Sandwich versus Bootstrap Standard Errors

In [1]:
```
import abc
import collections
import multiprocessing
import sys
from typing import Any, Callable, NamedTuple, Sequence, Tuple

from absl import app
from absl import flags
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
import seaborn as sns
import statsmodels.api as sm
from scipy import stats
import tensorflow as tf
from tensorflow.python.ops import gen_array_ops
from tensorflow.python.ops import gen_linalg_ops
from tensorflow.python.ops import parallel_for
pfor = sys.modules['tensorflow.python.ops.parallel_for.pfor']

tf.enable_v2_behavior()
np.set_printoptions(suppress=True)
```

In [2]:
```
@pfor.RegisterPForWithArgs('MatrixBandPart', gen_array_ops.matrix_band_part)
@pfor.RegisterPForWithArgs('MatrixDiag', gen_array_ops.matrix_diag)
def _convert_matrix_diag(pfor_input, op_type, op_func):
    del op_type
    return pfor.wrap(op_func(*[x.t for x in pfor_input.inputs]), True)

@pfor.RegisterPForWithArgs('MatrixSetDiag', gen_array_ops.matrix_set_diag)
@pfor.RegisterPForWithArgs('MatrixTriangularSolve', gen_linalg_ops.matrix_triangul
ar_solve)
def _convert_matrix_solve(pfor_input, op_type, op_func):
    del op_type
    pfor_input.stack_inputs()
    return pfor.wrap(op_func(*[x.t for x in pfor_input.inputs]), True)
```

Data

In [3]:
```
orthodont_data = pd.read_csv('../hw4/orthodont.csv')
orthodont_data = orthodont_data.set_index('Subject')
orthodont_data.head(8)
```

Out[3]:

Subject	distance	age	Sex
M01	26.0	8	Male
M01	25.0	10	Male
M01	29.0	12	Male
M01	31.0	14	Male
M02	21.5	8	Male
M02	22.5	10	Male
M02	23.0	12	Male
M02	26.5	14	Male

In [4]:
```
def make_covariates(data_frame):
    age = (data_frame['age'] - 8).values
    is_female = (data_frame['Sex'] == 'Female').values.astype(np.float64)
    return np.column_stack((
        np.ones(len(data_frame)),
        age,
        is_female,
        age*is_female,
    ))

def make_response(data_frame):
    return data_frame['distance'].values

X = tf.convert_to_tensor(
    [make_covariates(orthodont_data.loc[i]) for i in np.unique(orthodont_data.inde
x)],
    tf.float32)
y = tf.expand_dims(tf.convert_to_tensor(
    [make_response(orthodont_data.loc[i]) for i in np.unique(orthodont_data.index
)],
    tf.float32), -1)
```

Cluster Correlation Structure

In [5]:
```
def make_covariance_homoscedastic(log_variance):
    """Makes diagonal homoscedastic covariance structure."""
    return tf.exp(log_variance)*tf.eye(4)
```

In [6]:
```
def make_covariance_exchangeable(log_covariance_params):
    """Makes heteroscedastic, exchangeble covariance structure."""
    standard_errors = tf.exp(log_covariance_params[:-1])  # First entries are stan
dard errors.
    rho = tf.exp(log_covariance_params[-1])  # Last entry is correlation.
    correlation = tf.ones((4, 4), dtype=tf.float32)*rho + tf.eye(4)*(1. - rho)
    return correlation*standard_errors*tf.expand_dims(standard_errors, -1)
```

