ASI Final Assignment

https://github.com/mspronesti/advanced-statistical-inference

Load the Dataset

In [5]:
```
from google.colab import drive
drive.mount('/content/drive')

%cd /content/drive/MyDrive/
```

```
Drive already mounted at /content/drive; to attempt to forcibly remount, call drive.mo
unt("/content/drive", force_remount=True).
/content/drive/MyDrive
```

In [6]:
```
# load from kaggle using kaggle.json config file from drive
# assumption: kaggle.json is located under the main root in your drive

###################################
# If you run this notebook multiple
# times, comment the following
# lines after the very first one,
# not to delete and re-download
# the dataset again
###################################

import os
os.environ["KAGGLE_CONFIG_DIR"]='/content/drive/My Drive'
!kaggle competitions download -c santander-customer-transaction-prediction
!unzip -p santander-customer-transaction-prediction.zip train.csv > train.csv
!rm santander-customer-transaction-prediction.zip
```

```
Downloading santander-customer-transaction-prediction.zip to /content/drive/My Drive
 94% 235M/250M [00:03<00:00, 128MB/s]
100% 250M/250M [00:03<00:00, 70.2MB/s]
```

0. Data Exploration

A) Download and import the Santander dataset. The labels of the test data are not publicly available, so create your own test set by randomly choosing half of the instances in the original training set

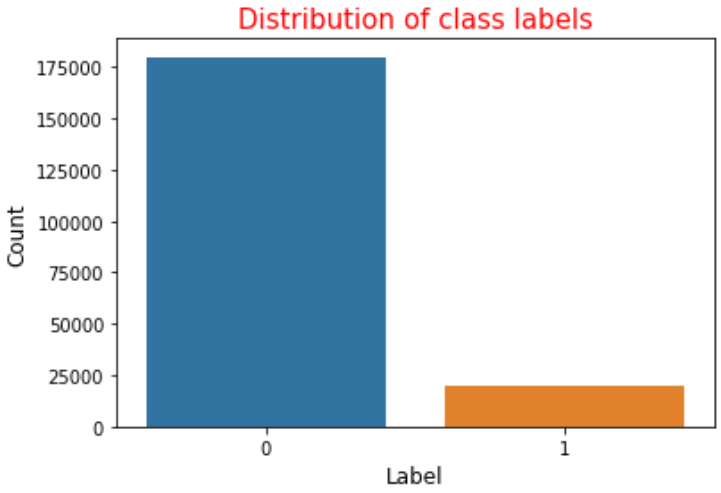
In [ ]:
```
import pandas as pd
# import modin.pandas as pd
import numpy as np
from sklearn.model_selection import train_test_split

data = pd.read_csv('train.csv')

# drop the ID code and split data and labels
df_data = data.drop(columns=['target', 'ID_code'])
df_target = data['target']

# split the dataset
X_train, X_test, y_train, y_test = \
  train_test_split(df_data, df_target, test_size=0.5, shuffle=True, random_state=42)

X_train = X_train.to_numpy()
X_test = X_test.to_numpy()

y_train = y_train.to_numpy()
y_test = y_test.to_numpy()
```

B) Comment on the distribution of class labels and the dimensionality of the input and how these may affect the analysis.

The Santander Customer Transaction dataset is characterized binary labels, so that we can evaluate the distribution of the class labels simply summing them and dividing by the number of samples

In [8]:
```
import matplotlib.pyplot as plt
import seaborn as sb

ones_percentage = np.sum(y_train) / len(y_train)
print('1s percentage = %f' % ones_percentage)
print('0s percentage = %f' % (1. - ones_percentage))

# plot the label distribution
ax = sb.countplot(x='target', data=data)
ax.set_xlabel("Label", size=12)
ax.set_ylabel("Count", size=12)
ax.set_title("Distribution of class labels",  color='r', size=15)
plt.show()
```

```
1s percentage = 0.099600
0s percentage = 0.900400
```



Hence the dataset is pretty unbalanced, with one class being present almost 10 times more than the other.

Opting to use the dataset as it is forces us to discard the accuracy as a valuable metrics as a dummy model always outputting 0 is going to have 90% accuracy.

1. Bayesian Linear Regression

A) Implement Bayesian linear regression

In [9]:
```
import numpy as np
from numpy.linalg import inv as inverse

#####################################################
## Bayesian Linear Regression utils                ##
#####################################################

def build_features(x, K):
    # assert K is legit
    assert isinstance(K, (int, np.int32, np.int64)) and K > 0
    # first column of the matrix (the bias)
    ones = np.ones(x.shape[0])
    # following columns containing the Kth powers of the feature
    power_stack = np.column_stack(tuple(x ** k for k in range(1, K+1)))
    return np.column_stack((ones, power_stack))

def sklearn_build_features(x, K):
  from sklearn.preprocessing import PolynomialFeatures
```

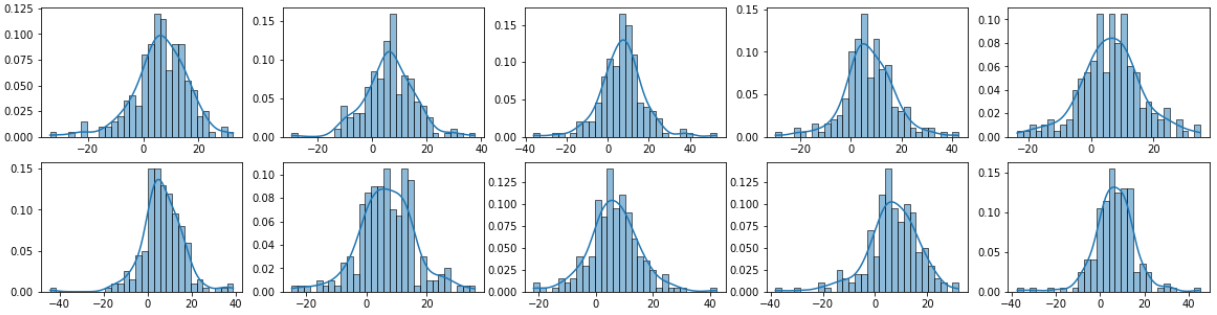
```
  poly = PolynomialFeatures(K)
  return poly.fit_transform(x)

def compute_posterior(X, y, sw2, sn2):
    """
    Args:
      X: the design matrix compute previously
         (or the features, in ML terminology)
      y: labels
      sw2: sigma_w ^ 2
      sn2: sigma_n ^ 2
    """
    # just the definitions
    _, cov_size = X.shape
    # S is a diagonal matrix defined as (see above)
    # S = sw2 * np.eye(cov_size)
    # thus it's inverse is a diag matrix having entries
    # 1 / entry
    S_inv = 1/sw2 * np.eye(cov_size)

    Sigma_inv = 1/sn2 * X.T @ X + S_inv
    Sigma = inverse(Sigma_inv)
    # now the posterior covariance is just the inverse of \Sigma^-1, i.e. Sigma
    w_posterior_cov = Sigma
    w_posterior_mean = (1/sn2) * Sigma @ X.T @ y

    return (
        w_posterior_mean,
        w_posterior_cov
    )

def compute_predictive(Xt, w_mean, w_cov, sn2):
    def _compute_predictive_single_point(xt_i, w_mean, w_cov, sn2):
        # reasoning: see the identity to prove in the above question
        yt_i_mean = xt_i.T @ w_mean
        yt_i_var = sn2 + xt_i @ w_cov @ xt_i
        return yt_i_mean, yt_i_var

    yt_mean, yt_var = np.zeros(len(Xt)), np.zeros(len(Xt))
    for i, xt_i in enumerate(Xt):  # Loop on all the points
        yt_mean[i], yt_var[i] = _compute_predictive_single_point(
            xt_i, w_mean, w_cov, sn2
        )

    return yt_mean, yt_var


#####################################################
## Bayesian Linear Regression class                ##
#####################################################

class BayesianLinearRegression:
  """Bayesian Linear Regression class"""
  def __init__(self, sw2, sn2):
    self.sw2_ = sw2
    self.sn2_ = sn2
    self.w_posterior_cov_ = None
    self.w_posterior_mean_ = None

  def fit(self, X, y, with_bias=False):
    """
    Fits the BLR and retrieves
    the fitted object

    Args:
      X:
        training data
        expected with bias term
      y:
        training samples

    Return:
```

```
      the fitted object
    """
    self.w_posterior_mean_, self.w_posterior_cov_ = \
     compute_posterior(X, y, self.sw2_, self.sn2_)
    return self

  def predict(self, X):
    """
    Predicts the labels for the test
    data X using the computed posterior

    Args:
      X: test data, expected with bias term

    Returns:
      predicted labels
    """
    return compute_predictive(X, self.w_posterior_mean_,
                              self.w_posterior_cov_, self.sn2_)
```

