MA 1018: Introduction to Scientific Computing
Additional Topics and Applications

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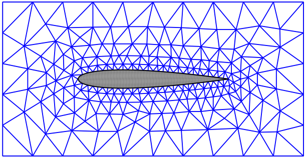
Additional topics

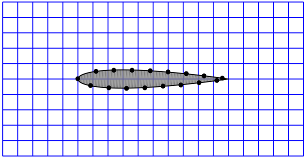
We will give a brief introduction to the following topics:

- **Computational science:** numerical methods for differential equations, computational fluid dynamics (CFD), etc.
- **Mathematical image processing:** variational image processing methods, computer vision, etc.
- **Data science:** clustering, classification, dimensionality reduction, and related machine learning techniques, etc.

Fluid-structure interaction (流體結構耦合) problem

- The primary issues for CFD are accuracy, computational efficiency, and the ability to handle complex geometries.
- The fluid-structure interaction problem describes the coupling of fluid and structure mechanics. It usually requires the modeling of complex geometric structure and moving boundaries. Thus, it is very challenging for conventional body-fitted approach.



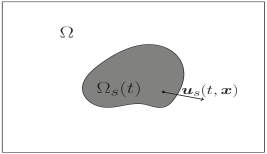


Incompressible Navier-Stokes equations

A simple one-way coupling FSI problem is flow over a stationary or moving solid body with a prescribed velocity.

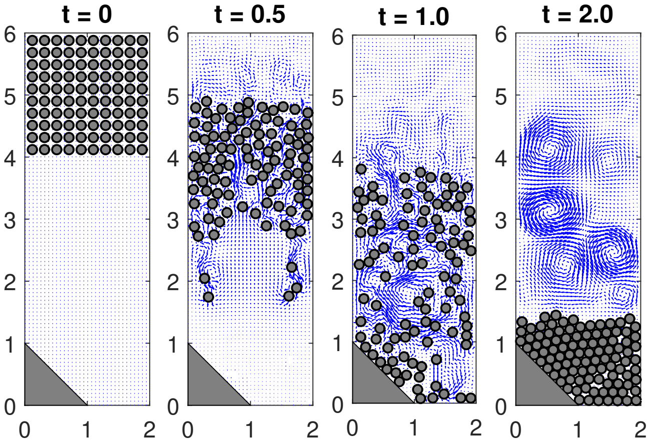
Let Ω be the fluid domain which encloses a rigid body positioned at $\overline{\Omega}_s(t)$ *with a prescribed velocity* $\boldsymbol{u}_s(t,\boldsymbol{x})$. The FSI problem with initial value and no-slip boundary condition can be posed as follows:

$$
\begin{aligned}
\frac{\partial \boldsymbol{u}}{\partial t} - \nu\nabla^2\boldsymbol{u} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + \nabla p &= \boldsymbol{f} \quad \text{in } (\Omega\setminus\overline{\Omega}_s)\times(0,T],\\
\nabla\cdot\boldsymbol{u} &= 0 \quad \text{in } (\Omega\setminus\overline{\Omega}_s)\times(0,T],\\
\boldsymbol{u} &= \boldsymbol{u}_b \quad \text{on } \partial\Omega\times[0,T],\\
\boldsymbol{u} &= \boldsymbol{u}_s \quad \text{on } \partial\Omega_s\times[0,T],\\
\boldsymbol{u} &= \boldsymbol{u}_0 \quad \text{in } (\Omega\setminus\overline{\Omega}_s)\times\{t=0\},
\end{aligned}
$$



