

化学反応の数値

平良和昭

化学反応速度論への 半群論的アプローチ

講演の目標

- 化学反応論における**反応拡散方程式**の数学的研究を通して、**非線型解析学**を概観すること。

研究の目的

- 化学反応論で良く知られている実験データを**数学的に**解明すること。
- **フランク・カメネツキーのパラメータ**の**臨界値**（例えば**発火点**、**消火点**）の**数値解析**を**実際に行うための理論的な裏付け**を与えること。

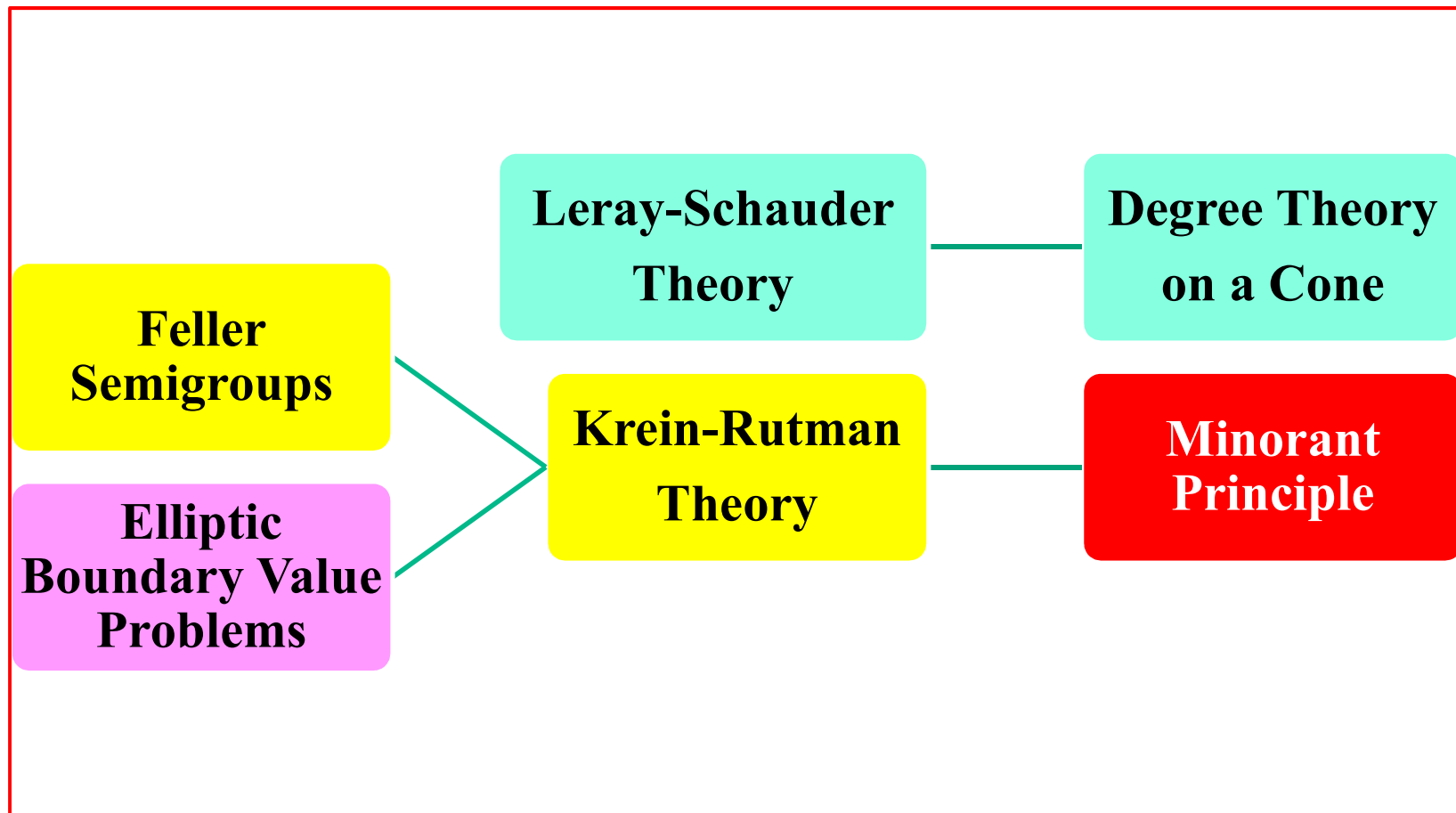
結論

- フランク・カメネツキーのパラメータの臨界値（例えば発火点、消火点）と一般ロバン境界条件との関連を解明した。

Bird's-Eye View

Fields	Subjects	Studied by
•Linear Algebra	•Markov Chains •Transition Matrices	Perron and Frobenius
•Probability	•Markov Processes •Green Operators	Feller and Dynkin
•Functional Analysis	•Minorant Principle •Eigenvalues	Krein and Rutman

My Approach to Chemical Reactions



文 献

General References

Brown, R.F. (2014): A topological introduction to nonlinear analysis, 3rd edition (Springer, Cham)

Chang, K.-C. (2005): Methods in nonlinear analysis (Springer-Verlag, Berlin)

My Work

Taira, K. (2016): Bifurcation curves in a combustion problem with general Arrhenius reaction-rate laws, *Annali dell'Universita di Ferrara*, Vol. 62, No. 2, 337-371

反應擴散方程式

化学反応と温度の関係

- 化学反応が進む
- 反応熱により、領域の温度が上昇
- 化学反応がさらに進む(アウレニウスの法則)
- 一方で、熱拡散が起こる
- 領域の境界で、境界条件(等温条件、断熱条件)を課す(ニュートンの冷却の法則)

アレニウスの法則

◆ 化学反応速度論におけるアレニウスの法則は、指数関数型の非線型項に対応している。

アレニウス

◆ **Svante August Arrhenius (1859-1927)**

スウェーデンの化学者

1903年ノーベル化学賞（電解質溶液における電離説）

Svante August Arrhenius



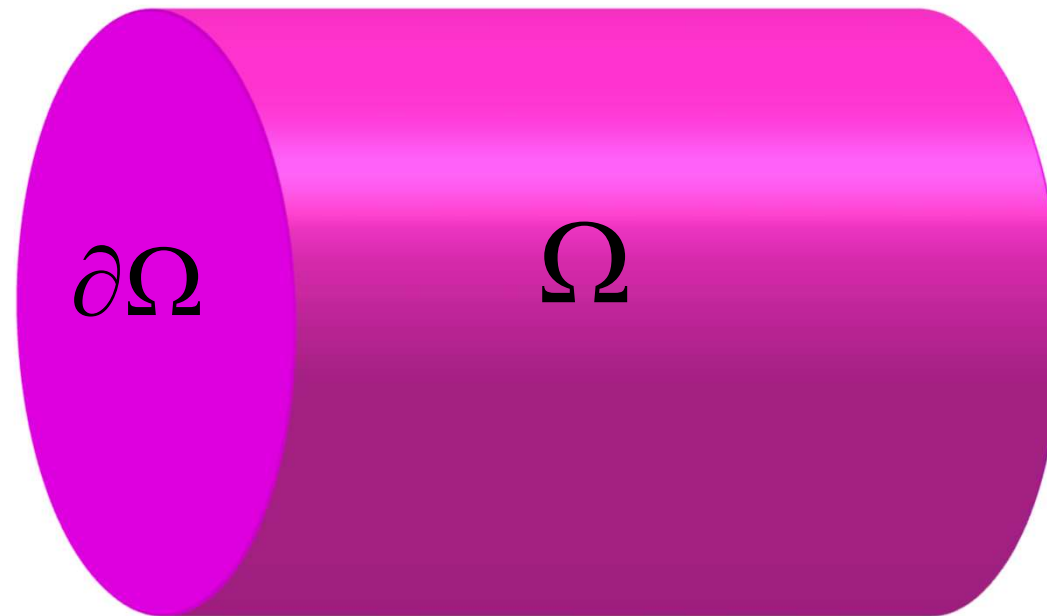
ニュートンの冷却の法則

◆ 熱の交換は容器表面の内と外との温度差に比例するというニュートンの冷却の法則は、一般ロバン境界条件に対応している。

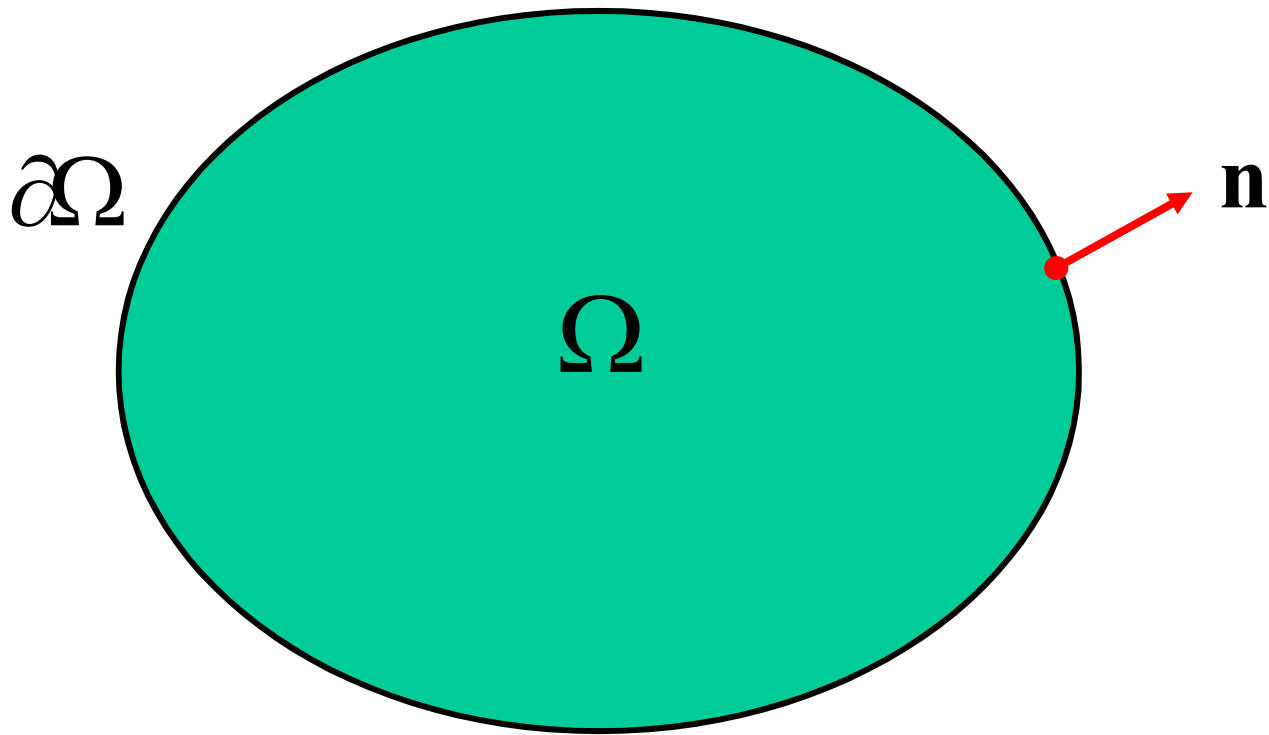
反応拡散方程式

(放物型初期値・境界値問題)

有界領域(フラスコ)



有界領域



反應擴散問題

$$\frac{\partial u}{\partial t} = \Delta u + \lambda(1 + \varepsilon u)^m \exp\left[\frac{u}{1 + \varepsilon u}\right] \quad \text{in } \Omega \times (0, \infty),$$

$$a \frac{\partial u}{\partial \mathbf{n}} + (1 - a)u = 0 \quad \text{on } \partial\Omega \times (0, \infty),$$

$$u|_{t=0} = u_0 \quad \text{in } \Omega.$$

Here:

$$0 \leq m < 1$$

各項の解釈

Simple Arrhenius rate law

$$\frac{\partial u}{\partial t} = \lambda \exp\left[\frac{u}{1 + \varepsilon u}\right] \quad \text{in } \Omega \times (0, \infty)$$

$$m = 0$$

Bimolecular rate law

$$\frac{\partial u}{\partial t} = \lambda(1 + \varepsilon u)^{\frac{1}{2}} \exp\left[\frac{u}{1 + \varepsilon u}\right] \quad \text{in } \Omega \times (0, \infty)$$

$$m = \frac{1}{2}$$

活性化エネルギー

$$\frac{1}{\varepsilon}$$

- 化学反応が起こるために、越えなければならないエネルギーの山

活性化エネルギー(敷居エネルギー)

- 活性化エネルギーの山が**高ければ**、化学反応は**ゆっくり**と進行する。
- 活性化エネルギーの山が**低ければ**、化学反応は**速やか**に進行する。

フランク・カメネツキーのパラメータ

λ

◆ 化学反応物の(無次元化された)発熱量

境界条件

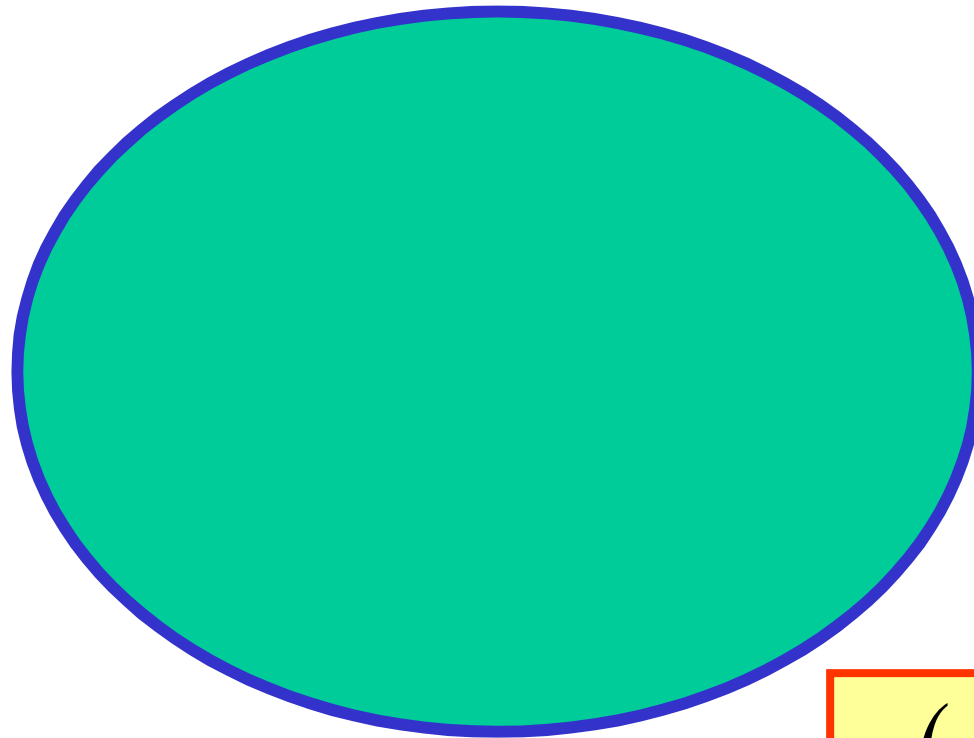
ニュートンの冷却の法則

$$\left[\frac{\partial u}{\partial \mathbf{n}} \right] = - \left(\frac{1-a}{a} \right) [u] \quad \text{on } \partial\Omega \times (0, \infty)$$

$$0 \leq a(x) \leq 1 \quad \text{on } \partial\Omega$$

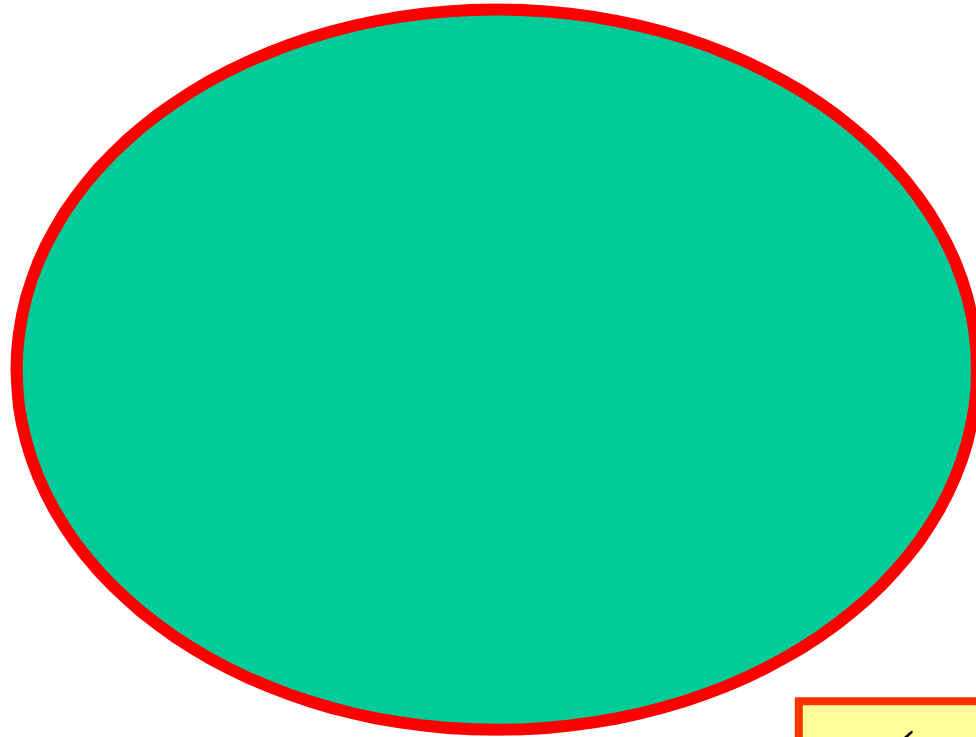
熱の交換（左辺）は容器表面の内と外との温度差（右辺）に比例する

等温(冷却)条件



$$a(x) \equiv 0$$

断热(保温)条件



$$a(x) \equiv 1$$

定常問題 (橢円型境界値問題)

