Introduction to STAN

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Outline

- Step back: The big picture so far
- Case study: Analyzing a cyclist's daily travel times
- Introduction to STAN
- Mixture models in STAN

Step back: The big picture so far

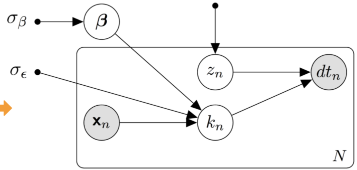
- Probability and statistics recap
  - Probability theory at the center of everything that we do
  - Allows to capture uncertainty
- Probabilistic graphical models (PGMs)
  - Intuitive and compact way of representing the structure of a prob. model
  - Relationships between variables and conditional independencies
  - How the joint distribution factorizes
- Generative processes
  - A "story" of how the observed data was generated
  - Explicit description of how the different variables in the model are related
  - Complementary to PGM representation: more detailed, but less intuitive
- Joint probability distribution and Bayesian inference
  - Joint probability of the model: central object for all computations
  - Bayesian inference: model $+$ data $\rightarrow$ patterns
  - Important concepts: likelihood, prior, posterior, conjugate prior, etc.

Step back: The big picture so far

- Everything is related...

$$p(\boldsymbol{\beta}, \mathbf{z}, \mathbf{k}, \mathbf{dt}) =$$
$$p(\boldsymbol{\beta}|\sigma_\beta) \prod_{n=1}^{N} p(k_n|\mathbf{x}_n, \boldsymbol{\beta}, \sigma_\epsilon)\, p(z_n|\pi)\, p(dt_n|z_n, k_n)$$

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 $k_n \sim \mathcal{N}(\mathbf{x}_n^T\boldsymbol{\beta}, \sigma_\epsilon)$
   3. If $z_n = 1$, $dt_n = k_n$,
      - otherwise $dt_n = 0$



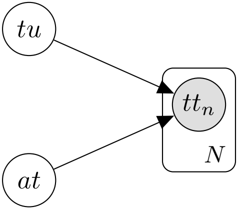
Case study: Analyzing a cyclist's daily travel times

- Suppose that you commute to work everyday by bicycle
- As a methodic cycler, you keep track of your daily travel times (tt)

$$\mathcal{D} = \{tt_1, \ldots, tt_N\}$$

- Based on your collected data, you start building a (simple) PGM to understand your cycling behaviour

tt_n - travel time in the n^{th} day
at - average travel-time
tu - traffic uncertainty



- Making it a bit more formal...

$$tt_n \sim \mathcal{N}(tt_n | at, tu)$$

Case study: Analyzing a cyclist's daily travel times

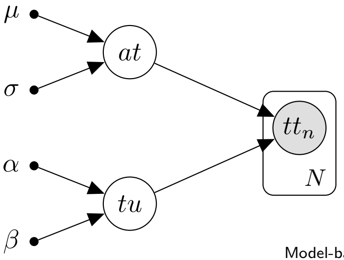
- We have our likelihood

$$tt_n \sim \mathcal{N}(tt_n|at, tu)$$

- Time to specify the priors

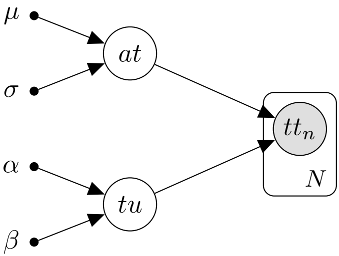
$$at \sim \mathcal{N}(at|\mu, \sigma^2)$$
$$tu \sim \mathcal{IG}(tu|\alpha, \beta)$$

- We chose conjugate priors (for all the advantages explained before)
  However, STAN does not care about conjugacy!
- More complete representation of the model