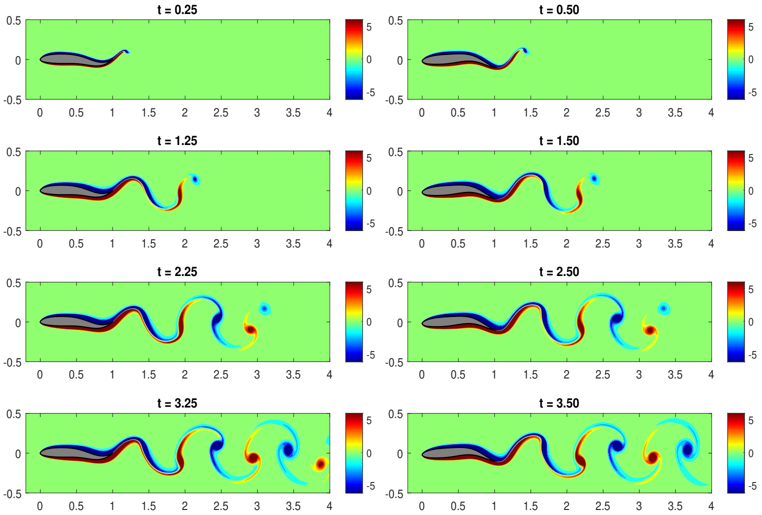
where $\boldsymbol{u}$ is the velocity field, p the pressure (divided by a constant density ρ), ν the kinematic viscosity, $\boldsymbol{f}$ the density of body force.

Sedimentation of multiple particles



The sedimentation of multiple particles and the flow field visualization at time $t = 0, 0.5, 1.0,$ *and* 2.0

Flow past a swimming fish-like solid body



The instantaneous vorticity contours of the FSI problem of flow past a swimming fish-like solid body

Mathematical image processing

Tony F. Chan (陳繁昌): *Image processing and computational mathematics,* Davis Centre, University of Waterloo, October 7th, 2015.

https://www.youtube.com/watch?v=zZN_L8ntO9I

Image processing has emerged not only as an application domain where computational mathematics provides ideas and solutions but also in spurring new research directions, *"a new Computational Fluid Dynamics!"*

We briefly introduce the variational method/energy functional minimization approach to 2-D image processing.

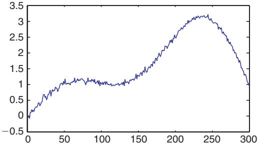
Total variation (總變差)

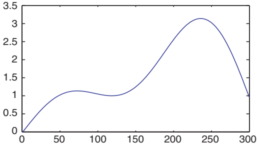
Let $u : [a,b] \to \mathbb{R}$. Let $\mathcal{P}_n = \{x_0 = a, x_1, \cdots, x_n = b\}$ be an arbitrary partition of $\overline{\Omega} := [a,b]$ and $\Delta x_i = x_i - x_{i-1}$. The total variation of u is

$$\begin{aligned} \|u\|_{TV(\Omega)} &:= \sup_{\mathcal{P}_n} \sum_{i=1}^{n} |u(x_i) - u(x_{i-1})| = \sup_{\mathcal{P}_n} \sum_{i=1}^{n} \left| \frac{u(x_i) - u(x_{i-1})}{\Delta x_i} \right| \Delta x_i \\ &= \int_\Omega |u'(x)|\, dx, \quad \text{if } u \text{ is smooth.} \end{aligned}$$

Denoising is the problem of removing noise from an image:

$$\text{minimize} \left(\int_\Omega |u'(x)|\, dx + \text{ some data fidelity term} \right).$$





1-D example

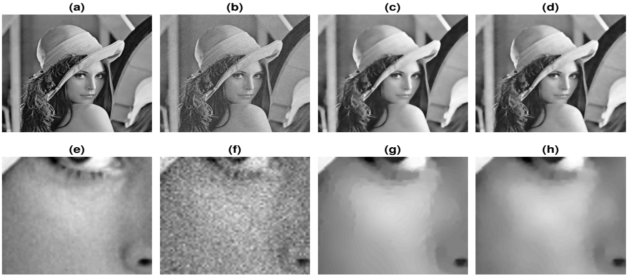
ROF total-variation model vs. adaptive diffusivity model

