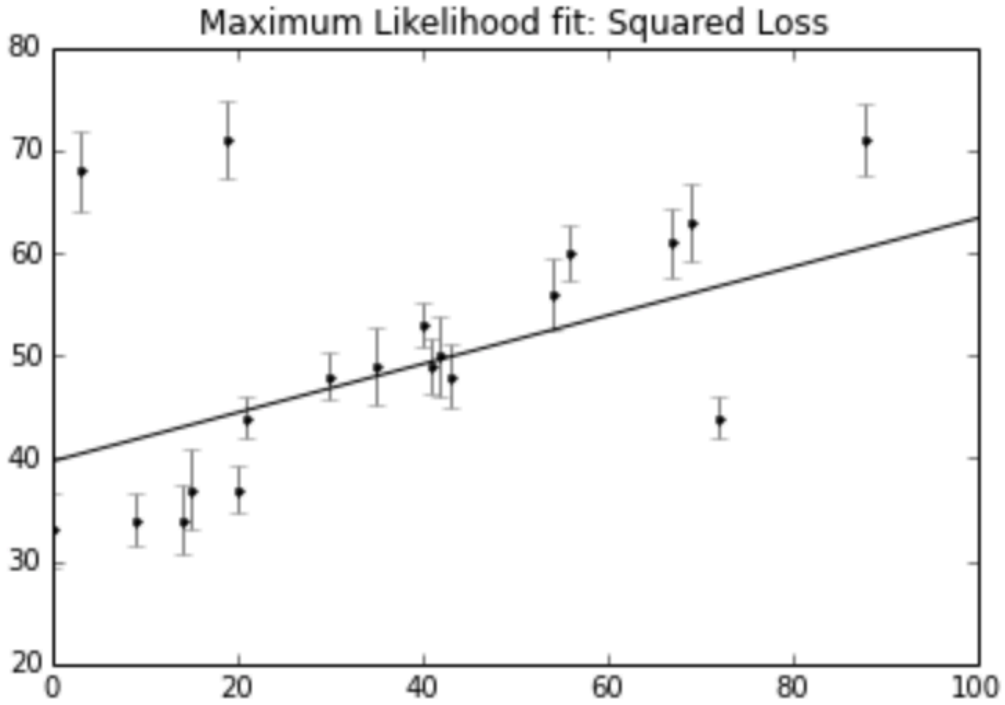
- Suppose we have data that can be fit to a linear regression, apart from a few outlier points
- It is always better to understand the underlying generative model of outliers
- But suppose we just want to identify them



Let us model this as a Gaussian

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

- We get a poor fit to the data (we will discuss more formally what that means in the next lecture)

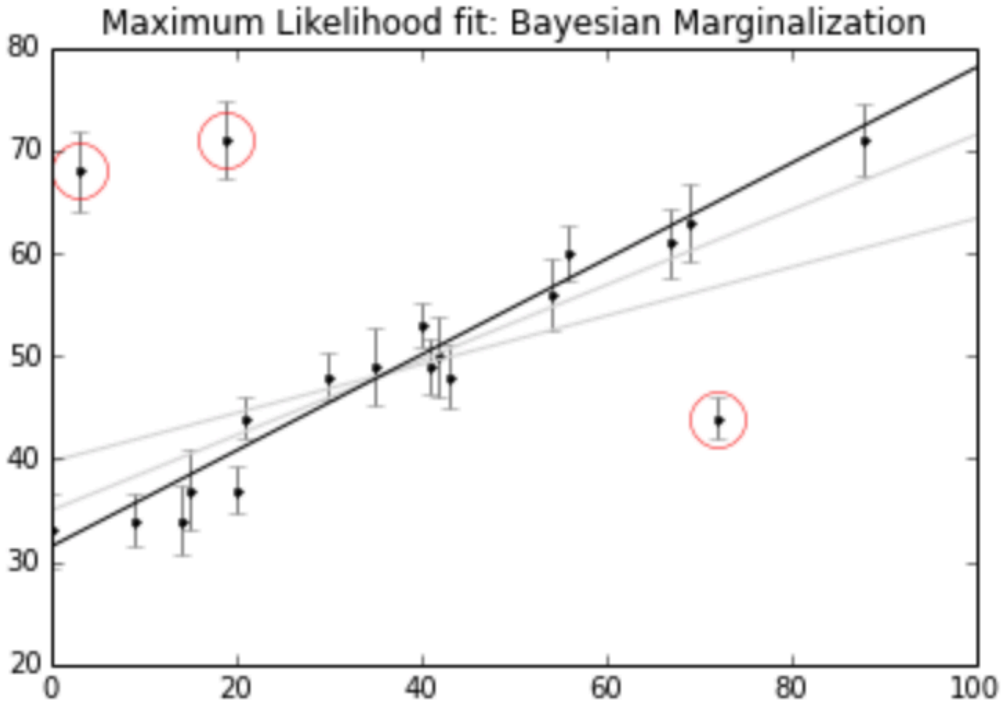


Let us model this as a Gaussian

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

- 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 g_i: 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



