Optimization with Constraints

Why Constraints?

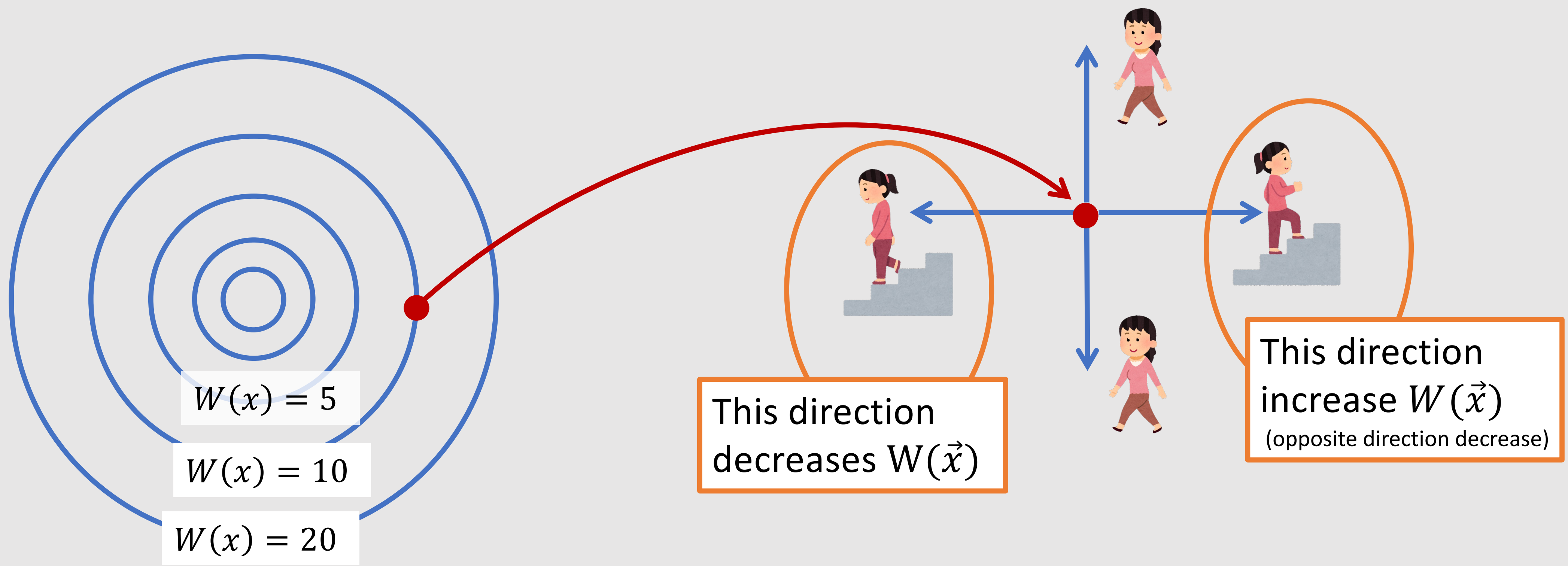
- Solid deformation
  - Non penetration constraints

