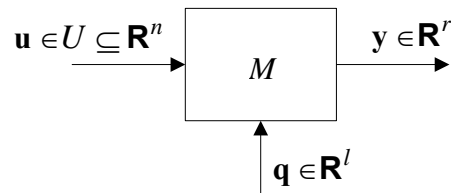


Optimization

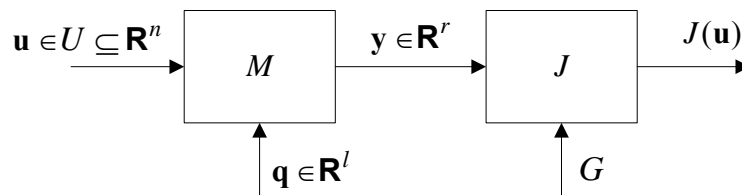
- We study parameter optimization algorithms.

(1) Generic problem definition

- Basic ingredients: M, U, G



- Model (M): (parameterized) mathematical representation of "plant"
- $y = M(\mathbf{u})$ (deterministic optimization) or $y = M(\mathbf{u}, \mathbf{q})$ (stochastic optimization with \mathbf{q} random vector)
- Admissible decisions (U): admissible range of values of parameters



- Goal (G): a performance index or objective (function) expressed as a function of $\mathbf{u} \in U \subseteq \mathbf{R}^n$
- Performance index, $J : \mathbf{R}^n \rightarrow \mathbf{R}$ or $J : U \rightarrow \mathbf{R}$
- Generic optimization problem is

$$\min_{\mathbf{u} \in U} J(\mathbf{u}).$$

(1) An element $\mathbf{u}^* \in U$ which achieves the min above is optimal and $J^* = J(\mathbf{u}^*)$ is the optimal or minimal value. We say $\mathbf{u}^* \in \arg \min_{\mathbf{u} \in U} J(\mathbf{u})$.

(2) $\mathbf{u}^* \in U$ is not necessarily unique.

(3) $\mathbf{u}^* \in U$ may not exist. If we are not sure about its existence, we write

$$J^* = \inf_{\mathbf{u} \in U} J(\mathbf{u}) \text{ or } J^* = \sup_{\mathbf{u} \in U} J(\mathbf{u}).$$

(4) $\min_{\mathbf{u} \in U} J(\mathbf{u}) = -\max_{\mathbf{u} \in U} \{-J(\mathbf{u})\}$ and $\max_{\mathbf{u} \in U} J(\mathbf{u}) = -\min_{\mathbf{u} \in U} \{-J(\mathbf{u})\}$.

(2) Existence of optimal elements

- (Compactness theorem) Suppose $U \subseteq \mathbf{R}^n$ is nonempty and compact and $J:U \rightarrow \mathbf{R}$ is continuous. Then an optimal element $\mathbf{u}^* \in U$ exists, i.e., $J^* = J(\mathbf{u}^*) = \min_{\mathbf{u} \in U} J(\mathbf{u})$.
- Without compactness we need coercivity or convexity for existence of the optimal elements.
- Suppose a function $J:\mathbf{R}^n \rightarrow \mathbf{R}$ is continuous. J is coercive if $\lim_{\|\mathbf{u}\| \rightarrow \infty} J(\mathbf{u}) \rightarrow +\infty$, i.e., J blows up uniformly in every direction.
- (Coercivity theorem) Suppose $U \subseteq \mathbf{R}^n$ is nonempty and closed and $J:U \rightarrow \mathbf{R}$ is continuous and coercive. Then an optimal element $\mathbf{u}^* \in U$ exists, i.e., $J^* = J(\mathbf{u}^*) = \min_{\mathbf{u} \in U} J(\mathbf{u})$.

(3) Uniqueness of the optimum

- (Convex set) A set $U \subseteq \mathbf{R}^n$ is convex if $\forall \mathbf{u}, \mathbf{v} \in U$ and $\forall \lambda \in [0, 1]$, $(1-\lambda)\mathbf{u} + \lambda\mathbf{v} \in U$.
- (Convex function) A function $J:\mathbf{R}^n \rightarrow \mathbf{R}$ is (strictly, with $<$) convex if $\forall \mathbf{u}, \mathbf{v} \in U$ and $\forall \lambda \in [0, 1]$, $J[(1-\lambda)\mathbf{u} + \lambda\mathbf{v}] \leq (1-\lambda)J(\mathbf{u}) + \lambda J(\mathbf{v})$.
- J is concave if $-J$ is convex.
- (Hessian lemma) Suppose J is continuously differentiable on an open convex set U . Then, $J(\mathbf{u})$ is convex iff the Hessian matrix $\nabla^2 J(\mathbf{u})$ is positive semidefinite at each point $\mathbf{u} \in U$ where

$$\nabla^2 J(\mathbf{u}) := \begin{bmatrix} \frac{\partial^2 J}{\partial u_1^2} & \frac{\partial^2 J}{\partial u_1 \partial u_2} & \cdots & \frac{\partial^2 J}{\partial u_1 \partial u_n} \\ \frac{\partial^2 J}{\partial u_2 \partial u_1} & \frac{\partial^2 J}{\partial u_2^2} & \cdots & \frac{\partial^2 J}{\partial u_2 \partial u_n} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial^2 J}{\partial u_n \partial u_1} & \frac{\partial^2 J}{\partial u_n \partial u_2} & \cdots & \frac{\partial^2 J}{\partial u_n^2} \end{bmatrix}.$$

- If J is convex, the optimum is unique.