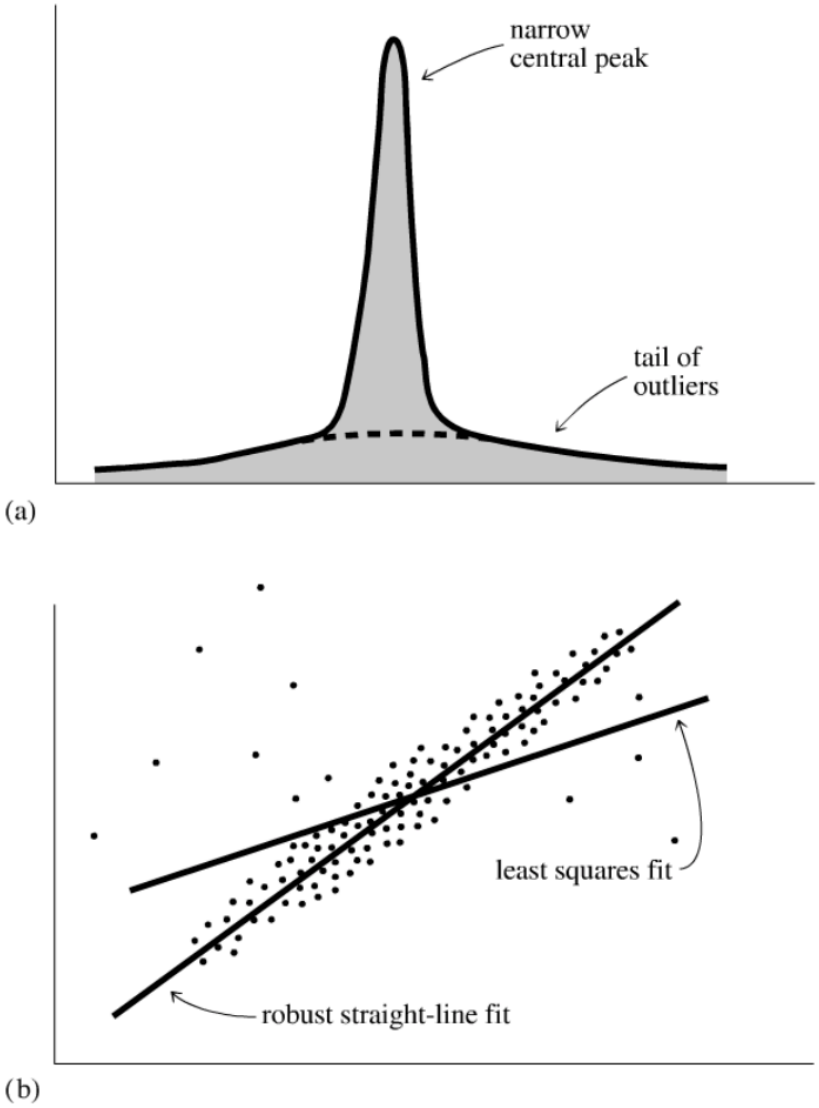
Note that this may not be what we want: outliers may be a source of information, so labeling them and discarding may destroy useful information

Pooling

- In previous example we have assumed each event has its own g_i 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
- 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

Alternatives: Robust Analysis

- So far we used L2 norm, justified by Gaussian error distribution, as in 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 is equivalent to changing the norm



Error PDF

- Suppose we know PDF of the error P

$$P = \prod_{i=0}^{N-1} \{\exp[-\rho(y_i, y\{x_i|\mathbf{a}\})]\,\Delta y\}$$

- 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**

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

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

M-Estimators and Norms

- Gaussian (L2) $\rho(z) = \frac{1}{2}z^2 \qquad \psi(z) = z$
- Laplace (double exponential, L1) $\rho(x) = |z| \qquad \psi(z) = \mathrm{sgn}(z)$
- Lorentzian (Cauchy) $\rho(z) = \log\left(1 + \frac{1}{2}z^2\right) \qquad \psi(z) = \frac{z}{1 + \frac{1}{2}z^2}$
- 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-χ^2 with n degrees of freedon
- Norms: Lp norm defined as
- L2: ridge, L1: lasso

$$\|Z\|_p = \left(\sum_{i=1}^{N} |Z_i|^p\right)^{1/p}$$

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
- We will work this out in the context of Wiener filter when we discuss Fourier methods.
- Here we want to compare L1 and L2 norms

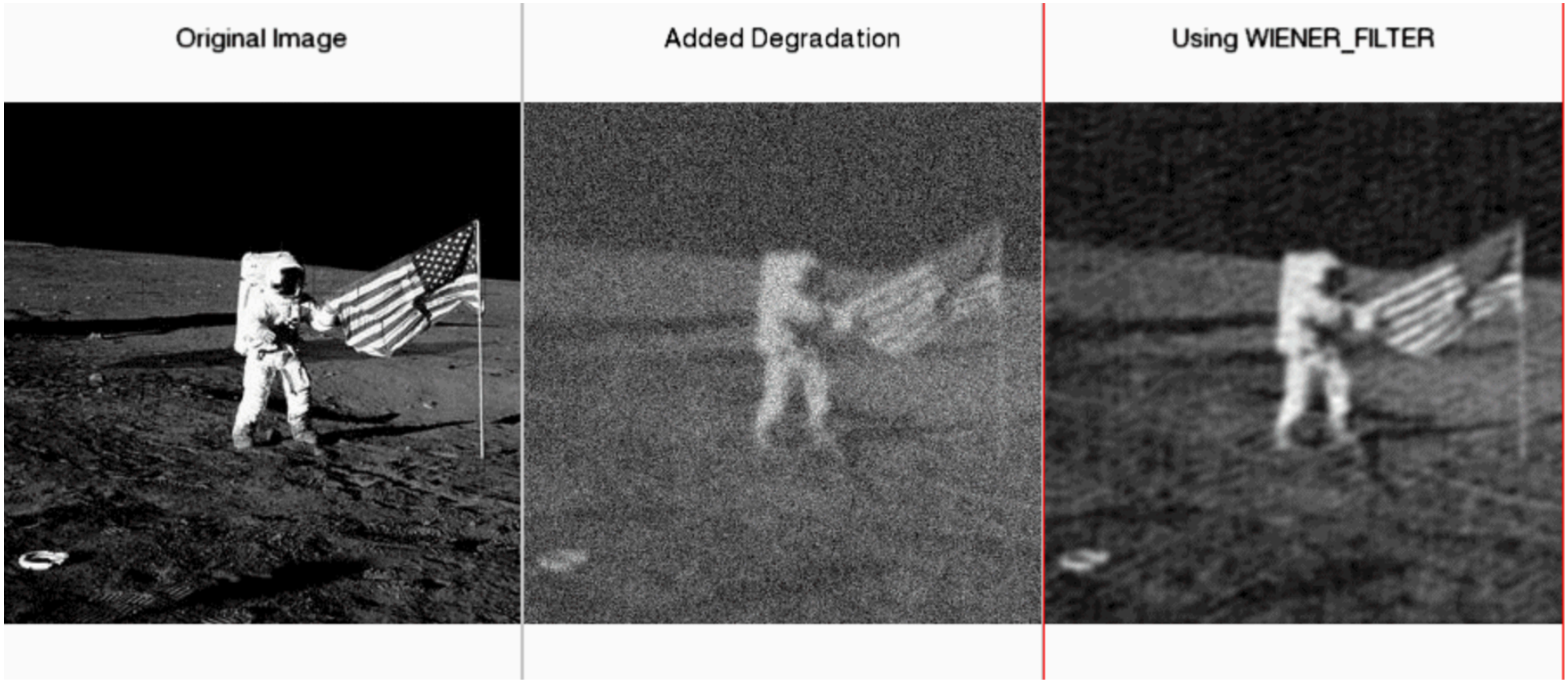
Tikhonov (ridge, L2) Regularization

- We use L2 norm and add it to linear least squares

$$\|A\mathbf{x} - \mathbf{b}\|^2 + \|\Gamma\mathbf{x}\|^2$$

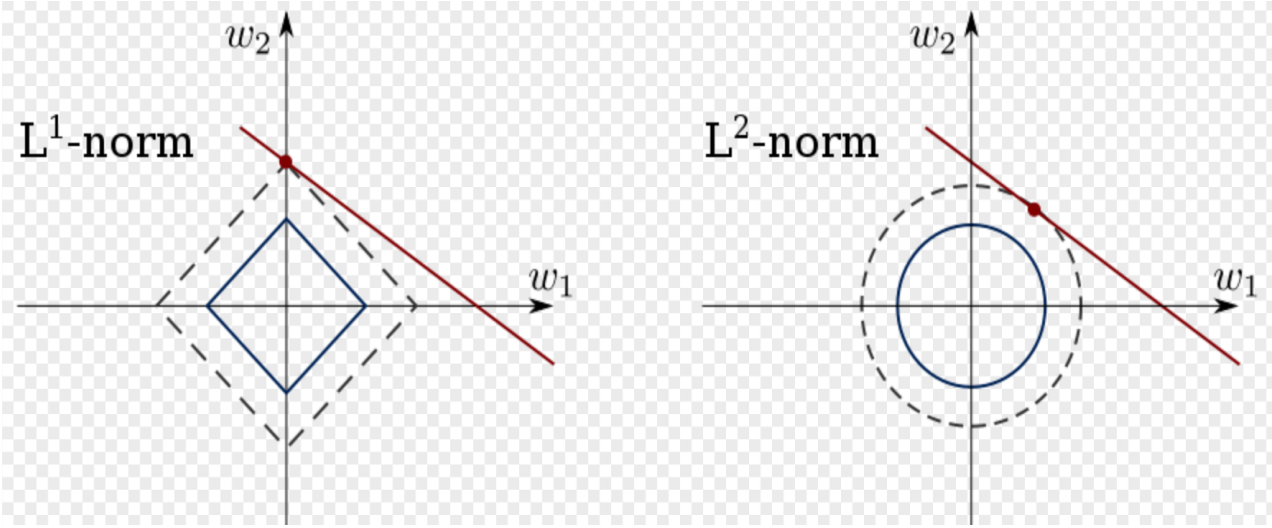
- Γ can be a general matrix, but for L2 $\Gamma = \alpha I$
- Normal equation solution $\hat{x} = (A^\top A + \Gamma^\top \Gamma)^{-1} A^\top \mathbf{b}$
- SVD solution: $A = U\Sigma V^\top \qquad \hat{x} = VDU^\top b \qquad D_{ii} = \dfrac{\sigma_i}{\sigma_i^2 + \alpha^2}$
- We see that regularization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

Wiener Filtering (Fourier L2)



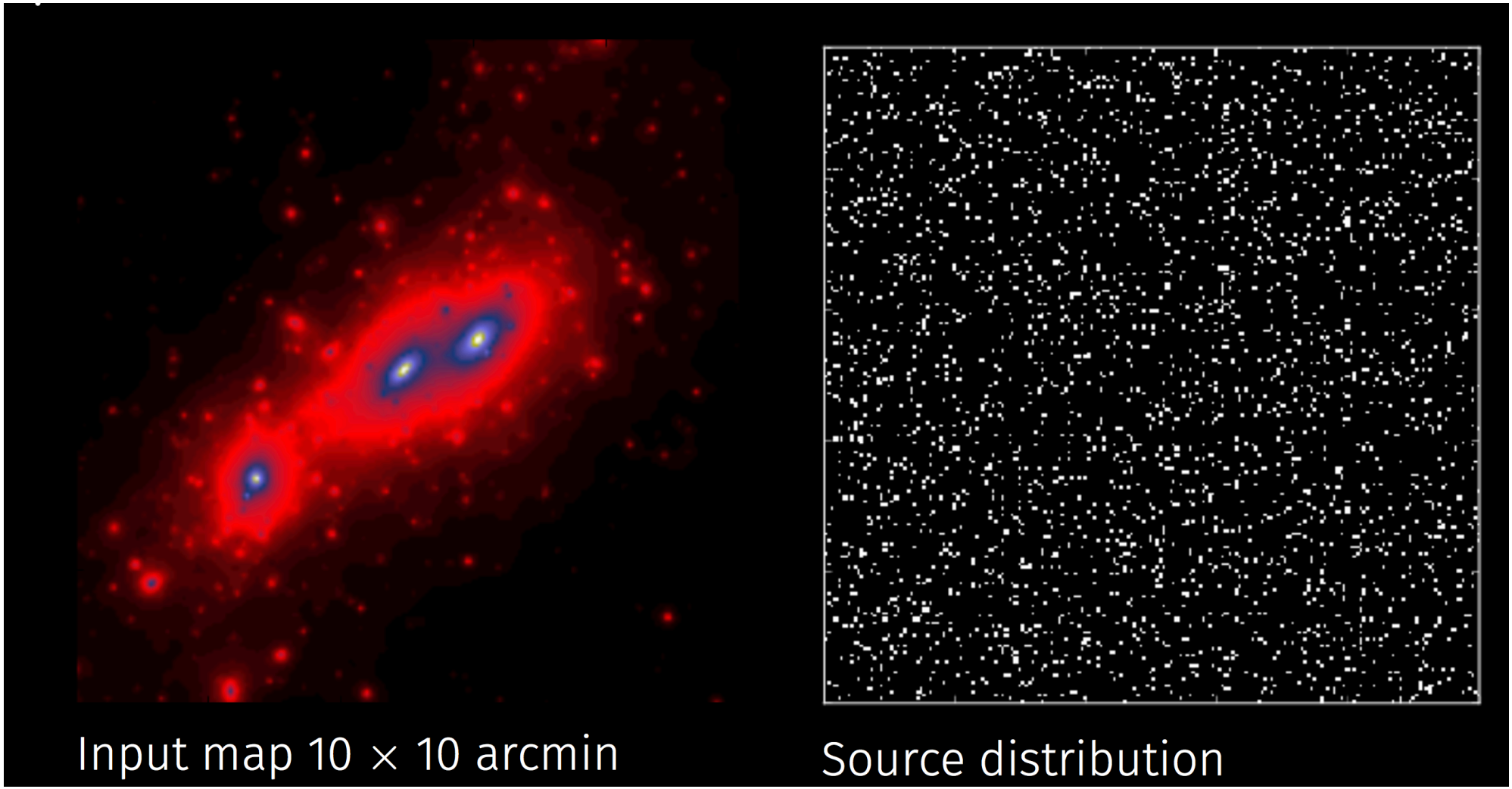
L1 vs. L2 Norm for Regularization

- Suppose we have just one linear relation and 2 parameters: we must regularize. We want to find w_1 and w_2 subject to their linear relation $E_{11}w_1+E_{12}w_2 = c_1$ (normal eq., red line) and minimizing the norm L1 or L2