B) Describe any pre-processing that you suggest for this data

To discuss an appropriate pre-processing, let's plot the training data first

In [10]:
```
figs, axs = plt.subplots(2, 5, figsize=(20, 5))
axs = axs.flatten()

for i, ax in enumerate(axs):
    sb.histplot(X_train[i], bins=30, kde=True, stat='probability', ax=ax)
    ax.set(ylabel="")
    title = f"w_{i}"

plt.show()
```

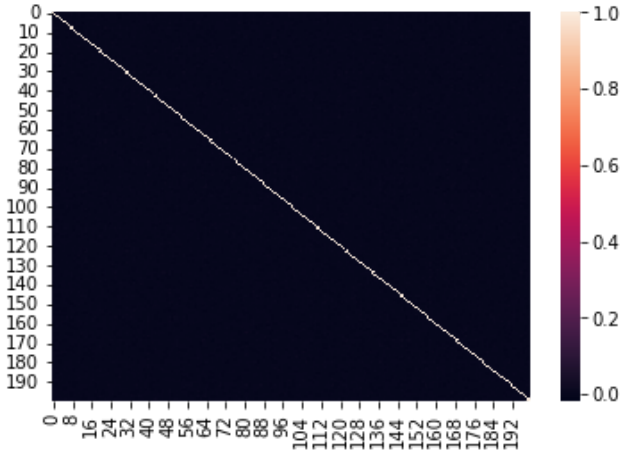


From the above plots, we can notice how the features follow a gaussian-like distribution. Hence, we should first standardize the data ($\mu = 0,\ \sigma^2 = 1$)

In [11]:
```
from sklearn.preprocessing import StandardScaler

sc = StandardScaler()
sc.fit(X_train)
X_train = sc.transform(X_train)
X_test = sc.transform(X_test)
```

We could also consider reducing the number of features using a dimensionality reduction technique. To this purpose, let's briefly study the correlation between the 200 features

In [12]:
```
corr_mat = pd.DataFrame(X_train).corr()
plt.subplots()
sb.heatmap(corr_mat)
plt.show()
```

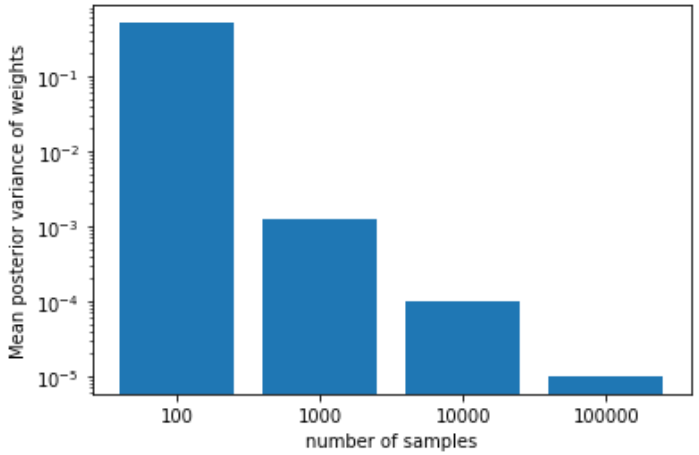


The heatmap reveals that all the features are important, hence I will proceed keeping all of them.

C) Treat class labels as continuous and apply regression to the training data. Also, calculate and report the posterior variance of the weights

In [13]:
```
sn2 = 1
sw2 = 1
K = 1

X = build_features(X_train, K)

# samples to iterate over
samples = [100, 1000, 10000, 100000]
# list to store the means of the posterior covariances
w_posterior_cov_means = []

for i in samples:
  _, w_posterior_cov = compute_posterior(X[0:i], y_train[0:i], sn2, sw2)
  mean_var = np.mean(np.diag(w_posterior_cov))
  w_posterior_cov_means.append(mean_var)

plt.bar(x=range(len(samples)), height=w_posterior_cov_means)
plt.yscale('log')
plt.xlabel('number of samples')
plt.ylabel('Mean posterior variance of weights')
plt.xticks(range(len(samples)), samples)
```

Out[13]:
```
([<matplotlib.axis.XTick at 0x7f63099822d0>,
  <matplotlib.axis.XTick at 0x7f63058a7990>,
  <matplotlib.axis.XTick at 0x7f63058a7750>,
  <matplotlib.axis.XTick at 0x7f630586f7d0>],
 [Text(0, 0, '100'),
  Text(0, 0, '1000'),
  Text(0, 0, '10000'),
  Text(0, 0, '100000')])
```



In [14]:
```
blr = BayesianLinearRegression(sw2, sn2)
```

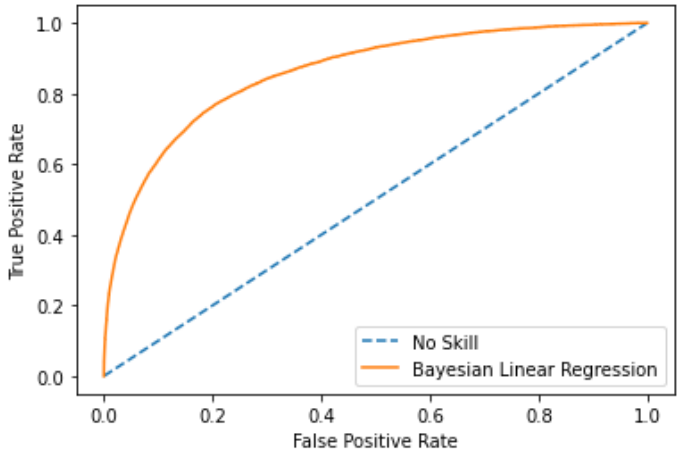
```
# evaluate the posterior
blr.fit(X, y_train)

# bayesian prediction on train
y_mean_tr, y_var_tr = blr.predict(X)

# bayesian prediction on test
X_test_ = build_features(X_test, K)
y_mean, y_var = blr.predict(X_test_)
```

