In [1]:
```
# Imports
import pymc3 as pm
import numpy.random as npr
import numpy as np
import matplotlib.pyplot as plt
import matplotlib as mpl
from collections import Counter
import seaborn as sns
import missingno as msno

# Set plotting style
# plt.style.use('fivethirtyeight')
sns.set_style('white')
sns.set_context('poster')

%load_ext autoreload
%autoreload 2
%matplotlib inline
%config InlineBackend.figure_format = 'retina'

import warnings
warnings.filterwarnings('ignore')
```

In [2]:
```
import pyqrcode as pq
icon = pq.create('https://ericmjl.github.io/bayesian-stats-talk')
icon.png('images/qrcode.png', scale=6)
```

# Bayesian Statistical Analysis with PyMC3

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PyCon 2017, Portland, OR

- HTML Notebook on GitHub: **ericmjl**.github.io/**bayesian-stats-talk** (https://ericmjl.github.io/bayesian-stats-talk)
- Twitter: @ericmjl (https://twitter.com/ericmjl)

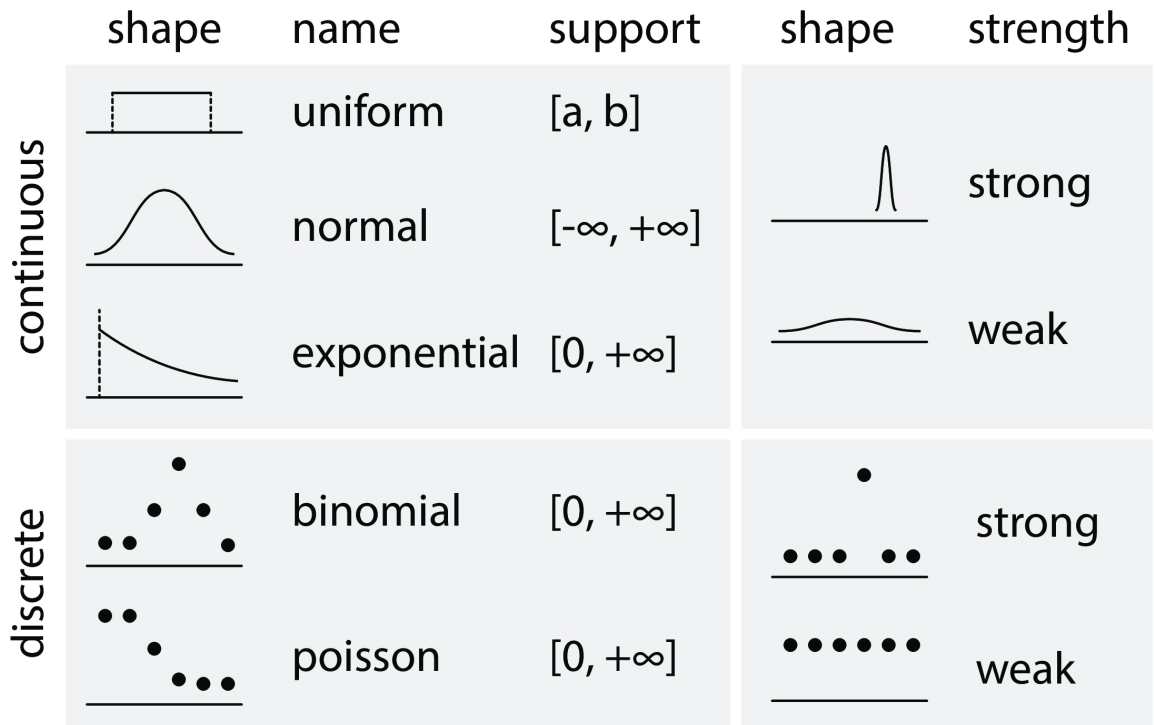
## talk features

- **minimal field jargon:** let's focus on the mechanics of analysis, rather than the terminology. *e.g. won't explain A/B testing, spike & slab regression, conjugate distributions...*
- **pareto principle:** the basics will get you to 80% of what you'll need
- **enjoy the talk:** focus on Bayes, get code later!

## assumed knowledge

- familiarity with Python:
  - objects & methods
  - context manager syntax

- knowledge of basic stats terminology:
  - mean
  - variance
  - interval




## the obligatory Bayes rule slide

$$P(H|D) = \frac{P(D|H)P(H)}{P(D)}$$

- $P(H|D)$: Probability that the hypothesis is true given the data.
- $P(D|H)$: Probability of the data arising given the hypothesis.
- $P(H)$: Probability that the hypothesis is true, globally.
- $P(D)$: Probability of the data arising, globally.

## bayesian thinking

update beliefs having seen the evidence

## `pymc3`

- Library of **statistical distributions**, **sampling algorithms**, and **syntax** for specifying statistical models
- Everything in Python!

### computation-powered Bayesian stats

- Bayesian statistics was infeasible because of **complicated integrals** needed to compute **posterior distributions**.
- **M**arkov **C**hain **M**onte **C**arlo (MCMC) sampling enables us to **estimate shape of posterior distributions**; calculus not required.

# common statistical analysis problems

- **parameter estimation**: "is the true value equal to X?"

- **comparison between experimental groups**: "are the treatments different from the control(s)?"

# problem type 1: parameter estimation

"is the true value equal to X?"

OR

"given the data, for the parameter of interest, what is the probability distribution over the possible values?"

# example 1: the obligatory coin toss problem

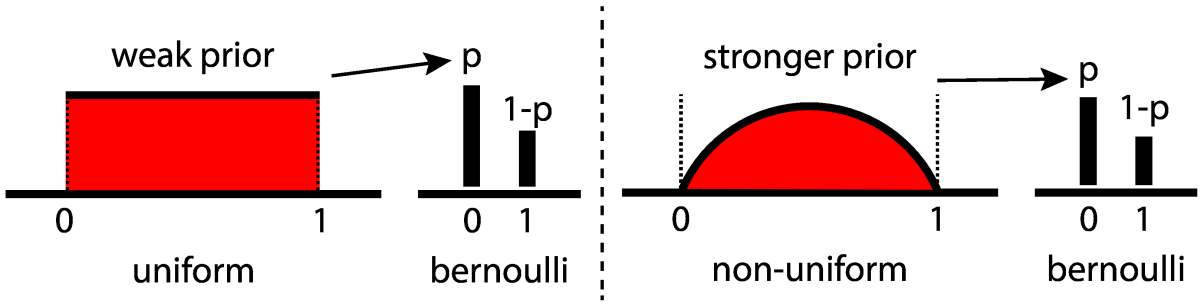
I tossed my coin $n$ times, and it came up as heads $h$ times. Is it biased?

## parameterized problem

"I want to know $p$, the probability of tossing heads. Given $n$ tosses and $h$ observed heads, is it probable that the value of $p$ is close to $0.5$ , say, in the interval $[0.48, 0.52]$?"

