Chapter 3
Bilevel Optimization

Convex Optimization for Machine Learning & Computer Vision
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Outline

- Arise of hyperparameters in variational methods.
- Bilevel optimization.
- Implicit function from lower-level problem.
- Adjoint-based solver.

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Training regularization parameters for denoising

A denoising oracle $z \mapsto u$:

$$u \in \arg\min_{\widehat{u}\colon \Omega \to \mathbb{R}} \sum_{l=1}^{L} \alpha_l \|K_l \widehat{u}\|_1 + \frac{1}{2}\|\widehat{u} - z\|^2.$$

- $\{K_l\}$ are given analysis filters (typically overcomplete).
- The regularization weights $\{\alpha_l\}$ are hyperparameters.

Figure: BSDS500 dataset. Left: clean data $\{\bar{u}_i\}$; Right: noisy data $\{z_i\}$.

$$\min_{\{\alpha_l\}} \; J(\{u_i\}) = \frac{1}{N}\sum_{i=1}^{N} \|u_i - \bar{u}_i\|^2$$

$$\text{s.t.} \;\; u_i \in \arg\min_{\widehat{u}} \sum_{l=1}^{L} \alpha_l \|K_l \widehat{u}\|_1 + \frac{1}{2}\|\widehat{u} - z_i\|^2.$$

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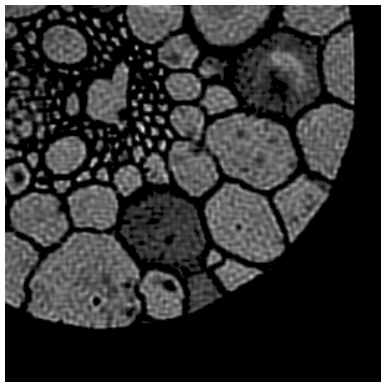
Calibrating blurring kernel

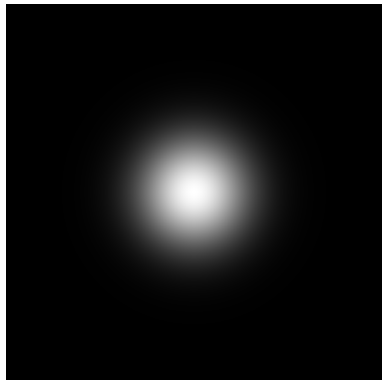
A deblurring oracle $z \mapsto u$:

$$u \in \arg\min_{\widehat{u}:\,\Omega\to\mathbb{R}} \alpha\|\nabla\widehat{u}\|_1 + \frac{1}{2}\|h \star \widehat{u} - z\|^2.$$

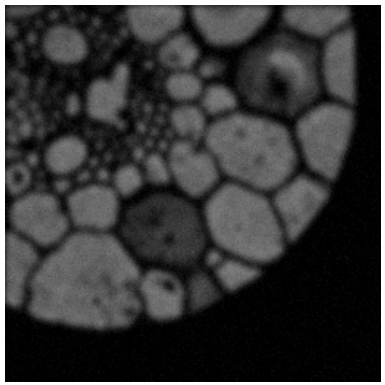
- For simplicity, α and ∇ are fixed.
- $\star$ denotes 2D convolution: $(h \star u)_{i,j} = \sum_{i',j'} h_{i-i',j-j'} u_{i',j'}$.
- The blurring kernel h is a hyperparameter.



clean image $\bar{u}_i$



blurring kernel h



blurred image z_i

$$\min_{\{\alpha_l\}} J(\{u_i\}, h) = \frac{1}{N}\sum_{i=1}^{N} \|u_i - \bar{u}_i\|^2 + R(h)$$

$$\text{s.t. } u_i \in \arg\min_{\widehat{u}} \alpha\|\nabla\widehat{u}\|_1 + \frac{1}{2}\|h \star \widehat{u} - z_i\|^2.$$

- The regularization term R enforces structures on h.

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Bilevel optimization

- A generic **bilevel optimization** model:

$$\min_{u,\,h} \; J(u,h)$$
$$\text{s.t.} \;\; u \in \arg\min_{\widehat{u}} H(\widehat{u},h).$$

  - The **lower-level** problem is an oracle / classifier / predictor (on u), which is dependent on hyperparameter h.
  - The **upper-level** problem is a supervisor, which trains the lower-level model (i.e. hyperparameter h).

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- Hyperparameter h may arise from:
  - Parameters / freedoms in the oracle (e.g. regularization weights).
  - Unknowns / uncertainties from modeling (e.g. blurring kernel).

