10.34: Numerical Methods Applied to Chemical Engineering

Lecture 12:
Constrained Optimization
Equality constraints and Lagrange multipliers

Recap

- Unconstrained optimization
- Newton-Raphson methods
- Trust-region methods

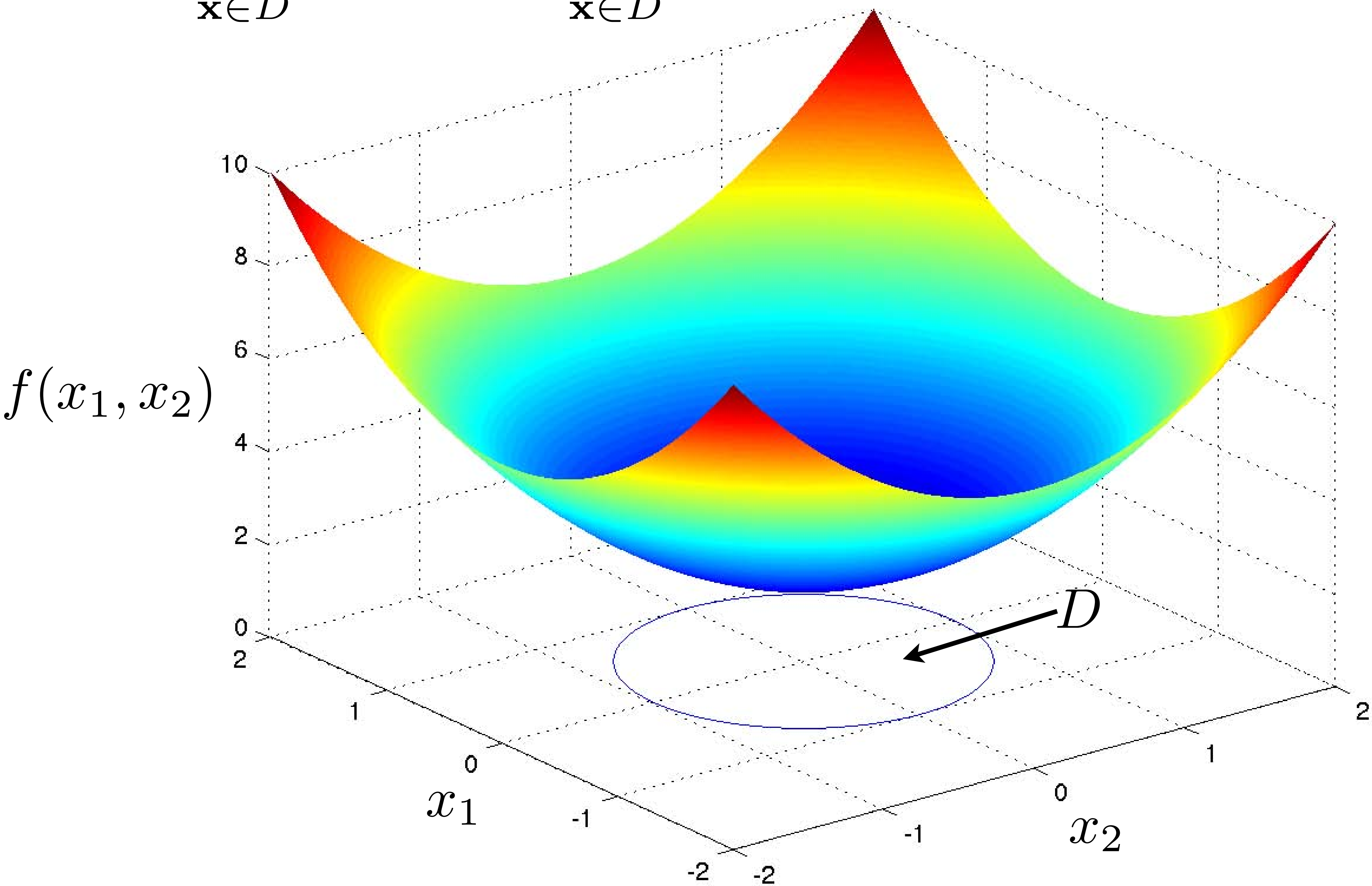
Midterm Exam

- Expect 3 problems
- Comprehensive exam:
  - Linear algebra
  - Systems of nonlinear equations
  - Optimization

Constrained Optimization

- Problems of the sort:

$$\min_{\mathbf{x} \in D} f(\mathbf{x}) \qquad \arg\min_{\mathbf{x} \in D} f(\mathbf{x})$$



Constrained Optimization

- Problems of the sort:

$$\min_{\mathbf{x} \in D} f(\mathbf{x}) \qquad \arg\min_{\mathbf{x} \in D} f(\mathbf{x})$$

- The feasible set can be described in terms of two types of constraints:
  - Equality constraints: $\mathcal{D} = \{\mathbf{x} : \mathbf{c}(\mathbf{x}) = 0\}$
  - Inequality constraints: $\mathcal{D} = \{\mathbf{x} : \mathbf{h}(\mathbf{x}) \geq 0\}$

Constrained Optimization

- Problems of the sort:

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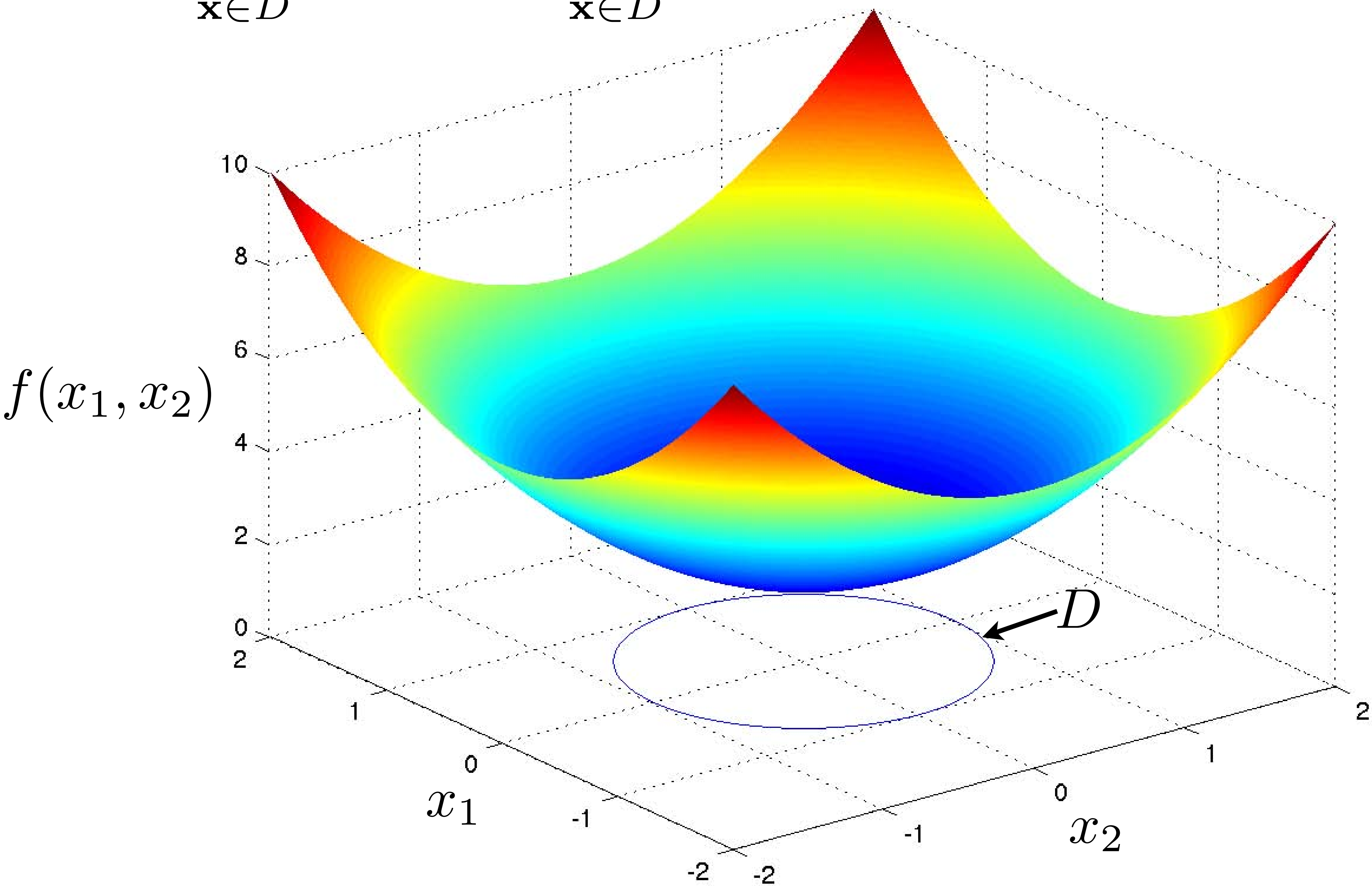

Constrained Optimization

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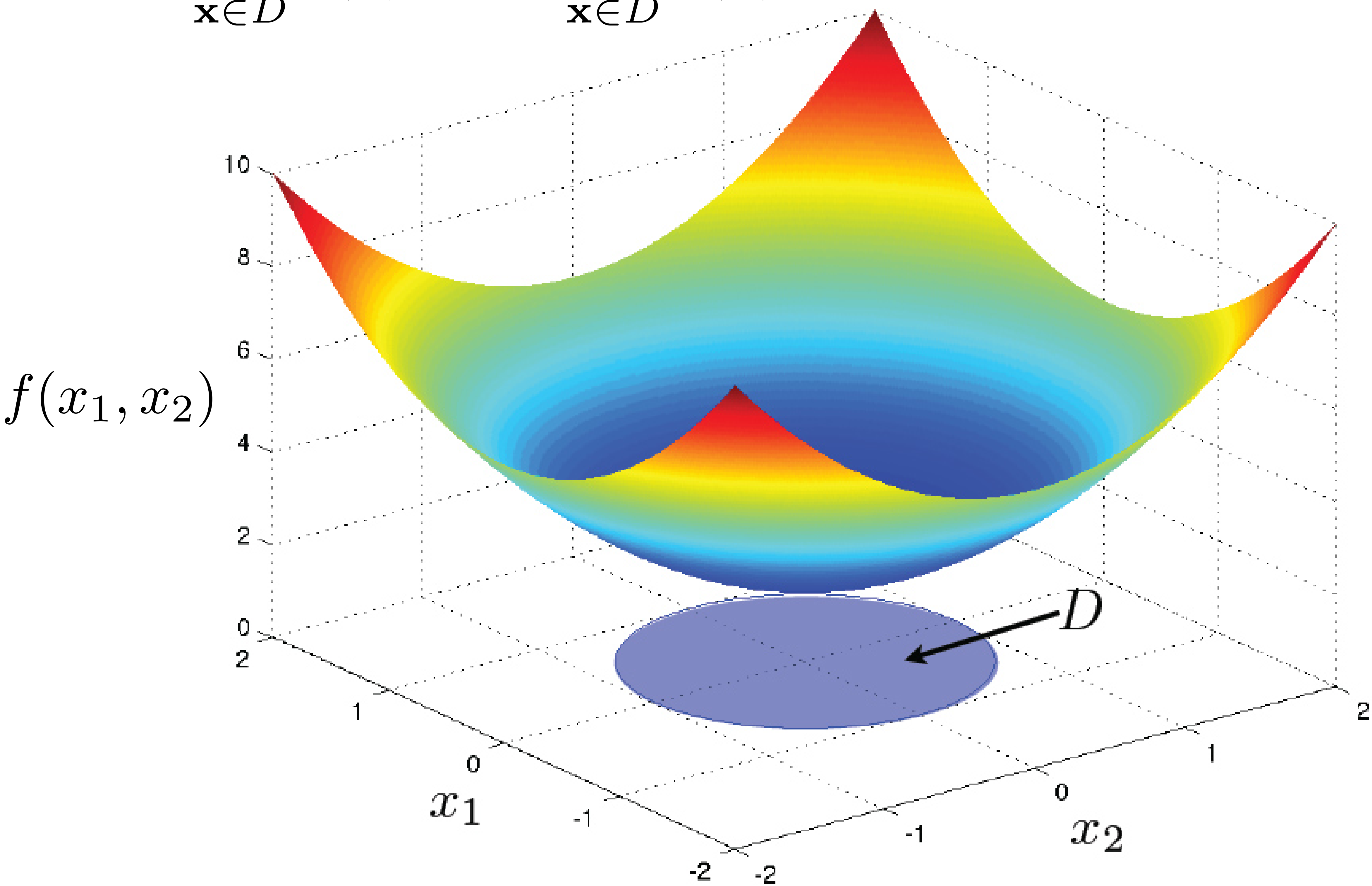

Constrained Optimization

- Problems of the sort:

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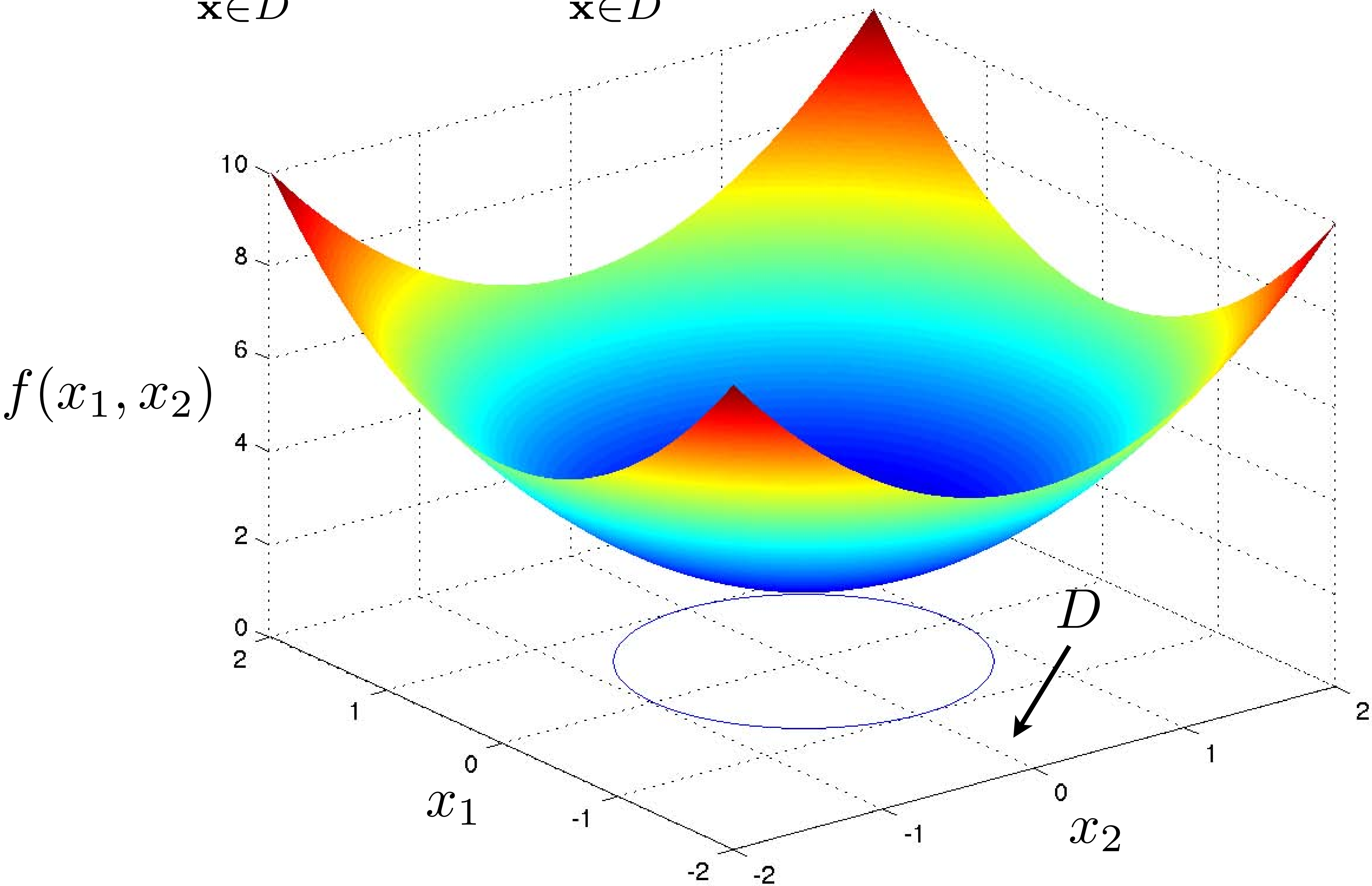


Constrained Optimization

- Examples:
  - minimize: $E(\mathbf{v}, \mathbf{x}) = \frac{1}{2}m\|\mathbf{v}\|_2^2 + m\mathbf{g}^T\mathbf{x}$
  - subject to: $\|\mathbf{x} - \mathbf{x}_0\|_2 = L$

Constrained Optimization

- Examples:
  - minimize: $f(\mathbf{x}) = \mathbf{c}^T\mathbf{x}$
  - subject to: $\mathbf{A}\mathbf{x} - \mathbf{b} \leq 0$
    $\mathbf{x} \geq 0$

Constrained Optimization

- In general:
  - minimize: $f(\mathbf{x})$
  - subject to: $\mathbf{c}(\mathbf{x}) = 0$
    $\mathbf{h}(\mathbf{x}) \geq 0$
- One approach is to approximate the problem as unconstrained – penalty methods:
  - minimize:

$$F(\mathbf{x}) = f(\mathbf{x}) + \frac{1}{2\mu}\left(\|\mathbf{c}(\mathbf{x})\|_2^2 + \sum_{i=1}^{N} H(-h_i(\mathbf{x}))h_i(\mathbf{x})^2\right)$$

  - as $\mu \to 0$
  - with $H(x \geq 0) = 1, H(x < 0) = 0$

Equality Constraints

- Method of Lagrange multipliers
  - minimize: $f(\mathbf{x})$
  - subject to: $c(\mathbf{x}) = 0$
- What are the necessary conditions for defining a minimum?
  - Taylor expansion of $f(\mathbf{x})$ in some direction with $\|\mathbf{d}\|_2 \ll 1$:

$$f(\mathbf{x}+\mathbf{d}) = f(\mathbf{x}) + \mathbf{g}(\mathbf{x})^T\mathbf{d} + \ldots$$

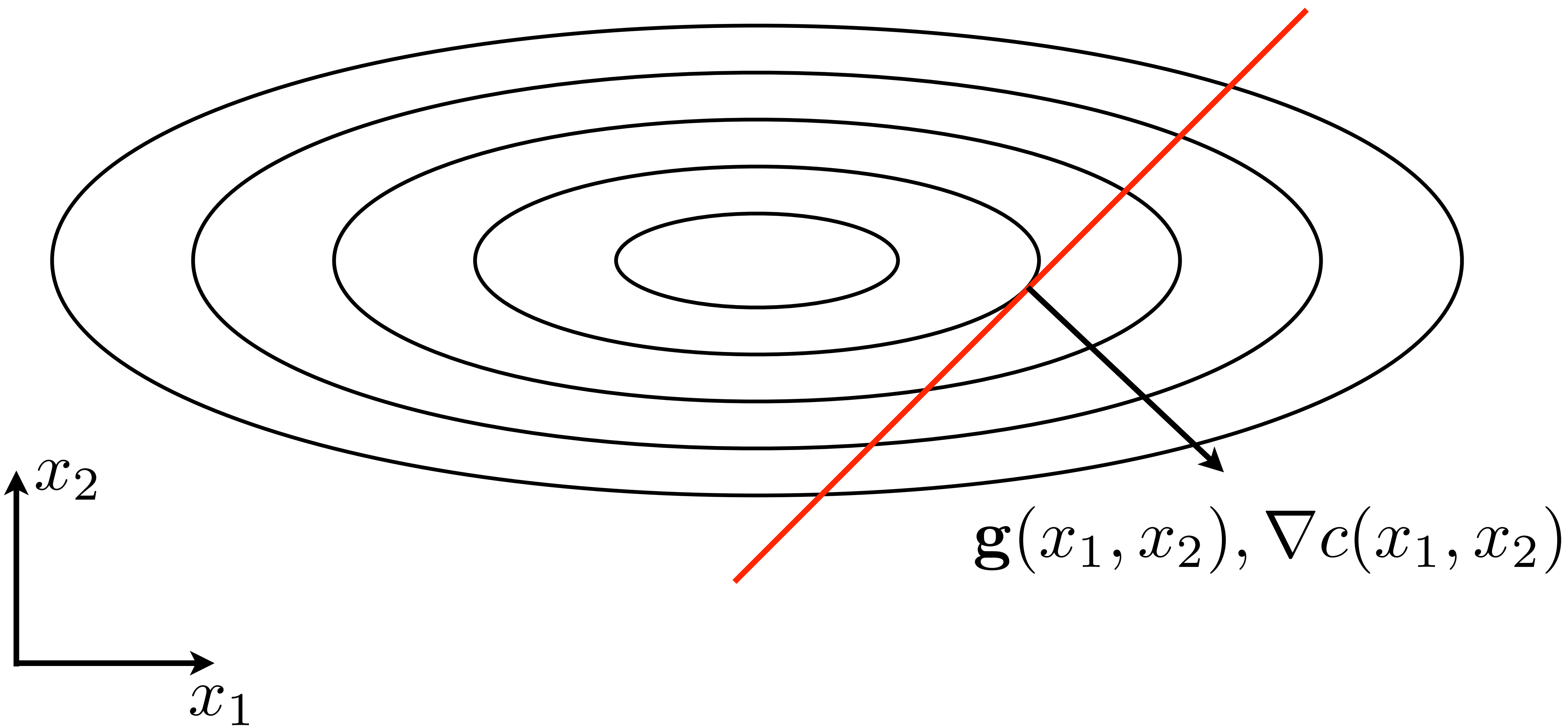
    - either $\mathbf{g}(\mathbf{x}) = 0$ or $\mathbf{g}(\mathbf{x}) \perp \mathbf{d}$ at the minimum
  - For equality constraints, $c(\mathbf{x}) = 0$, and $c(\mathbf{x}+\mathbf{d}) = 0$
    - Taylor expansion of $c(\mathbf{x})$ in the same direction:

$$c(\mathbf{x}+\mathbf{d}) = c(\mathbf{x}) + \nabla c(\mathbf{x}) \cdot \mathbf{d} + \ldots \Rightarrow \mathbf{d} \perp \nabla c(\mathbf{x})$$

  - Therefore, $\mathbf{g}(\mathbf{x}) \parallel \nabla c(\mathbf{x}) \Rightarrow \mathbf{g}(\mathbf{x}) - \lambda \nabla c(\mathbf{x}) = 0$

Equality Constraints

- Example
  - minimize: $f(x_1, x_2) = x_1^2 + 10x_2^2$
  - subject to: $c(x_1, x_2) = x_1 - x_2 - 3 = 0$
    - Contours of the function and the constraint



Equality Constraints

- Method of Lagrange multipliers
  - minimize: $f(\mathbf{x})$
  - subject to: $c(\mathbf{x}) = 0$
- A solution to the equality constrained problem satisfies:

$$\begin{pmatrix} \mathbf{g}(\mathbf{x}) - \lambda \nabla c(\mathbf{x}) \\ c(\mathbf{x}) \end{pmatrix} = 0$$

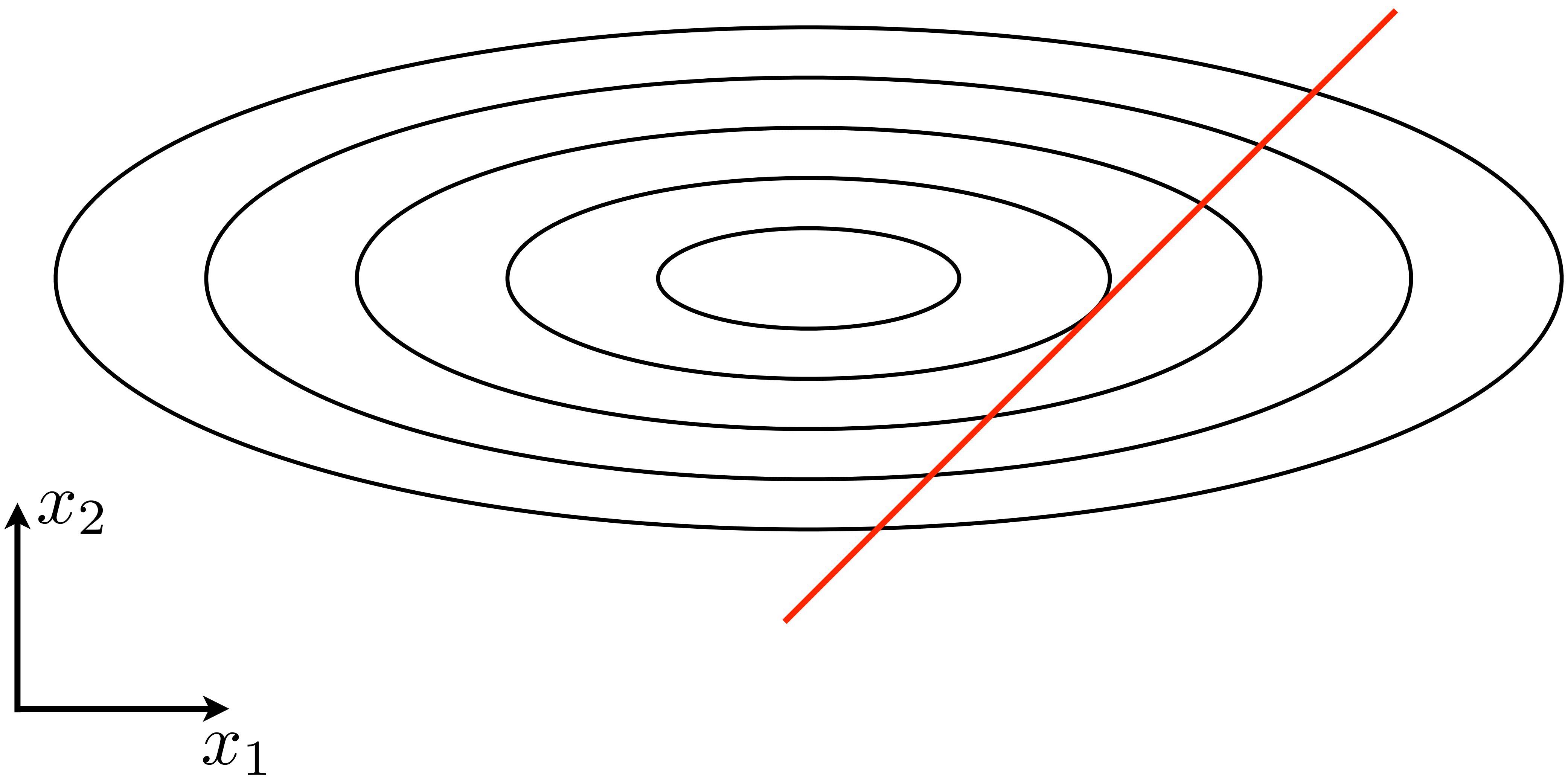
  - For the unknowns: $\mathbf{x}, \lambda$
  - λ is called a Lagrange multiplier
  - The solution set $(\mathbf{x}, \lambda)$ is a critical point of:

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) - \lambda c(\mathbf{x})$$

    - called the "Lagrangian"

Equality Constraints

- Example
  - minimize: $f(x_1, x_2) = x_1^2 + 10x_2^2$
  - subject to: $c(x_1, x_2) = x_1 - x_2 - 3 = 0$
    - Contours of the function and the constraint



Equality Constraints

- Method of Lagrange multipliers
  - minimize: $f(\mathbf{x})$
  - subject to: $\mathbf{c}(\mathbf{x}) = 0$
- What are the necessary conditions for defining a minimum?
  - Taylor expansion of $f(\mathbf{x})$ in some direction with $\|\mathbf{d}\|_2 \ll 1$:

$$f(\mathbf{x}+\mathbf{d}) = f(\mathbf{x}) + \mathbf{g}(\mathbf{x})^T\mathbf{d} + \ldots$$

    - either $\mathbf{g}(\mathbf{x}) = 0$ or $\mathbf{g}(\mathbf{x}) \perp \mathbf{d}$ at the minimum
  - For equality constraints, $\mathbf{c}(\mathbf{x}) = 0$, and $\mathbf{c}(\mathbf{x}+\mathbf{d}) = 0$
    - Taylor expansion of $\mathbf{c}(\mathbf{x})$ in the same direction:

$$\mathbf{c}(\mathbf{x}+\mathbf{d}) = \mathbf{c}(\mathbf{x}) + \mathbf{J}_c(\mathbf{x})\mathbf{d} + \ldots$$

    - The direction belongs to what set of vectors?

Equality Constraints

- Method of Lagrange multipliers
  - minimize: $f(\mathbf{x})$
  - subject to: $\mathbf{c}(\mathbf{x}) = 0$
- What are the necessary conditions for defining a minimum?
  - Taylor expansion of $f(\mathbf{x})$ in some direction with $\|\mathbf{d}\|_2 \ll 1$:

$$f(\mathbf{x} + \mathbf{d}) = f(\mathbf{x}) + \mathbf{g}(\mathbf{x})^T \mathbf{d} + \dots$$

    - either $\mathbf{g}(\mathbf{x}) = 0$ or $\mathbf{g}(\mathbf{x}) \perp \mathbf{d}$ at the minimum
  - If $\mathbf{J}_c(\mathbf{x})\mathbf{d} = 0$ and $\mathbf{g}(\mathbf{x}) \perp \mathbf{d}$,
    - then $\mathbf{g}(\mathbf{x})$ at the minimum belongs to what set of vectors?

    - Therefore:

Equality Constraints

- Method of Lagrange multipliers
  - minimize: $f(\mathbf{x})$
  - subject to: $\mathbf{c}(\mathbf{x}) = 0$
- What are the necessary conditions for defining a minimum?
  - Taylor expansion of $f(\mathbf{x})$ in some direction with $\|\mathbf{d}\|_2 \ll 1$:

$$f(\mathbf{x} + \mathbf{d}) = f(\mathbf{x}) + \mathbf{g}(\mathbf{x})^T \mathbf{d} + \ldots$$

    - either $\mathbf{g}(\mathbf{x}) = 0$ or $\mathbf{g}(\mathbf{x}) \perp \mathbf{d}$
  - If $\mathbf{J}_c(\mathbf{x})\mathbf{d} = 0$ and $\mathbf{g}(\mathbf{x}) \perp \mathbf{d}$,
    - then $\mathbf{g}(\mathbf{x})$ at the minimum belongs to what set of vectors?

    - Therefore:

Equality Constraints

- Method of Lagrange multipliers
  - minimize: $f(\mathbf{x})$
  - subject to: $\mathbf{c}(\mathbf{x}) = 0$
- A solution to the equality constrained problem satisfies:

$$\begin{pmatrix} \mathbf{g}(\mathbf{x}) - \mathbf{J}_c(\mathbf{x})^T \boldsymbol{\lambda} \\ \mathbf{c}(\mathbf{x}) \end{pmatrix} = 0$$

  - For the unknowns: $\mathbf{x}, \boldsymbol{\lambda}$
  - $\boldsymbol{\lambda}$ is a vector of Lagrange multiplier
  - The solution set $(\mathbf{x}, \boldsymbol{\lambda})$ is a critical point of:

$$L(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) - \mathbf{c}(\mathbf{x})^T \boldsymbol{\lambda}$$

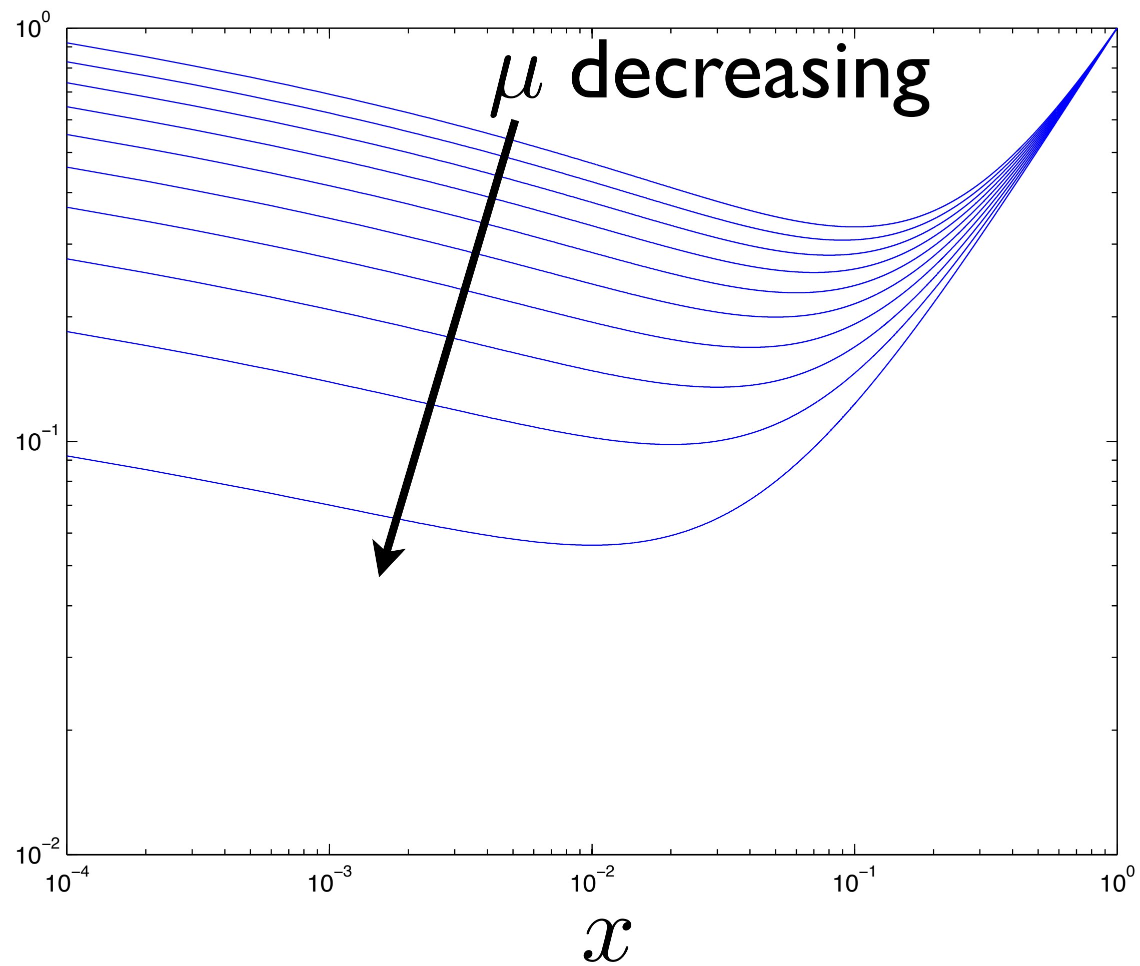
    - called the "Lagrangian"

Inequality Constraints

- Interior point methods
  - minimize: $f(\mathbf{x})$
  - subject to: $\mathbf{h}(\mathbf{x}) \geq 0$
- Rewrite as unconstrained optimization by using a barrier:
  - minimize: $$f(\mathbf{x}) - \mu \sum_{i=1}^{N} \log(h_i(\mathbf{x}))$$
  - as $\mu \to 0^+$
- For $h_i(\mathbf{x}) \to 0$, the objective function becomes large
  - This creates a barrier from which an unconstrained optimization scheme may not escape.
- Determining the minimum of this new objective function for progressively weaker barriers ($\mu \to 0^+$) is important.
  - How can this be done reliably?

Inequality Constraints

- Interior point methods, example
  - minimize: x
  - subject to: $x \geq 0$
- Rewrite as unconstrained optimization by using a barrier:
  - minimize: $x - \mu \log(x)$



Inequality Constraints

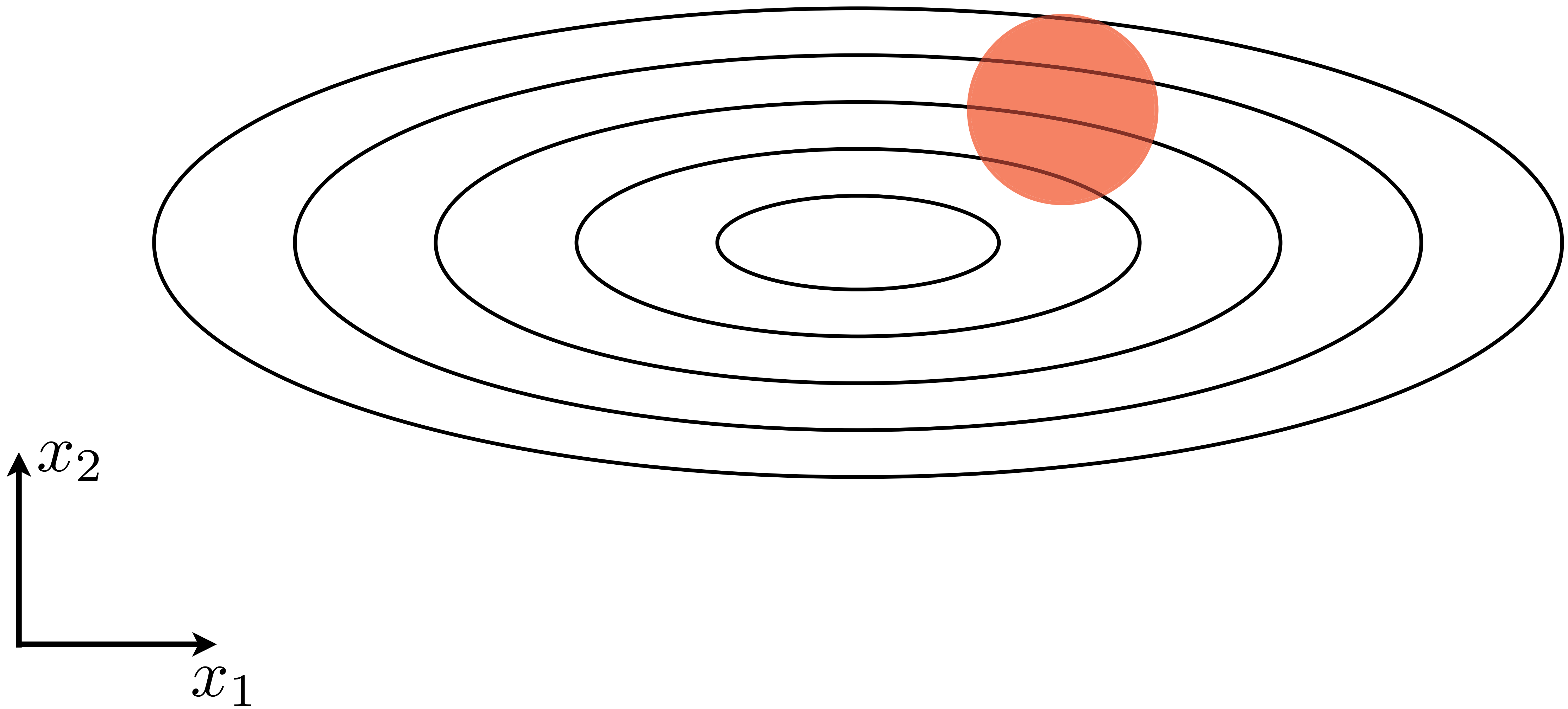
- Interior point methods:
  - minimize: $f(\mathbf{x})$
  - subject to: $\mathbf{h}(\mathbf{x}) \geq 0$
- Rewrite as unconstrained optimization by using a barrier:
  - minimize: $f(\mathbf{x}) - \mu \sum_{i=1}^{N} \log(h_i(\mathbf{x}))$
  - as $\mu \to 0^+$
- Why a logarithmic barrier?
- The minimum of the unconstrained problem is found where:

Inequality Constraints

- Interior point methods:
  - minimize: $f(\mathbf{x})$
  - subject to: $\mathbf{h}(\mathbf{x}) \geq 0$
- Rewrite as unconstrained optimization by using a barrier:
  - minimize: $f(\mathbf{x}) - \mu \sum_{i=1}^{N} \log(h_i(\mathbf{x}))$
  - as $\mu \rightarrow 0^+$
- Use ___________ to study a sequence of barrier parameters
- Stop ___________ when:

Inequality Constraints

- Example:
  - minimize: $f(x_1, x_2) = x_1^2 + 10x_2^2$
  - subject to: $h(x_1, x_2) = 1 - (x_1 - 2)^2 - (x_2 - 2)^2 \geq 0$
    - Contours of the function and the constraint



Inequality Constraints

```
f = @(x) x(1)^2 + 10 * x(2)^2;
grad_f = @(x) [ 2*x(1); 20*x(2) ];
H_f = @(x) [ 2 0; 0 20 ];

h = @(x) 1 - ( x(1) - 2 )^2 - ( x(2) - 2 )^2;
grad_h = @(x) [ -2*(x(1)-2); -2*(x(2)-2) ];
H_h = @(x) [ -2 0; 0 -2 ];

phi = @(x,mu) f( x ) - mu * log( h( x ) );
grad_phi = @(x,mu) grad_f( x ) - mu / h( x ) * grad_h( x );
H_phi = @(x,mu) H_f( x ) - mu / h( x ) * H_h( x ) + mu / h( x )^2 * grad_h( x ) * grad_h( x )';

x = [ 2; 2 ];

for mu = [ 1:-0.01:0.01 ]

    while ( norm( grad_phi( x, mu ) ) > 1e-8 )

        x = x - H_phi( x, mu ) \ grad_phi( x, mu );

    end;

end;
```

Inequality Constraints

- Example:
  - minimize: $f(x_1, x_2) = x_1^2 + 10x_2^2$
  - subject to: $h(x_1, x_2) = 1 - (x_1 - 2)^2 - (x_2 - 2)^2 \geq 0$
    - Contours of the function and the constraint