Model comparison example

For $\cot^{-1}\phi \in (1, 4)$

- $\phi \sim \mathrm{TruncatedNormal}(\mu_\phi, \sigma_\phi, 0, 90)$
- $\phi \sim \mathrm{Uniform}(\cot^{-1}4, \cot^{-1}1)$
- $\cot(\phi) \sim \mathrm{Uniform}(1, 4)$

[1]
```
import numpy as np
import scipy.stats as st
import pandas as pd
import pymc3 as pm
import theano.tensor as tt
import matplotlib.pyplot as plt
import seaborn as sns
```

```
Could not import matplotlib.animation 'ascii' codec can't decode byte
0xc2 in position 90: ordinal not in range(128)
```

[2]
```
cot = lambda phi: 1 / np.tan(np.radians(phi))
acot = lambda a: np.degrees(np.arctan(1 / a))
```

Define some core values to ensure consistent samples:

Dataset creation

We'll create a series of mock datasets, each corresponding to a different possible reality. We choose to truncate each dataset to between $\cot^{-1}4$ and $\cot^{-1}1$.

The normally distributed dataset is chosen to be close to the cot-uniform dataset.

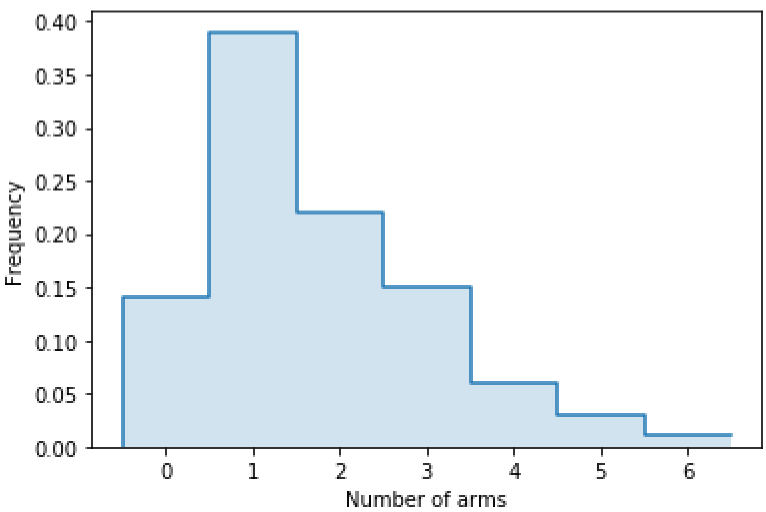
[3]
```
np.random.seed(0)

# number of galaxies in the sample
N_GALS = 100
# Mean number of arms per galaxy
MU_N_ARMS = 1.7
```

```
# normal_dataset
MU_PHI = 14.76377094845352
# inter-galaxy pitch angle std (between galaxies in the sample)
SD_PHI = 12.775146676186282
# intra-galaxy pitch angle std (between arms in the galaxy)
SD_GAL = 10
```

[4]

```
# generate a number of arms for each galaxy
n_arms = st.poisson(MU_N_ARMS).rvs(N_GALS)
# and an array of galaxy index for each arm
gal_arm_map = np.concatenate([
    np.tile(i, n_arms[i])
    for i in range(len(n_arms))
])
def get_arm_pas(gal_pa, n=1, sd=SD_GAL, lower=0, upper=90):
    a = (lower - gal_pa) / SD_PHI
    b = (upper - gal_pa) / SD_PHI
    return st.truncnorm(a, b, loc=gal_pa, scale=sd).rvs(n)
```



First, `normal_dataset` consists of galaxies with pitch angles drawn from a Normal distribution

[6]