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- An **implicit function approach**:
  - Ideally, lower-level problem $\Leftrightarrow$ **implicit function** $h \mapsto u$.
  - In this scenario, bilevel problem $\rightsquigarrow$ reduced problem:

$$\min_{h} J(u(h),h).$$

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Problem settings

$$\min_{u\in\mathbb{R}^n,\, h\in\mathbb{R}^m} \; J(u,h)$$
$$\text{s.t.} \;\; u \in \arg\min_{\widehat{u}} f(\widehat{u},h) + g(\widehat{u}),$$

- The upper-level objective $J : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$ is continuously differentiable.
- The lower-level objective is the sum of a differentiable $f : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$ and a non-differentiable function $g : \mathbb{R}^n \to \mathbb{R}$.
- Assume f and g are proper, convex, lsc in u for any $h \Rightarrow$

$$\boxed{\begin{aligned}\min_{u\in\mathbb{R}^n,\, h\in\mathbb{R}^m} \; & J(u,h)\\ \text{s.t.} \;\; & 0 \in F(u,h) + G(u)\end{aligned}}$$

  with $F(u,h) = \nabla_u f(u,h),\;\; G(u) = \partial g(u)$.
- Further assume $F(\cdot,h)$ is μ-strongly monotone for any $h \in \mathbb{R}^m$, i.e.

$$\langle u - v, F(u,h) - F(v,h)\rangle \geq \mu\|u-v\|^2, \;\; \forall u, v \in \mathbb{R}^n.$$

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Implicit function

Theorem (implicit function under strong monotonicity)

There exists a (single-valued) Lipschitz continuous implicit function $h \mapsto u$ s.t. (u, h) satisfies $0 \in F(u, h) + G(u)$.

Proof: on board.

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Proof: on board.

Remarks

Implicit function can be obtained without assuming strong monotonicity of $F(\cdot, h)$.

Theorem (generalized implicit function theorem)

Let (u_0, h_0) be a point that satisfies $0 \in F(u, h) + G(u)$, where F is continuously differentiable and G is a *closed* set-valued map. Assume $\exists$ neighborhoods $U_\xi \ni 0,\ U_u \ni u_0$ s.t.

$$\xi \in U_\xi \mapsto \left\{u : \xi \in F(u_0, h_0) + \nabla_u F(u_0, h_0)^\top (u - u_0) + G(u)\right\} \cap U_u$$

is a Lipschitz function. Then $\exists$ nighborhoods $V_h \ni h_0,\ V_u \ni u_0$ s.t. $h \in V_h \mapsto u \in V_u$ with $0 \in F(u, h) + G(u)$ is a Lipschitz implicit function.

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Sensitivity analysis

- How to perform gradient descent on bilevel optimization?
- Solve the **linearized bilevel problem** for $(\delta u, \delta h)$:

$$\begin{aligned} \min_{\delta u,\, \delta h} \quad & \nabla_u J(u,h)^\top \delta u + \nabla_h J(u,h)^\top \delta h \\ \text{s.t.} \quad & (\delta u, -\nabla_u F(u,h)^\top \delta u - \nabla_h F(u,h)^\top \delta h) \in T_{\text{gph}\, G}(u, -F(u,h)). \end{aligned}$$

- The constraint on $(\delta u, \delta h)$ is called the **sensitivity equation**, which is motivated by the characterization:

$$0 \in F(u,h) + G(u) \quad \Leftrightarrow \quad (u, -F(u,h)) \in \text{gph}\, G.$$

- gph G is the **graph** of G, i.e.

$$\text{gph}\, G = \{(u,v) \in \mathbb{R}^n \times \mathbb{R}^n : v \in G(u)\}.$$

- $T_C(\theta)$ is the **tangent cone** of a closed set C at $\theta \in C$, i.e.

$$T_C(\theta) = \left\{ \eta : \exists \{t^k\} \subset \mathbb{R}_+,\ \{\theta^k\} \subset C \ \text{ s.t. } t^k \to 0^+,\ \frac{\theta^k - \theta}{t^k} \to \eta \right\}.$$

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- Case study: $G(\cdot) = \partial \|\cdot\|_1$ and $F(u,h) = (u-h)/\alpha$.

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Adjoint-based solver

- Further assume G is (single-valued) differentiable function.
- The linearized bilevel problem reduces to:

$$\begin{aligned} \min_{\delta u,\, \delta h} \quad & \nabla_u J(u,h)^\top \delta u + \nabla_h J(u,h)^\top \delta h \\ \text{s.t.} \quad & 0 = \nabla_u F(u,h)^\top \delta u + \nabla_h F(u,h)^\top \delta h + \nabla G(u)^\top \delta u. \end{aligned}$$

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- Hence, its solution provides a gradient descent direction:

$$\delta h = -\nabla_h J(u,h) + \nabla_h F(u,h)[\nabla_u F(u,h) + \nabla G(u)]^{-1} \nabla_u J(u,h).$$

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- Let $\frac{\partial u}{\partial h}$ be the Jacobian of the implicit function $h \mapsto u$. Then

$$-[\nabla_u F(u,h) + \nabla G(u)]^{-1} = \left(\frac{\partial u}{\partial h}\right)^\top.$$

For this reason, $-[\nabla_u F(u,h) + \nabla G(u)]^{-1} \nabla_u J(u,h)$ is called the **adjoint state**.

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- Hence, its solution provides a gradient descent direction:

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- To complete one iteration, $h \leftarrow h + \tau \delta h$ for properly chosen step size τ; update u by solving the lower-level problem.

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