STAT 207: Optimization

Optimization considers the problem

$$\begin{aligned} \text{minimize } & f(x) \\ \text{subject to constraints on } & x \end{aligned}$$

- Maximization or minimization
- Exact or iterative solutions

Why is optimization important in statistics?

- Parameter Estimation:
  - Maximum likelihood estimation (MLE).
  - Maximum a posteriori (MAP) estimation in Bayesian framework.
- Model Selection:
  - AIC/BIC;
  - LASSO, penalized regression.
- Machine learning:
  - Training neural networks involves minimizing a loss function + certain regularizations.

Commonly used optimization methods:

- Newton type algorithms
- Quasi-Newton algorithm
- Expectation-maximization (EM) algorithm
- Majorization-minimization (MM) algorithm
- Gradient Descent

Basic results

Suppose $f(x)$ is differentiable on the open set U:

- differential $df(x)$

- gradient $\nabla f(x)$

- second differential (Hessian) $d^2 f(x) = \nabla^2 f(x)$

(Fermat) Suppose a differentiable function $f(x)$ has a local minimum at the point y of the open set U. Then $\nabla f(x)$ vanishes at y.

- Stationary point y: $\nabla f(y) = 0$

NAS Proposition 11.2.3 Suppose a twice continuously differentiable function $f(x)$ has a local minimum at the point y of the open set U. Then $d^2 f(x)$ is positive semidefinite at y. Conversely, if y is a stationary point and $d^2 f(y)$ is positive definite, then y is a local minimum.

- A function f is coercive if $\lim_{\|x\|_2 \to \infty} f(x) = \infty$.

Example: $f(x) = \frac{1}{2} x^T A x + b^T x + c$, where A is positive definite.

Example Show that the sample mean and sample variance are the MLE of the theoretical mean and variance of a random sample $y_1, y_2, .., y_n$ from a multivariate normal distribution.

Convexity

A function $f : R^n \to R$ is **convex** if

- $\text{dom} f$ is a convex set: $\alpha x + (1 - \alpha) y \in \text{dom} f$ for all $x, y \in \text{dom} f$ and any $\alpha \in (0, 1)$, and

- $f(\alpha x + (1 - \alpha) y) \leq \alpha f(x) + (1 - \alpha) f(y)$ for all $x, y \in \text{dom} f$ and any $\alpha \in (0, 1)$.

f is **strictly convex** if the inequality is strict for all $x \neq y$ and α.

Supporting hyperplane inequality A differentiable function f is convex if and only if

$$f(y) \geq f(x) + df(x)(y - x)$$

for all $x, y \in \mathrm{dom} f$.

Second-order condition for convexity A twice differentiable function f is convex if and only if $\nabla^2 f(x)$ is PSD for all $x \in \mathrm{dom} f$. It is strictly convex if and only if $\nabla^2 f(x)$ is PD for all $x \in \mathrm{dom} f$.

Convexity and global optima

Suppose f is a convex function.

- Any stationary point y, i.e., $\nabla f(y) = 0$, is a global minimum. (Proof: By supporting hyperplane inequality, $f(x) \geq f(y) + \nabla f(y)^\top (x - y) = f(y)$ for all $x \in \mathrm{dom}\, f$.)
- Any local minimum is a global minimum.
- The set of (global) minima is convex.
- If f is strictly convex, then the global minimum, if exists, is unique.

Example: Least squares estimate. $f(\beta) = \frac{1}{2} \|y - X\beta\|_2^2$ has Hessian $\nabla^2 f = X^\top X$ which is positive semidefinite. So f is convex and any stationary point (solution to the normal equation) is a global minimum. When X is rank deficient, the set of solutions is convex.

Jensen's inequality

If h is convex and W a random vector taking values in $\mathrm{dom} f$, then

$$\mathbb{E}[h(\mathbf{W})] \geq h[\mathbb{E}(\mathbf{W})],$$

provided both expectations exist. For a strictly convex h, equality holds if and only if $W = \mathbf{E}(W)$ almost surely.

Proof: Take $x = W$ and $\mathbf{y} = \mathbf{E}(\mathbf{W})$ in the supporting hyperplane inequality.

Information inequality

Let f and g be two densities with respect to a common measure μ and $f, g > 0$ almost everywhere relative to μ. Then

$$\mathbb{E}_f[\log(f)] \geq \mathbb{E}_f[\log(g)],$$

with equality if and only if f=g almost everywhere on μ.

Proof: Apply Jensen's inequality to the convex function $-\ln(t)$ and random variable W=$g(X)/f(X)$ where X~f.