## prior

- prior belief about parameter: $p \sim Uniform(0, 1)$
- likelihood function: $data \sim Bernoulli(p)$




In [3]:
```
# Make the data needed for the problem.
from random import shuffle
total = 30
n_heads = 11
n_tails = total - n_heads
tosses = [1] * n_heads + [0] * n_tails
shuffle(tosses)
```

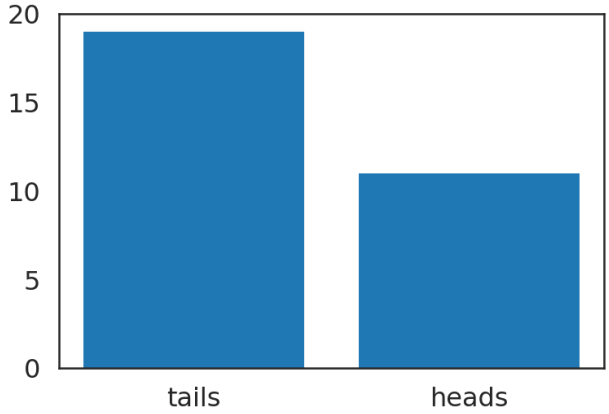
## data

In [4]:
```
print(tosses)
```

```
[1, 0, 0, 1, 1, 0, 1, 0, 0, 0, 0, 0, 0, 1, 0, 1, 1, 1, 0, 1, 0, 0, 0, 1, 1,
0, 0, 0, 0, 0]
```

In [5]:
```
def plot_coins():
    fig = plt.figure()
    ax = fig.add_subplot(1,1,1)
    ax.bar(list(Counter(tosses).keys()), list(Counter(tosses).values()))
    ax.set_xticks([0, 1])
    ax.set_xticklabels(['tails', 'heads'])
    ax.set_ylim(0, 20)
    ax.set_yticks(np.arange(0, 21, 5))
    return fig
```

In [6]:
```
fig = plot_coins()
plt.show()
```




## code

In [7]:
```
# Context manager syntax. `coin_model` is **just**
# a placeholder
with pm.Model() as coin_model:
    # Distributions are PyMC3 objects.
    # Specify prior using Uniform object.
    p_prior = pm.Uniform('p', 0, 1)

    # Specify likelihood using Bernoulli object.
    like = pm.Bernoulli('likelihood', p=p_prior,
                        observed=tosses)
                        # "observed=data" is key
                        # for likelihood.
```

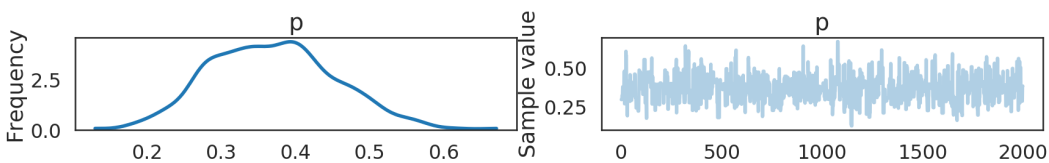
## MCMC Inference Button (TM)

In [8]:
```
with coin_model:
    # don't worry about this:
    step = pm.Metropolis()

    # focus on this, the Inference Button:
    coin_trace = pm.sample(2000, step=step)
```

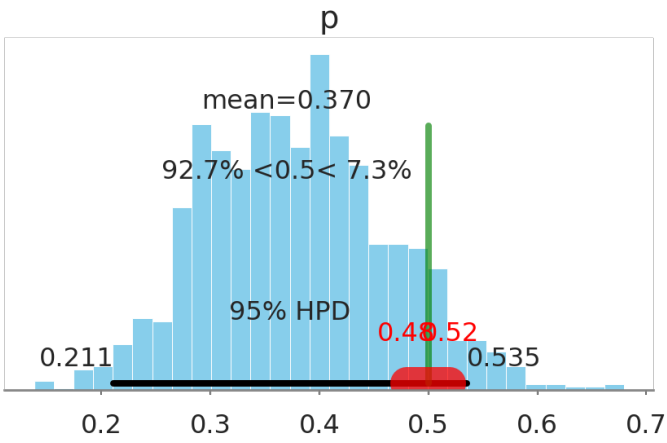
```
100%|██████████| 2500/2500 [00:00<00:00, 5844.85it/s]
```

## results

In [9]:
```
pm.traceplot(coin_trace)
plt.show()
```



In [10]:
```
pm.plot_posterior(coin_trace[100:], color='#87ceeb',
                  rope=[0.48, 0.52], point_estimate='mean',
                  ref_val=0.5)
plt.show()
```




- **95% highest posterior density (HPD)** encompasses the **region of practical equivalence (ROPE)**.
- GET MORE DATA!

# pattern

1. parameterize your problem using statistical distributions
2. justify your model structure
3. write model in PyMC3, hit the **Inference Button**™
4. interpret based on posterior distributions
5. (optional) with new information, modify model structure.

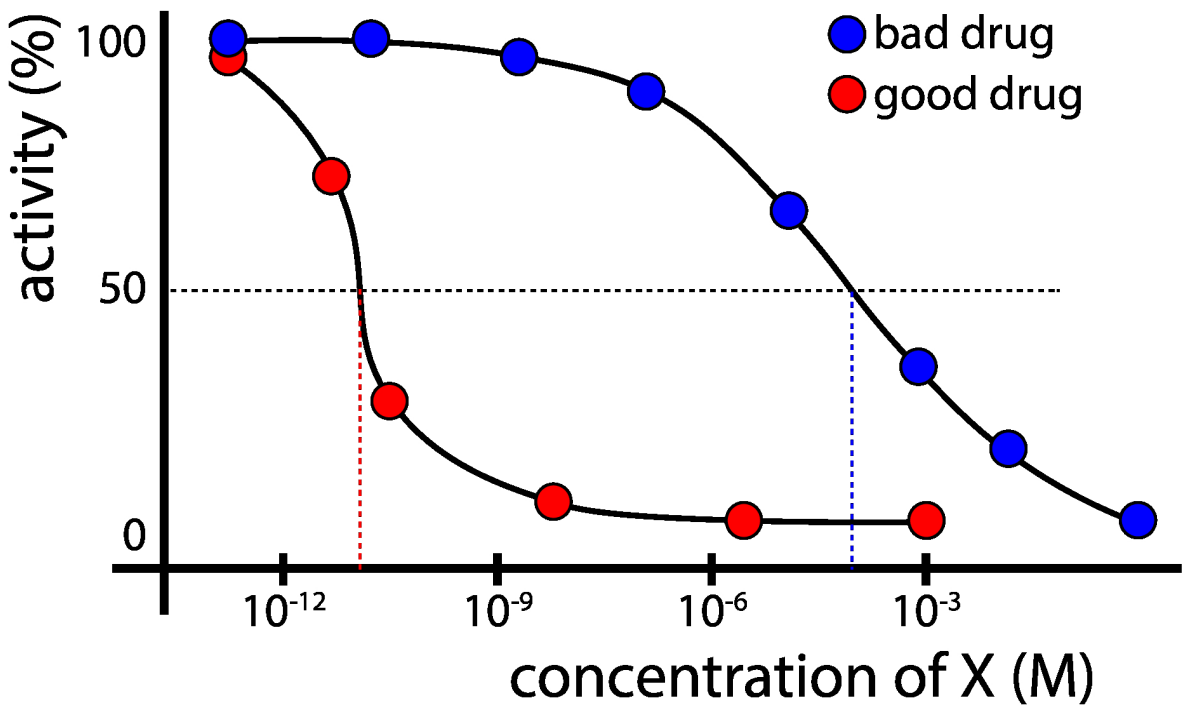
# example 2: the chemical activity problem

I have a newly developed molecule X; how good is X in stopping flu replication?