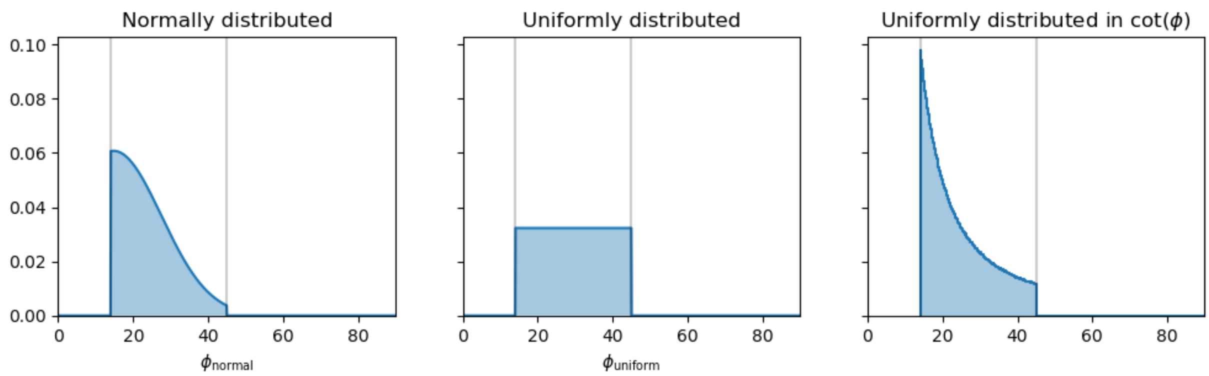
```
normal_dist = st.truncnorm(
    a=(acot(4)-MU_PHI) / SD_PHI, b=(acot(1) - MU_PHI) / SD_PHI,
    loc=MU_PHI, scale=SD_PHI
)
normal_dataset = normal_dist.rvs(N_GALS)
normal_arms = np.concatenate([
    get_arm_pas(gal_pa, n)
    for n, gal_pa in zip(n_arms, normal_dataset)
])
```

Second, the dataset with ϕ uniform between $\cot^{-1}(4) \simeq 14.35°$ and $\cot^{-1}(4) \simeq 57.3°$, which will be called the `uniform_dataset`

```
[7]
uniform_dist = st.uniform(loc=acot(4), scale=(acot(1) - acot(4)))
uniform_dataset = uniform_dist.rvs(N_GALS)
uniform_arms = np.concatenate([
    get_arm_pas(gal_pa, n)
    for n, gal_pa in zip(n_arms, uniform_dataset)
])
```

Finally, we have the dataset that is uniform for $\cot\phi \in [1, 4]$, `cot_uniform_dist`

```
[8]
__cot_uniform_dist = st.uniform(loc=1, scale=4 - 1)
def cot_uniform_dist_rvs(N):
    return acot(__cot_uniform_dist.rvs(N))
cot_uniform_dataset = cot_uniform_dist_rvs(len(n_arms))
cot_uniform_arms = np.concatenate([
    get_arm_pas(gal_pa, n)
    for n, gal_pa in zip(n_arms, cot_uniform_dataset)
])
```



The simple way

Given a distribution of galaxy pitch angles, we want to ask *"does this data look like it has been drawn from this distribution?"* We can achieve this using the Kolmogorov-Smirnov test. Note that the null hypothesis is that the dataset **is** drawn from the distribution being tested, so we are interested in small p-values.

```
[60]
types = ('Normal', 'Uniform', 'Cot Uniform')
```

```python
output = pd.DataFrame(
    [], dtype=float,
    index=[f'{i} Dataset' for i in types],
    columns=[f'{i} Model' for i in types],
)
for dataset, dataset_type in zip(
    (normal_dataset, uniform_dataset, cot_uniform_dataset),
    (f'{i} Dataset' for i in types)
):
    p_norm = st.truncnorm.fit(
        dataset,
        (acot(4)-15) / 10, (acot(1) - 15) / 10, loc=20, scale=10
    )
    p_uniform = st.uniform.fit(dataset)
    p_cot_uniform = st.uniform.fit(cot(dataset))
    output.loc[dataset_type] = (
        st.kstest(dataset, st.truncnorm(*p_norm).cdf).pvalue,
        st.kstest(dataset, st.uniform(*p_uniform).cdf).pvalue,
        st.kstest(
            cot(dataset),
            st.uniform(*p_cot_uniform).cdf
        ).pvalue,
    )
display(output.round(2))
```