Important applications of information inequality: M-estimation, EM algorithm.

\vspace{50mm}

Optimization with Equality Constraints

- Suppose the objective function $f(x)$ to be minimized is continuously differentiable and defined on R^n.

- The gradient direction $\nabla f(x) = df(x)^T$ is the direction of steepest ascent of $f(x)$ near the point x.

- The following linear approximation is often used

  $$f(x+su) = f(x) + sdf(x)u + o(s),$$

  for a unit vector u and a scalar s.

Lagrange multipliers

The Lagrangian function

$$\mathcal{L}(x,w) = f(x) + \sum_{i=1}^{m} w_i g_i(x),$$

where $f(x)$ is the objective function to minimize, $g_i(x) = 0$ are equality constraints.

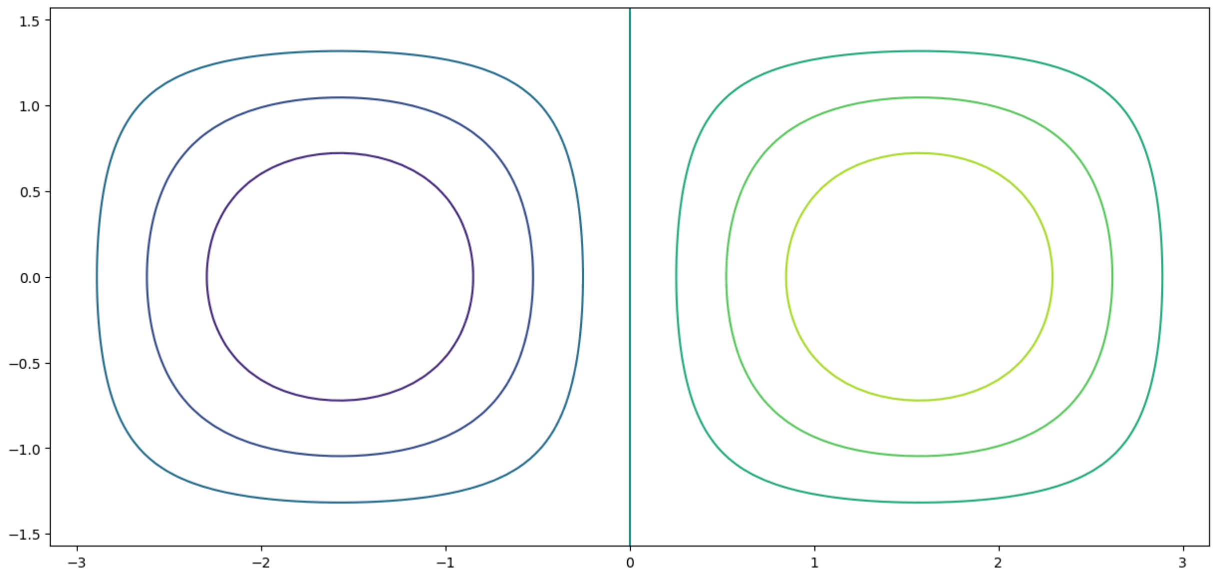
Gradient

\begin{center}
\includegraphics[width=0.9\textwidth]{gradient.png}
\end{center}

In [3]:

```
import numpy as np
import matplotlib.pyplot as plt

# Define the function
def f(x, y):
    return np.sin(x) * np.cos(y)

# Define the range of x and y
x = np.linspace(-np.pi, np.pi, 100)
y = np.linspace(-np.pi/2, np.pi/2, 100)

# Create a grid of (x, y) coordinates
X, Y = np.meshgrid(x, y)

# Compute the function values at the grid points
Z = f(X, Y)
```

```python
# Set up the plot
fig, ax = plt.subplots(figsize=(15, 7))

# Plot the level curves
ax.contour(X, Y, Z)

# Show the plot
plt.show()
```



Proposition 11.3.1 (Lagrange) Suppose the continuously differentiable function $f(x)$ has a local minimum at the feasible point y and that the constraint functions $g_1(x), \ldots, g_m(x)$ are continuously differentiable with linearly independent gradient vectors $\nabla g_i(y)$ at y. Then

- there exists a multiplier vector λ such that (y, λ) is a stationary point of the Lagrangian.

Furthermore, if $f(x)$ and all $g_i(x)$ are twice continuously differentiable, then

- $v^T \nabla^2 L(y) v \geq 0$ for every tangent vector v at y.