REML Loss

In [7]:
```
def solve_beta(X, y, weights):
    projected_X = tf.reduce_sum(tf.matmul(tf.tensordot(tf.transpose(X, [0, 2, 1]),
weights, 1), X), 0)
    projected_y = tf.reduce_sum(tf.matmul(tf.tensordot(tf.transpose(X, [0, 2, 1]),
weights, 1), y), 0)
    return tf.linalg.cholesky_solve(tf.linalg.cholesky(projected_X), projected_y)

def loss_fn(X, y, covariance):
    weights = tf.linalg.cholesky_solve(tf.linalg.cholesky(covariance), tf.eye(4))
    beta = solve_beta(X, y, weights)
    residuals = y - tf.tensordot(X, beta, 1)
    weighted_squared_error = tf.matmul(
        tf.tensordot(tf.transpose(residuals, [0, 2, 1]), weights, 1), residuals)
    loss = tf.reduce_mean(weighted_squared_error) + tf.linalg.logdet(covariance)
    reml_loss = tf.reduce_sum(tf.matmul(tf.tensordot(tf.transpose(X, [0, 2, 1]), w
eights, 1), X), 0)
    return loss + tf.linalg.logdet(reml_loss) / tf.cast(tf.shape(y)[0], tf.float32
)
```

Optimization

Minimizes REML loss with Newton-Raphson algorithm

In [8]:
```
class CovarianceSpec(NamedTuple('CovarianceSpec', [
    ('initial_params', np.array),
    ('make_covariance', Callable[[tf.Tensor], tf.Tensor]),
])):
    """Encapsulates covariance parameters."""

def fit(X, y, covariance_spec):
    covariance_params = tf.Variable(covariance_spec.initial_params)
    for i in range(16):
        with tf.GradientTape(persistent=True) as outer_tape:
            with tf.GradientTape() as inner_tape:
                loss = loss_fn(X, y, covariance_spec.make_covariance(covariance_pa
rams))
            gradients = inner_tape.gradient(loss, covariance_params)
        hessian = outer_tape.jacobian(gradients, covariance_params,
                                      parallel_iterations=4, experimental_use_pfor
=False)
        covariance_params.assign_add(tf.reshape(
            tf.linalg.cholesky_solve(tf.linalg.cholesky(hessian), -tf.expand_dims(
gradients, -1)),
            covariance_params.shape))
    return covariance_params
```

In [9]:
```
log_variance = fit(
    X, y,
    CovarianceSpec(initial_params=[0.], make_covariance=make_covariance_homoscedas
tic))
tf.sqrt(tf.exp(log_variance)).numpy()
```

```
WARNING: Logging before flag parsing goes to stderr.
W0222 05:03:56.179281 140456376928000 deprecation.py:323] From /usr/local/lib/pyt
hon3.5/dist-packages/tensorflow/python/ops/math_grad.py:80: colocate_with (from t
ensorflow.python.framework.ops) is deprecated and will be removed in a future ver
sion.
Instructions for updating:
Colocations handled automatically by placer.
W0222 05:03:56.192803 140456376928000 deprecation.py:323] From /usr/local/lib/pyt
hon3.5/dist-packages/tensorflow/python/ops/array_grad.py:425: to_int32 (from tens
orflow.python.ops.math_ops) is deprecated and will be removed in a future versio
n.
Instructions for updating:
Use tf.cast instead.
```

Out[9]:
```
array([2.256949], dtype=float32)
```

Standard Error Estimates

The ML covariance estimate assumes that the covariance model is correct.

In [10]:
```
def ml_covariance(X, weights):
    covariance = tf.reduce_sum(tf.matmul(tf.tensordot(tf.transpose(X, [0, 2, 1]),
weights, 1), X), 0)
    return tf.linalg.cholesky_solve(tf.linalg.cholesky(covariance), tf.eye(tf.shap
e(covariance)[0]))
```

In [11]:
```
reml_weights = tf.linalg.cholesky_solve(
    tf.linalg.cholesky(make_covariance_homoscedastic(log_variance)), tf.eye(4))

reml_estimates = pd.DataFrame(collections.OrderedDict([
    ('Estimate', tf.squeeze(solve_beta(X, y, reml_weights)).numpy()),
    ('REML Standard Error', tf.sqrt(tf.linalg.diag_part(ml_covariance(X, reml_weig
hts))).numpy()),
]), index=['$\\hat\\beta_{i}$'.format(i=i) for i in range(4)])

reml_estimates
```