D) Suggest a way to discretize predictions and display the confusion matrix on the test data and report accuracy

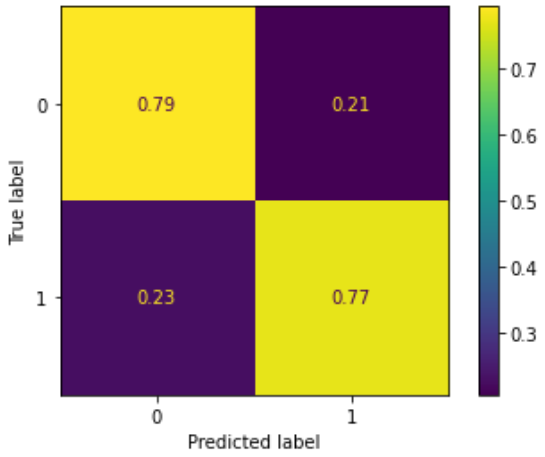
To discretize the prediction we need to find a cutoff point that maximize the score. As already declared, using the accuracy for unbalanced data is not recommended, as we will end up with a very low sensitivity. To have a better understanding of the results we can exploit the ROC curve and the AUC score so that our final discretization is gonna depend on the optimal threshold

$$y_{pred\_i} = \begin{cases} 0 \text{ if } \hat{y} < opt\_threshold \\ 1 \text{ if } \hat{y} \geq opt\_threshold \end{cases}$$

In [15]:
```
from sklearn.metrics import (
    confusion_matrix,
    ConfusionMatrixDisplay,
    roc_curve,
    roc_auc_score,
    accuracy_score,
    f1_score
)

def display_roc_cm_scores(y_test, y_pred, label=""):
  fpr, tpr, thresholds = roc_curve(y_test, y_pred)

  plt.plot([0,1], [0,1], linestyle='--', label='No Skill')
  plt.plot(fpr, tpr,  label=label)
  plt.xlabel('False Positive Rate')
  plt.ylabel('True Positive Rate')
  plt.legend()
  plt.show()

  optimal_idx = np.argmax(tpr - fpr)
  optimal_threshold = thresholds[optimal_idx]

  print("\nOptimal threshold %.2f" % optimal_threshold )

  y_pred = y_pred >= optimal_threshold

  print("Accuracy score: %f" % accuracy_score(y_test, y_pred))
  print("F1 score: %f" % f1_score(y_test, y_pred))
  print("AUC: %f" % roc_auc_score(y_test, y_pred))

  # plot the confusion matrix
  cm = confusion_matrix(y_test, y_pred)

  sensitivity = cm[0,0] / (cm[0,0] + cm[0,1])
  specificity = cm[1,1] / (cm[1,0] + cm[1,1])

  print("Sensitivity: %f" % sensitivity)
  print("Specificity: %f\n" % specificity)

  # normalized confusion matrix
  disp = ConfusionMatrixDisplay(confusion_matrix=cm/cm.sum(axis=1)[:, np.newaxis])
  disp.plot()


display_roc_cm_scores(y_test, y_mean, "Bayesian Linear Regression")
```




```
Optimal threshold 0.18
Accuracy score: 0.791270
F1 score: 0.428153
AUC: 0.782173
Sensitivity: 0.793583
Specificity: 0.770763
```



2. Logistic Regression

A) The goal is to implement a Bayesian logistic regression classifier; assume a Gaussian prior on the parameters. As a first step, implement a Markov chain Monte Carlo inference algorithm to infer parameters

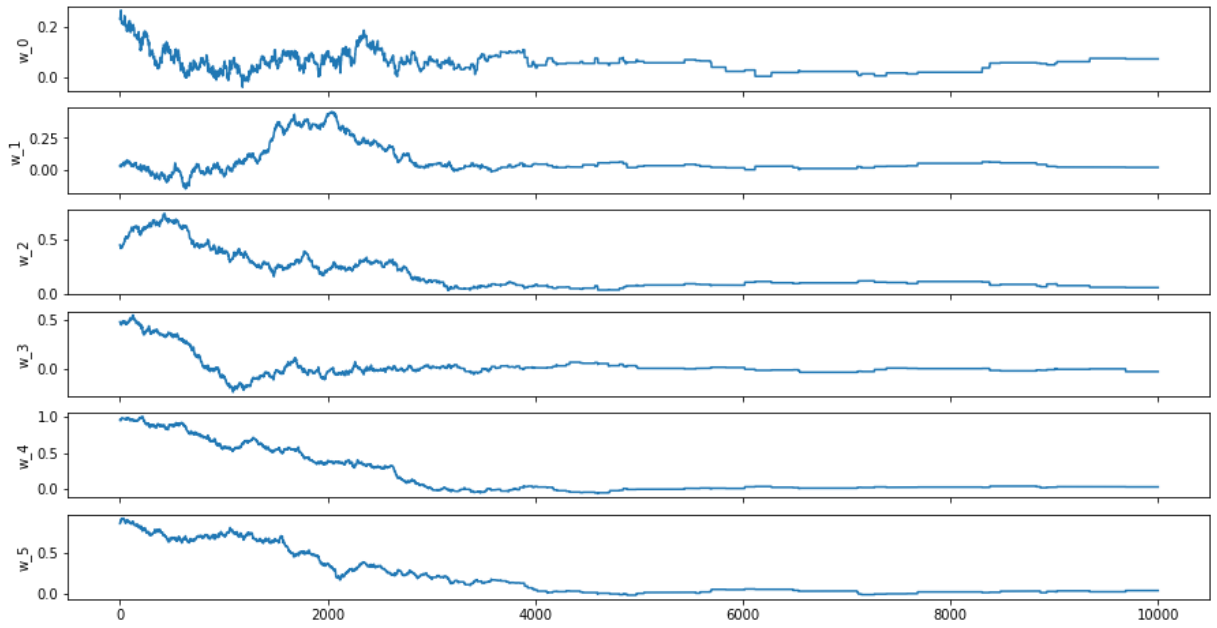
In [16]:

```
from tqdm import tqdm

#####################################################
##             MCMC utils                          ##
#####################################################

X = X_train
y = y_train

def logistic(z):
    return 1 / (1 + np.exp(-z))

def bernoulli_density(y, p, jitter=1e-10):
    return y.T * np.log(p + jitter) + (1 - y).T * np.log(1 - p + jitter)

def gaussian_density(x, mean=0, var=1):
    return - .5 * np.log(2 * np.pi * var) - .5 * (x - mean)**2 / var

def logposterior(w, X, y):
    # compute model output
    # and feed it to the logistic regression
    p = logistic(X @ w)
    # apply bernoulli to get
```

```
    # the log likelihood point by point
    log_lik = bernoulli_density(y, p)
    prior = gaussian_density(w)
    # add the summations because the above computations
    # are point by point
    return np.sum(log_lik) + np.sum(prior)

def rw_mh_step(w_prev, step_size):
    # step size used for the covariance
    # see slide 32
    # x ~ N(mu, sigma^2) <=> x ~ sigma * eps + mu
    # being eps ~ N(0,1)
    # in other words we sample from a normal distribution with 0 mean
    # and variance 1 and then we multiply it by the std-dev (i.e. step size)
    # and we add mu
    ws_tilde = np.random.multivariate_normal(
      mean = w_prev,
      cov = step_size * np.eye(len(w_prev))
    )
    # in this scenario , mu = w_prev and the standard deviation is
    # step_size
    #ws_tilde = ws_tilde * step_size + w_prev
    # compute the acceptance ratio
    # notice that the second term is = 1 because of symmetry in Gaussians

    # the difference is because we're dealing with logs and then we reconvert to exps
    # equivalently we could do exp of both and then divide
    ratio = logposterior(ws_tilde, X, y) - logposterior(w_prev, X, y)
    ratio = np.exp(ratio)
    # acceptance
    return ws_tilde if ratio >= 1 or ratio >= np.random.uniform(0, 1) else w_prev

def run_sampling(w, n_samples, step_size=1, burn_in=0):
    w = np.atleast_1d(w)
    samples = np.empty((n_samples, *w.shape))
    for i in tqdm(range(n_samples)):
        w = rw_mh_step(w, step_size)
        samples[i] = w

    return samples[burn_in:, :]
```