Credit: Damnsoft 09 @ Wikipedia

- Fluid
  - incompressibility constraints: vortex

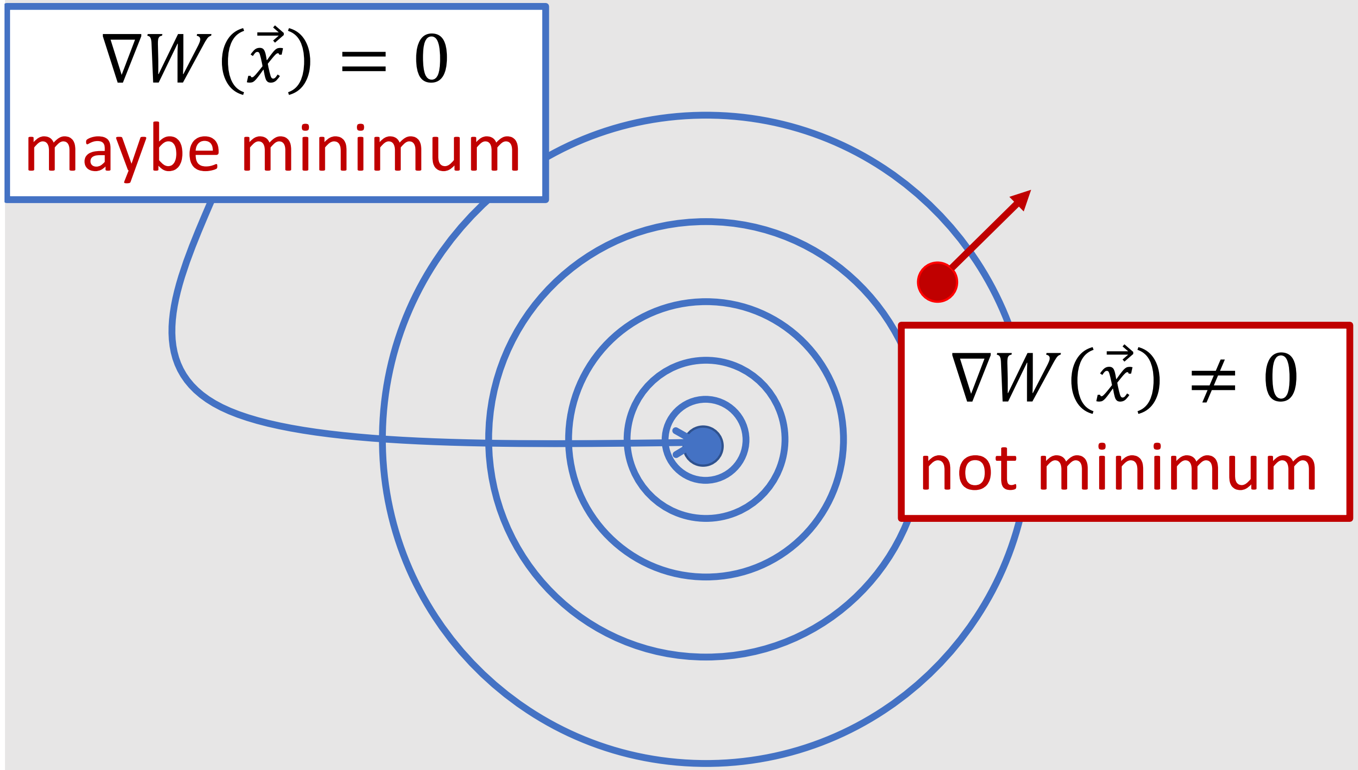
Credit: Astrobob @ Wikipedia

Not Minimum If Its Gradient is not Zero



Maybe **Minimum if Gradient is** **Zero**

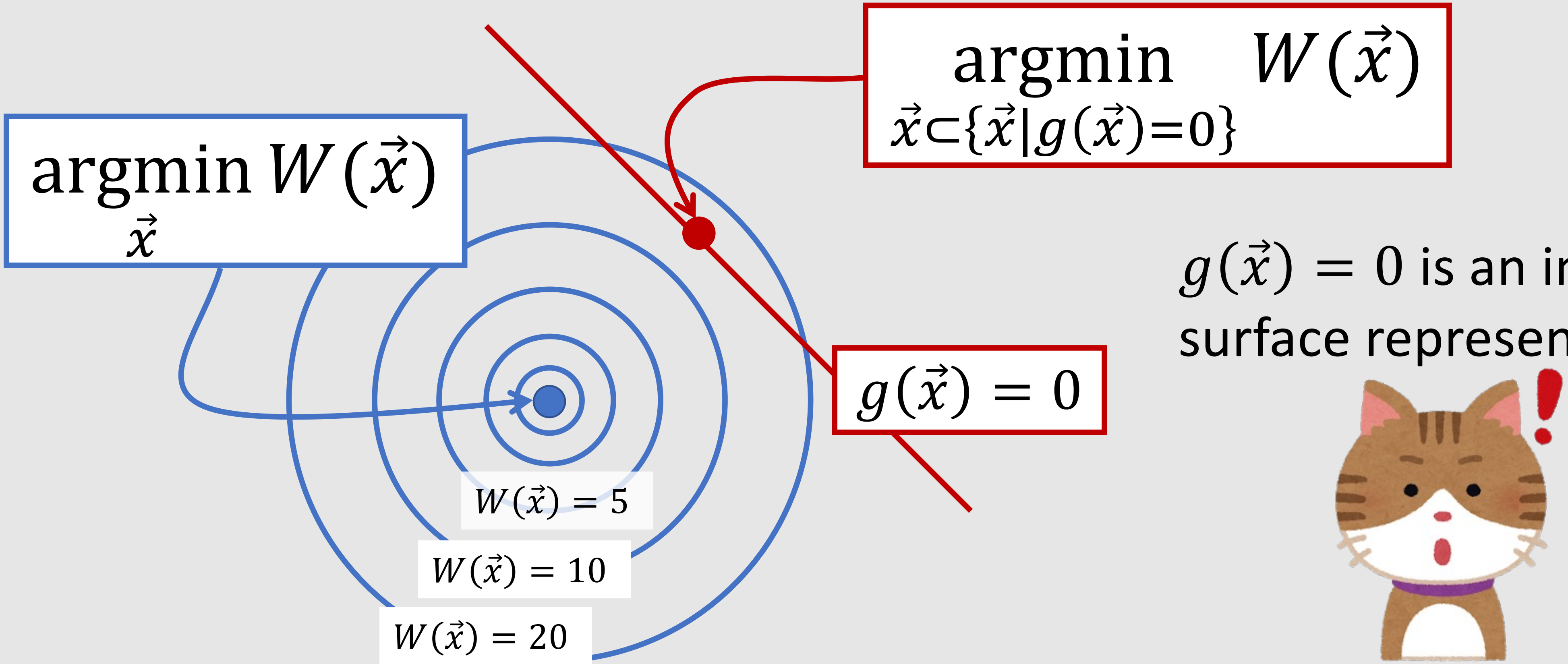
- Find a candidate where the gradient is zero $\nabla W(\vec{x}) = 0$



find the root of gradient!