Conversely, if (y, λ) is a stationary point of the Lagrangian and $v^T \nabla^2 L(y) v > 0$ for every nontrivial tangent vector v at y, then

- y represents a local minimum of $f(x)$ subject to the constraints.

Example Quadratic Programming with Equality Constraints

Minimizing a quadratic function

$$q(x) = \frac{1}{2} x^T A x + b^T x + c$$

on $\mathbb{R}^n$ subject to the m linear equality constraints

$$v_i^T x = d_i, \quad i = 1, .., m$$

is one of the most important problems in nonlinear programming.

To minimize $q(x)$ subject to the constraints, we introduce the Lagrangian

$$L(x, \lambda) = \frac{1}{2} x^T A x + b^T x + c + \sum_{i=1}^{m} \lambda_i (v_i^T x - d_i) = \frac{1}{2} x^T A x + b^T x + c + \lambda^T (V x - d)$$

A stationary point of $L(x, \lambda)$ is determined by the equations

$$\begin{gathered} Ax + b + V^T \lambda = 0, \\ Vx = d, \end{gathered}$$

whose formal solution amounts to

$$\begin{pmatrix} x \\ \lambda \end{pmatrix} = \begin{pmatrix} A & V^T \\ V & 0 \end{pmatrix}^{-1} \begin{pmatrix} -b \\ d \end{pmatrix}.$$

The inverse exists thanks to the following proposition.

Proposition 11.3.2 Let A be an $n \times n$ positive definite matrix and V be an $m \times n$ matrix. Then the matrix

$$M = \begin{bmatrix} A & V^\top \\ V & 0 \end{bmatrix}$$

has inverse

$$M^{-1} = \begin{bmatrix} A^{-1} - A^{-1} V^\top (V A^{-1} V^\top)^{-1} V A^{-1} & -(V A^{-1} V^\top)^{-1} V A^{-1} \\ -A^{-1} V^\top (V A^{-1} V^\top)^{-1} & (V A^{-1} V^\top)^{-1} \end{bmatrix}$$

if and only if V has linearly independent rows $v_{t_1}, \ldots, v_{t_m}$.

Additional **Example 11.3.4**

Optimization with Inequality Constraints

Minimize an objective function $f_0(x)$ subject to the mixed constraints

$$\begin{gathered} h_i(x) = 0, \quad 1 \leq i \leq p \\ f_j(x) \leq 0, \quad 1 \leq j \leq m. \end{gathered}$$

A constraint $f_j(x)$ is

- active at the feasible point x provided $f_j(x) = 0$;
- it is inactive if $f_j(x) < 0$.

To avoid redundant constraints, we need

- linear independence of the gradients of the equality constraints,
- and a restriction on the active inequality constraints.

Duality

- The Lagrangian is

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) = f_0(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i f_i(\mathbf{x}) + \sum_{i=1}^{p} \nu_i h_i(\mathbf{x}).$$

The vectors $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_m)^\top$ and $\boldsymbol{\nu} = (\nu_1, \ldots, \nu_p)^\top$ are called the Lagrange multiplier vectors or dual variables.

- The **Lagrange dual function** is the minimum value of the Lagrangian over $\mathbf{x}$:

$$g(\boldsymbol{\lambda}, \boldsymbol{\nu}) = \inf_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) = \inf_{\mathbf{x}} \left(f_0(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i f_i(\mathbf{x}) + \sum_{i=1}^{p} \nu_i h_i(\mathbf{x}) \right).$$

- Denote the optimal value of the original problem by p^*. For any $\boldsymbol{\lambda} \succeq 0$ and any $\boldsymbol{\nu}$, we have

$$g(\boldsymbol{\lambda}, \boldsymbol{\nu}) \leq p^*.$$

Proof: For any feasible point $\widetilde{\mathbf{x}}$,

$$\mathcal{L}(\widetilde{\mathbf{x}}, \boldsymbol{\lambda}, \boldsymbol{\nu}) = f_0(\widetilde{\mathbf{x}}) + \sum_{i=1}^{m} \lambda_i f_i(\widetilde{\mathbf{x}}) + \sum_{i=1}^{p} \nu_i h_i(\widetilde{\mathbf{x}}) \leq f_0(\widetilde{\mathbf{x}})$$

because the second term is non-positive and the third term is zero. Then,

$$g(\boldsymbol{\lambda}, \boldsymbol{\nu}) = \inf_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\nu}) \leq \mathcal{L}(\widetilde{\mathbf{x}}, \boldsymbol{\lambda}, \boldsymbol{\nu}) \leq f_0(\widetilde{\mathbf{x}}).$$

- Since each pair (λ, ν) with $\lambda \succeq 0$ gives a lower bound to the optimal value p^*, it is natural to ask for the best possible lower bound the Lagrange dual function can provide. This leads to the **Lagrange dual problem**

$$\max_{\lambda \succeq 0} g(\lambda, \nu),$$

  which is a convex problem regardless of whether the primal problem is convex or not.