(4) Local minimum

- Suppose $U \subseteq \mathbf{R}^n$ is open and $J:U \rightarrow \mathbf{R}$. A point $\mathbf{u}^* \in U$ is a strong local minimum of J over U if $J(\mathbf{u}) > J(\mathbf{u}^*)$ for all $\mathbf{u} \in U$ in some (open) neighbor of \mathbf{u}^* .
- A weak local minimum is defined with \geq .
- (Theorem) Suppose $U \subseteq \mathbf{R}^n$ is open and $J:U \rightarrow \mathbf{R}$ and $\mathbf{u}^* \in U$. \mathbf{u}^* is a strong local minimum if $\nabla J(\mathbf{u}^*) = 0$ and $\nabla^2 J(\mathbf{u}^*) > 0$ (positive definite), where the gradient

$$\nabla J(\mathbf{u}^*) = \left[\frac{\partial J}{\partial u_1} \quad \frac{\partial J}{\partial u_2} \quad \dots \quad \frac{\partial J}{\partial u_n} \right]^T.$$

(5) Steepest descent algorithm

- Let $J:\mathbf{R}^n \rightarrow \mathbf{R}$ is differentiable and $\mathbf{v} \in \mathbf{R}^n$ is given with $\mathbf{v} \neq \mathbf{0}$. The directional derivative at a given point $\bar{\mathbf{u}} \in \mathbf{R}^n$ in the direction of \mathbf{v} is

$$\left. \frac{dJ}{d\mathbf{v}} \right|_{\bar{\mathbf{u}}} = [\nabla J(\bar{\mathbf{u}})]^T \hat{\mathbf{v}} \quad \text{where} \quad \hat{\mathbf{v}} = \frac{\mathbf{v}}{\|\mathbf{v}\|}.$$

- Note that J is decreasing in the negative gradient direction since with $\mathbf{v} = -\nabla J(\mathbf{u})$,

$$\left. \frac{dJ}{d\mathbf{v}} \right|_{\bar{\mathbf{u}}} = -[\nabla J(\bar{\mathbf{u}})]^T \frac{\nabla J(\bar{\mathbf{u}})}{\|\nabla J(\bar{\mathbf{u}})\|} = -\|\nabla J(\bar{\mathbf{u}})\| \leq 0.$$

- $\mathbf{v} = -\frac{\nabla J(\mathbf{u})}{\|\nabla J(\mathbf{u})\|}$ is the direction of maximal decrease.

- (Steepest descent algorithm)

(1) Initial guess, \mathbf{u}^0 .

(2) Iterate with $\mathbf{u}^{k+1} = \mathbf{u}^k - h \frac{\nabla J(\mathbf{u}^k)}{\|\nabla J(\mathbf{u}^k)\|}$ for $k = 1, 2, \dots$ with $h > 0$ being the algorithm

step size.

(3) Stopping criterions may include

smallness of $|J(\mathbf{u}^{k+1}) - J(\mathbf{u}^k)|$,

smallness of $\|\mathbf{u}^{k+1} - \mathbf{u}^k\|$,

smallness of $\|\nabla J(\mathbf{u}^k)\|$,

condition on $\nabla^2 J(\mathbf{u}^k)$,

some criteria for N consecutive times,

and combinations of above.

- Step size
 - (1) Fixed step size
 - (2) Dynamic step size by line search (uniform search, sequential search, dichotomous search, golden section method, Fibonacci search)
- Criticism of steepest descent algorithm
 - (1) Myopic
 - (2) Possible oscillation
 - (3) May require multiple restarts to avoid a local minimum
 - (4) Slow convergence
- Good performance when \mathbf{u}^0 is far away from the optimum.

