Physics-informed regularization: Solving PDEs

Contents


```python
import numpy as np
np.set_printoptions(precision=3)
import matplotlib.pyplot as plt
%matplotlib inline
import seaborn as sns
sns.set(rc={"figure.dpi":100, "savefig.dpi":300})
sns.set_context("notebook")
sns.set_style("ticks")

import scipy
import scipy.stats as st
import urllib.request
import os

def download(
    url : str,
    local_filename : str = None
):
    """Download a file from a url.

    Arguments
    url            -- The url we want to download.
    local_filename -- The filemame to write on. If not
                      specified
    """
    if local_filename is None:
        local_filename = os.path.basename(url)
    urllib.request.urlretrieve(url, local_filename)
```

Objectives

- Learn how to solve PDEs with neural networks.

This notebook replicates some of the results of Lagaris et al. 1998).

```python
import numpy as np
import torch
import torch.nn as nn

# This is useful for taking derivatives:
def grad(outputs, inputs):
    return torch.autograd.grad(outputs, inputs, grad_outputs=torch.ones_like(outputs),
create_graph=True)[0]
```

Example: Solving PDEs

consider a PDE of the form:

$$\frac{\partial^2}{\partial x^2}\Psi(x,y) + \frac{\partial^2}{\partial y^2}\Psi(x,y) = f(x,y),$$

on $(x,y) \in [0,1]^2$ with Dirichlet boundary conditions:

$$\Psi(0,y) = f_0(y),$$

$$\Psi(1,y) = f_1(y),$$

$$\Psi(x,0) = g_0(x),$$

and

$$\Psi(x,1) = g_1(x).$$

We write:

$$\hat{\Psi}(x,y;\theta) = A(x,y) + x(1-x)y(1-y)N(x,y;\theta),$$

where $A(x,y)$ is chosen to satisfy the boundary conditions:

$$A(x,y) = (1-x)f_0(y) + xf_1(y) + (1-y)\{g_0(x) - [(1-x)g_0(0) + xg_0(1)]\} + y\{g_1(x) - [(1-x)g_1(0) + xg_1(1)]\}.$$

The loss function that we need to minimize is:

$$L(\theta) = \int_{[0,1]^2} \left\{ \frac{\partial^2}{\partial x^2}\hat{\Psi}(x,y;\theta) + \frac{\partial^2}{\partial y^2}\hat{\Psi}(x,y;\theta) - f(x,y) \right\}^2 dxdy.$$

Here is code that solves the same problem:

```python
class PDEProblemDC(object):
    """
    A class representing PDE with DC boundary.

    :param rhs:               The right hand side of the equation.
                              This must be a function with signature rhs((x,y))
                              where t is time and y is the state of the system.
    :param f0:                Left boundary conditon.
    :param f1:                Right boundary condition.
    :param g0:                Bottom boundary conditon.
    :param g1:                Top boundary condition.
    :param net:               A neural network for representing the solution. This must have
                              two-dimensional input and one-dimensional output.
    """

    def __init__(self, rhs, f0, f1, g0, g1, net):
        self._rhs = rhs
        self._f0 = f0
        self._f1 = f1
        self._g0 = g0
        self._g1 = g1
        self._net = net
        # This implements a function that satisfies the boundary conditions exactly
        g00 = self.g0(torch.zeros((1,)))[0]
        g01 = self.g0(torch.ones((1,)))[0]
        g10 = self.g1(torch.zeros((1,)))[0]
        g11 = self.g1(torch.ones((1,)))[0]
        def A(x):
            res = (1.0 - x[:, 0]) * self.f0(x[:, 1])
            res += x[:, 0] * self.f1(x[:, 1])
            res += (1.0 - x[:, 1]) * (self.g0(x[:, 0]) - ((1.0 - x[:, 0]) * g00 + x[:, 0] * g01))
            res += x[:, 1] * (self.g1(x[:, 0]) - ((1.0 - x[:, 0]) * g10 + x[:, 0] * g11))
            return res
        self._A = A
        self._solution = lambda x: self.A(x) + x[:, 0] * (1.0 - x[:, 0]) * x[:, 1] * (1.0 - x[:, 1]) * self.net(x)[:, 0]

    @property
    def rhs(self):
        return self._rhs

    @property
    def f0(self):
        return self._f0

    @property
    def f1(self):
        return self._f1

    @property
    def g0(self):
        return self._g0

    @property
    def g1(self):
        return self._g1

    @property
    def A(self):
        return self._A

    @property
    def net(self):
        return self._net

    @property
    def solution(self):
        """
        Return the solution function.
        """
        return self._solution

    def squared_residual_loss(self, X):
        """
        Returns the squared residual loss at spatial locations X.

        :param T:    Must be a 1D torch tensor.
        """
        X.requires_grad = True
        sol = self.solution(X)
        A = self.A(X)
        sol_x = grad(sol, X)
```