Case study: Analyzing a cyclist's daily travel times

- Complete representation of the model

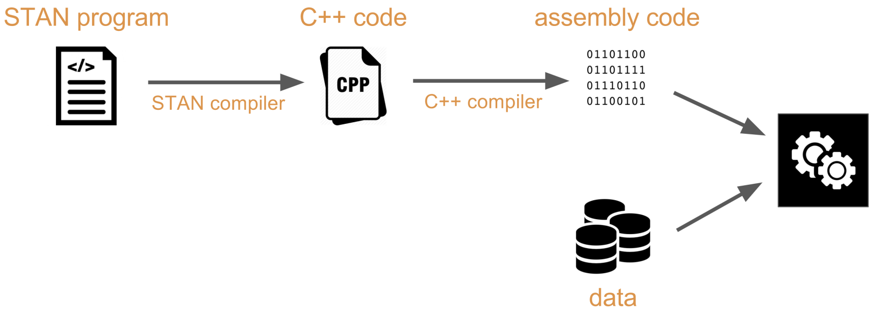


- Corresponding generative process

  1. Draw average travel time $at \sim \mathcal{N}(at|\mu, \sigma^2)$
  2. Draw traffic uncertainty $tu \sim \mathcal{IG}(tu|\alpha, \beta)$
  3. For each day $n \in \{1, \ldots, N\}$
     (a) Draw travel time $tt_n \sim \mathcal{N}(tt_n|at, tu)$

- This generative process description is what STAN relies on!

STAN Workflow



- The top part is completely **seamless** to the user!
- The user needs only to:
  - Specify STAN program (based on the generative process)
  - Assemble data in a Python dictionary
  - Call one of STAN's inference methods
  - Extract and interpret the results

Building blocks of a STAN program

```
functions {
      // Define functions (optional)
}
data {
      // Declare the input data to the model (observed variables)
}
transformed data {
       // Apply transformations to the data (optional)
}
parameters {
       // Declare latent variables in the model (to be inferred)
}
transformed parameters {
       // Apply transformations to the latent variables (optional)
}
model {
       // Specify the model (generative process)
}
generated quantities {
       // Generate data from the model (e.g. predictions for testset)
}
```

Building blocks of a STAN program

- Going back to our case study of cyclist travel times...
- **Data block**: where we declare the input data to the model (observed variables)

```
data {
   int<lower=1> N;  // number of samples
   vector[N] tt;    // observed travel times
}
```

  - We can specify constraints on the inputs (sanity checks)
    E.g. N must be positive

- **Parameters block**: where we declare the latent variables in the model

```
parameters {
   real at;             // average travel time
   real<lower=0> tu;  // traffic uncertainty
}
```

  - We can also specify constraints on the latent variables
    E.g. the traffic uncertainty tu (variance of a Gaussian) must be positive

Building blocks of a STAN program

- **Model block**: where we specify the model (generative process)

```
model {
   at ~ normal(12, 10); // prior on the avg travel times
   tu ~ cauchy(0, 10);  // prior on the traffic uncertainty
   for (n in 1:N) {
      tt[n] ~ normal(at, tu);  // likelihood
   }
}
```

  - We placed an informative prior on at (you should do this whenever you can!)
  - In STAN, the second parameter of "`normal(12, 10)`" is a standard deviation and not a variance! So, the variance is actually $10^2 = 100$
  - *Cauchy* distribution is often recommended as a prior for variances[1]
    - It has a bell-shape like the Gaussian, but fatter tails
    - Due to the positive constraint on tu, this is effectively a *half-Cauchy*
  - We can make the "for" loop more efficient (*vectorization*)

```
tt ~ normal(at, tu);  // likelihood
```

[1] See STAN best practices online

Case study: Analyzing a cyclist's daily travel times

- Putting everything together...

```
data {
    int<lower=1> N;   // number of samples
    vector[N] tt;     // observed travel times
}
parameters {
    real at;              // average travel time
    real<lower=0> tu;   // traffic uncertainty
}
model {
    at ~ normal(12, 10);  // prior on the avg travel times
    tu ~ cauchy(0, 10);   // prior on the traffic uncertainty
    tt ~ normal(at, tu);  // likelihood
}
```

- The model is specified! Let's now look at the data...

Note

"model" block encodes the (log) joint distribution (used by STAN for inference)!