In [ ]:
```
_, n_feats = X.shape

# MH params
w_init = np.random.rand(n_feats)
n_samples = 10000
step_size = 1e-4

# metropolis sampler (temporary keep all the samples - no burn_in specified -,
# then discard according to the trace plots)
samples = run_sampling(w_init, n_samples, step_size)
```

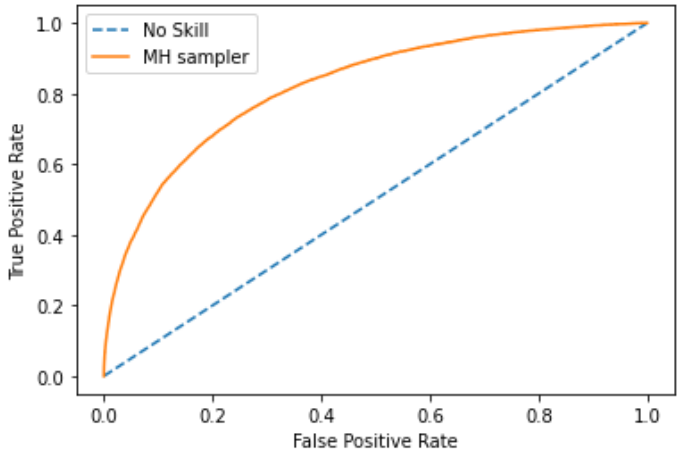
In [18]:
```
fig, axes_tuple = plt.subplots(6, 1, figsize=[15, 8], sharex=True)

for i, ax in enumerate(axes_tuple):
  ax.plot(list(range(0, samples.shape[0])), samples[:, i])
  ax.set_ylabel(f'w_{i}')

plt.show()
```



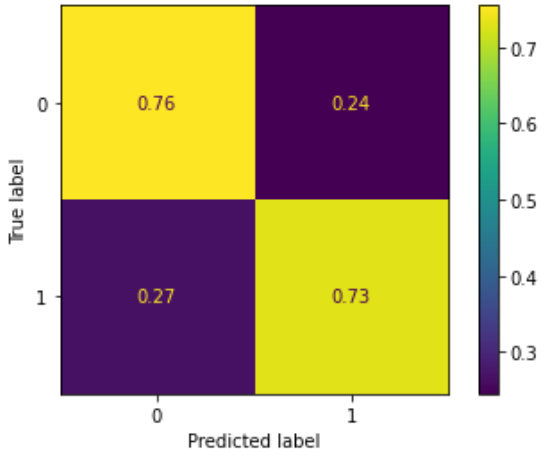
In [19]:
```
# Introduce a burn-in
samples_ = samples[4000:, :]

# now predict
def predict(Xt, samples):
    # see slide 81 for the formula
    # too much RAM required for this
    #return np.mean(logistic(samples @ Xt.T), axis=0)
    n_samples = samples.shape[0]

    sum = 0
    for i in tqdm(range(n_samples)):
      sum += logistic(Xt @ samples[i])

    return 1/n_samples * sum

y_mh_pred = predict(X_test, samples_)
```

```
100%|██████████| 6000/6000 [01:37<00:00, 61.66it/s]
```

In [20]:
```
display_roc_cm_scores(y_test, y_mh_pred, "MH sampler")
```




```
Optimal threshold 0.58
Accuracy score: 0.752880
F1 score: 0.375486
AUC: 0.743967
Sensitivity: 0.755147
Specificity: 0.732788
```



B) Implement the variational approximation we studied in the course to obtain an approximation to the posterior over model parameters

In [21]:

```python
import jax
import jax.numpy as jnp
from typing import NamedTuple
from functools import partial

####################################
##  Variational Inference utils    ##
####################################

class GaussianDiagonal(NamedTuple):
    mean: jnp.array
    log_var: jnp.array

def jnp_bernoulli_density(y, p, jitter=1e-10):
    # bernoully log density rewritten using jax numpy
    return y * jnp.log(p + jitter ) + (1 - y) * jnp.log(1 - p + jitter)

def sample_gaussian_diagonal(rng, params):
    mean, log_var = params
    # extract variance taking the exp
    # from log variance
    var = jnp.exp(log_var)
    sigma = jnp.sqrt(var)

    eps = jax.random.normal(
        key=rng,
        shape=mean.shape
    )
    return mean + sigma * eps

def kl_diag_diag(q_params, p_params):
    assert isinstance(q_params, GaussianDiagonal)
    assert isinstance(p_params, GaussianDiagonal)
    mean_q, log_var_q = q_params
    mean_p, log_var_p = p_params

    var_p = jnp.exp(log_var_p)
    var_q = jnp.exp(log_var_q)
    kl = .5 * jnp.sum(
        log_var_p - log_var_q + (var_q + jnp.square(mean_q - mean_p)) / var_p - 1
      )
    return kl

def model(w, X):
    # nested to avoid overwriting
    # the other "logistic", which
    # uses numpy
    def _logistic(z):
      return 1 / (1 + jnp.exp(-z))

    return _logistic(X @ w)
```

```
###
# elbo function
###

def create_elbo_fn(sample_fn, likelihood_fn, kl_divergence_fn):
    """Create a function to compute the ELBO, given the function to sample
    from the posterior, the likelihood function and the KL divergence
    """

    @partial(jax.vmap, in_axes=[0, None, None, None])
    def likelihood_sample_fn(rng, q_params, X, y):
        """Compute the likelihood with one Monte Carlo sample of the posterior
        The function is decorated to vectorize multiple MC samples automatically
        """
        # Get one sample of w using the sample_fn and the parameters of q
        # So afterwards  we expect the sample_gaussian_diagonal as sample_fn
        w = sample_fn(rng, q_params)
        # Predict the output using the sample before
        yp = model(w, X)
        # Compute the likelihood and return it
        return likelihood_fn(y, yp)

    def elbo_fn(q_params, p_params, rng, X, y, Nmc=1):
        """Computes the ELBO with multiple samples"""
        # Split the random seed in Nmc times
        rng = jax.random.split(rng, Nmc)

        # Compute the values of the likelihood
        likelihood_vals = likelihood_sample_fn(rng, q_params, X, y)
        # Compute the expectation (i.e. take the mean)
        expected_likelihood = jnp.mean(jnp.sum(likelihood_vals, axis=1))
        # Compute the KL divergence
        kl = kl_divergence_fn(q_params, p_params)
        # Compute the ELBO
        elbo = expected_likelihood - kl
        # Return the ELBO and its two term (used later for logging)
        return elbo, (expected_likelihood, kl)

    return elbo_fn

elbo_fn = create_elbo_fn(
    sample_fn=sample_gaussian_diagonal,
    kl_divergence_fn=kl_diag_diag,
    likelihood_fn=jnp_bernoulli_density
)
```