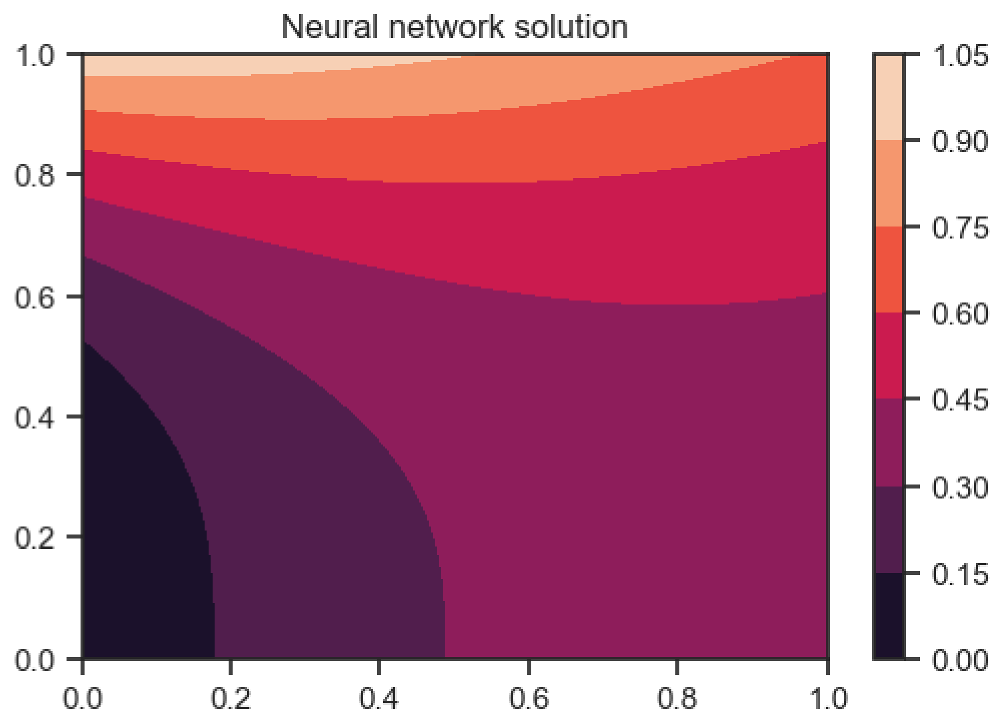
```
        # Get the second derivatives
        sol_xx = grad(sol_x[:, 0], X)[:, 0]
        sol_yy = grad(sol_x[:, 1], X)[:, 1]
        rhs = self.rhs(X)
        return torch.mean((sol_xx + sol_yy - rhs) ** 2)

    def solve_lbfgs(self, X_colloc, max_iter=10):
        """
        Solve the problem by minimizing the squared residual loss.

        :param T_colloc: The collocation points used to solve the problem.
        """
        optimizer = torch.optim.LBFGS(self.net.parameters())

        # Run the optimizer
        def closure():
            optimizer.zero_grad()
            l = self.squared_residual_loss(X_colloc)
            l.backward()
            return l
        for i in range(max_iter):
            res = optimizer.step(closure)
            print(res)


def plot_contour(ex, true_sol):
    """Plot the contour of the true solution and the approximation."""
    xx = np.linspace(0, 1, 64)
    X, Y = np.meshgrid(xx, xx)
    X_flat = torch.Tensor(np.hstack([X.flatten()[:, None], Y.flatten()[:, None]]))
    Z_flat = ex.solution(X_flat).detach().numpy()
    Z_t_flat = true_sol(X_flat)
    Z_t_flat = Z_t_flat.detach().numpy()
    Z = Z_flat.reshape(64, 64)
    Z_t = Z_t_flat.reshape(64, 64)
    fig, ax = plt.subplots()
    c = ax.contourf(X, Y, Z)
    ax.set_title("Neural network solution")
    plt.colorbar(c)
    fig, ax = plt.subplots()
    c = ax.contourf(X, Y, Z_t)
    ax.set_title("True solution")
    plt.colorbar(c)
```

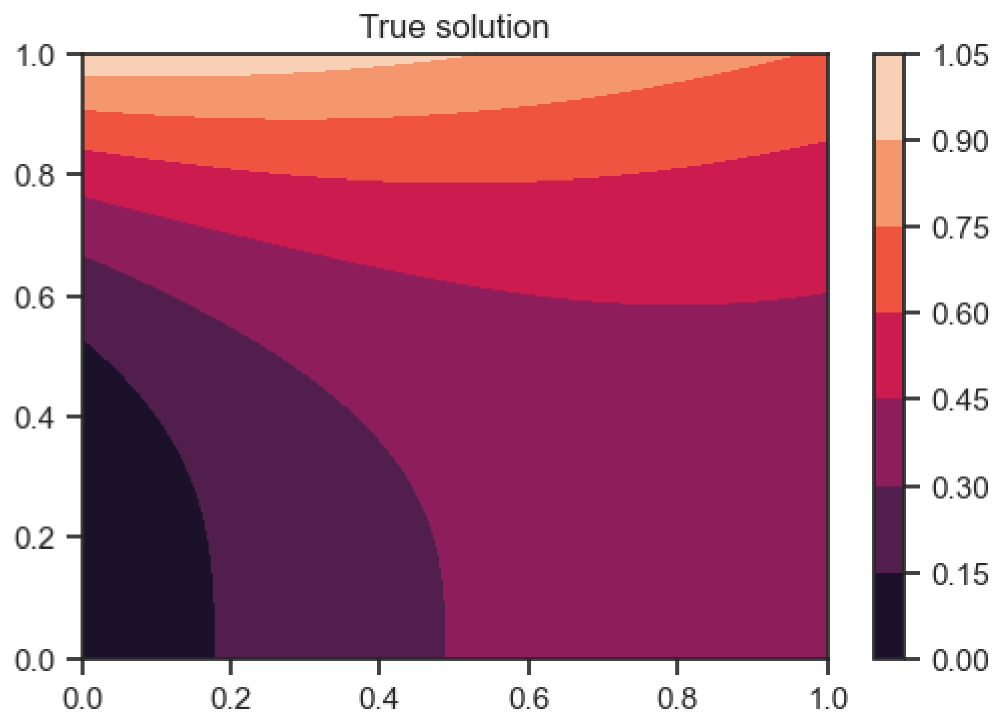
And here is how to solve it with neural networks:

```
# Problem 5 of Lagaris
rhs = lambda x: torch.exp(-x[:, 0]) * (x[:, 0] - 2.0 + x[:, 1] ** 3 + 6.0 * x[:, 1])
f0 = lambda x2: x2 ** 3
f1 = lambda x2: (1.0 + x2 ** 3) * np.exp(-1.0)
g0 = lambda x1: x1 * torch.exp(-x1)
g1 = lambda x1: torch.exp(-x1) * (x1 + 1.0)
ex5 = PDEProblemDC(rhs, f0, f1, g0, g1,
                   nn.Sequential(nn.Linear(2, 10), nn.Sigmoid(), nn.Linear(10,1,
bias=False)))
x = np.linspace(0, 1, 10)
X, Y = np.meshgrid(x, x)
X_flat = torch.Tensor(np.hstack([X.flatten()[:, None], Y.flatten()[:, None]]))
ex5.solve_lbfgs(X_flat)
```

```
tensor(0.0107, grad_fn=<MeanBackward0>)
tensor(0.0001, grad_fn=<MeanBackward0>)
tensor(9.8839e-05, grad_fn=<MeanBackward0>)
tensor(1.4855e-05, grad_fn=<MeanBackward0>)
tensor(6.9040e-06, grad_fn=<MeanBackward0>)
tensor(1.5973e-06, grad_fn=<MeanBackward0>)
tensor(6.9797e-07, grad_fn=<MeanBackward0>)
tensor(5.1638e-07, grad_fn=<MeanBackward0>)
tensor(4.4831e-07, grad_fn=<MeanBackward0>)
tensor(4.4608e-07, grad_fn=<MeanBackward0>)
```

```
ex5_true_sol = lambda x: torch.exp(-x[:, 0]) * (x[:, 0] + x[:, 1] ** 3)
plot_contour(ex5, ex5_true_sol)
```

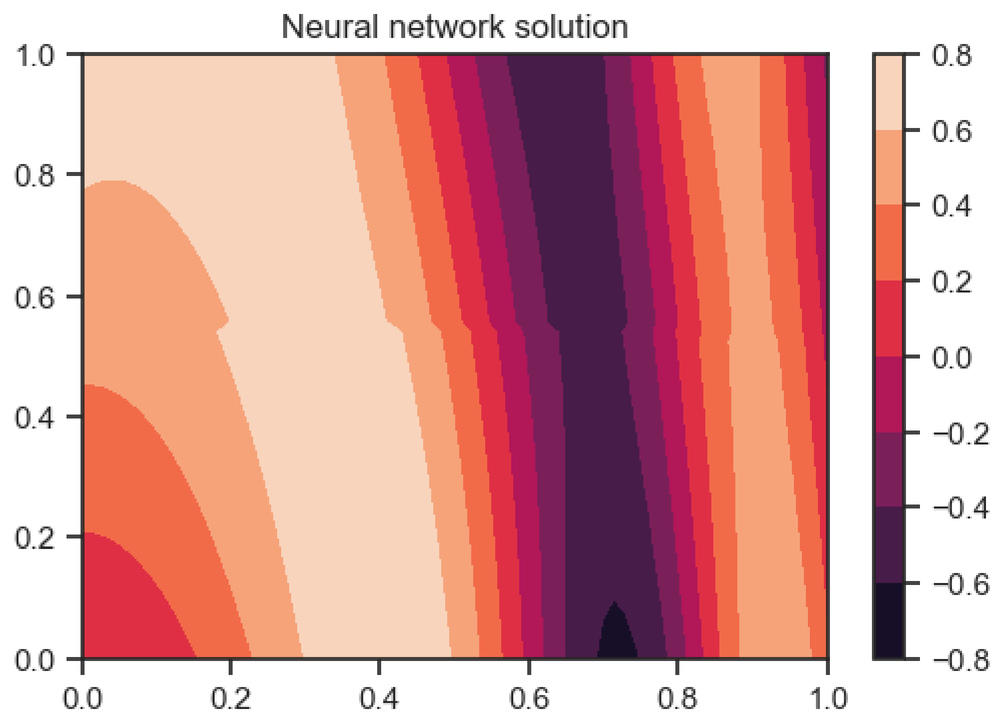


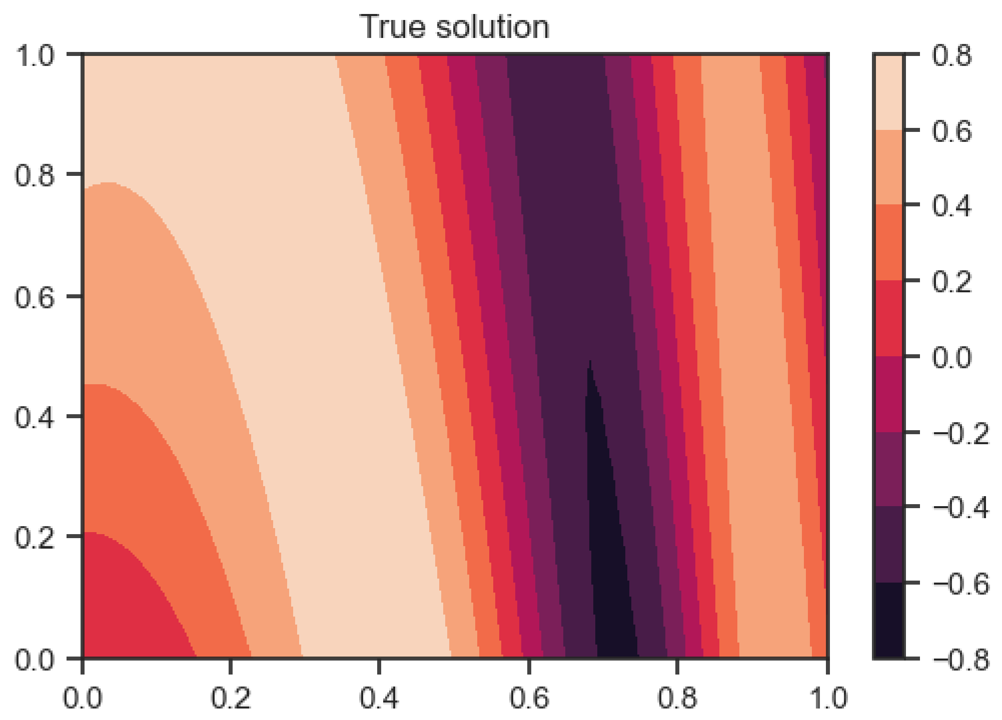



```
# Problem 6 of Lagaris
a = 3.0
def rhs(x):
    tmp1 = torch.exp(-(a * x[:, 0] + x[:, 1]) / 5.0)
    tmp2 = (-4.0 / 5.0 * a ** 3 * x[:, 0] - 2.0 / 5.0 + 2.0 * a ** 2) * torch.cos(a ** 2 *
x[:, 0] ** 2 + x[:, 1])
    tmp2 += (1.0 / 25.0 - 1.0 - 4.0 * a ** 4 * x[:, 0] ** 2 + a ** 2 / 25.0) * torch.sin(a
** 2 * x[:, 0] ** 2 + x[:, 1])
    return tmp1 * tmp2
ex6_true_sol = lambda x: torch.exp(-(a * x[:, 0] + x[:, 1]) / 5.0) * torch.sin(a ** 2 *
x[:, 0] ** 2 + x[:, 1])
f0 = lambda x2: ex6_true_sol(torch.stack((torch.zeros_like(x2), x2), dim=1))
f1 = lambda x2: ex6_true_sol(torch.stack((torch.ones_like(x2), x2), dim=1))
g0 = lambda x1: ex6_true_sol(torch.stack((x1, torch.zeros_like(x1)), dim=1))
g1 = lambda x1: ex6_true_sol(torch.stack((x1, torch.ones_like(x1)), dim=1))
net = nn.Sequential(nn.Linear(2, 10), nn.Sigmoid(), nn.Linear(10, 1, bias=False))
ex6 = PDEProblemDC(rhs, f0, f1, g0, g1, net)
x = np.linspace(0, 1, 10)
X, Y = np.meshgrid(x, x)
X_flat = torch.Tensor(np.hstack([X.flatten()[:, None], Y.flatten()[:, None]]))
# Does not always work because of local minima.
# Try multiple times.
ex6.solve_lbfgs(X_flat, max_iter=10)
```

```
tensor(28.7037, grad_fn=<MeanBackward0>)
tensor(28.6589, grad_fn=<MeanBackward0>)