Input data to STAN

- Recall our data block:

```
data {
   int<lower=1> N;  // number of samples
   vector[N] tt;    // observed travel times
}
```

- In Python, we wrap input data in a **dictionary** object

```
cyclist_dat = {'N': 14,
               'tt': [13,17,16,32,12,13,28,12,14,18,36,16,16,31]}
```

- Dictionary keys must match **exactly** the names in the data block declaration!

Inference with STAN

- Recall that STAN provides two types of inference methods
  - Markov chain Monte Carlo (MCMC) - the No U-Turn Sampler (NUTS)
  - Automatic Differentiation Variational Inference (ADVI) - a combination of variational and stochastic...
- We begin by compiling the model (regardless of the inference method)

```
sm = pystan.StanModel(model_code=model_definition)
```

- Run MCMC (NUTS) to compute the posterior distribution of the latent variables (inference)

```
fit = sm.sampling(data=data, iter=1000, chains=4)
```

- Or use ADVI (typically much faster, but still experimental)

```
fit = sm.vb(data=data, iter=10000)
```

Coming soon to STAN...

Riemannian manifold Hamiltonian Monte Carlo (RHMC), expectation propagation, and streaming (stochastic) variational inference, etc.

Interpreting the output of STAN

- We can print a summary of the results using

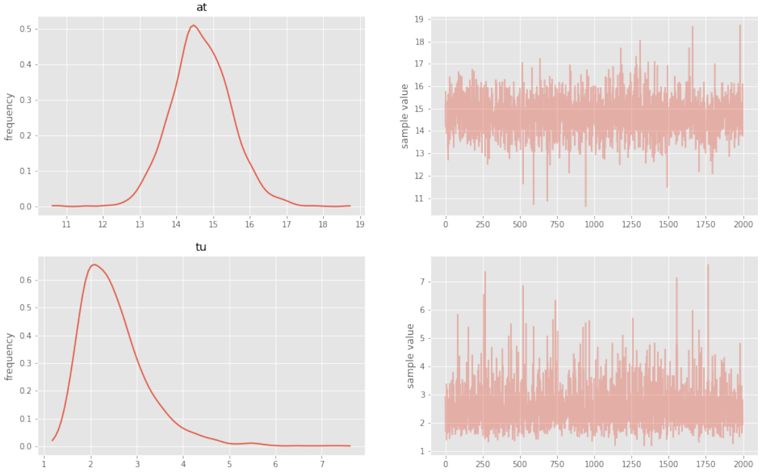
```
print(fit)
```

```
Inference for Stan model: anon_model_257f22c9ec6a2127b7174a37ecde293c.
4 chains, each with iter=1000; warmup=500; thin=1;
post-warmup draws per chain=500, total post-warmup draws=2000.

       mean se_mean   sd   2.5%    25%    50%    75%  97.5% n_eff Rhat
at    14.67    0.03 0.83  13.14  14.15  14.64  15.21  16.33   874  1.0
tu     2.53    0.03 0.75   1.54   1.99   2.38   2.86   4.39   735 1.01
lp__ -12.64    0.04 1.13 -15.63 -13.05 -12.31 -11.86 -11.53   635 1.01

Samples were drawn using NUTS at Mon Jan 29 15:18:04 2018.
For each parameter, n_eff is a crude measure of effective sample size,
and Rhat is the potential scale reduction factor on split chains (at
convergence, Rhat=1).
```

- Make sure to check the diagnostics provided!
  - The value of *Rhat* should be close to 1 (or slightly higher)
  - The number of effective samples (*n_eff*) should not be small

Interpreting the output of STAN

- We can plot the posterior distributions using `fit.plot()`



- Extract the samples from the posterior distribution:

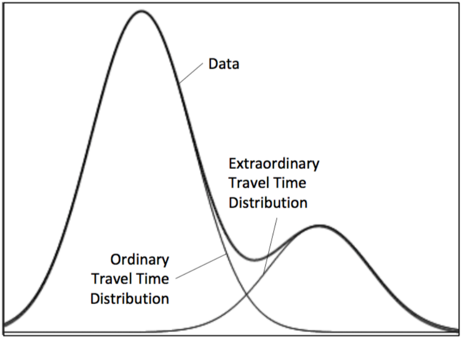
```
samples = fit.extract(permuted=True)
```

Playtime!