Let $f : \overline{\Omega} \subset \mathbb{R}^2 \to \mathbb{R}$ be a given noisy image. Rudin-Osher-Fatemi (1992) proposed the model:

$$\min_{u \in \mathcal{V}} \left(\int_{\Omega} |\nabla u| + \frac{\lambda}{2} (u - f)^2 \, d\boldsymbol{x} \right), \quad \lambda > 0.$$

Hsieh-Shao-Yang (2018) proposed an adaptive model to alleviate *the staircasing effect:*

$$\min_{u \in \mathcal{V}} \left(\int_{\Omega} \frac{1}{2} \varphi(|\nabla u^*|) |\nabla u|^2 + \frac{\lambda}{2} (u - f)^2 \, d\boldsymbol{x} \right), \quad \lambda > 0.$$



A variational model for image contrast enhancement

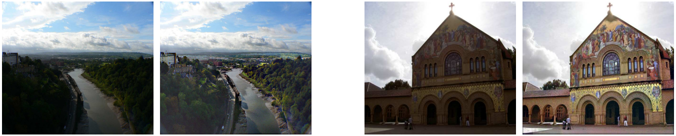
Hsieh-Shao-Yang (2020): for every $f \in \{f_R, f_G, f_B\}$, we solve

$$\min_{u \in \mathcal{V}} \left(\int_\Omega |\nabla u - \nabla h_c| \, d\boldsymbol{x} + \frac{\lambda}{2} \int_\Omega (u - g_c)^2 \, d\boldsymbol{x} \right),$$

where the adaptive functions g_c and h_c are defined as

$$g_c(\boldsymbol{x}) := \begin{cases} \alpha \bar{f}, & \boldsymbol{x} \in \Omega_d, \\ f(\boldsymbol{x}), & \boldsymbol{x} \in \Omega_b, \end{cases} \qquad h_c(\boldsymbol{x}) := \begin{cases} \beta f(\boldsymbol{x}), & \boldsymbol{x} \in \Omega_d, \\ f(\boldsymbol{x}), & \boldsymbol{x} \in \Omega_b. \end{cases}$$

Numerical methods: *(i) Euler-Lagrange equation + solving IBVP; (ii) direct discretization + split Bregman iterations.*



Numerical results by the split Bregman iterations

Chan-Vese segmenation model: nonconvex minimization

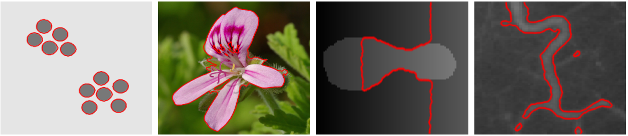
Chan-Vese (1999) modified Mumford-Shah model (1989): two-phase

$$\min_{c_1,c_2,\mathcal{C}} \left(\mu|\mathcal{C}| + \nu|\Omega_{\text{in}}| + \lambda_1 \int_{\Omega_{\text{in}}} (f(\boldsymbol{x}) - c_1)^2 + \lambda_2 \int_{\Omega_{\text{out}}} (f(\boldsymbol{x}) - c_2)^2 \right).$$

In terms of H, δ, and the level set function ϕ, we have

$$\min_{c1,c2,\phi} \Big(\mu \int_\Omega \delta(\phi(\boldsymbol{x}))|\nabla\phi(\boldsymbol{x})| + \nu \int_\Omega H(\phi(\boldsymbol{x})) + \lambda_1 \int_\Omega (f(\boldsymbol{x}) - c_1)^2 H(\phi(\boldsymbol{x}))$$
$$+\lambda_2 \int_\Omega (f(\boldsymbol{x}) - c_2)^2 (1 - H(\phi(\boldsymbol{x}))) \Big).$$

Numerical method: *an alternating iterative scheme (region averages + solving IBVP of the Euler-Lagrange equation)*