	Normal Model	Uniform Model	Cot Uniform Model
Normal Dataset	0.77	0.00	0.68
Uniform Dataset	0.08	0.48	0.00
Cot Uniform Dataset	0.04	0.00	0.63

We can display this more clearly by stating whether we can reject the null hypothesis (that the data could be from this distribution) at the 10% level:

	Normal Model	Uniform Model	Cot Uniform Model
Normal Dataset	Accept	Reject	Accept
Uniform Dataset	Reject	Accept	Reject
Cot Uniform Dataset	Reject	Reject	Accept

Even at the relatively high 10% level we struggle to reject the possibility that the data was drawn from an incorrect distribution.

Model defininion using Pymc3

An alternative approach is to use Bayesian inference to perform model comparison, either using LOO cross-validation, or Bayes Factors between models (though this is tricky to compute). The problem we will have with LOO is that as we are simply testing which is the most appropriate posterior to use, our models could fit any theoretical distribution, meaning they are not as robust as they ought to be for proper model comparison.

Define the Normal model using `pymc3`:

[11]

```
def make_normal_model(arms, gal_arm_map, name='Normal'):
    with pm.Model(name) as model:
        # one global mean
        mu_phi_scaled = pm.LogitNormal(
            'mu_phi_scaled',
            mu=0, sigma=1.5,
            testval=0.29
        )

        # one global variance
        mu_phi = pm.Deterministic('mu_phi', 90 * mu_phi_scaled)

        # We need to separate inter- and intra- galaxy stds
        # due to galaxy pitch angle sample truncation
        sigma_phi = pm.InverseGamma(
            'sigma_phi',
            alpha=2, beta=20,
            testval=5
        )
        sigma_gal = pm.InverseGamma(
            'sigma_gal',
            alpha=2, beta=20,
            testval=5
        )

        phi_gal = pm.TruncatedNormal(
            'phi_gal',
            mu=mu_phi, sigma=sigma_phi,
            lower=acot(4), upper=acot(1),
            shape=max(gal_arm_map) + 1
        )
```

```
        phi_arm = pm.TruncatedNormal(
            'phi_arm',
            mu=phi_gal[gal_arm_map], sd=sigma_gal,
            lower=0, upper=90,
            shape=len(arms),
            observed=arms,
        )
    return model
```

Define the Uniform model

```
[12]  def make_uniform_model(arms, gal_arm_map, name='Uniform'):
          with pm.Model(name) as model:
              phi_gal = pm.Uniform(
                  'phi_gal',
                  lower=acot(4), upper=acot(1),
                  shape=max(gal_arm_map) + 1
              )
              # intra-galaxy dispersion
              sigma_gal = pm.InverseGamma(
                  'sigma_gal',
                  alpha=2, beta=20, testval=5
              )
              phi_arm = pm.TruncatedNormal(
                  'phi_arm',
                  mu=phi_gal[gal_arm_map], sd=sigma_gal,
                  lower=0, upper=90,
                  observed=arms,
              )
          return model
```

And finaly the Cot-Uniform model

```
[13]  def make_cot_uniform_model(arms, gal_arm_map,
                                     name='CotUniform'):
          with pm.Model(name) as model:
              cot_phi = pm.Uniform(
                  'cot_phi_gal',
                  lower=1, upper=4,
                  shape=max(gal_arm_map) + 1
              )
              phi_gal = pm.Deterministic(
                  'phi_gal', 180 / np.pi * tt.arctan(1 / cot_phi)
              )
              # intra-galaxy dispersion
```

```python
        sigma_gal = pm.InverseGamma(
            'sigma_gal',
            alpha=2, beta=20, testval=5
        )
        phi_arm = pm.TruncatedNormal(
            'phi_arm',
            mu=phi_gal[gal_arm_map], sd=sigma_gal,
            lower=0, upper=90,
            observed=arms,
        )
    return model
```

Inference

We'll test each model against the Normally-distributed sample, and perform some basic model comparison