- The basics of STAN and PyStan (Section 1 of the notebook)
- First STAN model: Cyclist's daily travel times (Sections 2.1 and 2.2)
  - See "4 - Probabilistic Programming with STAN.ipynb" notebook
  - Only until Section 2.2 (inclusive)!
  - Expected duration: 45 minutes

Case study: Analyzing a cyclist's daily travel times

- A single Gaussian distribution might not be the best choice...
  - Ocasional extraordinary circumstances (e.g. flat tire or a road closed by construction) often add a substantial amount to the usual travel time



Case study: Analyzing a cyclist's daily travel times

- Mixture model with two Gaussians
  - First Gaussian models the travel time of ordinary trips

$$\mathcal{N}(at_o, tu_o)$$

  - Second Gaussian models abnormal travel times

$$\mathcal{N}(at_a, tu_a)$$

  - Latent Bernoulli variable z_n indicates which mixture component was responsible for the each outcome tt_n

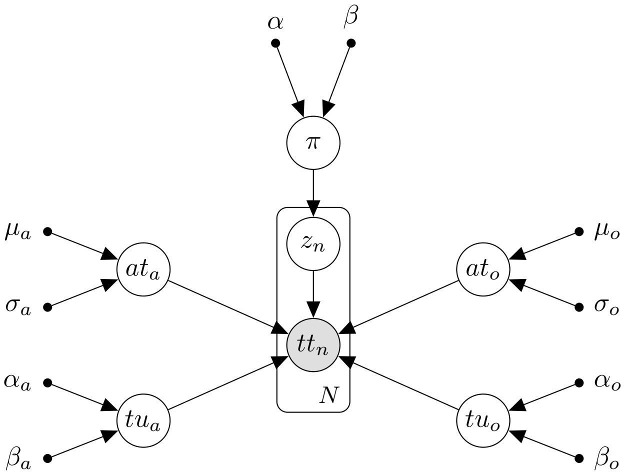
$$z_n \sim \text{Bernoulli}(z_n|\pi)$$

  - Variable π controls mixing proportions, where $\pi \sim \text{Beta}(\pi|\alpha, \beta)$
- The likelihood becomes

$$\begin{aligned} p(tt_n|at_o, tu_o, at_a, tu_a) &= p(z_n = 1)\,\mathcal{N}(at_o, tu_o) + p(z_n = 0)\,\mathcal{N}(at_a, tu_a) \\ &= \pi\,\mathcal{N}(at_o, tu_o) + (1 - \pi)\,\mathcal{N}(at_a, tu_a) \end{aligned}$$

Case study: Analyzing a cyclist's daily travel times

- The graphical model becomes



Case study: Analyzing a cyclist's daily travel times

- Corresponding generative process

  1. Draw average travel time for ordinary days $at_o \sim \mathcal{N}(at_o|\mu_o, \sigma_o^2)$
  2. Draw traffic uncertainty for ordinary days $tu_o \sim \mathcal{IG}(tu_o|\alpha_o, \beta_o)$
  3. Draw average travel time for abnormal days $at_a \sim \mathcal{N}(at_a|\mu_a, \sigma_a^2)$
  4. Draw traffic uncertainty for abnormal days $tu_a \sim \mathcal{IG}(tu_a|\alpha_a, \beta_a)$
  5. Draw mixing proportions $\pi \sim \text{Beta}(\pi|\alpha, \beta)$
  6. For each day $n \in \{1, \ldots, N\}$
     (a) Decide type of day $z_n \sim \text{Bernoulli}(z_n|\pi)$
     (b) If $z_n = 1$
         Draw ordinary travel time $tt_n \sim \mathcal{N}(tt_n|at_o, tu_o)$
     (c) If $z_n = 0$
         Draw abnormal travel time $tt_n \sim \mathcal{N}(tt_n|at_a, tu_a)$

Playtime!

- Mixture model of cyclist's daily travel times (Sections 2.3 and 2.4)
- K-means clustering (Part 2 of the notebook)
    - See “4 - Probabilistic Programming with STAN.ipynb" notebook
    - Expected duration: 45 minutes