反應擴散問題

$$-\Delta u = \lambda (1 + \varepsilon u)^m \exp\left[\frac{u}{1 + \varepsilon u}\right] \quad \text{in } \Omega$$

$$a \frac{\partial u}{\partial \mathbf{n}} + (1 - a) u = 0 \quad \text{on } \partial\Omega$$

發見的考察

非線形項

$$f(t) = (1 + \varepsilon t)^m \exp\left[\frac{t}{1 + \varepsilon t}\right]$$

$$0 \leq m < 1$$

反應擴散問題

$$\begin{cases} -\Delta u = \lambda f(u) & \text{in } \Omega \\ a \frac{\partial u}{\partial \mathbf{n}} + (1-a)u = 0 & \text{on } \partial\Omega \\ u > 0 & \text{in } \Omega \end{cases}$$

$$0 \leq a(x) \leq 1 \quad \text{on } \partial\Omega$$

非線形問題への 一般的なアプローチ

非線形問題の線形化近似

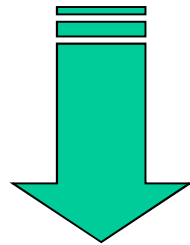
微分積分学	非線形関数解析学
曲線 $y = f(x)$	非線形方程式 $y = F(x)$
$f'(x_0) \neq 0$	$DF(x_0)$ 全単射
曲線 $y = f(x)$ は、点 x_0 の近くでは、直線 $y = f(x_0) + f'(x_0)(x - x_0)$ で近似される。	非線形方程式 $y = F(x)$ は、点 x_0 の近くでは、線形方程式 $y = F(x_0) + DF(x_0)(x - x_0)$ で近似される。

非線形問題の解法(1)

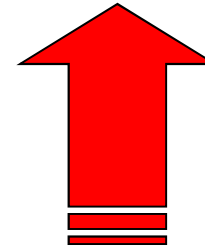
非線形問題

自明解のみ

線形化



逆関数定理



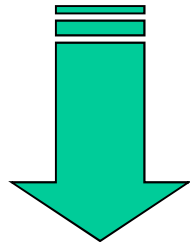
線形化問題が一意的可解的

非線形問題の解法(2)

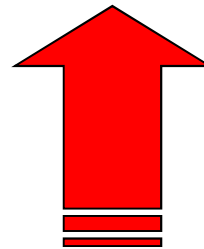
非線形問題

非自明解の存在

線形化



固有関数からの摂動



線形化問題の固有値が代数的に単純

固有値の重複度

- 幾何的重複度 = 固有空間の次元
- 代数的重複度 = 一般化固有空間の次元

幾何的單純性 (ジョルダン標準形)

$$\begin{pmatrix} \lambda & 1 & \cdot & \cdot & 0 \\ 0 & \lambda & 1 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \lambda & 1 \\ 0 & 0 & \cdot & \cdot & \lambda \end{pmatrix}$$

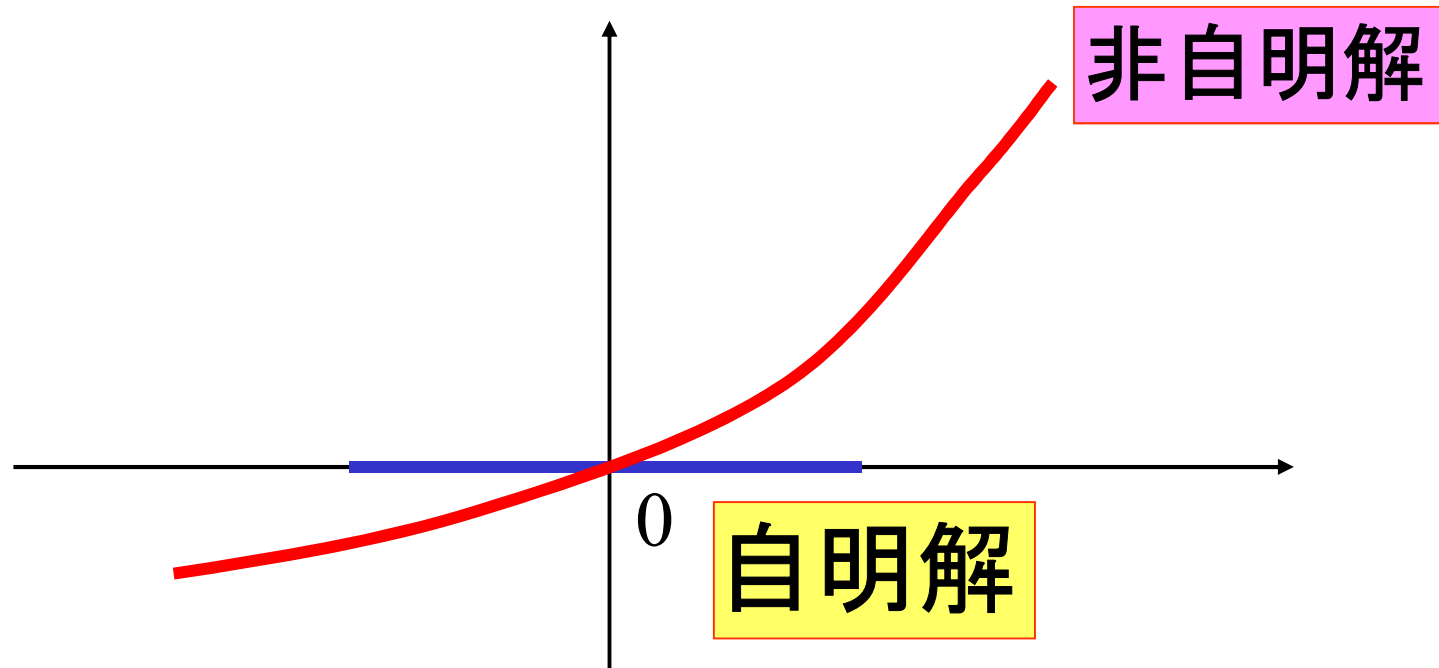
代数的単純性 (ジョルダン標準形)

$$\begin{pmatrix} \lambda & 0 & \cdot & \cdot & 0 \\ 0 & \mu & 1 & \cdot & 0 \\ \cdot & 0 & \mu & \cdot & \cdot \\ \cdot & \cdot & \cdot & \mu & 1 \\ 0 & 0 & \cdot & \cdot & \mu \end{pmatrix}$$

非線形問題の解法(3)

- ◆ 非線形問題の非自明解は、線形化問題の固有値から分岐する。
- ◆ 代数的に単純な固有値は、強い安定性を持ち、非自明な分岐解を固有関数からの摂動によって構成できる。

解の局所分岐ダイアグラム



Perron-Frobenius theorem
and
Markov Chains

Transition Matrix of a Markov Chain

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdot & \cdot & a_{1n} \\ a_{21} & a_{22} & \cdot & \cdot & a_{2n} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ a_{n-11} & a_{n-12} & \cdot & \cdot & a_{n-1n} \\ a_{n1} & a_{n2} & \cdot & \cdot & a_{nn} \end{pmatrix}$$

$$a_{ij} > 0$$

$$\sum_{j=1}^n a_{ij} = 1, \quad \sum_{j=1}^n a_{ji} = 1$$

Example

$$A = \begin{pmatrix} a & 1 - a \\ 1 - a & a \end{pmatrix}$$

$$0 < a < 1$$

Eigenvalues and Eigenvectors

Eigenvalues	Eigenvectors
1	$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$
$2a - 1$ $ 2a - 1 < 1$	$\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

Frobenius Root (1)

$$A \mathbf{f} = \mathbf{1} \mathbf{f}, \quad \mathbf{f} = \begin{pmatrix} 1 \\ 1 \\ \cdot \\ \cdot \\ 1 \end{pmatrix}$$

F r o b e n i u s r o o t 1

a l g e b r a i c a l l y s i m p l e e i g e n v a l u e

Frobenius Root (2)

$${}^t A \mathbf{f} = 1 \mathbf{f}, \quad \mathbf{f} = \begin{pmatrix} 1 \\ 1 \\ \cdot \\ \cdot \\ 1 \end{pmatrix}$$

Frobenius root 1

algebraically simple eigenvalue

Frobenius Root (3)

$$1 = \lim_{n \rightarrow \infty} \|A^n\|^{1/n} \quad (\text{Spectral Radius})$$

The Perron-Frobenius Theorem

$$T = (t_{ij}), \quad t_{ij} > 0.$$

Then :

$$(i) \quad r = \lim_{n \rightarrow \infty} \|T^n\|^{1/n} > 0. \quad (\text{spectral radius})$$

r is a **unique eigenvalue** of T

having **positive eigenvector**.

r is **algebraically simple**.

(ii) r is an algebraically simple eigenvalue of $T^* = (t_{ji})$ with a positive eigenvector.

セミヨ-ノフ近似式

固有值問題

$$\begin{cases} -\Delta \varphi_1 = \lambda_1 \varphi_1 & \text{in } \Omega \\ a \frac{\partial \varphi_1}{\partial \mathbf{n}} + (1-a) \varphi_1 = 0 & \text{on } \partial\Omega \\ \varphi_1 > 0 & \text{in } \Omega \end{cases}$$

正值解の候補 (1)

$$\mathbf{u} = C(\lambda)\varphi_1$$

正值解の候補 (2)

$$\begin{cases} -\Delta \mathbf{u} = \lambda_1 C(\lambda) \varphi_1 \\ \lambda f(\mathbf{u}) = \lambda f(C(\lambda) \varphi_1) \end{cases}$$

\Leftrightarrow

$$\lambda = \lambda_1 \frac{C(\lambda) \varphi_1}{f(C(\lambda) \varphi_1)} = \lambda_1 \frac{\mathbf{u}}{f(\mathbf{u})}$$

Semenov Approximations

$$v(t) = \frac{t}{f(t)} = \frac{t}{(1 + \varepsilon t)^m \exp\left[\frac{t}{1 + \varepsilon t}\right]}$$

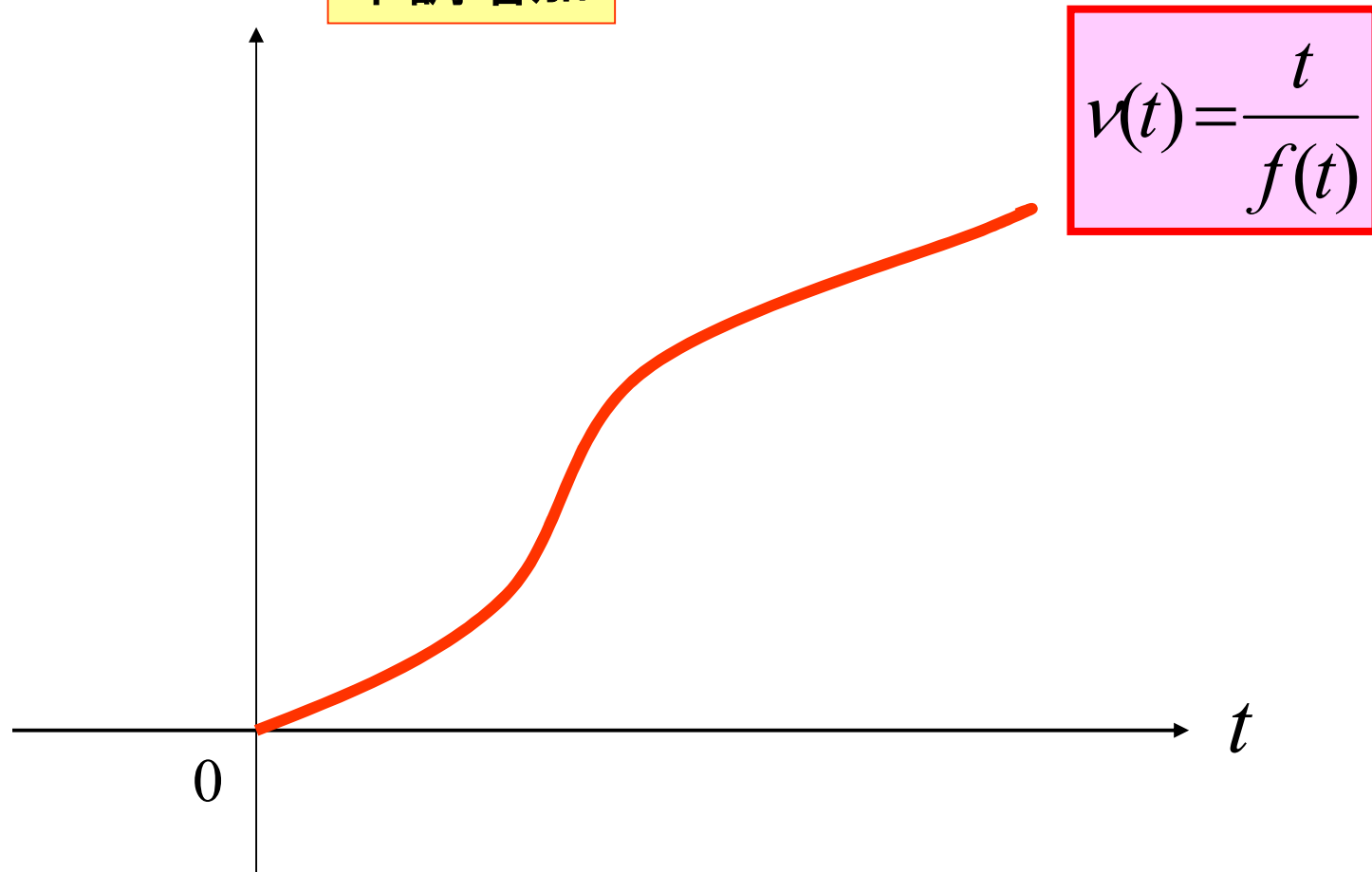
$$f(t) = (1 + \varepsilon t)^m \exp\left[\frac{t}{1 + \varepsilon t}\right]$$

$$\varepsilon \geq \left(\frac{1}{1 + \sqrt{1 - m}} \right)^2$$

\Rightarrow

$v(t) = \frac{t}{f(t)}$ **is increasing for all $t \geq 0$.**

単調増加



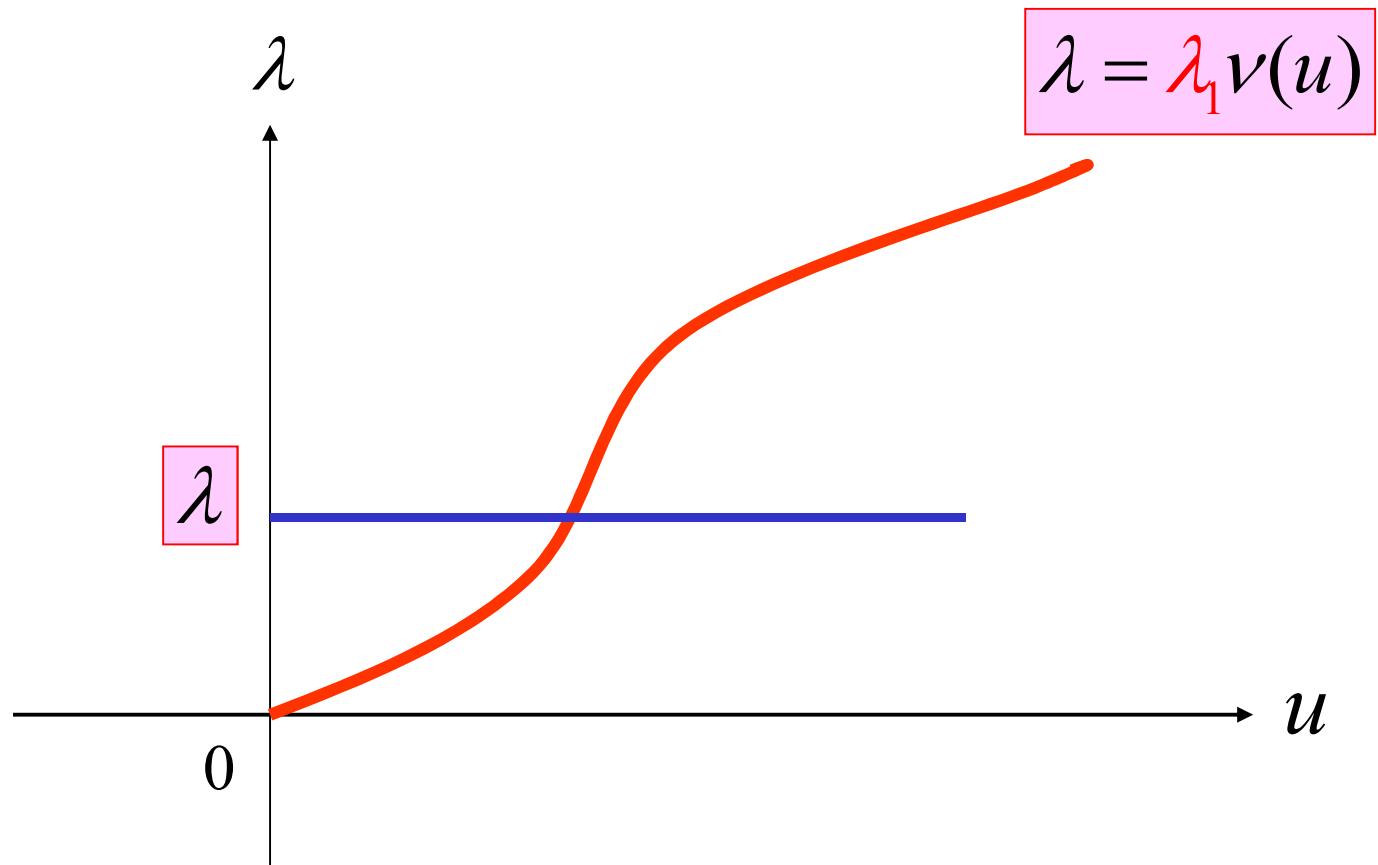
$$v(t) = \frac{t}{f(t)}$$

正值解の形

$$\begin{cases} -\Delta u = \lambda f(u) & \text{in } \Omega \\ a \frac{\partial u}{\partial \mathbf{n}} + (1-a)u = 0 & \text{on } \partial\Omega \\ u > 0 & \text{in } \Omega \end{cases}$$

