PGM foundations - Part 2

Priors, Generative processes and Mixture models

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Outline

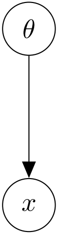
- PGMs in continuous domain
- Generative processes
- Mixture models

PGM in continuous domain

- Thus far, we've been using only discrete variables
- Conditional Probability Tables
- Extension to continuous domain is almost trivial...
- But with it, some concepts become more relevant
  - Prior
  - Conjugate prior

PGMs in continuous domain

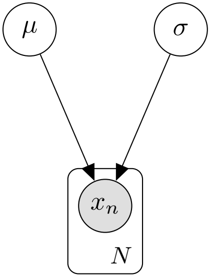
- General form



- We use functions instead of tables
- Typically, each function is a well-known distribution (or combination of them)
- Every distribution is parameterized by a set θ

PGMs in continuous domain

- Guassian distribution

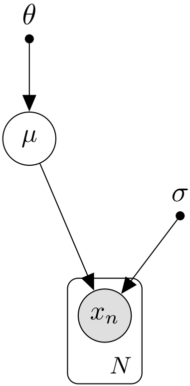


- A well-known example is the Gaussian (or *Normal)* distribution
- In this PGM, we assume to have observations x_n, that follow a Gaussian distribution
- It has two parameters (mean μ, variance σ^2)
- Inference
  - It has a well-known log likelihood function

PGMs in continuous domain

- A Graphical Model allows for a full Bayesian treatment:
  - We can assign *priors* to the parameters
  - We can use domain knowledge
  - Good to prevent overfitting
  - What would be the form of those priors?

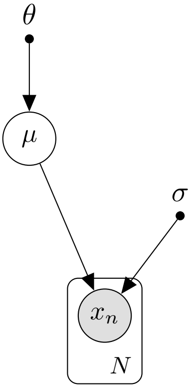
Gaussian distribution case



- To simplify, let's assume we know σ but not μ
- Can we pick *any* distribution, $D(\mu|\theta)$?
- Our joint distribution would become:

$$p(\mu, \mathbf{x}|\theta, \sigma) = D(\mu|\theta) \prod_{n=1}^{N} p(x_n|\mu, \sigma)$$

Gaussian distribution case



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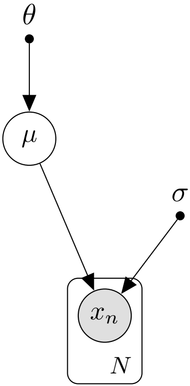

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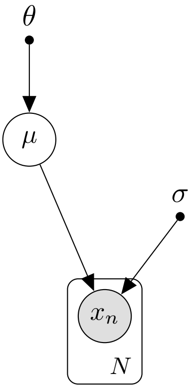

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  - If $D(\mu|\theta)$ is normal, then $p(\mu, \mathbf{x})$ is normal too!
- If $p(\mu, \mathbf{x})$ is not a known distribution, we may have trouble deriving it (analytically)...

Conjugate priors

- For many known distributions, there is a corresponding *conjugate prior*, P, that preserves its form under multiplication. I.e., if we have distribution L and its conjugate prior P_0, we should have

$$P_1 = L \times P_0$$

- where P_1 has the same form as P_0
- For example, the Beta distribution is the conjugate prior of Bernoulli; and we've seen that the Normal is the conjugate for the mean of the Normal (when variance is known).
- If we have a known closed form for model, inference is generally more efficient!
- **This is great for online learning (why?)!**

Conjugate priors

- We usually use a table

Discrete distributions [edit]

Likelihood	Model parameters	Conjugate prior distribution	Prior hyperparameters	Posterior hyperparameters	Interpretation of hyperparameters[note 1]	Posterior predictive[note 2]
Bernoulli	*p* (probability)	Beta	$\alpha,\, \beta$	$\alpha + \sum_{i=1}^{n} x_i,\, \beta + n - \sum_{i=1}^{n} x_i$	$\alpha - 1$ successes, $\beta - 1$ failures[note 1]	$p(\tilde{x} = 1) = \frac{\alpha'}{\alpha' + \beta'}$
Binomial	*p* (probability)	Beta	$\alpha,\, \beta$	$\alpha + \sum_{i=1}^{n} x_i,\, \beta + \sum_{i=1}^{n} N_i - \sum_{i=1}^{n} x_i$	$\alpha - 1$ successes, $\beta - 1$ failures[note 1]	$\operatorname{BetaBin}(\tilde{x} \mid \alpha', \beta')$ (beta-binomial)
Negative binomial with known failure number, *r*	*p* (probability)	Beta	$\alpha,\, \beta$	$\alpha + \sum_{i=1}^{n} x_i,\, \beta + rn$	$\alpha - 1$ total successes, $\beta - 1$ failures[note 1] (i.e., $\frac{\beta - 1}{r}$ experiments, assuming r stays fixed)	
Poisson	λ (rate)	Gamma	$k,\, \theta$	$k + \sum_{i=1}^{n} x_i,\, \frac{\theta}{n\theta + 1}$	k total occurrences in $\frac{1}{\theta}$ intervals	$\operatorname{NB}(\tilde{x} \mid k', \theta')$ (negative binomial)
			$\alpha,\, \beta$[note 3]	$\alpha + \sum_{i=1}^{n} x_i,\, \beta + n$	α total occurrences in β intervals	$\operatorname{NB}\left(\tilde{x} \mid \alpha', \frac{1}{1 + \beta'}\right)$ (negative binomial)
Categorical	$\boldsymbol{p}$ (probability vector), *k* (number of categories; i.e., size of $\boldsymbol{p}$)	Dirichlet	$\boldsymbol{\alpha}$	$\boldsymbol{\alpha} + (c_1, \ldots, c_k)$, where c_i is the number of observations in category *i*	$\alpha_i - 1$ occurrences of category *i*[note 1]	$p(\tilde{x} = i) = \frac{\alpha_i{}'}{\sum_i \alpha_i{}'} = \frac{\alpha_i + c_i}{\sum_i \alpha_i + n}$

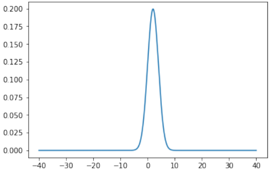
Figure: From Wikipedia

Some conjugate priors to remember...

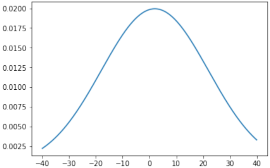
Likelihood	**Prior**
Normal with known variance	Normal
Normal with known mean	Inverse Gamma
Multivariate normal, known mean	Inverse Wishart
Multivariate normal, unknown mean and variance	Normal-inverse-Wishart
Exponential	Gamma
Bernoulli	Beta
Mulitnomial	Dirichlet
Poisson	Gamma

Last note on priors

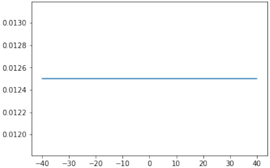
- Depending on what you know of the problem (or the constraints you want to impose...):



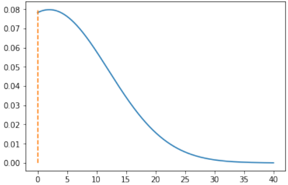
Proper informative prior



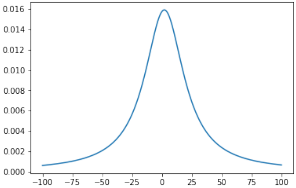
Proper weakly informative prior



Inproper uninformative prior



Proper bounded prior



Proper uninformative prior (notice scale and fat tails)

Playtime!

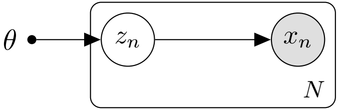
- Open notebook "3-PGM fundamentals.ipynb"
- Do part 1 (est. duration=30 min)

Generative processes

- By now, you understand that you can combine variables in multiple ways in your graphical model
- On the other hand, you may be overwhelmed about where to start doing your own
  - Small models, with few variables, are simple
  - What if you have a lot of variables, assumptions, domain knowledge?...
- You need to think from a generative perspective...

"Generative story" of data

- How is a data point generated?



- Given a parameter θ
- For $n = 1..N$, do
  1. Draw a random latent variable, $z_n \sim p(z|\theta)$
  2. Given z_n, generate x_n such that $x_n \sim p(x|\theta, z_n)$
- In fact, this resembles a program structure!

A more complex example - Dwell time prediction

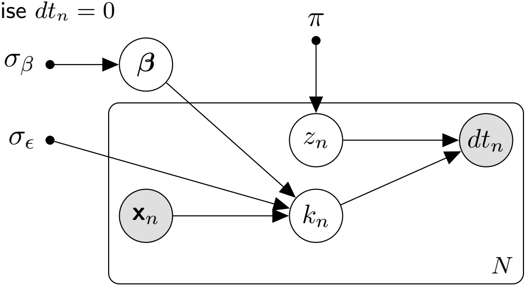
For a given bus stop, that serves a single line, can we predict the amount of time the next bus will be stopped there to load/unload passengers (the *dwell* time)?

- Our dataset contains $\{x_n = \{0, 1\}$-representing peak/non-peak hour, dt_n - dwell time$\}$.
- Notice that, sometimes, the bus does not stop at all!
- When it stops, we measure the duration as dt

Dwell time prediction

Given N, σ_β, σ_ϵ and π

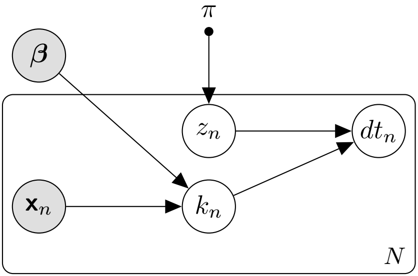
1. Draw a pair of parameters[1], $\boldsymbol{\beta} \sim \mathcal{N}(\mathbf{0}, I\sigma_\beta)$
2. For $n = 1..N$
   1. Draw one value for z_n, such that $z_n \sim Bern(\pi)$.
      - If $z_n = 1$, the bus has stopped ($z_n = 0$ otherwise).
      - Distributed as Bernoulli, with parameter π
   2. Draw one value for k_n, such that $k_n \sim \mathcal{N}(\beta_0 + \beta_1 x_n, \sigma_\epsilon)$
   3. If $z_n = 1$, $dt_n = k_n$,
      - otherwise $dt_n = 0$



[1] We need two values for β, one for the intercept, another for the peak/non-peak information.

Dwell time prediction

- After you define your model, you need to estimate it. I.e. infer the following:
    - Distribution of $\boldsymbol{\beta}$
    - Optimal values of σ_ϵ, σ_β, and π (we defined them as constants!)
- Of course, when you have them, you can make your predictions!
- Your model will look different:



"Generative story" of data

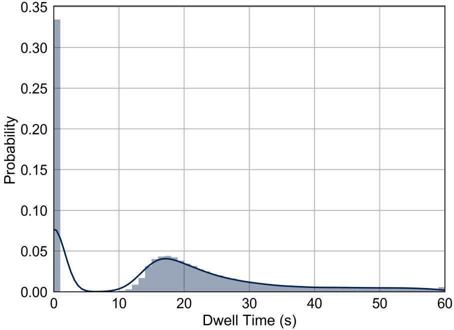
- Set up the building blocks, as per available knowledge
- Easy to change data distributions inside the model
- Can be used to *actually* generate data!
    - Ancestral sampling

Playtime!

- Open notebook "3-PGM fundamentals.ipynb"
- Do part 2 (est. duration=30 min)

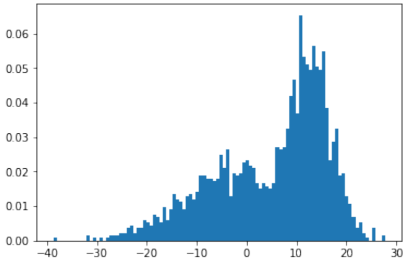
Mixture models

- A PGM is composed of observed and latent variables, parameters, constants.
- In this course, we'll approach some examples from this very large family
- Mixture models are pervasive in data modelling in general
- Problem:
    - Sub-populations of data
    - Data generated from combination/competition of multiple sources
    - Number of sources usually discrete and finite

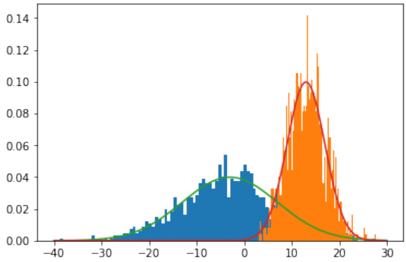


The canonical example: Gaussian Mixture

- What we observe



- What really happens



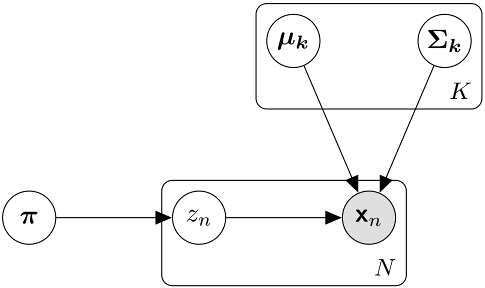
Generative story

Given:

- A dataset with N points (or vectors) $(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n)$ and a value K

1. Draw $\boldsymbol{\pi}$, and $(\boldsymbol{\mu_k}, \boldsymbol{\Sigma_k})$ for all K gaussians
2. For $n = 1, 2, ..., N$
   1. Draw $z_n \sim Multinomial(\boldsymbol{\pi})$
      - $\boldsymbol{\pi}$ is a vector $(1 \times K)$ with the probabilities of each class
   2. Define $k = z_n$. Generate $\mathbf{x}_n$, from the k-th Gaussian,

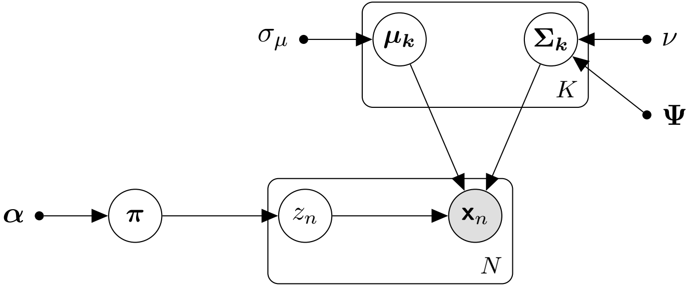
$$\mathbf{x}_n \sim \mathcal{N}(\boldsymbol{\mu_k}, \boldsymbol{\Sigma_k})$$



Note: in practice we need to be exhaustive

...particularly in probabilistic programming (e.g. STAN)

- $\boldsymbol{\pi} \sim Dir(\boldsymbol{\alpha})$
- $\boldsymbol{\mu_k} \sim \mathcal{N}(\mathbf{0}, I\sigma_\mu)$
- $\boldsymbol{\Sigma_k} \sim \mathcal{W}^{-1}(\boldsymbol{\Psi}, \nu)$
    - Typically, $\nu =$ number of dimensions, and $\boldsymbol{\Psi} = I$



Playtime!

- Open notebook "3-PGM fundamentals.ipynb"
- Do part 3 (est. duration=45 min)

The problem of inference

- ...your last exercise should show that we need efficient inference methods
  - Complex distribution (e.g. involving log of sum; an unknown form; etc.)
  - High dimensionality (e.g. more than a couple of parameters is often too many!)
  - Continuous dimensions instead of discrete
- Two general approaches:
  - Exact inference
  - Approximate Inference
- Before we get practical (i.e. STAN), we need to understand a bit how inference can be done
  - Important to manipulate STAN and understand its output
- STAN uses Approximate Inference (we'll talk about it today)
- In a later class, we'll get more detailed (in both Exact and Approx.).

Conclusions

- PGMs are extremely flexible. They can combine:
  - Discrete and continuous variables
  - Parametric and non-parametric models
  - Informative and non-informative priors
  - Online learning with conjugate priors
  - Partial and complete data
- Think in a generative way helps design a model

References

- (Koller and Friedman, 2009) Koller, D., and Friedman, N. Probabilistic graphical models: principles and techniques. MIT press. (2009).