Optimization 101
Mathematical Preliminaries

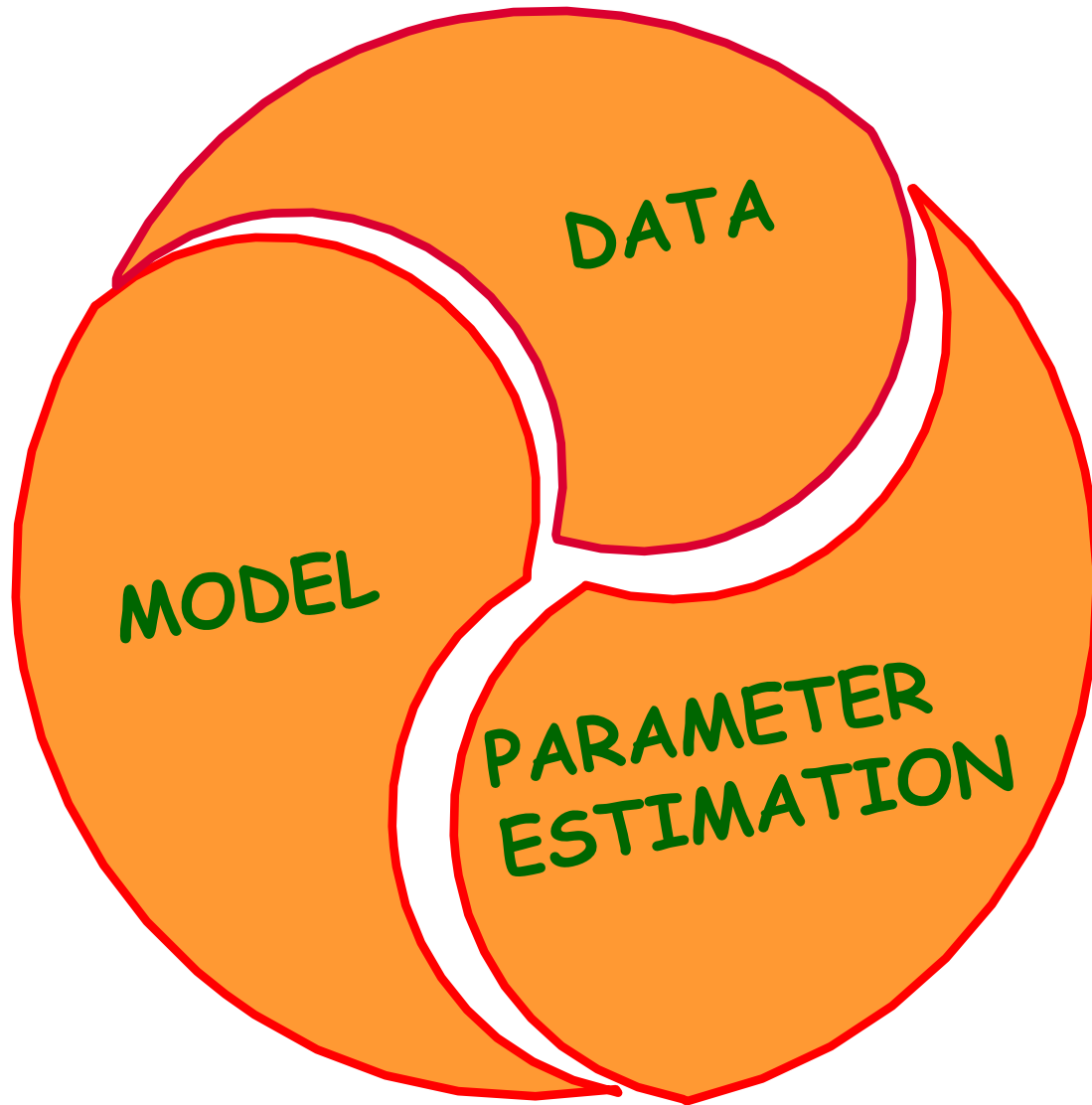**Dr. Nagiza F. Samatova**
Department of Computer Science
North Carolina State University
and
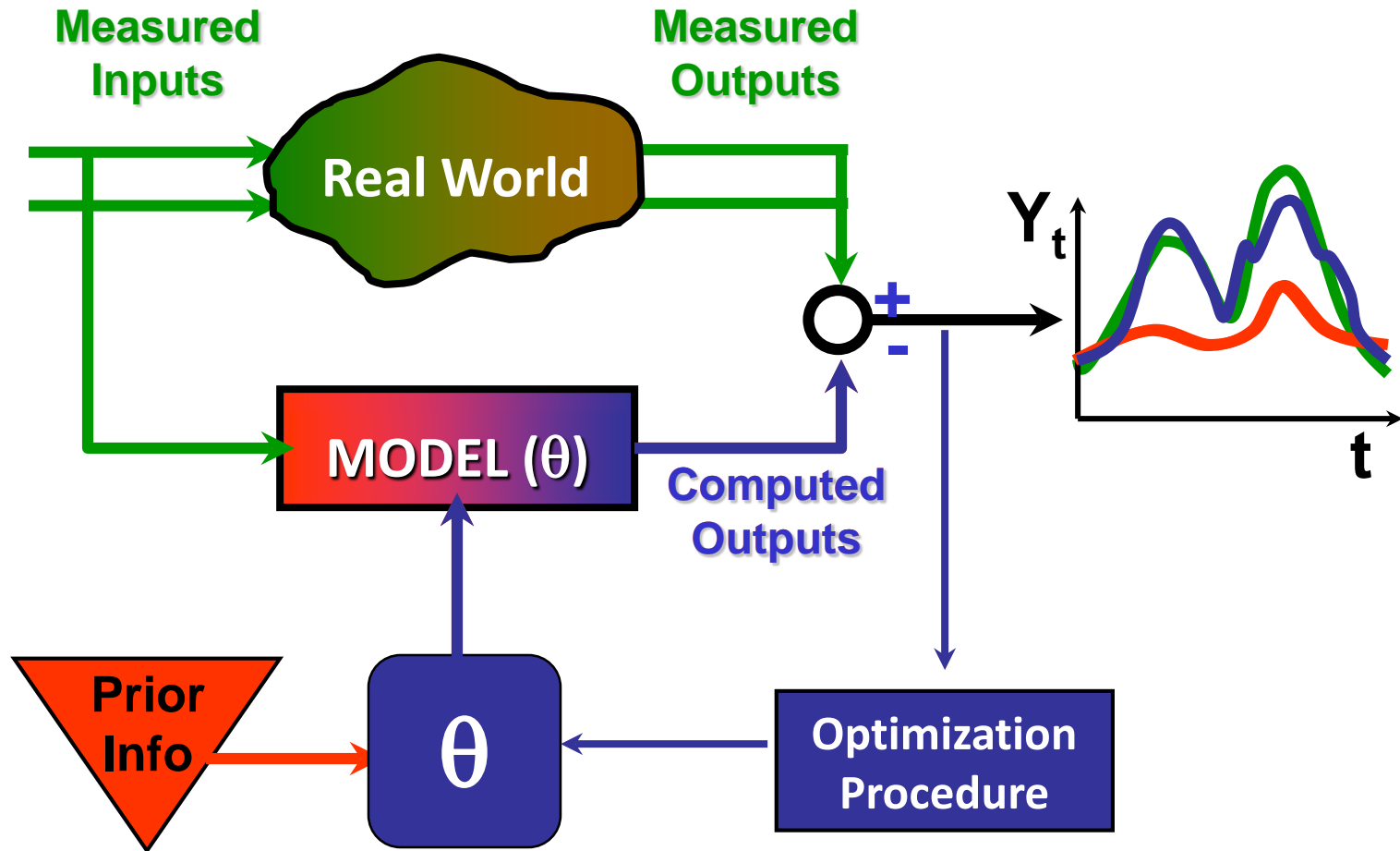Computer Science and Mathematics Division
Oak Ridge National Laboratory