## experiment

- test a range of concentrations of X, measure flu activity
- compute **$IC_{50}$**: the concentration of X that causes the replication rate of the virus to be halved.

## data



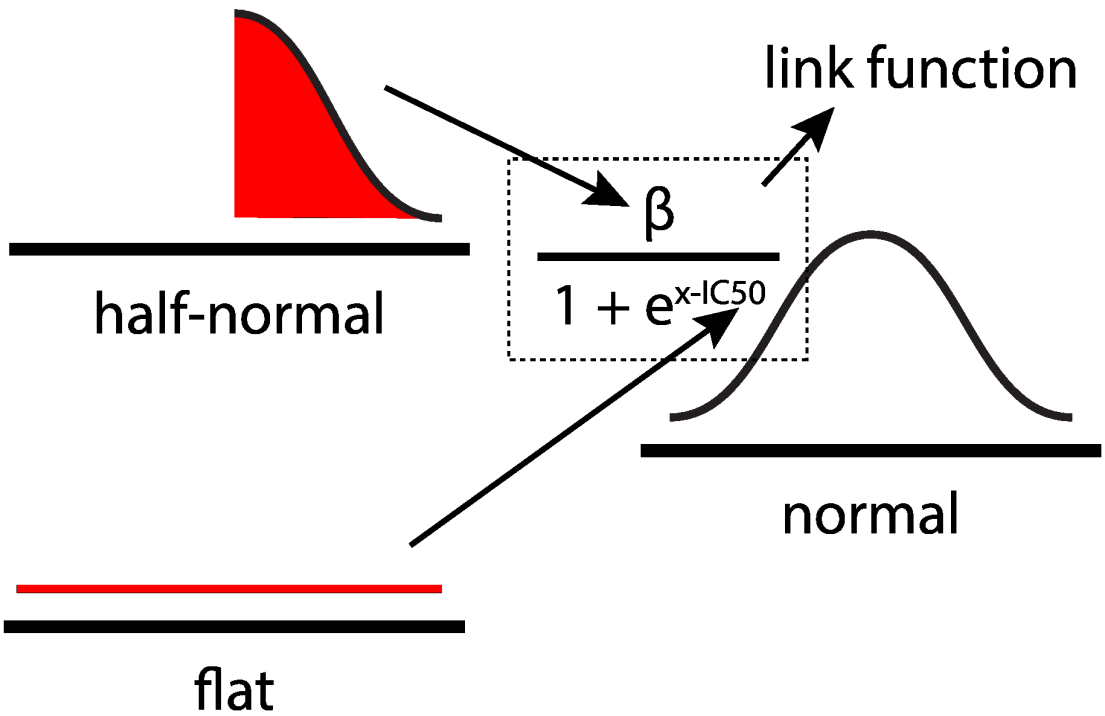

In [11]:
```
import numpy as np
chem_data = [(0.00080, 99),
(0.00800, 91),
(0.08000, 89),
(0.40000, 89),
(0.80000, 79),
(1.60000, 61),
(4.00000, 39),
(8.00000, 25),
(80.00000, 4)]

import pandas as pd

chem_df = pd.DataFrame(chem_data)
chem_df.columns = ['concentration', 'activity']
chem_df['concentration_log'] = chem_df['concentration'].apply(lambda x:np.lo
g10(x))
# df.set_index('concentration', inplace=True)
```

## parameterized problem

given the data, what is the **$IC_{50}$** value of the chemical, and the uncertainty surrounding it?

## prior

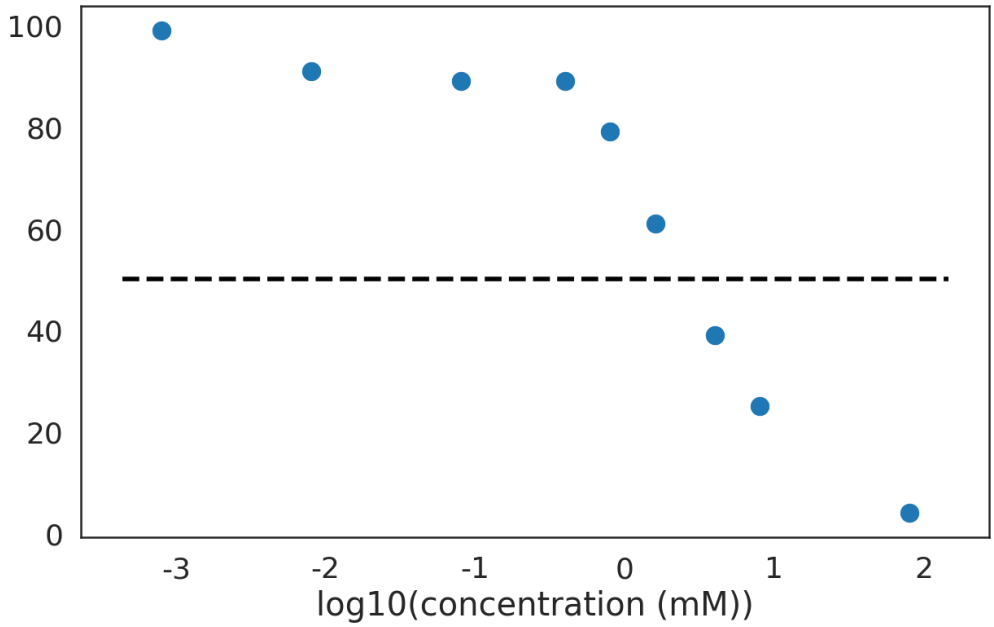
- measurement function from domain knowledge: $m = \frac{\beta}{1+e^{x-IC_{50}}}$
- prior belief about constant to be estimated: $\beta \sim HalfNormal(100^2)$
- prior belief about parameter of interest: $log(IC_{50}) \sim ImproperFlat$
- likelihood function: $data \sim N(m, 1)$




## data

In [12]:
```
def plot_chemical_data(log=True):
    fig = plt.figure(figsize=(10,6))
    ax = fig.add_subplot(1,1,1)
    if log:
        ax.scatter(x=chem_df['concentration_log'], y=chem_df['activity'])
        ax.set_xlabel('log10(concentration (mM))', fontsize=20)
    else:
        ax.scatter(x=chem_df['concentration'], y=chem_df['activity'])
        ax.set_xlabel('concentration (mM)', fontsize=20)
    ax.set_xticklabels([int(i) for i in ax.get_xticks()], fontsize=18)
    ax.set_yticklabels([int(i) for i in ax.get_yticks()], fontsize=18)

    plt.hlines(y=50, xmin=min(ax.get_xlim()), xmax=max(ax.get_xlim()), lines
tyles='--',)
    return fig
```

In [13]:
```
fig = plot_chemical_data(log=True)
plt.show()
```




## code

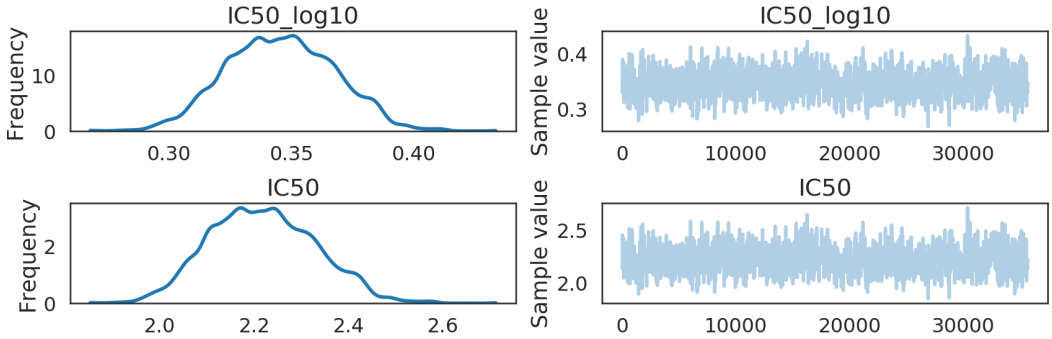
In [14]:
```
with pm.Model() as ic50_model:
    beta = pm.HalfNormal('beta', sd=100**2)
    ic50_log10 = pm.Flat('IC50_log10')  # Flat prior
    # MATH WITH DISTRIBUTION OBJECTS!
    measurements = beta / (1 + np.exp(chem_df['concentration_log'].values -
                                      ic50_log10))

    y_like = pm.Normal('y_like', mu=measurements,
                       observed=chem_df['activity'])
    # Deterministic transformations.
    ic50 = pm.Deterministic('IC50', np.power(10, ic50_log10))
```

## MCMC Inference Button (TM)

In [15]:
```
with ic50_model:
    step = pm.Metropolis()
    ic50_trace = pm.sample(100000, step=step)
```

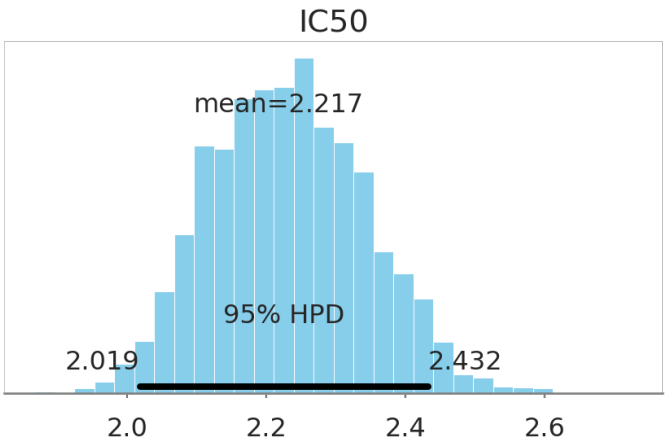
```
38%|▉▉▉▉       | 37984/100500 [00:06<00:10, 6081.47it/s]
```

In [16]:
```
pm.traceplot(ic50_trace[2000:], varnames=['IC50_log10', 'IC50'])  # live: sa
mple from step 2000 onwards.
plt.show()
```




## results

In [17]:
```
pm.plot_posterior(ic50_trace[4000:], varnames=['IC50'],
                  color='#87ceeb', point_estimate='mean')
plt.show()
```




The $IC_{50}$ of the chemical is between approx. [2 mM, 2.4 mM] (95% HPD). It's kind of a bad chemical; uncertainty doesn't matter much here, because of the scale of badness...

# problem type 2: comparison between treatment groups

"are my experimental treatments different from my controls?"

# example 1: the drug IQ problem

does a drug treatment affect IQ scores?

(documented in Kruschke, 2013, example modified from PyMC3 documentation)

In [18]:
```
drug = [  99.,  110.,  107.,  104.,  103.,  105.,  105.,  110.,   99.,
        109.,  100.,  102.,  104.,  104.,  100.,  104.,  101.,  104.,
        101.,  100.,  109.,  104.,  105.,  112.,   97.,  106.,  103.,
        101.,  101.,  104.,   96.,  102.,  101.,  100.,   92.,  108.,
         97.,  106.,   96.,   90.,  109.,  108.,  105.,  104.,  110.,
         92.,  100.]

placebo = [  95.,  105.,  103.,   99.,  104.,   98.,  103.,  104.,  102.,
         91.,   97.,  101.,  100.,  113.,   98.,  102.,  100.,  105.,
         97.,   94.,  104.,   92.,   98.,  105.,  106.,  101.,  106.,
        105.,  101.,  105.,  102.,   95.,   91.,   99.,   96.,  102.,
         94.,   93.,   99.,   99.,  113.,   96.]

def ECDF(data):
    x = np.sort(data)
    y = np.cumsum(x) / np.sum(x)

    return x, y

def plot_drug():
    fig = plt.figure()
    ax = fig.add_subplot(1,1,1)
    x_drug, y_drug = ECDF(drug)
    ax.plot(x_drug, y_drug, label='drug, n={0}'.format(len(drug)))
    x_placebo, y_placebo = ECDF(placebo)
    ax.plot(x_placebo, y_placebo, label='placebo, n={0}'.format(len(placeb
o)))
    ax.legend()
    ax.set_xlabel('IQ Score')
    ax.set_ylabel('Cumulative Frequency')
    ax.hlines(0.5, ax.get_xlim()[0], ax.get_xlim()[1], linestyle='--')

    return fig
```

In [19]:
```
# For my own curiosity: from a frequentist point of view, is there a "statis
tically significant" difference
# between the two treatments?

from scipy.stats import ttest_ind

ttest_ind(drug, placebo)
```

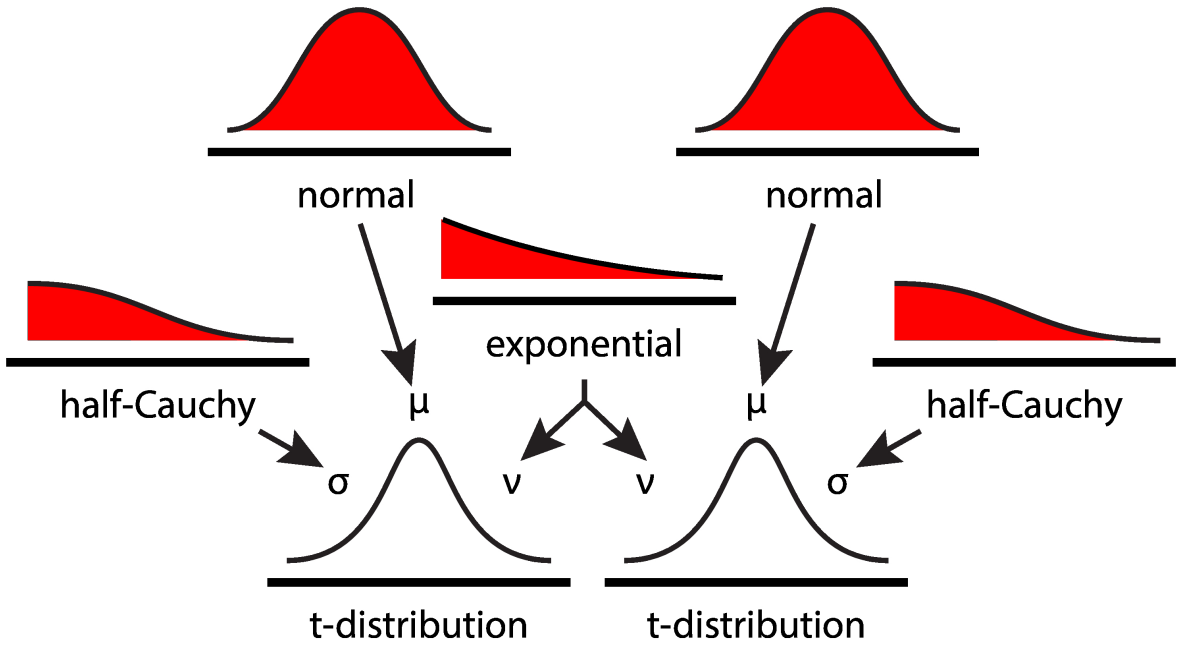
Out[19]:
```
Ttest_indResult(statistic=2.2806701634329549, pvalue=0.025011500508647616)
```