\Leftrightarrow

$$\lambda = \lambda_1 \frac{u}{f(u)} = \lambda_1 v(u)$$



$$0 < \varepsilon < \left(\frac{1}{1 + \sqrt{1 - m}} \right)^2$$

\Rightarrow

$v(t) = \frac{t}{f(t)}$ has a local **maximum** at $t = t_1(\varepsilon)$

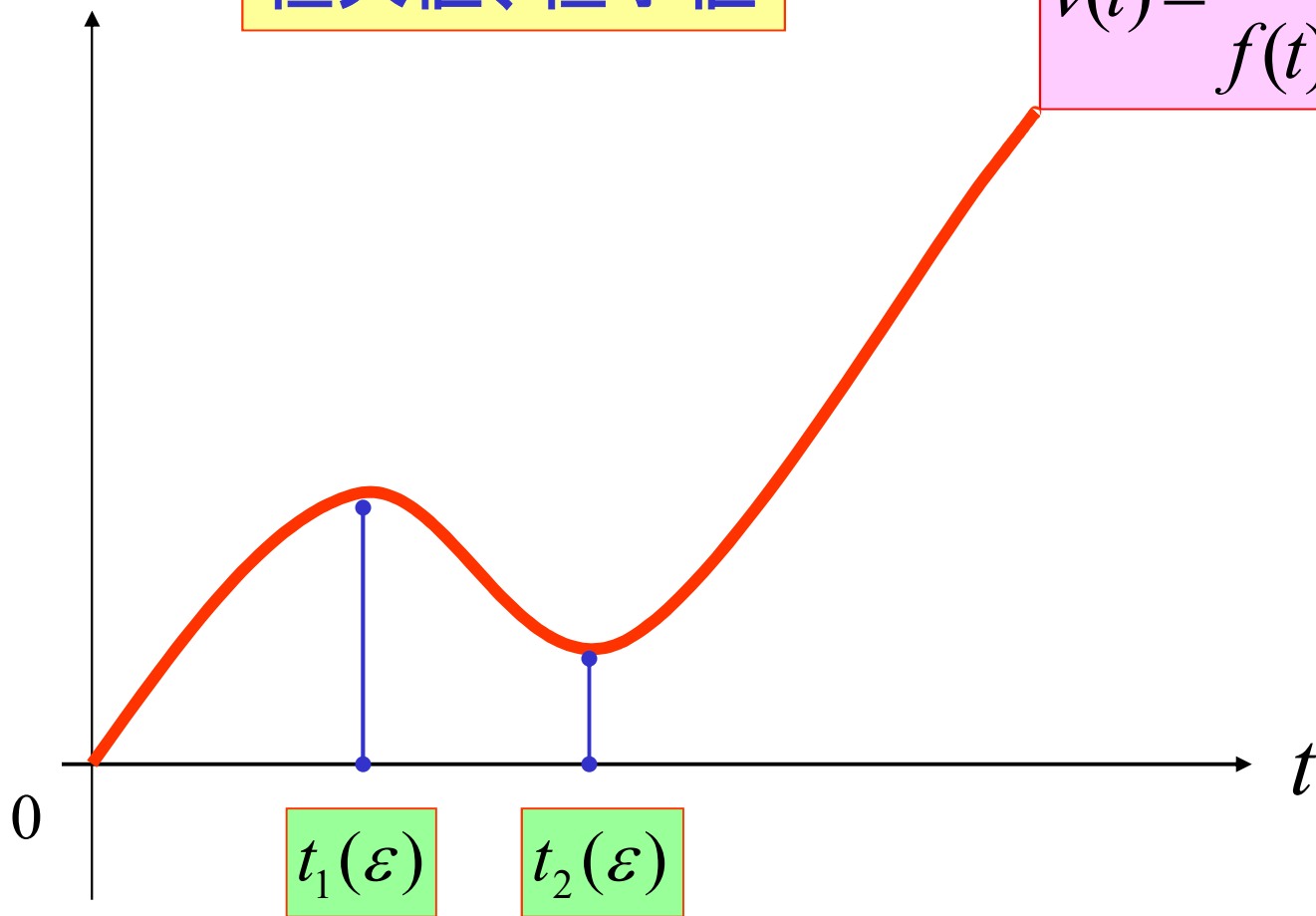
$v(t) = \frac{t}{f(t)}$ has a local **minimum** at $t = t_2(\varepsilon)$

$$t_1(\varepsilon) = \frac{1 + (m-2)\varepsilon - \sqrt{m^2\varepsilon^2 + 2(m-2)\varepsilon + 1}}{2(1-m)\varepsilon^2}$$

$$t_2(\varepsilon) = \frac{1 + (m-2)\varepsilon + \sqrt{m^2\varepsilon^2 + 2(m-2)\varepsilon + 1}}{2(1-m)\varepsilon^2}$$

極大値、極小値

$$v(t) = \frac{t}{f(t)}$$

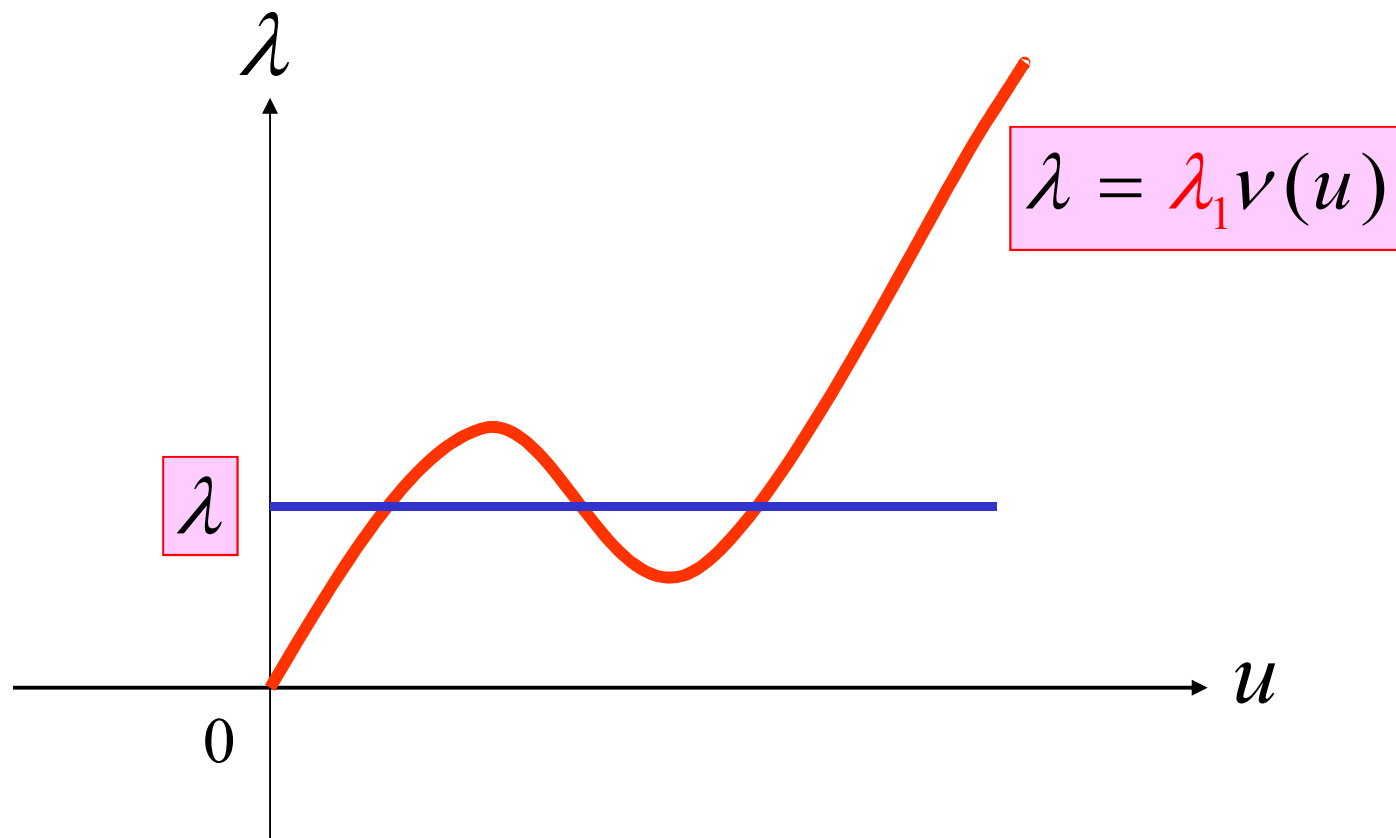


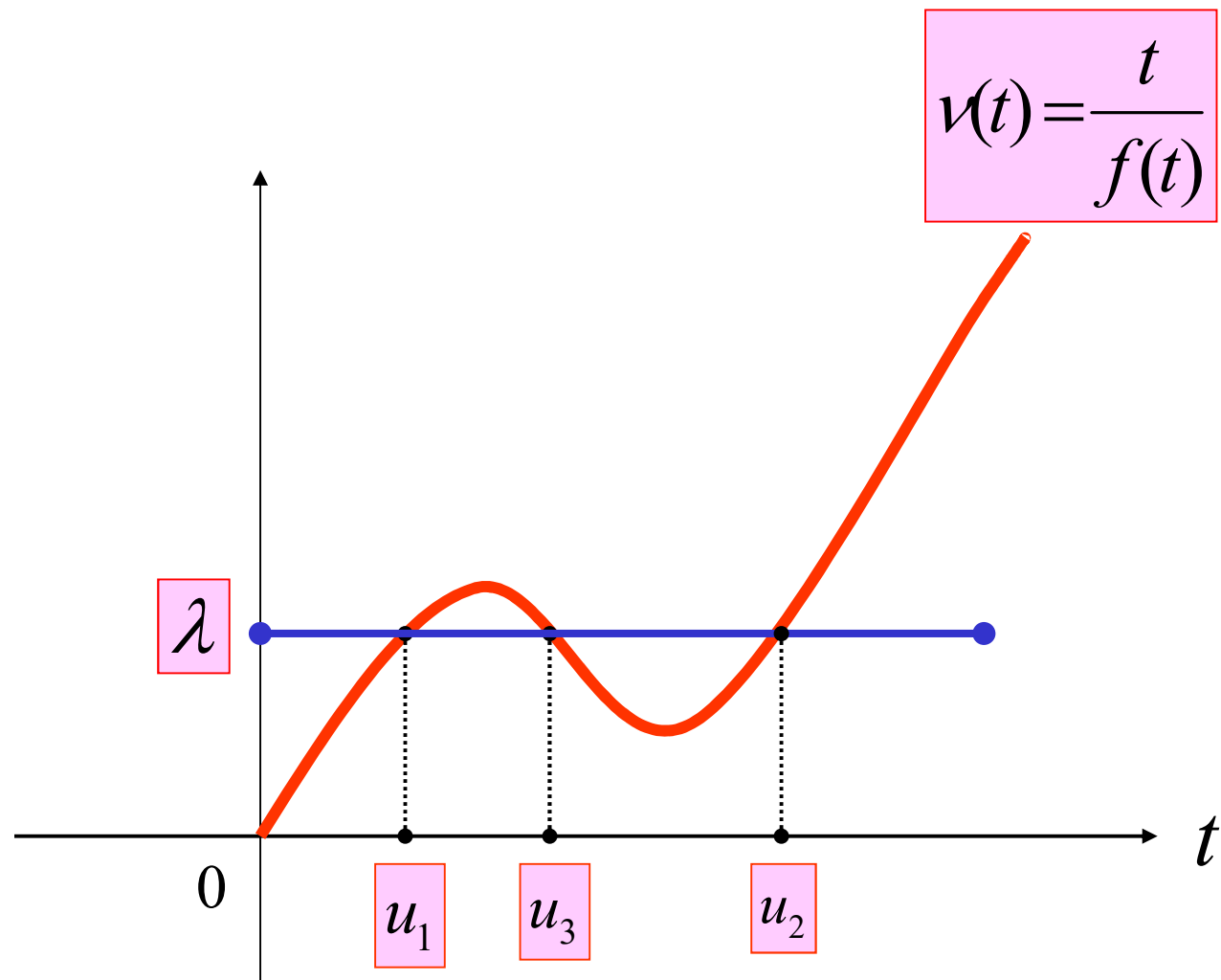
正值解の形

$$\begin{cases} -\Delta u = \lambda f(u) & \text{in } \Omega \\ a \frac{\partial u}{\partial \mathbf{n}} + (1-a)u = 0 & \text{on } \partial\Omega \\ u > 0 & \text{in } \Omega \end{cases}$$

\Leftrightarrow

$$\lambda = \lambda_1 \frac{u}{f(u)} = \lambda_1 v(u)$$





化学反応の数理

証明の概略

証明の概略 (その1)

Leray-Schauder Theory

文献

Leray, J., Schauder, J.(1934):

Topologie et equations fonctionelles.

**Ann. Sci. Ecole Norm. Sup. Vol. 51,
45-78.**

Bird's-Eye View

Existence Theorems	Finite-dimensional case	Nonlinear Analysis
Positive Solutions	Perron-Frobenius (Linear Algebra)	Krein-Rutmann (Minorant Principle)
Non-trivial Solutions	Brouwer Degree (Topology)	Leray-Schauder Degree (Degree Theory)

Schauder's Fixed-Point Theorem

Brouwer's Fixed-Point Theorem

A continuous f of a **closed, bounded convex** set Ω in \mathbb{R}^n into itself has a fixed point :

$$\exists x_0 \in \Omega \text{ such that } f(x_0) = x_0$$

Schauder's Fixed-Point Theorem

Let X be a real Banach space and Ω a **closed, bounded convex subset** of X .

If f is a **compact map** of Ω into itself, then it has a fixed point in Ω :

$\exists x_0 \in \Omega$ such that $f(x_0) = x_0$

写像度の有用性(1)

- The **Leray-Schauder degree** is an important **topological tool** introduced by Leray and Schauder in the study of **nonlinear partial differential equations**.

写像度の有用性(2)

- The **nontriviality** of the degree guarantees the **existence of a fixed point** of the **compact mapping** in the domain.
(Kronecker's existence theorem)

写像度の有用性(3)

- It should be emphasized that the more precisely we **know the degree** the sharper we can estimate **the number of fixed points**.
- This opens a door to the study of **multiple solutions** in nonlinear analysis.

Kronecker's Existence Theorem

Let X be a real Banach space and Ω a **bounded, open subset** of X with boundary $\partial\Omega$.