- We denote the optimal value of the Lagrange dual problem by d^*, which satisfies the weak duality

$$d^* \le p^*.$$

The difference $p^* - d^*$ is called the optimal duality gap.

- If the primal problem is convex, that is

$$\begin{aligned} \min_{\mathbf{x}} \quad & f_0(\mathbf{x}) \\ \text{subject to} \quad & f_i(\mathbf{x}) \le 0, \quad i = 1, \ldots, m, \\ & \mathbf{A}\mathbf{x} = \mathbf{b}, \end{aligned}$$

with $f_0, \ldots, f_m$ convex, we usually (but not always) have strong duality, i.e., $d^* = p^*$.

- The conditions under which strong duality holds are called constraint qualifications. A commonly used one is Slater's condition: There exists a point in the relative interior of the domain such that

$$\begin{aligned} f_i(\mathbf{x}) < 0, \quad i = 1, \ldots, m, \\ \mathbf{A}\mathbf{x} = \mathbf{b}. \end{aligned}$$

Such a point is also called **strictly feasible**.

KKT (Karush, Kuhn, and Tucker) Conditions

- "One of the great triumphs of 20th century applied mathematics."
- Original paper: Nonlinear Programming by Kuhn and Tucker 1951

Nonconvex problems

- Assume $f_0, \ldots, f_m, h_1, \ldots, h_p$ are differentiable. Let $\mathbf{x}^*$ and $(\boldsymbol{\lambda}^*, \boldsymbol{\nu}^*)$ be any primal and dual optimal points with zero duality gap, i.e., strong duality holds.
- Since $\mathbf{x}^*$ minimizes $L(\mathbf{x}, \boldsymbol{\lambda}^*, \boldsymbol{\nu}^*)$ over $\mathbf{x}$, its gradient vanishes at $\mathbf{x}^*$, we have the Karush-Kuhn-Tucker (KKT) conditions:
  - Stationarity

$$\nabla f_0(\mathbf{x}^*) + \sum_{i=1}^m \boldsymbol{\lambda}_i^* \nabla f_i(\mathbf{x}^*) + \sum_{i=1}^p \boldsymbol{\nu}_i^* \nabla h_i(\mathbf{x}^*) = \mathbf{0}.$$

  - Primal feasibility

$$\begin{aligned} f_i(\mathbf{x}^*) \le 0, \quad i = 1, \ldots, m \\ h_i(\mathbf{x}^*) = 0, \quad i = 1, \ldots, p \end{aligned}$$

  - Dual feasibility

$$\boldsymbol{\lambda}^* \geq \mathbf{0},$$

- Complementary slackness

$$\boldsymbol{\lambda}^* \cdot \mathbf{f}(\mathbf{x}^*) = 0$$

- The fourth condition (complementary slackness) follows from:

$$f_0(\mathbf{x}^*) = \inf_{\mathbf{x}}\{f_0(\mathbf{x}) + \sum_{i=1}^{m} \boldsymbol{\lambda}_i^* f_i(\mathbf{x}) + \sum_{i=1}^{p} \boldsymbol{\nu}_i^* h_i(\mathbf{x})\}$$

Since $\sum_{i=1}^{m} \boldsymbol{\lambda}_i^* f_i(\mathbf{x}^*) = 0$ and each term is non-positive, we have $\boldsymbol{\lambda}_i^* f_i(\mathbf{x}^*) = 0$, $i = 1, \ldots, m$.

- To summarize, for any optimization problem with differentiable objective and constraint functions for which strong duality obtains, any pair of primal and dual optimal points must satisfy the KKT conditions.

Convex problems

- When the primal problem is convex, the KKT conditions are also sufficient for the points to be primal and dual optimal.
- If f_i are convex and h_i are affine, and $(\tilde{x}, \tilde{\lambda}, \tilde{\nu})$ satisfy the KKT conditions, then $\tilde{x}$ and $(\tilde{\lambda}, \tilde{\nu})$ are primal and dual optimal, with zero duality gap.
- The KKT conditions play an important role in optimization. Many algorithms for convex optimization are conceived as, or can be interpreted as, methods for solving the KKT conditions.

Python Implementations

- scipy.optimize
- Duke lectures

In [ ]: