9. The Bootstrap

Let $X_1, \dots, X_n \sim F$ be random variables distributed according to F, and

$$T_n = g(X_1, \dots, X_n)$$

be a **statistic**, that is, any function of the data. Suppose we want to know $\mathbb{V}_F(T_n)$, the variance of T_n.

For example, if $T_n = n^{-1} \sum_{i=1}^n X_i$ then $\mathbb{V}_F(T_n) = \sigma^2 / n$ where $\sigma^2 = \int (x - \mu)^d F(x)$ and $\mu = \int x dF(x)$.

9.1 Simulation

Suppose we draw iid samples $Y_1, \dots, Y_B \sim G$. By the law of large numbers,

$$\overline{Y}_n = \frac{1}{B} \sum_{j=1}^B Y_j \xrightarrow{\text{P}} \int y dG(y) = \mathbb{E}(Y)$$

as $B \rightarrow \infty$. So if we draw a large sample from G, we can use the sample mean to approximate the mean of the distribution.

More generally, if h is any function with finite mean then, as $B \rightarrow \infty$,

$$\frac{1}{B} \sum_{j=1}^B h(Y_j) \xrightarrow{\text{P}} \int h(y) dG(y) = \mathbb{E}(h(Y))$$

In particular, for functions $a(Y_j) = Y_j^2$ and $b(Y_j) = Y_j$,

$$\frac{1}{B} \sum_{j=1}^B (Y_j - \overline{Y}) = \frac{1}{B} \sum_{j=1}^B Y_j^2 - \left(\frac{1}{B} \sum_{j=1}^B Y_j \right)^2 \xrightarrow{\text{P}} \int y^2 dG(y) - \left(\int y dG(y) \right)^2 = \mathbb{V}(Y)$$

So we can use the sample variance of the simulated values to approximate $\mathbb{V}(Y)$.

9.2 Bootstrap Variance Estimation

To simulate from the distribution of a statistic T_n when the data is assumed to have distribution $\hat{F}_n$, we simulate $X_1^*, \dots, X_n^*$ from $\hat{F}_n$ and then compute the statistic over these values, $T_n^* = g(X_1^*, \dots, X_n^*)$.

$$\begin{array}{rlcccc} \text{Real world} & F & \Longrightarrow & X_1, \ldots, X_n & \Longrightarrow & T_n = g(X_1, \ldots, X_n) \\ \text{Bootstrap world} & \hat{F}_n & \Longrightarrow & X_1^*, \ldots, X_n^* & \Longrightarrow & T_n^* = g(X_1^*, \ldots, X_n^*) \end{array} \quad \begin{array}{r} (1) \\ (2) \end{array}$$

Drawing an observation from $\hat{F}_n$ is equivalent to drawing one point at random from the original data set.

Bootstrap Variance Estimation

1. Draw $X_1^*, \ldots, X_n^* \sim \hat{F}_n$.
2. Compute $T_n^* = g(X_1^*, \ldots, X_n^*)$.
3. Repeat steps 1 and 2, B times, to get $T_{n,1}^*, \ldots, T_{n,B}^*$.
4. Let

$$v_{\text{boot}} = \frac{1}{B} \sum_{b=1}^B \left(T_{n,b}^* - \frac{1}{B} \sum_{r=1}^B T_{n,r}^* \right)^2$$

9.3 Bootstrap Confidence Intervals

Normal Interval.

$$T_n \pm z_{\alpha/2} \hat{\text{se}}_{\text{boot}}$$

where $\hat{\text{se}}_{\text{boot}}$ is the bootstrap estimate of the standard error. This is not accurate unless the distribution of T_n is close to Normal.

Pivotal Intervals.

Let $\theta = T(F)$, $\hat{\theta}_n = T(\hat{F}_n)$ and define the **pivot** $R_n = \hat{\theta}_n - \theta$. Let $\hat{\theta}_{n,1}^*, \ldots, \hat{\theta}_{n,B}^*$ define bootstrap replications of $\hat{\theta}_n$. Let $H(r)$ denote the CDF of the pivot:

$$H(r) = \mathbb{P}_F(R_n \leq r)$$

Define the interval $C_n^* = (a, b)$ where

$$a = \hat{\theta}_n - H^{-1}\left(1 - \frac{\alpha}{2}\right) \quad \text{and} \quad b = \hat{\theta}_n - H^{-1}\left(\frac{\alpha}{2}\right)$$

Then,

$$
\begin{aligned}
\mathbb{P}(a \leq \theta \leq b) &= \mathbb{P}(a - \hat{\theta}_n \leq \theta - \hat{\theta}_n \leq b - \hat{\theta}_n) & (3)\\
&= \mathbb{P}(\hat{\theta}_n - b \leq \hat{\theta}_n - \theta \leq \hat{\theta}_n - a) & (4)\\
&= \mathbb{P}(\hat{\theta}_n - b \leq R_n \leq \hat{\theta}_n - a) & (5)\\
&= H(\hat{\theta}_n - a) - H(\hat{\theta}_n - b) & (6)\\
&= H\left(H^{-1}\left(1 - \frac{\alpha}{2}\right)\right) - H\left(H^{-1}\left(\frac{\alpha}{2}\right)\right) & (7)\\
&= 1 - \frac{\alpha}{2} - \frac{\alpha}{2} = 1 - \alpha & (8)
\end{aligned}
$$

Hence C_n^* is an exact $1 - \alpha$ confidence interval for θ.

Unfortunately, a and b depend on the unknown distribution H, but we can form a bootstrap estimate for it:

$$\hat{H}(r) = \frac{1}{B} \sum_{b=1}^{B} I(R^*_{n,b} \leq r)$$

where $R^*_{n,b} = \hat{\theta}^*_{n,b} - \hat{\theta}_n$.

Let r^*_β denote the β sample quantile of $(R^*_{n,1}, \dots, R^*_{n,B})$, and let θ^*_β denote the β sample quantile of $(\theta^*_{n,1}, \dots, \theta^*_{n,B})$. Note that $r^*_\beta = \theta^*_\beta - \hat{\theta}_n$. It follows an approximate $1 - \alpha$ confidence interval $C_n = (\hat{a}, \hat{b})$ where

$$
\begin{aligned}
\hat{a} &= \hat{\theta}_n - \hat{H}^{-1}\left(1 - \frac{\alpha}{2}\right) &&= \hat{\theta}_n - r^*_{1-\alpha/2} = 2\hat{\theta}_n - \theta^*_{1-\alpha/2} & (9)\\
\hat{b} &= \hat{\theta}_n - \hat{H}^{-1}\left(\frac{\alpha}{2}\right) &&= \hat{\theta}_n - r^*_{\alpha/2} = 2\hat{\theta}_n - \theta^*_{\alpha/2} & (10)
\end{aligned}
$$

The $1 - \alpha$ **bootstrap pivotal confidence** is

$$C_n = \left(2\hat{\theta}_n - \hat{\theta}^*_{1-\alpha/2},\ 2\hat{\theta}_n - \hat{\theta}^*_{\alpha/2}\right)$$

Theorem 9.3. Under weak conditions on $T(F)$,

$$\lim_{n \rightarrow \infty} \mathbb{P}_F\left(T(F) \in C_n\right) \rightarrow 1 - \alpha$$

Percentile Intervals.

The **bootstrap percentile interval** is defined by

$$C_n = \left(\theta^*_{\alpha/2},\ \theta^*_{1-\alpha/2}\right)$$

9.5 Technical Appendix

The Jacknife

This method is less computationally expensive than bootstraping, but it is less general -- it does *not* produce consistent estimates of the standard errors of the sample quantiles.

Let $T_n = T(X_1, \dots, X_n)$ be a statistic and let $T_{(-i)}$ denote the statistic with the i-th observation removed. Let $\overline{T}_n = n^{-1} \sum_{i=1}^n T_{(-1)}$. The jacknife estimate of $\mathbb{V}(T_n)$ is

$$v_{\text{jack}} = \frac{n-1}{n} \sum_{i=1}^n \left(T_{(-i)} - \overline{T}_n \right)^2$$

and the jacknife estimate of the standard error is $\hat{\text{se}}_{\text{jack}} = \sqrt{v_{\text{jack}}}$.

Under suitable conditions on T it can be shown that $v_{\text{jack}} / \mathbb{V}(T_n) \xrightarrow{\text{P}} 1$.

Justification for the Percentile Interval

Suppose there exists a monotone transformation $U = m(T)$ such that $U \sim N(\phi, c^2)$ where $\phi = m(\theta)$.

Let $U_t^* = m(\theta^*_{n,b})$. Let u_β^* be the sample quantile of the U_b^*'s. Since a monotone transformation preserves quantiles, we have that $u^*_{\alpha/2} = m(\theta^*_{\alpha/2})$.

Also, since $U \sim N(\phi, c^2)$ the $\alpha/2$ quantile of U is $\phi - z_{\alpha/2} c$. Hence $u^*_{\alpha/2} = \phi - z_{\alpha/2} c$. Similarly, $u^*_{1-\alpha/2} = \phi + z_{\alpha/2} c$.

Therefore,

$$\begin{aligned}
\mathbb{P}(\theta^*_{\alpha/2} \leq \theta \leq \theta^*_{1-\alpha/2}) &= \mathbb{P}(m(\theta^*_{\alpha/2}) \leq m(\theta) \leq m(\theta^*_{1-\alpha/2})) && (11) \\
&= \mathbb{P}(u^*_{\alpha/2} \leq \phi \leq u^*_{1-\alpha/2}) && (12) \\
&= \mathbb{P}(U - c z_{\alpha/2} \leq \phi \leq U + c z_{1-\alpha/2}) && (13) \\
&= \mathbb{P}\left(-z_{\alpha/2} \leq \frac{Y - \phi}{c} \leq z_{1-\alpha/2} \right) && (14) \\
&= 1 - \alpha && (15)
\end{aligned}$$

9.6 Exercises

Exercise 9.6.1. Consider the data in example 9.6.

- Find the plug-in estimate of the correlation coefficient.
- Estimate the standard error using the bootstrap.
- Find a 95% confidence interval using all three methods.

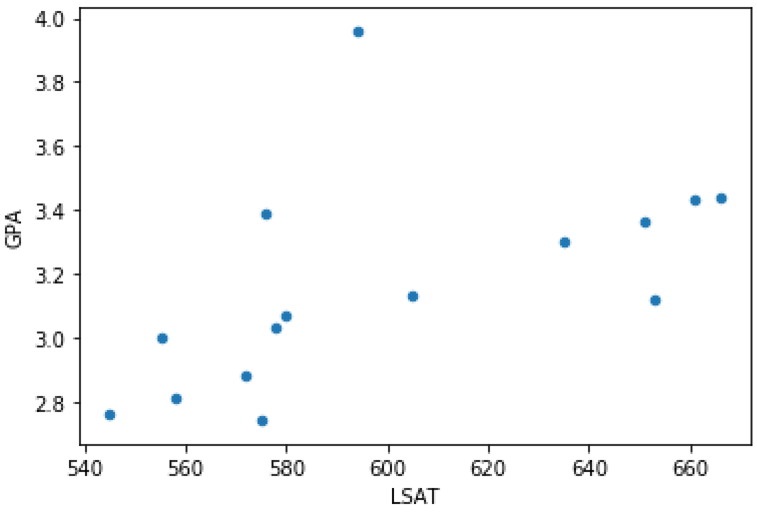
In [1]:
```
# Data from example 9.6:

LSAT = [576, 635, 558, 578, 666, 580, 555, 661, 651, 605, 653, 575, 545, 572, 594]
GPA = [3.39, 3.30, 2.81, 3.03, 3.44, 3.07, 3.00, 3.43, 3.36, 3.13, 3.12, 2.74, 2.76, 2.88, 3.96]
```

In [2]:
```
import math
import numpy as np
import pandas as pd
from tqdm import tqdm_notebook
%matplotlib inline

df = pd.DataFrame({'LSAT': LSAT, 'GPA': GPA})
df.plot.scatter(x='LSAT', y='GPA')
```

Out[2]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x16cf9d8cfd0>
```



In [3]:
```
# Plug-in estimates for mean and correlation

X = df['LSAT'].to_numpy()
Y = df['GPA'].to_numpy()

def corr(X, Y):
    mu_x = X.mean()
    mu_y = Y.mean()

    return sum((X - mu_x) * (Y - mu_y)) / math.sqrt(sum((X - mu_x)**2) * sum((Y - mu_y)**2))


theta_hat = corr(X, Y)

print('Estimated correlation coefficient: %.4f' % corr(X, Y))
```

```
Estimated correlation coefficient: 0.5459
```

In [4]:
```
# Bootstrap for SE of correlation coefficient

nx = len(X)
ny = len(Y)

B = 1000000
t_boot = np.empty(B)
for i in tqdm_notebook(range(B)):
    xx = np.random.choice(X, nx, replace=True)
    yy = np.random.choice(Y, ny, replace=True)
    t_boot[i] = corr(xx, yy)

se = t_boot.std()

print('Estimated SE of correlation coefficient: %.4f' % se)
```

```
Estimated SE of correlation coefficient: 0.2674
```

In [5]:
```
# Confidence intervals obtained from bootstrap

from scipy.stats import norm

z = norm.ppf(.975)

normal_conf = (theta_hat - z * se, theta_hat + z * se)
percentile_conf = (np.quantile(t_boot, .025), np.quantile(t_boot, .975))
```

```
pivotal_conf = (2*theta_hat - np.quantile(t_boot, 0.975), 2*theta_hat - np.quantile(t_boot, .025))

print('95%% confidence interval (Normal): \t %.3f, %.3f' % normal_conf)
print('95%% confidence interval (percentile): \t %.3f, %.3f' % percentile_conf)
print('95%% confidence interval (pivotal): \t %.3f, %.3f' % pivotal_conf)
```

```
95% confidence interval (Normal):       0.022, 1.070
95% confidence interval (percentile):   -0.503, 0.522
95% confidence interval (pivotal):      0.569, 1.594
```

Exercise 9.6.2. (Computer Experiment). Conduct a simulation to compare the four bootstrap confidence interval methods.

Let $n = 50$ and let $T(F) = \int (x-\mu)^3 dF(x)/\sigma^3$ be the skewness. Draw $Y_1, \dots, Y_n \sim N(0,1)$ and set $X_i = e^{Y_i}$, $i = 1, \dots, n$. Construct the four types of bootstrap 95% intervals for $T(F)$ from the data $X_1, \dots, X_n$. Repeat this whole thing many times and estimate the true coverage of the four intervals.

In [6]:
```
import numpy as np
from tqdm import tqdm_notebook
from scipy.stats import norm

def create_data(n=50):
    y = norm.rvs(size=n)
    return np.exp(y)

def skewness(x):
    n = len(x)
    mu = sum(x) / n
    var = sum((x - mu)**2) / n
    return sum((x - mu)**3 / (n * var**(3/2)))

def bootstrap_values(x, B=10000, show_progress=True):
    n = len(x)
    t_boot = np.empty(B)
    iterable = tqdm_notebook(range(B)) if show_progress else range(B)
    for i in iterable:
        xx = np.random.choice(x, n, replace=True)
        t_boot[i] = skewness(xx)

    return t_boot

def bootstrap_intervals(theta_hat, t_boot, alpha=0.05):
    se = t_boot.std()

    z = norm.ppf(1 - alpha/2)
```

```
    q_half_alpha = np.quantile(t_boot, alpha/2)
    q_c_half_alpha = np.quantile(t_boot, 1 - alpha/2)

    normal_conf = (theta_hat - z * se, theta_hat + z * se)
    percentile_conf = (q_half_alpha, q_c_half_alpha)
    pivotal_conf = (2*theta_hat - q_c_half_alpha, 2*theta_hat - q_half_alpha)

    return normal_conf, percentile_conf, pivotal_conf
```

In [7]:
```
# Creating the data
x = create_data(n=50)
```

In [8]:
```
# Nonparametric Bootstrap
theta_hat = skewness(x)
t_boot = bootstrap_values(x, B=100000)

normal_conf, percentile_conf, pivotal_conf = bootstrap_intervals(theta_hat, t_boot, alpha=0.05)

print('95%% confidence interval (Normal): \t %.3f, %.3f' % normal_conf)
print('95%% confidence interval (percentile): \t %.3f, %.3f' % percentile_conf)
print('95%% confidence interval (pivotal): \t %.3f, %.3f' % pivotal_conf)
```

```
95% confidence interval (Normal):       1.032, 2.638
95% confidence interval (percentile):   1.154, 2.757
95% confidence interval (pivotal):      0.912, 2.515
```

Note: parametric bootstrap is only covered in chapter 10. The below assumes that "four types of bootstrap" in the exercise refers to the 3 types of nonparametric bootstrap covered in chapter 9, plus parametric bootstrap from chapter 10.

For the parametric bootstrap, assume $X = e^Y$ where $Y \sim N(\mu, \sigma^2)$. Then

$$\mathbb{E}(X) = \mathbb{E}(e^Y) = \int_{-\infty}^{\infty} e^y \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{y-\mu}{\sigma}\right)^2} dy = \frac{1}{\sigma\sqrt{2\pi}} \int e^{y-\frac{1}{2}\left(\frac{y-\mu}{\sigma}\right)^2} dy = e^{\mu+\sigma^2/2} \tag{16}$$

$$\mathbb{E}(X^2) = \mathbb{E}(e^{2Y}) = e^{2\mu+(2\sigma)^2/2} = e^{2\mu+2\sigma^2} \tag{17}$$

Solving the two equations for the moments we get parameter estimates:

$$\hat{\mu}_Y = 4\log\mathbb{E}(X) - \log\mathbb{E}(X^2) \tag{18}$$

$$\hat{\sigma}_Y = \sqrt{\log\mathbb{E}(X^2) - 2\log\mathbb{E}(X)} \tag{19}$$

From these parameter estimates, we can generate bootstrap samples: sample values for $Y_i \; N(\hat{\mu}_Y, \hat{\sigma}^2_Y)$, calculate $X_i = Y_i$, and calculate the statistic $T(X_i)$ on each sample generated this way.

In [9]:
```
# Parametric bootstrap
# Assume X = e^Y, Y ~ N(\mu, \sigma^2)

def estimate_parameters(x):
    log_e_x = np.log(x.mean())
    log_e_x2 = np.log((x**2).mean())

    mu_Y_hat = 4 * log_e_x - log_e_x2
    sigma_Y_hat = np.sqrt(log_e_x2 - 2 * log_e_x)

    return mu_Y_hat, sigma_Y_hat

def bootstrap_skewness_parametric(mu, sigma, n, B = 10000, show_progress=True):
    t_boot = np.empty(B)
    iterable = tqdm_notebook(range(B)) if show_progress else range(B)
    for i in iterable:
        xx = np.exp(norm.rvs(size=n, loc=n, scale=sigma))
        t_boot[i] = skewness(xx)

    return t_boot

def bootstrap_parametric_intervals(mu, t_boot, alpha=0.05):
    se = t_boot.std()
    z = norm.ppf(1 - alpha/2)

    return (theta_hat - z * se, theta_hat + z * se)
```

In [10]:
```
mu_X_hat = x.mean()
mu_Y_hat, sigma_Y_hat = estimate_parameters(x)
t_boot = bootstrap_skewness_parametric(mu_Y_hat, sigma_Y_hat, 50, B=100000)

parametric_normal_conf = bootstrap_parametric_intervals(mu_X_hat, t_boot, alpha=0.05)
print('95%% confidence interval (Parametric Normal): \t %.3f, %.3f' % parametric_normal_conf)
```

```
95% confidence interval (Parametric Normal):     -0.181, 3.851
```

In [11]:
```
# Repeat nonparametric bootstrap many times
n_experiments = 10

normal_conf = np.empty((n_experiments, 2))
```

```
percentile_conf = np.empty((n_experiments, 2))
pivotal_conf = np.empty((n_experiments, 2))

for i in tqdm_notebook(range(n_experiments)):
    theta_hat = skewness(x)
    t_boot_experiment = bootstrap_values(x, B=100000, show_progress=False)
    normal_conf[i], percentile_conf[i], pivotal_conf[i] = bootstrap_intervals(theta_hat, t_boot_experiment, alpha=0.05)
```

In [12]:

```
print('Normal confidence lower bound: \t\t mean %.3f, SE %.3f' %
      (normal_conf[:, 0].mean(), normal_conf[:, 0].std()))
print('Normal confidence upper bound: \t\t mean %.3f, SE %.3f' %
      (normal_conf[:, 1].mean(), normal_conf[:, 1].std()))

print('Percentile confidence lower bound: \t mean %.3f, SE %.3f' %
      (percentile_conf[:, 0].mean(), percentile_conf[:, 0].std()))
print('Percentile confidence upper bound: \t mean %.3f, SE %.3f' %
      (percentile_conf[:, 1].mean(), percentile_conf[:, 1].std()))

print('Pivotal confidence lower bound: \t mean %.3f, SE %.3f' %
      (pivotal_conf[:, 0].mean(), pivotal_conf[:, 0].std()))
print('Pivotal confidence upper bound: \t mean %.3f, SE %.3f' %
      (pivotal_conf[:, 1].mean(), pivotal_conf[:, 1].std()))
```

```
Normal confidence lower bound:          mean 1.031, SE 0.001
Normal confidence upper bound:          mean 2.639, SE 0.001
Percentile confidence lower bound:      mean 1.154, SE 0.002
Percentile confidence upper bound:      mean 2.762, SE 0.005
Pivotal confidence lower bound:         mean 0.907, SE 0.005
Pivotal confidence upper bound:         mean 2.515, SE 0.002
```

In [13]:

```
# Repeat parametric bootstrap many times

n_experiments = 10
parametric_normal_conf = np.empty((n_experiments, 2))

for i in tqdm_notebook(range(n_experiments)):
    mu_X_hat = x.mean()
    mu_Y_hat, sigma_Y_hat = estimate_parameters(x)
    t_boot = bootstrap_skewness_parametric(mu_Y_hat, sigma_Y_hat, 50, B=100000, show_progress=False)
    parametric_normal_conf[i] = bootstrap_parametric_intervals(mu_X_hat, t_boot, alpha=0.05)
```

In [14]:
```
print('Parametric Normal confidence lower bound: \t mean %.3f, SE %.3f' %
      (parametric_normal_conf[:, 0].mean(), parametric_normal_conf[:, 0].std()))
print('Parametric Normal confidence upper bound: \t mean %.3f, SE %.3f' %
      (parametric_normal_conf[:, 1].mean(), parametric_normal_conf[:, 1].std()))
```

```
Parametric Normal confidence lower bound:        mean -0.185, SE 0.003
Parametric Normal confidence upper bound:        mean 3.854, SE 0.003
```

Exercise 9.6.3. Let $X_1, \dots, X_n \sim t_3$ where $n = 25$. Let $\theta = T(F) = (q_{.75} - q_{.25})/1.34$ where q_p denotes the p-th quantile. Do a simulation to compare the coverage and length of the following confidence intervals for θ:

- Normal interval with standard error from the bootstrap
- Bootstrap percentile interval

Remark: the jacknife does not give a consistent estimator of the variance of a quantile.

Solution. We will assume that t_3 represents a t-distribution with shape parameter 3.

In [15]:
```
import numpy as np
from scipy.stats import t
from tqdm import tqdm_notebook

n = 25
X = t.rvs(3, size=25)
```

In [16]:
```
def T(x):
    return (np.quantile(x, 0.75) - np.quantile(x, 0.25)) / 1.34
```

In [17]:
```
theta_hat = T(X)
```

In [18]:
```
# Run bootstrap

B = 1000000
t_boot = np.empty(B)
for i in tqdm_notebook(range(B)):
    xx = np.random.choice(X, n, replace=True)
    t_boot[i] = T(xx)

se_boot = t_boot.std()

alpha = 0.05
z = norm.ppf(1 - alpha/2)
q_half_alpha = np.quantile(t_boot, alpha/2)
```

```
q_c_half_alpha = np.quantile(t_boot, 1 - alpha/2)

normal_conf = (theta_hat - z * se_boot, theta_hat + z * se_boot)
percentile_conf = (q_half_alpha, q_c_half_alpha)

print('95%% confidence interval (Normal): \t %.3f, %.3f' % normal_conf)
print('95%% confidence interval (percentile): \t %.3f, %.3f' % percentile_conf)
```

```
95% confidence interval (Normal):        0.032, 2.089
95% confidence interval (percentile):    0.605, 2.378
```

Exercise 9.6.4. Let $X_1, \dots, X_n$ be distinct observations (no ties). Show that there are

$$\binom{2n-1}{n}$$

distinct bootstrap samples.

Hint: Imagine putting n balls into n buckets.

Solution.

Each bootstrap sample (random draws with replacement) will select a_i copies of X_i, where $0 \leq a_i \leq n$ and $\sum_{i=1}^n a_i = n$, for integer a_i. Each bootstrap sample is uniquely represented by this sequence of variables, and each sequence of variables uniquely determines a bootstrap sample -- so the number of distinct bootstrap samples is equal to the number of solutions to this equation, that is, the number of partitions of n into n buckets.

Lets write a_i explicitly in base 1, representing it as a_i consecutive copies of the digit 1:

$$
\begin{aligned}
0_{10} &= \text{empty string}_1 && (20) \\
1_{10} &= 1_1 && (21) \\
2_{10} &= 11_1 && (22) \\
3_{10} &= 111_1 && (23) \\
4_{10} &= 1111_1 && (24) \\
&\vdots && (25)
\end{aligned}
$$

So a solution for

$$a_1 + a_2 + \cdots + a_n = n$$

is uniquely represented by a sequence of $2n-1$ symbols, being n digits 1 and $n-1$ plus signs. For example, if $a_1=3$, $a_2=0$, $a_3=1$, then we write

$$111++1+\cdots=n$$

The number of such solutions is then obtained by choosing n of the $2n-1$ symbols to be digit 1 -- that is, $\binom{2n-1}{n}$.

Exercise 9.6.5. Let $X_1,\dots,X_n$ be distinct observations (no ties). Let $X_1^*,\dots,X_n^*$ denote a bootstrap sample and let $\overline{X}^*_n = n^{-1}\sum_{i=1}^n X_i^*$. Find:

- $\mathbb{E}(\overline{X}^*_n | X_1,\dots,X_n)$
- $\mathbb{V}(\overline{X}^*_n | X_1,\dots,X_n)$
- $\mathbb{E}(\overline{X}^*_n)$
- $\mathbb{V}(\overline{X}^*_n)$

Solution.

(a)

$$\mathbb{E}(\overline{X}^*_n | X_1,\dots,X_n) = \mathbb{E}\left(n^{-1}\sum_{i=1}^n X_i\right) = n^{-1}\sum_{i=1}^n \mathbb{E}(X_i) = \mathbb{E}(X) \tag{26}$$

(b)

$$\begin{aligned}
\mathbb{V}(\overline{X}^*_n|X_1,\dots,X_n) &= \mathbb{E}((\overline{X}^*_n)^2|X_1,\dots,X_n) - \mathbb{E}(\overline{X}^*_n|X_1,\dots,X_n)^2 && (27)\\
&= \mathbb{E}\left(\left(n^{-1}\sum_{i=1}^n X_i\right)^2\right) - \mathbb{E}\left(n^{-1}\sum_{i=1}^n X_i\right)^2 && (28)\\
&= n^{-2}\mathbb{E}\left(\sum_{i=1}^n X_i^2 + \sum_{i=1}^n \sum_{j=1, j\neq i}^n X_i X_j\right) - \mathbb{E}(X)^2 && (29)\\
&= n^{-2}\sum_{i=1}^n \mathbb{E}(X_i^2) + n^{-2}\sum_{i=1}^n \sum_{j=1, j\neq i}^n \mathbb{E}(X_i X_j) - \mathbb{E}(X)^2 && (30)\\
&= n^{-1}(\mathbb{V}(X) + \mathbb{E}(X)^2) + n^{-2}\sum_{i=1}^n \sum_{j=1, j\neq i}^n \mathbb{E}(X_i)\mathbb{E}(X_j) - \mathbb{E}(X)^2 && (31)\\
&= n^{-1}(\mathbb{V}(X) + \mathbb{E}(X)^2) + n^{-1}(n-1)\mathbb{E}(X)^2 - \mathbb{E}(X)^2 && (32)\\
&= \frac{1}{n}\mathbb{V}(X) && (33)
\end{aligned}$$

(c)

$$\mathbb{E}(\overline{X}^*_n) = \mathbb{E}\left(n^{-1}\sum_{i=1}^n X_i^*\right) = n^{-1}\sum_{i=1}^n \mathbb{E}(X_i^*) = \mathbb{E}(X) \quad (34)$$

(d)

$$\begin{aligned}
\mathbb{V}(\overline{X}^*_n) &= \mathbb{E}((\overline{X}^*_n)^2) - \mathbb{E}(\overline{X}^*_n)^2 && (35)\\
&= \mathbb{E}\left(\left(n^{-1}\sum_{i=1}^n X_i^*\right)^2\right) - \mathbb{E}(X)^2 && (36)\\
&= n^{-2}\sum_{i=1}^n \sum_{j=1}^n \mathbb{E}(X_i^* X_j^*) - \mathbb{E}(X)^2 && (37)
\end{aligned}$$

Now, the same value X_k may have been sampled twice in $\mathbb{E}(X_i^* X_j^*)$. This always happens when $i = j$, and this happens with probability $1/n$ when $i \neq j$. Thus,

$$
\begin{aligned}
\mathbb{V}(\overline{X}^*_n) &= n^{-2}\left(\sum_{i=1}^n \mathbb{E}(X_i^2) + \sum_{i=1}^n \sum_{j=1, j\neq i}^n \left(\frac{1}{n}\mathbb{E}(X_i^2) + \left(1 - \frac{1}{n}\right)\mathbb{E}(X_i)\mathbb{E}(X_j)\right)\right) - \mathbb{E}(X)^2 && (38)\\
&= n^{-1}\mathbb{E}(X^2) + n^{-2}(n-1)\mathbb{E}(X^2) + n^{-2}(n-1)^2 E(X)^2 - \mathbb{E}(X)^2 && (39)\\
&= n^{-2}(2n-1)\left(\mathbb{E}(X^2) - \mathbb{E}(X)^2\right) && (40)\\
&= \frac{2n-1}{n^2}\mathbb{V}(X) && (41)
\end{aligned}
$$

Exercise 9.6.6. (Computer Experiment). Let $X_1, \dots, X_n \sim N(\mu, 1)$. Let $\theta = e^{\mu}$and let $\hat{\theta} = e^{\overline{X}}$ be the mle. Create a dataset (using $\mu = 5$) consisting of $n = 100$ observations.

(a) Use the bootstrap to get the se and 95% confidence interval for θ.

(b) Plot a histogram of the bootstrap replications for the parametric and non-parametric bootstraps. These are estimates of the distribution of $\hat{\theta}$. Compare this to the true sampling distribution of $\hat{\theta}$.

In [19]:

```
import numpy as np
import pandas as pd
from scipy.stats import norm
from tqdm import tqdm_notebook
%matplotlib inline

X = norm.rvs(loc=5, scale=1, size=100)
```

In [20]:

```
# Get estimated value

theta_hat = np.exp(X.mean())

# Run nonparametric bootstrap

B = 1000000
t_boot_nonparam = np.empty(B)
n = len(X)
for i in tqdm_notebook(range(B)):
    xx = np.random.choice(X, n, replace=True)
    t_boot_nonparam[i] = np.exp(xx.mean())

se_boot = t_boot_nonparam.std()

alpha = 0.05
```

```
z = norm.ppf(1 - alpha/2)
normal_conf = (theta_hat - z * se_boot, theta_hat + z * se_boot)

print('95%% confidence interval (Normal): \t %.3f, %.3f' % normal_conf)
```

```
95% confidence interval (Normal):        104.486, 160.228
```

In [21]:

```
# Run parametric bootstrap

mu_hat = X.mean()
theta_hat = np.exp(mu_hat)

B = 1000000
t_boot_param = np.empty(B)
n = len(X)
for i in tqdm_notebook(range(B)):
    xx = norm.rvs(size=n, loc=mu_hat, scale=1)
    t_boot_param[i] = np.exp(xx.mean())

se_boot_param = t_boot_param.std()

alpha = 0.05
z = norm.ppf(1 - alpha/2)
normal_conf_param = (theta_hat - z * se_boot_param, theta_hat + z * se_boot_param)

print('95%% confidence interval (Parametric Normal): \t %.3f, %.3f' % normal_conf_param)
```

```
95% confidence interval (Parametric Normal):     106.225, 158.490
```

For the true sampling distribution,

$$\overline{X} = \frac{1}{n} \sum_{i=1}^n X_i \sim \frac{1}{n} N(n\mu, n) = N(\mu, n^{-2})$$

so the distribution of $\hat{\theta}$ is the distribution of $e^{\overline{X}}$. Its CDF is:

$$\mathbb{P}\left(\hat{\theta} \leq t\right) = \mathbb{P}\left(e^{\overline{X}} \leq t\right) = \mathbb{P}\left(\overline{X} \leq \log t\right) = F_{\overline{X}}(\log t)$$

In [22]:

```
import numpy as np
from scipy.stats import norm
from matplotlib import pyplot
```

```python
bins = np.linspace(50, 250, 500)
```

In [23]:

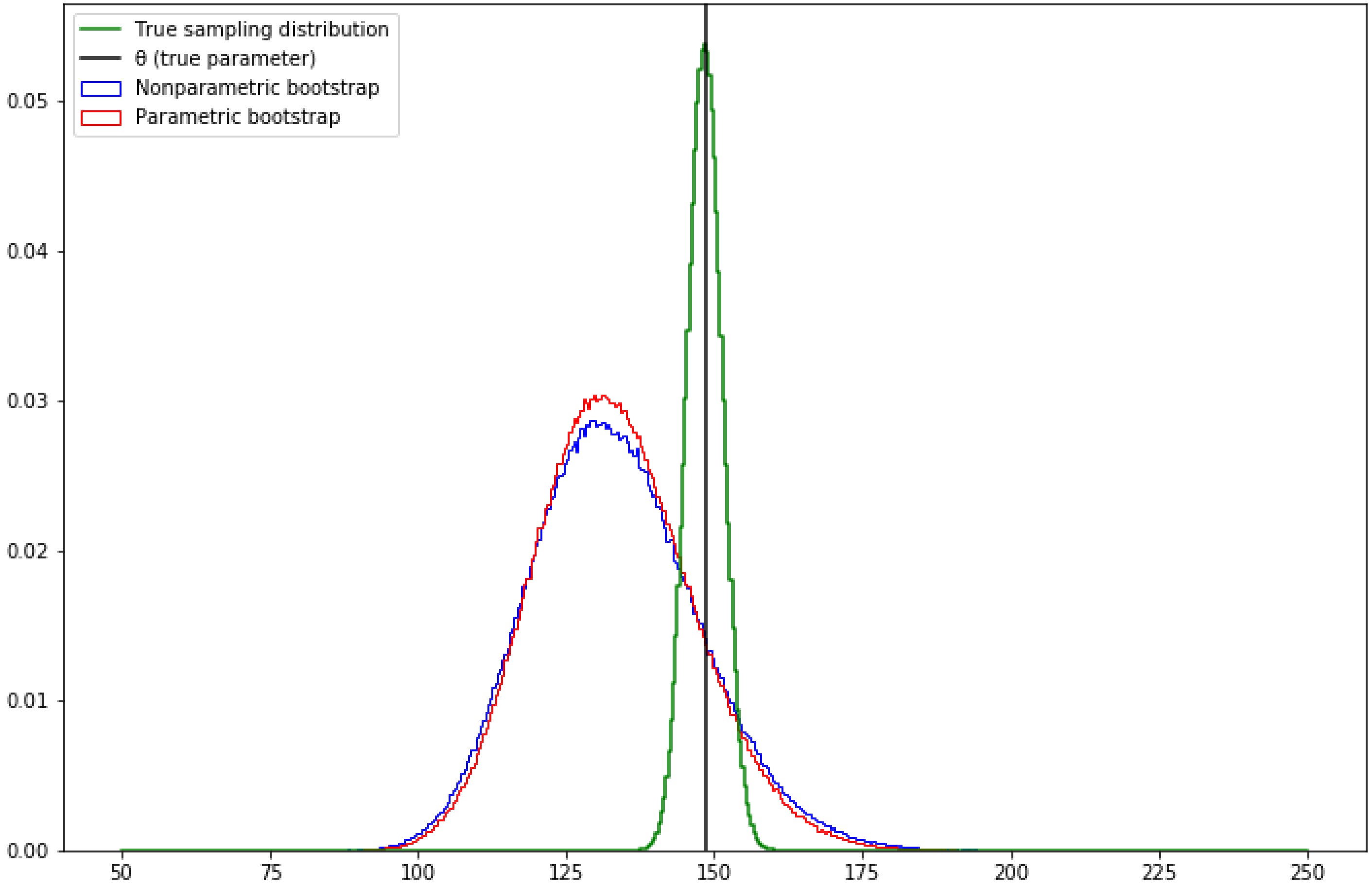
```python
# Generate the CDF for theta, calculate it for each bin, and include the differences between bins