Out[11]:

	Estimate	REML Standard Error
$\hat{\beta}_0$	22.615610	0.472075
$\hat{\beta}_1$	0.784380	0.126167
$\hat{\beta}_2$	-1.406521	0.739599
$\hat{\beta}_3$	-0.304834	0.197666

Sandwich

In [12]:
```
def sandwich_covariance(X, y, weights):
    bread = ml_covariance(X, weights)
    left_meat = tf.tensordot(tf.transpose(X, [0, 2, 1]), weights, 1)
    right_meat =  tf.transpose(left_meat, [0, 2, 1])
    residuals = y - tf.tensordot(X, solve_beta(X, y, weights), 1)
    residuals = tf.matmul(residuals, tf.transpose(residuals, [0, 2, 1]))
    meat = tf.reduce_sum(tf.matmul(tf.matmul(left_meat, residuals), right_meat), 0
)
    return tf.matmul(tf.matmul(bread, meat), bread)
```

In [13]:
```
sandwich_covariance_estimate = sandwich_covariance(
    X, y,
    tf.linalg.cholesky_solve(tf.linalg.cholesky(
        make_covariance_homoscedastic(log_variance)), tf.eye(X.shape[-1])))
sandwich_covariance_estimate.numpy()
```

Out[13]:
```
array([[ 0.28468183, -0.02929138, -0.28468183,  0.02929138],
       [-0.02929133,  0.00967223,  0.02929132, -0.00967223],
       [-0.2846818 ,  0.02929136,  0.5987651 , -0.02658853],
       [ 0.02929131, -0.00967222, -0.02658838,  0.01365793]],
      dtype=float32)
```

In [14]:
```
reml_estimates['Sandwich Standard Error'] = np.sqrt(np.diag(sandwich_covariance_es
timate.numpy()))

with open('reml_estimates.tex', 'w') as f:
    f.write(reml_estimates.to_latex(escape=False))

reml_estimates
```

Out[14]:

	Estimate	REML Standard Error	Sandwich Standard Error
$\hat{\beta}_0$	22.615610	0.472075	0.533556
$\hat{\beta}_1$	0.784380	0.126167	0.098347
$\hat{\beta}_2$	-1.406521	0.739599	0.773799
$\hat{\beta}_3$	-0.304834	0.197666	0.116867

Bootstrap

In [15]:
```
class SamplingStrategy(abc.ABC):
    @abc.abstractmethod
    def __call__(self, clusters: Tuple[tf.Tensor, tf.Tensor]):
        pass

class ClusterSampler(SamplingStrategy):
    def __call__(self, clusters):
        shape = tf.shape(clusters[0]).numpy()
        sample = np.random.choice(shape[0], shape[0], replace=True)
        return tuple([tf.gather(item, sample) for item in clusters])

class IndependentSampler(SamplingStrategy):
    def __call__(self, clusters):
        size = tf.reduce_prod(tf.shape(clusters[0])[:-1]).numpy()
        sample = np.random.choice(size, size, replace=True)
        return tuple([self._sample(item, sample) for item in clusters])

    def _sample(self, tensor: tf.Tensor, indices: np.array):
        original_shape = tf.shape(tensor)
        tensor = tf.reshape(tensor, (len(indices), -1))
        return tf.reshape(tf.gather(tensor, indices), original_shape)

class HierarchicalSampler(SamplingStrategy):
    def __call__(self, clusters):
        shape = tf.shape(clusters[0]).numpy()
        size = 1
        samples = []
        for s in shape[:-1]:
            size *= s
            samples.append(np.random.choice(s, size, replace=True))

        sample = []
        for i in range(len(samples[-1])):
            indices = [samples[-1][i]]
            for j in range(len(shape) - 3, -1, -1):
                indices.append(samples[j][i//s])
            sample.append(tuple(reversed(indices)))
        return tuple([tf.reshape(tf.gather_nd(item, sample), item.shape) for item
in clusters])
```

In [16]:
```
def _bootstrap_sample(args):
    X, y, covariance_spec = args
    covariance_params = fit(X, y, covariance_spec)
    covariance = covariance_spec.make_covariance(covariance_params)
    weights = tf.linalg.cholesky_solve(tf.linalg.cholesky(covariance), tf.eye(tf.s
hape(covariance)[0]))
    return solve_beta(X, y, weights)

def bootstrap(X, y, covariance_spec, sampler, num_trials):
    args = (sampler((X, y)) + (covariance_spec,) for _ in range(num_trials))
    pool = multiprocessing.Pool(4)
    estimates = list(pool.imap_unordered(_bootstrap_sample, args, 4))
    pool.close()
    return np.squeeze(np.array(estimates))
```

In [17]:
```
#bootstrap_samples_cluster = bootstrap(
#    X, y,
#    CovarianceSpec(initial_params=[0.],
#                   make_covariance=make_covariance_homoscedastic),
#    sampler=ClusterSampler(), num_trials=2048)
#np.save('bootstrap_samples_cluster', bootstrap_samples_cluster)
bootstrap_samples_cluster = np.load('bootstrap_samples_cluster.npy')
```

In [18]:
```
#bootstrap_samples_independent = bootstrap(
#    X, y,
#    CovarianceSpec(initial_params=[0.],
#                   make_covariance=make_covariance_homoscedastic),
#    sampler=IndependentSampler(), num_trials=2048)
#np.save('bootstrap_samples_independent', bootstrap_samples_independent)
bootstrap_samples_independent = np.load('bootstrap_samples_independent.npy')
```

In [19]:
```
#bootstrap_samples_hierarchical = bootstrap(
#    X, y,
#    CovarianceSpec(initial_params=[0.],
#                   make_covariance=make_covariance_homoscedastic),
#    sampler=HierarchicalSampler(), num_trials=2048)
#np.save('bootstrap_samples_hierarchical', bootstrap_samples_hierarchical)
bootstrap_samples_hierarchical = np.load('bootstrap_samples_hierarchical.npy')
```

In [20]:
```
bootstrap_standard_errors = pd.DataFrame(collections.OrderedDict([
    ('Cluster Resampling', np.std(bootstrap_samples_cluster, ddof=1, axis=0)),
    ('Independent Resampling', np.std(bootstrap_samples_independent, ddof=1, axis=
0)),
    ('Hierarchical Resampling', np.std(bootstrap_samples_hierarchical, ddof=1, axi
s=0)),
]), index=reml_estimates.index)

with open('bootstrap_standard_errors.tex', 'w') as f:
    f.write(bootstrap_standard_errors.to_latex(escape=False))

bootstrap_standard_errors
```

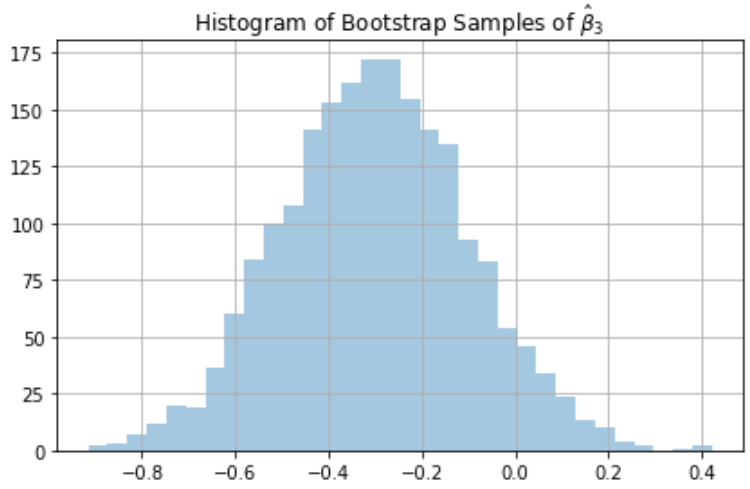
Out[20]:

	Cluster Resampling	Independent Resampling	Hierarchical Resampling
$\hat{\beta}_0$	0.527070	0.503651	0.672173
$\hat{\beta}_1$	0.100844	0.130554	0.153636
$\hat{\beta}_2$	0.786734	0.723665	1.006702
$\hat{\beta}_3$	0.119974	0.198361	0.218498

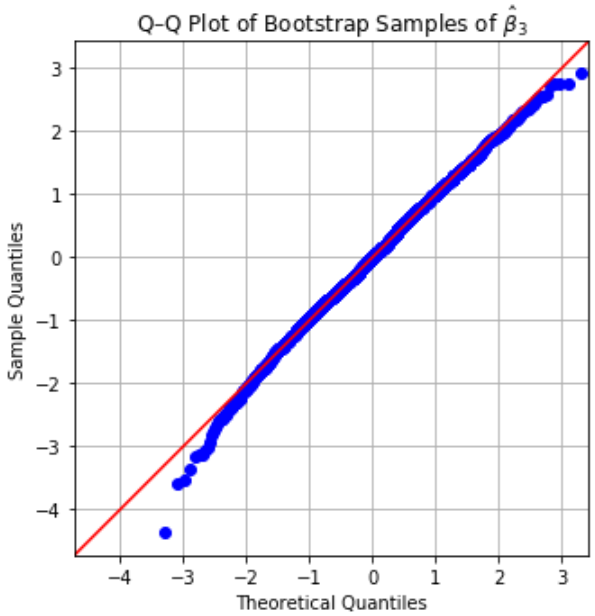
Diagnostic Plots

Check if the distribution of samples is normal.

In [21]:
```
fig = plt.figure(figsize=(6,4))
ax = fig.gca()
ax.grid(True)
sns.distplot(bootstrap_samples_independent[:,3], kde=False, ax=ax)
ax.set_title('Histogram of Bootstrap Samples of $\\hat\\beta_3$')
fig.tight_layout()
fig.savefig('hist_bootstrap_cluster.pdf', bbox_inches='tight')
```



In [22]:
```
fig = plt.figure(figsize=(5,5))
ax = fig.gca()
sm.qqplot(bootstrap_samples_cluster[:,3],
          line='45', ax=ax, fit=True)
ax.grid(True)
ax.set_title('Q–Q Plot of Bootstrap Samples of $\\hat\\beta_3$')
ax.set_aspect('equal')
fig.tight_layout()
fig.savefig('qq_bootstrap_cluster.pdf', bbox_inches='tight')
```



REML Exchangeable Test

Should agree with numbers from Chapter 2, slides 73 and 75.

In [23]:
```
log_exchangeable_covariance_params = fit(
    X, y,
    CovarianceSpec(initial_params=[0., 0., 0., 0., -1.],
                   make_covariance=make_covariance_exchangeable))
tf.exp(log_exchangeable_covariance_params).numpy()
```

Out[23]:
```
array([2.3867779 , 2.058272  , 2.4678187 , 2.19673   , 0.63528943],
      dtype=float32)
```

In [24]:
```
solve_beta(X, y, tf.linalg.cholesky_solve(
    tf.linalg.cholesky(
        make_covariance_exchangeable(log_exchangeable_covariance_params)),
    tf.eye(X.shape[-1])))
```

Out[24]:
```
<tf.Tensor: id=87610, shape=(4, 1), dtype=float32, numpy=
array([[22.485374  ],
       [ 0.79431295],
       [-1.2507197 ],
       [-0.3155596 ]], dtype=float32)>
```

In [25]:
```
tf.sqrt(tf.linalg.diag_part(
    ml_covariance(X, tf.linalg.cholesky_solve(
        tf.linalg.cholesky(
            make_covariance_exchangeable(log_exchangeable_covariance_params)),
        tf.eye(X.shape[-1]))))).numpy()
```

Out[25]:
```
array([0.5308524 , 0.07701091, 0.8316859 , 0.12065291], dtype=float32)
```