Model Construction

Src: Soroosh Sorooshian, UC Irvine

The Concept of Model Calibration

"Calibration: constraining the model to be consistent with observations"

Src: Soroosh Sorooshian, UC Irvine

Calibration Components

Objective Function

Search Algorithm

Sensitivity Analysis
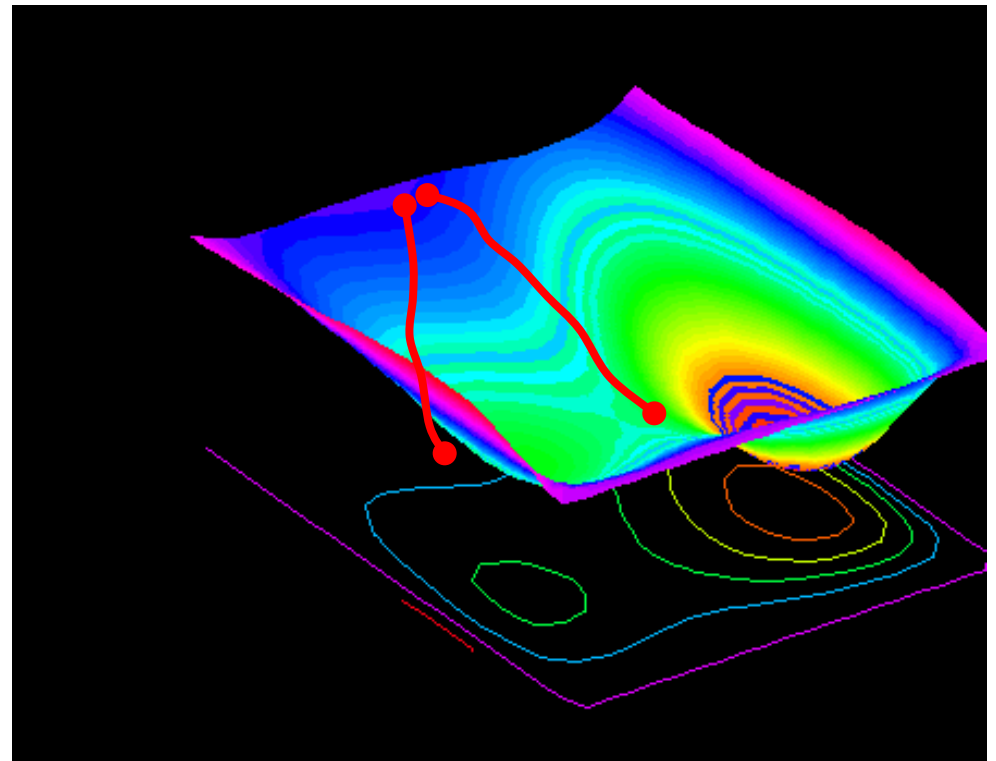
Problems with identifiability