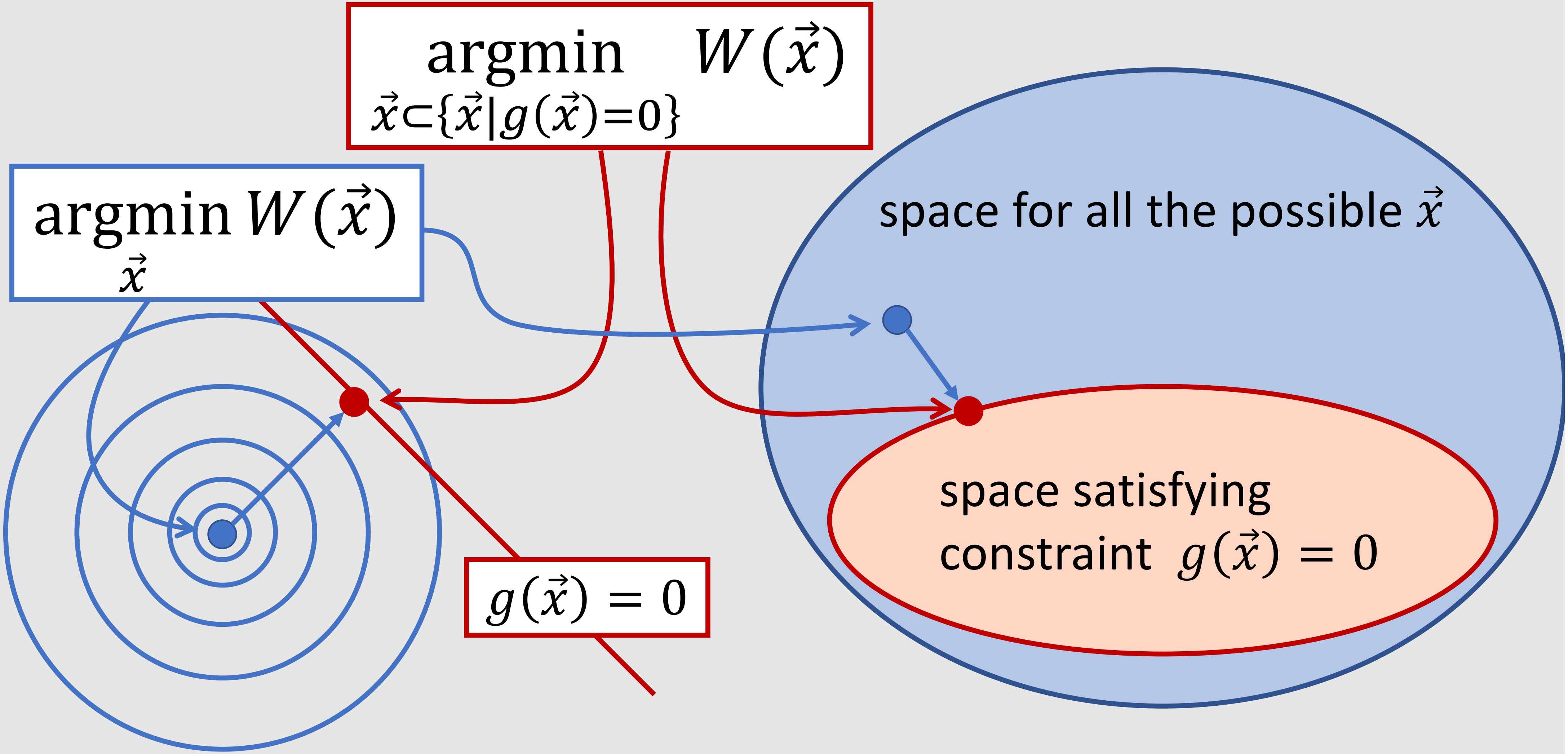
Optimization with Constraint

- Find a point $\vec{x}$ where the function $W(\vec{x})$ is minimized while satisfying $g(\vec{x}) = 0$



$g(\vec{x}) = 0$ is an implicit surface representation

Abstract View of the Solution Space

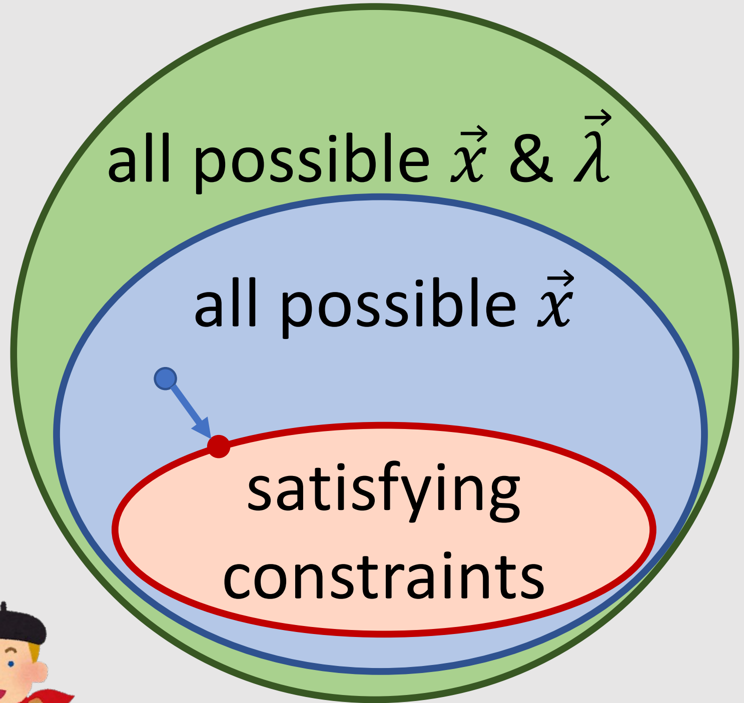


Three Approaches to Handle Constraints

- ***Degree of Freedom (DoF) elimination***
  - Optimization in the constraint space
  - Find minimum in

- ***Penalty method***
  - Approximate constraint as energy
  - Find minimum in

- ***Lagrange multiplier method***
  - Chose gradient parallel to the constraint's gradient
  - Find extremum in

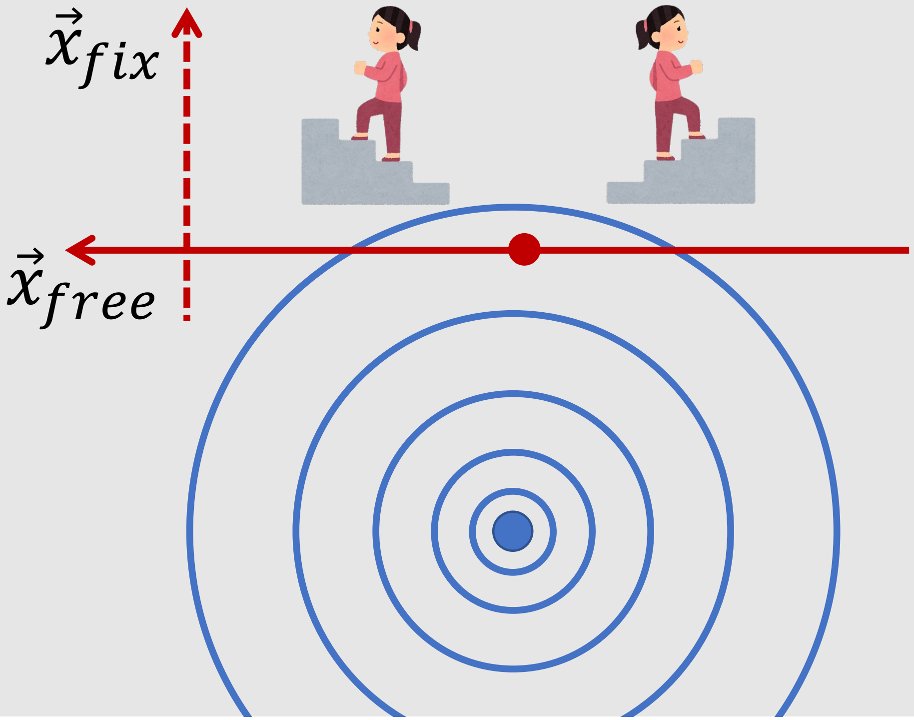


Degree of Freedom (DoF) Elimination

Degree of Freedom (DoF) Elimination

- Some DoF is fixed $\vec{x} = \{\vec{x}_{free}, \vec{x}_{fix}\}$

walk only on the line to find the minimum



$$dW(\vec{x}_{free}, \vec{x}_{fix}) = 0$$

$$\nabla W \cdot \begin{pmatrix} d\vec{x}_{free} \\ \boxed{d\vec{x}_{fix}} \end{pmatrix} = 0$$

$$\boxed{= 0}$$

Newton Method for DoF Elimination

- Update, Gradient and Hessian for Free/Fix DoF

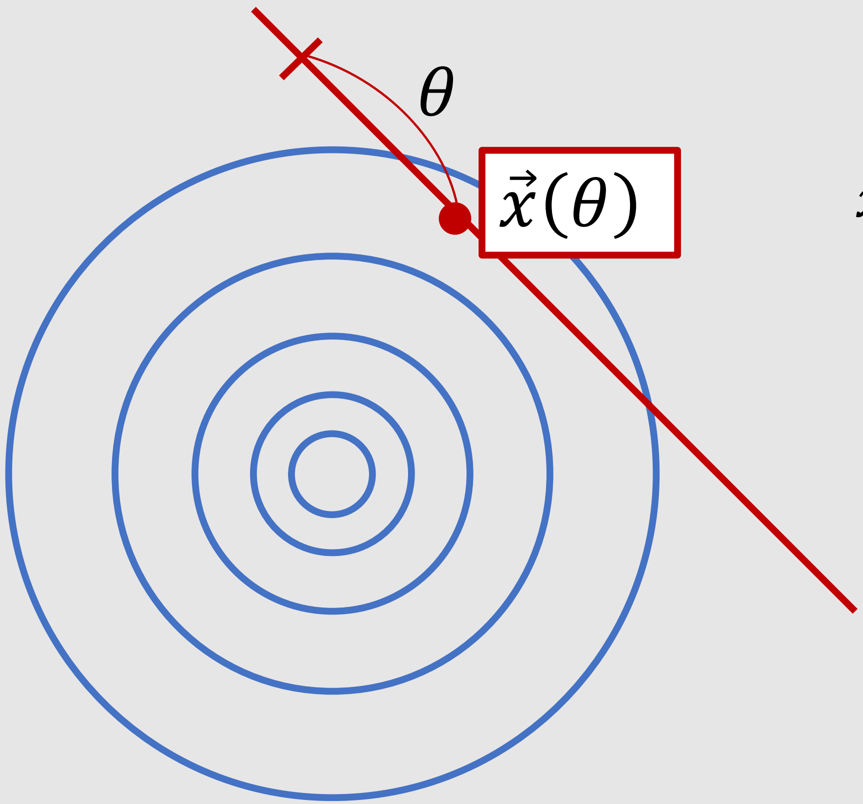
$$\nabla W = \begin{pmatrix} \nabla W_{free} \\ \nabla W_{fix} \end{pmatrix} \qquad \nabla^2 W = \begin{bmatrix} \nabla^2 W_{free,free} & \nabla^2 W_{free,fix} \\ \nabla^2 W_{fix,free} & \nabla^2 W_{fix,fix} \end{bmatrix}$$