In [22]:
```
p_params = GaussianDiagonal(jnp.zeros(n_feats), jnp.zeros(n_feats))
q_params = GaussianDiagonal(jnp.zeros(n_feats), jnp.zeros(n_feats))
rng = jax.random.PRNGKey(0)

elbo, (likelihood, kl) = elbo_fn(q_params, p_params, rng, X, y)
print("ELBO =", elbo)
print("Likelihood =", likelihood)
print("KL =", kl)
```

```
ELBO = -560005.1
Likelihood = -560005.1
KL = 0.0
```

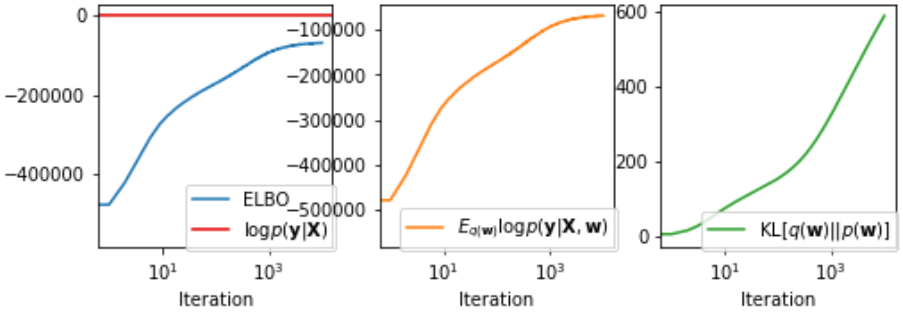
In [23]:
```
# Optimization via GD, see lab4 part 5 for details on the implementation
def sg_update(params, gradients, learning_rate=1e-3):
    updated_params = jax.tree_map(lambda p, g: p + learning_rate * g, params, gradients
    return updated_params

grad_elbo_fn = jax.grad(elbo_fn, has_aux=True)
grad_elbo_fn = jax.jit(grad_elbo_fn, static_argnames=("Nmc"))
```

In [24]:
```
elbo_summary = []
lik_summary = []
kl_summary = []
```

```
import math
lr = 1e-5

for i in tqdm(range(10000), desc="Training ELBO"):
    rng, rng2 = jax.random.split(rng)

    q_params_grad, (likelihood, kl) = grad_elbo_fn(q_params, p_params, rng, X_train, y_
    q_params = sg_update(q_params, q_params_grad, lr)

    lik_summary.append(likelihood)
    kl_summary.append(kl)
    elbo_summary.append(likelihood - kl)
```

```
Training ELBO: 100%|██████████| 10000/10000 [11:46<00:00, 14.16it/s]
```

In [25]:
```
fig, (ax0, ax1, ax2) = plt.subplots(1, 3, figsize=[8, 2.5])

ax0.plot(elbo_summary, label="ELBO")
ax1.plot(
    lik_summary,
    color="tab:orange",
    label=r"$E_{q(\mathbf{w})} \log p(\mathbf{y}|\mathbf{X},\mathbf{w})$",
)
ax2.plot(
    kl_summary,
    color="tab:green",
    label=r"$\mathrm{KL}[{q(\mathbf{w})}||{p(\mathbf{w})}]$",
)

ax0.semilogx()
ax1.semilogx()
ax2.semilogx()

ax0.axhline(-0.4, color="xkcd:red", label=r"$\log p(\mathbf{y}|\mathbf{X})$")
ax0.legend(bbox_to_anchor=(1.05, -0.05), loc="lower right")
ax1.legend(bbox_to_anchor=(1.05, -0.05), loc="lower right")
ax2.legend(bbox_to_anchor=(1.05, -0.05), loc="lower right")

ax0.set_xlabel("Iteration")
ax1.set_xlabel("Iteration")
ax2.set_xlabel("Iteration")

plt.show()
```



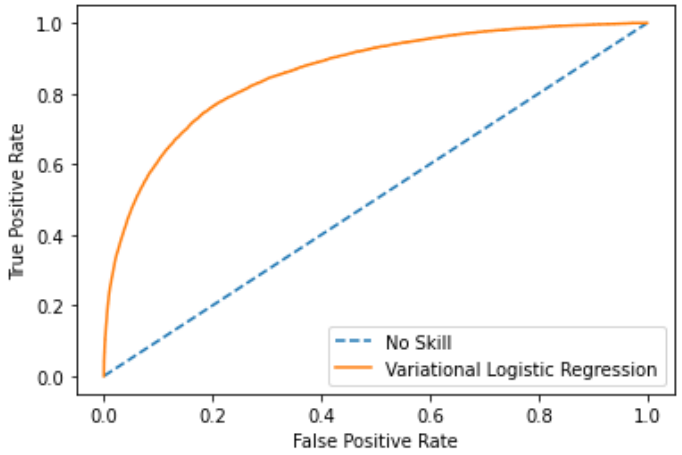
C) Based on samples from the posterior over model parameters, write a function that computes the predictive distribution, and write the necessary functions to evaluate classification metrics such as the log-likelihood on test data and error rate

In [26]:
```
def predict_y(sample_fn, q_params, Xt, rng, Nmc=10):
    """Compute the outputs of the model by sampling the posterior,
    then take the expectation
    """

    def predict_y_single(rng):
        w = sample_fn(rng, q_params)
        yp = model(w, Xt)
        return yp
```

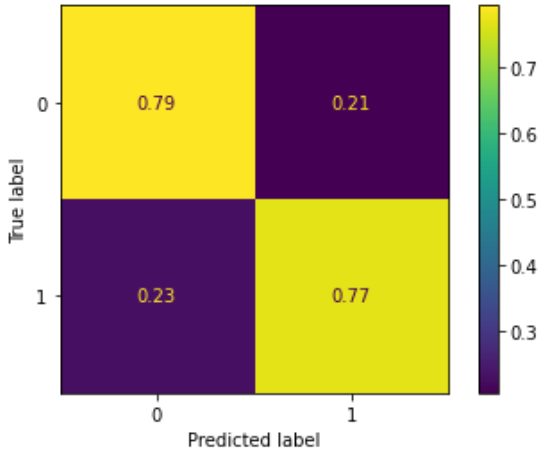
```
    rng = jax.random.split(rng, Nmc)
    Xt = jnp.atleast_1d(Xt)
    yp = jax.vmap(predict_y_single)(rng)
    # Take the mean
    yp = jnp.mean(yp, axis=0)
    return yp

y_vi_pred = predict_y(sample_gaussian_diagonal, q_params, X_test, rng, Nmc=1000)
print(y_vi_pred)
```

```
[0.22269455 0.35306793 0.35117713 ... 0.3983956  0.65481454 0.8160562 ]
```

In [27]:
```
display_roc_cm_scores(y_test, y_vi_pred, "Variational Logistic Regression")
```




```
Optimal threshold 0.58
Accuracy score: 0.791520
F1 score: 0.428195
AUC: 0.781963
Sensitivity: 0.793951
Specificity: 0.769974
```



D) Comment on the tuning of the Metropolis-Hastings algorithm, and how to guarantee that samples are representative of samples of the posterior over model parameters

The tuning of the Metropolis-Hastings algorithm required finding the best values for the following two hyper-parameters:

- step size
- number of samples.