tensor(28.7512, grad_fn=<MeanBackward0>)
tensor(28.7028, grad_fn=<MeanBackward0>)
tensor(28.7028, grad_fn=<MeanBackward0>)
tensor(28.7028, grad_fn=<MeanBackward0>)
tensor(28.7028, grad_fn=<MeanBackward0>)
tensor(28.7353, grad_fn=<MeanBackward0>)
tensor(28.7353, grad_fn=<MeanBackward0>)
tensor(28.7941, grad_fn=<MeanBackward0>)
```

```
plot_contour(ex6, ex6_true_sol)
```





Questions

Feel free to skip this as it can be hard if you are not expert with Python.

- Add a method to the class `PDEProblemDC` that uses stochastic gradient descent to solve the same problems. Once you are done, rerun the problems above with your code.
- According to the Dirchlet principle, the solution of the PDE:

$$\frac{\partial^2}{\partial x^2}\Psi(x,y) + \frac{\partial^2}{\partial y^2}\Psi(x,y) = f(x,y),$$

minimizes the energy functional:

$$J[\Psi] = \int_{[0,1]^2}\left[\frac{1}{2}\parallel \nabla\Psi \parallel^2 + \Psi f\right]dxdy,$$

subject to the boundary conditions. This means that you can solve the problem by minimizing the loss function:

$$J(\theta) = \int_{[0,1]^2}\left[\frac{1}{2}\parallel \nabla\hat{\Psi}(x,y;\theta) \parallel^2 + \hat{\Psi}(x,y;\theta)f(x,y)\right]dxdy.$$

Add this functionality to the class `PDEProblemDC`.

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