- Update only $d\vec{x}_{free}$ (while $d\vec{x}_{fix} = 0$) to achieve $\nabla W_{free} = 0$

$$d\vec{x} = \begin{pmatrix} d\vec{x}_{free} \\ d\vec{x}_{fix} \end{pmatrix} = \begin{bmatrix} \nabla^2 W_{free,free} & 0 \\ 0 & I \end{bmatrix}^{-1} \begin{pmatrix} \nabla W_{free} \\ 0 \end{pmatrix}$$

DoF Elimination for General Constraint

Parameterize solution $\vec{x}(\theta)$ such that constraints naturally satisfy



$$\underset{\vec{x}\subset\{\vec{x}|g(\vec{x})=0\}}{\operatorname{argmin}} W(\vec{x}) \Rightarrow \underset{\theta}{\operatorname{argmin}} W(\vec{x}(\theta))$$

e.g., $g(\vec{x}) = x + y + 2 = 0$

$$\Rightarrow \begin{cases} x = +\theta - 1 \\ y = -\theta - 1 \end{cases}$$

Minimize Parameterized Solution

$$\underset{\theta}{\operatorname{argmin}}\, W(\vec{x}(\theta))$$

Newton-Raphson method

$$d\theta = -\left[\frac{\partial^2 W}{\partial \theta^2}\right]^{-1}\left(\frac{\partial W}{\partial \theta}\right)$$

find the root of gradient!

$$\frac{\partial W}{\partial \theta} = \frac{\partial W}{\partial \vec{x}}\frac{\partial \vec{x}}{\partial \theta} \text{ and } \frac{\partial^2 W}{\partial \theta^2} = \left(\frac{\partial \vec{x}}{\partial \theta}\right)^T \frac{\partial^2 W}{\partial \vec{x}^2}\left(\frac{\partial \vec{x}}{\partial \theta}\right)$$