[14]

```python
# hierarchial models can be tricky to fit
with make_normal_model(normal_arms, gal_arm_map) as normal_model:
    normal_trace = pm.sample(target_accept=0.95)
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Multiprocess sampling (2 chains in 2 jobs)
NUTS: [Normal_phi_gal, Normal_sigma_gal, Normal_sigma_phi,
Normal_mu_phi_scaled]
Sampling 2 chains: 100%|██████████| 2000/2000 [01:14<00:00,
26.89draws/s]
The estimated number of effective samples is smaller than 200 for some
parameters.
```

[15]

```python
with make_uniform_model(normal_arms, gal_arm_map) as
uniform_model:
    uniform_trace = pm.sample(target_accept=0.95)
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Multiprocess sampling (2 chains in 2 jobs)
NUTS: [Uniform_sigma_gal, Uniform_phi_gal]
Sampling 2 chains: 100%|██████████| 2000/2000 [00:32<00:00,
62.25draws/s]
```

[16]

```python
with make_cot_uniform_model(normal_arms, gal_arm_map) as
cot_uniform_model:
    cot_uniform_trace = pm.sample(target_accept=0.95)
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Multiprocess sampling (2 chains in 2 jobs)
NUTS: [CotUniform_sigma_gal, CotUniform_cot_phi_gal]
Sampling 2 chains: 100%|██████████| 2000/2000 [00:27<00:00,
73.86draws/s]
```

Now perform the comparison!

[46]

```python
pm.compare({normal_model: normal_trace, uniform_model:
uniform_trace, cot_uniform_model: cot_uniform_trace}, ic='LOO')
```

```
/Users/tlingard/anaconda3/lib/python3.6/site-
packages/pymc3/stats.py:558: FutureWarning: arrays to stack must be
passed as a "sequence" type such as list or tuple. Support for non-
sequence iterables such as generators is deprecated as of NumPy 1.16 and
will raise an error in the future.
  ics.append((n, ic_func(t, m, pointwise=True)))
/Users/tlingard/anaconda3/lib/python3.6/site-
packages/pymc3/stats.py:300: UserWarning: Estimated shape parameter of
Pareto distribution is
        greater than 0.7 for one or more samples.
        You should consider using a more robust model, this is because
        importance sampling is less likely to work well if the marginal
        posterior and LOO posterior are very different. This is more
likely to
        happen with a non-robust model and highly influential
observations.
  happen with a non-robust model and highly influential
observations.""")
/Users/tlingard/anaconda3/lib/python3.6/site-
packages/pymc3/stats.py:300: UserWarning: Estimated shape parameter of
Pareto distribution is
        greater than 0.7 for one or more samples.
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        importance sampling is less likely to work well if the marginal
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/Users/tlingard/anaconda3/lib/python3.6/site-
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Pareto distribution is
        greater than 0.7 for one or more samples.
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        importance sampling is less likely to work well if the marginal
```
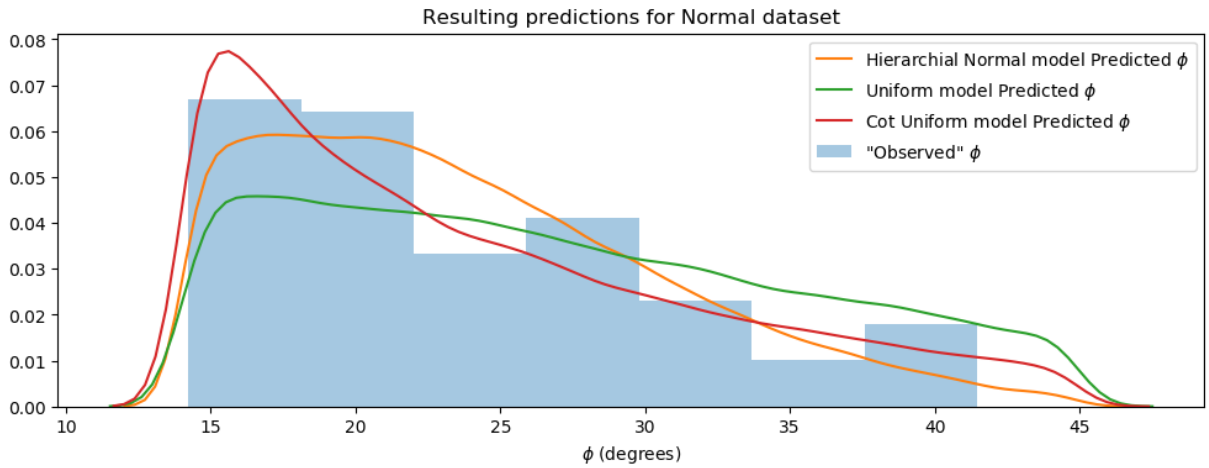

```
        posterior and LOO posterior are very different. This is more
likely to
        happen with a non-robust model and highly influential
observations.
  happen with a non-robust model and highly influential
observations.""")
```

