Stan Part 2

More Complex Models

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SCHOOL of DATA SCIENCE

Outline

- Stan Review
- Complex Models in Stan

Go to resources, download Stan + R file

Stan Review

<u>Data Block –</u>

- Define each piece of data that goes into your model.
- Not only do you input data here, you should also input hyperparameters and auxillary values.
  - Like sample size, or any other counts.
- Must provide exact type and constraints on the values.

```
data {
        int<lower=0> N;
        vector[N] y;
}
parameters {
        real mu;
        real<lower=0> sigma;
}
model {
        y ~ normal(mu, sigma);
}
```

Stan Review

<u>Parameters Block –</u> lowest level here (not transformations)

- Define the parameters in your model.
- Provide the type and constraints
- No transformed/functions of parameters, that goes into the transformed parameters block.

```
data {
        int<lower=0> N;
        vector[N] y;
}
parameters {
        real mu;
        real<lower=0> sigma;
}
model {
        y ~ normal(mu, sigma);
}
```

Stan Review

Model Block –

- This is where you specify the prior distributions and the likelihoods.
- You can use any data, parameters or transformed parameters in these calculations.
- Stan processes code in order. So, you need to specify priors, then specify your likelihoods.

think order reading down ↓

```
data {
        int<lower=0> N;
        vector[N] y;
}
parameters {
        real mu;
        real<lower=0> sigma;
}
model {                    E[x]   stndv
        y ~ normal(mu, sigma);
}
```

All stan models result in posterior value

Just est mu, sigma of a normal dist

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Linear Regression in Stan

i = obsv #

vector prod

$$y_i = \boldsymbol{x}_{\mathbf{i}}\boldsymbol{\beta} + \varepsilon_i$$

– classic model

Dist of outcome given params matters

Dist of X_i = not matter, treat as fixed + known

which is $\varepsilon_i \sim N(0, \sigma^2)$

Consider the humble linear regression. First, let's determine what counts as data here:

- y – vector of length N, taking real values with no constraints
- $\mathbf{X}$ – Matrix of dimensions $N \times p$, real values with no constraints.

→ Dist not matter

Auxiliary information:

- N – number of observations. Positive integer.
- p – number of predictor variables. Positive integer.

set these bc stan not read these off the matrix

Go into data block

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Data Block for Linear Regression

- y – vector of length N, taking real values with no constraints
- $\mathbf{X}$ – Matrix of dimensions $N \times p$, real values with no constraints.

Auxiliary information:

- N – number of observations. Positive integer.
- p – number of predictor variables. Positive integer.

```
data {
	int<lower=0> N;
	int<lower=0> p;
	vector[N] y;
	matrix[N, p] X;
}
```

Linear Regression in Stan

$$y_i = \boldsymbol{x}_{\mathbf{i}}\boldsymbol{\beta} + \varepsilon_i$$
$$\varepsilon_i \sim N(0, \sigma^2)$$

Now, what about the parameters?

- $\vec{\boldsymbol{\beta}}$ – vector of length p, real values, no constraints
- σ^2 - positive real value.

β_0 = callup vector so $\vec{\beta}$ is not pt'l
in $\vec{X}$

$$X = \begin{bmatrix} 1 & x_1 & x_2 & x_3 & \cdots \\ 1 & \vdots & \vdots & \vdots & \\ 1 & \vdots & \vdots & \vdots & \cdots \end{bmatrix}$$

```
data {
        int<lower=0> N;
        int<lower=0> p;
        vector[N] y;
        matrix[N, p] X;
}
parameters {
        vector[p] betas;
        real<lower=0> sigma;
}
```

vectors default to real vals

↳ next slide

If want to express like $y = B_0 + \vec{X}\vec{B} + \varepsilon$ would add real B_0 into parameters

Priors for Linear Regression in Stan

Multivariate prior on $\boldsymbol{\beta}$ – would like

- Needs to cover the real line
- Let's use independent normals.
- Note: Stan is vectorized, so that prior spec applies the same prior to all βs