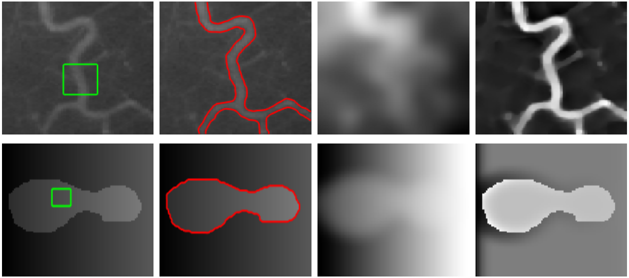
Numerical results by an alternating iterative scheme

Adaptive model for intensity inhomogeneous images

Liao-Yang-You (2022) proposed an entropy-weighted local intensity clustering-based model starting from *the bias field model:* $f = bI + n$*:*

$$\min_{\mathcal{C},b,\boldsymbol{c}} \left(\mu \, |\mathcal{C}| + \int_{\Omega} E_r(\boldsymbol{y}) \sum_{i=1}^{n} \int_{\Omega_i} K(\boldsymbol{y}-\boldsymbol{x}) \big(f(\boldsymbol{x}) - b(\boldsymbol{y}) c_i\big)^2 \, d\boldsymbol{x} \, d\boldsymbol{y} \right).$$

Numerical method: *a new alternating iterative scheme, called iterative convolution-thresholding (ICT) scheme.*



initial contour, segmented result, bias field b, and corrected image f / b

Sparse representation and dictionary learning

SR problem: *Given a signal vector* $\boldsymbol{x} \in \mathbb{R}^m$ *and a dictionary matrix* $\boldsymbol{D} \in \mathbb{R}^{m\times n}$, $n \gg m$, *we seek a coefficient vector* $\boldsymbol{z}^* \in \mathbb{R}^n$ *such that*

$$\boldsymbol{z}^* = \arg\min_{\boldsymbol{z}} \left(\frac{1}{2} \|\boldsymbol{x} - \boldsymbol{D}\boldsymbol{z}\|_2^2 + \lambda \|\boldsymbol{z}\|_1 \right), \qquad \lambda > 0.$$

SDL problem: *Let* $\{\boldsymbol{x}_i\}_{i=1}^N \subset \mathbb{R}^m$ *be a given dataset of signals. We seek a dictionary matrix* $\boldsymbol{D} = [\boldsymbol{d}_1, \boldsymbol{d}_2, \cdots, \boldsymbol{d}_n] \in \mathbb{R}^{m\times n}$ *together with the sparse coefficient vectors* $\{\boldsymbol{z}_i\}_{i=1}^N \subset \mathbb{R}^n$ *that solve the minimization problem:*

$$\min_{\boldsymbol{D},\{\boldsymbol{z}_i\}} \left(\frac{1}{2} \sum_{i=1}^N \|\boldsymbol{x}_i - \boldsymbol{D}\boldsymbol{z}_i\|_2^2 + \lambda \sum_{i=1}^N \|\boldsymbol{z}_i\|_1 \right)$$
$$\text{subject to } \|\boldsymbol{d}_k\|_2 \le 1,\ \forall\, 1 \le k \le n, \qquad \lambda > 0.$$

Numerical method: *alternating direction method of multipliers (ADMM).*

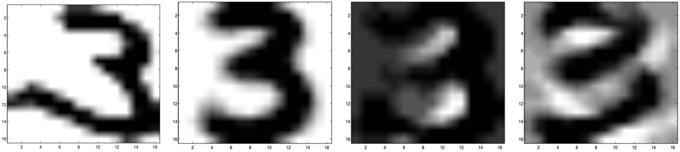
Application in single image inpainting

Single image inpainting: *we use the complete patches to train the dictionary, recover the incomplete patches by the sparse representation.*

