Data Science For Engineers
NPTEL PMRF Live Sessions

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Three Pillars of Data Science

1. **Linear Algebra**
2. **Statistics**
3. **Optimization**

Components of an Optimization Problem

- **Objective function** $f(x)$: to minimize or maximize
- **Decision variables** x: what we can control
- **Constraints**: restrictions on the variables

$$\text{minimize } f(x) \quad \text{subject to } g(x) \leq 0,\ h(x) = 0$$

Univariate Optimization

Univariate optimization treats functions of a single variable.

- **Local minimum:** lowest in a neighborhood
- **Global minimum:** lowest over entire domain
- **Convex functions:**
- **Non-convex functions:**

Finding a Minimum

- $f(x) = x^2 - 2x + 3$
- $f(x) = x^3 - 3x^2 + 6x + 1.$

First-Order Necessary Condition: $f'(x^*) = 0.$

Second-Order Sufficient Condition: $f''(x^*) > 0.$

Example

Find minima of $f(x) = 3x^3 - 4x^2 - 12x + 3$

Multivariate Optimization

Extension to Multiple Variables

- Contour plots: constant function value curves
- Iterative methods choose a direction and a step size
- Steepest descent direction: direction of maximum decrease

$$x^{k+1} = x^k + \alpha^k s^k$$

contour plots

For $f(x_1, x_2) = x_1^2 + x_2^2$: What will be the contour plot?

Gradient and Hessian Matrix

Gradient: $\nabla f = [\partial f/\partial x_1, ..., \partial f/\partial x_n]^T$.

Hessian: $H = [\partial^2 f/\partial x_i \partial x_j]$

Positive definite matrix

How do we know if the Hessian matrix is positive definite?

Practice question

For $f(x_1, x_2) = 3x_1^2 + 2x_1x_2 + 4.8x_2^2 - 5.4x_1 - 2x_2$

Gradient Descent

1. Initialize x^0
2. Compute gradient $\nabla f(x^k)$
3. Update $x^{k+1} = x^k - \alpha^k \nabla f(x^k)$
4. Check convergence (How do we check convergence?)
5. Repeat

Practice questions

1. Find the gradient of $f(x_1, x_2) = 3x_1^2 + x_1x_2 + 2x_2^2 - 5x_1 - 6x_2$.
2. Find the critical point(s) of $f(x_1, x_2) = 2x_1^2 + 3x_2^2 - 4x_1 - 12x_2 + 8$.
3. Compute the Hessian for $f(x_1, x_2) = 2x_1^2 + x_1x_2 + 3x_2^2$.
4. One iteration of GD for $f(x_1, x_2) = x_1^2 + x_2^2$ at $(2, 5)$ with $\alpha = 0.01$.
5. Check if $H = \begin{bmatrix} 5 & 2 \\ 2 & 6 \end{bmatrix}$ is positive definite.
6. Find the minimum of $f(x_1, x_2) = 2x_1^2 + 3x_2^2 + 4x_1 - 12x_2 + 7$.
7. For $f(x) = (x-3)^4 + (x-3)^2$, find all critical points.
8. Solve $\nabla f = 0$ for $f(x_1, x_2) = 2x_1^2 + 3x_1x_2 + x_2^2 - 4x_1 - 6x_2$.
9. Perform 3 GD iterations for $f(x_1, x_2) = x_1^2 + x_2^2$ starting at $(1, 3)$ with $\alpha = 0.1$.