def theta_cdf(x):
    return norm.cdf(np.log(x), loc=5, scale=1/50)

theta_cdf_bins = list(map(theta_cdf, bins))
theta_cdf_bins_delta = np.empty(len(bins))
theta_cdf_bins_delta[0] = 0
theta_cdf_bins_delta[1:] = np.diff(theta_cdf_bins)
```

In [24]:

```python
pyplot.figure(figsize=(12, 8))
pyplot.hist(t_boot_nonparam, bins, label='Nonparametric bootstrap', color='blue', histtype='step', density=True)
pyplot.hist(t_boot_param, bins, label='Parametric bootstrap', color='red', histtype='step', density=True)
pyplot.step(bins, theta_cdf_bins_delta, color='green', label='True sampling distribution')
pyplot.axvline(x=np.exp(5), color='black', label='θ (true parameter)')
pyplot.legend(loc='upper left')
pyplot.show()
```



Exercise 9.6.7. Let $X_1, \dots, X_n \sim \text{Uniform}(0, \theta)$. The mle is $\hat{\theta} = X_{\text{max}} = \max\{X_1, \dots, X_n\}$. Generate a dataset of size 50 with $\theta = 1$.

(a) Find the distribution of $\hat{\theta}$. Compare the true distribution of $\hat{\theta}$ to the histograms from the parametric and nonparametric bootstraps.

(b) This is a case where the nonparametric bootstrap does very poorly. In fact, we can prove that this is the case. Show that, for parametric bootstrap $\mathbb{P}(\hat{\theta}^* = \hat{\theta}) = 0$ but for the nonparametric $\mathbb{P}(\hat{\theta}^* = \hat{\theta}) \approx 0.632$.

Hint: show that $\mathbb{P}(\hat{\theta}^* = \hat{\theta}) = 1 - (1 - (1/n))^n$ then take the limit as n gets large.

In [25]:
```
import numpy as np

X = np.random.uniform(low=0, high=1, size=50)
```

In [26]:
```
# Nonparametric bootstrap

theta_hat = X.max()

B = 1000000
t_boot_nonparam = np.empty(B)
n = len(X)
for i in tqdm_notebook(range(B)):
    xx = np.random.choice(X, n, replace=True)
    t_boot_nonparam[i] = xx.max()

se_boot = t_boot_nonparam.std()

alpha = 0.05
z = norm.ppf(1 - alpha/2)
normal_conf = (theta_hat - z * se_boot, theta_hat + z * se_boot)

print('95%% confidence interval (Normal): \t %.3f, %.3f' % normal_conf)
```

```
95% confidence interval (Normal):        0.959, 1.037
```

In [27]:
```
# Run parametric bootstrap

theta_hat = X.max()

B = 1000000
t_boot_param = np.empty(B)
n = len(X)
for i in tqdm_notebook(range(B)):
    xx = np.random.uniform(low=0, high=theta_hat, size=50)
    t_boot_param[i] = xx.max()

se_boot_param = t_boot_param.std()

alpha = 0.05
z = norm.ppf(1 - alpha/2)
normal_conf_param = (theta_hat - z * se_boot_param, theta_hat + z * se_boot_param)

print('95%% confidence interval (Parametric Normal): \t %.3f, %.3f' % normal_conf_param)
```

```
95% confidence interval (Parametric Normal):     0.960, 1.036
```

For the true sampling distribution,

$$\hat{\theta} = \max\{X_1, \dots X_n\}$$

Its CDF is

$$\mathbb{P}(\hat{\theta} \leq x) = \prod_{i=1}^n \mathbb{P}(X_i \leq x) = F_{\text{Uniform}(0,\theta)}(x)^n$$

where

$$F_{\text{Uniform}(0,\theta)}(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ \frac{x}{\theta} & \text{if } 0 < x \leq \theta \\ 1 & \text{if } \theta < x \end{cases}$$

In [28]:

```
bins = np.linspace(0.75, 1.05, 200)
```

In [29]:

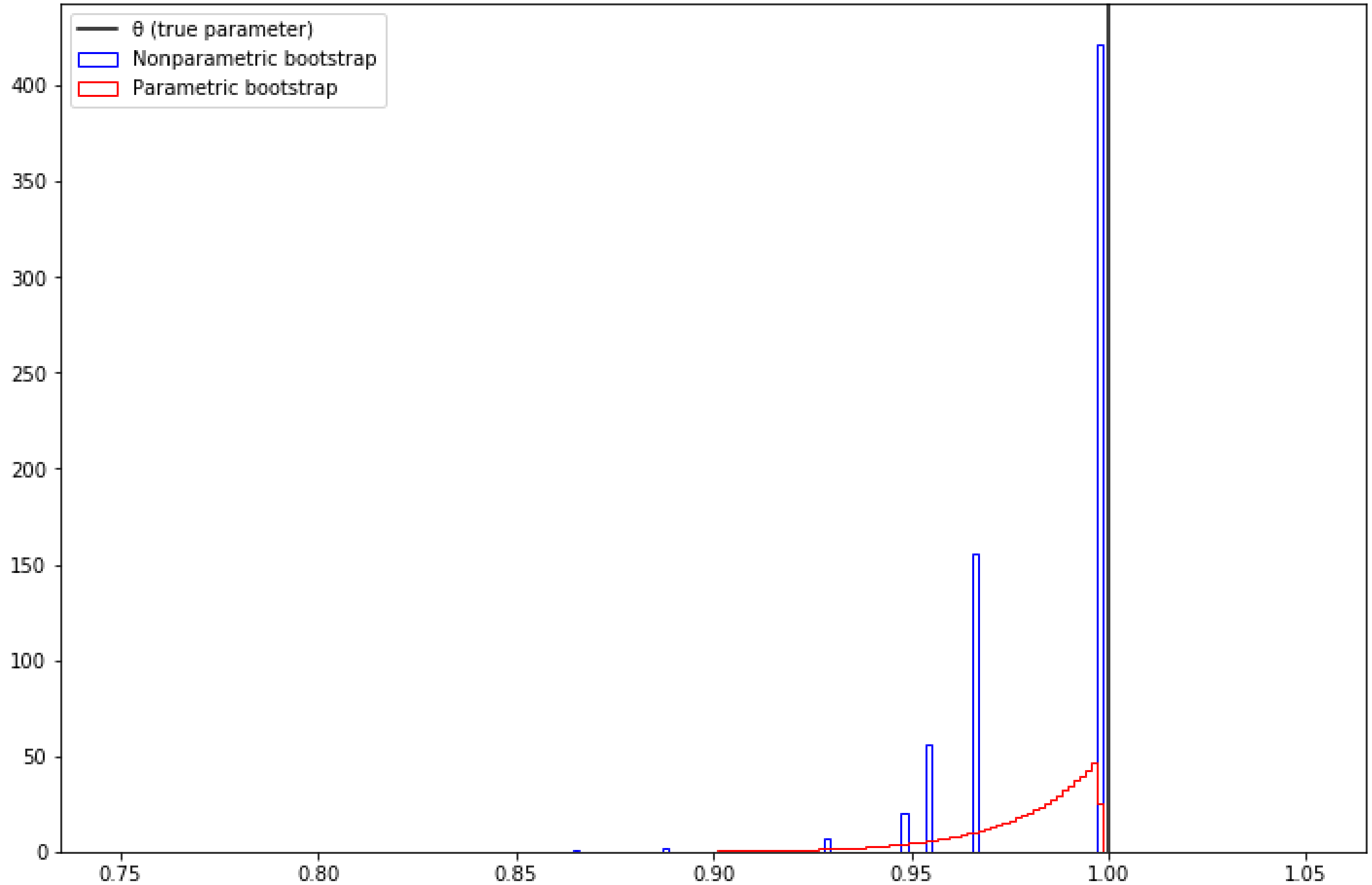
```
# Generate the CDF for theta, calculate it for each bin, and include the differences between bins

def theta_cdf(x):
    if x <= 0:
        return 0
    if x >= 1:
        return 1
    return x**50

theta_cdf_bins = list(map(theta_cdf, bins))
theta_cdf_bins_delta = np.empty(len(bins))
theta_cdf_bins_delta[0] = 0
theta_cdf_bins_delta[1:] = np.diff(theta_cdf_bins)
```

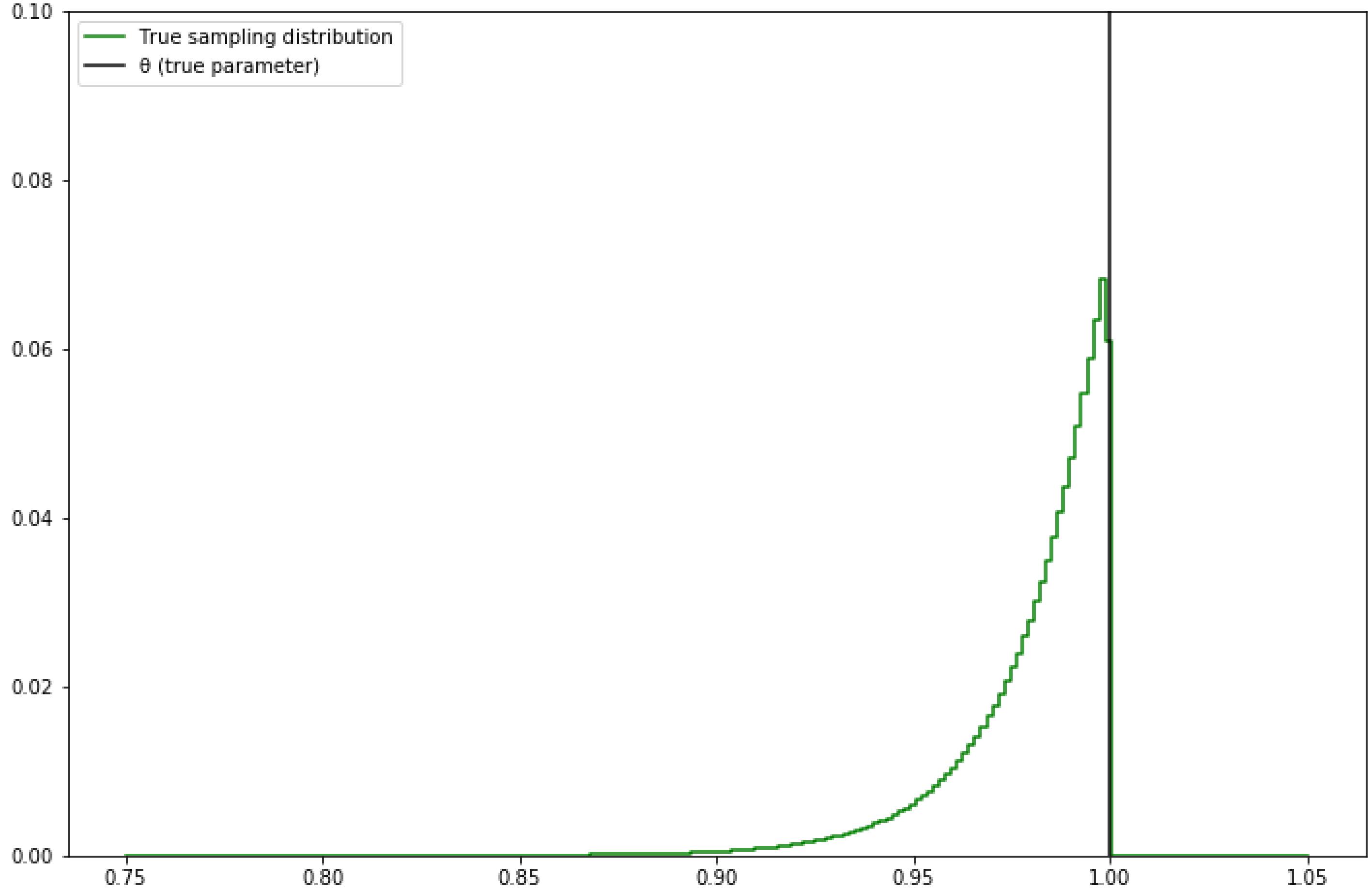
In [30]:

```
pyplot.figure(figsize=(12, 8))
pyplot.hist(t_boot_nonparam, bins, label='Nonparametric bootstrap', color='blue', histtype='step', density=True)
pyplot.hist(t_boot_param, bins, label='Parametric bootstrap', color='red', histtype='step', density=True)
pyplot.axvline(x=1, color='black', label='θ (true parameter)')
pyplot.legend(loc='upper left')
pyplot.show()
```



In [31]:

```
pyplot.figure(figsize=(12, 8))
pyplot.step(bins, theta_cdf_bins_delta, color='green', label='True sampling distribution')
pyplot.axvline(x=1, color='black', label='θ (true parameter)')
pyplot.legend(loc='upper left')
pyplot.ylim(0, 0.1)
pyplot.show()
```



(b)

For the parametric bootstrap process, the estimated parameter $\hat{\theta}^*$ is used on each k-th bootstrap sampling $\{X_{k1}, X_{k2}, \dots, X_{kn}\}$. But each variable X_{kj} is sampled from $\text{Uniform}(0, \hat{\theta}^*)$, which is a continuous distribution -- so the probability of obtaining exactly a sample at the boundaries is 0, and $\mathbb{P}(X_{kj} < \hat{\theta}^*) = 1$. Since the bootstrap functional of each draw, $T(F_n) = \max(F_n)$ is the largest drawn value in each sample, its values will also always be under $\hat{\theta}$, thus the estimated parameter via parametric bootstraping will aywals be under $[\hat{\theta}$, and $\mathbb{P}(\hat{\theta} * = \hat{\theta}) = 0$.

For the nonparametric bootstrap process, the estimated parameter $\hat{\theta}^*$ is the maximum value with a point mass in the empirical distribution function $\hat{F}$. Each bootstrap resample may or may not include that value when drawing from this sample -- if $\max\{X_1, \dots, X_n\} \in \{X_{k1}, \dots, X_{kn}\}$ then the estimated functional for that bootstrap sample will be the estimated parameter $\hat{\theta}^*$, otherwise it will necessarily be smaller.

Thus, the probability that $\mathbb{P}(\hat{\theta}* = \hat{\theta})$ is the probability that the largest element on the original data is included in a resampling with replacement. That turns out to be one minus the probability that it never gets included, so, $\mathbb{P}(\hat{\theta}* = \hat{\theta}) = 1 - (1 - (1/n))^n$. But $\lim_{n \to \infty}(1 + x/n)^n = e^x$, so the given probability goes to $1 - e^{-1} \approx 0.632$.

Exercise 9.6.8. Let $T_n = \overline{X}_n^2$, $\mu = \mathbb{E}(X_1)$, $\alpha_k = \int |x - \mu|^k dF(x)$ and $\hat{\alpha}_k = n^{-1} \sum_{i=1}^n |X_i - \overline{X}_n|^k$. Show that

$$v_{\text{boot}} = \frac{4\overline{X}_n^2 \hat{\alpha}_2}{n} + \frac{4\overline{X}_n \hat{\alpha}_3}{n^2} + \frac{\hat{\alpha}_4}{n^3}$$

Solution.

First, we rewrite the sample mean in terms of an expression containing the central moments. Let $S_n = n^{-1} \sum_{i=1}^n (X_i - \overline{X}_n) = 0$. Then:

$$\overline{X}_n = S_n + \overline{X}_n = \frac{1}{n} \sum_{i=1}^n (X_i - \overline{X}_n) + \overline{X}_n$$

The bootstrap variance, $\mathbb{V}\left(\overline{X}_n^2\right)$, can be expressed as

$$\mathbb{V}\left(\overline{X}_n^2\right) = \mathbb{E}\left(\overline{X}_n^4\right) - \mathbb{E}\left(\overline{X}_n^2\right)^2$$

Note that $\overline{X}_n$ is the mean of the distribution, and can be treated as constant when taking expectations.

We now have:

$$\begin{aligned}
\mathbb{E}\left(\overline{X}_n^4\right) &= \mathbb{E}\left((S_n + \overline{X}_n)^4\right) && (42) \\
&= \mathbb{E}\left(S_n^4 + 4S_n^3\overline{X}_n + 6S_n^2\overline{X}_n^2 + 4S_n\overline{X}_n^3 + \overline{X}_n^4\right) && (43) \\
&= \mathbb{E}(S_n^4) + 4\overline{X}_n\mathbb{E}(S_n^3) + 6\overline{X}_n^2\mathbb{E}(S_n^2) + 4\overline{X}_n^3\mathbb{E}(S_n) + \overline{X}_n^4 && (44)
\end{aligned}$$

Then, computing the moments of S_n,

$$\mathbb{E}(S_n) = 0 \tag{45}$$

$$\mathbb{E}(S_n^2) = \mathbb{E}\left(n^{-2}\left(\sum_i X_i - \overline{X}_n\right)^2\right) = \frac{\hat{\alpha}_2}{n} \tag{46}$$

$$\mathbb{E}(S_n^3) = \mathbb{E}\left(n^{-3}\left(\sum_i X_i - \overline{X}_n\right)^3\right) = \frac{\hat{\alpha}_3}{n^2} \tag{47}$$

$$\mathbb{E}(S_n^4) = \mathbb{E}\left(n^{-4}\left(\sum_i X_i - \overline{X}_n\right)^4 + n^{-2}n^{-4}\sum_i \sum_{j \neq i} (X_i - \overline{X}_n)^2 (X_j - \overline{X}_n)^2\right) = \frac{\hat{\alpha}_4 + \hat{\alpha}_2^2}{n^3} \tag{48}$$

and finally

$$\mathbb{E}\left(\overline{X}_n^2\right)^2 = \mathbb{E}\left(\overline{X}_n^2 + S_n\right)^2 = \overline{X}_n^4 + 2\overline{X}_n^2 \frac{\hat{\alpha}_2}{n} + \frac{\hat{\alpha}_2^2}{n^2}$$

Putting everything together,

$$v_{\text{boot}} = \mathbb{E}\left((S_n + \overline{X}_n)^4\right) - \mathbb{E}\left(\overline{X}_n^2 + S_n\right)^2 \tag{49}$$

$$= \mathbb{E}(S_n^4) + 4\overline{X}_n \mathbb{E}(S_n^3) + 6\overline{X}_n^2 \mathbb{E}(S_n^2) + 4\overline{X}_n^3 \mathbb{E}(S_n) + \overline{X}_n^4 - \left(\overline{X}_n^4 + 2\overline{X}_n^2 \frac{\hat{\alpha}_2}{n} + \frac{\hat{\alpha}_2^2}{n^2}\right) \tag{50}$$

$$= \frac{\hat{\alpha}_4 + \hat{\alpha}_2^2}{n^3} + 4\overline{X}_n \frac{\hat{\alpha}_3}{n^2} + 6\overline{X}_n^2 \frac{\hat{\alpha}_2}{n} + 0 + \overline{X}_n^4 - \overline{X}_n^4 - 2\overline{X}_n^2 \frac{\hat{\alpha}_2}{n} - \frac{\hat{\alpha}_2^2}{n^2} \tag{51}$$

$$= \frac{4\overline{X}_n^2 \hat{\alpha}_2}{n} + \frac{4\overline{X}_n \hat{\alpha}_3}{n^2} + \frac{\hat{\alpha}_4}{n^3} \tag{52}$$

Reference and discussion: https://stats.stackexchange.com/q/26082