DoF Elimination Use Cases

Fixing deformation in XYZ direction

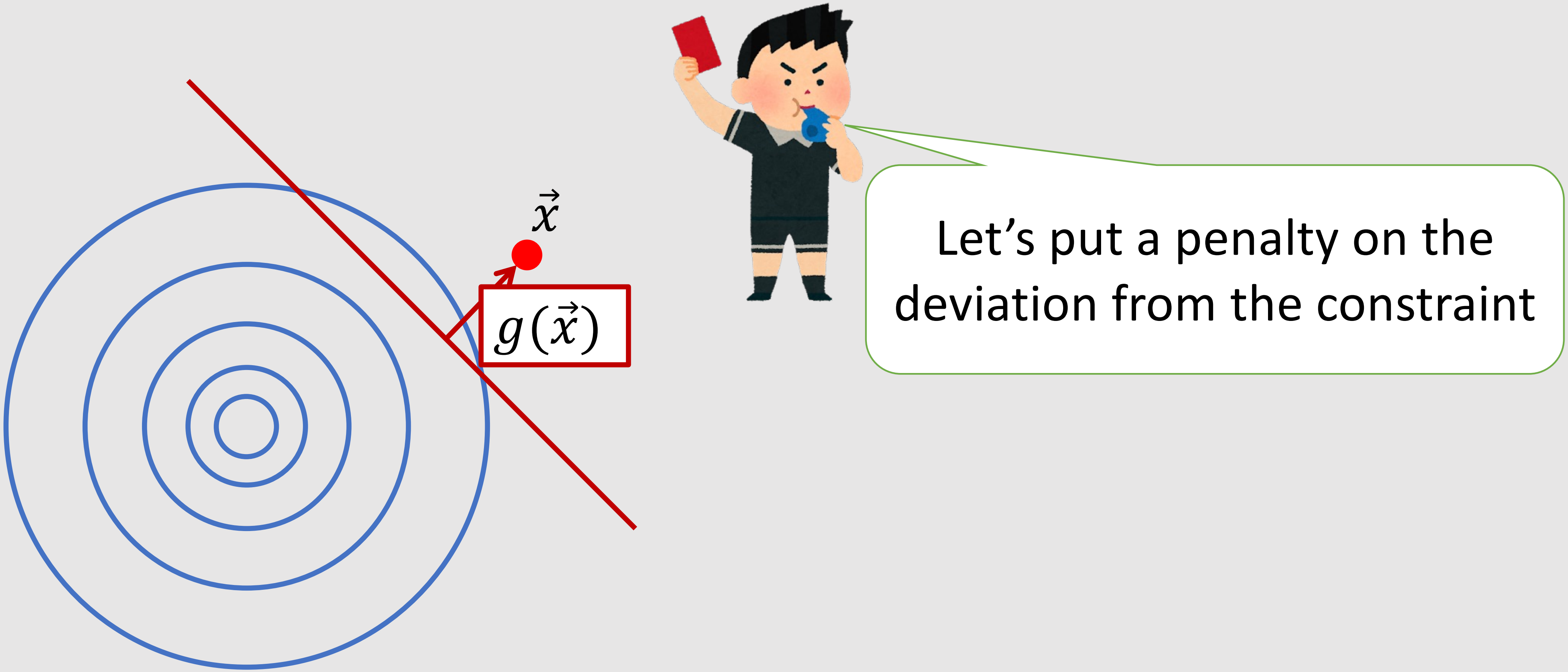
Optimization for rotation

Vortex method for fluid simulation

Penalty Method (Soft Constraint)

ペナルティー法

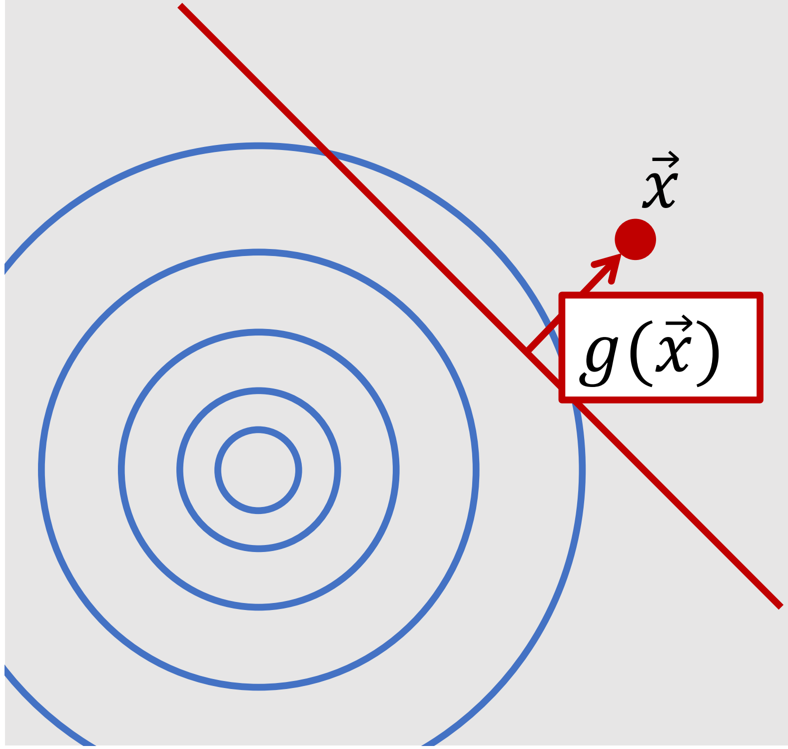
Deviation from Constraints is $g(\vec{x})$



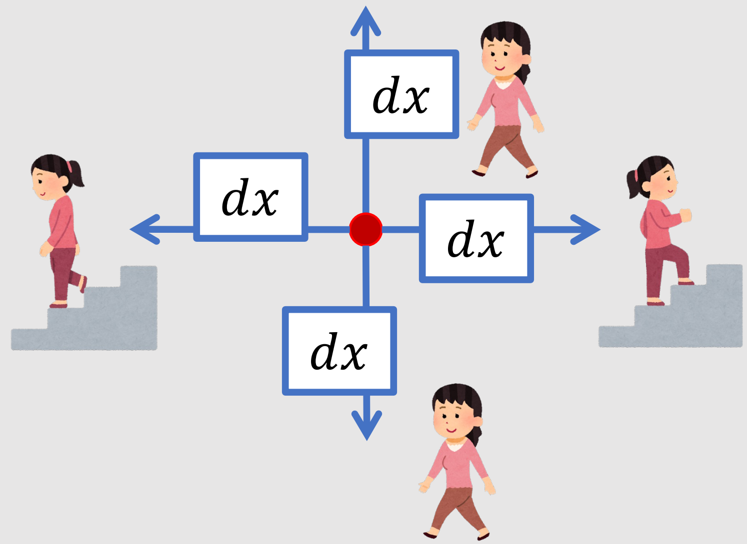
Penalty Method: Constraint as Energy

- Adding additional energy to encourage constraint

minimize $W(\vec{x}) + \alpha g^2(\vec{x})$ ➡ If α is large, $g(\vec{x})$ becomes small



$d\vec{x}$ can be all the direction



Linear System for Penalty Method

$$\boxed{\underset{\vec{x}}{\operatorname{argmin}}\, W(\vec{x}) + \alpha g^2(\vec{x})}$$

find the root of gradient!

