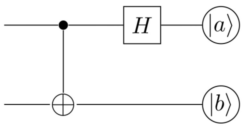
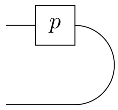
Exercise 7.1 (Bell circuit, part 2)
Generalize Exercise 4.1 by proofing the following equivalence for all $a, b \in \{0,1\}$, where p is the identity matrix, X, iY or Z (depending on a and b). The circuit thus generates one of the Bell states. Hint: See also Exercise 4.2(d).

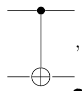
$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$



$=\ \frac{1}{\sqrt{2}}$



$\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{pmatrix} \hat{=}$



,

from 4.2d

$|a\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$
$|b\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$(H \cdot |a\rangle) \otimes |b\rangle = \left(\frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix}\right) \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}$

$\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \hat{=} \underline{\underline{\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}} = \underline{\underline{\frac{1}{\sqrt{2}} I}}$

$|a\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$
$|b\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$(H \cdot |a\rangle) \otimes b = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}$

$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} \hat{=} \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \underline{\underline{\frac{1}{\sqrt{2}} X}}$

$|a\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$
$|b\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$(H \cdot |a\rangle) \otimes |b\rangle = \left(\frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ -1 \end{pmatrix}\right) \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix}$

$\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix} \hat{=} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \underline{\underline{\frac{1}{\sqrt{2}} Z}}$

$|a\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$
$|b\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$(H \cdot |a\rangle) \otimes |b\rangle = \left(\frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 \\ -1 \end{pmatrix}\right) \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}$

$\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} \hat{=} \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \underline{\underline{\frac{1}{\sqrt{2}} iY}}$

exercise7.2_template

June 13, 2022

[1]:
```
import numpy as np
import matplotlib.pyplot as plt
```

[2]:
```
# Implementation of Exercise 5.2 (a)

def single_mode_matricization(T, j):
    """
    Matricization of numpy array `T` by partitioning into j-th dimension and␣
 ↪the remaining dimensions.
    """
    assert j < T.ndim
    # bring j-th dimension to the front
    T = np.transpose(T, [j] + list(range(j)) + list(range(j + 1, T.ndim)))
    T = np.reshape(T, (T.shape[0], -1)) # size of second dimension is inferred
    return T
```

[3]:
```
# Implementation of Exercise 5.2 (b)

def single_mode_product(A, T, j):
    """
    Compute the j-mode product between the matrix `A` and tensor `T`.
    """
    T = np.tensordot(A, T, axes=(1, j))
    # original j-th dimension is now 0-th dimension; move back to j-th place
    T = np.transpose(T, list(range(1, j + 1)) + [0] + list(range(j + 1, T.
 ↪ndim)))
    return T
```

[4]:
```
class TuckerTensor(object):
    """
    Tucker format tensor.
    """
    def __init__(self, Ulist, C):
        self.Ulist = [np.array(U) for U in Ulist]
        # core tensor
        self.C = np.array(C)
        # dimension consistency checks
```

```
        assert len(self.Ulist) == self.C.ndim
        for j in range(self.C.ndim):
            assert self.Ulist[j].shape[1] == C.shape[j]

    @property
    def shape(self):
        """Logical dimensions."""
        return tuple([U.shape[0] for U in self.Ulist])

    @property
    def ndim(self):
        """Number of logical dimensions."""
        return len(self.Ulist)

    def as_full_tensor(self):
        """
        Construct the Tucker format tensor as full (dense) array.

        Note: Should only be used for debugging and testing.
        """
        T = self.C
        for j in range(T.ndim):
            # apply Uj to j-th dimension
            T = single_mode_product(self.Ulist[j], T, j)
        return T
```