As regards the former, I obtained the best performance using 10^{-4}.

As for the latter, I initially performed a random walk on 10^4 samples and, displaying the trace plots, I applied a burnin of 4000 samples corresponding roughly to the point in the traces where they become stationary.

E) Comment on the tuning of the variational inference algorithm, and discuss the behavior of the optimization with respect to the choice of the optimizer/step-size.

The variational inference algorithm tries to minimize the ELBO, which is composed by the expected log-likelihood and the KL between the prior distribution and the distribution approximation

$$\mathcal{L}(\theta) = \underbrace{\mathbb{E}_{q_\theta} \log p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w})}_{\text{Expected loglikelihood}} - \mathrm{KL}[q_\theta(\boldsymbol{w})||p(\boldsymbol{w})] \tag{1}$$

However, the analytic evaluation is generally untractable so that we typically resort to sampling techniques using the reparametrization trick, i.e. drawing N_{MC} samples from q_θ:

$$\mathbb{E}_{q_\theta} \log p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w}) \approx \frac{1}{N_{\mathrm{MC}}} \sum_{\tilde{\boldsymbol{w}}_i \sim q_\theta} \log p(\boldsymbol{y}|\boldsymbol{X}, \tilde{\boldsymbol{w}}_i) \tag{2}$$

The hyperparameters to tune are therefore:

- N_{mc} : the number of MonteCarlo samples
- n_{iter} : the number of iterations of the ELBO algorithm
- lr : the learning rate used for the iterative optimization

As for the learning rate, to avoid big "bouncings" during the GD optimization process, we use small values. This is especially for the first iterations, where the KL distance between the approximation and the likelihood is high.

Employing a grid search, I tried the following values:

- lr = [1e-2, 1e-3, 1e-4, 1e-5]
- N_{mc} = [10, 100, 1000, 10000]
- n_{iter} = [1000, 10000]

Achieving the best performances with lr = 1e-5, N_{mc} = 1000 and n_{iter} = 10 000.

A further analysis might be conduced using a different optimizer, e.g. Adam (not reported for notebook length constraints)

In [ ]:
```
def adam_update(params, gradients, m, v, t, beta1=.9, beta2=.999, lr=1e-3, eps=1e-8):
    """
    Adam update step

    Args:
      m:
        first moment
      v:
        second moment
      t:
        iteration number
      beta1:
        gradient running average
        coefficient
      beta2:
        square gradient running average
        coefficient
      lr:
        learning rate
      eps:
        numerical stability coeff (not to divide by 0)
    """
    mt = jax.tree_map(lambda m, g: beta1 * m + (1. - beta1) * g,
                      m, gradients)

    vt = jax.tree_map(lambda v, g: beta2 * v + (1. - beta2) * g ** 2,
```

```
                        v, gradients)
    m_hat = jax.tree_map(lambda m:  m / (1. - beta1 ** (t+1))
                             , mt)
    v_hat = jax.tree_map(lambda v: v / (1 - beta2 ** (t+1))
                             , vt)

    updated_params = jax.tree_map(lambda p, m, v: \
                                  p + lr * m / (jnp.sqrt(v) + eps)\
                                  , params, m_hat, v_hat)

    return updated_params, mt, vt
```

F) Report the error metrics implemented in point 2.C. above and the confusion matrix on the test data. Discuss logistic regression performance with respect to the performance of Bayesian linear regression.

The error metrics and the confusion matrics both for the logistic regression and the Bayesian linear regression are reported in the respective sections and synthesized in the following table:

Score	Bayesian Linear Regression	Metropolis-Hastings	Variational Inference
Accuracy	0.791	0.775	0.791
Sensitivity	0.794	0.783	0.794
Specificity	0.770	0.714	0.770
F1 score	0.428	0.391	0.428
AUC	0.782	0.714	0.782

Looking at these results we can notice that, despite a lower error rate for linear regression, the number of false positives is the highest of the analyzed cases. Therefore as suggested in question B, the imbalanced dataset and the number of features (especially if considered uncorrelated) has a big impact when evaluating the model.

G) Compare the uncertainties on predictions obtained by the Metropolis-Hastings algorithm and variational inference. First, compare the log-likelihood on test data as a global metric to assess which inference method yields better uncertainty quantification. Second, pick a few test points for which the mean of the predictive distribution is

- (a) around 0.5
- (b) giving a correct prediction
- (c) giving a wrong prediction

and visualize/discuss what the predictive distribution looks like. Discuss the difference between the Metropolis-Hastings algorithm and variational inference.

In [28]:
```
def logistic_loglik(y, y_tilde):
    ll = y * np.log(y_tilde + 1e-10) + (1 - y)* np.log(1 - y_tilde + 1e-10)
    return np.mean(ll)
```

In [29]:
```
print("VI Logistic Regression log-likelihood: %f" % logistic_loglik(y_test, y_vi_pred))
print("MH Logistic Regression log-likelihood: %f" % logistic_loglik(y_test, y_mh_pred))
```

```
VI Logistic Regression log-likelihood: -0.659882
MH Logistic Regression log-likelihood: -0.671641
```

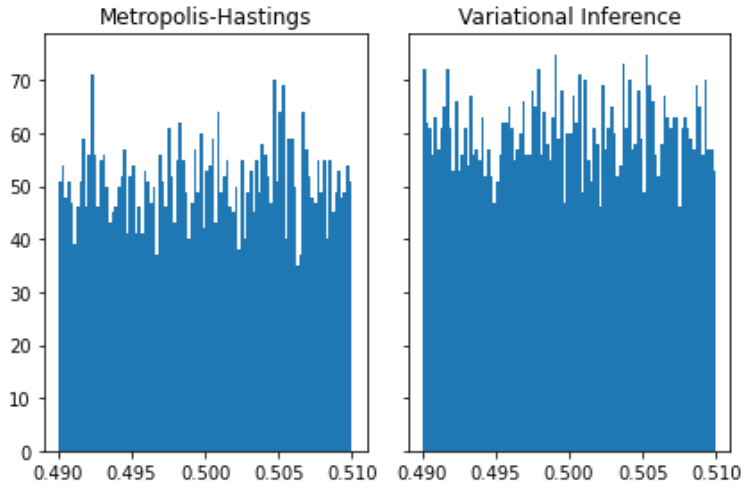
Then the two predictors seem to work equally well in terms of log-likelihood.