Minimize $W + g$ with Newton's method:

$$d\vec{x} = -[\nabla^2 W + \underbrace{\alpha \nabla^2 g^2}_{2\nabla g \cdot \nabla g + 2\nabla^2 g}]^{-1}(\nabla W + \underbrace{\alpha \nabla g^2}_{2g\nabla g})$$

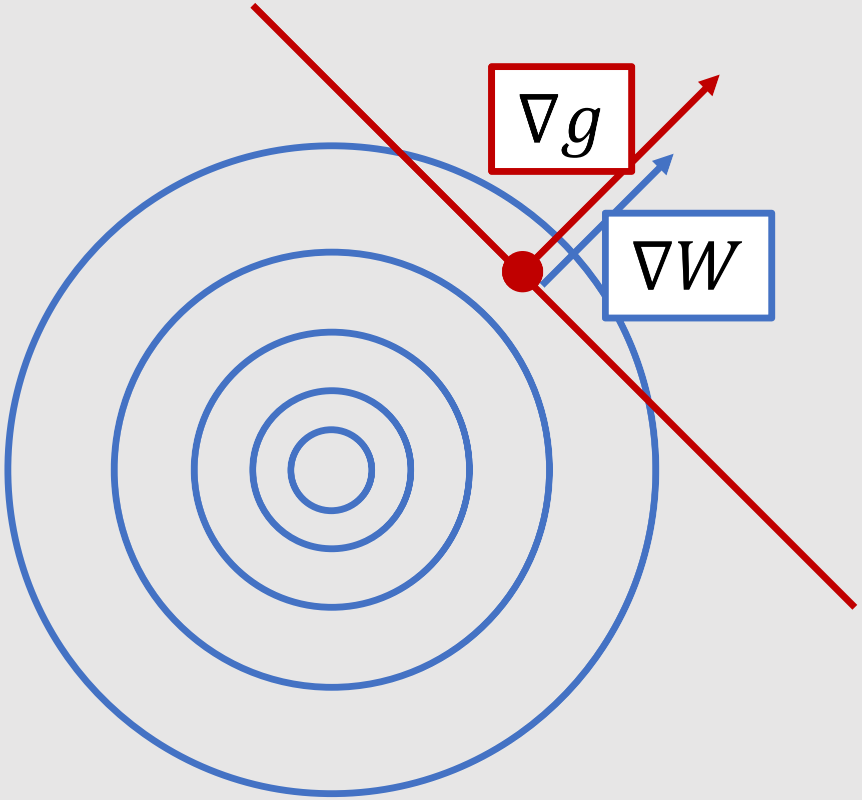
Lagrange Multiplier Method

ラグランジュ未定乗数法

je ne sais quoi!