A map $K : \bar{\Omega} = \Omega \cup \partial\Omega \rightarrow X$ is **compact** and

$$\deg(I - K, p, \Omega) \neq 0$$

\Rightarrow

$\exists x_0 \in \bar{\Omega}$ such that $(I - K)x_0 = p$

ルレイ・シャウダーの写像度 (有限次元版)

写像度の導入(1)

$\Omega \subset \mathbf{R}^n$ 有界開集合

$$f = (f_1, f_2, \dots, f_n) : \bar{\Omega} = \Omega \cup \partial\Omega \rightarrow \mathbf{R}^n$$

C^1 級関数

写像度の導入(2)

f の ヤコビ 行列 式

$$J_f(x) := \begin{vmatrix} \frac{\partial f_1}{\partial x_1} & \cdot & \cdot & \frac{\partial f_1}{\partial x_n} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \frac{\partial f_n}{\partial x_1} & \cdot & \cdot & \frac{\partial f_n}{\partial x_n} \end{vmatrix}, \quad x \in \overline{\Omega}$$

$$n = 1 \implies J_f(x) = f'(x), \quad x \in \overline{\Omega}$$

写像度の導入(3)

$$p \in \mathbf{R}^n, \quad f(x) = p$$

(1) $f(x)$ の 正 則 値

$$\stackrel{\text{def}}{\Leftrightarrow} J_f(x) \neq 0$$

(2) $f(x)$ の 臨 界 値

$$\stackrel{\text{def}}{\Leftrightarrow} J_f(x) = 0$$

写像度の導入(4)

$p \in \mathbf{R}^n$, $f(x)$ の正則値の場合 :

$\text{deg}(f, p, \Omega)$

$$\stackrel{\text{def}}{=} \begin{cases} \sum_{f(x)=p} \text{sgn } J_f(x) & \text{if } f^{-1}(p) \neq \emptyset, \\ 0 & \text{if } f^{-1}(p) = \emptyset \end{cases}$$

Here :

$$\text{sgn } J_f(x) = \frac{J_f(x)}{|J_f(x)|}$$

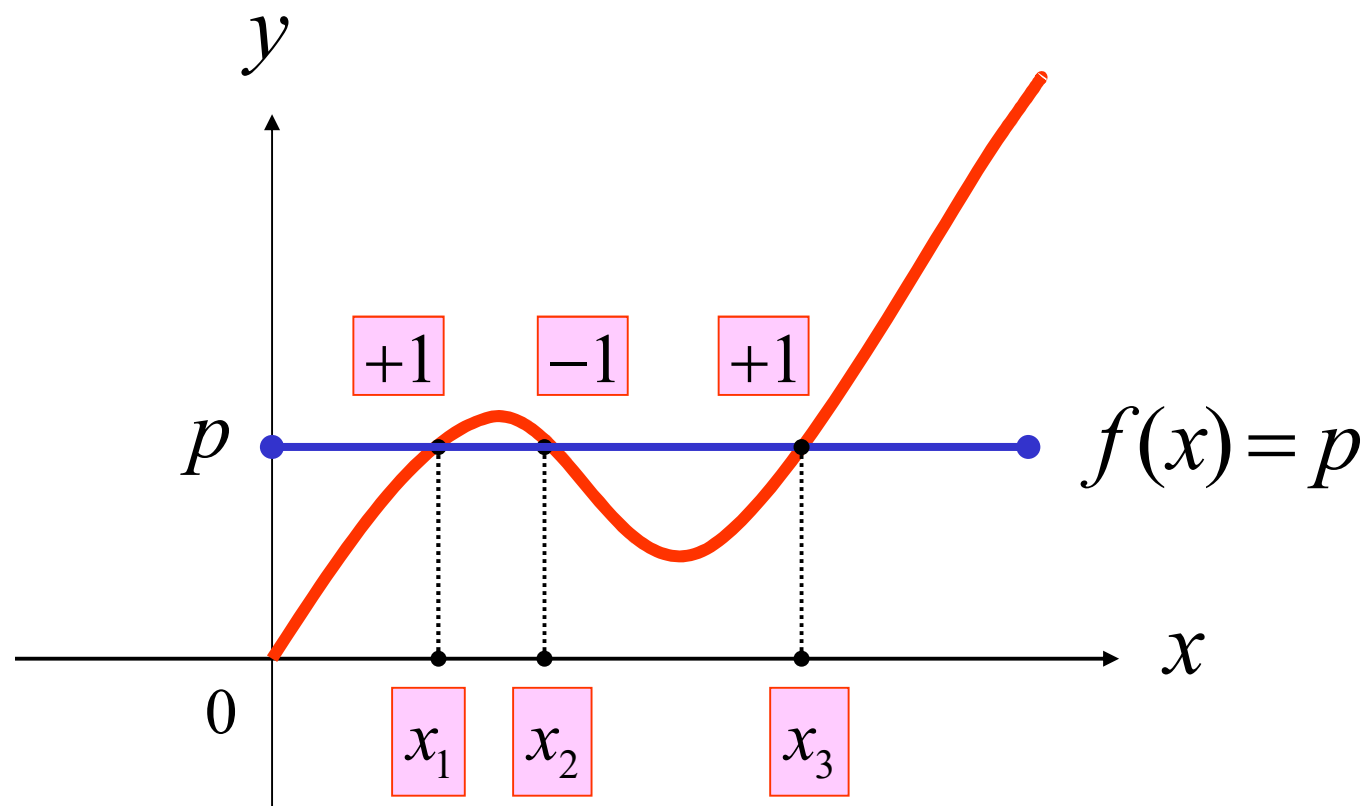
写像度の計算例(1)

$\Omega \subset \mathbf{R}$ 有界開集合

$f : \overline{\Omega} \rightarrow \mathbf{R}^1$ C^1 級関数

$$J_f(x) = f'(x), \quad x \in \overline{\Omega}$$

写像度の計算例(2)



写像度の計算例(3)

$$\begin{aligned} \deg(f, p, \Omega) &= \operatorname{sgn} f'(x_1) + \operatorname{sgn} f'(x_2) + \operatorname{sgn} f'(x_3) \\ &= 1 + (-1) + 1 \\ &= 1 \end{aligned}$$

中間値の定理

$$\varphi(x) := f(x) - p$$

\Rightarrow

$$\varphi(-1) = f(-1) - p < 0$$

$$\varphi(1) = f(1) - p > 0$$

\Rightarrow

$\exists x_0 \in (-1, 1)$ **such that**

$$\varphi(x_0) = f(x_0) - p = 0$$

(Intermediate Value Theorem)

写像度による存在証明

$f(x)$ is continuous on $I = [-1, 1]$

$f(I) \subseteq I, \quad p \in I$

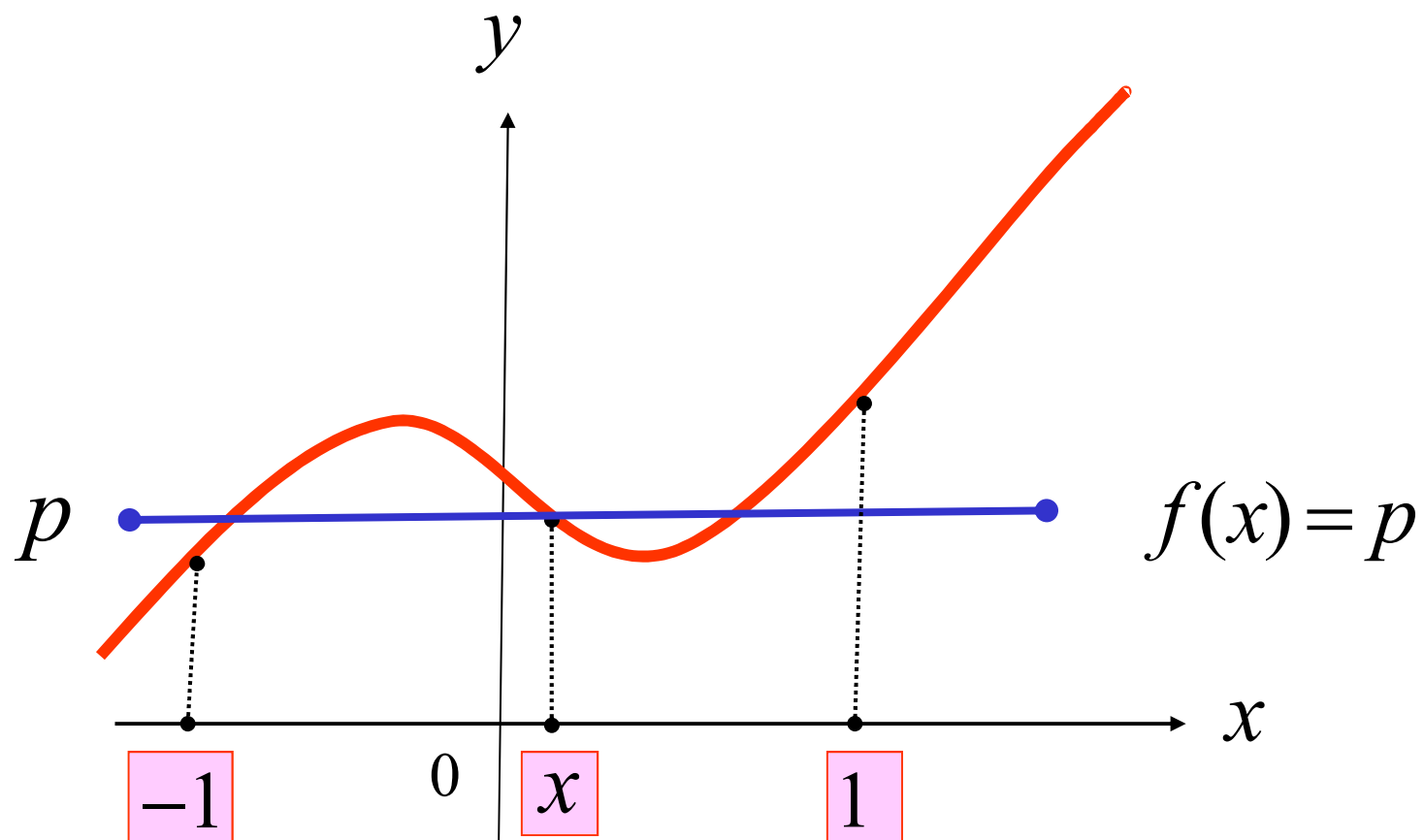
$$f(-1) - p < 0$$

$$f(1) - p > 0$$

\Rightarrow

$\exists x_0 \in I$ such that $f(x_0) = p$

写像度による証明(1)



写像度による証明(2)

$f(x) = p$ となる $x \in I$
の個数は奇数

$$\deg(f, p, \Omega)$$

$$= \operatorname{sgn} f'(x_1) + \operatorname{sgn} f'(x_2) + \operatorname{sgn} f'(x_3)$$

$$= 1 + (-1) + 1$$

$$= 1 \neq 0$$

写像度による証明(3)

$$I = [-1, 1]$$

$$\partial I = \{-1\} \cup \{1\}$$

$$f(\partial I) \neq p$$

$$\deg(f, p, \Omega) \neq 0$$

$$\Rightarrow \exists x_0 \in I \text{ such that } f(x_0) = p$$

Leray-Schauder Topological Degree

Sard's Lemma

$\Omega \subset \mathbf{R}^n$ 有界開集合

$f : \bar{\Omega} = \Omega \cup \partial\Omega \rightarrow \mathbf{R}^n$ C^1 級関数

\Rightarrow

臨界値の集合は \mathbf{R}^n の中で測度ゼロ

Compact Mapping

X a real Banach space

Ω a **bounded, open subset** of X

with boundary $\partial\Omega$

A continuous map $f : \Omega \rightarrow X$ is **compact**

if it maps **bounded sets** in Ω into

relatively compact sets of X

Characterization of Compact Mappings

A continuous map $f : \Omega \rightarrow X$ is **compact**

\Leftrightarrow

f is a **uniform limit** of mappings

whose ranges lie in **finite - dimensional subspaces**

Leray-Schauder Degree (1)

Let X be a real Banach space

Ω bounded open set in X

$K : \overline{\Omega} \rightarrow X$ compact map

$$x - Kx \neq p, \quad \forall x \in \partial\Omega$$

Leray-Schauder Degree (2)

$K : \bar{\Omega} \rightarrow X$ **compact map**

$$(1) K(\bar{\Omega}) \subseteq X_n$$

$$(2) p \in X_n$$

X_n **finite - dimensional subspace of X**

\Rightarrow

$$\deg(I - K, p, \Omega) := \deg(I - K, p, \Omega \cap X_n)$$

Leray-Schauder Degree (3)

$K : \bar{\Omega} \rightarrow X$ **compact map**

$K_n : \bar{\Omega} \rightarrow X_n$

$$\sup_{x \in \bar{\Omega}} \|Kx - K_n x\| \leq \frac{1}{n}$$

\Rightarrow

$$\deg(I - K, p, \Omega) := \lim_{n \rightarrow \infty} \deg(I - K_n, p, \Omega \cap X_n)$$

写像度の基本的性質

- (1) ホモトピー不変性
- (2) 正規性
- (3) 領域に関する加法性
- (4) 存在性

(1) Homotopy Invariance

Ω a **bounded open subset of X**

$K : \overline{\Omega} \times [0, 1] \rightarrow \mathbf{R}^n$ **compact**

$$x - K(x, t) \neq p, \quad 0 \leq \forall t \leq 1, \forall x \in \partial\Omega$$

\Rightarrow

$\deg(I - K(\cdot, t), p, \Omega)$ **is independent of t**

(1) ホモトピー不変性

$h(x, t) : \bar{\Omega} \times [0, 1] \rightarrow \mathbf{R}^n$ 連続関数

$h(\cdot, t) : \bar{\Omega} \rightarrow \mathbf{R}^n$ C^2 関数

$$h(x, t) \neq p, \quad \forall x \in \partial\Omega, 0 \leq \forall t \leq 1$$

\Rightarrow

$\deg(h(\cdot, t), p, \Omega)$ t について不変

(2) ホモトピー不変性

$h(x, t) : \bar{\Omega} \times [0, 1] \rightarrow \mathbf{R}^n$ 連続関数

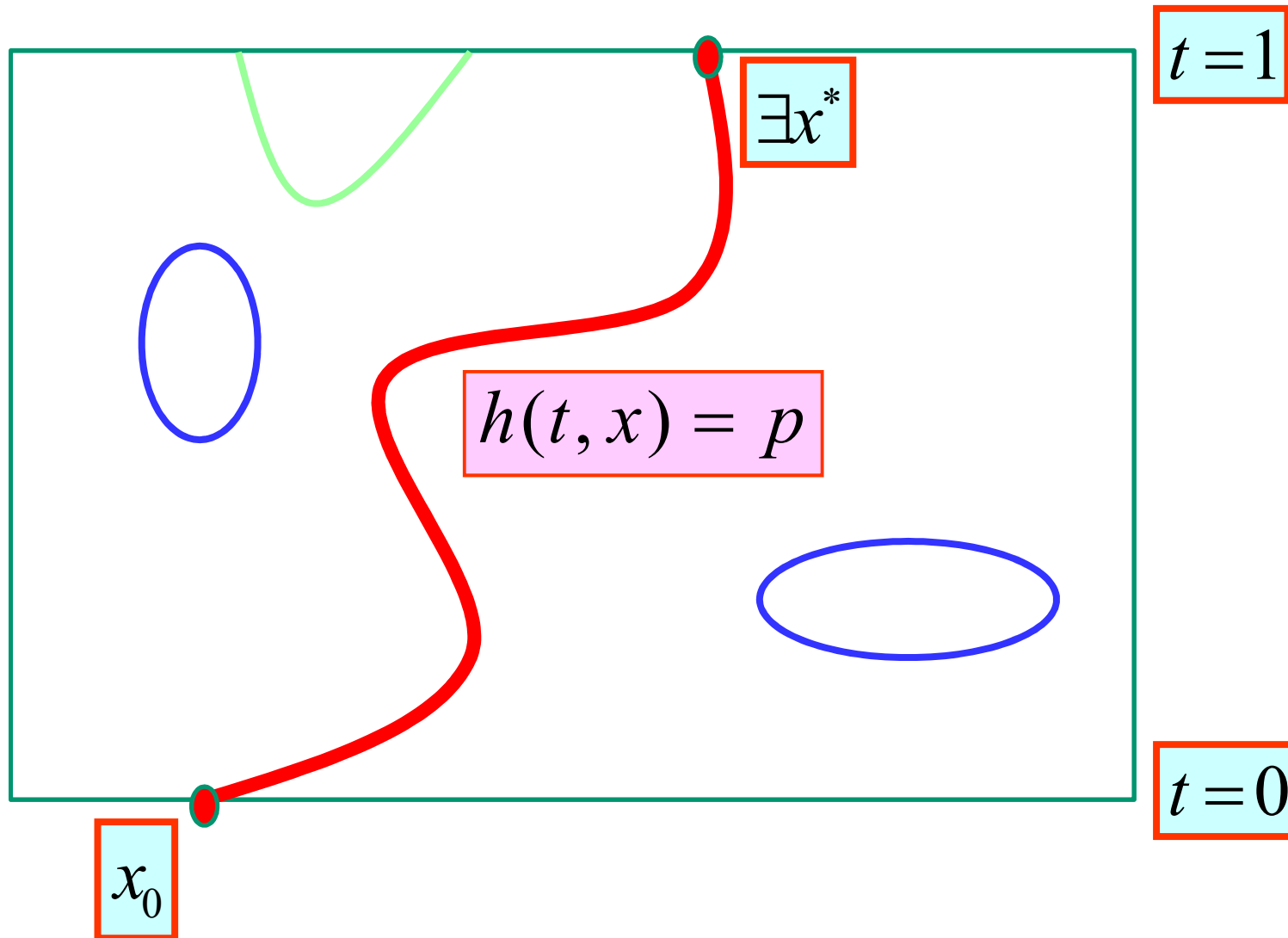
$$\begin{cases} f_0 = h(\cdot, 0) : \bar{\Omega} \rightarrow \mathbf{R}^n \\ f_1 = h(\cdot, 1) : \bar{\Omega} \rightarrow \mathbf{R}^n \end{cases}$$

$$h(x, t) \neq p, \quad \forall x \in \partial\Omega, 0 \leq \forall t \leq 1$$

\Rightarrow

$$\deg(f_0, p, \Omega) = \deg(f_1, p, \Omega)$$

$$h(x, t) \neq p, \quad \forall x \in \partial\Omega, 0 \leq \forall t \leq 1$$



(2) Normalization

$$\deg(I, p, \Omega) = \begin{cases} 1 & \text{if } p \in \Omega \\ 0 & \text{if } p \notin \Omega \end{cases}$$

(2) 正規性

$$f(x) = x - x_0, \quad x_0 \in \Omega$$

\Rightarrow

$$\deg(f, 0, \Omega) = 1$$

(3) Translation Invariance

$$\deg(I - K, p, \Omega) = \deg(I - K - p, 0, \Omega)$$

(4) Domain Additivity

$$\Omega_1, \Omega_2 \subseteq \Omega, \quad \Omega_1 \cap \Omega_2 = \emptyset$$

$$x - Kx \neq p, \quad \forall x \in \overline{\Omega} \setminus (\Omega_1 \cup \Omega_2)$$

\Rightarrow

$$\deg(I - K, p, \Omega)$$

$$= \deg(I - K, p, \Omega_1) + \deg(I - K, p, \Omega_2)$$

(3) 領域に関する加法性

$$\Omega_1, \Omega_2 \subseteq \Omega, \quad \Omega_1 \cap \Omega_2 = \emptyset$$

$$f(x) \neq p, \quad \forall x \in \overline{\Omega} \setminus (\Omega_1 \cup \Omega_2)$$

\Rightarrow

$$\deg(f, p, \Omega)$$

$$= \deg(f, p, \Omega_1) + \deg(f, p, \Omega_2)$$

Kronecker's Existence Theorem

Let X be a real Banach space and Ω a **bounded, open subset** of X with boundary $\partial\Omega$.