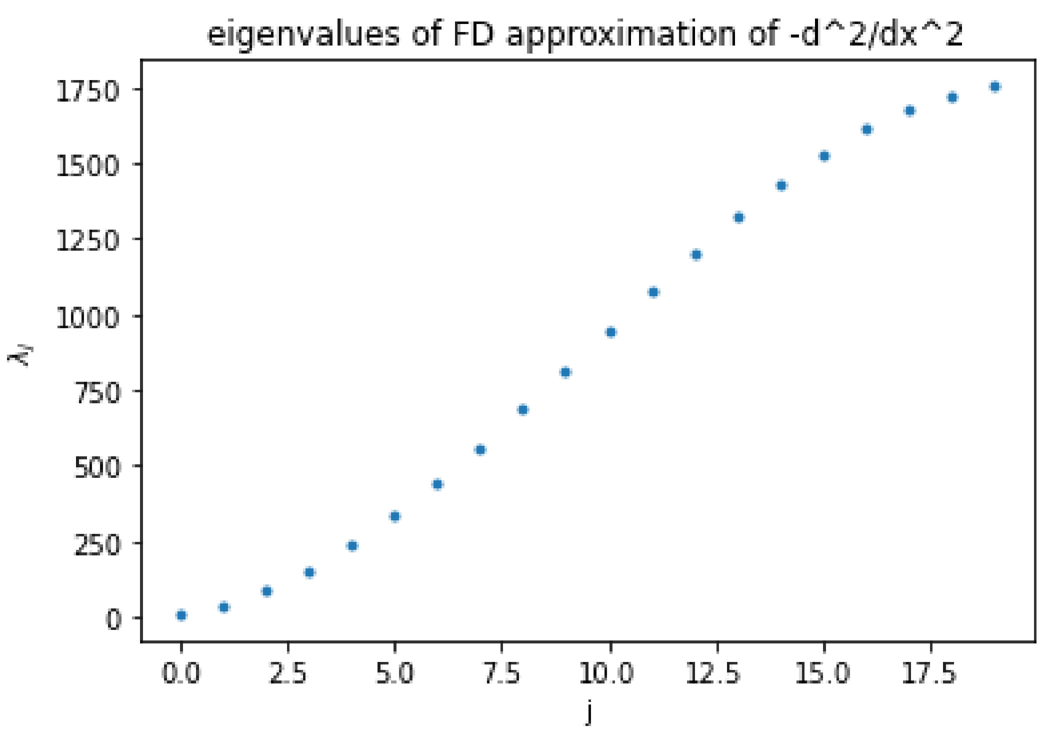
[5]:

```
# Implementation of Exercise 5.2 (d)

def higher_order_svd(T, max_ranks):
    """
    Compute the higher-order singular value decomposition
    (Tucker format approximation) of the NumPy array `T`.
    """
    assert T.ndim == len(max_ranks)
    Ulist = []
     list = []
    for j in range(T.ndim):
        A = single_mode_matricization(T, j)
        U,  , Vh = np.linalg.svd(A, full_matrices=False)
          = U.shape[1]
        if max_ranks[j] > 0:
            # truncate in case max_ranks[j] <
              = min( , max_ranks[j])
        Ulist.append(U[:, : ])
         list.append( )
    # form the core tensor
    C = T
```

```
    for j in range(C.ndim):
        # apply Uj^\dagger to j-th dimension
        C = single_mode_product(Ulist[j].conj().T, C, j)
    return TuckerTensor(Ulist, C), list
```

[6]:
```
def fd_second_derivative_zero_boundary(n):
    """
    Finite difference discretization of -d^2/dx^2 on [0, 1] with zero boundary␣
 ↪conditions.
    """
    a = np.full(n-1, 2)
    b = np.full(n-2, -1)

    return n**2 * (np.diag(a) + np.diag(b, 1) + np.diag(b, -1))
```

[7]:
```
n = 21

A = fd_second_derivative_zero_boundary(n)

# visualize eigenvalues
plt.plot(np.linalg.eigvalsh(A), '.')
plt.xlabel("j")
plt.ylabel(r"$\lambda_j$")
plt.title("eigenvalues of FD approximation of -d^2/dx^2");
```



[8]:

```python
# A is symmetric and all eigenvalues are larger than zero, i.e., A is positive␣
↪definite
min(np.linalg.eigvalsh(A))
```

[8]: 9.851211269436485

[9]:

```python
# as short test, this should be zero:
abs(min(np.linalg.eigvalsh(A)) - 9.851211269436485)
```

[9]: 0.0

[10]:

```python
# `L` operator as full matrix, as reference and for tests
L = (
    np.kron(np.kron(A,                    np.identity(len(A))), np.
↪identity(len(A))) +
    np.kron(np.kron(np.identity(len(A)), A                   ), np.
↪identity(len(A))) +
    np.kron(np.kron(np.identity(len(A)), np.identity(len(A))), A                  ␣
↪  ))
print(L.shape)
```

```
(8000, 8000)
```

[11]:

```python
def quadratic_form_tucker_isometry(A, phi: TuckerTensor, j):
    """
    Construct the square matrix `K` which expresses <phi, L phi> with
    L = A x I x ... x I + ... + I x ... x I x A
    in dependence of the j-th isometry `phi.Ulist[j]`, such that
    <phi, L phi> = <u_j, K u_j> with u_j = phi.Ulist[j].flatten().
    """
    n_u = len(phi.Ulist)
    indices = [i for i in range(n_u) if i != j]

    I = np.eye(A.shape[0])
    K = np.tensordot(phi.C, phi.C, axes=(indices, indices))
    K = np.kron(A, K)

    for i in indices:
        M = phi.Ulist[i].transpose().dot(A).dot(phi.Ulist[i])
        MC = np.tensordot(M, phi.C, ([1], [i]))
        MC = np.moveaxis(MC, 0, i)
        K += np.kron(I, np.tensordot(phi.C, MC, axes=(indices, indices)))

    return K
```

[12]:
```python
# test of `quadratic_form_tucker_isometry`
kdim_test = (2, 3, 4)
test = TuckerTensor([np.linalg.qr(np.random.randn(n-1, kdim_test[j]))[0] for j␣
↪in range(3)], np.random.standard_normal(kdim_test))
tvec = np.reshape( test.as_full_tensor(), -1)
utest = [np.reshape( test.Ulist[j], -1) for j in range(3)]
# reference value
L ref = np.dot( tvec, L @  tvec)
# relative error should be zero up to numerical rounding errors
err = [abs(np.dot(utest[j], quadratic_form_tucker_isometry(A,  test, j) @␣
↪utest[j]) -  L ref) / abs( L ref) for j in range(3)]
err
```

[12]: [0.0, 1.7098997634721596e-16, 0.0]

[13]:
```python
def linear_form_tucker_isometry(phi: TuckerTensor, b: TuckerTensor, j):
    """
    Construct the vector `g` which expresses <phi, b>
    in dependence of the j-th isometry `phi.Ulist[j]`, such that
    <phi, b> = <u_j, g> with u_j = phi.Ulist[j].flatten().
    """
    # all but j-th dimension
    jcompl = list(range(j)) + list(range(j + 1, phi.ndim))
    g = phi.C
    for k in jcompl:
        g = single_mode_product(b.Ulist[k].T @ phi.Ulist[k], g, k)
    g = b.Ulist[j] @ np.tensordot(b.C, g, axes=(jcompl, jcompl))
    assert g.shape == phi.Ulist[j].shape
    return np.reshape(g, -1)
```

[14]:
```python
def quadratic_form_tucker_core(A, phi: TuckerTensor):
    """
    Construct the square matrix `K` which expresses <phi, L phi> with
    L = A x I x ... x I + ... + I x ... x I x A
    in dependence of the core tensor `phi.C`, such that
    <phi, L phi> = <c, K c> with c = phi.C.flatten().
    """
    K = np.zeros((phi.C.size, phi.C.size))
    for j in range(phi.ndim):
        K1 = np.identity(1)
        for k in range(phi.ndim):
            K1 = np.kron(K1, phi.Ulist[k].T @ A @ phi.Ulist[k] if k == j else␣
↪np.identity(phi.Ulist[k].shape[1]))
        K += K1
    return K
```

[15]:

```python
def linear_form_tucker_core(phi: TuckerTensor, b: TuckerTensor):
    """
    Construct the vector `g` which expresses <phi, b>
    in dependence of the core tensor `phi.C`, such that
    <phi, b> = <c, g> with c = phi.C.flatten().
    """
    # construct temporary Tucker format tensor
    Alist = [phi.Ulist[j].T @ b.Ulist[j] for j in range(phi.ndim)]
    g = TuckerTensor(Alist, b.C).as_full_tensor()
    return np.reshape(g, -1)
```

[16]:

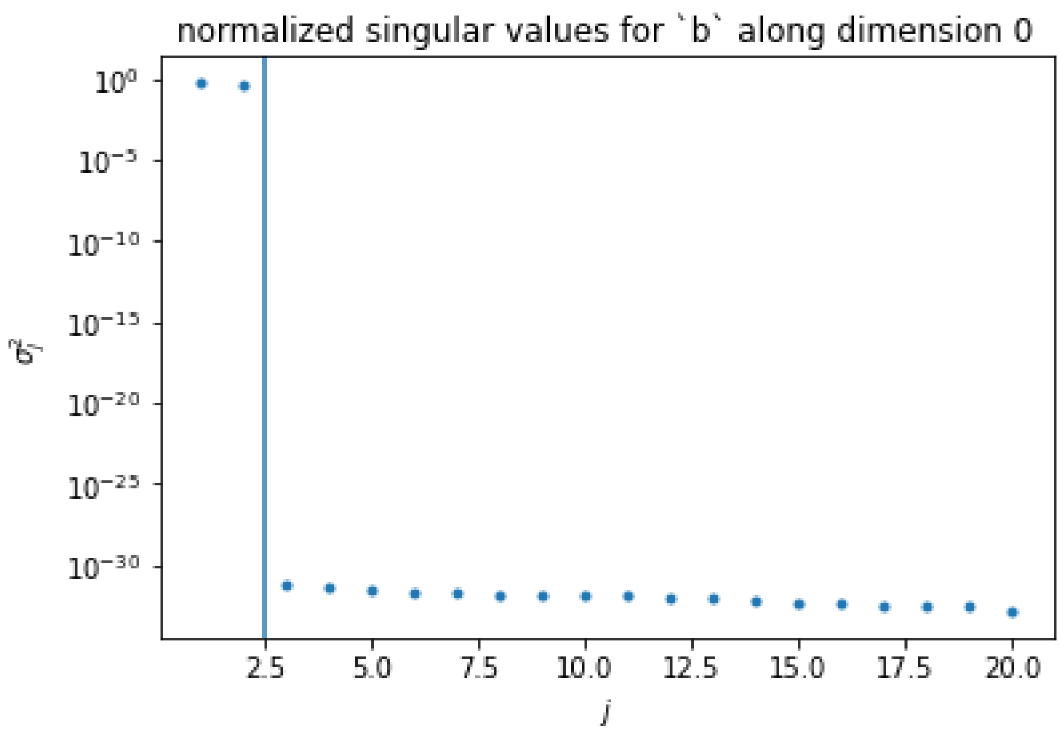
```python
def factorized_tucker_als_step(A, phi: TuckerTensor, b: TuckerTensor):
    """
    Alternating Least Squares (ALS) optimization step of a Tucker format tensor
 `phi`
    for target function 1/2 <phi, L phi> - <phi, b> with
    L = A x I x ... x I + ... I x ... x I x A.
    """
    assert phi.ndim == b.ndim
    # optimize U matrices one-by-one
    for j in range(phi.ndim):
        # construct least squares terms for Ulist[j]
        K = quadratic_form_tucker_isometry(A, phi, j)
        g = linear_form_tucker_isometry(phi, b, j)
        Ujnext = np.reshape(np.linalg.solve(K, g), phi.Ulist[j].shape)
        # perform QR decomposition to ensure Ulist[j] remains an isometry
        phi.Ulist[j], R = np.linalg.qr(Ujnext, mode='reduced')
        # absorb R into core tensor
        phi.C = single_mode_product(R, phi.C, j)
    # optimize core tensor
    K = quadratic_form_tucker_core(A, phi)
    g = linear_form_tucker_core(phi, b)
    phi.C = np.reshape(np.linalg.solve(K, g), phi.C.shape)
    # result is stored in updated `phi`
```

[17]:

```python
# construct `b` tensor

bfull = np.array([[[np.sin(3*np.pi*(i + j + k)/n) for k in range(1, n)] for j
 in range(1, n)] for i in range(1, n)])
print("bfull.shape:", bfull.shape)

# keep only 2 singular values along each dimension
b, listb = higher_order_svd(bfull, [2, 2, 2])

print("b Tucker approximation error:", np.linalg.norm(np.reshape(b.
 as_full_tensor() - bfull, -1)) / np.linalg.norm(np.reshape(bfull, -1)))
```

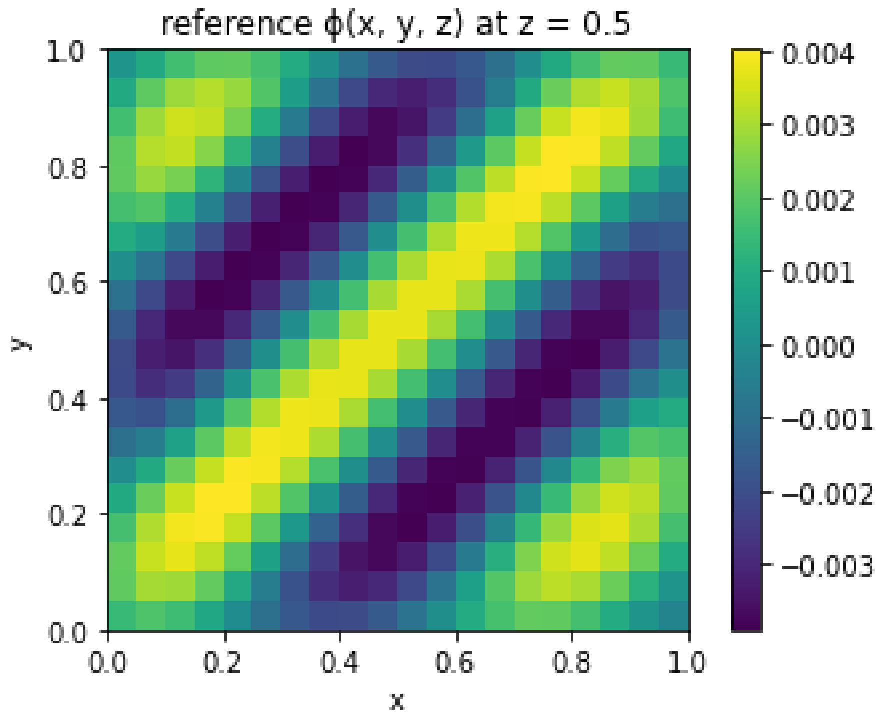
```
bfull.shape: (20, 20, 20)
b Tucker approximation error: 8.336626324261062e-16
```

[18]:
```
# show some singular values from HOSVD of `b`
plt.semilogy(range(1, len( listb[0]) + 1),  listb[0]**2 / np.sum( listb[0]**2),␣
 ↪'.')
plt.axvline(x=2.5)
plt.ylabel("$\\sigma_j^2$")
plt.xlabel("$j$")
plt.title("normalized singular values for `b` along dimension 0");
plt.show()
```

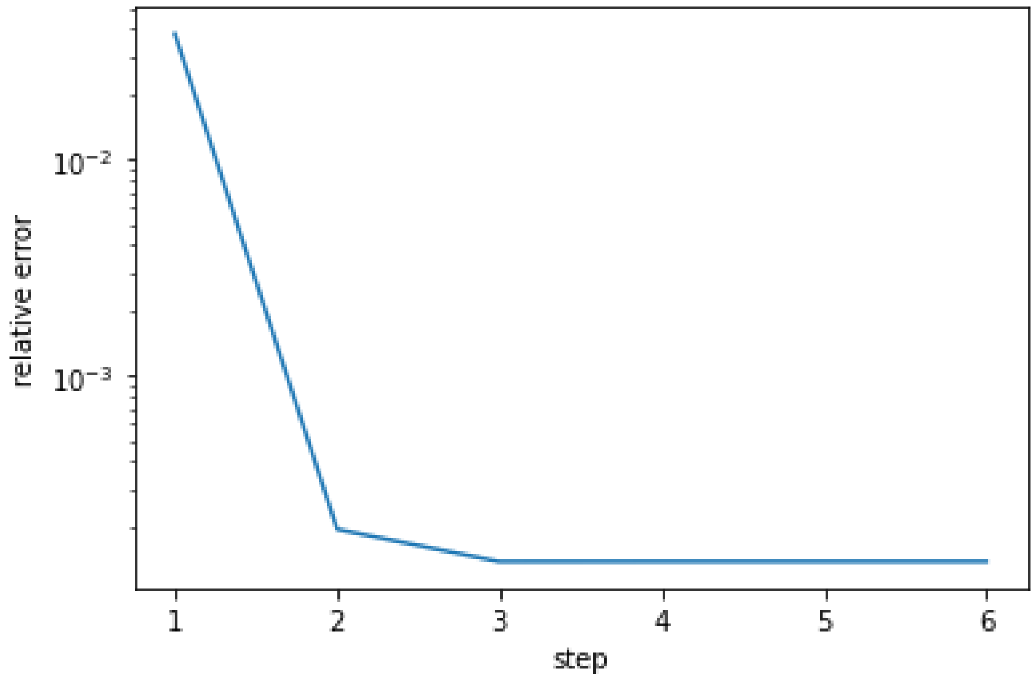


[19]:
```
# reference solution
print("Solving reference linear system...")
 ref = np.reshape(np.linalg.solve(L, np.reshape(bfull, -1)), bfull.shape)
print("done.")
print(" ref.shape:",  ref.shape)
plt.imshow( ref[:, :, n//2], extent=[0,1,0,1])
plt.xlabel("x")
plt.ylabel("y")
plt.title("reference  (x, y, z) at z = 0.5")
plt.colorbar()
plt.show()
```

```
Solving reference linear system…
done.
 ref.shape: (20, 20, 20)
```



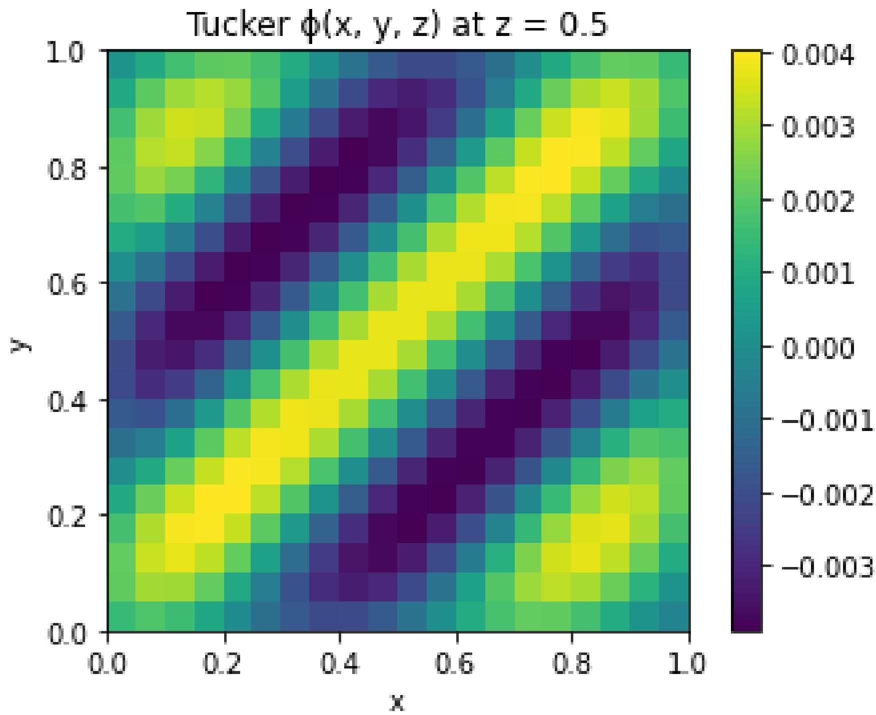

```
[20]: # run optimization

# initial tensor
np.random.seed(42)
k = 4
 = TuckerTensor([np.linalg.qr(np.random.randn(n-1, k), mode='reduced')[0] for␣
↪_ in range(3)], np.random.randn(k, k, k))

numiter = 6
errlist = []
for i in range(numiter):
    factorized_tucker_als_step(A,  , b)
    errlist.append(np.linalg.norm( .as_full_tensor() - ref) / np.linalg.
↪norm( ref))

plt.semilogy(range(1, numiter + 1), errlist)
plt.xlabel("step")
plt.ylabel("relative error")
plt.show()
```



[21]:
```
# core tensor
 .C.shape
```

[21]: (4, 4, 4)

[22]:
```
# visualize Tucker format approximation (should be visually indistinguishable␣
 ↪from reference solution)
 full =  .as_full_tensor()
plt.imshow( full[:, :, n//2], extent=[0,1,0,1])
plt.xlabel("x")
plt.ylabel("y")
plt.title("Tucker  (x, y, z) at z = 0.5")
plt.colorbar()
plt.show()
```


Tucker ϕ(x, y, z) at z = 0.5
y
x
0.0
0.2
0.4
0.6
0.8
1.0
0.004
0.003
0.002
0.001
0.000
−0.001
−0.002
−0.003