Src: Soroosh Sorooshian, UC Irvine

The Ideal case: Convex Optimization

Parameter **R**

Objective Function

True Parameter Set

Parameter X

Created By G-H Park

Src: Soroosh Sorooshian, UC Irvine
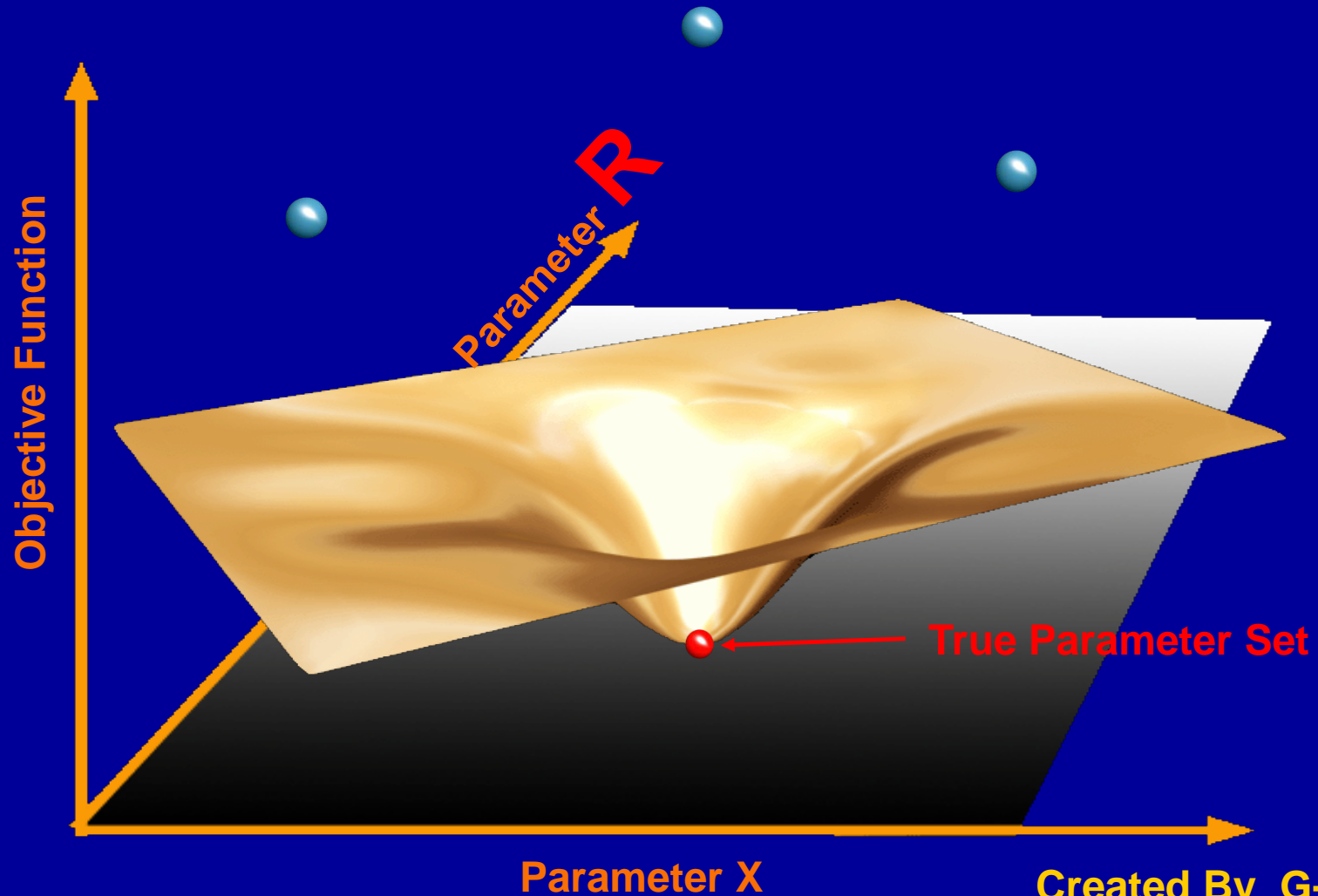
Difficulties in Global Optimization

Objective Function

Parameter Z

Parameter X

True Parameter Set

Parameter Estimation
(non-convex, multi-optima)

Global Optimum

Objective Function

Parameter Z

Parameter X

Src: Soroosh Sorooshian, UC Irvine

Difficulties in Optimization

1.- Regions of Attraction *More than one main convergence region*

2.- Local Optima *Many small "pits" in each region*

Duan, Gupta, and Sorooshian, 1992, WRR

Src: Soroosh Sorooshian, UC Irvine

Difficulties in Optimization

1.- Regions of Attraction *More than one main convergence region*

2.- Local Optima *Many small "pits" in each region*

3.- Roughness *Rough surface with discontinuous derivatives*

Duan, Gupta, and Sorooshian, 1992, WRR
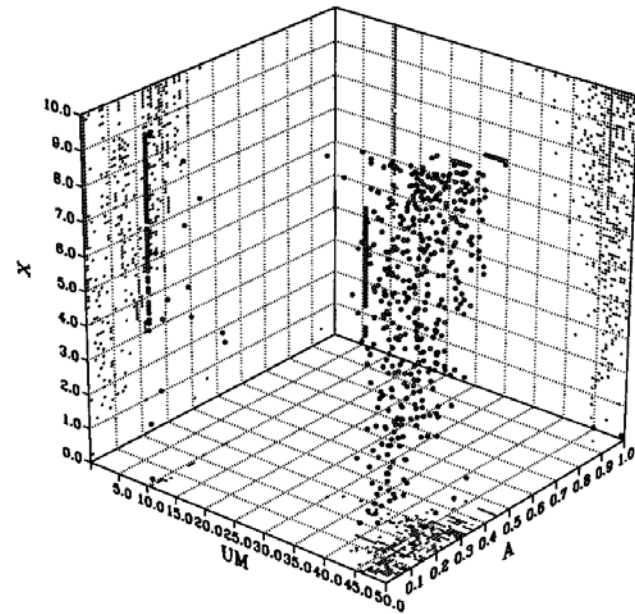
Src: Soroosh Sorooshian, UC Irvine
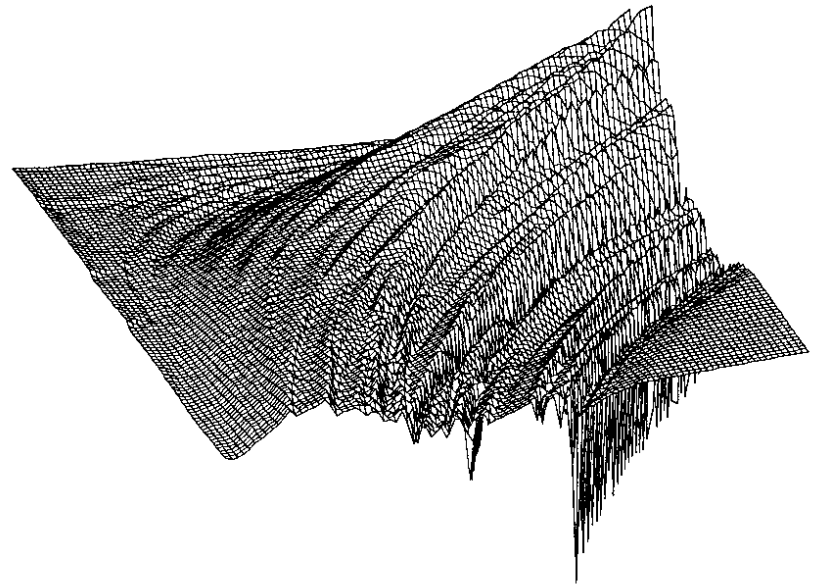
Difficulties in Optimization