In [30]:
```
pred_mh_0_5 = y_mh_pred[(y_mh_pred >= .49) & (y_mh_pred <= .51)]
pred_vi_0_5 = y_vi_pred[(y_vi_pred >= .49) & (y_vi_pred <= .51)]

n_bins = 100
# Metropolis Hastings
fig, axs = plt.subplots(1, 2, sharey=True, tight_layout=True)
```

```
axs[0].hist(pred_mh_0_5, bins=n_bins)
axs[0].title.set_text('Metropolis-Hastings')

# Variational Inference
axs[1].hist(pred_vi_0_5, bins=n_bins)
axs[1].title.set_text('Variational Inference')
plt.plot()
```

Out[30]:

```
[]
```

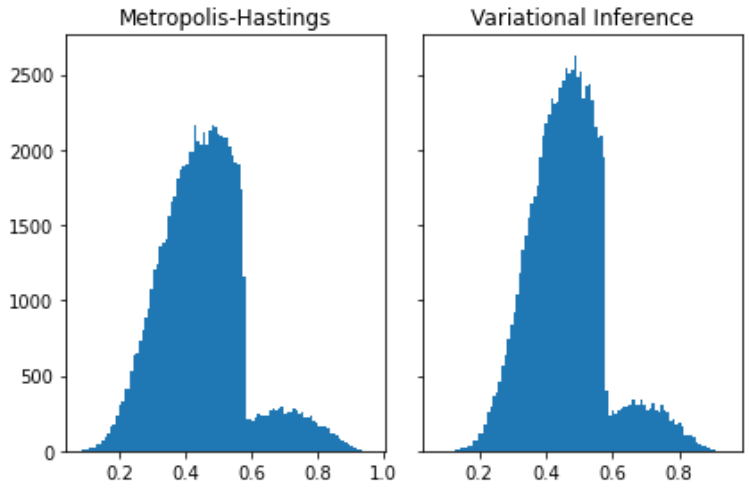


In [44]:

```
# correct preds
y_mh_discrete = y_mh_pred >= .58 # hardcoded threshold, computed above
pred_mh_correct = y_mh_pred[y_test == y_mh_discrete]

y_vi_discrete = y_vi_pred >= .58   # hardcoded threshold, computed above
pred_vi_correct = y_vi_pred[y_test == y_vi_discrete]

n_bins = 100
# Metropolis Hastings
fig, axs = plt.subplots(1, 2, sharey=True, tight_layout=True)
axs[0].hist(pred_mh_correct, bins=n_bins)
axs[0].title.set_text('Metropolis-Hastings')

# Variational Inference
axs[1].hist(pred_vi_correct, bins=n_bins)
axs[1].title.set_text('Variational Inference')
plt.plot()
```

Out[44]:

```
[]
```

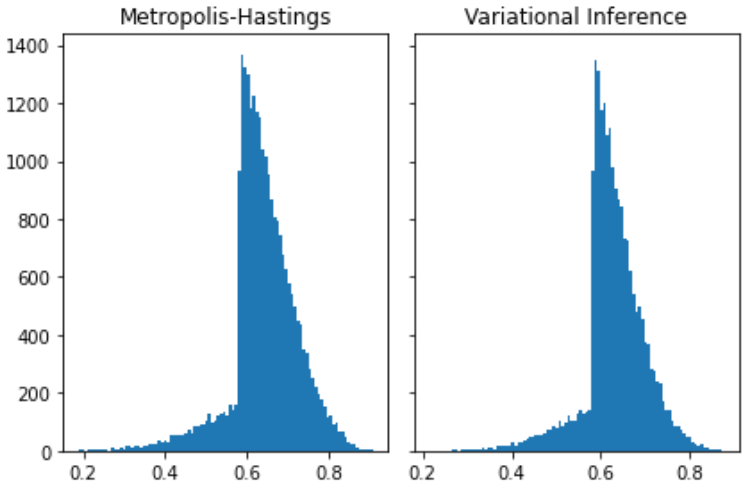


In [45]:

```
# wrong preds
pred_mh_wrong = y_mh_pred[y_test != y_mh_discrete]
pred_vi_wrong = y_vi_pred[y_test != y_vi_discrete]

n_bins = 100
# Metropolis Hastings
```

```
fig, axs = plt.subplots(1, 2, sharey=True, tight_layout=True)
axs[0].hist(pred_mh_wrong, bins=n_bins)
axs[0].title.set_text('Metropolis-Hastings')

# Variational Inference
axs[1].hist(pred_vi_wrong, bins=n_bins)
axs[1].title.set_text('Variational Inference')
plt.plot()
```

Out[45]: []



From the above results and plot we can notice that the log likelihood is almost the same for both the models. In addition, plot (b) seems to be skewed towards the "0" class while plot (c) shows, for both the models, how the majority of misclassified points stands over the threshold of 0.5 as a result of the unbalanced dataset.

3. Bonus Questions

Implement the Laplace approximation and compare the predictive mean and variance with the ones obtained by other approximations

Super brief thought process

Calling H the Hessian matrix, we want to implement the following approximation to the posterior

$$q(w) \backsim N(w|w_{MAP}, S_N)$$

being w_{MAP} the maximum aposteriori solution, i.e. the w which maximes $p(w|y, X)$ evaluated via numerical optimization, e.g. Newton-Raphson method (see slides 15) and S_N the inverse of

$$S_N^{-1} = -\nabla\nabla log\, p(w|X, y)$$

i.e. the inverse of the matrix of the second derivatives of the log likelihood, which is nothing but the Hessian H.

Hence

- use a numerical method to compute w_{MAP} (e.g. NR)
- compute the Hessian
- invert the Hessian
- draw N samples from a Gaussian multivariate having w_{MAP} as mean and H^{-1} as variance, being N an hyperparameter, e.g. 100
- use the N samples to make the prediction

I propose two implementations:

- a from scratch version (follows the above steps)
- a `scipy`-based version (described below)

"Hand made" (from scratch) version

In [33]:
```
def logposterior_grad(X, y, w, prior_mean, prior_cov):
    """Computes the gradient of the log posterior"""
    p = logistic(X @ w)
    # retrieve the grad
    return X.T @ (y - p) + inverse(prior_cov) @ (w - prior_mean)

def logposterior_hessian(X, y, w, prior_cov):
    """Computes the hessian of the logposterior"""
    p = logistic(X @ w)
    hess = (X.T * (p * (1 - p))) @ X + inverse(prior_cov)
    return hess
```

In [34]:
```
def newton_raphson_gd(X, y, w, prior_mean, prior_cov, lr=1e-2, tol=1e-5, max_iter=100):
    """Inefficient implementation from wikipedia "dummy-version" pseudocode"""
    # hyper-parameters set by hand
    loss = 1e5
    losses = []
    w_opt = 0

    for i in range(max_iter):

        # find the next step length.
        grad = logposterior_grad(X, y, w, prior_mean, prior_cov)
        hess = logposterior_hessian(X, y, w, prior_cov)

        # update the coefficient for next step
        w_new = w + lr * inverse(hess) @ grad

        # check convergence
        loss_new = logposterior(w, X, y)
        if abs(loss_new - loss) < tol:
            break
        else:
            losses.append(loss_new)
            loss, w = loss_new, w_new

        w_opt = w_new

    return w_opt, losses
```