(6) Generalized Newton-Raphson

- Pretend J is quadratic near \mathbf{u}^k and $\mathbf{u}^{k+1} = \mathbf{u}^k + \Delta\mathbf{u}$. Then,

$$J(\mathbf{u}^k + \Delta\mathbf{u}) = J(\mathbf{u}^k) + [\nabla J(\mathbf{u}^k)]^T \Delta\mathbf{u} + \frac{1}{2}(\Delta\mathbf{u})^T \nabla^2 J(\mathbf{u}^k) \Delta\mathbf{u} + \text{h.o.t.}$$

where h.o.t. is 0 from the quadratic assumption. Now we optimize w.r.t. $\Delta\mathbf{u}$, i.e., let

$$\frac{\partial J(\mathbf{u}^k + \Delta\mathbf{u})}{\partial \Delta\mathbf{u}} = \nabla J(\mathbf{u}^k) + \nabla^2 J(\mathbf{u}^k) \Delta\mathbf{u} = 0$$

and

$$\Delta\mathbf{u} = -[\nabla^2 J(\mathbf{u}^k)]^{-1} \nabla J(\mathbf{u}^k).$$

- (*Generalized Newton algorithm*)

- (1) Initial guess, \mathbf{u}^0 .
- (2) Iterate with $\mathbf{u}^{k+1} = \mathbf{u}^k - [\nabla^2 J(\mathbf{u}^k)]^{-1} \nabla J(\mathbf{u}^k)$ for $k = 1, 2, \dots$
- (3) Check the conditioning of the matrix $[\nabla^2 J(\mathbf{u}^k)]^{-1}$.
- (4) Stopping criterions

- Good performance near the optimum but computationally expensive

(7) Gauss-Newton algorithm

- Computation of Hessian is often too expensive or impossible.
- Approximate Hessian as $[\nabla^2 J(\mathbf{u}^k)] \approx [\nabla J(\mathbf{u}^k)]^T \nabla J(\mathbf{u}^k)$.
- In order to handle the ill-conditioning problem of $[\nabla J(\mathbf{u}^k)]^T \nabla J(\mathbf{u}^k)$, use *Levenberg-*

Marquardt method where $[\nabla^2 J(\mathbf{u}^k)] \approx \left\{ [\nabla J(\mathbf{u}^k)]^T \nabla J(\mathbf{u}^k) + \delta \mathbf{I} \right\} = \tilde{\mathbf{H}}$ for some positive constant δ .

- (Gauss-Newton algorithm)

(1) Initial guess, \mathbf{u}^0 .

(2) Iterate with $\mathbf{u}^{k+1} = \mathbf{u}^k - \tilde{\mathbf{H}}^{-1} \nabla J(\mathbf{u}^k)$ for $k = 1, 2, \dots$

(3) Check the conditioning of the matrix $\left\{ [\nabla J(\mathbf{u}^k)]^T \nabla J(\mathbf{u}^k) \right\}^{-1}$ and adjust δ if necessary.

(4) Stopping criterions

(8) Conjugate direction (gradient) algorithm

- Let \mathbf{A} be an $n \times n$ positive definite symmetric matrix. A pair of nonzero vectors $\mathbf{x}, \mathbf{y} \in \mathbf{R}^n$ are mutually conjugate w.r.t. \mathbf{A} if $\mathbf{x}^T \mathbf{A} \mathbf{y} = 0$.

- Orthogonality is a special case with $\mathbf{A} = \mathbf{I}$.

- Eigenvectors of \mathbf{A} are mutually conjugate.

- If $\{\mathbf{v}^k\}_{k=0}^{n-1}$ are mutually conjugate, then they are linearly independent.

- Conjugate direction was found to be better than the steepest direction in many cases. There are many possible conjugate directions.

- (Conjugate direction algorithm in general)

(1) Initial guess, \mathbf{u}^0 .

(2) Iterate with $\mathbf{u}^{k+1} = \mathbf{u}^k + h_k \frac{\mathbf{v}^k}{\|\mathbf{v}^k\|}$ for $k = 1, 2, \dots$ with $h_k > 0$ being the algorithm

step size.

(3) Stopping criterions

- (Conjugate direction algorithm - Fletcher Reeves)

(1) Initial guess, \mathbf{u}^0 and $\mathbf{v}^0 = -\nabla J(\mathbf{u}^0)$.

(2) Iterate with $\mathbf{u}^{k+1} = \mathbf{u}^k + h_k \frac{\mathbf{v}^k}{\|\mathbf{v}^k\|}$ for $k = 1, 2, \dots$ with $h_k > 0$ being the algorithm

step size. Compute $\mathbf{v}^{k+1} = -\nabla J(\mathbf{u}^{k+1}) + \frac{\|\nabla J(\mathbf{u}^{k+1})\|^2}{\|\nabla J(\mathbf{u}^k)\|^2} \mathbf{v}^k$.

(3) Stopping criterions

- In conjugate direction algorithm, we have the following condition.

$$\mathbf{v}^k \perp \nabla J(\mathbf{u}^{k+1}) \quad \text{or} \quad (\mathbf{v}^k)^T \nabla J \left(\mathbf{u}^k + h_k \frac{\mathbf{v}^k}{\|\mathbf{v}^k\|} \right) = 0.$$