Positive Real Valued prior on σ^2

- Let's use a half Cauchy here
- Because σ is constrained at 0, this leads to a half Cauchy

- use variable names not hard coded, put vars in data section

```
model {
        betas ~ normal(0,10);
        sigma ~ cauchy(0,5);
}
```

weakly uninformative

bc in prev slide var is ≥ 0

no defined E[X] → use Cauchy for variance to be uninformative

Model for Linear Regression in Stan

$$y_i = \boldsymbol{x}_{\mathbf{i}}\boldsymbol{\beta} + \varepsilon_i$$
$$\varepsilon_i \sim N(0, \sigma^2)$$

(A) Mean $= \vec{X}\vec{\beta}$

Var $= \sigma^2$ bc adding scalar which only changes $E[\,]$

What is the likelihood here:

- y_i is distributed as a normal variable with mean $\boldsymbol{x}_{\mathbf{i}}\boldsymbol{\beta}$
- Why? Think about rules of expectations.

```
model {
        betas ~ normal(0,10);
        sigma ~ cauchy(0,5);
        y ~ normal(X * betas, sigma);
}
```

n×p, p

mean

order matters

n×p · p

Note: for $E[\,]$

$E[a+X] = a + E[X]$

Here $E[y] = E[X\beta + \varepsilon] = E[\varepsilon] + X\beta = X\beta$

$= (A)$

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All Together

```
data {
	int<lower=0> N;
	int<lower=0> p;
	vector[N] y;
	matrix[N, p] X;
}
parameters {
	vector[p] betas;
	real<lower=0> sigma;
}
model {
	betas ~ normal(0,10);
	sigma ~ cauchy(0,5);
	y ~ normal(X * betas, sigma);
}
```

All Together

Generated data with the following:

- 1 intercept of value 2, 2 predictors with betas of .5 and 1.5.
- Sigma is .5
- 200 observations.

within stds

Summary function applied to fit model - 1st 3 columns

	mean	se_mean	sd
betas[1]	2.006755	0.000572	0.036063
betas[2]	0.47539	0.00057	0.036495
betas[3]	1.519859	0.000524	0.03538
sigma	0.500919	0.000406	0.025694
lp__	38.25616	0.030454	1.404715

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Generalized Linear Model

y was a continuous variable, which meant that linear regression is appropriate.

- How about if y is dichotomous?
- Or a count?

Stan makes changing the response distribution very easy.

```
data {
        int<lower=0> N;
        int<lower=0> p;
        array[N] int<lower=0, upper=1> y;
        matrix[N, p] X;
}
parameters {
        vector[p] betas;
}
model {
        betas ~ normal(0,10);
        //For a logistic regression
        y ~ bernoulli_logit(X * betas);
}
```

Logistic regression

Assume: y = Bernoulli

$P(y=1) = \text{invLogit}(X\vec{\beta})$

(not put in sigma bc error rolled into that prob)

Generalized Linear Model

y was a continuous variable, which meant that linear regression is appropriate.

- How about if y is dichotomous?

want model

$\boxed{E(Y) = \lambda}$

- Or a count? Poisson (λ) $Var = \frac{1}{\lambda}$

Stan makes changing the response distribution very easy.

```
data {
        int<lower=0> N;
        int<lower=0> p;
        array[N] int<lower=0> y;
        matrix[N, p] X;
}
parameters {
        vector[p] betas;
}
model {
        betas ~ normal(0,10);
        //For a Poisson regression
        //0 is for intercept, as that is in
        //the betas
        y ~ poisson_log_glm(X, 0, betas);
}
```

param intercept but have intercept in $X_{n \times p}$ so $= 0$

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Generalized Linear Model

Estimates - not quite, but ok, is expected, w/in stdv range

Generated 1000 observations:

- Betas: 0, .25, -.25
- Outcome, logistic y.