Other applications: *single image super-resolution, image fusion, ...*

Data science: classification of handwritten digits

- The image of one digit is a 16×16 real matrix, representing gray scale. It can also be represented as a vector in $\mathbb{R}^{256}$, by stacking the columns of the matrix.
- A set of n digits (say, handwritten 3's) can then be represented by a matrix $\boldsymbol{A} \in \mathbb{R}^{256 \times n}$.
- *The columns of $\boldsymbol{A}$ span a subspace of $\mathbb{R}^{256}$. We can compute an approximate basis of this subspace using the SVD $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^\top$. Note that $\{\boldsymbol{u}_1, \boldsymbol{u}_2, \cdots, \boldsymbol{u}_{256}\}$ is a basis of $\mathbb{R}^{256}$.*



(left) digit 3 and (right) three basis vectors for 3's

Classification of handwritten digits (cont'd)

- Let $\boldsymbol{b}$ be a vector representing an unknown digit. We now want to classify the unknown digit as one of the digits 0–9.
- Given a set of approximate basis vectors for 3's, $\boldsymbol{u}_1, \boldsymbol{u}_2, \cdots, \boldsymbol{u}_k$, we can determine whether $\boldsymbol{b}$ is a 3 by checking if there is a linear combination of the basis vectors, $\sum_{j=1}^{k} x_j \boldsymbol{u}_j$, such that

$$\boldsymbol{b} - \sum_{j=1}^{k} x_j \boldsymbol{u}_j$$

is small in some measure.

- This classification of handwritten digits problem can be mathematically formulated as follows:

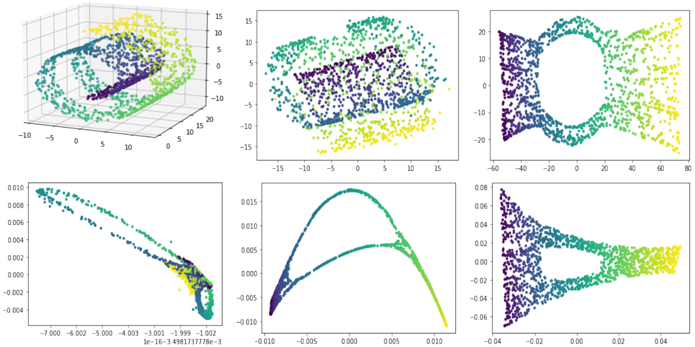
$$\min_{0 \le i \le 9} \left(\min_{x_j^{(i)}, j=1,2,\cdots,k} \|\boldsymbol{b} - \sum_{j=1}^{k} x_j^{(i)} \boldsymbol{u}_j^{(i)} \|_* \right), \quad \text{for some norm } \| \cdot \|_*.$$

Dimensionality reduction methods

- *Linear dimensionality reduction methods*
  - Principal component analysis (PCA)
  - Linear discriminant analysis (LDA)
  - Classical multidimensional scaling (MDS)
- *Non-linear dimensionality reduction methods (manifold learning)*
  - Isometric mapping (Isomap)
  - Diffusion maps
  - Laplacian eigenmap (LE)
  - Locally linearly embedding (LLE)

Swiss roll with a hole

Swiss roll with a hole: $n = 1500$, $m = 3$, and $d = 2$



Top row: Swiss roll with a hole, classical MDS, and Isomap
Bottom row: diffusion map, LE, and LLE

U-net for medical image segmentation

Let $\boldsymbol{v} \in \mathbb{R}_{+}^{m \times n}$ be a grayscale image of size $m \times n$ to be segmented. The CNN can be formulated as a parameterized nonlinear operator $\mathcal{N}_{\Theta}$ with parameter set Θ, expressed as $\boldsymbol{v}^{(K)} = \mathcal{N}_{\Theta}(\boldsymbol{v}) \in \mathbb{R}_{+}^{m \times n \times \ell}$, where ℓ denotes the number of classes:

$$\begin{cases} \boldsymbol{v}^{(0)} &= \boldsymbol{v}, \\ \widetilde{\boldsymbol{v}}^{(k)} &= \mathcal{T}_{\Theta^{(k-1)}}(\boldsymbol{v}^{(k-1)}), \\ \boldsymbol{v}^{(k)} &= \mathcal{A}^{(k)}(\widetilde{\boldsymbol{v}}^{(k)}), \qquad \text{for } k = 1 : K, \end{cases}$$

where $\mathcal{A}^{(k)}$ represents an activation function (e.g., sigmoid, ReLU, softmax), a sampling operation (e.g., downsampling, upsampling), or a composition of such operations, and the affine transformation is defined by

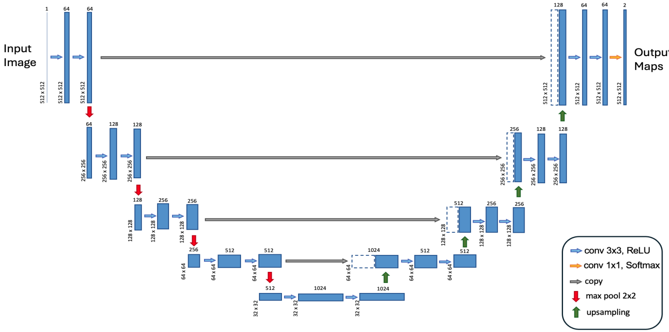
$$\mathcal{T}_{\Theta^{(k-1)}}(\boldsymbol{v}) = \boldsymbol{W}^{(k-1)} * \boldsymbol{v} + \boldsymbol{b}^{(k-1)}.$$

The complete set of network parameters is defined as $\Theta = \{\Theta^{(k)} = (\boldsymbol{W}^{(k)}, b^{(k)}) \mid k = 0 : K-1\}$.

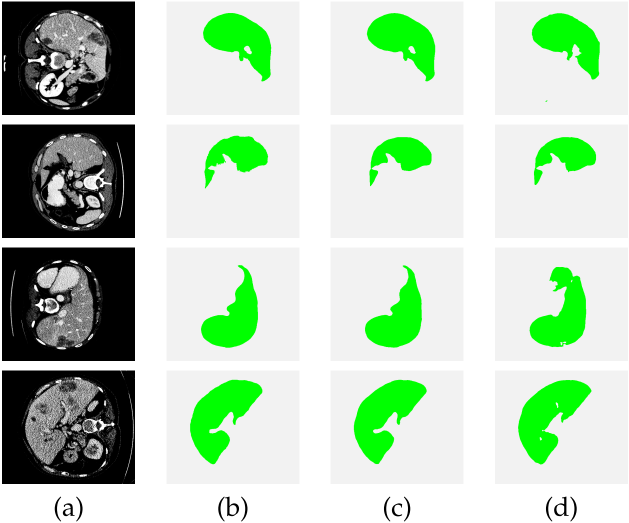
U-Net architecture for two-phase liver image segmentation

Given P grayscale training images $\boldsymbol{V} = [v_1, v_2, \cdots, v_P]$, $v_i \in \mathbb{R}_+^{m\times n}$, ground truth segmentations $\boldsymbol{U} = [\boldsymbol{U}_1, \boldsymbol{U}_2, \cdots, \boldsymbol{U}_P]$, $\boldsymbol{U}_i \in \{0,1\}^{m\times n\times \ell}$, the training objective is to learn a parameter set Θ^* that minimizes a specified loss function $\mathcal{L}(\mathcal{N}_\Theta(\boldsymbol{V}), \boldsymbol{U})$,

$$\Theta^* = \arg\min_{\Theta} \mathcal{L}(\mathcal{N}_\Theta(\boldsymbol{V}), \boldsymbol{U}).$$



Liver segmentation results



Representative liver segmentation results: (a) CT image; (b) Ground truth; (c) VR-U-Net; (d) U-Net