A map $K : \bar{\Omega} = \Omega \cup \partial\Omega \rightarrow X$ is **compact** and

$$x - Kx \neq p, \quad \forall x \in \partial\Omega$$

$$\deg(I - K, p, \Omega) \neq 0$$

\Rightarrow

$\exists x_0 \in \Omega$ such that $(I - K)x_0 = p$

(4) 解の存在性

$$\deg(f, p, \Omega) \neq 0$$

$$\Rightarrow \exists x_0 \in \Omega \text{ such that } f(x_0) = p$$

Fixed Point Existence Theory

Finite-Dimensional Example (Index Theorem)

Let A be a real **non-singular** matrix in \mathbf{R}^n

$$T = I - A$$

\Rightarrow

$$\deg T := \operatorname{sgn}(\det A) = (-1)^\beta$$

$$\beta = \sum_{\lambda > 1} n_\lambda(T)$$

Example (1)

$$A = \begin{pmatrix} a & 1 \\ 0 & b \end{pmatrix}, \quad ab \neq 0$$

$$T = I - A = \begin{pmatrix} 1 - a & -1 \\ 0 & 1 - b \end{pmatrix}$$

\Rightarrow

$$\text{deg } T := \text{sgn}(ab) = (-1)^\beta$$

$$\beta = \sum_{\lambda > 1} n_\lambda(T)$$

Example (2)

$$\det(\lambda I - T)$$

$$= (\lambda - (1 - a))(\lambda - (1 - b))$$

$$\lambda > 1 \Leftrightarrow 1 - a > 1, 1 - b > 1$$

$$\Leftrightarrow a < 0, b < 0$$

Example (3)

a	b	$\deg T$	β	$(-1)^\beta$
+	+	+1	0	+1
+	-	-1	1	-1
-	+	-1	1	-1
-	-	+1	2	+1

Leray-Schauder Index

Leray-Schauder Index (1)

Let X be a real Banach space

Ω a bounded open set in X

$$\phi : \overline{\Omega} = \Omega \cup \partial\Omega \rightarrow X$$

$$\phi \in C^1(\Omega, X)$$

$$\phi(x) \neq 0, \forall x \in \partial\Omega$$

$$K = I - \phi : \overline{\Omega} \rightarrow X \text{ compact}$$

Leray-Schauder Index (2)

$$\begin{cases} x_0 \text{ **isolated solution of } \phi(x) = 0 \\ D\phi(x_0) = I - DK(x_0) \text{ **invertible} \end{cases}****$$

\Rightarrow

$$i(\phi, 0, x_0) := \deg(I - K, 0, B(x_0, \varepsilon))$$

Index Theorem

$$\phi : \overline{\Omega} = \Omega \cup \partial\Omega \rightarrow X$$

$$\phi \in C^1(\Omega, X)$$

$$\phi(x) \neq 0, \forall x \in \partial\Omega$$

$$K = I - \phi : \overline{\Omega} \rightarrow X \text{ compact}$$

\Rightarrow

$$i(\phi, 0, x_0) = (-1)^\beta, \quad \beta = \sum_{\lambda_j > 1} \beta_j$$

Schaefers Fixed Point Theorem

Let X be a real Banach space

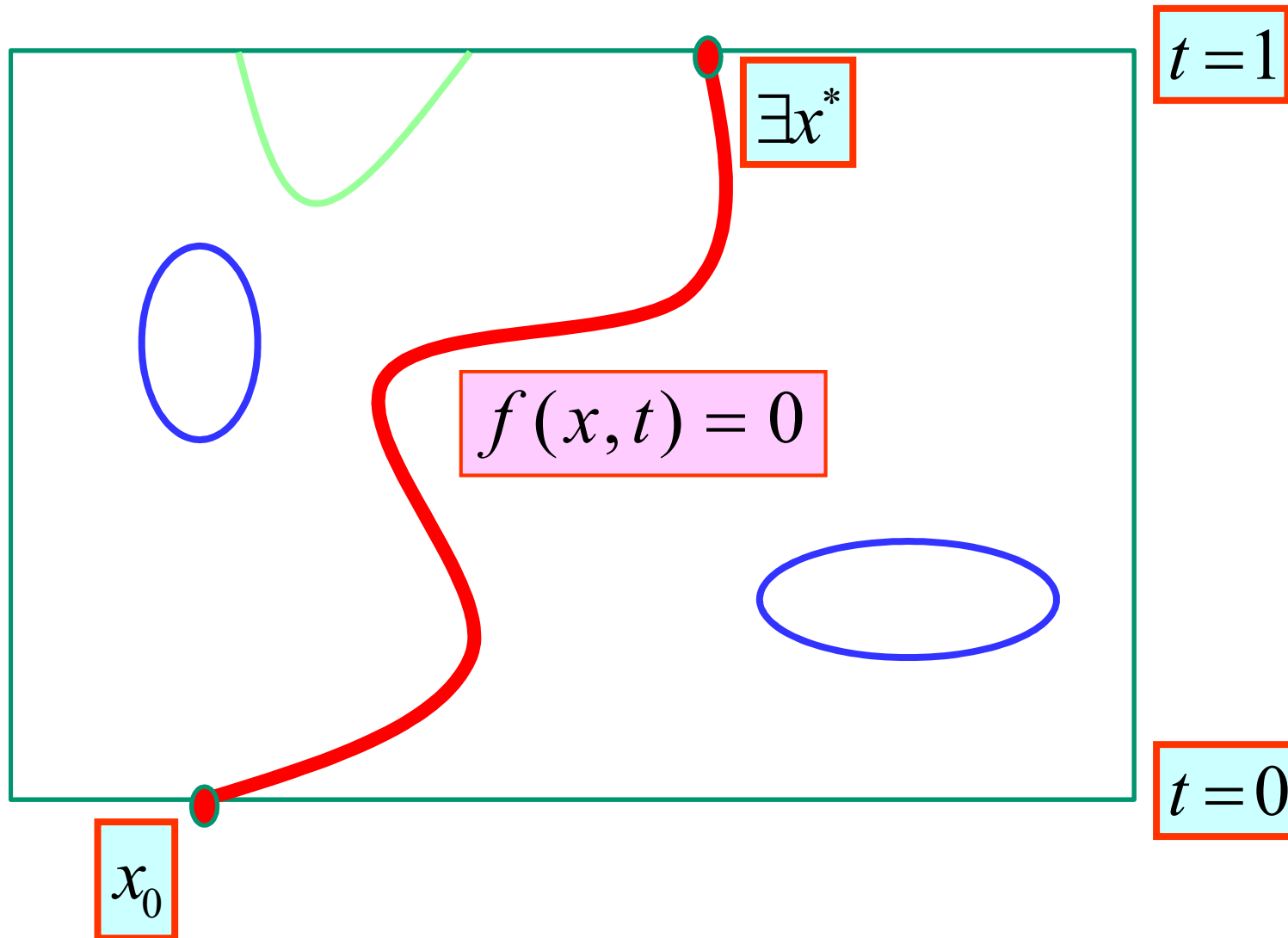
$H : X \times [0,1] \rightarrow X$ **a compact map**

$$H(x, 0) = 0$$

$S = \{x \in X : \exists t, x = H(x, t)\}$ **is bounded**

$\Rightarrow \exists x^* \in X$ **such that** $H(x^*, 1) = x^*$

$$f(x, t) := x - (1 - t)x_0 - H(x, t)$$



化学反応の数理

証明の概略 (その2)

アイデアの背景 (線形代数)

Perron-Frobenius理論

と

Markov鎖

推移確率行列 (Markov 連鎖)

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdot & \cdot & a_{1n} \\ a_{21} & a_{22} & \cdot & \cdot & a_{2n} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ a_{n-11} & a_{n-12} & \cdot & \cdot & a_{n-1n} \\ a_{n1} & a_{n2} & \cdot & \cdot & a_{nn} \end{pmatrix}$$

$$a_{ij} > 0$$

$$\sum_{j=1}^n a_{ij} = \sum_{k=1}^n a_{kj} = 1$$

Frobenius 根 (1)

$$A \mathbf{f} = 1 \mathbf{f}, \quad \mathbf{f} = \begin{pmatrix} 1 \\ 1 \\ \cdot \\ \cdot \\ 1 \end{pmatrix}$$

Frobenius 根 1 は、
代数的に単純な固有値

Frobenius 根 (2)

$$1 = \lim_{n \rightarrow \infty} \|A^n\|^{1/n} \quad (\text{Spectral Radius})$$

The Perron-Frobenius Theorem

$$T = (t_{ij}), \quad t_{ij} > 0.$$

Then :

$$(i) \quad r = \lim_{n \rightarrow \infty} \|T^n\|^{1/n} > 0. \quad (\text{spectral radius})$$

r is a **unique eigenvalue** of T

having **positive eigenvector**.

r is **algebraically simple**.

(ii) r is an algebraically simple eigenvalue of $T^* = (t_{ji})$ with a positive eigenvector.

Perron-Frobenius定理 の 無限次元版

代数的単純性の 解析的な判定条件

Krein-Rutman

の理論

文献

- **Krein and Rutman: Linear operators leaving invariant a cone in a Banach space, Amer. Math. Soc. Transl. 10 (1962), 199-325**

強正值性 (積分核版)

Strong Positivity (1)

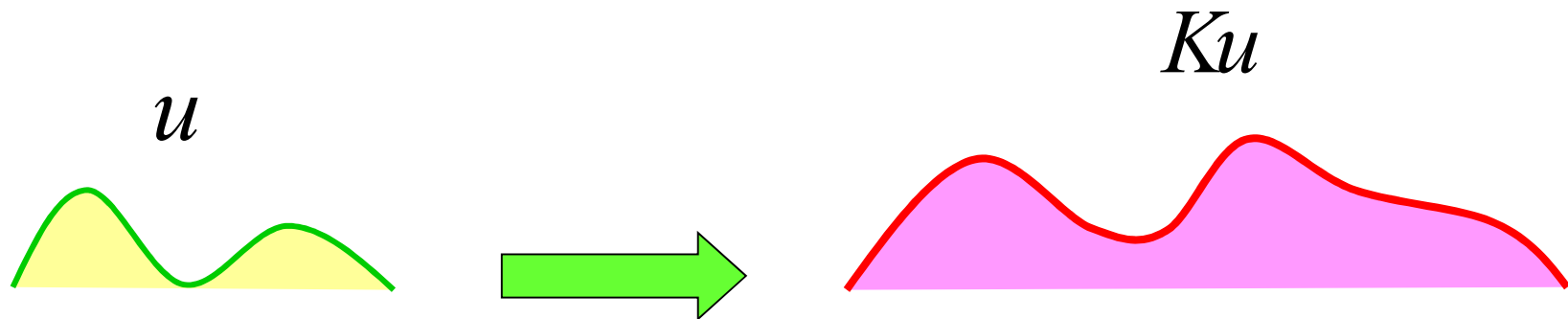
$$Ku(x) = \int k(x, y)u(y)dy$$

$$k(x, y) > 0$$

\Leftrightarrow

$$u(x) \geq 0 \Rightarrow Ku(x) > 0 \quad \text{strongly positive}$$

Strong Positivity (2)



順序付き Banach 空間論

順序付きベクトル空間

V is an **ordered vector space**

def

\Leftrightarrow

- (i) (V, \leq) is an ordered set.
- (ii) V is a real vector space.
- (iii) The ordering \leq is **linear** :

$$(a) \ x, y \in V, x \leq y \Rightarrow x + z \leq y + z, \forall z \in V.$$

$$(b) \ x, y \in V, x \leq y \Rightarrow \alpha x \leq \alpha y, \forall \alpha \geq 0.$$

順序付き Banach 空間

E is an **ordered Banach space**

def

\Leftrightarrow

(i) E is a Banach space.

(ii) (E, \leq) is an ordered vector space.

(iii) $P := \{x \in E : x \geq 0\}$, **positive cone**, is closed.

(a) $x, y \in P \Rightarrow \alpha x + \beta y \in P, \forall \alpha, \beta \geq 0$.

(b) $P \cap (-P) = \{0\}$.

Example (1)

$$Y = C(\overline{\Omega}),$$

$$u \leq v \stackrel{\text{def}}{\Leftrightarrow} u(x) \leq v(x), \forall x \in \overline{\Omega}$$

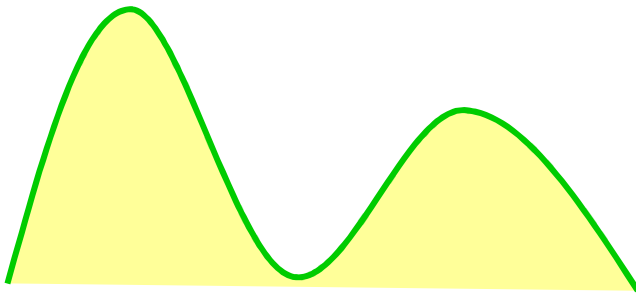


$$P_Y = \{u \in C(\overline{\Omega}) : u \geq 0 \text{ on } \overline{\Omega}\},$$

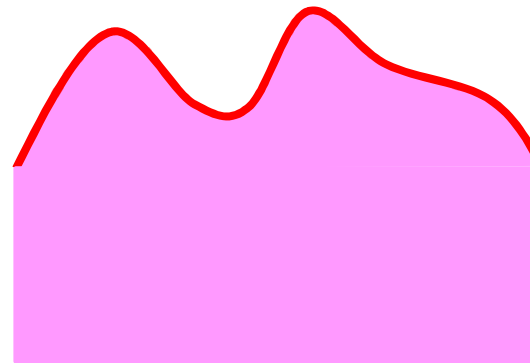
$$\text{Int}(P_Y) = \{u \in C(\overline{\Omega}) : u > 0 \text{ on } \overline{\Omega}\}$$

Example (2)

$u \in P_Y$



$u \in \text{Int}(P_Y)$



Strong Positivity

$$Ku(x) = \int_{\Omega} k(x, y)u(y)dy$$

$$k(x, y) > 0$$

\Leftrightarrow

$$u(x) \geq 0 \Rightarrow Ku(x) > 0 \quad \text{strongly positive}$$

$$K(P \setminus \{0\}) \subset \text{Int}(P)$$

コンパクト性 (関数解析版)

Characterization of Compact Operators

A continuous operator $T : X \rightarrow Y$ is **compact**

\Leftrightarrow

T is a **uniform limit** of operators

whose ranges lie in **finite - dimensional subspaces**

(of finite rank)

Perron-Frobenius の定理

コンパクト性

強正値性

連続化

Krein-Rutman の理論

The Krein-Rutman Theorem (1)

Let (E, P) be an ordered Banach space with non - empty interior, and assume that $K : E \rightarrow E$ is **strongly positive and compact**.

$$K (P \setminus \{0\}) \subset \text{Int} (P)$$

The Krein-Rutman Theorem (2)

(i) $r = \lim_{n \rightarrow \infty} \|K^n\|^{1/n} > 0$, (spectral radius)

r is a **unique eigenvalue** of K

having a **positive eigenfunction**.

r is **algebraically simple**.

(ii) r is also an algebraically simple

eigenvalue of the adjoint $K^* : E^* \rightarrow E^*$

with a positive eigenfunction.

Krein-Rutman理論

と

Markov過程

半群的アプローチ の方針

Hille-Yosida の 半群理論

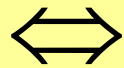
Bird's-Eye View (1)



Bird's-Eye View (2)

$$T_t = e^{t\mathcal{A}}$$

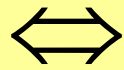
Kolmogorov



Parabolic Theory

Hille - Yosida \Updownarrow

$$(\alpha I - \mathcal{A})^{-1}$$



Feller

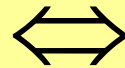
Elliptic Theory

Brownian Motion

Case

Bird's-Eye View (1-dimensional case)

$$\frac{1}{\sqrt{2\pi t}} e^{-\frac{(x-y)^2}{2t}}$$

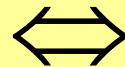


$$e^{\frac{1}{2} t \frac{d^2}{dx^2}}$$

Laplace \Updownarrow

\Updownarrow Hille - Yosida

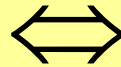
$$\frac{1}{\sqrt{2\alpha}} e^{-\sqrt{2\alpha}|x-y|}$$



$$\left(\alpha - \frac{1}{2} \frac{d^2}{dx^2} \right)^{-1}$$

Bird's-Eye View (2)

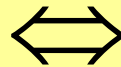
$$\frac{\partial}{\partial t} - \frac{1}{2} \frac{d^2}{dx^2}$$



Heat Equation



$$\alpha - \frac{1}{2} \frac{d^2}{dx^2}$$



Sturm-Liouville

Bird's-Eye View



Riesz-Markov-Dynkin Representation Theorem

$$T_t f(x) = \int_K \exists! p_t(x, dy) f(y), \quad \forall f \in C(K)$$

\Leftrightarrow

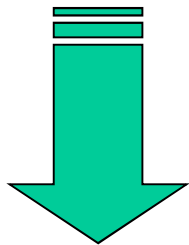
$$0 \leq p_t(x, \cdot) \leq 1, \quad \forall t \geq 0, \quad \forall x \in K$$

Riesz-Markov Representation Theorem

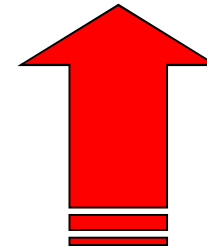
$$(\alpha I - A)^{-1} f(x) = \int_{\bar{D}} \exists! G_{\alpha}(x, dy) f(y)$$

Transition Probability and Green kernel

$$p_t(x, dy)$$



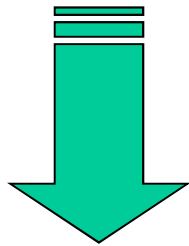
Laplace Transform



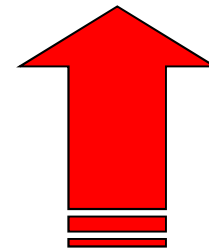
$$G_\alpha(x, dy) = \int_0^\infty e^{-\alpha t} p_t(x, dy) dt$$

Hille-Yosida Theory (1)

$$T_t = e^{tA}$$



Laplace Transform



$$(\alpha I - A)^{-1} = \int_0^{\infty} e^{-\alpha t} e^{tA} dt = \int_0^{\infty} e^{-\alpha t} T_t dt$$

Hille-Yosida Theory (2)

$$e^{tA} = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} e^{\alpha t} (\alpha I - A)^{-1} d\alpha$$

$$(\alpha I - A)^{-1} = \int_0^{\infty} e^{-\alpha t} e^{tA} dt$$

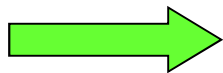
$T_t = e^{tA}$: **Semigroup**

$(\alpha I - A)^{-1}$: **Resolvent (Green operator)**

Feller 半群 の理論

連続関数空間上の半群理論

$$Y = C(\overline{\Omega}),$$
$$u \leq v \stackrel{\text{def}}{\Leftrightarrow} u(x) \leq v(x), \forall x \in \overline{\Omega}$$



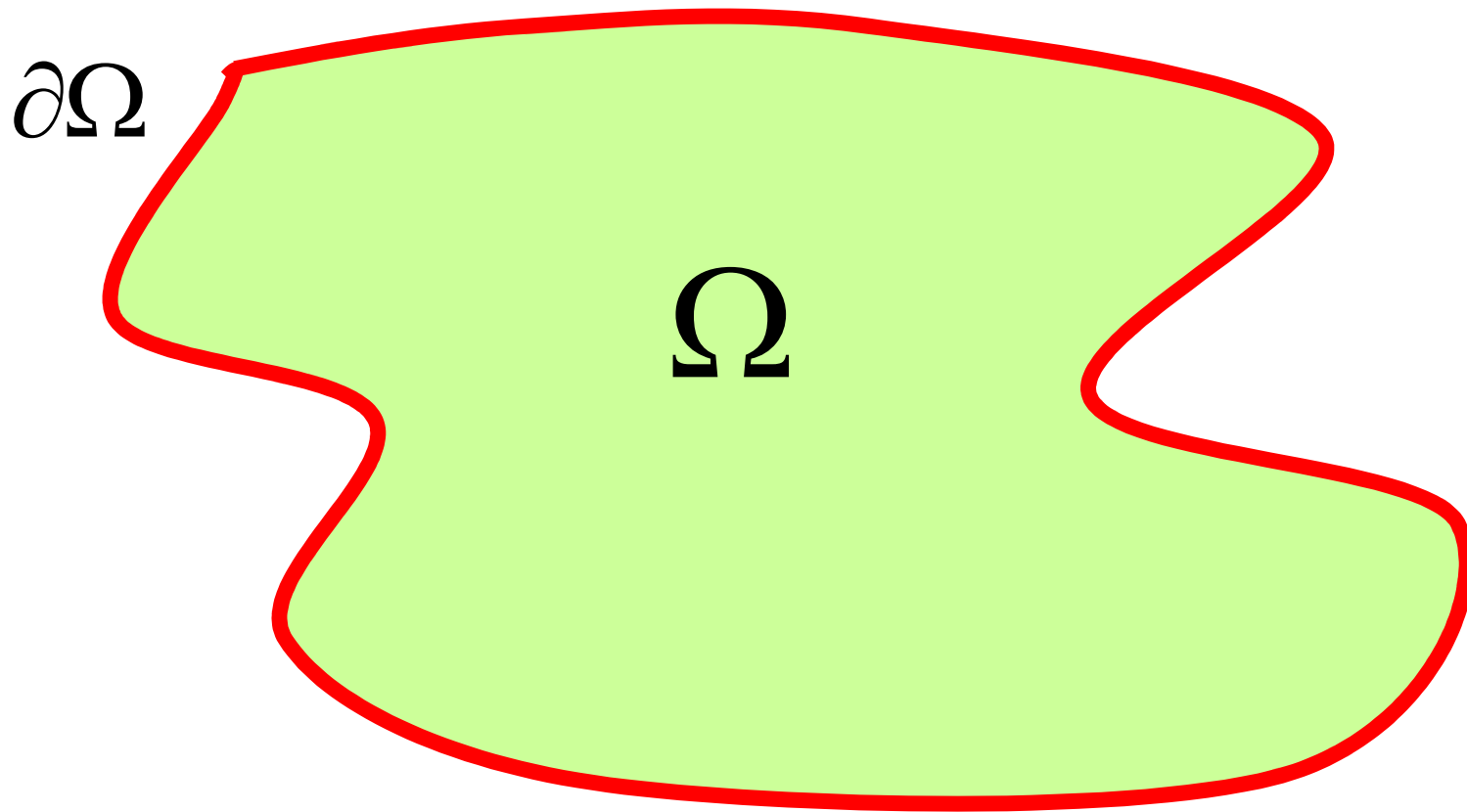
$$P_Y = \{u \in C(\overline{\Omega}) : u \geq 0 \text{ on } \overline{\Omega}\},$$
$$\text{Int}(P_Y) = \{u \in C(\overline{\Omega}) : u > 0 \text{ on } \overline{\Omega}\}$$

William Feller

William Feller (1906-1970)
Croatian–American Mathematician



有界領域



関数空間(一般の場合)

$C(\bar{\Omega})$ = space of real - valued, continuous functions
on the **closure** $\bar{\Omega} = \Omega \cup \partial\Omega$

with the maximum norm

$$\|u\| = \max_{x \in \bar{\Omega}} |u(x)|.$$

Riesz-Markov-Dynkin Representation Theorem

$$T_t f(x) = \int_K \exists! p_t(x, dy) f(y), \quad \forall f \in C(K)$$

\Leftrightarrow

$$0 \leq p_t(x, \cdot) \leq 1, \quad \forall t \geq 0, \forall x \in K$$

Feller 半群 (一般の場合)

A family of bounded linear operators

$$\{T_t\}_{t \geq 0}$$

is called a **Feller semigroup** if it satisfies the following three conditions :

$$(1) T_{t+s} = T_t \cdot T_s, \quad \forall t, s \geq 0.$$

$$(2) \lim_{s \downarrow 0} \|T_{t+s} f - T_t f\| = 0, \quad \forall f \in C(\bar{\Omega}).$$

$$(3) \forall f \in C(\bar{\Omega}), 0 \leq f \leq 1 \text{ on } \bar{\Omega} \Rightarrow 0 \leq T_t f \leq 1 \text{ on } \bar{\Omega}.$$

Hille・吉田の生成定理

The operator

$$\mathbf{A} : C(\bar{\Omega}) \rightarrow C(\bar{\Omega})$$

generates a Feller semigroup if it satisfies
the following four conditions :

(a) $D(\mathbf{A})$ is dense in $C(\bar{\Omega})$.

(b) $\exists! u \in D(\mathbf{A})$ such that $(\alpha - \mathbf{A})u = f$, $\forall f \in C(\bar{\Omega})$.

(c) $\forall f \in C(\bar{\Omega})$, $f \geq 0$ on $\bar{\Omega} \Rightarrow (\alpha - \mathbf{A})^{-1} f \geq 0$ on $\bar{\Omega}$.

(d) $\|(\alpha - \mathbf{A})^{-1}\| \leq \frac{1}{\alpha}$, $\forall \alpha > 0$.

Green 作用素

$$u = G_{\alpha}^0 f = (\alpha - A)^{-1} f$$

Strong Positivity

$$\mathbf{G}_\alpha^0 f(x) = \int_\Omega G_\alpha(x, y) f(y) dy$$

$$\boxed{G_\alpha(x, y) > 0}$$

\Leftrightarrow

$$f(x) \geq 0 \Rightarrow \mathbf{G}_\alpha^0 f(x) > 0 \quad \text{strongly positive}$$

The Hille-Yosida-Ray Theorem

The operator

$$A : C(\overline{\Omega}) \rightarrow C(\overline{\Omega})$$

generates a Feller semigroup if it satisfies the following three conditions :

(a) $D(A)$ is dense in $C(\overline{\Omega})$.

(b) $\exists u \in D(A)$ such that $(\alpha - A)u = f$, $\forall f \in C(\overline{\Omega})$.

(c) **If $u \in D(A)$ attains its positive maximum at a point $x_0 \in \overline{\Omega}$, then $Au(x_0) \leq 0$.**

最大値の原理 (ソボレフ空間版)

劣調和関数の最大値の原理

- 劣調和(下に凸)関数は、その最大値を**境界の点**でとる。(最大値の原理)
- 劣調和関数が、内部の点で最大値をとれば、**定数**である。(強最大値の原理)

Weak Maximum Principle (Aleksandrov-Bakel'man)

Assume that :

$$\begin{cases} u \in C(\bar{D}) \cap W_{\text{loc}}^{2,N}(D), \\ (\alpha - W)u(x) \leq 0 \text{ for a.a. } x \in D. \end{cases}$$

Then :

$$\sup_D u \leq \sup_{\partial D} u^+.$$

Strong Maximum Principle

Assume that

$$\left\{ \begin{array}{l} u \in C(\bar{D}) \cap W_{\text{loc}}^{2,N}(D), \\ (\alpha - W)u(x) \leq 0 \text{ for a.a. } x \in D, \\ M = \sup_D u \geq 0. \end{array} \right.$$

Then :

$\exists x_0 \in D$ such that $u(x_0) = M \Rightarrow u(x) \equiv M, \forall x \in D.$

Fixed Point Index Theory

Fixed point index theory

Existence Theorems	Methods	Studied by
Non-trivial Solutions	Degree Theory	Leray-Schauder (1934)
Positive Solutions	Fixed Points in a Positive Cone	Leggett-Williams (1982)

正值錐上の 写像度理論

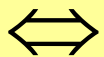
Retracts and Retractions

Let X be a **metric space**

A **non - empty subset** $A \subseteq X$

is a **retract** of X

def

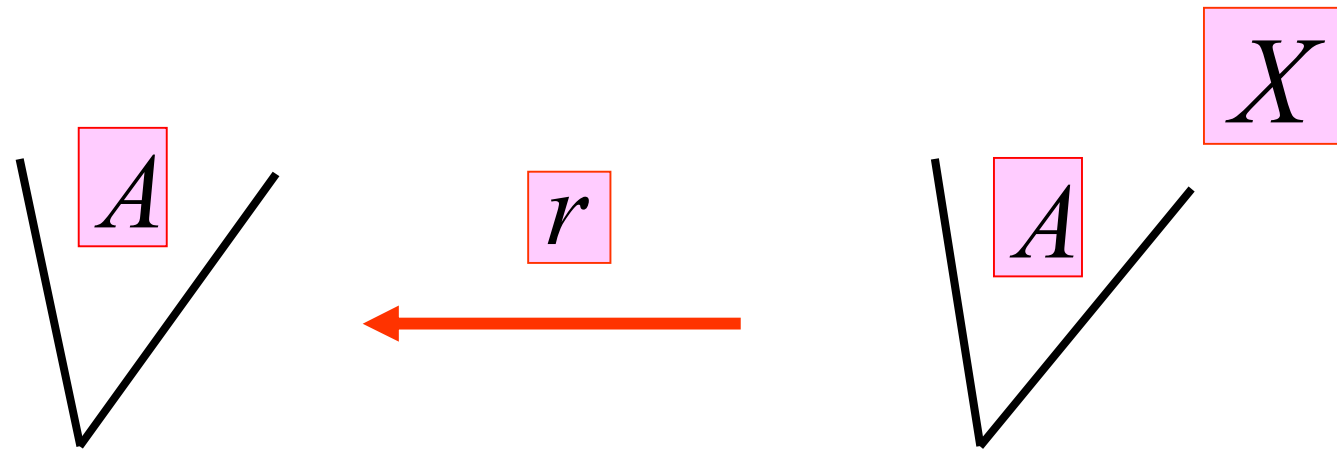


$\exists r : X \rightarrow A$ **continuous map** such that

$r|_A =$ **the identity map** on A

r is a **retraction**

レトラクトとレトラクション



$\exists r : X \rightarrow A$ **continuous map**

$r|_A =$ **the identity map on A**

Theorem (Dugundji)

Let E be a Banach space.

Every non - empty **closed convex** subset of E is a **retract** of E .

Ordered Banach Space

E is an **ordered Banach space** :

(i) E is a Banach space.

(ii) (E, \leq) is an ordered vector space.

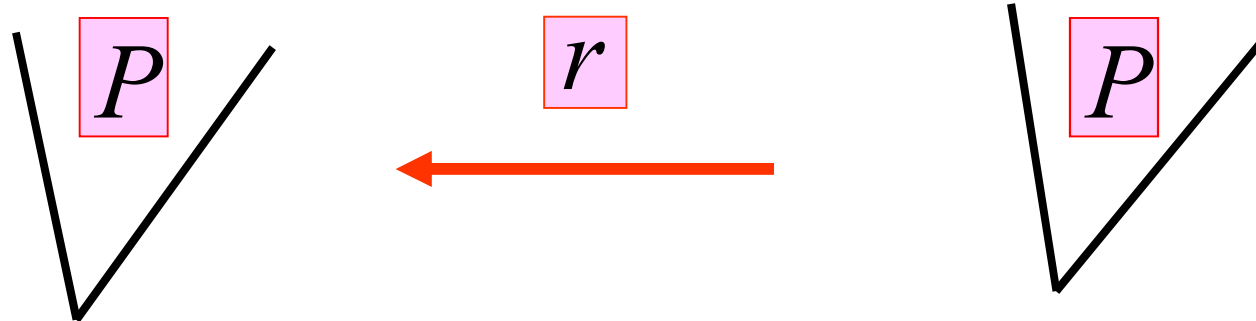
(iii) $P := \{x \in E : x \geq 0\}$, **positive cone**, is closed.

(a) $x, y \in P \Rightarrow \alpha x + \beta y \in P, \forall \alpha, \beta \geq 0$.

(b) $P \cap (-P) = \{0\}$.

レトラクトとレトラクション

$$E = C(\bar{\Omega})$$

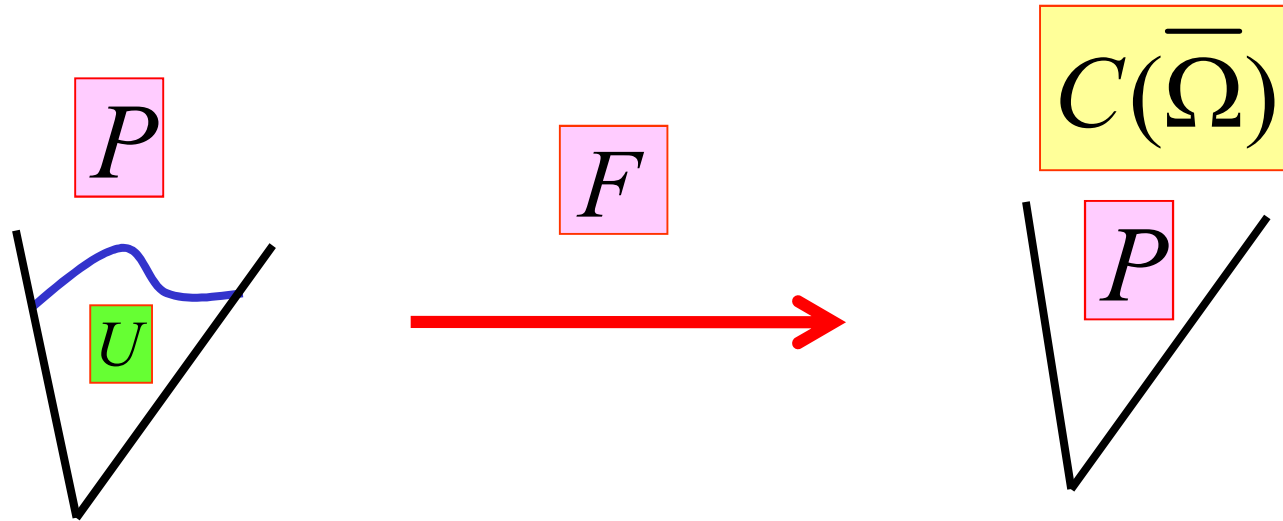


$\exists r : C(\bar{\Omega}) \rightarrow P$ **continuous map**

$r|_P =$ **the identity map on P**

$$P = \{u \in C(\bar{\Omega}) : u \geq 0\}$$

正值錐上の写像度(1)

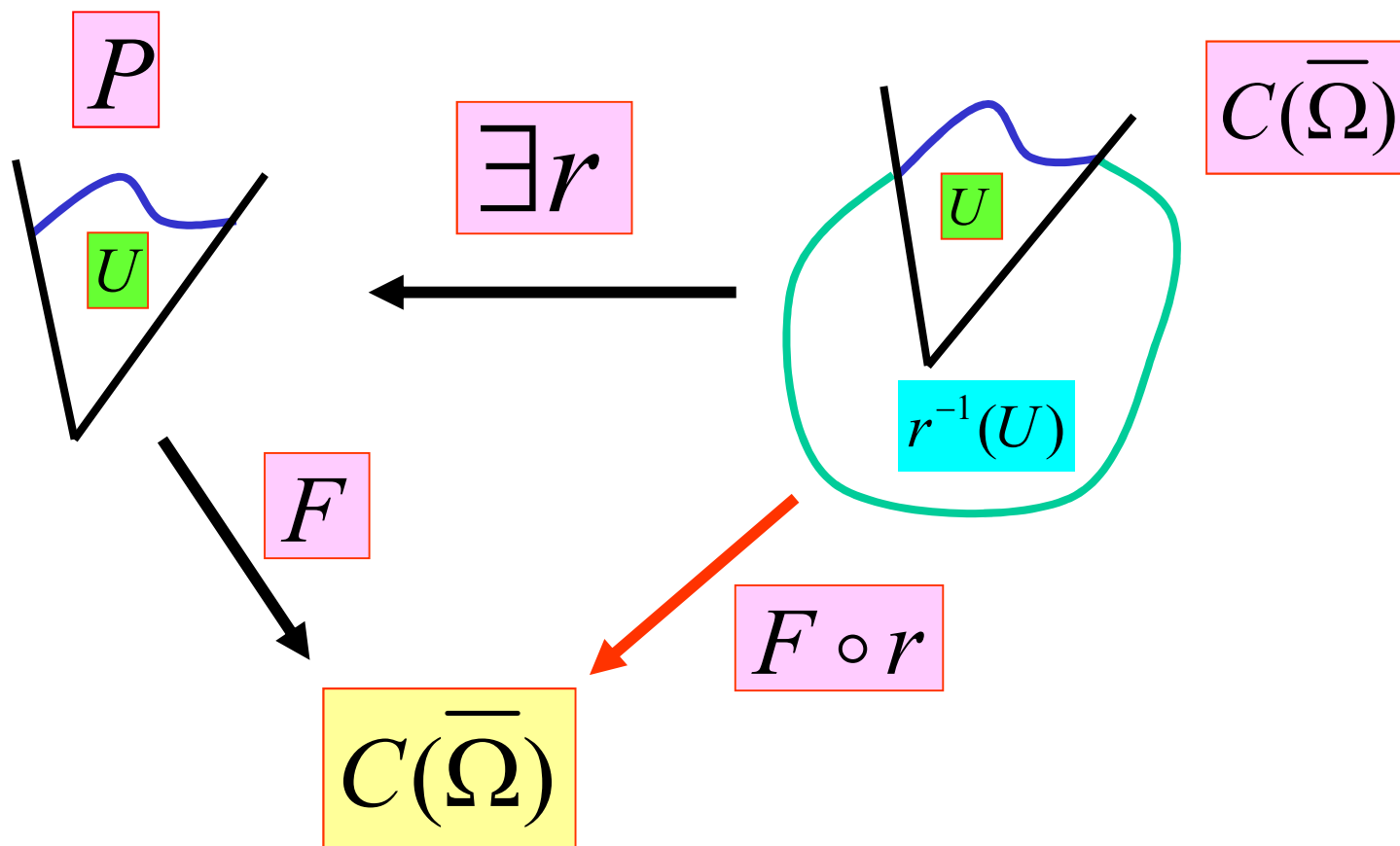


$U \subseteq P$ **open subset**

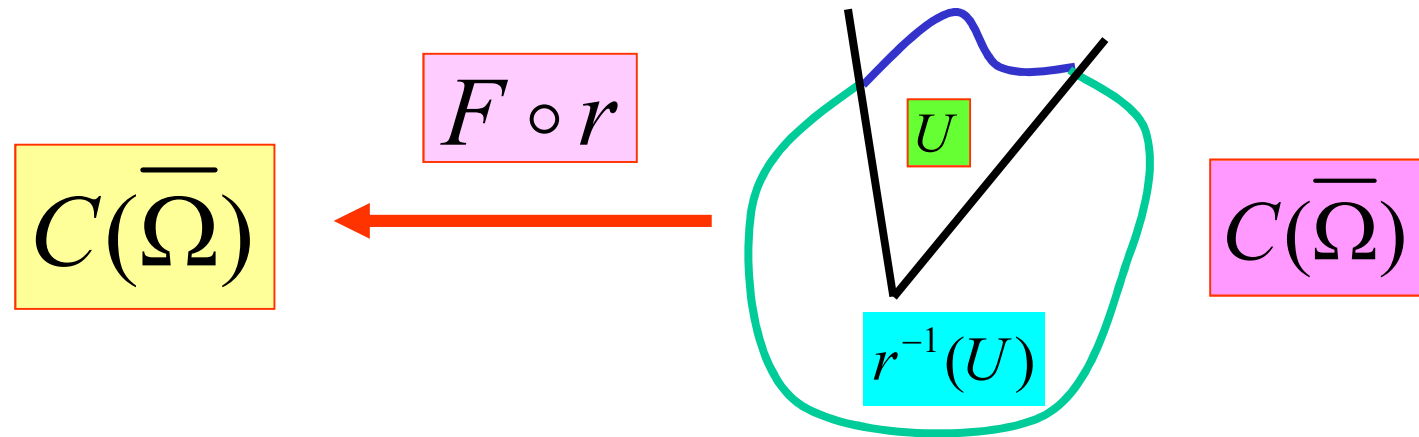
$F : \overline{U} \rightarrow P, \overline{F(U)}$ **compact**

$u \neq F(u), \quad \forall u \in \partial U$

正值錐上の写像度(2)



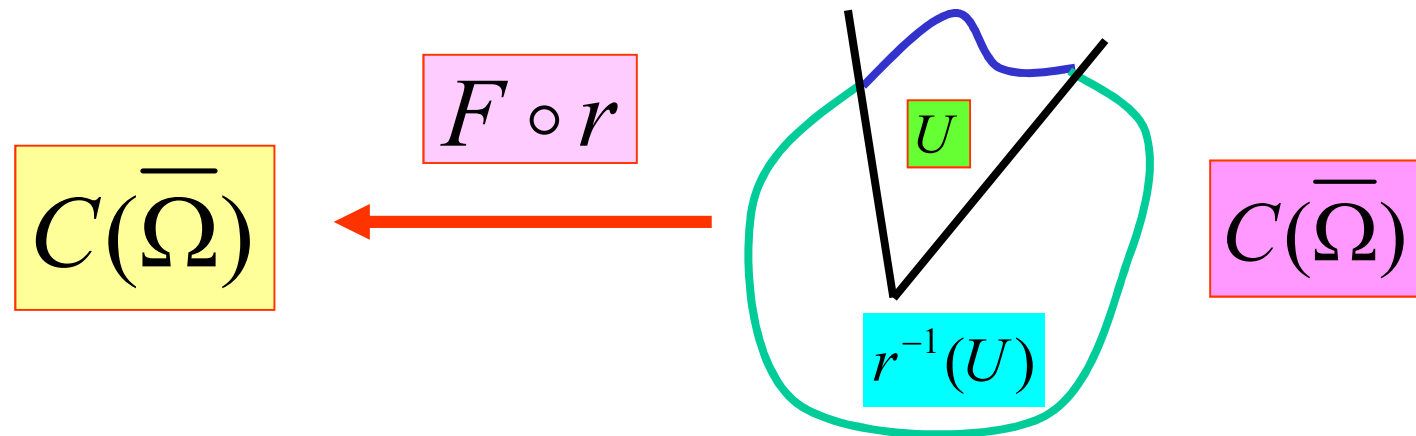
正值錐上の写像度(3)



$$i(F, U) := \deg(I - F \circ r, r^{-1}(U), 0)$$

Leray - Schauder degree with respect to 0 of $I - F \circ r$ defined on $\overline{r^{-1}(U)}$.

正值錐上の写像度(4)



$$u \neq F(u), \quad \forall u \in \partial U$$

\Rightarrow

$$i(F, U) := \deg(I - F \circ r, r^{-1}(U), 0)$$

Leray - Schauder degree with respect to 0 of $I - F \circ r$ defined on $\overline{r^{-1}(U)}$.

Leggett-Williams Theory

多重正值解の 存在定理

多重不動点の存在定理(1)

(X, Q, \geq) an ordered Banach space

The positive cone Q has non - empty interior

$\eta : Q \rightarrow [0, \infty)$ a **continuous and concave** functional

$G : Q_\tau = \{w \in Q : \|w\| \leq \tau\} \rightarrow Q$ a **compact** mapping

such that

$$\|G(w)\| < \tau, \quad \forall w \in Q_\tau, \quad \|w\| = \tau$$

多重不動点の存在定理(2)

Assume : $0 < \exists \delta < \tau, \exists \sigma > 0$ such that

$$W = \left\{ w \in \overset{\circ}{Q}_\tau : \eta(w) > \sigma \right\} \neq \emptyset$$

$$\|G(w)\| < \delta, \quad \forall w \in Q_\delta, \quad \|w\| = \delta$$

$$\eta(w) < \sigma, \quad \forall w \in Q_\delta$$

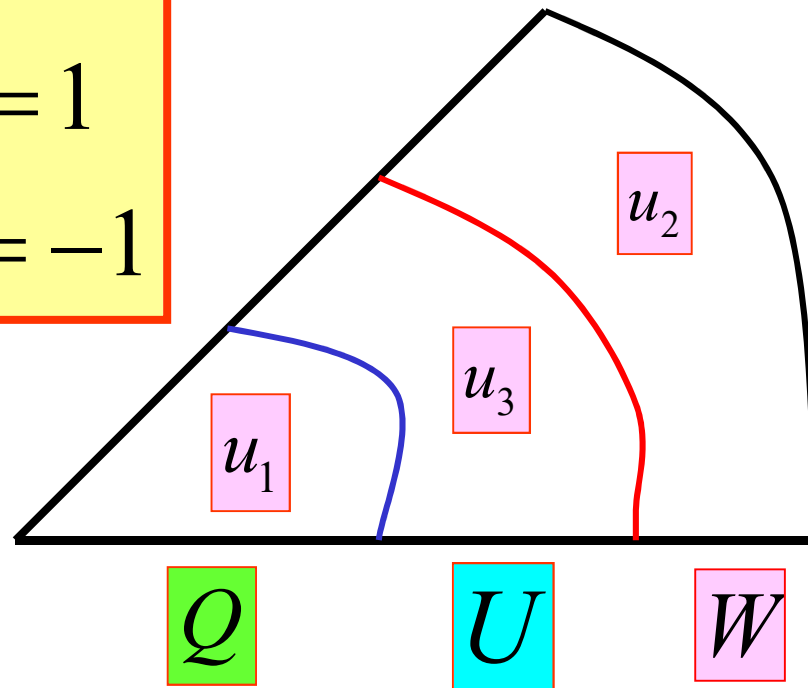
$$\eta(G(w)) > \sigma, \quad \forall w \in Q_\tau, \quad \eta(w) = \sigma$$

\Rightarrow

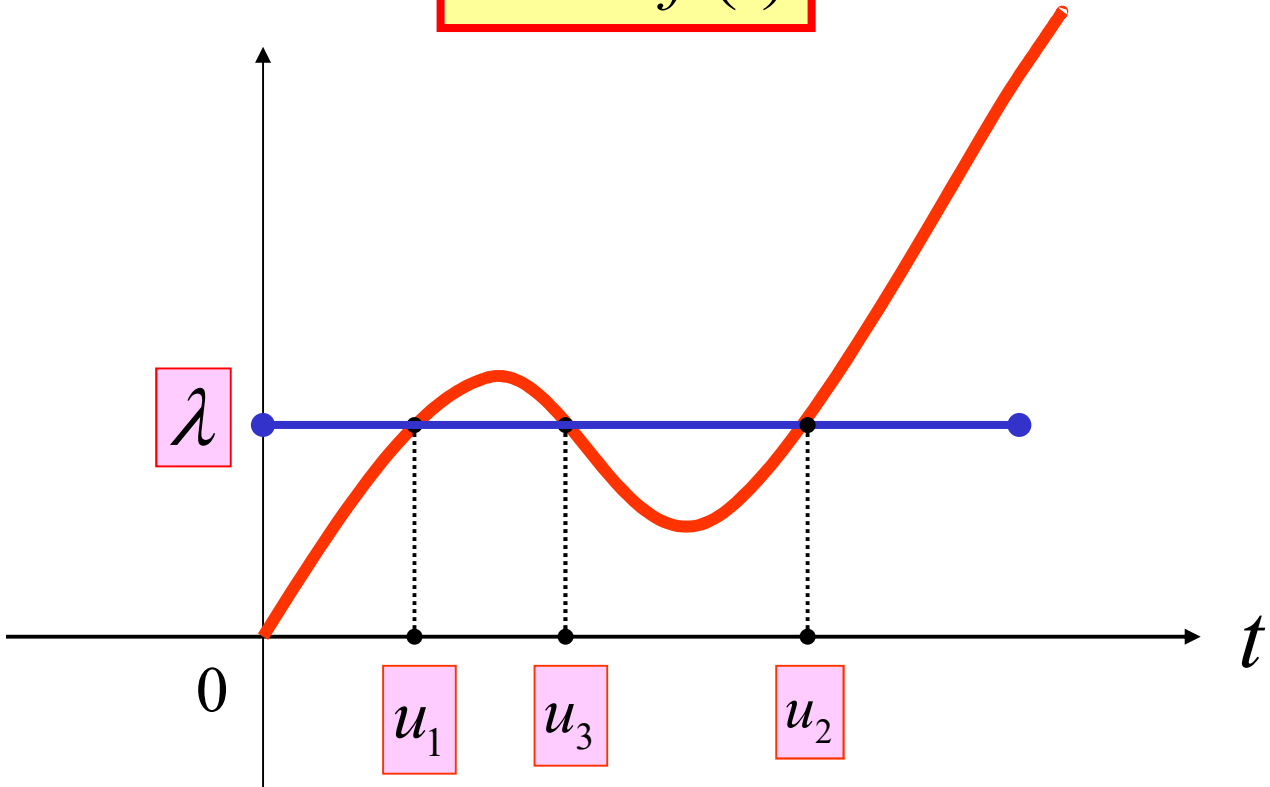
G has at least **three distinct fixed points**