	mean	se_mean	sd
betas[1]	-0.10199	0.00097	0.063958
betas[2]	0.250536	0.001123	0.066339
betas[3]	-0.20258	0.001138	0.066409
lp__	-682.011	0.026912	1.248414

Generated 1000 observations:

- Betas: 2, 3, -2 → this pattern: pos, pos, neg
  int   1st pred   last pred
- Outcome: Poisson y.
- Note: Coefficients are in log form.

	mean	se_mean	sd
betas[1]	pos ✓ 0.52455	0.000543	0.027194
betas[2]	pos ✓ 0.803861	0.000385	0.019549
betas[3]	neg ✓ -0.51686	0.000396	0.01998
lp__	1090.908	0.030559	1.250715

so fit bc pattern

Training/Testing in Stan

Cross-validation is an important component of any DS stack.

- Train our model on some set of data.
- Test the performance of our model on a new set of data.

In Bayes, we can compute the posterior predictive distribution:

- Given our posteriors, what are our predictions for a new set of data.

uncertainty in ↗

In Stan:

- We can input our new data as part of our data block.
- Then use the generated quantities block to sample our predictions.

to calc pred for testing

Training/Testing in Stan

In Stan:

- We can input our new data as part of our data block.
- Then use the generated quantities block to sample our predictions.

Generated quantities:

- No impact on model fit.
- Can be extracted with `extract` in R

– entire traces for all params

Exp

```
data {
        int<lower=0> N;
        int<lower=0> Nt
        int<lower=0> p;
        vector[N] y;
        matrix[N, p] X;
        matrix[N_t, p] X_tilde;
        matrix[N_t, p] Y_tilde;

}
//Parameters and model block are the same
generated quantities {
        vector[N_t] tilde_y = X_tilde * betas;
        vector[N_t] error = Y_tilde - tilde_y;
}
```

→ # training

→ # testing

training

~~matrix~~ vector

→ no impact on model fit

pred val:

not take into account error

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Training/Testing in Stan

Linear regression:

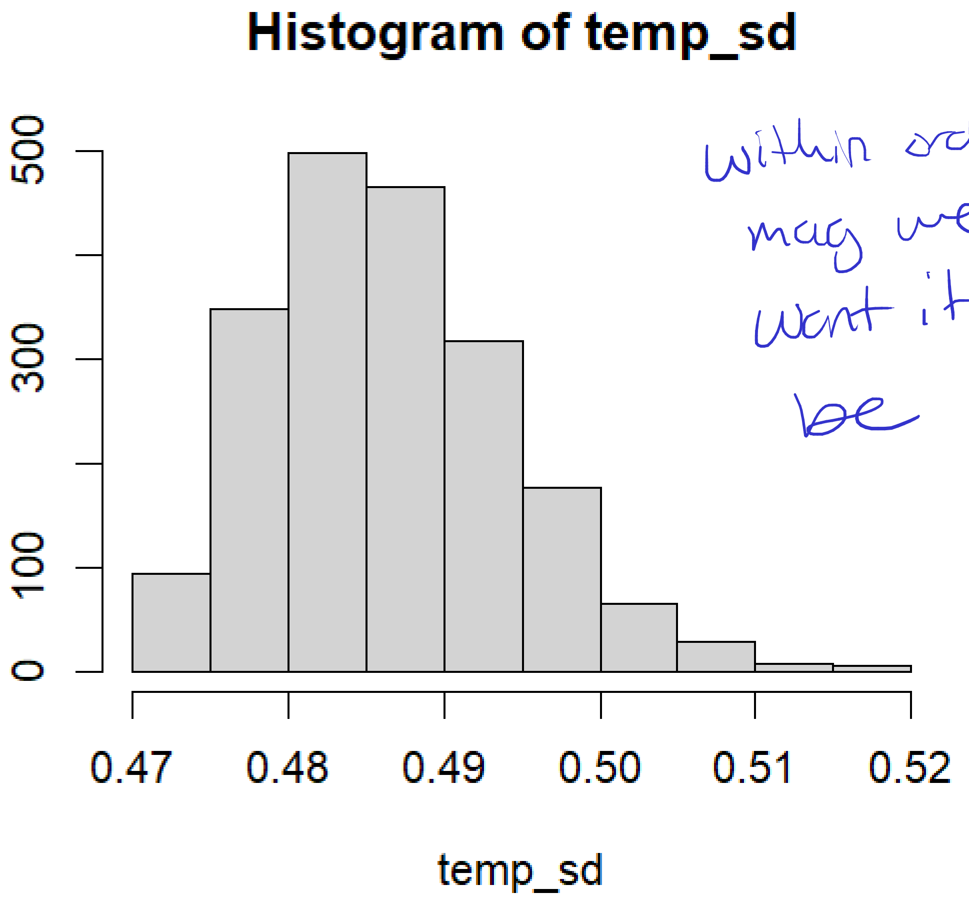
- 50 testing samples

Plot the distribution of estimated testing error standard deviations

- This should be approximately .5

Slight underestimate of testing error residual…

- Result of the prior choice with small sample (100 training)



within order mag we want it to be

K-Fold Validation in Stan

- You can program a random split procedure into any Stan model.
- First, we need to define a user function that can generate permutations of the data.

functions block-

- Define user functions in C++ type notation.

```
functions {                    new function ↓ (vect indices + permute)
  array[] int permutation_rng(int N) {
    array[N] int y;            return array
    for (n in 1 : N) {
      y[n] = n;                take 1st n samples
    }
    vector[N] theta = rep_vector(1.0 / N, N);   prob of selection
    for (n in 1 : size(y)) {
      int i = categorical_rng(theta);
      int temp = y[n];         ← reassign
      y[n] = y[i];             ← swap      this permutes
      y[i] = temp;
    }
    return y;
  }                            ↳ new set of permuted indices
}
```

K-Fold Validation in Stan

Next, we need to use that function:

- In the transformed data block, we use the permutation function to define testing and training sets.

Equiv to selecting at random n traing and n testing

```
data {
  int<lower=0> N;
  int<lower=0> p;
  matrix[N,p] x;
  vector[N] y;
  int<lower=0, upper=N> N_test;
}
transformed data {
int N_train = N - N_test;
array[N] int permutation = permutation_rng(N);
matrix[N_train,p] x_train = x[permutation[1 : N_train],];
vector[N_train] y_train = y[permutation[1 : N_train]];
matrix[N_test,p] x_test = x[permutation[N_train + 1 : N],];
vector[N_test] y_test = y[permutation[N_train + 1 : N]];
}
```

do opperations on data

subset of data

everything left over

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K-Fold Validation in Stan

Next, we need to use that function:

- In the transformed data block, we use the permutation function to define testing and training sets.

get view uncertainty in pred

This setup will compile into a model that randomly selects N_test testing cases each time its run.

Gives diff fold when run model

```
model {
    // Same priors as before
    betas ~ normal(0,10);
    sigma ~ cauchy(0,5);
    y_train ~ normal(x_train*betas, sigma);
}
generated quantities {
  vector[N_test] y_test_sim =
        as_vector(normal_rng(x_test*betas,
sigma));
  vector[N_test] err = y_test_sim -
x_test*betas;
}
```

using training

simulated predictions

post predicted dist in full

generate normal var for every w/ mean and sigma

Summary and Important Concepts

Stan is a strongly typed language: Be careful as to how you define different variables.

New Block Types:

- functions – User defined functions.
- transformed data – Manipulations of provided data.
- transformed parameters – Manipulations of parameters.
- generated quantities – Any output you want after the model is done. (call fitting done)
  - Usually for predictive distributions…

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Next Time

No class 10/8 and 10/10 (I'm away at a conference)

- Review course materials!
- Play around with Stan!

No class 10/15 – University Reading Days!

Next Class: 10/17

- Midterm Review! – He will be here

<u>Midterm: 10/22</u>