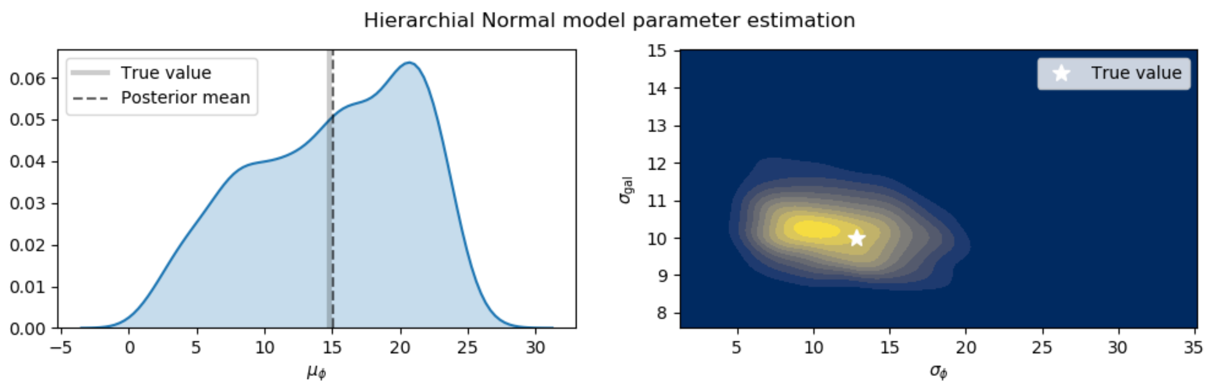
	LOO	pLOO	dLOO	weight	SE	dSE	shape_
Normal	1315.53	34.56	0	0.86	17.09	0	1
CotUniform	1317.54	40.43	2.01	0.08	17.23	3.58	1
Uniform	1329.74	43.74	14.21	0.06	16.34	7.96	1

We can see that the Hierarchial Normal model is preferred here, though as the models are only vaguely specified we end up with a lot of warnings.

What does the posterior on Galaxy pitch angle look like for the different models?



Hierarchial model results



It looks like the model has found the most likely solution, but with slight issues with spread and divergences.

Cot-uniform dataset

Can we still identify the correct model for the cot-uniform dataset?