Lagrange Multiplier Method

- At minimum point, two gradients $\nabla W, \nabla g$ should be parallel



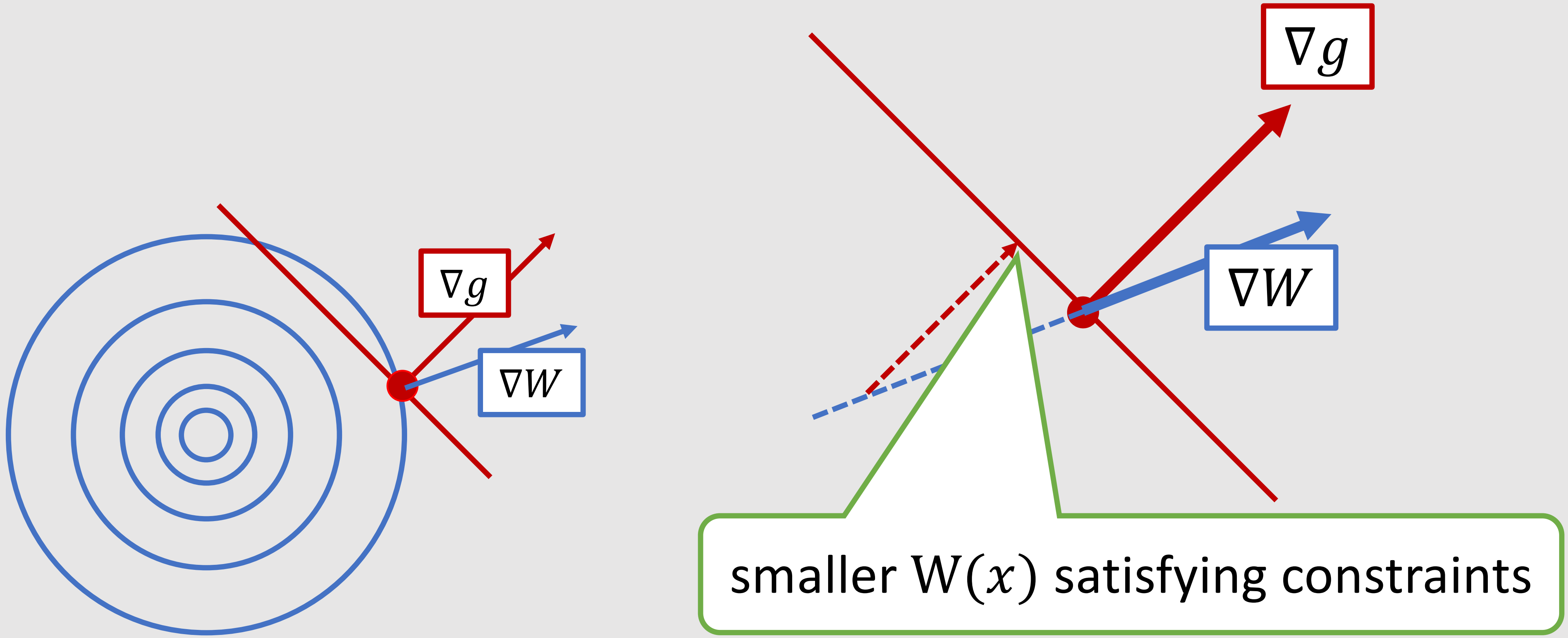
$$\nabla W \parallel \nabla g$$

$$\Downarrow$$

$$\exists \lambda \neq 0 \;\; s.t. \; \nabla W = \lambda \nabla g$$

Why Parallel at Constrained Minimum?

- If $\nabla W, \nabla g$ are not parallel, smaller $W(x)$ exists satisfying constraints



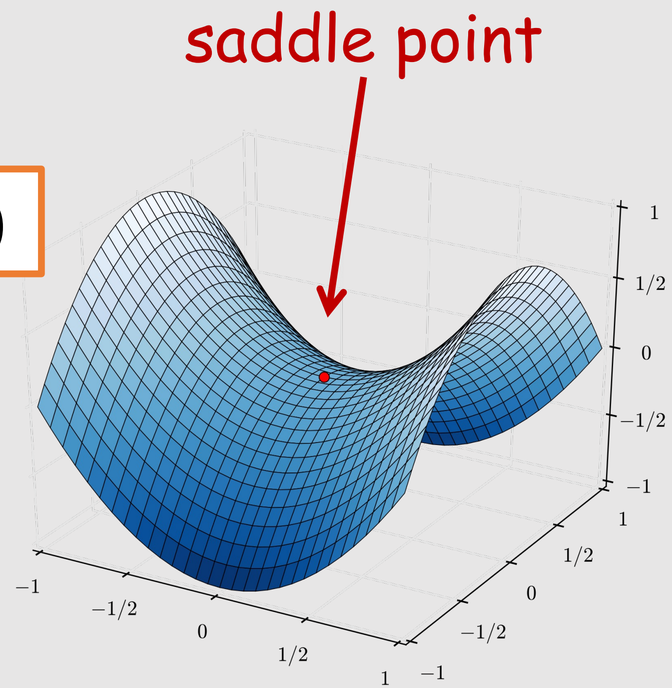
Find Saddle Point not Minima for LM Method

- We changed minimization problem to saddle point finding problem

$$\boxed{\nabla W(\vec{x}) = \lambda \nabla g(\vec{x})}$$

$$\boxed{\nabla \overline{W}(\vec{x},\lambda) = 0 \; where \; \overline{W}(\vec{x},\lambda) = W(\vec{x}) - \lambda g(\vec{x})}$$

Don’t minimize $\overline{W}\ (\vec{x},\lambda)$. Find where the gradient is zero using the Newton method

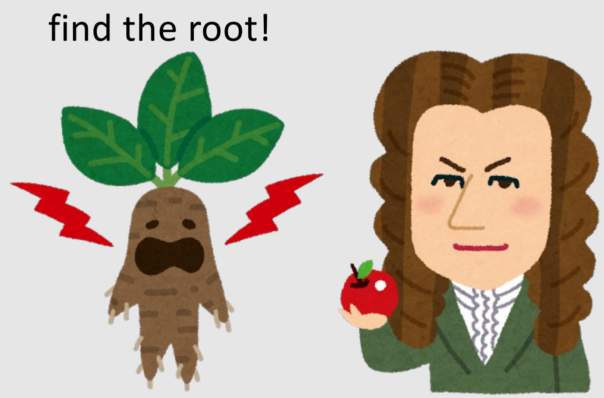


Credit: Nicoguaro @ Wikipedia

Lin. System for Lagrange Multiplier Method

$$\begin{pmatrix} \nabla W(\vec{x}) - \lambda \nabla g(\vec{x}) \\ -g(\vec{x}) \end{pmatrix} = H(\vec{x}, \lambda) = 0$$

Newton-Raphson method



$$\begin{aligned} \begin{pmatrix} d\vec{x} \\ d\lambda \end{pmatrix} &= -[\nabla H]^{-1} H \\ &= -\begin{bmatrix} \nabla^2 W(\vec{x}) - \lambda \nabla^2 g(\vec{x}) & -\nabla g(\vec{x}) \\ -\nabla g(\vec{x}) & 0 \end{bmatrix} \begin{pmatrix} \nabla W(\vec{x}) - \lambda \nabla g(\vec{x}) \\ -g(\vec{x}) \end{pmatrix} \end{aligned}$$

Let’s Practice Lagrange Multiplier Method

Maximize $f(x, y) = x + y$ where $g(x, y) = x^2 + y^2 - 1 = 0$

check it out!