1.- Regions of Attraction *More than one main convergence region*

2.- Local Optima *Many small "pits" in each region*

3.- Roughness *Rough surface with discontinuous derivatives*

4.- Flatness *Flat near optimum with significantly different parameter sensitivities*

5.- Shape *Long and curved ridges*

Duan, Gupta, and Sorooshian, 1992, WRR

Src: Soroosh Sorooshian, UC Irvine
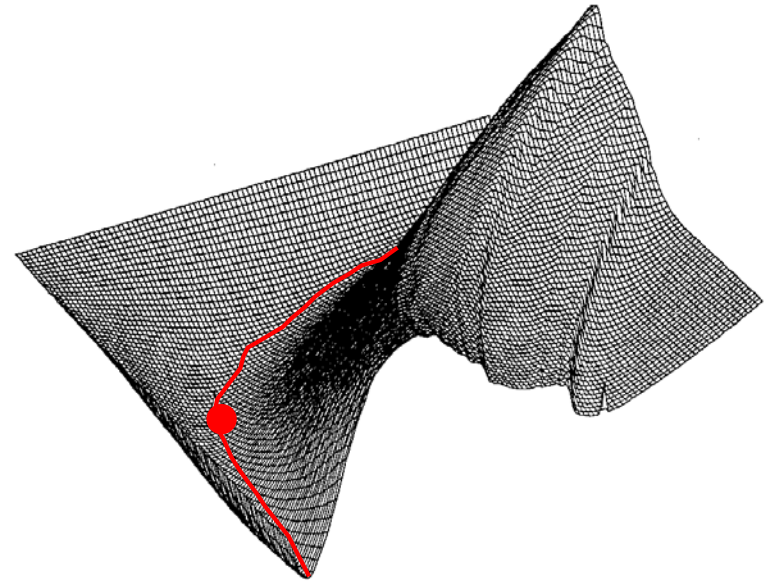
Mathematical Optimization Subfields

- **Linear programming**
- **Integer programming**
- **Quadratic programming**
- **Nonlinear programming**
- **Convex programming**
- **Semidefinite programming**
- **Stochastic programming**
- **Combinatorial optimization**
- **Dynamic programming**
- **....**

Optimization Problem: General Formulation

GIVEN:

    Objective function: $f : \mathbb{R}^d \rightarrow \mathbb{R}$

   cost function, energy function

$$f(x) = f(x_1, x_2, ..., x_d)$$

  Subject to constraints:

     Equality constraints: $g_i(x) = 0, \ i = 1, 2, ..., p$

 and/or

    Inequality constraints: $h_i(x) \leq 0, \ i = 1, 2, ..., q$

SOLVE:

  Minimization problem: $f(x_{min}) = \min_{x \in \mathbb{R}^d} f(x_1, x_2, ..., x_d)$

  Maximization problem: $f(x_{max}) = \max_{x \in \mathbb{R}^d} f(x_1, x_2, ..., x_d)$

Solving Strategies

Optimization

Constrained

Unconstrained

Equality

Inequality

Lagrange Method

Lagrange Method
w/ bounded Lagrangian
multipliers

1. Stationary points, x^*:

$$\frac{df}{dx}\bigg|_{x=x^*} = 0$$

2. Min. stationary points, x^*:

$$\frac{d^2 f}{dx^2}\bigg|_{x=x^*} < 0$$

3. Max. stationary points, x^*:

$$\frac{d^2 f}{dx^2}\bigg|_{x=x^*} > 0$$

4. Saddle stationary points, x^*:
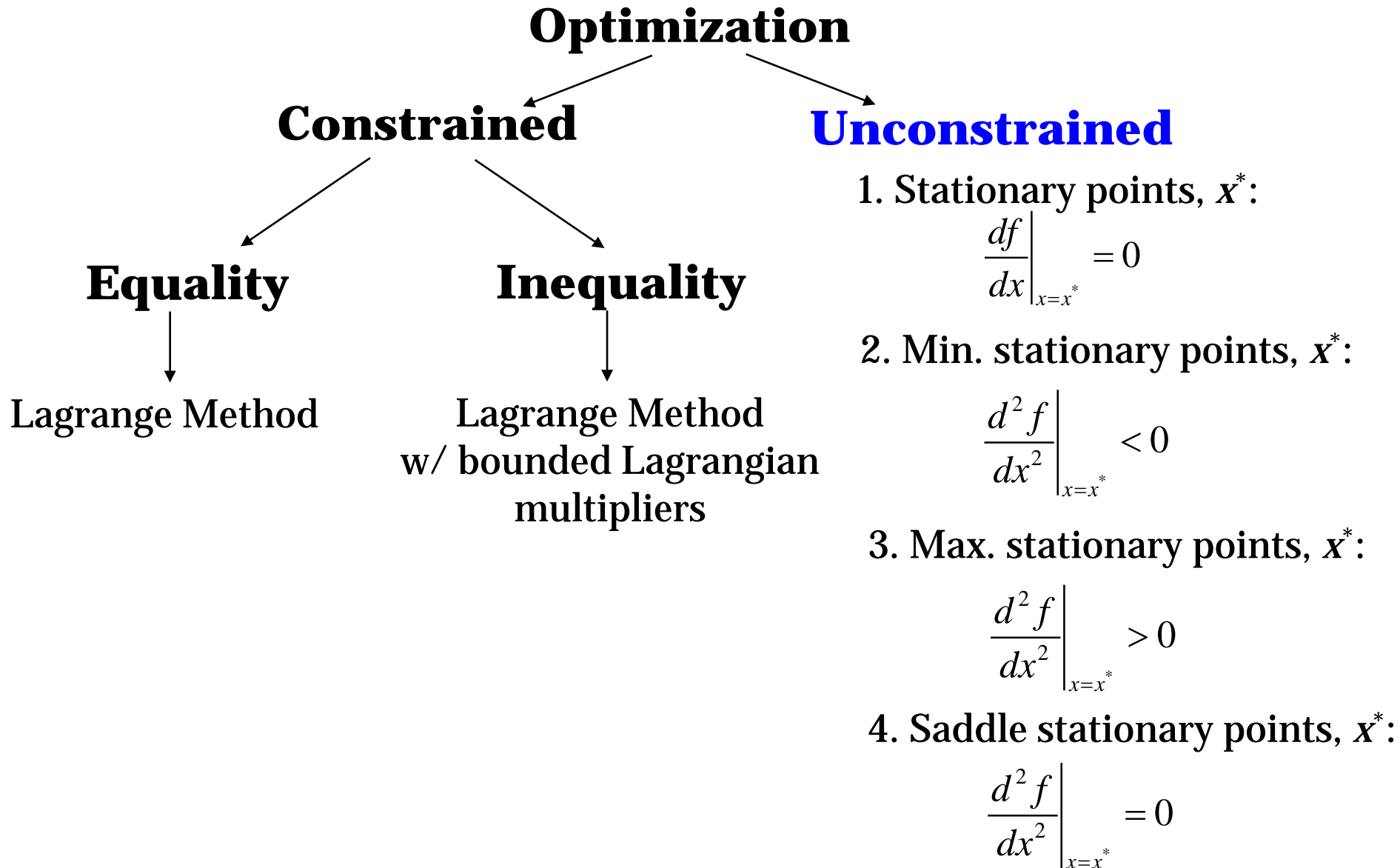
$$\frac{d^2 f}{dx^2}\bigg|_{x=x^*} = 0$$

Solving Strategies

Optimization

Constrained

Equality

Lagrange Method

Inequality

Lagrange Method
w/ bounded Lagrangian
multipliers

Unconstrained

1. Stationary points, x^*:

$$\left.\frac{df}{dx}\right|_{x=x^*} = 0$$

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3. Max. stationary points, x^*:

$$\left.\frac{d^2 f}{dx^2}\right|_{x=x^*} > 0$$

4. Saddle stationary points, x^*:

$$\left.\frac{d^2 f}{dx^2}\right|_{x=x^*} = 0$$

Unconstrained Optimization, *d*=1

$$f: \mathbb{R}^d \rightarrow \mathbb{R}$$
$$f(x) \rightarrow min \text{ or } f(x) \rightarrow max$$

1. **Stationary** points, x^*:

$$\left. \frac{df}{dx} \right|_{x=x^*} = 0$$

2. **Min**. stationary points, x^*:
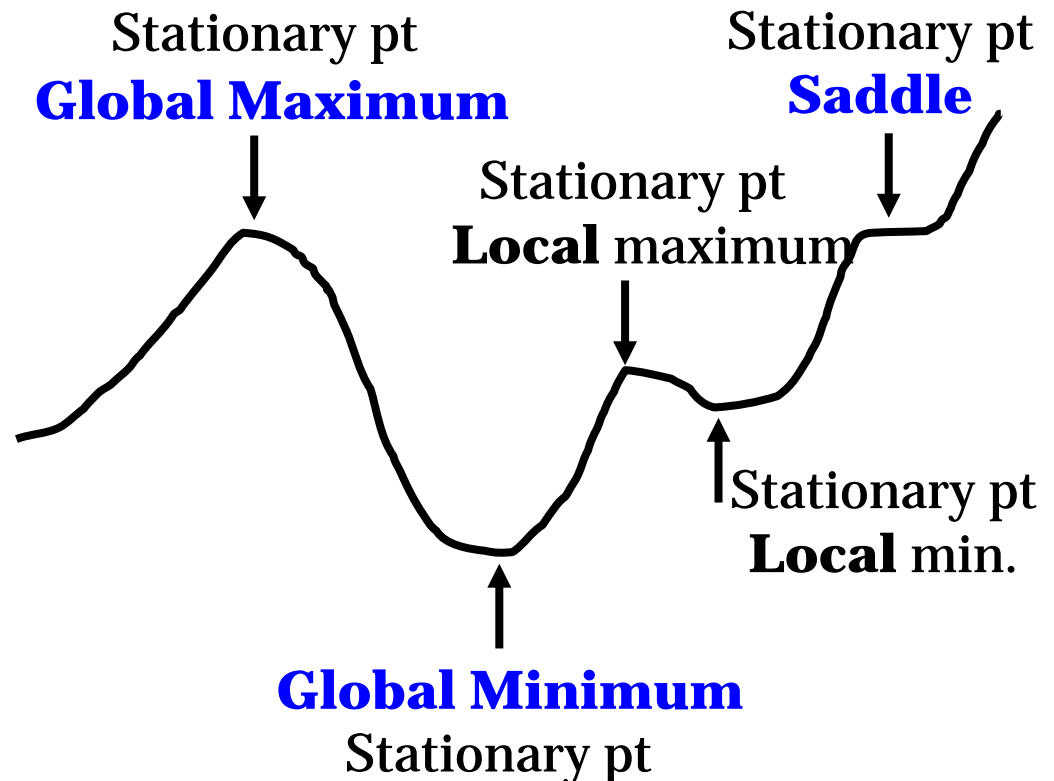
$$\left. \frac{d^2 f}{dx^2} \right|_{x=x^*} < 0$$

3. **Max**. stationary points, x^*:

$$\left. \frac{d^2 f}{dx^2} \right|_{x=x^*} > 0$$

4. **Saddle** stationary points, x^*:

$$\left. \frac{d^2 f}{dx^2} \right|_{x=x^*} = 0$$

Stationary pt
Global Maximum

Stationary pt
Saddle

Stationary pt
Local maximum

Stationary pt
Local min.

Global Minimum
Stationary pt

Unconstrained Multivariate Optimization, *d*>1

$$f: \mathbb{R}^d \to \mathbb{R}, d > 1$$
$$f(x_1, x_2, \ldots, x_d) \to min \text{ or}$$
$$f(x_1, x_2, \ldots, x_d) \to max$$

1. **Stationary** points, x^*:

$$\left. \frac{\partial f}{\partial x_j} \right|_{x_j = x_j^*} = 0, \ \ \forall j = 1, 2, \ldots, d \ \longleftarrow \ \text{partial derivatives}$$

2. **Hessian matrix**, $H(x)$

$$H(x) = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x_1 \partial x_1} & \dfrac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_1 \partial x_d} \\ \dfrac{\partial^2 f}{\partial x_2 \partial x_1} & \dfrac{\partial^2 f}{\partial x_2 \partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_2 \partial x_d} \\ \cdots & \cdots & \cdots & \cdots \\ \dfrac{\partial^2 f}{\partial x_d \partial x_1} & \dfrac{\partial^2 f}{\partial x_d \partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_d \partial x_d} \end{bmatrix}$$

Hessian matrix

3. **Min**. stationary points, x^*:

$$\left. x^T H(x) x \right|_{x = x^*} > 0 \ \longleftarrow \ \text{positive definite } \boldsymbol{H}$$

4. **Max**. stationary points, x^*:

$$\left. x^T H(x) x \right|_{x = x^*} < 0$$

5. **Saddle** stationary points, x^*:

$$\longleftarrow \ \text{indefinite } \boldsymbol{H}$$

Ex: Unconstrained Multivariate Case, *d=2*

GIVEN:

Objective function: $f: \mathbb{R}^2 \rightarrow \mathbb{R}, d = 2$

$$f(x, y) = 3x^2 + 2y^3 - 2xy$$

Subject to constraints:

Equality constraints: *None*

and/or

Inequality constraints: *None*

SOLVE:

Minimization problem: $f(x_{min}, y_{min}) = \min_{(x,y)\in\mathbb{R}^2} f(x, y)$

Maximization problem: $f(x_{max}, y_{max}) = \max_{(x,y)\in\mathbb{R}^2} f(x, y)$

Ex: Hessian Matrix

$$f(x,y) = 3x^2 + 2y^3 - 2xy$$

1. Stationary points, p^*:

$$\left.\frac{\partial f}{\partial p_j}\right|_{p_j=p_j^*} = 0, \ \forall j = 1, 2, \ldots, d \ \longleftarrow \ \text{partial derivatives}$$

$$H(x,y) = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x \partial x} & \dfrac{\partial^2 f}{\partial x \partial y} \\ \dfrac{\partial^2 f}{\partial y \partial x} & \dfrac{\partial^2 f}{\partial y \partial y} \end{bmatrix}$$

$$\begin{cases} \dfrac{\partial f}{\partial x} = 6x - 2y = 0 \\ \dfrac{\partial f}{\partial y} = 6y^2 - 2x = 0 \end{cases}$$

$$\Longrightarrow \quad p_1^* = (x_1^*, y_1^*) = (0,0)$$

$$p_2^* = (x_2^*, y_2^*) = (\frac{1}{27}, \frac{1}{9})$$

2. Hessian matrix, $H(x,y)$

$$H(x,y) = \begin{bmatrix} 6 & -2 \\ -2 & 12y \end{bmatrix}$$

3. Min. stationary points, p^*:

$$\left. p^T H(p) p \right|_{p=p^*} > 0 \ \longleftarrow \ \text{positive definite } H$$

$$\left. (x,y)^T \begin{bmatrix} 6 & -2 \\ -2 & 12\frac{1}{9} \end{bmatrix} (x,y) \right|_{(x,y)=(\frac{1}{27},\frac{1}{9})} = 4x^2 - 2xy + 4y^2/3 = 4(x - \frac{y}{4})^2 + 13\frac{y^2}{4} > 0 \ \Longrightarrow \ p_{\min}^* = (\frac{1}{27}, \frac{1}{9})$$

Analytical vs. Numerical Solution

- **Analytical solutions:**
  - First and second derivatives exist
- **Numerical methods:**
  - Derivatives can NOT be solved analytically
  - Such cases are abundant

Classes of Numerical Methods

- **Based on smoothness of the objective function:**
  - **First order methods**
  - **Second order methods**
  - **Combinatorial methods**
  - **Derivative-free methods**
- **Actual methods:**
  - **Newton's method**
  - **Gradient descent method** **(aka steepest descent/ascent)**
  - **Conjugate gradient method**
  - **Quasi-Newton method**
  - **Simplex method**
  - **Ellipsoid method**
  - **...**

Newton's Method – Univariate Case

Based on **quadratic** approximation to the function $f(x)$.