## experiment

- randomly assign participants to two treatment groups:
  - `+drug` vs. `-drug`
- measure IQ score for each participant

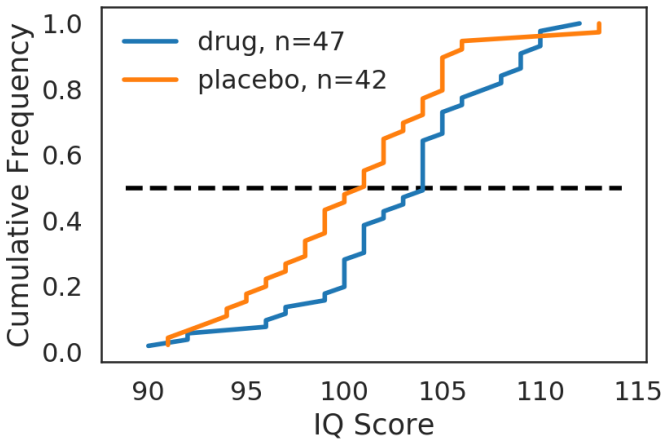
## priors

- measured data are t-distributed: $data \sim StudentsT(\mu, \sigma, \nu)$
- means are normally distributed: $\mu \sim N(0, 100^2)$
- degrees of freedom are exponentially-distributed: $\nu \sim Exp(30)$
- variance is positively-distributed: $\sigma \sim HalfCauchy(100^2)$




## data

In [20]:
```
fig = plot_drug()
plt.show()
```




## code

In [21]:
```
y_vals = np.concatenate([drug, placebo])
labels = ['drug'] * len(drug) + ['placebo'] * len(placebo)

data = pd.DataFrame([y_vals, labels]).T
data.columns = ['IQ', 'treatment']
```

In [22]:
```
with pm.Model() as kruschke_model:
    # Focus on the use of Distribution Objects.
    # Linking Distribution Objects together is done by
    # passing objects into other objects' parameters.
    mu_drug = pm.Normal('mu_drug', mu=0, sd=100**2)
    mu_placebo = pm.Normal('mu_placebo', mu=0, sd=100**2)
    sigma_drug = pm.HalfCauchy('sigma_drug', beta=100)
    sigma_placebo = pm.HalfCauchy('sigma_placebo', beta=100)
    nu = pm.Exponential('nu', lam=1/29) + 1

    drug_like = pm.StudentT('drug', nu=nu, mu=mu_drug,
                            sd=sigma_drug, observed=drug)
    placebo_like = pm.StudentT('placebo', nu=nu, mu=mu_placebo,
                               sd=sigma_placebo, observed=placebo)
    diff_means = pm.Deterministic('diff_means', mu_drug - mu_placebo)
    pooled_sd = pm.Deterministic('pooled_sd',
                                 np.sqrt(np.power(sigma_drug, 2) +
                                         np.power(sigma_placebo, 2) / 2))
    effect_size = pm.Deterministic('effect_size',
                                   diff_means / pooled_sd)
```

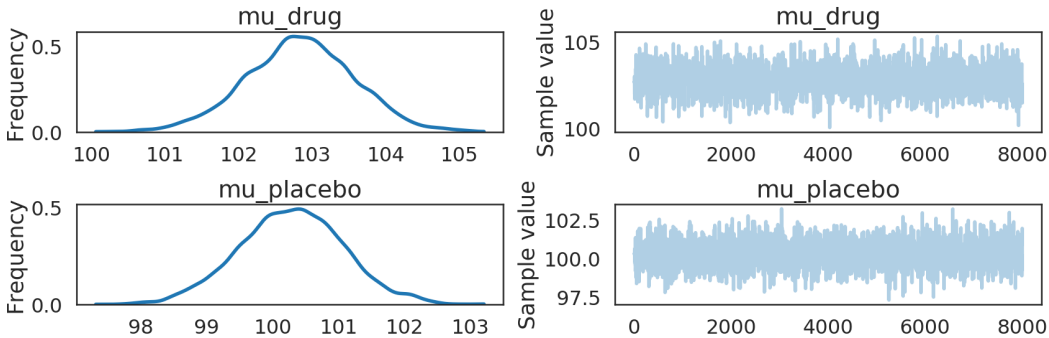
## MCMC Inference Button (TM)

In [23]:
```
with kruschke_model:
    kruschke_trace = pm.sample(10000, step=pm.Metropolis())
```

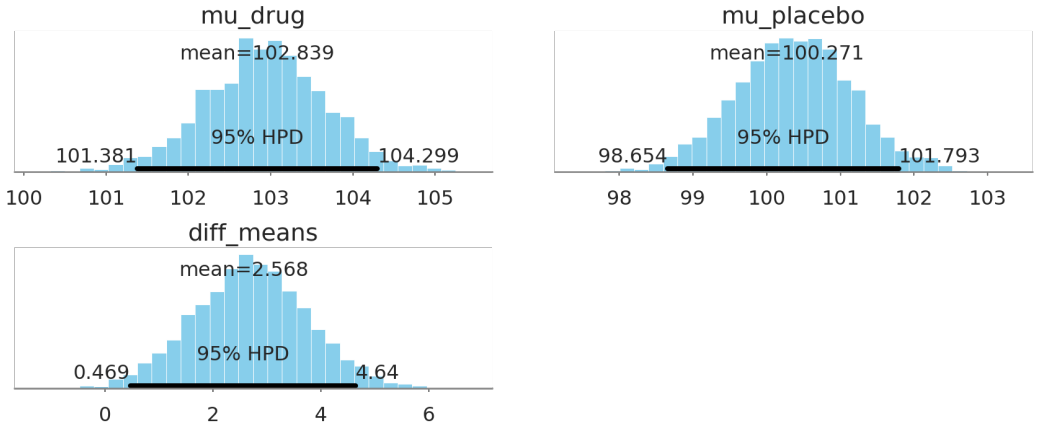
```
100%|██████████| 10500/10500 [00:05<00:00, 1851.26it/s]
```

## results

In [24]:
```
pm.traceplot(kruschke_trace[2000:],
             varnames=['mu_drug', 'mu_placebo'])
plt.show()
```



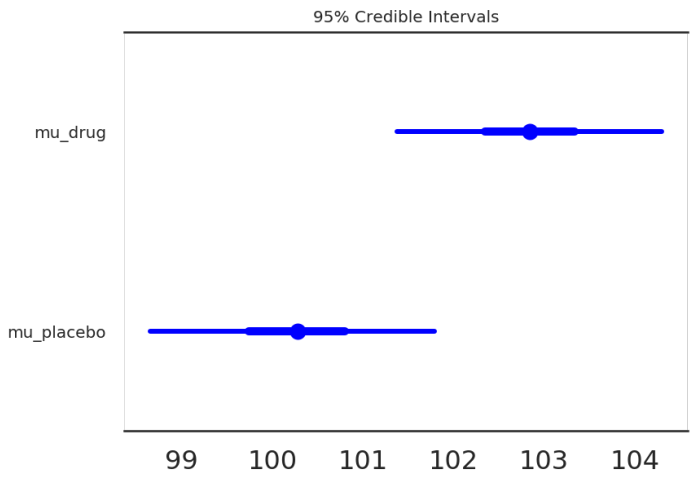
In [25]:
```
pm.plot_posterior(kruschke_trace[2000:], color='#87ceeb',
            varnames=['mu_drug', 'mu_placebo', 'diff_means'])
plt.show()
```




- Difference in mean IQ: [0.5, 4.6]
- Frequentist p-value: $0.02$ (!!!!!!!!)

In [26]:
```
def get_forestplot_line(ax, kind):
    widths = {'median': 2.8, 'iqr': 2.0, 'hpd': 1.0}
    assert kind in widths.keys(), f'line kind must be one of {widths.keys
()}'
    lines = []
    for child in ax.get_children():
        if isinstance(child, mpl.lines.Line2D) and np.allclose(child.get_lw
(), widths[kind]):
            lines.append(child)
    return lines

def adjust_forestplot_for_slides(ax):
    for line in get_forestplot_line(ax, kind='median'):
        line.set_markersize(10)

    for line in get_forestplot_line(ax, kind='iqr'):
        line.set_linewidth(5)

    for line in get_forestplot_line(ax, kind='hpd'):
        line.set_linewidth(3)

    return ax
```

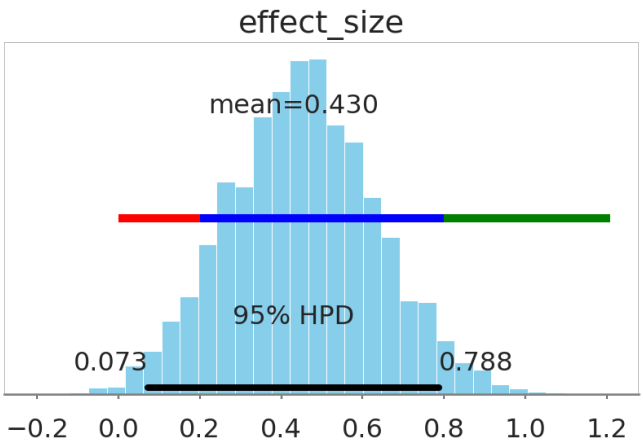
In [27]:
```
pm.forestplot(kruschke_trace[2000:],
              varnames=['mu_drug', 'mu_placebo'])
ax = plt.gca()
ax = adjust_forestplot_for_slides(ax)
plt.show()
```




**Forest plot**: 95% HPD (thin line), IQR (thicker line), and median (dot) of the posterior distribution on the same axes, allowing us to directly compare the treatment and control.

In [28]:
```
def overlay_effect_size(ax):
    height = ax.get_ylim()[1] * 0.5
    ax.hlines(height, 0, 0.2, 'red', lw=5)
    ax.hlines(height, 0.2, 0.8, 'blue', lw=5)
    ax.hlines(height, 0.8, ax.get_xlim()[1], 'green', lw=5)
```

In [29]:
```
ax = pm.plot_posterior(kruschke_trace[2000:],
                       varnames=['effect_size'],
                       color='#87ceeb')
overlay_effect_size(ax)
```




- Effect size (Cohen's d, none to small, medium, large) could be anywhere from essentially nothing to large (95% HPD [0.0, 0.77]).
- Improvement in IQ is 0-4 points.
- The drug is very likely inconsequential.
- No evidence of **biological significance**.

# example 2: the phone sterilization problem

compared to two commonly-used treatments, do my "fancy methods" sterilize my phone better?

## the experiment design

- randomly assign phones to one of six groups: 4 "fancy" methods + 2 "control" methods.
- swab phone before and after treatment, grow bacteria
- **count** number of bacteria colonies formed, compare counts before and after

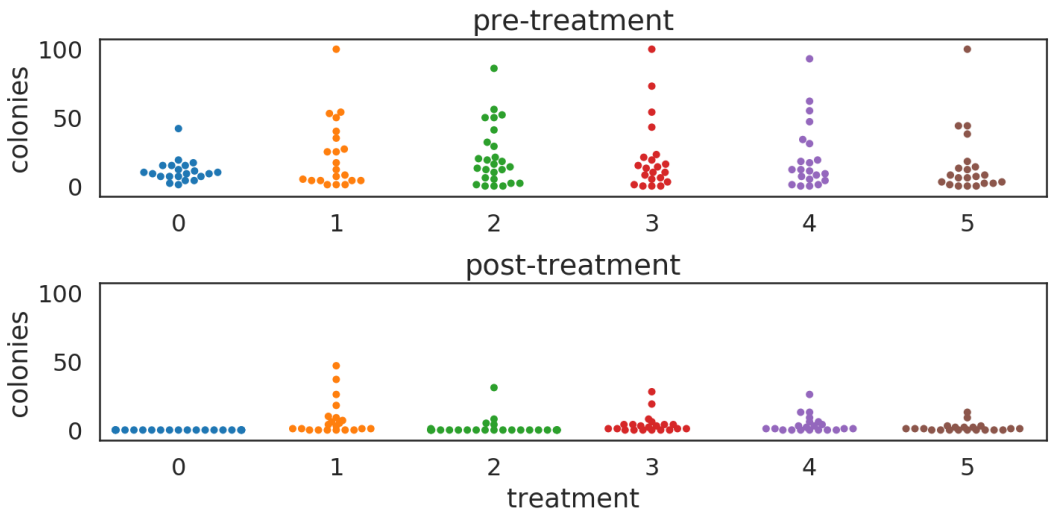
In [30]:
```
renamed_treatments = dict()
renamed_treatments['FBM_2'] = 'FM1'
renamed_treatments['bleachwipe'] = 'CTRL1'
renamed_treatments['ethanol'] = 'CTRL2'
renamed_treatments['kimwipe'] = 'FM2'
renamed_treatments['phonesoap'] = 'FM3'
renamed_treatments['quatricide'] = 'FM4'

# Reload the data one more time.
data = pd.read_csv('datasets/smartphone_sanitization_manuscript.csv', na_val
ues=['#DIV/0!'])
del data['perc_reduction colonies']

# Exclude cellblaster data
data = data[data['treatment'] != 'CB30']
data = data[data['treatment'] != 'cellblaster']

# Rename treatments
data['treatment'] = data['treatment'].apply(lambda x: renamed_treatments[x])

# Sort the data according to the treatments.
treatment_order = ['FM1', 'FM2', 'FM3', 'FM4', 'CTRL1', 'CTRL2']
data['treatment'] = data['treatment'].astype('category')
data['treatment'].cat.set_categories(treatment_order, inplace=True)
data['treatment'] = data['treatment'].cat.codes.astype('int32')
data = data.sort_values(['treatment']).reset_index(drop=True)
data['site'] = data['site'].astype('category').cat.codes.astype('int32')

data['frac_change_colonies'] = ((data['colonies_post'] - data['colonies_pre
'])
                                / data['colonies_pre'])
data['frac_change_colonies'] = pm.floatX(data['frac_change_colonies'])
del data['screen protector']

# Change dtypes to int32 for GPU usage.
def change_dtype(data, dtype='int32'):
    return data.astype(dtype)

cols_to_change_ints = ['sample_id', 'colonies_pre', 'colonies_post',
                       'morphologies_pre', 'morphologies_post', 'phone ID']

cols_to_change_floats = ['year', 'month', 'day', 'perc_reduction morph',
                         'phone ID', 'no case',]

for col in cols_to_change_ints:
    data[col] = change_dtype(data[col], dtype='int32')

for col in cols_to_change_floats:
    data[col] = change_dtype(data[col], dtype='float32')

data.dtypes


# # filter the data such that we have only PhoneSoap (PS-300) and Ethanol (E
T)
# data_filtered = data[(data['treatment'] == 'PS-300') | (data['treatment']
== 'QA')]
# data_filtered = data_filtered[data_filtered['site'] == 'phone']
# data_filtered.sample(10)
```

```
Out[30]: sample_id                 int32
         treatment                 int32
         colonies_pre              int32
         colonies_post             int32
         morphologies_pre          int32
         morphologies_post         int32
         year                    float32
         month                   float32
         day                     float32
         perc_reduction morph    float32
         site                      int32
         phone ID                float32
         no case                 float32
         frac_change_colonies    float64
         dtype: object
```

## data

In [31]:
```
def plot_colonies_data():
    fig = plt.figure(figsize=(10,5))
    ax1 = fig.add_subplot(2,1,1)
    sns.swarmplot(x='treatment', y='colonies_pre', data=data, ax=ax1)
    ax1.set_title('pre-treatment')
    ax1.set_xlabel('')
    ax1.set_ylabel('colonies')
    ax2 = fig.add_subplot(2,1,2)
    sns.swarmplot(x='treatment', y='colonies_post', data=data, ax=ax2)
    ax2.set_title('post-treatment')
    ax2.set_ylabel('colonies')
    ax2.set_ylim(ax1.get_ylim())
    plt.tight_layout()
    return fig
```

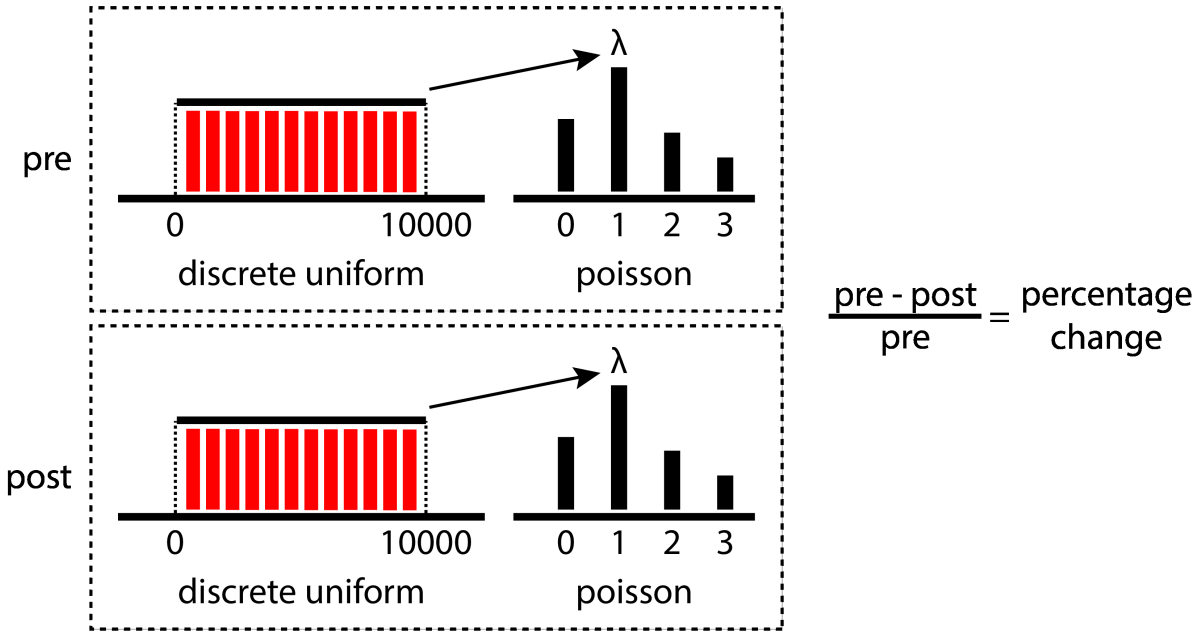
In [32]:
```
fig = plot_colonies_data()
plt.show()
```



## priors

Counts are **Poisson** distributed. Thus...

- Count likelihoods are Poisson distributed: $data_i^j \sim Poisson(\mu_i^j), j \in [pre, post], i \in [1, 2, 3...]$
- Priors for Poisson parameters are discrete uniform distributed: $\mu_i^j \sim DiscreteUniform(0, 10^4), j \in [pre, post], i \in [1, 2, 3...]$
- Sterilization efficacy is measured by percentage change, defined as: $\frac{mu_{pre} - mu_{post}}{mu_{pre}}$




## code

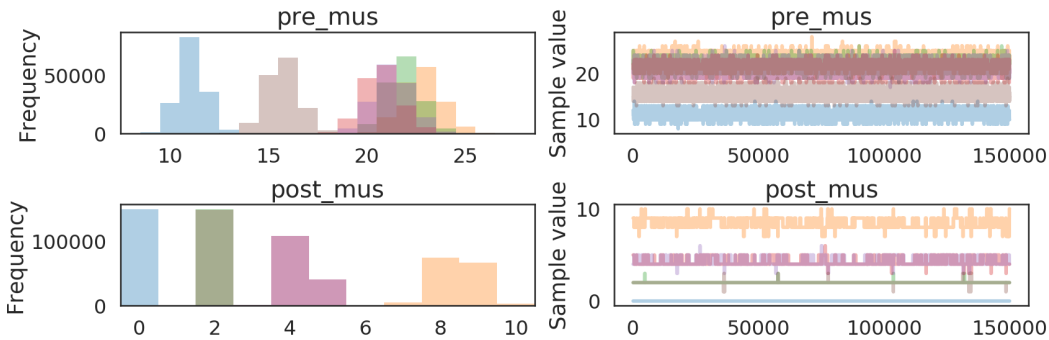
In [33]:
```
with pm.Model() as poisson_estimation:

    mu_pre = pm.DiscreteUniform('pre_mus', lower=0, upper=10000,
                                shape=len(treatment_order))
    pre_mus = mu_pre[data['treatment'].values]  # fancy indexing!!
    pre_counts = pm.Poisson('pre_counts', mu=pre_mus,
                            observed=pm.floatX(data['colonies_pre']))

    mu_post = pm.DiscreteUniform('post_mus', lower=0, upper=10000,
                                 shape=len(treatment_order))
    post_mus = mu_post[data['treatment'].values]  # fancy indexing!!
    post_counts = pm.Poisson('post_counts', mu=post_mus,
                             observed=pm.floatX(data['colonies_post']))

    perc_change = pm.Deterministic('perc_change',
                                   100 * (mu_pre - mu_post) / mu_pre)
```

## MCMC Inference Button (TM)

In [34]:
```
with poisson_estimation:
    poisson_trace = pm.sample(200000)
```

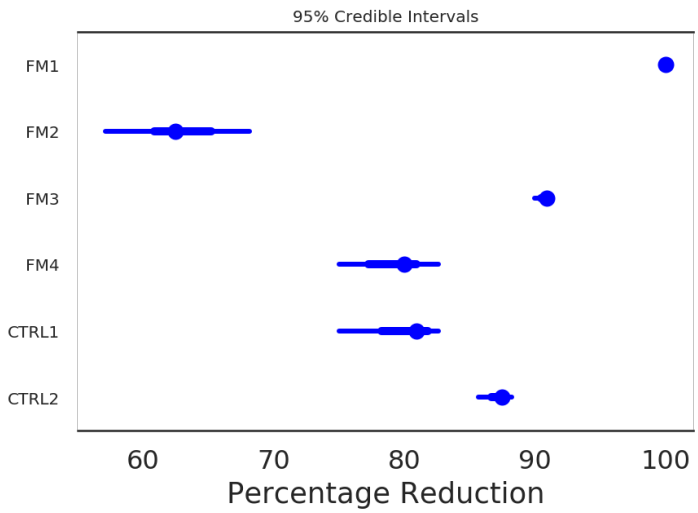
```
Assigned Metropolis to pre_mus
Assigned Metropolis to post_mus
100%|██████████| 200500/200500 [00:37<00:00, 5330.33it/s]
```

In [35]:
```
pm.traceplot(poisson_trace[50000:], varnames=['pre_mus', 'post_mus'])
plt.show()
```




## results

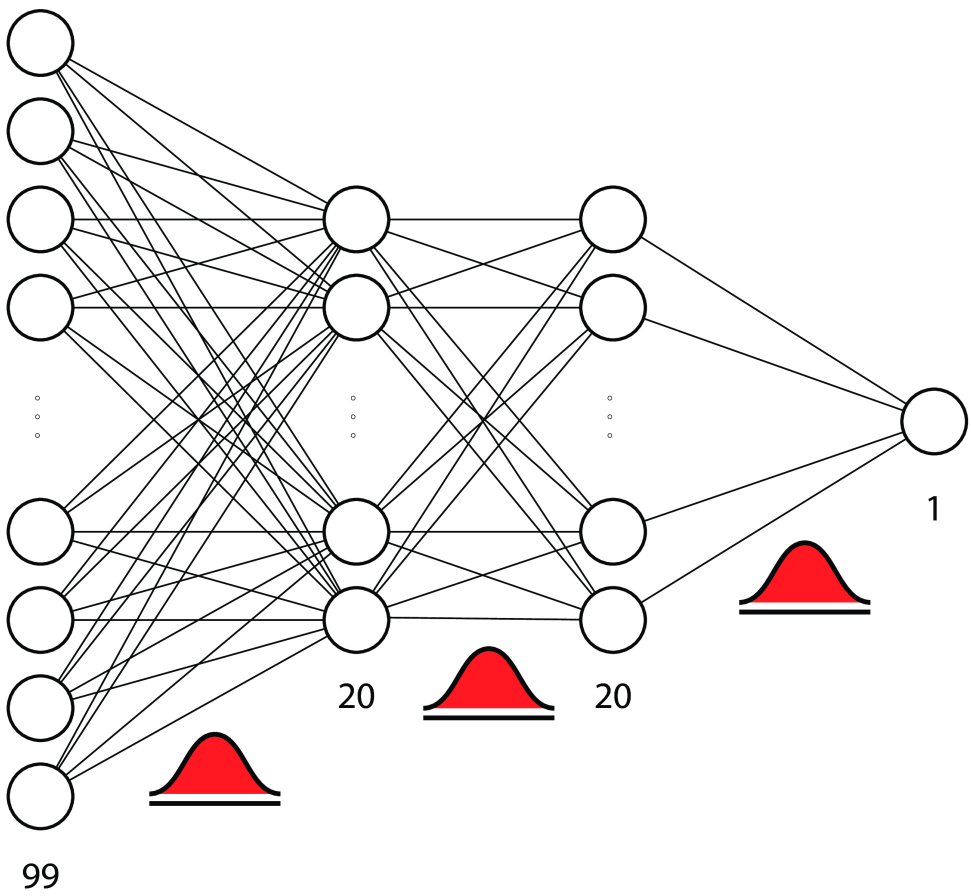
In [36]:
```
pm.forestplot(poisson_trace[50000:], varnames=['perc_change'],
              ylabels=treatment_order, xrange=[0, 110])
plt.xlabel('Percentage Reduction')

ax = plt.gca()
ax = adjust_forestplot_for_slides(ax)
```




# problem type 3: complicated stuff

# example: bayesian neural networks

a.k.a. bayesian deep learning




Forest Cover Notebook (https://github.com/ericmjl/bayesian-analysis-recipes/blob/master/multiclass-classification-neural-network.ipynb)

## concepts featured

- Parameter Estimation:
  - **Coin Toss:** Priors & Posteriors
  - **$IC_{50}$:** Link functions & Deterministic computations
- Control vs. Treatment:
  - **Drug IQ:** One treatment vs. one control
  - **Phone Sterilization:** Multiple treatments vs. multiple controls.
- Bayesian Neural Nets:
  - **Forest Cover:** Parameter priors & Approximate inference.

## pattern

1. parameterize your problem using statistical distributions
2. justify your model structure
3. write model in PyMC3, hit the **Inference Button™**
4. interpret based on posterior distributions
5. (optional) with new information, modify model structure.

## bayesian estimation

- write a **descriptive** model for how the data were generated.
  - original bayes: do this **before** seeing your data.
  - empirical bayes: do this **after** seeing your data.
- estimate **posterior distributions** of model parameters of interest.
- **deterministically compute** posterior distributions of derived parameters.

## resources

- John K. Kruschke's books (https://sites.google.com/site/doingbayesiandataanalysis/), paper (http://www.indiana.edu/~kruschke/BEST/), and video (https://www.youtube.com/watch?v=fhw1j1Ru2i0&feature=youtu.be).
- Statistical Re-thinking book (http://xcelab.net/rm/statistical-rethinking/)
- Jake Vanderplas' blog post (http://jakevdp.github.io/blog/2014/03/11/frequentism-and-bayesianism-a-practical-intro/) on the differences between Frequentism and Bayesianism.
- PyMC3 examples & documentation (https://pymc-devs.github.io/pymc3/examples.html)
- Andrew Gelman's blog (http://andrewgelman.com/)
- Recommendations for prior distributions wiki (https://github.com/stan-dev/stan/wiki/Prior-Choice-Recommendations)
- Cam Davidson-Pilon's Bayesian Methods for Hackers (https://github.com/CamDavidsonPilon/Probabilistic-Programming-and-Bayesian-Methods-for-Hackers)
- My repository (https://github.com/ericmjl/bayesian-analysis-recipes) of Bayesian data analysis recipes.

## GO BAYES!

- Full notebook with bonus resources: https://github.com/ericmjl/bayesian-stats-talk (https://github.com/ericmjl/bayesian-stats-talk)
- Twitter: @ericmjl (https://twitter.com/ericmjl)
- Website: ericmjl.com (http://www.ericmjl.com)