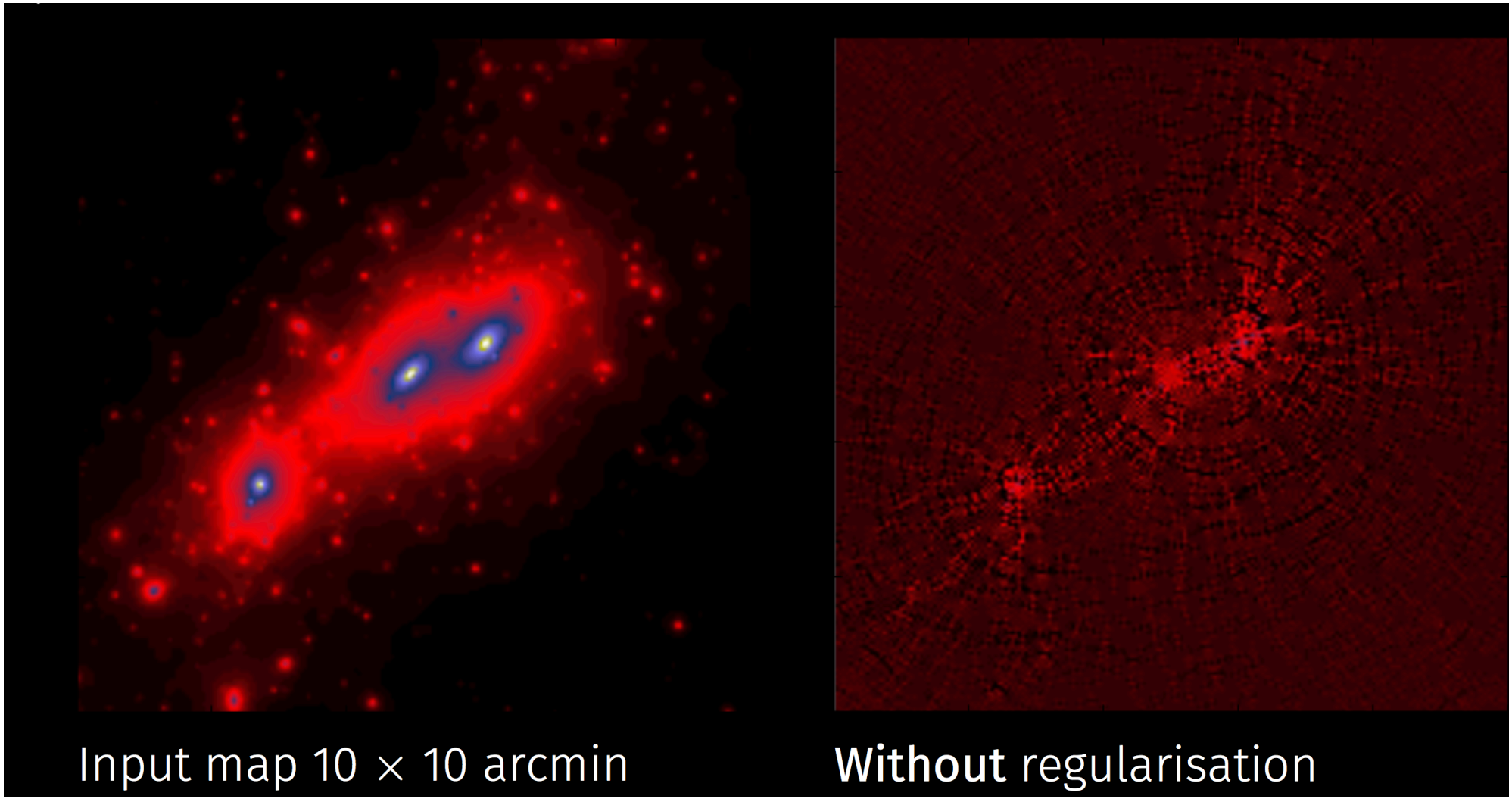
- We see that L1 norm is minimized at $w_1 = 0$: L1 norm enforces sparseness, L2 does not
- Bayesian view: Laplace distribution is sharply peaked at 0
- LASSO: can both regularize and reduce dimensionality (shrinkage)