1. **Taylor** series expansion of $f()$: $f(x) \approx f(x_0) + (x - x_0)f'(x_0) + \dfrac{(x - x_0)^2}{2}f''(x_0)$

2. Set the first-derivative of $f()$ to 0: $f'(x) = f'(x_0) + (x - x_0)f''(x_0) = 0$

3. Derive the update formula for x: $x = x_0 + \dfrac{f'(x_0)}{f''(x_0)}$

Newton's method – Algorithm

$1:$ Let x_0 be the initial point

$2:$ **while** $|f'(x_0)| > \varepsilon$ **do**

$3:$ $\quad x = x_0 + \dfrac{f'(x_0)}{f''(x_0)}$

$4:$ $\quad x_0 = x$

$5:$ **end while**

$6:$ return x

Newton's Method – Multivariate Case

Replace:

$$f'(x_1, x_2, ..., x_d) \rightarrow \nabla f(x_1, x_2, ..., x_d) =$$
$$= (\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, ..., \frac{\partial f}{\partial x_d})$$
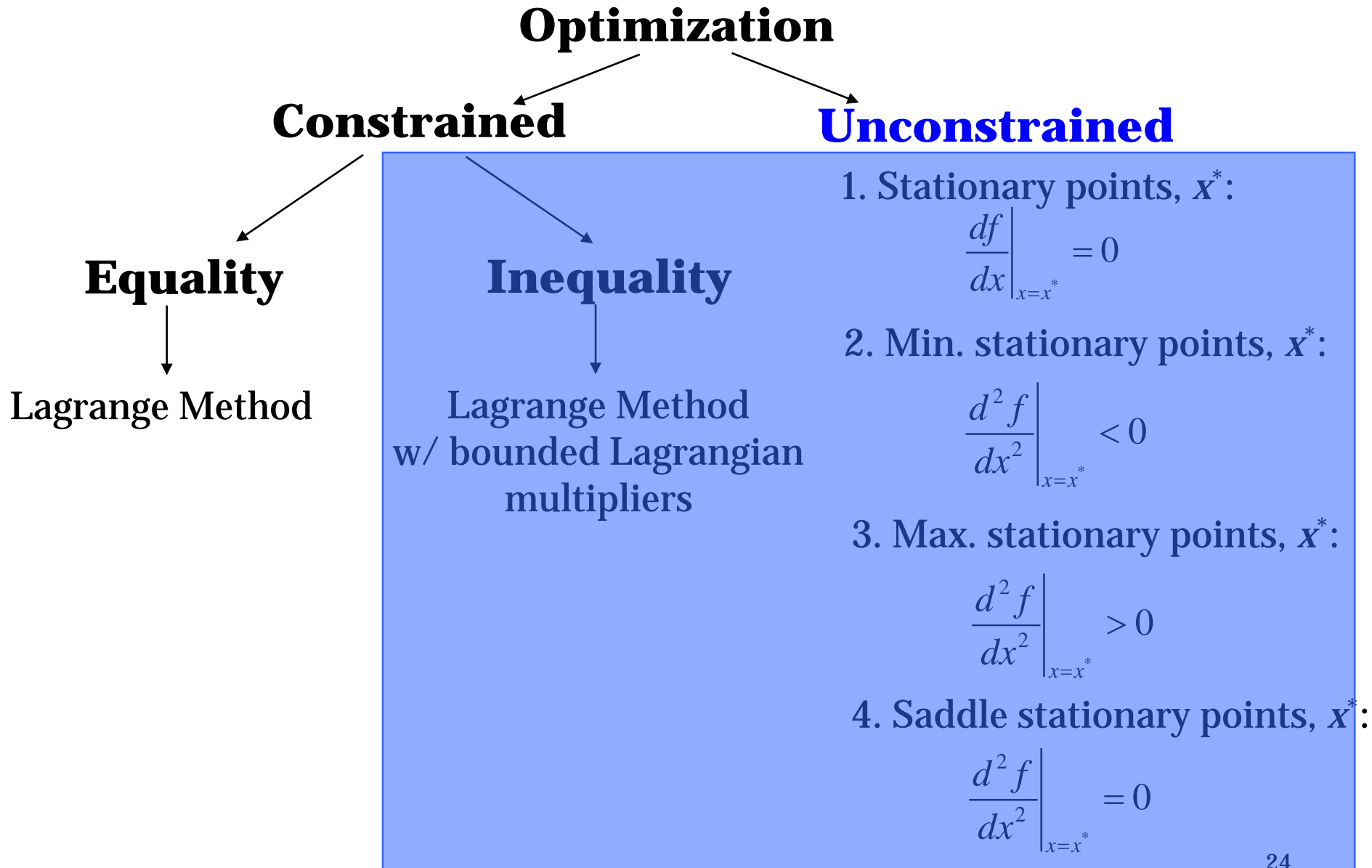
$\longleftarrow$ **gradient operator**

$$f''(x_1, x_2, ..., x_d) \rightarrow H(x_1, x_2, ..., x_d)$$

$\longleftarrow$ **Hessian matrix**

Update:

$$x = x_0 - H^{-1} \nabla f(x)|_{x=x_0}$$

Solving Strategies

Optimization

Constrained   **Unconstrained**

Equality   **Inequality**

Lagrange Method

Lagrange Method
w/ bounded Lagrangian
multipliers

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Constrained Optimization, Equality Constraints
The Lagrange Method

