BME 493/593, Spring 2019:
Computational Methods for Imaging Science
Assignment 5 (due April 22, 2019)

Instructions: The problems below require a mix of paper-and-pencil work and Python implementation using the Jetstream cloud resources[1]. Remember that, as stated in the syllabus, you should both

1. Submit a hard copy of your solutions (which will be collected on Monday, April 22 **before** the class starts), **and**

2. Upload a digital copy of your solutions on Canvas by 9:59 AM on Monday, April 22.

Please include generated results and figures of your code in the hard copy of your solutions. The digital copy uploaded on Canvas must be a scan (or *readable* cellphone picture) of the hard copy that you handed in at the beginning of class. The instructors will grade only the hard copy of your solutions. The digital copy uploaded on Canvas only serves as proof that the assignment was turned in on time. If you are late or miss class on the day the assignment is due, uploading your solution on Canvas before the due date ensures that your assignment is considered on time.

To access the Jetstream cloud computing resources follow the link `http://uvilla.github.io/cmis_labs/cloud.html` and use your wustl e-mail address (all lowercase and without `@wustl.edu`) as username and your student id as password.

For this assignment you will need the following files (that you can find inside the `cmis_lab/Assignment5` folder on the Jetstream cloud resources):

- `Poisson_SD.ipynb` illustrating the use of hIPPYlib/fenics for solving a determinisitc inverse problem for the coefficient field of a Poisson equation, using the steepest descent method;

- `Poisson_INCG.ipynb` illustrating the use of hIPPYlib/fenics for solving a determinisitc inverse problem for the coefficient field of a Poisson equation, using the inexact Newton Conjugate Gradient algorithm.

Problem 1: Frequency-domain inverse wave propagation problem Here we formulate and solve an inverse acoustic wave propagation problem in the frequency domain, which is governed by the Helmholtz equation. This is a problem of great practical relevance. Its applications include full waveform inversion in ultrasound computed tomography, seismic imaging, and non-destructive material quality control.

Let $\Omega \subset \mathbb{R}^d$ be a bounded domain ($d \in \{2, 3\}$) with boundary $\partial\Omega$. The idea is to propagate harmonic waves from multiple sources $f_j(\boldsymbol{x})$ ($j = 1, \dots, N_s$) at multiple frequencies ω_i ($i = 1, \dots, N_f$) into a medium and measure the amplitude $u_{ij}(\boldsymbol{x})$ of the reflected wavefields at points $\boldsymbol{x}_k$ ($k = 1, \dots, N_d$) for

[1] These resources were awarded to us by the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by the National Science Foundation.

each source and frequency, with the goal of inferring the soundspeed of the medium, $c(\boldsymbol{x})$. We can formulate this inverse problem as follows:

$$\min_m \mathcal{J}(m) := \frac{1}{2} \sum_i^{N_f} \sum_j^{N_s} \sum_k^{N_d} \int_\Omega (u_{ij}(m) - u_{ij}^{obs})^2 \, \delta(\boldsymbol{x} - \boldsymbol{x}_k) \, d\boldsymbol{x} + \frac{\beta}{2} \int_\Omega \nabla m \cdot \nabla m \, d\boldsymbol{x}$$

where $u_{ij}(\boldsymbol{x})$ depends on the medium parameter field $m(\boldsymbol{x})$, which is equal to $1/c(\boldsymbol{x})^2$, through the solution of Helmholtz problem

$$\begin{aligned} -\Delta u_{ij} - \omega_i^2 \, m \, u_{ij} &= f_j \quad \text{in } \Omega, \quad i = 1, \dots, N_f, \quad j = 1, \dots, N_s, \\ u_{ij} &= 0 \quad \text{on } \partial\Omega. \end{aligned}$$

In the problem above, $u_{ij}^{obs}(\boldsymbol{x})$ denotes given measurements (for frequency i and source j), u_{ij} is the amplitude of the acoustic wavefield, and $\beta > 0$ is the regularization parameter.

a) Derive an expression for the gradient of $\mathcal{J}$ with respect to the medium m using the Lagrangian method for a single source and frequency, i.e., for $N_f = N_s = 1$. Give both variational and strong forms of the gradient.

b) Derive an expression for the action of the Hessian in a direction $\hat{m}$ in the single source and frequency case. Give both variational and strong forms of the Hessian action.

c) Derive an expression for the gradient for an arbitrary number of sources and frequencies[2]. How many state and adjoint equations have to be solved for a single gradient computation?

Problem 2: Inverse diffusion problem We would like to solve the inverse problem for the diffusion equation we discussed in class, on the domain $\Omega = [0,1] \times [0,1]$:

$$\min_m \mathcal{J}(m) := \frac{1}{2} \int_\Omega (u(m) - u^{obs})^2 \, d\boldsymbol{x} + \frac{\gamma}{2} \int_\Omega \nabla m \cdot \nabla m \, d\boldsymbol{x}, \tag{1}$$

where the field $u(\boldsymbol{x})$ depends on the diffusivity $e^m(\boldsymbol{x})$ through the solution of

$$\begin{aligned} -\nabla \cdot (e^m \nabla u) &= 0 \quad \text{in } \Omega, \\ e^m \nabla u \cdot \boldsymbol{n} &= j \quad \text{on } \partial\Omega, \end{aligned} \tag{2}$$

where $\gamma > 0$ is the regularization parameter, and $j(\boldsymbol{x})$ is a boundary source term. We synthesize the measurement data $u^{obs}(\boldsymbol{x})$ by solving the forward diffusion equation with $m(x,y) = \ln 2$ for $(x - 0.5)^2 + (y - 0.5)^2 \leq 0.04$ and $m(x,y) = \ln 9$ otherwise. Noise is added to this *data* to simulate actual instrument noise.

Please only include the code for question (d).

a) Run the `Poisson_SD.ipynb` notebook and report the number of steepest descent iterations for a discretization of the domain with 8×8, 16×16, 32×32, 64×64 pixels. Discuss how the number of iterations changes as the parameter dimension increases. Is steepest descent method scalable with respect to the parameter dimension?

[2] Hint: Every state equation with solution u_{ij} has a corresponding adjoint variable p_{ij}. The Lagrangian functional now involves the sum over all state equations.

b) Run the `Poisson_INCG.ipynb` notebook and report the number of inexact Newton and of total CG iterations for a discretization of the domain with 8×8, 16×16, 32×32, 64×64 pixels. Discuss how the number of iterations changes as the parameter dimension increases. Is inexact Newton-CG method scalable with respect to the parameter dimension?

c) Run the `Poisson_INCG.ipynb` notebook and report the generalized eigenvalues and eigenvectors of the Hessian misfit at the solution of the inverse problem for a discretization of the domain with 8×8, 16×16, 32×32, 64×64 pixels. What do you observe?

d) Since the coefficient m is discontinuous, a better choice of regularization is total variation rather than Tikhonov regularization, to prevent an overly smooth reconstruction. Use $\beta = 0.1$ to make the non-differentiable TV regularization term differentiable. In other words, your regularization functional should be:

$$\mathcal{R}_{TV}^{\beta} := \int_{\Omega} (\nabla m \cdot \nabla m + \beta)^{\frac{1}{2}} \, d\boldsymbol{x}.$$

- Modify the implementation in `Poisson_SD.ipynb` to include total variation regularization and plot the result for a reasonably chosen regularization parameter[3].
- **Extra credits:** Modify the implementation in `Poisson_INCG.ipynb` and plot the result for the value of γ found above.

[3] Either experiment manually with a few values for γ or use the L-curve criterion or Morozov's discrepancy principle.