写像度の計算

$$\begin{aligned}i(F, Q) &= 1 \\i(F, W) &= 1 \\i(F, U) &= -1\end{aligned}$$



$$v(t) = \frac{t}{f(t)}$$

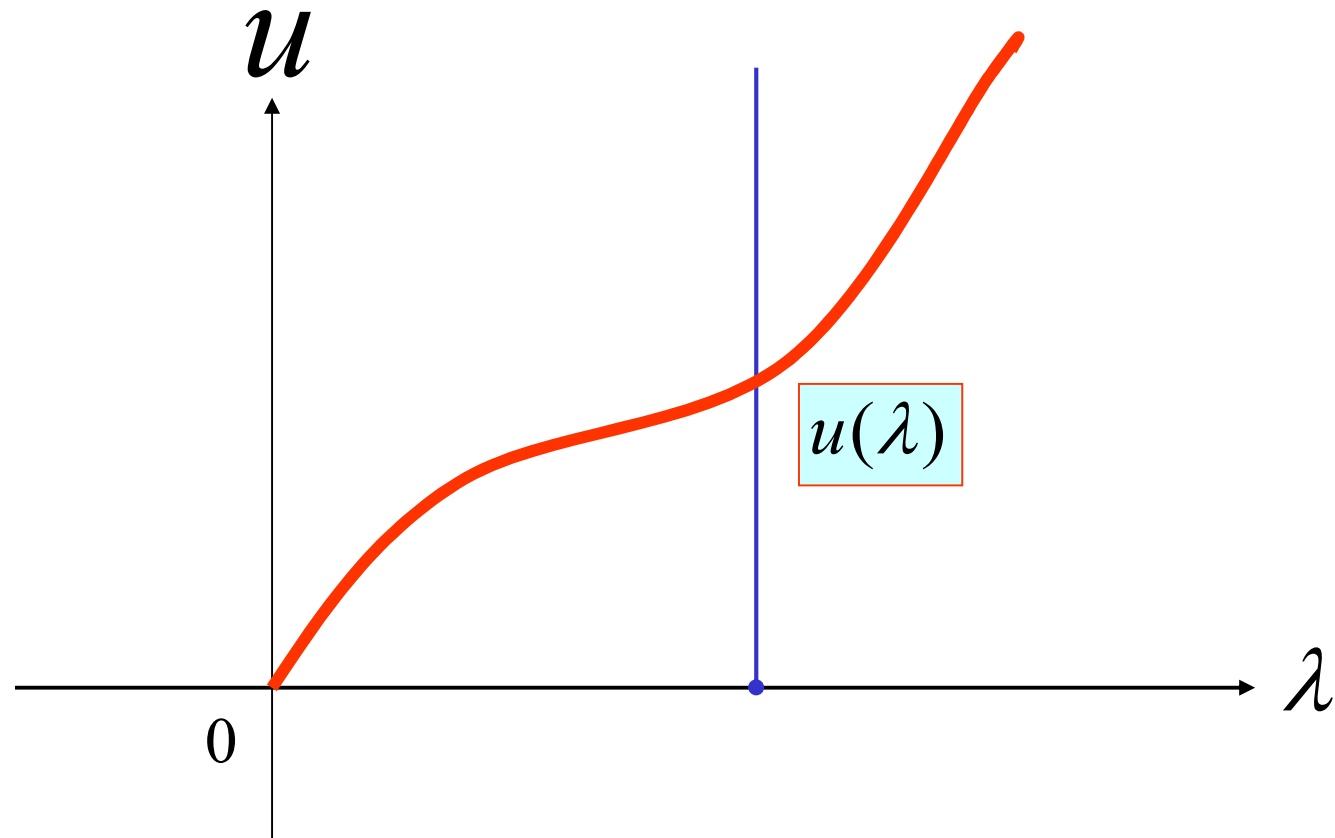


反応速度論への 応用

低い活性化エネルギー

$$\varepsilon \geq \left(\frac{1}{1 + \sqrt{1 - m}} \right)^2$$

低い活性化エネルギー

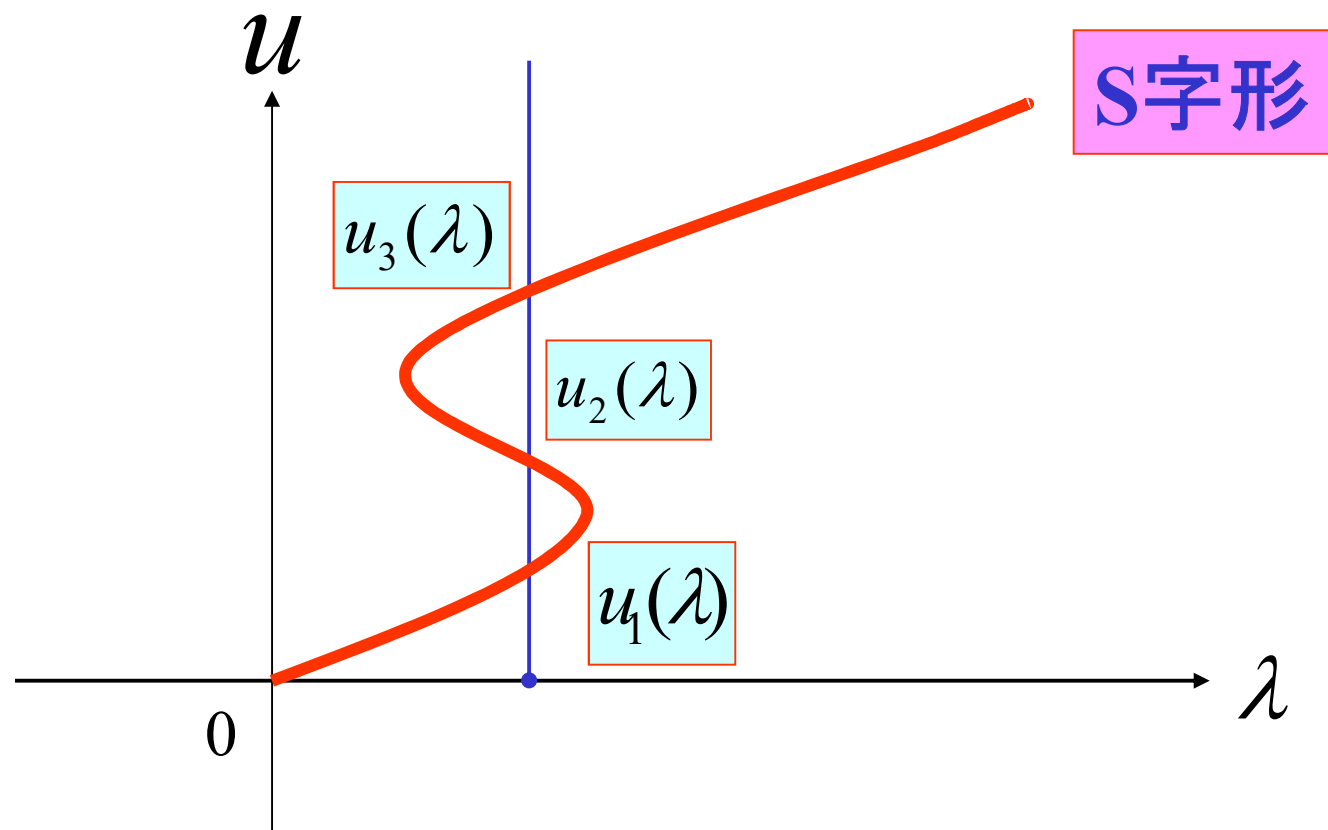


化学反応は連続的に進行する。

高い活性化エネルギー

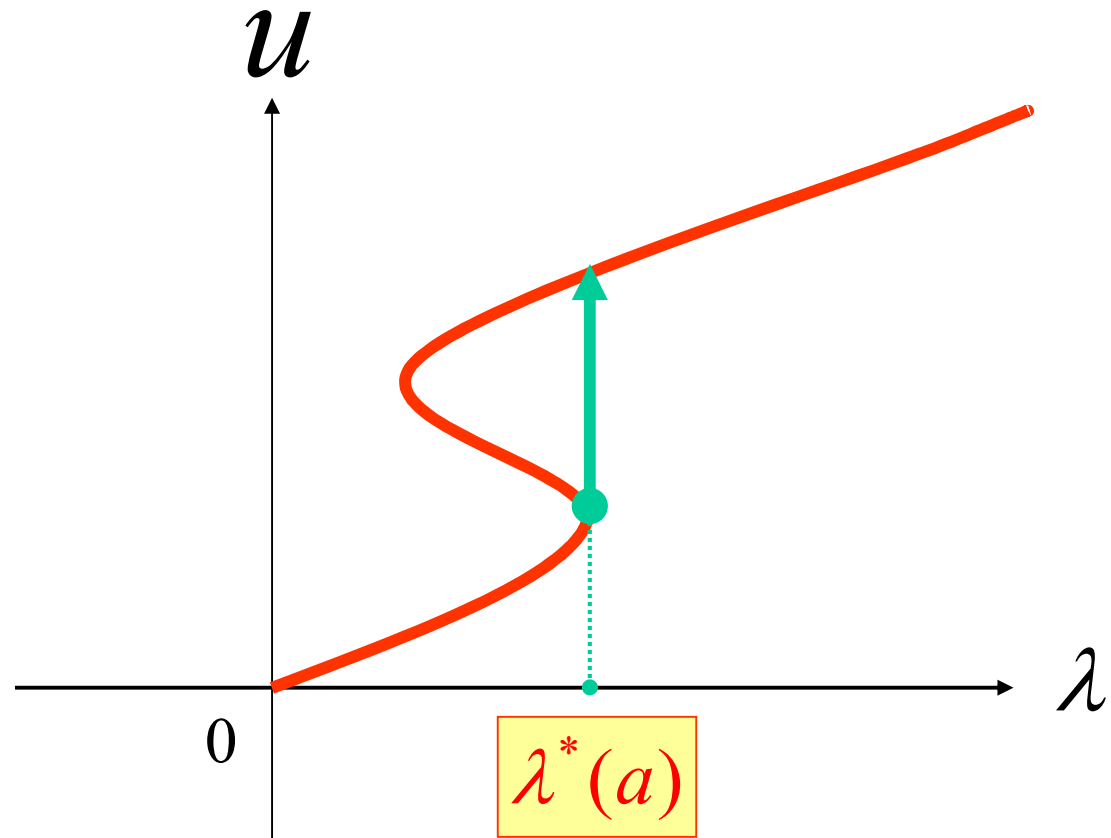
$$0 < \varepsilon \ll \left(\frac{1}{1 + \sqrt{1 - m}} \right)^2$$

高い活性化エネルギー

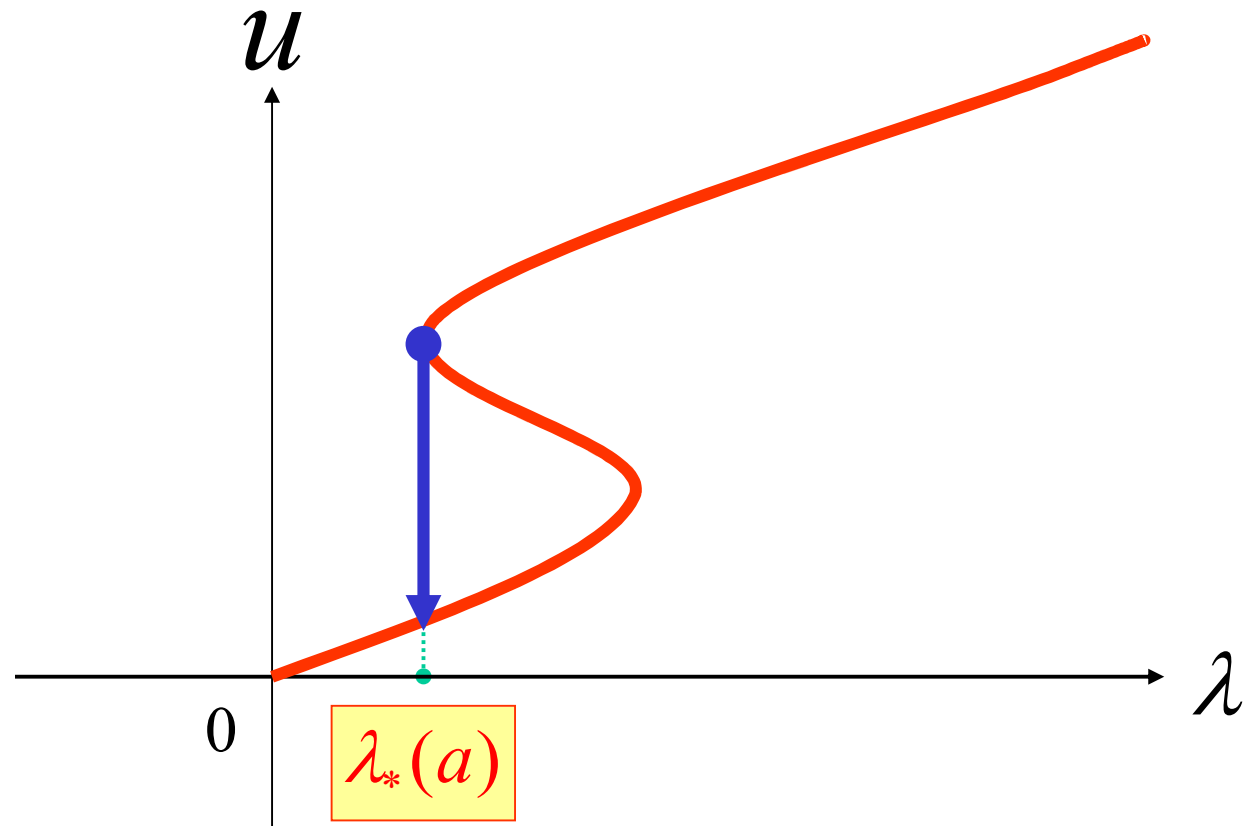


化学反応は不連続的に進行する。

発火点 (熱爆発)



消火点 (温度失活)



発火点の比較定理 (1)

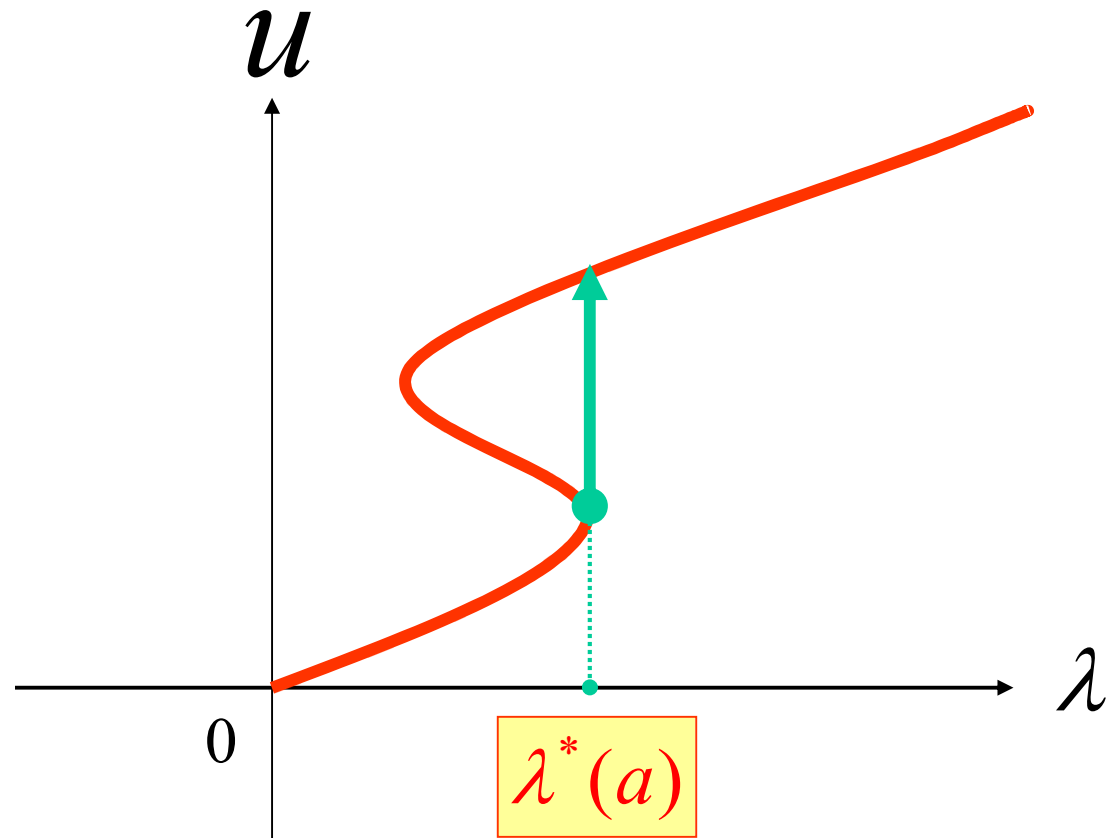
発火点	境界条件
$\lambda^*(a)$	$a \frac{\partial u}{\partial \mathbf{n}} + (1-a)u = 0$
$\lambda^*(1)$	$\frac{\partial u}{\partial \mathbf{n}} = 0$
$\lambda^*(0)$	$u = 0$

発火点の比較定理 (2)

$$\lambda^*(1) < \lambda^*(a) < \lambda^*(0)$$

- 発火温度は、**保温条件**の場合が**一番低く**(火がつきやすく)、**冷却条件**の場合が**一番高い**(火がつきにくい)。

発火点 (熱爆発)



消火点の比較定理 (1)

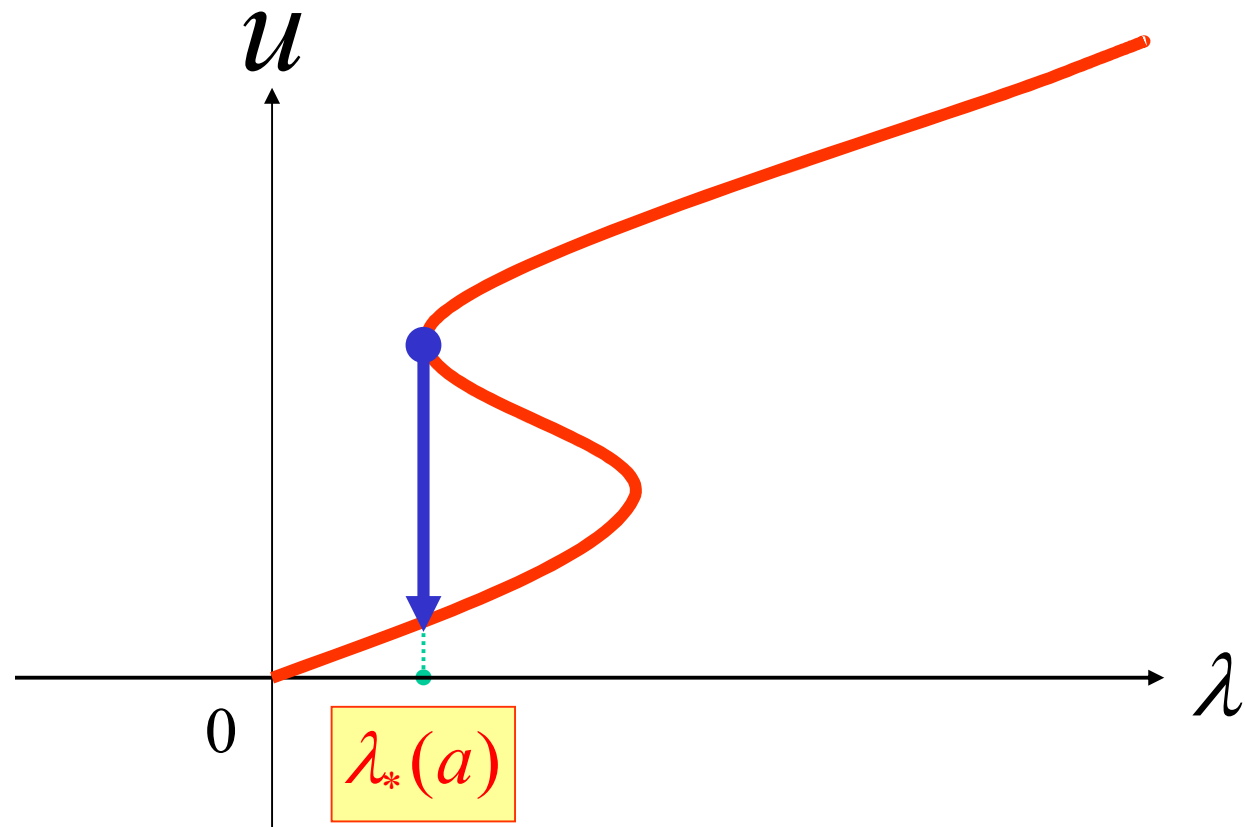
消火点	境界条件
$\lambda_*(a)$	$a \frac{\partial u}{\partial \mathbf{n}} + (1-a)u = 0$
$\lambda_*(1)$	$\frac{\partial u}{\partial \mathbf{n}} = 0$
$\lambda_*(0)$	$u = 0$

消火点の比較定理 (2)

$$\lambda_*(1) < \lambda_*(a) < \lambda_*(0)$$

- 消火温度は、**保温条件**の場合が**一番低く**(火が消えにくく)、**冷却条件**の場合が**一番高い**(火が消えやすい)。

消火点 (温度失活)



今後の 数値解析的問題

パラメータの数値解析

$\lambda^*(a)$ (発火点)

$\lambda_*(a)$ (消火点)

発火点の数値解析

(2000: 皆本, 中尾, 山本)

ε	$\lambda^*(0)$
0.01	3.359
0.02	3.399
0.20	4.51

END