Example: Image sampled at discrete points

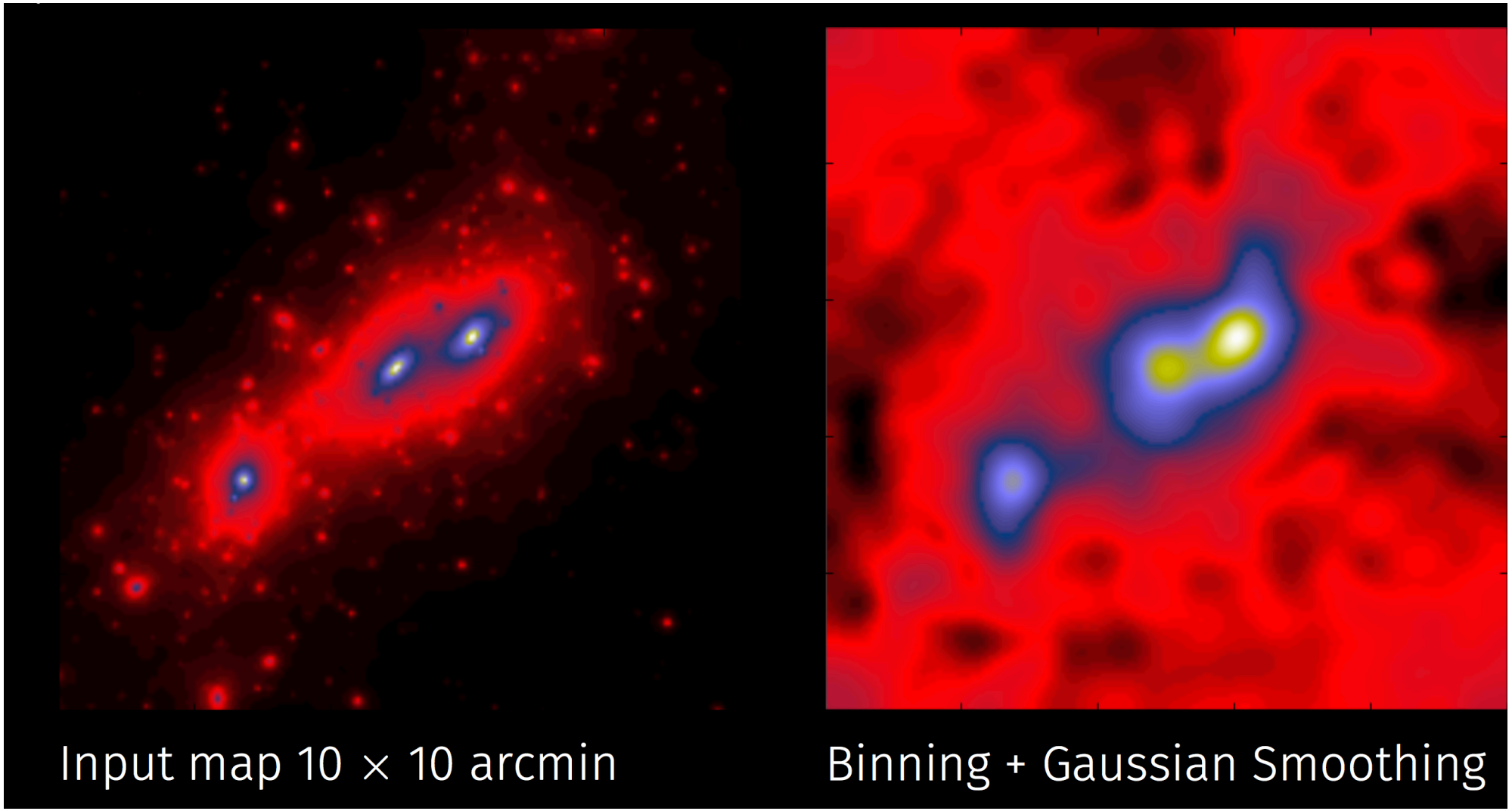


Credit: F. Lanusse

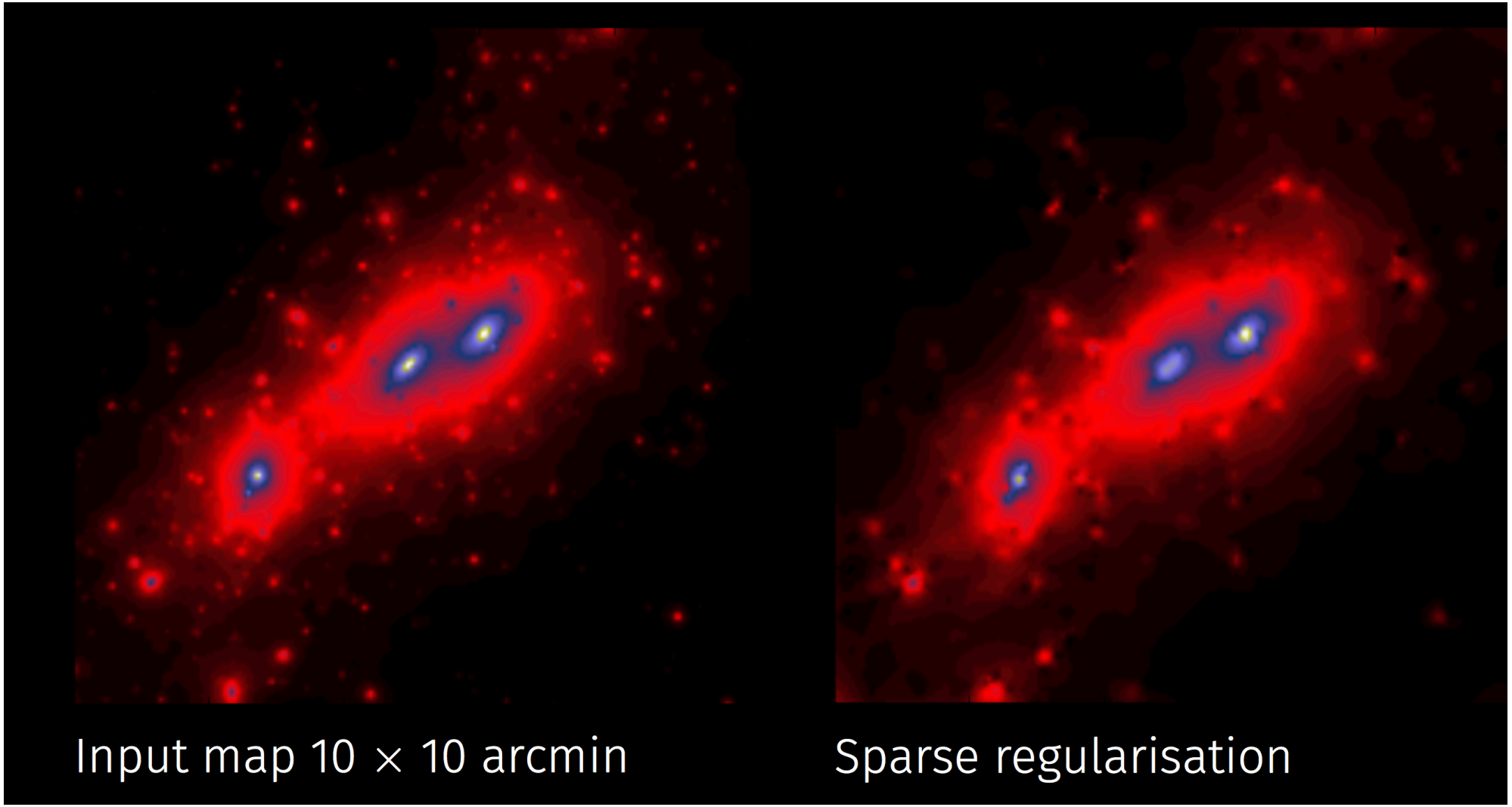
No Regularization Reconstruction



L2 Norm Regularization



L1 Norm Regularization



Posterior for Mixture Models

$$
\begin{aligned}
& p\left(\{\alpha_k, m_k, b_k\} | \{\hat{y}_i, \sigma_i, x_i\}\right) \\
& \propto \prod_i p\left(\hat{y}_i | \{\alpha_k, m_k, b_k\}, x_i, \sigma_i\right)\ p(\{\alpha_k, m_k, b_k\}) \\
& = \prod_i \sum_{a_i} p\left(\hat{y}_i, a_i | \{\alpha_k, m_k, b_k\}, x_i, \sigma_i\right)\ p(\{\alpha_k, m_k, b_k\}) \\
& = \prod_i \sum_{a_i} p\left(\hat{y}_i | \{\alpha_k, m_k, b_k\}, a_i, x_i, \sigma_i\right)\ p(a_i | \{\alpha_k, m_k, b_k\})\ p(\{\alpha_k, m_k, b_k\}) \\