$$f : R^d \rightarrow R, \ d \geq 1$$

$$f(x_1, x_2, ..., x_d) \rightarrow \min$$

subject to: $g_i(x_1, x_2, ..., x_d) = 0, \ i = 1, 2, .., p$

1. Define the **Lagrangian**: $\quad L(x, \lambda) = f(x) + \sum_{i=1}^{p} \lambda_i g_i(x)$

Lagrangian multipliers

2. Set the first-derivatives to 0:

$$\frac{\partial L}{\partial x_j} = 0, \ \forall j = 1, 2, ..., d$$

$$\frac{\partial L}{\partial \lambda_i} = 0, \ \forall j = 1, 2, ..., p$$

3. Solve the ($d+p$) equations in Step 2
   to obtain stationary point x^* and
   the corresponding values for λ_i's

Example

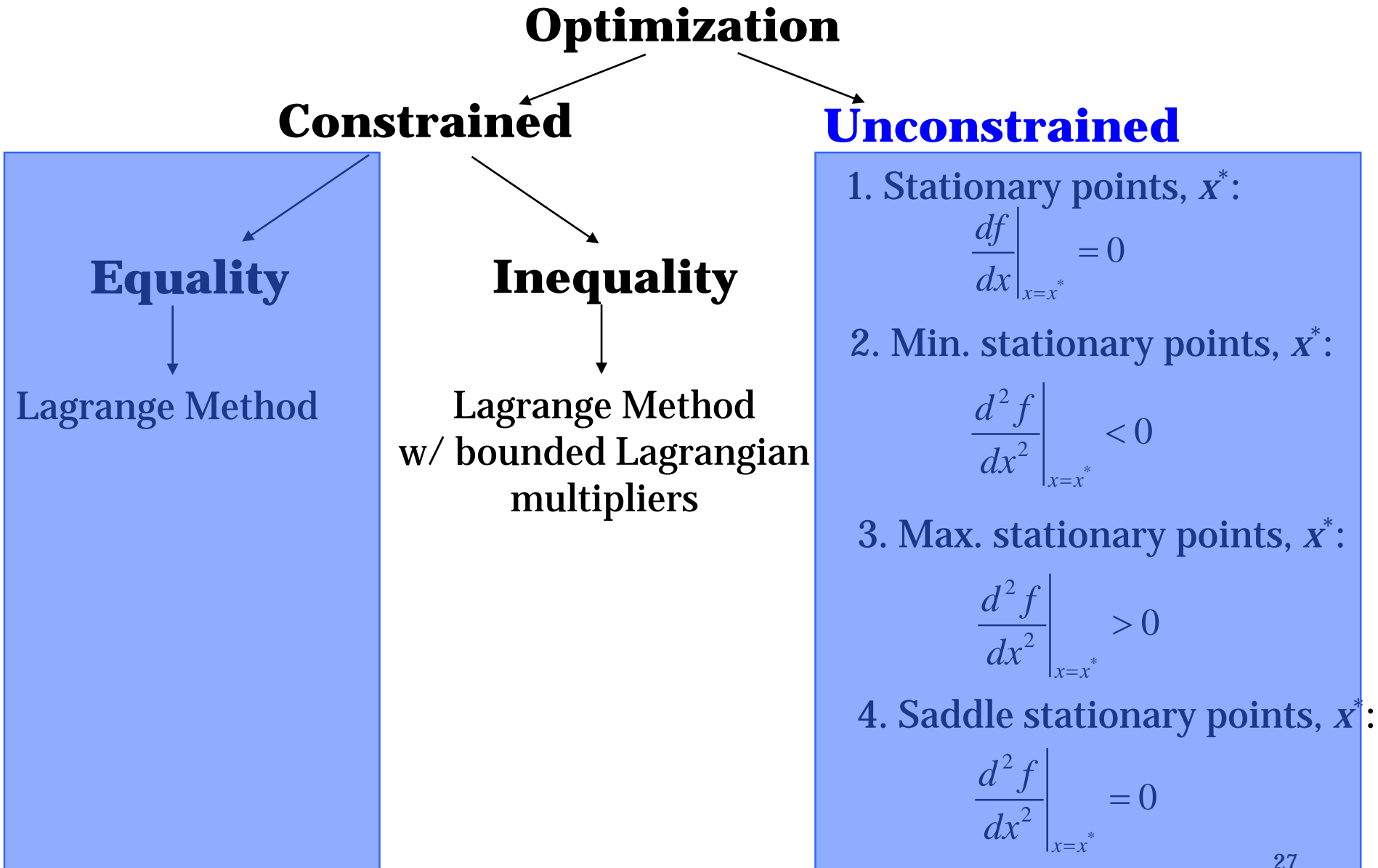Objective function: $f(x, y) = x + 2y \rightarrow \min$

Subject to the constraint: $g(x, y) = x^2 + y^2 - 4 = 0$

$$L(x, \lambda) = f(x) + \sum_{i=1}^{p} \lambda_i g_i(x)$$

$$\frac{\partial L}{\partial x_j} = 0, \ \forall j = 1, 2, ..., d$$

$$\frac{\partial L}{\partial \lambda_i} = 0, \ \forall j = 1, 2, ..., p$$

Solving Strategies

Optimization

Constrained   **Unconstrained**

Equality

Lagrange Method

Inequality

Lagrange Method
w/ bounded Lagrangian
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$$\left.\frac{d^2 f}{dx^2}\right|_{x=x^*} = 0$$

Constrained Optimization, Inequality Constraints

$$f : R^d \rightarrow R, \ d \geq 1$$
$$f(x_1, x_2, ..., x_d) \rightarrow \min$$
$$\text{subject to: } h_i(x_1, x_2, ..., x_d) \leq 0, \ i = 1, 2, .., q$$

1. Define the **Lagrangian**:

$$L(x, \lambda) = f(x) + \sum_{i=1}^{q} \lambda_i h_i(x)$$

2. Set **Karush-Kuhn-Tucker** (KKT) conditions:

$$\frac{\partial L}{\partial x_j} = 0, \ \forall j = 1, 2, ..., d$$

$$h_i(x) \leq 0, \ \forall i = 1, 2, ..., q$$

$$\lambda_i \geq 0, \ \forall i = 1, 2, ..., q$$

$$\lambda_i h_i(x) = 0, \ \forall i = 1, 2, ..., q$$

The Lagrange multipliers are no longer unbounded in the presence of inequality constraints.

3. Solve the system in Step 2
to obtain stationary point x^* and
the corresponding values for λ_i's

Example

Objective function: $f(x, y) = (x-1)^2 + (y-3)^2 \rightarrow \min$

Subject to the constraints: $h_1(x, y) = x + y - 2 \leq 0$

$h_2(x, y) = x - y \leq 0$

$$L(x, \lambda) = f(x) + \sum_{i=1}^{q} \lambda_i h_i(x)$$

$$\frac{\partial L}{\partial x_j} = 0,\ \forall j = 1, 2, ..., d$$

$$\lambda_i h_i(x) = 0,\ \forall i = 1, 2, ..., q$$

$$h_i(x) \leq 0,\ \forall i = 1, 2, ..., q$$

$$\lambda_i \geq 0,\ \forall i = 1, 2, ..., q$$