STAT/BIOST 571: Homework 5

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Problem 1: Sandwich and bootstrap standard error estimates (10 points)

As on slide 2.76, fit the model

$$EY_{ij} = \beta_0 + \beta_1(Age_{ij} - 8) + \beta_2 Gender_i + \beta_3(Age_{ij} - 8) \times Gender_i$$

to the dental data by using REML, but use a homoscedastic covariance models with no correlation.

(a) Calculate sandwich-based standard error estimates for $\hat{\beta}_3$ that account for clustering by subject. Write your own code for this, using matrix algebra.

	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

Table 1: Parameter estimates using REML with a homoscedastic covariance models with no correlation.

Solution: The REML estimates can be found in Table 1. REML standard errors were calculated assuming that covariance model is specified correctly by taking the square root of the diagonal $\left(\sum_{i=1}^n X_i^\intercal \hat{\Sigma}_{\text{REML}}^{-1} X_i\right)^{-1}$, where $\hat{\Sigma}_{\text{REML}} = \hat{\alpha} I_m$, since cluster sizes are equal and there is only one covariance parameter on the diagonal.

Sandwich covariance estimates can be obtained by

$$\hat{\Sigma}_{\text{Sandwich}} = \left(\sum_{i=1}^n X_i^\intercal \hat{\Sigma}_{\text{REML}}^{-1} X_i\right)^{-1} \left(\sum_{i=1}^n X_i^\intercal \hat{\Sigma}_{\text{REML}}^{-1} \hat{\Sigma}_{\text{Empirical}} \hat{\Sigma}_{\text{REML}}^{-1} X_i\right) \left(\sum_{i=1}^n X_i^\intercal \hat{\Sigma}_{\text{REML}}^{-1} X_i\right)^{-1},$$

where the empirical covariance estimate is $\hat{\Sigma}_{\text{Empirical}} = \frac{1}{n} \sum_{i=1}^n \left(Y_i - X_i\hat{\beta}\right)\left(Y_i - X_i\hat{\beta}\right)^\intercal$ since we assume each cluster has the same covariance structure.

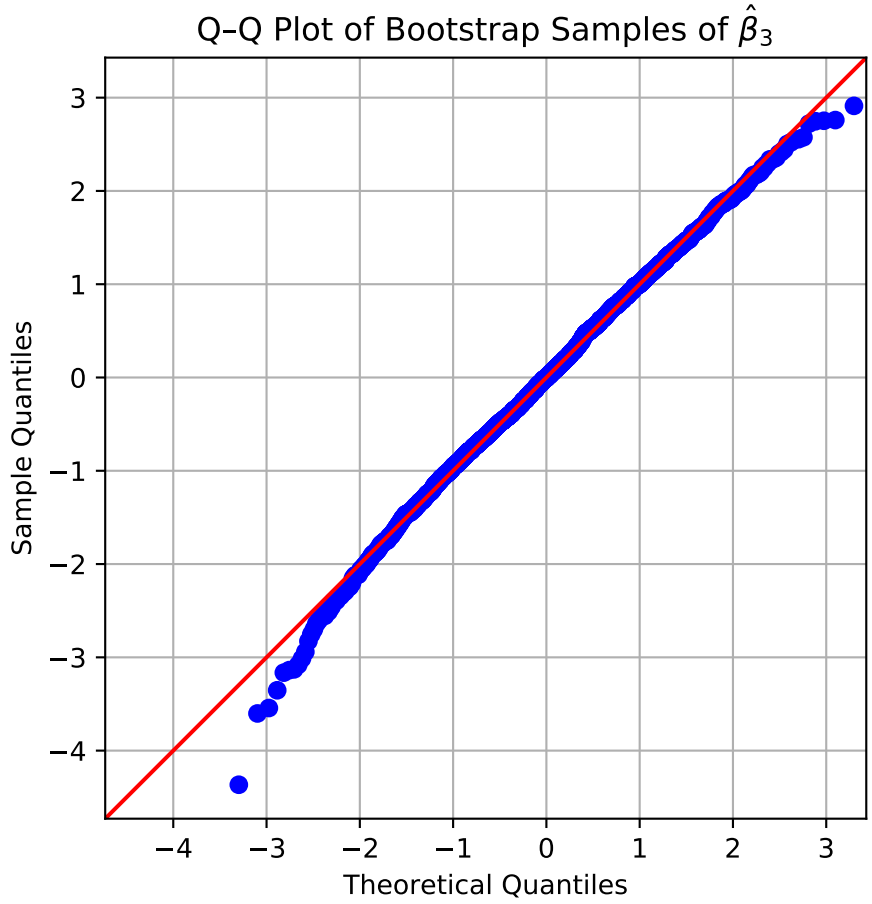


Figure 1: Bootstrap Q–Q plot for $\hat{\beta}_3$ when resampling clusters.

Using $\hat{\Sigma}_{\text{Sandwich}}$ for to get the standard error of $\hat{\beta}_3$, we obtain a smaller standard error $\boxed{0.11686716}$ since we can exploit within cluster correlation to get a better estimate.

(b) Calculate bootstrap standard error estimates for $\hat{\beta}_3$ by resampling clusters. Describe the results of some basic diagnostics you can do to provide confidence that bootstrap intervals are valid for this dataset and that you have simulated a sufficient number of draws to accurately approximate true bootstrap intervals?

Solution: The bootstrap standard error for $\hat{\beta}_3$ when resampling clusters is $\boxed{0.11997406,}$ which is similar to the sandwich estimate.

This was calculated by taking the square root of the sample variance of the of the boostrap samples for $\hat{\beta}_3$. 2,048 samples were taken. Normality of the samples was checked by using a Q–Q plot in Figure 1 and a histogram in Figure 2. The distribution in the histrogram does look normal, and the fit in the Q–Q plot is quite good, so we can be confident that the distribution of the samples is indeed normal.

Indeed, if $\hat{\beta}_3$ is our REML estimate, $\hat{\sigma}$ is our bootstrap standard error, and Φ is the CDF for the standard normal, then the interval $\left[\hat{\beta}_3 - \Phi^{-1}(0.975)\,\hat{\sigma}, \hat{\beta}_3 + \Phi^{-1}(0.975)\,\hat{\sigma}\right]$ contains

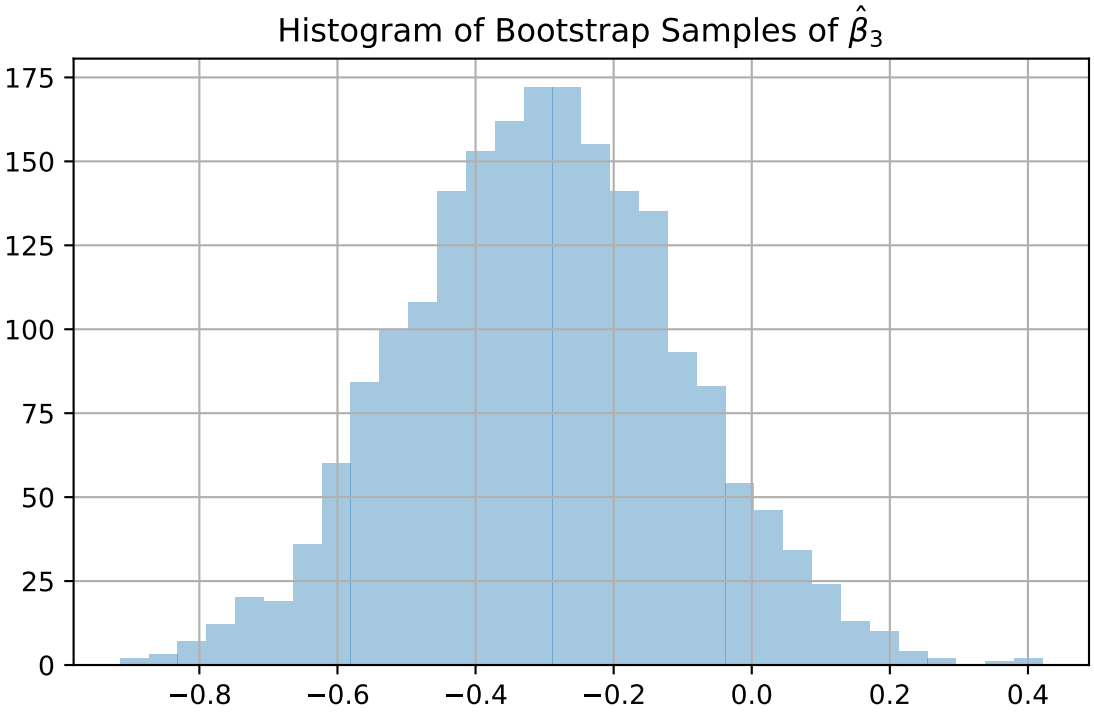


Figure 2: Bootstrap histogram for $\hat{\beta}_3$ when resampling clusters.

94.97% of the bootstrap samples, so the interval is quite accurate.

(c) Calculate bootstrap standard error estimates for $\hat{\beta}_3$ based on resampling observations without regard to cluster and resampling both clusters and observations within clusters.

Solution: The results can be seen in Table 2. Independent sampling is done without regard to clusters. In hierarchical sampling, clusters are sampled, and then, observations within clusters are sampled.

When sampling without regard to clusters, the standard error for $\hat{\beta}_3$ is $\boxed{0.198361,}$ which is similar to the REML standard error in Table 1.

	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

Table 2: Standard errors calculated with the bootstrap with various sampling strategies. 2,048 samples were collected each time.

When resampling both clusters and observations within clusters, the standard error for $\hat{\beta}_3$ is $\boxed{0.218498,}$ which is quite large.

(d) Discuss any differences between your sandwich standard error estimates and the three versions of bootstrap standard errors.

Solution: See Table 1 for the sandwich estimates and Table 2 for the bootstrap estimates.

When only resampling clusters, the standard errors are similar to those of the sandwich-based standard errors. This is not surprising since our equation for the sandwich estimate is accounting for the within-cluster correlation in calculating $\hat{\Sigma}_{\text{Empirical}}$ and summing over the clusters.

When resampling without regard to clusters, the standard errors are similar to those of the REML model. This makes sense since in our REML model, we're assuming homoscedastic covariance models with no correlation, which means we're assuming that our observations are independent of each other.

When resampling both clusters and observations within clusters, we get large, inaccurate standard errors. This is because the cluster sizes $m = 4$ are quite small, so the asymptotics are not kicking in.

Appendix

Code for generating the tables and figures is attached in the subsequent pages.

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
```

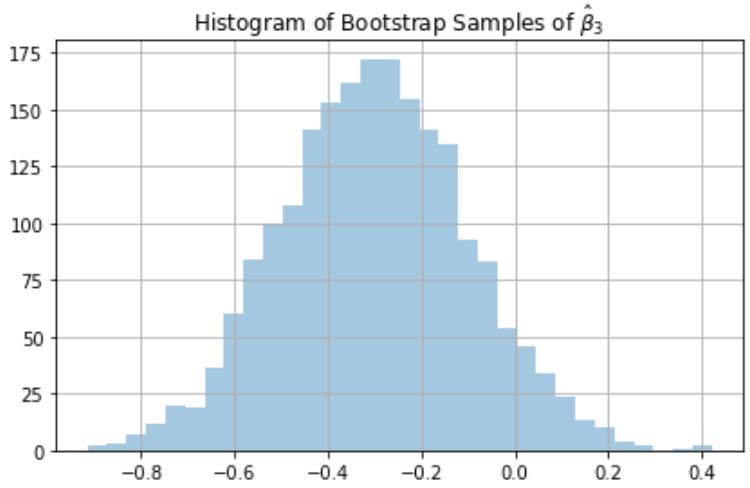
Out[20]:

	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

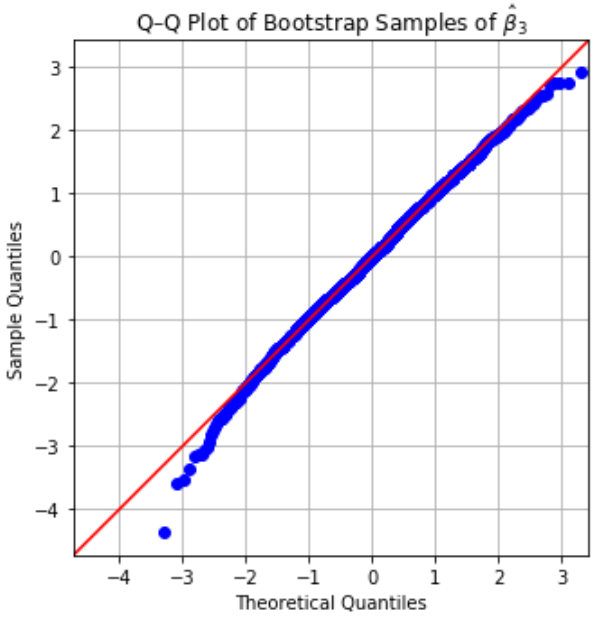
Diagnostic Plots

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)
```