& = \prod_i \sum_{a_i} p\left(\hat{y}_i | m_{a_i}, b_{a_i}, x_i, \sigma_i\right)\ p(a_i | \{\alpha_k\})\ p(\{\alpha_k, m_k, b_k\}) \\
& = \prod_i p(\{\alpha_k, m_k, b_k\}) \sum_{a_i} \alpha_k\ \mathcal{N}(\hat{y}_i - m_{a_i} x_i - b_{a_i}; \sigma_i^2)
\end{aligned}
$$

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

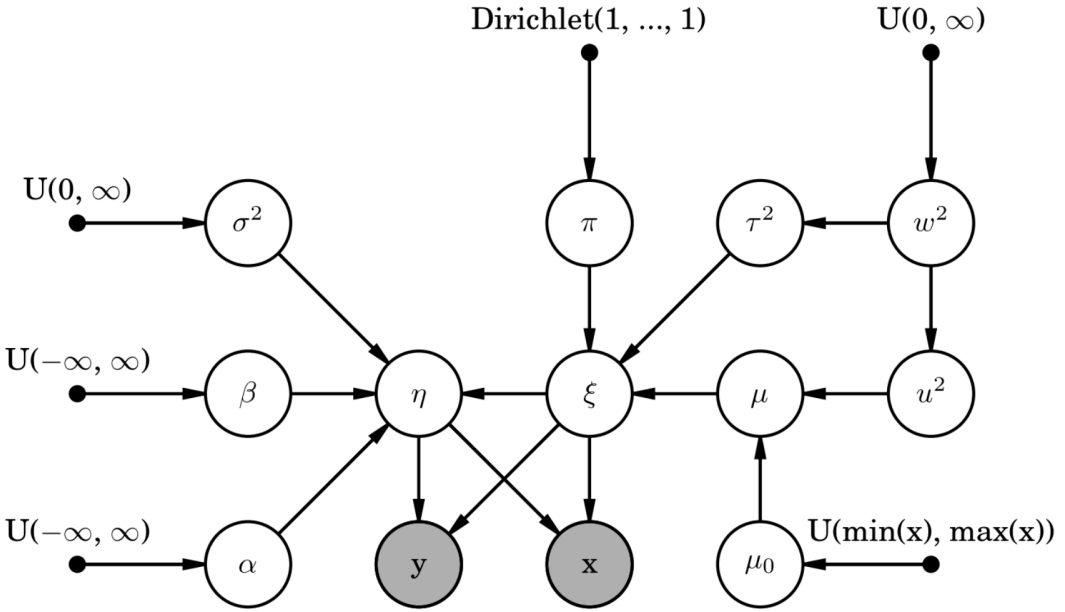
Here, (*alpha*, *beta*) are the regression coefficients, *epsilon* is the intrinsic random scatter about the regression, *xerr* is the measurement error in *x*, and *yerr* is the measurement error in *y*. *epsilon* is assumed to be normally-distributed with mean zero and variance *sigsqr*. *xerr* and *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): uniform between x and y
Dirichlet distribution f:

$$f(x_1,\ldots,x_K;\alpha_1,\ldots,\alpha_K) = \frac{1}{\mathrm{B}(\boldsymbol{\alpha})}\prod_{i=1}^{K} x_i^{\alpha_i-1}$$

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

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
- 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 general approach to outliers is robust analysiswith 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

Literature

- *Numerical Recipes*, Press et al., Chapter 15
- *Bayesian Data Analysis,* Gelman et al. , Chapter 5