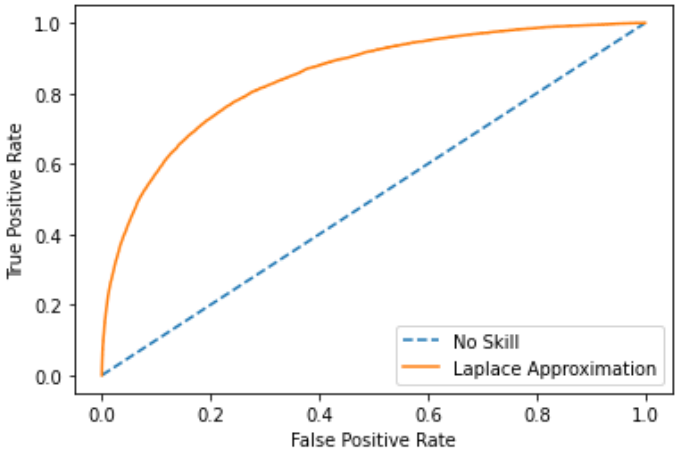
In [35]:
```
def laplace_approx(X, y, prior_mean, prior_cov, lr = 1e-2, max_iter = 10):
    _, n_feats = X.shape
    w_init = 1e-3 * np.ones(n_feats)
    posterior_mean, _ = newton_raphson_gd(X, y, w_init, prior_mean, prior_cov, lr, max_

    hess = logposterior_hessian(X, y, posterior_mean, prior_cov)
    posterior_var = inverse(hess)

    return (
       posterior_mean,
       posterior_var
    )
```

In [36]:
```
_, n_feats = X.shape
prior_variance = 1e2 * np.eye(n_feats)
prior_mean = np.zeros(n_feats)

w_map, s_n = laplace_approx(X_train, y_train, prior_mean, prior_variance)
```

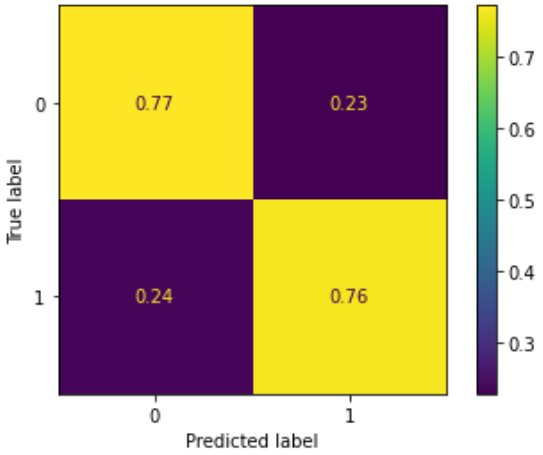
In [37]:
```
samples = np.random.multivariate_normal(w_map, s_n, 100)

y_laplace = predict(X_test, samples)
```

```
100%|██████████| 100/100 [00:01<00:00, 64.57it/s]
```

In [38]:
```
display_roc_cm_scores(y_test, y_laplace, "Laplace Approximation")
```




```
Optimal threshold 0.51
Accuracy score: 0.769670
F1 score: 0.401756
AUC: 0.766655
Sensitivity: 0.770437
Specificity: 0.762872
```



Scipy version

This version employes `scipy.optimize.minimize` to compute w_{MAP} and S_N and now it reduces to the previous approach.

In [39]:
```
import scipy

w_init = np.zeros(n_feats)

def neg_logposterior(w, X, y):
    y_hat = logistic(X @ w)
    log_ll = bernoulli_density(y,y_hat)
    prior = gaussian_density(w)

    return - (np.sum(log_ll) + np.sum(prior))

def laplace_approx_scipy(X, y, w_init):
  # solve using scipy
  solution = scipy.optimize.minimize(
      neg_logposterior,
      w_init,
      args=(X, y),
      method='BFGS',
      options={'disp':True, 'maxiter':10}
  )
```

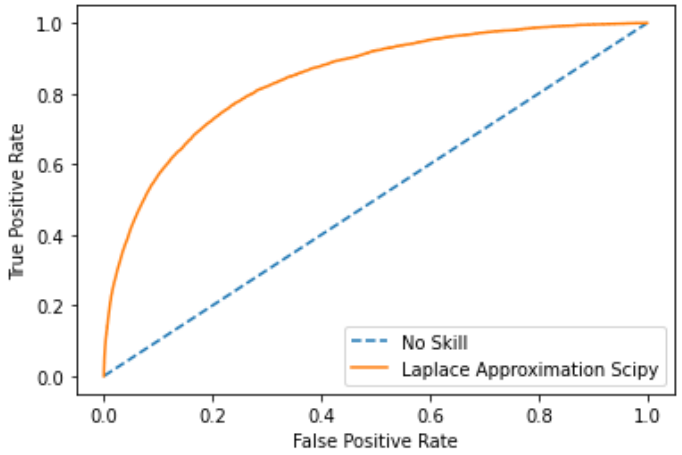
```
    # retrieve w_map and H^-1
    return solution.x, solution.hess_inv
```

In [40]:
```
w_map_scipy, hess_scipy = laplace_approx_scipy(X_train, y_train, w_init)
```

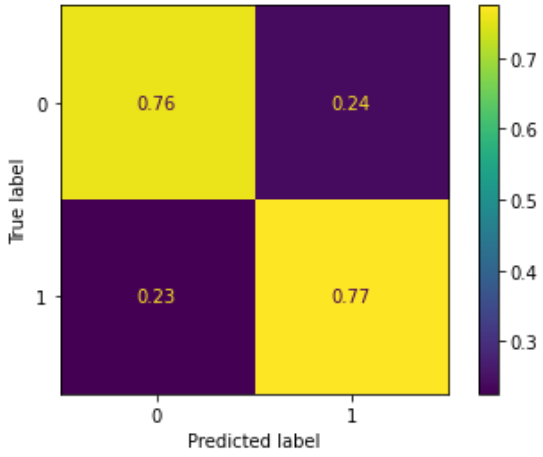
```
Warning: Maximum number of iterations has been exceeded.
         Current function value: 66768.740503
         Iterations: 10
         Function evaluations: 4848
         Gradient evaluations: 24
```

In [41]:
```
# now we do as above (draw samples > predict > display metrics)
samples = np.random.multivariate_normal(w_map_scipy, hess_scipy,  5000)

y_laplace_scipy = predict(X_test, samples)

display_roc_cm_scores(y_test, y_laplace_scipy, "Laplace Approximation Scipy")
```

```
100%|██████████| 5000/5000 [01:19<00:00, 63.05it/s]
```




```
Optimal threshold 0.51
Accuracy score: 0.759440
F1 score: 0.394848
AUC: 0.765951
Sensitivity: 0.757784
Specificity: 0.774117
```



Suggest what can be done to improve performances

As already mentioned, the dataset is highly imbalanced, with one class present roughly 10 times more than the other. This might play a key role in the results obtained while tackling this problem.

We might then consider rebalancing it using one of the following approaches:

- Undersampling: select an handful of the sample belonging to the majority class to rebalance the distributions
- SMOTE: create synthetic data starting from the data of the minority class

In addition, for the Variational Infernece implementation, using a numeric approach to compute the bernoulli density (e.g. the popular log sum trick) might improve the performances, avoiding the log function "exploding".