[47]

```
# hierarchial models can be tricky to fit
with make_normal_model(cot_uniform_arms, gal_arm_map) as
normal_model2:
    normal_trace2 = pm.sample(target_accept=0.95)
with make_uniform_model(cot_uniform_arms, gal_arm_map) as
uniform_model2:
    uniform_trace2 = pm.sample(target_accept=0.95)
with make_cot_uniform_model(cot_uniform_arms, gal_arm_map) as
cot_uniform_model2:
    cot_uniform_trace2 = pm.sample(target_accept=0.95)
pm.compare({normal_model2: normal_trace2, uniform_model2:
uniform_trace2, cot_uniform_model2: cot_uniform_trace2},
ic='LOO')
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Multiprocess sampling (2 chains in 2 jobs)
NUTS: [Normal_phi_gal, Normal_sigma_gal, Normal_sigma_phi,
Normal_mu_phi_scaled]
The acceptance probability does not match the target. It is
0.902747183008485, but should be close to 0.95. Try to increase the
number of tuning steps.
The estimated number of effective samples is smaller than 200 for some
parameters.
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Multiprocess sampling (2 chains in 2 jobs)
NUTS: [Uniform_sigma_gal, Uniform_phi_gal]
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Multiprocess sampling (2 chains in 2 jobs)
NUTS: [CotUniform_sigma_gal, CotUniform_cot_phi_gal]
/Users/tlingard/anaconda3/lib/python3.6/site-
packages/pymc3/stats.py:558: FutureWarning: arrays to stack must be
passed as a "sequence" type such as list or tuple. Support for non-
sequence iterables such as generators is deprecated as of NumPy 1.16 and
will raise an error in the future.
```

```
  ics.append((n, ic_func(t, m, pointwise=True)))
/Users/tlingard/anaconda3/lib/python3.6/site-
packages/pymc3/stats.py:300: UserWarning: Estimated shape parameter of
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        happen with a non-robust model and highly influential
observations.
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/Users/tlingard/anaconda3/lib/python3.6/site-
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        posterior and LOO posterior are very different. This is more
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/Users/tlingard/anaconda3/lib/python3.6/site-
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        importance sampling is less likely to work well if the marginal
        posterior and LOO posterior are very different. This is more
likely to
        happen with a non-robust model and highly influential
observations.
  happen with a non-robust model and highly influential
observations.""")
```
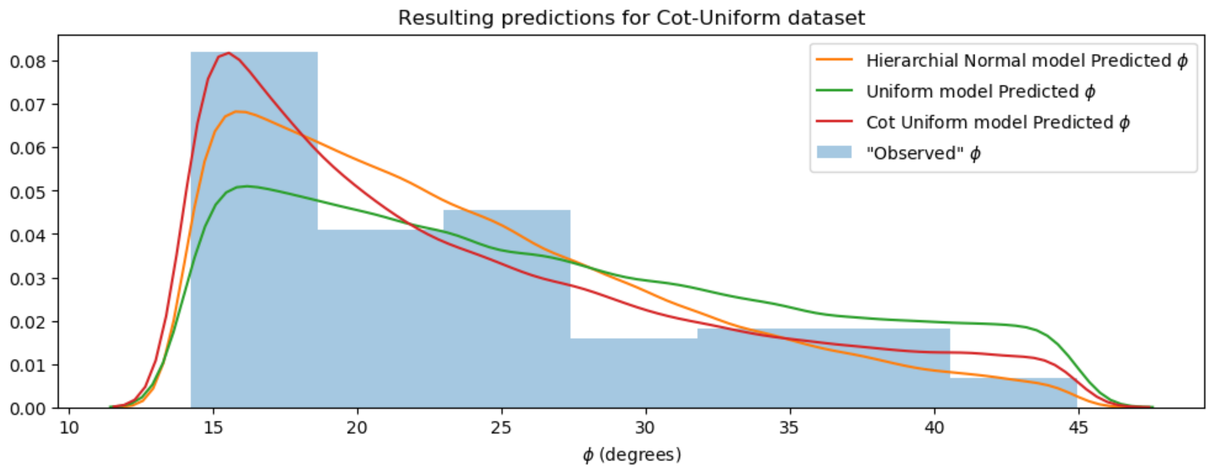

	LOO	pLOO	dLOO	weight	SE	dSE	shape_
CotUniform	1304.77	43.05	0	0.83	16.25	0	1
Normal	1307.57	37.47	2.8	0	16.32	2.88	1
Uniform	1315.62	45.26	10.85	0.17	14.8	8.13	1


Resulting predictions for Cot-Uniform dataset
Hierarchial Normal model Predicted ϕ
Uniform model Predicted ϕ
Cot Uniform model Predicted ϕ
"Observed" ϕ
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
10
15
20
25
30
35
40
45
ϕ (degrees)

Yes we can!!